Coastal marine heatwaves: Understanding extreme forces

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The Earth is not dying, it is being killed. And the people who are killing it have names and addresses.



-Utah Phillips



KEYWORDS

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eawater temperature from regional to global scale is central to many measures of biodiversity and continues to aid our understanding of the evolution and ecology of biological assemblages. Therefore, a clear understanding of the relationship between marine biodiversity and thermal structures is critical for effective conservation planning. In the anthropocene, an epoch characterised by anthropogenic forcing on the climate system, future patterns in biodiversity and ecological functioning may be estimated from projected climate scenarios however; absent from many of these scenarios is the inclusion of extreme thermal events, known as marine heatwaves (MHWs). There is also a conspicuous absence in knowledge of the drivers for all but the most notorious of these events.

Before the drivers of MHWs along the coast of South Africa could be determined, it was first necessary to validate the 129 in situ coastal seawater temperature time series that could be used to this end. In doing so it was found that time series created with older (longer), lower precision (0.5°C) instruments were more useful than newer (shorter) time series produced with high precision (0.001°C) instruments. With the in situ data validated, a history of the occurrence of MHWs along the coastline (nearshore) was created and compared against MHWs detected by remotely sensed data (offshore). This comparison showed that the forcing of offshore temperatures onto the nearshore was much lower than anticipated, with the rates of co-occurrence for events between the datasets along the coast ranging from 0.2 to 0.5. To accommodate this lack of consistency between datasets, a much larger mesoscale area was then taken around southern Africa when attempting to determine potential mesoscale drivers of MHWs along the coast. Using a self organising-map (SOM), it was possible to organise the synoptic scale oceanographic and atmospheric states during coastal MHWs into discernible groupings. It was found that the most common synoptic oceanographic pattern during coastal MHWs was Agulhas Leakage, and the most common atmospheric pattern was anomalously warm overland air temperatures. With these patterns known it is now necessary to calculate how often they occur when no MHW has been detected. This work may then allow for the development of predictive capabilities that could help mitigate the damage caused by MHWs.

November 2017



DECLARATION

declare that *Coastal marine heatwaves: Understanding extreme forces* is my own work, that it has not been submitted for any degree or examination in any other university, and that all the sources I have used or quoted have been indicated and acknowledged by complete references.

DATE: November 10th, 2017

UNIVERSITY of the WESTERN CAPE



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PREFACE

This PhD thesis through publication covers the research I have performed over the last three years. It also links to and interacts with the myriad of data products I've produced in the intersticing time. Whereas this printed body of work is static in nature, the data science upon which it has been built is not. Much of this work, and its continuation, may be found at my GitHub page: https://github.com/robwschlegel/.





CHAPTER

INTRODUCTION

Earth, meaning that, for all of the cunning and guile we may posses, we cannot divest ourselves from the resources of our birth place, our one inhabited planet. Because our home is not one static homogeneous entity, the benefits it affords us through space and time naturally differ. This utilisation of Earth's various ecosystems has provided a wide range of different products and services that humans have been able to exploit in their continuous march of progress from cave dwellers to cloud skimmers. Due to the importance of ecosystems, there have been a range of attempts at quantifying their 'value' to humanity with perhaps none having been more successful than the work performed by Costanza et al. (1997). In this ground-breaking study, monetary value was attached to the ecosystem services that may be extracted from specific areas of the planet. In this way, which pays direct homage to the avarice of humanity, it is possible to have a conversation about which parts of the planet may be optimally exploited for our benefit.

This is not to say that our dominance over the natural world should be assumed. Far from it. Humanity has raged against the bars of it's cradle for millennia, leading some to propose a new start of a new epoch, the 'Anthropocene' (Crutzen, 2002). A sardonic concept that belies control over the natural world. Rather, it is during this Anthropocene that not only have we begun to see the limits of our species' ability to overcome the barriers of the physical world, but how those barriers are beginning to fold in on us. The agency of humanity's destructive nature, like moths in a wardrobe, has gnawed away at the veil of deception we have, perhaps unknowingly, erected around ourselves. We begin now to view our world with a frank gaze with which we see, at every turn, ecosystems fraught with anthropogenic perturbations (e.g. Pasher et al., 2013; Hautier et al., 2015; Murray et al., 2015; Wakelin et al., 2015; Zhang et al., 2017). As our knowledge in this field of study grows, along with it rises a cacophony of pessimism on what, if anything, can actually be done to combat this issue (Kotiaho et al., 2015). And yet, this is only one small facet of the challenges that are ranged out ahead of us. The Holocene, the epoch preceding the Anthropocene, is noteworthy for the stability of it's climate, and how this afforded our species with the constancy we required to develop our civilisations (Dansgaard et al., 1993). Ironically, it is this very climatic stability that has

allowed us to raise ourselves up to great enough heights to sunder it. We are only now beginning to understand the depth of the impact that anthropogenic climate change will have on us, and the planet we must call home (IPCC, 2015). If we are fortunate enough to watch the dust settle, our only remark may be 'Et tu, Homo sapiens?'

Climate change

One of the first thorough explanations for how humans may effect a change in global climate patterns was first published by Sawyer (1972) in which it was outlined how the increased emission of CO₂ in the atmosphere could begin a feedback loop that may, by the year 2000, increase the global average temperature by 0.6°C. In the time since this has been introduced to our collective consciousness there have been a host of meetings and talks. Beginning perhaps in 1972 with the United Nations Conference on the Human Environment in Stockholm, Sweden, there was then a 20 year gap in global focus on this issue until 1992 when the Earth Summit was held in Rio De Janeiro. From that point onward, annual meetings have been organised by the United Nations Framework Convention on Climate Change (UNFCCC). The scientific base for these meetings has been provided by the Intergovernmental Panel on Climate Change (IPCC; IPCC, 1992, 1995, 2001, 2007, 2015)), which was established in 1988. Through these annual UNFCC meetings, supported by scientific research sourced by the IPCC, much progress has been made in identifying and better defining the problems that we as a human collective face with increasing urgency due to the anthropogenic forcing of our climate. These global summits, working groups, and collaborations were/are necessary to define the challenges before a group of people with disparate values, beliefs, and outlooks on life could begin to move forward in a unified direction. This is accomplished not only by making sense of all of the science swarming around the topic of climate change, but also by 'translating' this information into morsels that can be more easily digested by the minds of politicians and other policy makers.

The scope of global climate change, meaning specifically how historic climate patterns will be altered through anthropogenic forcing, is so vast as to be difficult for the human mind to grasp. Not simply the scale of the impact, but the complexity inherent in the interconnectivity of Earth systems being anthropogenically forced, and how those outcomes may affect the health of our planet. The introduction of 'planetary boundaries' by Rockström et al. (2009) was a leap forward in the structuring of this knowledge in a way that was directly relevant to the potential impact anthropogenic forcing may have. This concept, updated most recently by Steffen et al. (2015), aims to identify the several core (a)biotic processes on Earth that are instrumental for the continuation of life as we know it. Within each planetary boundary exists a safety level, based on the collective knowledge for each process, that should not be exceeded. Above these safe operating levels exists an area of uncertainty as to the risks posed by their exceedence. Determining an upper limit is difficult for most boundaries, but not all. The planetary boundary of biodiversity loss, as measured against expected background rates of species extinction, has assuredly been surpassed (Steffen et al., 2015). Likewise, the safe boundaries for the warming of the planet by greenhouse gas emissions and loading of the nitrogen cycle have also been surpassed. Of the several key boundaries identified in this work, Steffen et al. (2015) concluded that climate change and the integrity of the biosphere were centrally important to the continuation of a stable, Holocene-like climate, and that all other planetary boundaries operate within the continuation of these two primary boundaries. This means that whereas a planetary boundary, such as the mean saturation state of

aragonite in global surface seawater (one measure of pH, and an effect of ocean acidification), may have broad negative impacts on coral reefs (e.g. Hoegh-Guldberg et al., 2007), it is the loss of the biodiversity itself, or the warming of the atmosphere due to the same CO₂ that is lowering the oceans' pH levels, that may truly lead to the end of the Holocene. This example demonstrates that these boundaries are clearly inter-linked, and one may not research one boundary without considering others; however, the conclusion of Steffen et al. (2015), highlighting the importance of the changing global climate and biodiversity loss above everything else, directed the focus of this thesis in its effort to drive forward our understanding of the most ecologically threatening forces that South Africa faces, or may face.

Hot water

The work on planetary boundaries has been very productive in structuring our understanding of the threats we pose to ourselves via the destruction of the natural world; however, a centrally important criticism that may be made about the framework is that it has largely omitted the importance of the ocean in establishing the safe levels of operation for many of the planetary boundaries (Nash et al., 2017). Studies of anthropogenic impacts on ecosystems are generally split into land or sea, with each camp focussing predominantly on it's own area of expertise. Terrestrial ecosystems are more familiar to the general populace; however, marine ecosystems produce comparable levels of primary production (Chavez et al., 2011) and are most certainly at risk from a changing climate (Österblom et al., 2017). This has been seen in decreases to said primary productivity (Lewandowska et al., 2014), asymmetrical responses of predators and their prey leading to trophic 'turbulence' (Dell et al., 2014), and marine defaunation (McCauley et al., 2015). In conjunction with one another these changes may impact the food-web dynamics for every marine ecosystem on the planet (Hoegh-Guldberg and Bruno, 2010). Even more dire is the direct impact that climate change has on ecosystem forming species, particularly those found along the coast such as oysters, sea and salt marsh grasses, mangroves, and corals (Hoegh-Guldberg and Bruno, 2010). Rising temperatures may also allow for the increased spread of non-native species (Lord, 2017) and the outbreak of diseases (Altizer et al., 2013). In addition to these direct effects on biodiversity, the weakening of coastal marine ecosystems is problematic because several of them have the highest carbon sequestration rates on the planet (Mcleod et al., 2011) and the coastal ocean may increase the atmospheric CO₂ uptake of the global ocean by 24%. Within a South African context, a review by Mead et al. (2013) concluded that coastal ecosystems are at risk from anthropogenic climate change, and a review by Whitfield et al. (2016) concluded that changes in coastal biodiversity have also been observed. Given that these are critical planetary boundaries (Steffen et al., 2015), it was determined that impacts on the coastal ecosystems of South Africa should become the focus of this thesis.

It was then necessary to deduce which of the two critical planetary boundaries (Steffen et al., 2015) should become the primary focus of the investigation into the forces threatening coastal ecosystems. Referring to the literature on multi-dimensional studies of the physical forces acting on marine ecosystems, temperature is generally found to be either at, or near the top, of the list of the most fundamental drivers (e.g. Blanchette et al., 2008; Tittensor et al., 2010; Couce et al., 2012; Rodgers et al., 2015). Increases in global temperatures are one of the main focus points in climate science, and so a very large body of knowledge already exists on this topic (e.g. IPCC, 2015). Furthermore, temperature is relatively easy to measure compared to biotic indices and so may provide a more transparent appraisal of any threats posed. It is for these reasons, and my background in coastal temperature research, that I

decided to focus on the potential threats to South Africa's coastal ecosystems from climate change, rather than on biodiversity loss.

Even though an unprecedented amount of work has been done to unravel the potential negative impacts of climate change on the ocean, there remains an unending amount still to be done. In order to determine which aspect of climate change may be most relevant to coastal marine ecosystem health, it is necessary to first identify the different 'modes' of climate change and the threat level they pose. Once the most threatening mode of change has been deduced, one must then identify the different mechanisms driving this mode of change and how they may be defined, detected, characterised, and quantified. Only once the mechanisms responsible for the driving of the most dangerous mode of change have been identified will it be possible to develop effective adaptation strategies.

Modes of change

The anthropogenically forced warming of the climate, which has already negatively affected marine ecosystems with far-reaching consequences for humanity and natural ecological functioning (McCauley et al., 2015), may be divided into two 'modes'. Mode 1 is the familiar concept of the gradual long-term (decadal) trend in the rise of global mean sea surface temperatures (IPCC, 2015), which will continue for decades, if not centuries. Mode 2 is the changes in climate variability, manifested as increases in the frequency and severity of extreme events, which are now being acknowledged as a potentially greater threat (Thompson et al., 2013). These two different modes of climate change, the threats they may pose, and the knowledge that exists within South Africa for them are covered below.

Mode 1: decadal trends

Long-term (decadal) temperature trends are projected to have negative impacts on nearly all of Earth's systems and have thus far received the lion's share of focus in research (IPCC, 2015). In marine ecosystems, decadal temperature trends have been linked to changes in community structure (Bernardmo et al., 2015), fish stock collapse (Pershing et al., 2015), impacts on phenology (Asch, 2015) and the effects that may have on the timing of the arrival of migratory species (Ward et al., 2016). Model studies on the projection of decadal temperature trends have found possible changes in the spatial distribution and body size of pelagic species (Lefort et al., 2015), as well as an increased risk of extinction to both terrestrial and marine species (Urban, 2015). A meta-analysis of the effects of climate change on species distribution and phenology found the changes to be equitable to, or greater than those observed on land (Poloczanska et al., 2013). The long-term thermal trends along the coastlines of many parts of the world have been, or are being recorded (e.g. Freeland, 1990; Gómez-Gesteira et al., 2008; Shearman and Lentz, 2010) as generally greater than those reported for the open oceans (IPCC, 2015), meaning that coastal marine ecosystems around the world may be at greater risk of this mode of change than the open ocean.

Within a South African context, many researchers have contributed a very large body of work to the investigation of the effects/occurrence of climate change along the coast (e.g. Schumann et al., 1995; Rouault et al., 2010; Santos et al., 2012; Mead et al., 2013). This physical science base was used by Mead et al. (2013) for a review of the impacts on coastal marine ecosystems and biota in South Africa, which found that observed biotic changes may be linked to long-term temperature trends, though the predominant temperature trends along certain portions of the coastline are cooling, rather than warming. In a review by Whitfield

et al. (2016), changes in biodiversity could also be linked to long-term temperature trends. With all of this research dedicated to the investigation of long-term (decadal) trends in temperature on marine ecosystems it would appear conclusive that this is the most important mode of climate change to study. Recent work on the documentation of extreme events has begun to alter this perception.

Mode 2: extreme events

Extreme thermal events have been given a range of labels that may be broadly divided into two categories: cold-spells (*e.g.* Gunter, 1941; Lirman et al., 2011; Boucek et al., 2016) and heatwaves (*e.g.* Gordon et al., 1988; Stott et al., 2004; Perkins-Kirkpatrick et al., 2016). These rapid-onset extreme thermal events may begin, impact ecosystems, and end before they have been detected. Records of extreme events in the literature go back to the WWII era (Gunter, 1941), but only began to receive concerted attention roughly a decade ago when Jentsch et al. (2007) called the importance of this mode of climate change into focus. In the time since, steps have been taken towards understanding the drivers of these events, and the damage they may be causing. Extreme events have been linked to the formation of toxic algal blooms (McCabe et al., 2016), distributional shifts of intertidal alga (Harley and Paine, 2009), and of course the ever-ubiquitous bleaching of coral reefs (Schoepf et al., 2015). The importance of extreme events in the consideration of the effects of climate change on ecosystems is now beginning to be regarded as a necessity (Thompson et al., 2013). Furthermore, the long-term warming of the planet has been found to be increasing the likelihood of these extreme events (Diffenbaugh et al., 2017).

Within the context of South Africa, very little is known about extreme events. There have been very few prolific South African environmental scientists that have spent their energy/careers on the study of extreme climatic events for this region. Some thorough digging did turn up one recording of a potential extreme event having impacted the life cycle of the white mussel Donax serra Röding when surface water temperatures near Koeberg were significantly warmer than normal, inducing aseasonal sexual activity while inhibiting larval survival (Birkett and Cook, 1987). There is also anecdotal evidence that periods of prolonged warm surface water in False Bay damages kelp forests; however, as has been outlined above, the primary mode of climate change focussed on in South Africa's marine ecosystems has been long-term trends. Therefore, not only are the occurrence of extreme events almost completely undocumented, their potential impact on coastal ecosystems is virtually unknown. It is now becoming accepted that extreme thermal events pose the most proximate threat to ecosystems (Thompson et al., 2013), and this is why, of the two modes of climate change outlined here, I've chosen to focus on the latter. Linking the negative impacts of extreme events to biology is, unfortunately, beyond the scope of this thesis. But determining the causes of these extreme events is not.

Marine heatwaves (MHWs)

Historical context

Heatwaves have been gaining in notoriety over the past several years. The main reason for this likely being that we as humans can quite clearly determine for ourselves when a heatwave is occurring. It is not necessary for a meteorological service to inform us, as may be the case with more esoteric effects such as barometric pressure. Beyond this fact, it is also

something that can be, and is being quantified. Temperature, or more accurately heat content, is a very alluring field of study because it is a rather straightforward endeavour. As linear of a concept as one is able to find in the natural sciences. It goes up or down, but it cannot go side to side, though that may be a more poetic way of conceptualising climate change. Furthermore, as mentioned previously, temperature is generally found to be the most important abiotic variable for the structuring of marine ecosystems (*e.g.* Blanchette et al., 2008; Tittensor et al., 2010; Couce et al., 2012; Rodgers et al., 2015).

The term 'heatwave' has historically referred to atmospheric phenomena (Perkins and Alexander, 2013). One often finds vague definitions of these events, such as "a period of abnormally and uncomfortably hot [...] weather" (Glickman, 2000), but precise (though disparate) definitions based on statistical properties and other metrics of the temperature records that are relative to location and time of year have also been developed (e.g. Meehl, 2004; Alexander et al., 2006; Fischer and Schär, 2010; Fischer et al., 2011; Perkins and Alexander, 2013). Perkins-Kirkpatrick et al. (2016) give an excellent account of the history of the development of methods for the definition and measurement of these extreme events. It is, generally speaking, a rather new field of study, with few investigations into the development of statistical definitions of these extreme thermal events being more than a decade old, and much of the knowledge is being generated in Australia (Perkins-Kirkpatrick et al., 2016). It was not until Perkins and Alexander (2013) that a review of all of the definitions for heatwaves were catalogued and the first steps towards a globally acceptable definition of extreme atmospheric thermal events was developed. Based on the literature reviewed, Perkins and Alexander (2013) determined that an appropriate statistical definition of heatwaves should not be limited to static thresholds (e.g. 3°C above a given monthly mean), but rather should be pegged to percentiles. Specifically that the 90th percentile must be exceeded for at least three consecutive days. This simple outcome was a milestone in this work and has allowed it to grow into an international field of study for two primary reasons. The first was that this synthesis definition was simple to understand and to calculate. The second, and most important aspect of this work, was that one could apply this definition anywhere in the world. Because the definition now specifically focussed on daily values, this meant it was necessary to calculate daily climatologies, rather than basing these measurements on monthly climatologies (Schär et al., 2004). Due to advances in computing power the calculation of these daily climatologies and the implementation of the heatwave algorithm was not the issue it would have been a decade ago, which may have influenced the methodologies from which Perkins and Alexander (2013) synthesised their definition. A final aspect of the definition defined in 2013 was the consideration of the Excess Heat Factor (EHF) index. This was developed by Nairn and Fawcett (2013) and was designed to account for how warm an event may be in relation to the previous month in addition to the climatological 95th percentile used in a study.

As of Perkins and Alexander (2013), the world now had a very solid methodology for defining and measuring atmospheric heatwaves that could be applied to any time series anywhere in the world because it relied not on any global standard, but rather on the local daily climatology in question. This was a masterful stroke in science and its contribution to this field of research cannot be stressed enough. The only point of criticism to be levelled at it (somewhat unfairly) is that it only applied itself well to the definition of extreme thermal events in the atmosphere, but not as well in the ocean. In order to rectify this issue it was necessary to assemble an interdisciplinary task team because, just as with atmospheric science, many definitions for heatwaves had also surfaced in marine science (e.g. Mackenzie and Schiedek, 2007; Selig et al., 2010; Sura, 2011; Lima and Wethey, 2012; DeCastro et al., 2014).

Cold-spells, the other side of the extreme thermal event coin, have received much less attention throughout the preceding decades and perhaps for good reason. They have been shown to cause real ecological damage (Firth et al., 2015), but not to the same recorded extent as heatwaves (e.g. Wernberg et al., 2016). Additionally, in a warming planet, one may assume that the occurrence and severity of cold-spells are likely to decrease, and that heatwave counts and intensity should increase. These assumptions, coupled with the dramatic impact that extreme events have in the nearshore, make coastal marine heatwaves the most important facet of climate change to focus on within the problem that this PhD thesis aims to address.

Current definition

Building on the pioneering work of Perkins and Alexander (2013), Hobday et al. (2016) developed a statistical definition of what would constitute a 'marine heatwave' (MHW). Because this was based directly on the work of Perkins and Alexander (2013) it differed little in kind. In practice, the only concrete difference between the two was that MHWs must last for at least five consecutive days, with no more than a two day 'pause' in consecutive temperatures above the 90th percentile, as well as the removal of any consideration of EHF. Specifically, Hobday et al. (2016) defined a MHW as "a prolonged discrete anomalously warm water event that can be described by its duration, intensity, rate of evolution, and spatial extent", which was accompanied by statistical metrics that quantify the properties laid out in their definition. For example, the count of MHWs within a time series and their maximum and cumulative intensity are quantifiable parameters that can be calculated in an objective and consistent manner irrespective of geographical location. This also meant that because MHWs were compared against daily climatologies, an event could occur during any time of year, not just summer.

I have chosen to use the definition as well as the methodology laid out in Hobday et al. (2016) for the analysis of MHWs in this thesis. The algorithm developed by Hobday et al. (2016) requires daily time series data, and it isolates MHWs by first establishing the daily climatologies for the given time series. This is accomplished by finding the range of temperatures for any given day of the year, and then pooling these daily values further with the use of an 11-day moving window, across all years. From this pool are calculated two statistics of interest: the first is the average climatology for each day, and the second the 90th percentile threshold for each day. When the observed temperatures within a time series exceed this threshold for the required number of days it may be classified as a discrete event.

In order to calculate a MHW it is necessary to supply a climatology against which daily values may be compared. It is proscribed in Hobday et al. (2016) that this period be at least 30 years. By calculating MHWs against the daily climatologies in this way, the amount they differ from their localities may be quantified and compared across time and space — the implication is that this allows researchers to examine events from different variability regimes (*i.e.* regions of the world, seasons) and compare them with a consistent set of MHW metrics.

Impacts

Several large MHWs, and their ecological impacts, have been well documented. One of the first MHWs characterised occurred in 2003, and it negatively impacted as much as 80% of the Gorgonian fan colonies in the Mediterranean (Garrabou et al., 2009). A 2011 MHW is now known to have caused a permanent range contraction by roughly 100 km of the ecosystem

forming kelp species *Ecklonia radiata* in favour of the tropicalisation of reef fishes and seaweed turfs along the southern coast of Western Australia (Wernberg et al., 2016). The damage caused by MHWs is not confined to demersal organisms or coastal ecosystems, as demonstrated by a MHW in the North West Atlantic Ocean in 2012 that impacted multiple commercial fisheries (Mills et al., 2013). When extreme enough, such as 'The Blob' that persisted in the North West Pacific Ocean from 2014 to 2016, a MHW may negatively impact even marine mammals and seabirds (Cavole et al., 2016). Besides increases in mortality due to thermal stress, MHWs may also lead to outbreaks of disease in commercially viable species, such as that which occurred during the 2015/16 Tasman Sea event (Oliver et al., 2017a).

With all climate projections showing a warming planet, one could be forgiven for assuming that MCSs should become less frequent; however, examples of increased frequency in some specific localities do exist (*e.g.* Gershunov and Douville, 2008; Matthes et al., 2015). Lethality in marine ecosystems has been recorded for these events (Woodward, 1987), including mass kills of fish (Gunter, 1941, 1951; Holt and Holt, 1983) or invertebrates (Gunter, 1951; Crisp, 1964), the death of juvenile and sub-adult manatees (O'Shea et al., 1985; Marsh et al., 1986), as well as coral bleaching (Lirman et al., 2011). But it's not just the sudden lethality of MCSs that is a concern, species population distribution limits are often set by cold temperature boundaries, most specifically those ranging towards higher latitudes (Firth et al., 2011). It is for these reasons that impacts at the population level may aggregate into forcing on an entire ecosystem (*e.g.* Kreyling et al., 2008; Rehage et al., 2016). This ecosystem-wide impact of MCSs on a specific population has in fact been documented with ecosystem engineering mussels (Firth et al., 2011, 2015).

The temperature of the water at the surface of the ocean, better known as sea surface temperature (SST), is influenced largely by oceanic and atmospheric processes (Deser et al., 2010). How these processes are modulated from broad-scale to the more local-scale forcing required for a coastal MHW has yet to be determined. There is some strong documentation for the direct effect of atmospheric forcing that has lead to coastal MHWs (e.g. Garrabou et al., 2009) or MCSs (e.g. Gunter, 1941; Firth et al., 2011). This could lead one to hypothesise that coastal extreme events may be forced by anomalous atmospheric conditions; however, oceanographic influence on the formation of coastal MHWs has also been documented (Feng et al., 2013), meaning that no one clear pattern of forcing exists with regards to the cause of these events. Furthermore, atmosphere-ocean coupling is known to be affected by climate change, likely leading to conditions that will be favourable of upwelling and the winds that force that phenomenon (García-Reyes et al., 2015). This possible increase in upwelling may lead to detection of more MCSs simply because these cold temperatures caused by aseasonal upwelling will stand out against the historic climatologies. An additional consideration for the possible cause of MHWs is the abnormal advection of warm water onto the coast due to anomalous behaviour of nearby ocean currents (e.g. Mills et al., 2012; Feng et al., 2013; Benthuysen et al., 2014; Chen et al., 2014, 2015).

That ecosystem change may be effected by the two versions of extreme thermal events is clear. It is not known at all what impact these events are having along the coastline of South Africa, but they almost assuredly are having some. For this reason it would be useful for conservation and management purposes that a mechanistic understanding of their drivers be developed. Hobday et al. (2016) has done an immense service to the scientific community in the development of the MHWs algorithm, but the metrics that measure an extreme event do not actually reveal what the driver of that event may be. One must therefore develop a methodology and pursuant understanding of what these potential local-scale and/or

broad-scale drivers may be. This thesis aims to unravel the relationship of anomalous thermal events and their abiotic forcing mechanisms at different scales along the coast of South Africa.

Study area

The area of study for this thesis will focus on the coastline of South Africa, a roughly 3,000 km expanse. The annual mean (\pm standard deviation; SD) coastal seawater temperatures found there range from 12.3 \pm 1.2°C at the border with Namibia to 24.4 \pm 2.0°C at the Mozambican border. This coastline is particularly interesting as it is bordered by the Benguela and Agulhas currents (*e.g.* Roberts, 2005; Hutchings et al., 2009). These massive oceanographic features, taken in combination with other nearshore processes, affect the country's marine coastal ecosystems (Santos et al., 2012). In fact, these processes provide a natural laboratory along the coastline, allowing for a range of quantifiably different physical forces to be considered with regards to the formation of MHWs.

Ocean

The two major oceanographic features in the study area, the Agulhas and Benguela currents meet south of the subcontinent. There is no fixed border at which this occurs, rather these features fluctuate from a western-most border at the Cape Peninsula and an eastern-most border on the Agulhas Bank. These two monumental currents play an overwhelmingly important role along the coast, being the primary drivers behind most (a)biotic coastal processes (Roberts, 2005).

The Agulhas Current tends to retroflect back into the southern Indian Ocean (Hutchings et al., 2009) after moving south of the wide Agulhas Bank (Roberts, 2005), but it regularly influences the thermal regimes of the coastline as far as False Bay (Day, 1970). The Agulhas Current retroflection is largely influenced by interactions with the Benguela Current, an Eastern Boundary Upwelling System (EBUS) (Hutchings et al., 2009), but is not a constant feature and will, from time to time, force it's way through to the South Atlantic Ocean. When this occurs it is known as 'Agulhas Leakage' and spills warm saline bodies of water, typically eddies of some sort, into the Atlantic Ocean, where they go on to potentially influence much of Earth's climate via a complex network of teleconnections (Beal et al., 2011).

The statistical properties of the coastal waters tend to separate out into three distinct sections; 1) the cool temperate west coast, 2) the warm temperate south coast, and 3) the subtropical east coast (Smit et al., 2013). Though the west coast is classified as cool temperate (Hutchings et al., 2009), there are many points (e.g. Saldanha Bay) that often cross over into warm temperate thermal regimes for much of the year. In stark contrast to the cool west coast is the warm temperate east coast section. The dominating influence for this stretch of coast-line is the Agulhas Current, which moves tightly along the narrow continental shelf that is a trademark of this area (except for the Natal Bight) (Lüning et al., 1990). The thermal regime of the east coast is more homogeneous than anywhere else and is also characterised by much less annual variance than the other coastal sections in the study area. Situated between west and east one may find the south coast, which is largely dominated by the Agulhas Current, but experiences much more annual variance than the east coast.

Atmosphere

The atmosphere throughout the study area is dominated by two anticyclonic high pressure cells with quasi-stationary positions. The first of these, the South Indian Ocean High, may be found in the east, drawing warm, moist air towards the subcontinent (Van Heerden and Hurry, 1998). The second of these features, the South Atlantic Ocean High is situated to the west, drawing cool, dry air onto the west of the subcontinent (Van Heerden and Hurry, 1998). A third feature, the prevailing westerly winds, blows south of these two high pressure cells and tends to follow their annual migration north during winter and south over summer (Van Heerden and Hurry, 1998).

Besides the more predictable seasonal cycling of these features, solar heating over land in summer may allow for the development of pockets of low pressure, known as heat lows, that are absent during winter (Tyson and Preston-Whyte, 2000). These heat lows may then allow the two anticyclonic pressure cells to connect (Van Heerden and Hurry, 1998) across the subcontinent. During winter months, when the anticyclones have shifted north, the cold westerlies are able to have a greater impact on the weather of the southern tip of the subcontinent (Van Heerden and Hurry, 1998).

The temperatures in the atmosphere along the coastline are greatly influenced by either the Benguela Current (cold) on the west coast, or the Agulhas Current (warm) along the rest of the coastline (Van Heerden and Hurry, 1998). Conversely, the upwelling that is so typical of the west coast, and certain stretches of the south and east coast may be forced by atmospheric conditions (Lutjeharms et al., 2003; Roberts, 2005; Hutchings et al., 2009).

Remote vs. in situ

Temperature plays a large role in the structuring of biodiversity in the ocean (Schils and Wilson, 2006). Therefore, a clear understanding of the relationship between marine ecosystems and their thermal regimes is necessary for conservation planning, and in a time dominated by anthropogenic perturbations to the climate system, future patterns in biodiversity and ecological function may also be estimated from projected climate scenarios. Irrespective of the objectives of biogeographical studies or studies of climate change/variability, it is of paramount importance that the research is underpinned by reliable, accurate and precise temperature data. Unfortunately, not all data are created equal, and not all datasets are usable for a given task. Because the central aim of this thesis is the understanding of the drivers of coastal MHWs, it is necessary to ensure that temperature data are not only reliable, but appropriate for application to the monitoring of coastal thermal processes.

The collection of seawater temperature is either performed remotely, generally via satellites, or through more direct approaches, such as hand-held thermometers. I will cover these two different sources below, discussing their strengths and weaknesses.

Remote data

Good data are often difficult to obtain, and once obtained, it seems that they are even more difficult to maintain. To this end the scientific community tends towards the path of least resistance when using data not central to their hypotheses. In the natural sciences it is often abiotic data that are the victim of this nonchalance. This lack of scrutiny has led to decades of use of remotely-sensed gridded SST products for investigations into coastal ecology, phenology and oceanography. It is now known that these remotely-sensed data may be prone

to inaccuracies along the coast and that *in situ* data must be used in their place whenever possible (Smit et al., 2013); however, it is important to determine what exactly the limits of the use of these gridded data are as they are still a crucially important resource.

Remotely-sensed SST products are produced by a number of well-respected organisations around the globe. Cutting-edge technology is launched into space in order to gaze back down upon Earth and detect, amongst other things, the infra-red light being emitted by the ocean. This irradiance is then taken as a proxy for SST. Due to the distance at which these instruments are measuring the surface of the earth, a certain coarseness is unavoidable. This is best interpreted as the size of the pixels one sees in the final product. This gridding is necessary, and generally not an issue, as long as one is measuring phenomena in the open ocean.

Remotely-sensed SST products undergo a number of quality control and validation processes that are well documented (*e.g.* Reynolds and Smith, 1994; Brown et al., 1999; Martin et al., 2012), making their use more attractive as one must not be concerned with inconsistencies introduced into a study via these abiotic data. However, as previously mentioned, it has now come to light that the use of these data for coastal applications, as proposed for this thesis, is not recommended (Smit et al., 2013).

The extent of the bias in remotely-sensed SST over or under *in situ* measurements has not been well documented across the globe; therefore, there is little in the literature pertaining to this issue outside of a handful of papers that have looked at these discrepancies (Hughes et al., 2009; Smale and Wernberg, 2009; Castillo and Lima, 2010; Dufois and Rouault, 2012; Smit et al., 2013). As one would imagine, the idea that remotely-sensed SST values should be abandoned, or at least used with great care, for coastal science has been met with a certain measure of resistance from investigators who have built their careers upon the use and interpretation of satellite data. There are not currently any published rebuttals to the findings of Smit et al. (2013), though at conferences (such as GHRSST) the general sentiment is that remotely-sensed SST products may show a warm (or cold) bias, but they are still more useful when one is investigating broader swathes of the ocean. While it is my opinion that this statement is accurate, it serves to illustrate the underlying issue at the heart of this debate. Many of the researchers that are producing remotely-sensed SST products are mathematicians and engineers, not biologists/ecologists etc. To this end they often underestimate the importance of the localised events that the post-processing of these products is known to smooth out (Reynolds et al., 2007). In addition to this oversight in the cleaning algorithms that remotely-sensed data must face, the coarseness of the gridding of these products also leads to a phenomenon known as 'land bleed'. When a pixel overlaps both land and sea it is generally detected by the satellite and correctly thrown out. Depending on the size of the pixels, this then creates a very large 'shadow' along the coast of missing temperature data. It is within this shadow that many important coastal ecosystems may be found.

As one may have assumed, not all remotely-sensed products are created equal, and therefore not all of them demonstrate the same level of bias against *in situ* data. Smit et al. (2013) tested a range of remotely-sense products against *in situ* data along the coast of South Africa and found MODIS to have the least amount of bias. Meaning that if one is bereft of the use of *in situ* data for coastal studies, MODIS SST data should be the best choice. Overall, however, it is the the 1/4° NOAA Optimally Interpolated SST (OISST; Reynolds et al., 2007) product that is preferable for use in climate change studies. This is because even though the resolution of the temperature records is coarser spatially, the length of the product is much greater, dating back to late 1981, as opposed to late 1999 for MODIS data.

In situ data

The succour a well-maintained coastal *in situ* seawater temperature dataset would provide for the scientific community of South Africa would be very far-reaching, as much biological/ecological research requires coastal temperature data. The availability of such a dataset would also have an effect backward through time as an immense body of work would stand on perilously shaky legs, waiting for investigators to (in)validate decades of coastal research performed with temperature data that are now known to be biased (Smit et al., 2013).

Just such an in situ coastal seawater temperature dataset, known as the South African Coastal Temperature Network (SACTN), was constructed by Smit et al. (2013), following on from the initiation of the project by Roberts et al. (2011). At the time of this writing, the SACTN dataset consisted of 135 time series, ranging in length from less than 1 year to over 44 years, and covered the entire expanse of the South African coastline. Even though Smit et al. (2013) performed a thorough comparison of these data against multiple remotely-sensed products, the ability of the SACTN to be used instead of remotely-sensed SST products for nation-wide applications, as would be desirable, must be verified as the methods and standards that control for the collection of local in situ data from a single site may differ greatly. This is because seven different bodies (governmental, academic, and semi-private) contribute data to the SACTN, with each using its own instruments and methods for data collection. One particularly problematic outcome of this methodological sampling disparity is that, due to the prolific work of SAWS and KZNSB, two thirds of the SACTN time series were sampled with with hand-held thermometers, a manual recording process with a data precision of 0.500 °C. The current global standard is to use digital underwater temperature recorders (UTRs), having data precisions as fine as 0.001 °C (Jarraud, 2008).

Using these *in situ* temperature data *in lieu* of remotely-sensed SST data requires that the underlying characteristics of the contributing data sources are understood so that one may be certain how useful, reliable, or accurate these long-term measurements are for use in climate change studies such as those proposed in this thesis. To do so with the SACTN data would require that the measurement precisions and statistical characteristics of the data from the different contributing bodies be assessed against a rigorously defined methodology that would allow for the production of reproducible results. If one may be certain about the detection of decadal trends, one of the more elusive metrics in climate science, it would allow for more certainty in the ability to accurately detect shorter, if not larger signals, like MHWs.

It must also be mentioned that nearly all of the time series within the SACTN do not have meta-data records that meet the international standards for climate change research (Aguilar et al., 2003). Specifically there is a dearth in the recording of the instruments used for each time series, the drift of said instruments (Jarraud, 2008), who was sampling, and where the exact locations of samples were taken through time. It is at least known that all of the thermometer time series were sampled with thermometers, and the UTR time series with UTRs. Given these meta-data issues, work has been initiated to develop a nation wide standard of collection that has been under way since 2015. This includes but is not limited to: the recording of the serial numbers for each instrument used at each site, the upgrade from thermometers to UTRs, and the inclusion of digital data management techniques.

Problem statement

Extreme thermal events, known as MHWs, and detected with an algorithm defined by Hobday et al. (2016), have been shown to be responsible for ecosystem-wide damage to sections

of coastline throughout the world. It should therefore be assumed that these destructive events may be occurring along the coastline of South Africa as well, and a record of when they occurred and what their drivers were must be created. Several papers have been published on the causes of specific, high-profile MHWs (Garrabou et al., 2009; Feng et al., 2013; Pearce and Feng, 2013; Benthuysen et al., 2014; Bond et al., 2015; Oliver et al., 2017a), showing that a range of drivers may be responsible for events. Considering that the history of MHWs along the coast of South Africa has yet to be calculated, a methodology that is able to attribute the drivers of more than one event at a time would be desirable as it would otherwise not be practical to go through each event individually. The determination of the drivers for the events that have occurred along the coastline of South Africa will require that three problems be addressed. The first is that the *in situ* data to be used for the detection of coastal events must be validated. Next, the occurrence of events detected in situ along the coast must be compared against remotely sensed or modeled data from the same areas to determine the similarity between the sub-mesoscale coastal in situ data and the mesoscale remotely sensed or modeled data. It is necessary to quantify the potential relationship between these datasets because the final problem that needs to be addressed is the determination of how large the required scale is in order to understand the drivers of these events. Should the relationship between the datasets be weak, a much larger scale will need to be used in order to detect drivers that may be responsible for multiple events.

Aims

It was the Aim of the current chapter to provide a thorough review of the literature relevant to the following published studies and to provide context for the importance of the undertaking proposed. The research portions of the thesis are presented as three research papers in Chapters 2-4. The attendant aims, objectives and hypotheses for these studies are outlined in the following three subsections. The final chapter in this thesis will briefly recall the aims of the three studies and discuss the contributions to human knowledge made by them. It will then delve into the limitations to the research that have been clarified through hindsight, before concluding with ideas for further research.

As our societies move forward out of the information age and into the age of 'Big Data' it is necessary that our science follows suit. To this end, it is no longer acceptable to perform scientific enquiries with the 'business as usual' model. Specifically I am referring to the use of 'pointy-clicky' user interfaces. This encapsulates many things, the most inveterate being Microsoft Excel. This is an issue because it inhibits the proper production of reproducible research. This is not a contentious opinion to have, and yet so little scientific enquiry is performed with the use of command-line programming languages, at the express loss of reproducibility. By using a command line programming language, such as R (R Core Team, 2017), one may ensure that all steps taken in an analysis are known explicitly and may be reproduced with 100% confidence. I was employed as a research assistant for the year preceding this thesis and so was already competent in R; however, the further development of the knowledge and skills necessary to meet the demands of the published studies became an additional aim for this thesis. How this aim was further developed during each of the subsequent studies will be covered in turn.

Study 1

Before using the SACTN data for detecting coastal MHWs, it was necessary to perform additional quality control checks on them. Besides documenting the extent to which these data

adhere to the current global standard for climate change research (Jarraud, 2008), it was also useful to see how consistent with global change the coastline of South Africa is, with the assumption that many outliers would imply issues with the data. This can be accomplished by determining the decadal trends found in the time series. This then would allow for the verification of the SACTN data and their use for climate science.

The detection of these decadal trends, while interesting, is not a full study worthy of publishing. Therefore the primary aim of the first study was to determine not simply what the decadal trends are, but which variables of the SACTN time series most greatly affected a model's ability to detect the trends therein, and therefore which variables most greatly contribute to effective use of these data for climate change research. It was hypothesised that the properties most likely to have an influence on the detection of decadal trends would be: length, trend steepness, variance, proportion of missing data, and measurement resolution. The testing of this hypothesis will be made possible through a series of controlled experiments that allow one to pick out specific variables and manipulate them in isolation from the other variables within a time series.

A necessary objective for any time series analysis is that any dubious outliers or otherwise inconsistent time series must be addressed. The correcting of any such issues in the SACTN data will allow them to be compared with more fidelity against remotely-sensed SST data in the following studies. Once cleaned up, the data may then be divided into their respective coastal groupings via ordination/ hierarchical clustering methods, allowing for the following studies to appraise different regional effects within the data.

Taken together with the built-in fidelity to reproducible research, R also provides native support for version control capabilities. Most relevant to this thesis is the online resource GitHub ¹. This technology allows one to fully track and record all steps taken during the creation, implementation and editing of the code developed for an analysis. Furthermore, this resource was designed at its base to promote collaboration. Indeed, this is the reason it was initially created. A long-time staple of most tech related companies, it has been a long time coming, but finally this tool is making it's way into environmental sciences. The integration of the computer code written for this first study into Git was the first R related aim for this thesis.

Study 2

The primary aim of the second study was to determine the rates of co-occurrence of MHWs occurring along the coastline of South Africa between the nearshore (<400 m from spring low-tide) and offshore. The only dataset appropriate for the measurement of these nearshore temperatures is the South African Coastal Temperature Network (SACTN), as first detailed in Smit et al. (2013). Once the aim of the first study is achieved, that of validating the use of the SACTN, it will then be possible to begin to investigate the physical variables that could be forcing extreme thermal events along the coast. That Smit et al. (2013) were able to so succinctly show the massive biases between *in situ* and remotely-sensed data begged the questions: A) What is the nature of the difference in terms of its oceanographic drivers in space/time? B) How does mesoscale oceanic forcing influence seawater temperature properties/processes <400 m from the coastline? It was decided that an investigation seeking to answer these questions, taken with the historical records of the occurrence of every thermal event recorded along the coastline of South Africa for both data types would be an effective first step at determining what proximate thermal forces may be driving events along the

¹https://github.com

coast. To this end, the SACTN dataset and the 1/4° NOAA Optimally Interpolated SST (OISST; Reynolds et al., 2007) datasets shall be used to investigate the co-occurrence of marine heat waves (MHWs) and marine cold-spells (MCSs) with the methodology introduced by Hobday et al. (2016). This comparison will also serve as an example of a practical (citable) application of the SACTN. It will also allow for a novel approach to understanding the patterns of local oceanography along the South African coast and the implication anthropogenically forced climate change has for the changes in these patterns and long-term trend.

Besides allowing for the complete tracking of progress and providing the most comprehensive platform for digital collaboration available to our species, the pairing of R with Git also allows for complete transparency. This means that not only is every step in the workflow recorded in detail for the benefit of the author(s), but openness and seamless collaboration are performed automatically while allowing for the immediate dissemination of the work performed. The second R related aim for this thesis was to further develop my ability to collaborate with co-authors from around the world with these tools.

Study 3

It is hypothesised that much of the mesoscale activity happening along the coastline of South Africa does not link directly to the sub-mesoscale activity happening at the coastline. To investigate this hypothesis further required a quantified comparison of where along the coastline and under what conditions one may see agreement between sub-mesoscale and mesoscale phenomena. This was the aim of the third study and was achieved by comparing the historical *in situ* coastal MHW records against very large swathes of remotely-sensed products further from the coast. By looking for patterns in these synoptic scale states of both air and sea around South Africa during coastal MHWs measured *in situ*, combined with the knowledge gained from the completion of the previous aims, one may then arrive at the first findings that some common synoptic states do or do not exist between many individual events across time and space. This is the real prize as this information may then be taken by ecologists/conservationists and used to motivate for the development of effective conservation policies that are grounded in sound science.

In order to accomplish the objectives of the final study, my talents in R would need to ratchet up several notches. These objectives include the aggregation of very large remotely-sensed datasets for the creation and analysis of the synoptic states therein, the integration of several different statistical analyses into one seamless workflow, and the fully automated creation of complex atlas figures displaying a wide range of statistical outputs and visualisations. This then would be proper data science.

The benefits of the use of R and Git I have outlined above are not recent developments, rather they serve to address the traditional concerns of good scientific practice. The really exciting applications of this technology are still developing. This ranges from the abilities to immediately publish one's work as a simple blog, an entire website, or even a software package. These rather pedestrian developments only belie the limitless scope of developmental potential. Interactive web applications. Automatic enquiry. Fields of science that can take quantum leaps forward based on the seamless and automatic integration of citizen science with machine/deep learning. This PhD thesis only touched on some of the benefits that are represented by the tools I have learned to use. The next level of much of this work will be to see how large the future scope may rapidly and efficiently become. In order to allow for the planning of this eventuality, much focus was given towards the effective writing, development and storage of the code used for all of the analyses in this body of work.

Analyses

As the investigations performed throughout this thesis varied in their focus, it was necessary to employ several different analyses. The one common thread uniting all of them was that they were conducted in the programming language R (R Core Team, 2017). This ensures openness, accountability, and reproducibility for all work performed. It also allows for the tailoring of analyses after the articles from which they were inspired without having to use any 'out of the box' software. This is particularly relevant here as all of the different analyses central to this thesis, detailed below, are not available across any one specific software. With perhaps the exceptions of Python and MATLAB.

Trend modelling

There are two broad approaches to the modelling of trends in climate change research (IPCC, 2015). The first of these methods, the estimation of linear trends, is perhaps not the best measure of reality (*i.e.* true trends are almost never truly linear), but one is able to interpret and quantify the output of a linear model very easily. The other broad method of trend estimation, non-linear modelling, is a more realistic approach to trend estimation, and generally relies on complex statistical practices like higher-degree polynomials or non-parametric smoothing splines (Wood, 2006; Scinocca et al., 2010). Besides utilising statistics that are more opaque than those employed with linear modelling, the output of non-linear models is often difficult to interpret, and even more challenging to quantify. Taken by itself, a non-linear model of the decadal trend at a particular site is ideal; however, if one wishes to compare results between sites, or as is relevant to this thesis, between datasets, a linear model is required.

Both modelling types may be appropriately coerced to account for the serial autocorrelation of temperature time series that is often a criticism of climate science due to the effect this may have on trend estimation uncertainty (von Storch, 1999; Santer et al., 2008). One method that may correctly capture serial autocorrelation in linear modelling is Generalized Least Squares (GLS), with Generalized Additive Mixed Models (GAMM) being a non-linear alternative (Pinheiro and Bates, 2006; Wood, 2006). Because this thesis needs to be able to compare results between sites and datasets, it is necessary to use GLS for the modelling of any long-term trends. Furthermore, it is known that the model selected to detect a trend in a time series may greatly influence ones results (Franzke, 2012). For this reason it will be very important that not just the correct type of model, but also the correct correlation structures be used to maximize the model's ability to faithfully detect trends. This will be accomplished during the first study in this thesis.

Event detection

As outlined previously, the extreme thermal events along the coast of South Africa, which are central to this thesis, will be detected, quantified and recorded with the algorithm developed by Hobday et al. (2016). The events recorded in the *in situ* data from the SACTN will be compared against those detected in remotely-sensed data, allowing for additional insight into the bias seen between the different types of data. Due to the unique oceanography of the study area, this will allow for the consideration of nearshore influences as well as the forcing of two major ocean currents when looking for potential links between the different datasets.

The original algorithm constructed for Hobday et al. (2016) was done in the form of Python script². Because all of the work in this thesis was done exclusively in R, the R package 'RmarineHeatWaves' (Smit et al., 2017) was used to calculate the extreme events instead. A demonstration found within the R package shows that results do not differ from the Python code on which it is based. Recording the individual events is a rather straightforward task, but is not enough for the calculation of long-term trends. In order to provide the basis for these calculations, the metrics for the events must be aggregated into mean values based on the year in which they occur. With these annual values it is then possible to calculate long-term trends in extreme events.

Ordination

The final aim of this thesis seeks to show that there are recurrent patterns in air and/or sea during coastal MHWs. Before doing so it will be necessary to test the hypothesis that the synoptic patterns around South Africa do differ from 'normal' days when no extreme events are occurring. There are many potential ways to do this, but I posit here that the most effective method is through ordination. Specifically through the use of Nonmetric multidimensional scaling (NMDS). It should be noted up front that the goal of NMDS is not to perform some statistical analysis of the difference between days with and without extreme events. Indeed, NMDS does not provide any such result (e.g. a p-value). Rather it allows the user to visualise how all of the different values (days with or without events) differ from each other in a two dimensional space. And it is this final consideration that sets NMDS apart from other traditional ordination techniques, such as Principal Component Analysis (PCA). PCA determines different layers of variance and quantifies their orthogonal relationship to the most predominant of them, whereas NMDS simply squashes everything down to only two axes (Paliy and Shankar, 2016). This provides a 'what you see is what you get' output, ensuring that even though this technique is not commonly used in climate science, it is not overly difficult to understand. In addition to this ease of use, NMDS is also one of the most robust unconstrained ordination methods (Minchin, 1987).

I think this is a rather convincing argument for NMDS, but there is still one more reason/benefit for this analysis. The categorical variables attached to events may also be displayed on the results of the NMDS, known as a bi-plot, as vectors. The length and direction of the individual vectors may be taken together to infer yet another layer of information from this analysis. All of these ordination techniques are able to be carried out with the single R package 'vegan' (Oksanen et al., 2017). The appeal of reducing the variability of all of this data to only two dimensions is massive; however, it must be made very clear that the *x* and *y* axes of the resultant bi-plot do not relate to any specific variable from the data. The interpretation of the NMDS results requires expert knowledge on the part of the user to effectively pull out their meaning. In this case, whether or not 'normal' days are different from those during which a MHW occurred.

Clustering

There are many ways to cluster data and a complete summary of them would be beyond the scope of this introductory chapter. If one is interested in learning more, Jain (2010) provides a very comprehensive summary. The two most common systems of clustering in use today

²https://github.com/ecjoliver/marineHeatWaves

³https://github.com/ajsmit/RMarineHeatWaves

are K-means clustering and hierarchical cluster analysis (HCA). K-means clustering may be familiar to the reader from images of scatterplots with circles drawn around certain apparent clusters in the data. HCA produces the well known (perhaps notorious) dendrogram. In climate science, K-means clustering (*e.g.* Corte-Real et al., 1998; Burrough et al., 2001; Kumar et al., 2011) tends to win out over the use of HCA (*e.g.* Unal et al., 2003). That being said, they are both seemingly being replaced by the increasing popularity of self-organising maps (SOMs) (*e.g.* Cavazos, 2000; Hewitson and Crane, 2002; Morioka et al., 2010).

The first step of the SOM analysis, initialisation, is similar to K-means clustering in that the user specifies how many clusters (hereafter referred to as nodes) the computer must randomly assign all of the data into (Hewitson and Crane, 2002). This technique differs from more traditional techniques in that, upon iteratively finding better and better matches for each data point in one of the given clusters, the SOM algorithm also considers how well the newly formed clusters fit with one another (Hewitson and Crane, 2002). In this way the SOM algorithm is able to 'learn' how best to cluster the data within and between clusters, something not possible with other techniques. The benefit of this additional layer of competence is that one may now see the range of different patterns that may be present in the many synoptic states fed into the algorithm in a way that is visually accessible to the user (e.g. Gibson et al., 2017). It is this clustering of synoptic states within and between SOM nodes that will allow for the final aim of this thesis to be accomplished, the determination of predominant atmospheric and oceanographic states during coastal MHWs.

Contribution to knowledge

The current knowledge on climate change trends in the coastal waters surrounding South Africa have been almost exclusively derived from remotely-sensed gridded SST products (*e.g.* Schumann et al., 1995; Rouault et al., 2010). Newer remotely-sensed gridded SST products are approaching high enough resolutions for use in coastal waters; however, the longer running (older) products that could be used for the detection of long-term trends are not (*e.g.* Chao et al., 2009; Qiu et al., 2009; Vazquez-Cuervo et al., 2013). This, coupled with the work done by Smit et al. (2013), showing that remotely-sensed gridded SST data have a large warm bias in the nearshore when compared against coastal *in situ* data, motivate for the necessity of the calculation of decadal temperature trends in the nearshore with said *in situ* data. The initial aim of this thesis will act as a first step toward providing this crucial information.

The continued aggregation, refinement, and promotion of the SACTN will allow not only for the creation of these needed measurements of decadal temperature trends along the coast, they will also promote better science in coastal ecology. It is necessary that we shake off the historical use of satellite and/or model-generated temperature data for use in any enquiries along the coastline (e.g. Blanchette et al., 2008; Broitman et al., 2008; Tyberghein et al., 2012). This continues to be an issue either because investigators are not aware of the pitfalls that remotely-sensed data present, or they simply do not have access to a good *in situ* collected coastal seawater temperature dataset. The creation of just such a resource, the SACTN, will be ensured through the completion of this thesis.

The final and most substantial contribution to human knowledge that this thesis will make is in the understanding of which forces are driving coastal MHWs along the coastline of South Africa. This will be accomplished by combining a number of different statistical analyses, all outlined above, together in a novel way. The resultant patterns pulled out

by the novel methodology developed within this body of work may then be taken by ecologists/conservationists for focussed applications.

Research assumptions

The central assumption of this project was that remotely-sensed gridded SST and *in situ* time series may be compared. They are intrinsically different and therefore detractors of this new field of research will naturally incorporate this observation into their counterarguments against the findings of this thesis. It is also being assumed that for the purposes of nearshore investigations, *in situ* temperatures are more accurate than their SST counterparts. When one exceeds 400 m from the high tide line, the accuracy of SST values can be considered less biased (Smit et al., 2013). It is for this reason that the study area for this project has been confined to the nearshore (<400 m) strip of coastal water along South Africa.

An additional assumption to this research focussed on the forcing of extreme thermal events. Most research into the driving of MHWs around the world has shown that some mesoscale thermal oceanographic or atmospheric force, acting anomalously, had lead to the event in question (*e.g.* Garrabou et al., 2009; Feng et al., 2013; Pearce and Feng, 2013; Benthuysen et al., 2014; Oliver et al., 2017a). Some research has pointed towards other physical variables, such as sea level pressure (Bond et al., 2015), but for the purposes of this thesis it has been decided to focus predominantly on thermal influences. Outside of the types of variables driving these events, assumptions as to the scale of the forcing have also been made. Because little to no globally consistent understanding of the scope of the driving of events exists, especially along the coast, the second study in this thesis will focus on local causes, and the third study will look at a much larger synoptic scale, as required.

Conclusion

MHWs around the world have been documented to have caused extensive damage to coastal ecosystems. It may therefore be assumed that the same is happening in South Africa. For this reason, our knowledge of these extreme events within this country must be expanded upon. Currently nothing is known about these events in South Africa so the first step is to simply create a record of the occurrence of these events.

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In order to create a historic record of MHWs, the collection of *in situ* sampled seawater time series, in the form of the SACTN dataset, must be further developed and validated. Upon the validation of the SACTN and its use to document the occurrence of MHWs in South Africa, the proximate and distant forces that may be responsible for these events may then be determined.

The detection of forces responsible for extreme coastal events will represent an extensive body of work and so the application of these results to biotic endeavours will not be accomplished within this thesis. This is because the causes of these ecologically threatening events are difficult to determine. Once we do have knowledge on their drivers, this information will be invaluable to many fields of study. Most specifically to ecological investigations into the damage MHWs are causing along the coast.

The complete fabrication of the programming language R into this body of work will ensure its openness, reproducibility, and potential for future collaborations. The important knowledge generated in this thesis will, out of necessity, branch out into different fields of study.

To that end it is critical that the work done within this thesis is accessible to other research groups.

The ultimate goal that this research set out to meet was the application of the knowledge of the forcing of MHWs combined with forecasting of the mesoscale or synoptic scale patterns associated with these events to begin to develop a predictive model of MHWs. This will still be far off by the end of this thesis, but its realisation will have drawn nearer.



C H A P T E R

FIRST STUDY

Introduction

entral to the philosophy throughout this thesis are the conclussions in Smit et al. (2013). In this paper they revealed, using an amalgamation of coastal *in situ* time series from several different organisations, now referred to as the South African Coastal Temperature Network (SACTN), that remotely-sensed data along the coast display a strong yet inconsistent warm-bias. This makes their use for coastal oceanography/ecology ill-advised. More research was therefore required to be performed with the SACTN data to ensure their usability more broadly than just as a comparison tool against remotely-sensed data.

The first published study in this thesis by publication initially sought to determine the power of the decadal trends detected in the SACTN time series in order to show how useful these data would be for use across other fields of coastal science. This proved to be much more complicated than assumed for a number of reasons. The most notable of which was that one must have a base against which to calculate absolute zero in order to truly calculate the effect size that may then allow the determination of the power of a study. Because the only measure of temperature with absolute zero is Kelvin, this then makes the effect size of a decadal trend so minute in comparison to such a large temperature scale as to require hundreds to thousands of years of data. It was therefore necessary to think of a different approach to the validation of the SACTN data.

It was then that my supervisor and I decided to rather focus more on the constituent components of the SACTN time series, rather than the time series themselves. What this means was that we decided to see which parts of a time series (e.g. length, variance, precision) had the greatest effect on our ability to detect decadal trends. This was made possible through a controlled experiment in which the destruction and recombination of each time series was done in such a manner that the changing of each variable, and its resultant effect on the detection of the trend therein, could be quantified. This did not give us individual 'scores' for the usability of each time series, but it did inform us about the quality of the data more broadly. And for *in situ* collected data more broadly than that.

Climate Change in Coastal Waters: Time Series Properties Affecting Trend Estimation

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ABSTRACT

In South Africa, 129 in situ temperature time series of up to 43 years are used for investigations of the thermal characteristics of coastal seawater. They are collected with handheld thermometers or underwater temperature recorders (UTRs) and are recorded at precisions from 0.5° to 0.001°C. Using the natural range of seasonal signals and variability for 84 of these time series, their length, decadal trend, and data precision were systematically varied before fitting generalized least squares (GLS) models to study the effect these variables have on trend detection. The variables that contributed most to accurate trend detection, in decreasing order, were time series length, decadal trend, variance, percentage of missing data (% NA), and measurement precision. Time series greater than 30 years in length are preferred and although larger decadal trends are modeled more accurately, modeled significance (p value) is largely affected by the variance present. The risk of committing both type-1 and type-2 errors increases when \geq 5% NA is present. There is no appreciable effect on model accuracy between measurement precision of 0.1°-0.001°C. Measurement precisions of 0.5°C require longer time series to give equally accurate model results. The implication is that the thermometer time series in this dataset, and others around the world, must be at least two years longer than their UTR counterparts to be useful for decadal-scale climate change studies. Furthermore, adding older lower-precision UTR data to newer higher-precision UTR data within the same time series will increase their usefulness for this purpose.

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1. Introduction

The roughly 3000 km of South Africa's coastline is bordered by the Benguela and Agulhas Currents (e.g., Roberts 2005; Hutchings et al. 2009), which, in combination with other nearshore processes, affect the country's marine coastal ecosystems (Santos et al. 2012). A thorough understanding of these coastal processes is provided by several physical variables, with temperature being one of the main determinants (e.g., Blanchette et al. 2008; Tittensor et al. 2010; Couce et al. 2012). The statistical properties of in situ seawater temperature time series representing the whole coastline—such as the annual mean, minimum and maximum temperature, and the thermal range and variance characteristics—vary greatly among coastal sections due to the varying influence of the Benguela and Agulhas Currents. Based on these thermal properties, the coastline has been classified into a

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cool temperate west coast, a warm temperate south coast, and a subtropical east coast (Smit et al. 2013; Mead et al. 2013). That the ocean temperature of these regions is changing has been reported in recent years. For example, an increase of 0.55°–0.7°C decade⁻¹ has been reported in the Agulhas Current (Rouault et al. 2009, 2010), while the southern Benguela has decreased by 0.5°C decade⁻¹ during some parts of the year (Rouault et al. 2010).

The aforementioned climate change trends were derived from remotely sensed gridded sea surface temperature (SST) products. Whereas newer remotely sensed gridded SST products are approaching high enough resolutions for use in coastal waters, older longer products that could be used for the detection of long-term trends are not (e.g., Chao et al. 2009; Qiu et al. 2009; Vazquez-Cuervo et al. 2013). A study by Smit et al. (2013) has also shown that remotely sensed gridded SST data have a warm bias as large as 6°C when compared to coastal in situ data. Nevertheless, a widespread approach in coastal ecological research is to use satellite and/or model-generated temperature data as a

representation of SST along coastlines (e.g., Blanchette et al. 2008; Broitman et al. 2008; Tyberghein et al. 2012). Either the dangers of applying gridded SSTs to the coast are not widely known or in many places in the world there simply are no suitable in situ coastal temperature time series available. It is for this reason that we strongly recommended the use of in situ data to support research conducted within 400 m of the shoreline.

Where records of in situ coastal seawater temperature do exist, the reliability of many of these datasets that could be used in place of the remotely sensed SST data remains to be verified. Users of remotely sensed SST data benefit from it being refined through a number of welldocumented validation and quality control processes (e.g., Reynolds and Smith 1994; Brown et al. 1999; Martin et al. 2012), whereas the standards and methods with which local in situ data from a single dataset are collected and refined may differ greatly. For example, there are currently seven organizations and/or governmental departments (hereafter referred to as bodies) contributing coastal seawater temperature data to the South African Coastal Temperature Network (SACTN). These bodies use different methods and instruments to collect their data as no national standard has been set. One consequence of this methodological disparity is that two-thirds of the data were sampled with hand-held thermometers that are manually recorded at a data precision of 0.5°C, as opposed to the current generation of underwater temperature recorders (UTRs), which have an instrument precision as fine as 0.001°C. If these in situ temperature data are to be used together in lieu of remotely sensed SST data, it is important that the characteristics of the contributing data sources are written down at a precision of 0.5°C. Data at other lounderstood in terms of their ability to yield useful, reliable, and accurate long-term measurements for use in climate change studies.

This prompted us to examine the 129 in situ time series that comprise the SACTN. The range of measurement precisions and statistical characteristics of this dataset were used to guide a series of enquiry-driven analyses into the suitability of the time series to yield statistically significant and accurate assessments of decadal temperature change. The length, decadal trend, and data precision of each time series were adjusted in a systematic manner, and this forms the core of our analyses. Furthermore, the natural variability of each of the time series, which differ more or less predictably between coastlines variously affected by the Benguela and Agulhas Currents, was also entered into the analysis. Our aim was to assess the effect that each of these variables has on the ability of a model to produce a robust estimate of time series decadal trend. The effect gaps in the time series may have on the fitting of models was also

investigated as many of the time series used here have some missing data scattered throughout, which is unavoidable for a 20 year and greater time series that is sampled by hand by a single technician at each site.

The study provides a better understanding of some of the characteristics of a time series that are influential in the detection success of decadal trends in coastal ocean temperatures.

2. Methods

a. Data sources

Our study lies within the political borders of South Africa's coastline and the location of each point of collection may be seen in Fig. 1. Of these 129 time series, 43 are recorded with UTRs and the other 86 with hand-held mercury thermometers. The oldest currently running time series began on 1 January 1972; there are 11 total time series that started in the 1970s, 53 more started in the 1980s, 34 began in the 1990s, 18 in the 2000s, and 13 in the current decade.

The data are collected using two different methods and a variety of instruments. Hand-held mercury thermometers (which are being phased out in favor of alcohol thermometers or electronic instruments) are used in some instances at the shoreline, and represent seawater temperatures at the surface. At other places, predominantly along the country's east coast, data are collected with glass thermometers from small boats at the location of shark nets along the coast (Cliff et al. 1988). Whereas both types of thermometers allow for a measurement precision of 0.1°C, the recordings are calities are collected using delayed-mode instruments that are permanently moored shallower than 10 m, but generally very close to the surface below the low-water spring tide level.

Over the last 40+ years the electronic instruments used to measure coastal seawater temperatures have changed and improved. The previous standard was the Onset Hobo UTR with a thermal precision of 0.01°C. The new standard currently being phased in is the Starmon Mini UTR. These devices have a maximum thermal precision of 0.001°C ± 0.025°C (http://www. star-oddi.com/). Of the 43 UTR time series in this dataset, 30 were recorded at a precision of 0.001°C for their entirety, and 5 UTR time series include older data that were recorded at a precision of 0.01° or 0.1°C and so have been rounded down to match this level of precision. Eight additional UTR time series have data recorded at a precision of only 0.1°C.

The thermometer data are recorded manually and saved in an aggregated location at the head offices of the

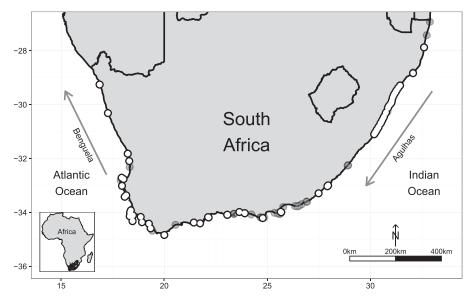


FIG. 1. Map of South Africa indicating the location of the 129 time series comprising the South African Coastal Temperature Network. The locations of the 84 time series used in this study are shown as solid white circles and the unused time series as gray-filled circles.

collecting bodies. UTRs are installed and maintained by divers and data are retrieved at least once annually. These data are digital and are downloaded to a hard drive at the respective head offices of the collecting bodies.

b. Data management

Each of the seven bodies contributing data to this study has its own method of data formatting. Steps are being taken toward a national standard as we move toward replacing all the thermometer recordings with UTR devices; however, as of the writing of this article, one does not yet exist. Data from each organization were formatted to a project-wide comma-separated values (CSV) format with consistent column headers before any statistical analyses were performed. This allowed for the same methodology to be used across the entire dataset, ensuring consistent analysis. Before analyzing the data, they were scanned for any values above 35°C or below 0°C. These data points were changed to NA, meaning not available, before including them in the SACTN dataset.

All analyses and data management performed in this paper were conducted with R version 3.3.1 (21 June 2016; http://www.r-project.org/). The script and data used to conduct the analyses and create the figures seen in this paper may be found at https://github.com/schrob040/Trend_Analysis.

Any time series with a temporal precision finer than one day were averaged into daily values before being aggregated into the SACTN. A series of additional checks were then performed (e.g., removing long stretches in the time series without associated temperature recordings)

and time series shorter than five calendar years, collected deeper than 10 m or missing more than 15% of their monthly values were removed. At the time of this analysis, this usable daily dataset consisted of 84 time series, consisting of 819 499 days of data; monthly averages were then made from these daily data to create the 26 924 temperature values available for use in this study.

c. Systematic analysis of time series

We used the 84 time series simply for their variance properties (composed of seasonal, interannual, decadal, and noise components), which reflect that of the thermal environment naturally present along the roughly 3000 km of South African coastline. Linear trends that may have been present in each time series were removed prior to the ensuing analysis by applying an ordinary least squares regression and keeping the detrended residuals as anomaly time series. In doing so we avoided the need to simulate a series of synthetic time series, whose variance components may not have been fully representative of that naturally present in coastal waters. These detrended anomaly time series (henceforth simply called time series) represent a range of time scales from 72 to 519 months in duration.

To each of the 84 time series, we artificially added linear decadal trends of 0.00° – 0.20° C decade⁻¹. In other words, we now had time series that captured the natural thermal variabilities around the coast, but with their decadal trends known a priori. The range of decadal trends was selected based around the global average of 0.124° C from Kennedy et al. (2011) and used in IPCC (2013). Furthermore, in order to represent the

instrumental precision of the instruments used to collect these time series, we rounded each of these (84 time series \times 5 decadal trends) to four levels of precision: 0.5°, 0.1°, 0.01°, and 0.001°C. Consequently, we had a pool of 1680 time series with which to work.

To gain further insight into the effect of time series length on trend detection, each time series was first shortened to a minimum length of 5 yr, starting in January so that the timing of the seasonal signal for each time series would be equitable. After fitting the model (see section 2d below) to all 1680 of the shortened time series, the next year of data for each time series was added and the models fitted again. This process was iterated until the full length of each time series was attained. For example, if a time series consisted of 12 full years of data, it would require 160 models (8 iterations of increasing length \times 5 decadal trends \times 4 levels of precision); similarly, 720 models would be applied to a 40-yr time series. Considering the 84 time series available, the total number of individual models required to capture each combination of variables quickly increased to 36 220.

Our approach of fitting models to each of the semiartificial time series that we generated allowed us to study the effect that the relevant variables (time series length, natural variability, added slope, and level of measurement precision) has on the ability of the time series model to faithfully detect the decadal thermal trend, which was known a priori. The primary results of interest in these analyses were the significance (*p* value) of the model fit, the accuracy of the decadal trend determined by the GLS model, and the error associated with the trend estimate.

d. Time series model

The selection of the appropriate model can greatly influence the ability to detect trends (Franzke 2012). Two broad approaches are widely used in climate change research (IPCC 2013). The first group of models estimates linear trends, and although linearity may not reflect reality (i.e., trends are very frequently nonlinear), these models do provide the convenience of producing an easy to understand decadal trend (e.g., 0.106°C decade⁻¹; Wilks 2011; IPCC 2013). The other group accommodates nonlinear trajectories of temperature through time by the use of higher-degree polynomial terms or nonparametric smoothing splines, but the inconvenience comes from not being able to easily compare models among sites (Wood 2006; Scinocca et al. 2010). Both groups of models can accommodate serially correlated residuals, which is often the cause for much criticism due to their effect on the uncertainty of the trend estimates (Von Storch 1999; Santer et al. 2008). For example, generalized least squares (GLS; yielding estimates of linear trends) and generalized additive mixed models (GAMM; nonlinear fitting with no trend estimate provided) can both capture various degrees of serial autocorrelation (Pinheiro and Bates 2006; Wood 2006). Although our exploratory analysis assessed two parameterizations of each of the model groups, we opted to proceed here with a GLS equipped with a second-order autoregressive [AR(2)] correlation structure fitted using restricted maximum likelihood (REML; Pinheiro and Bates 2006):

$$y_t = \beta_0 + \beta_1 x_t + \varepsilon_t,$$

where the lag-2 autocorrelated residuals are given by

$$\varepsilon_t = \phi_1 \varepsilon_{t-1} + \phi_2 \varepsilon_{t-2} + w_t$$

and the white noise series is

$$w_t \sim \text{i.i.d.} N(0, \sigma^2).$$

This approach is similar to that of the IPCC, although the latter uses an AR(1) error term (Hartmann et al. 2013). Another difference from the IPCC approach is that we nested the autoregressive component within a given year. This modeling approach allowed us to assess how various properties of the detrended time series would affect the models' ability to detect trends by comparing the estimates of the trends against the known artificially added trends.

3. Results

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The residuals for the base 84 detrended time series may be seen in Fig. 2. From these detrended time series the length, decadal trend, and precision variables were systematically manipulated as explained in the methods. It was found that the important variables affecting the accuracy of the slope detected by the GLS model, in decreasing order, were 1) time series length, 2) the size of the added decadal trend, 3) initial SD of the time series (after detrending but prior to adding artificial slopes), 4) the amount of spurious or missing data (NA), and 5) measurement precision. These variables influence the model fits in a systematic manner.

As would be expected, the size of the decadal trend estimated by the GLS increases in direct proportion to the decadal trend that we added and therefore knew a priori. What is especially noteworthy in this analysis is that time series of longer duration more often result in trend estimates converging with the actual trend than those of shorter length (Fig. 3). This effect is most evident from around 30 yr. Furthermore, how well the

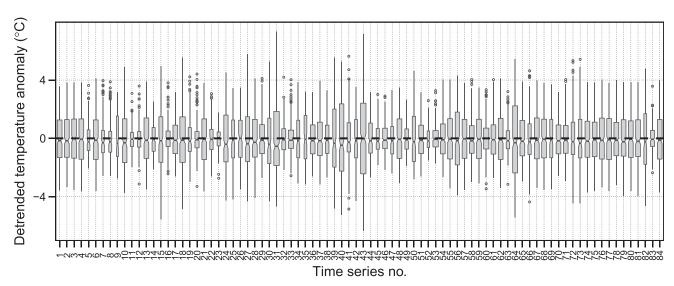


FIG. 2. Box-and-whisker plot summarizing the 84 temperature anomaly (°C) time series used in this study (i.e., after detrending) but before adding a decadal trend or rounding the data. The plot indicates the first and third quartiles as the extremities of the boxes, the median is shown as the horizontal line within each box, the minima and maxima are indicated by the whiskers, and the points are outliers.

estimated model trend converges with the actual trend is also very visible in the standard error (SE) of the trend estimate (Fig. 4): models fitted to short time series always have modeled trends with larger SE compared to longer ones. The strength of this correlation is r = 0.56 (p < 0.001) and it remains virtually unchanged as the added decadal trend increases. The p value of the fitted models also varies in relation to time series duration and to the steepness of the added decadal trend (Fig. 5). It is

usually the longer time series equipped with steeper decadal trends that are able to produce model fits with estimated trends that are statistically significant. Note, however, that this p value tests the null hypothesis that the estimated trend is no different from 0°C decade⁻¹ at $p \le 0.05$, and *not* that the slope is not different from the added trend. Taken together, these outcomes show that although our GLS model can very often result in trend estimates that *approach* the true trend, it is seldom that

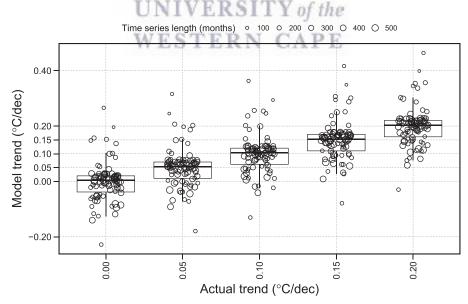


FIG. 3. The effect of time series length on the ability of the GLS model to accurately detect the trend added to each time series. The box-and-whisker plot shows the first and third quartiles as the extremities of the boxes, the median is shown as the horizontal line within each box, and the minima and maxima are indicated by the ends of the whiskers. Points indicate the spread of the actual data and their size are scaled according to the length of the time series they represent as shown at the top of the figure.

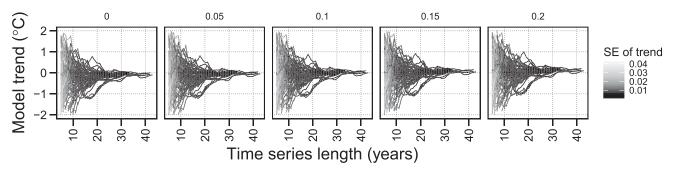


FIG. 4. The relationship between the length of a time series, the size of the modeled trend, and its SE. Each individual line shows the modeled trend for 1 of the 84 sites used in this analysis to which a model was fitted iteratively as the time series length was "grown" from 5 yr in length to the maximum duration available for the site. (left)–(right) The progressive effect that decadal trend has on this relationship (indicated by the numeral above each panel), and the gray-shaded bar shown on the right, is mapped to the SE of the trend.

those estimates are statistically significant in the sense that the estimated trends differ statistically from 0°C decade⁻¹.

The variance of the detrended data is another variable that can affect model fitting, but its only systematic influence concerns the SE of the trend estimate. Here, it acts in a manner that is entirely consistent across all a priori trends (Fig. 6). What we see is that as the variance of the data increases [represented here as standard deviation (SD)] the SE of the slope estimates increases too. Moreover, it does so disproportionately more for time series of shorter duration. Again, as we have seen with the estimated trend that converges to the true trend around 30 yr, so too does the initial SD of the data cease to be important in time series of around three decades in length.

The number of NAs permitted in any of our time series was limited to 15% per time series. Twenty-five of the 84 time series have less than 1% NA. An additional 45 time series have up to 5% NA, 10 have up to 10% NA, and 4 have up to 15% NA. The mean number of NA for the data is 2.65%. The relationship between % NA and the p value of the models is shown in Fig. 7. At 2.5% or fewer NA their presence does not have any discernible effect on resultant p values. Progressively increasing the number of NAs above 5%, however, leads to a drastic improvement of models fitted to series with no or gently increasing decadal trends (these generally have very large p values indicative of very poor fits, perhaps due to the presence of a very weak signal), and a significant deterioration of models fitted to data with steep decadal trends (for these data, the model generally fits better at low numbers of NA, as suggested by the larger number of p values that approach 0.05). In other words, the more missing values (NA) there are in a time series with no discernible decadal trend, the more likely a model is to erroneously detect one. On the other hand, model results from time series that do have

detectable decadal trends tend to produce fits that are not significantly different from 0°C decade⁻¹.

Regarding the effect that the level of measurement precision has on the GLS models, we see in Fig. 8 that decreasing the precision from 0.001° to 0.01°C has an undetectable effect on any differences in the modeled trends. The root-mean-square error (RMSE) between the slopes estimated from 0.001° and 0.01°C data is 0.001. The correspondence between the slopes estimated for data reported at 0.5°C compared to that at 0.001°C decreases to a RMSE of 0.03.

The effect of decreasing data measurement precision from 0.001° to 0.5°C has almost no appreciable effect on any of the measures of variance presented in this study. The effect of measurement precision on the accuracy of the modeled slope, however, becomes very pronounced going from 0.1° to 0.5°C. This effect is larger on smaller decadal trends. For example, at a trend of 0.05°C decade⁻¹, the deviation from the true value of models fitted to data with a precision of 0.1°C is negligible; however, the accuracy of the fitted model on data recorded at a precision of 0.5°C with a real trend of 0.05°C decade⁻¹ is 10.81% different on average (i.e., given a slope of 0.05°C decade⁻¹ the model detects slopes of 0.055°C decade⁻¹). This accuracy of the models improves to an average difference of 6.44% with a slope of 0.10°C decade⁻¹ and 2.24% at 0.15°C decade⁻¹ and decreases slightly to 2.30% at 0.20°C decade⁻¹. A precision of 0.5°C always provides clearly less accurate modeled trends than at higher precisions; however, the current analysis did not highlight one precision that consistently provides the most accurate estimate of the trends. This may, however, become determinable in an analysis of synthetic data with variance structures that are manipulated in a more consistent manner.

As the actual time series used to generate the data for this study are predominantly over 300 months in length and recorded at a data precision of 0.5°C, we would be

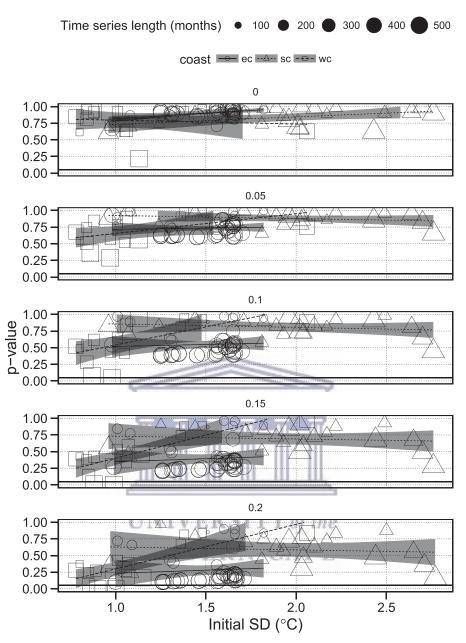


FIG. 5. The effect of the SD (°C) of the anomaly time series before adding a decadal trend (initial SD), or rounding the data to the different levels of precision, on the significance of the modeled trend. The sizes of the symbols are scaled in direct proportion to the time series length and are shown at the top of the figure. Time series belonging to the three South African coastal sections are represented using different symbols. The east coast (ec; circles) typically has the most stable thermal regime of the three coasts, with the south coast (sc; triangles) having the greatest amount of variance and the west coast (wc; squares) consisting of areas with both high and low variance. Linear models with 95% confidence intervals (indicated by the gray-shaded ribbons) have been fitted separately for each coastal section, and illustrate the interaction between initial SD in each group and the significance (*p* value) of the GLS models. (top)–(bottom) Increasing decadal trends are shown as indicated by the numerals above the panels.

remiss not to investigate the interaction between the increase in accuracy provided by a lengthy time series against the decrease caused by a data precision of 0.5°C. In other words, at what point does a model fitted to a

longer time series, with less precise measurements (e.g., those taken by thermometers and reported at a precision of 0.5°C), become as accurate as a time series with more precise measurements (e.g., UTRs)? Figure 8 shows how

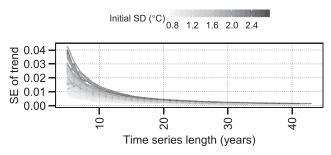


FIG. 6. The relationship between the effect of initial SD (°C) (i.e., the variance of the anomaly time series before adding artificial decadal trends; shown here as gray shades), on the SE of a modeled trend, controlled for by the length of the time series. The effect of the size of the added decadal trends on the relationship is imperceptible and therefore only a decadal trend of 0.2° C decade⁻¹ is presented.

varied the modeled trends become when a precision of 0.5°C is used, and we see here that when these low-resolution time series have a shallow slope of 0.05°C decade⁻¹, a fitted model requires 24 months of additional data on average to have a comparable level of accuracy to a model fitted to data recorded at a precision of 0.1°C. The difference in the required time series length necessary for accurate detection decreases to

16 months when a larger slope 0.20°C decade⁻¹ is present in the data.

An analysis with a large number of variables as shown here is bound to have a medley of complex interactions between the various statistics being measured; however, much of the range seen in the results of the GLS models can be well explained by the influence of one independent variable, or two operating in concert, as we have shown above. The most important of these variables has clearly been the length of the time series.

4. Discussion

The strongest finding of this analysis is that the accurate detection of long-term trends in time series primarily concerns the length of a dataset. But there are also a host of nuances resulting from time series length, the steepness of the decadal trend the model is asked to detect, the influence of the SD of a time series, the amount of missing values, and the precision at which the data have been measured or recorded that interact with one another and that must be considered.

Whereas time series with smaller variances (shown as SD in this study) generally produce model fits that are

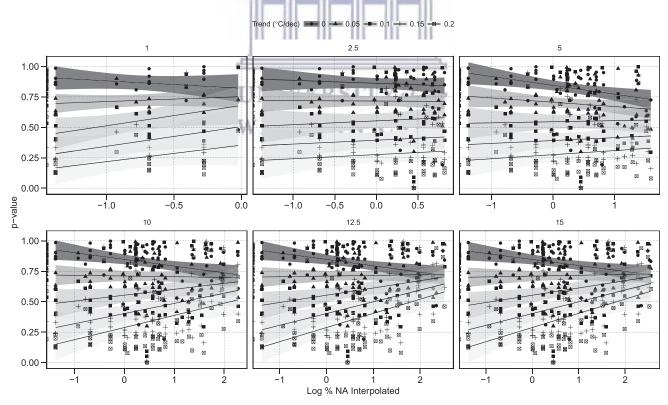


FIG. 7. The relationship between the amount of missing values ($\log \%$ NA) and the significance of a modeled trend (p value). Each panel shows the effect of an increasingly larger amount of missing values indicated above each panel by numerals (from top left to bottom right): 1, 2.5, 5, 10, 12.5, and 15. The fitted black lines and 95% confidence intervals (shown as gray-shaded bands) represent each of the five decadal trends assessed ($^{\circ}$ C decade $^{-1}$) shown using different black symbols: 0 (circles), 0.05 (triangles), 0.1 (squares), 0.15 (crosses), and 0.2 (squares with an \times symbol inside).

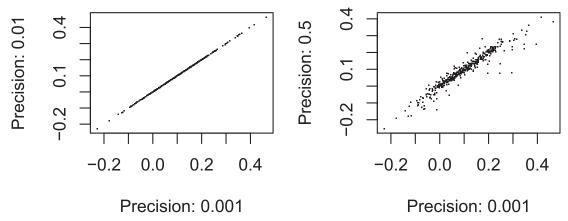


FIG. 8. Plots representing correlations of the modeled trends acquired at different levels of rounding, which can be interpreted as representations of different measurement precisions. (left) The effect of rounding from 0.001° to 0.01°C may be seen. (right) Rounding from a precision of 0.001°-0.5°C has a visibly greater effect on the deterioration of the correlation between the two sets of estimated trends.

statistically significant (i.e., with decadal trends that are significantly different from 0°C decade⁻¹ at p < 0.05) and with smaller SE of the estimated trends after shorter lengths of time, we also see that increasing a time series' length beyond 25 yr, but preferably beyond 30 yr, will increase the likelihood of detecting a decadal temperature change even in very variable datasets. Detecting temperature change in highly variable coastal environments, such as those around the coast of South Africa and many temperate coastal environments globally, will therefore benefit from access to the longest possible time series available. This phenomenon is demonstrated in Fig. 5, which uses symbols to show the time series binned by the three different coastal sections of South Africa (Smit et al. 2013). Of these three coastal sections measurements that are taken regularly. The inclusion of the east coast is known to have the most stable thermal regime (i.e., with the smallest variance), with the south coast having the greatest variance. Long time series at sites of low variance result in great improvements in our ability to detect significant climate change trends, and this effect is most obvious in time series with steeper decadal trends. The selection of sites for long-term monitoring must therefore account for the location of study and necessitate adequate planning to collect a long enough time series.

The detection of long-term trends requires long-term data, a fact that is already firmly established in climate change research (Ohring et al. 2005; IPCC 2013). The length of these time series is firmly under the control of the investigator with sufficient foresight and perseverance to plan the installation and management of new instrument networks that will yield usable results only after about three-quarters of a typical academic career has passed. Should such data already exist—and considering the scarcity of such long-term records that are already yielding benefits today—we must ensure that these sources of data are managed and curated with great care and diligence as they are practically irreplaceable. For this reason, it is essential that we understand the inherent strengths and weaknesses of such existing sources of data so that we may fully maximize their utility and extract from them the model coefficients needed to detect decadal temperature trends, and know the accuracy of these estimates to the best of our ability. There are many time series <20 yr in length that should be avoided, where possible, for trend analysis. These will mature with time and their maintenance needs to be ensured going forward.

Aside from length, the most powerful time series have too many missing values (NAs) in the datasets must be avoided. We have shown that permitting 5% NAs or more into our time series has a drastic and significant influence on the chance of committing a type-1 error (arriving at a false positive, i.e., detecting a trend when none exists) for time series with no or very gentle decadal trends. On the other hand, the inclusion of NAs in datasets with a decadal trend present tends to cause an increase in the probability of committing a type-2 error (i.e., finding false negatives). Although our modern UTR datasets generally have fewer NAs than we should be concerned about—therefore with a low chance of committing type-1 or type-2 errors—the presence of NAs may seriously compromise some of the time series that are still being collected by hand using hand-held thermometers.

We have demonstrated clearly that as the steepness of an expected decadal trend increases, the ability for it to be modeled accurately increases, too. Our GLS model is generally not able to detect trends that are

significantly different from 0°C decade⁻¹ unless a slope of 0.20°C decade⁻¹ exists. Very rarely were we able to produce significant model fits at shallower slopes. No trends with a slope <0.05°C decade⁻¹ were found to be significant in this study. Based on the relationship between SD and the added decadal trend, we see that time series with an SD of 1.5°C (the bulk of the time series here) and a decadal trend of 0.10°C decade⁻¹ should consist of roughly 640 months of data before our GLS model would regularly be able to detect a significant trend (p < 0.05). This finding is somewhat discouraging as most global analyses of decadal SST change based on gridded SST products estimate a trend closer to 0.1°C decade⁻¹ (e.g., IPCC 2013). This means that the trends present in most time series representative of very variable coastal environments that exhibit the same variance structure as that of our data are probably unlikely to be detected as significant, even if they do indeed exist. In other words, the chance of committing a type-2 error is probably very real for such systems, unless time series >50 yr are available.

As 50-yr coastal seawater temperature time series are probably very scarce, it is important to note that those measured at precisions of 0.1°-0.001°C require fewer months of data to detect long-term trends. Based on the data presented here, we calculated that time series measured at a low precision (0.5°C) may require as much as an additional 24 months of data to accurately detect long-term trends. One of the motivators for this paper was to investigate the effect measurement precision has on a time series' ability to produce results useful for investigations of long-term climate change, and to validate the use of the low-precision 0.5°C thermometer in a statistical sense. data. This is an important consideration as many studies investigating the effects of climate change (e.g., Grant et al. 2010; Scherrer and Körner 2010; Lathlean and Minchinton 2012) do use lower-precision 0.1°C data. Although the precision of much of our data is below the current standard of 0.1°C required for climate change research (Ohring et al. 2005; WMO 2008), the length of the thermometer time series makes them a valuable asset. The average length of the thermometer time series in the SACTN, from which the 84 time series used in this study were drawn, is 349 months. The average length of the UTR time series is 167 months. Given this difference in the lengths of the time series, even after correcting for the negative effect of low measurement precision, the time series collected with thermometers are currently more useful for climate change research than the UTR time series within the SACTN. Because time series with data precisions of 0.1°-0.001°C produce comparable results, newer higher-precision UTR data may be combined with older lower-precision UTR data within the

same time series without concern that the reduced overall data precision may have a negative impact on a model's ability to detect decadal trends. Extending time series in this way will serve to make them more dependable as length is the primary criterion through which one should initially assess the potential to accurately detect a decadal trend before refining ones assumptions with any statistical analyses. A time series with data precision finer than 0.1°C is therefore only necessary when an investigation requires that the decadal trend be known to an accuracy of 0.01°C or finer (e.g., Karl et al. 2015).

It is important to take note of the accuracy of the models, not only to focus on the significance of their results. Indeed, the p value given for the slope in a model does not show how well the model detects the true trend in the data (known a priori in this study); rather, it tells us if the detected trend is significantly different from 0°C decade⁻¹. This is not particularly useful for applying the results of climate change research more broadly to biotic interests. For example, of the 1344 models (84 base time series × 4 decadal trends × 4 levels of precision) fitted to time series with decadal trends ≥ 0.05 °C decade⁻¹, 317 of these were accurate to within 10% of the decadal trend known a priori, but not significant ($p \ge 0.05$). That a long-term trend does exist that may be accurately detected by a model and related to an observed change in the natural world—such as range expansion/contraction of coastal biota (Bolton et al. 2012; Straub et al. 2016; Wernberg et al. 2016)—is more important than whether or not the model can show if that trend is significantly different from 0°C decade⁻¹

We must mention also that much of the metadata pertaining to the older temperature records used here have over time been lost. As with the bulk of the International Comprehensive Ocean-Atmosphere Data Set (ICOADS; Freeman et al. 2016), in situ coastal seawater temperature monitoring that started in the 1970s in South Africa was not developed with climate change research in mind, and comprehensive records that keep track of details of the instruments used, calibration, their turnover, and changes in monitoring methods and locations and so forth are not always available as per modern requirements (Aguilar et al. 2003). For studies of climate change per se this is a serious limitation and it prevents us from knowing anything about the accuracy of the instruments or potential issues of drift (stability) that may have occurred. We do know, however, that all the time series sampled with thermometers were sampled only with thermometers, and vice versa for the UTR time series, ensuring that the precisions of the measured data used in this study are

correct. Moving forward with the further development of the SACTN and the establishment of a national standard of data collection and instrument maintenance, we are able to record and archive all these levels of pertinent metadata, allowing for the enforcement of SI traceability and the accurate measurement of instrument drift (WMO 2008). Nevertheless, the detrended anomaly time series used here were taken only for their variance properties, which we think accurately reflect those of the three different coastal sections. They provide a strong backbone for semiartificial time series, and we have shown how important insights about model fitting could be derived from these data.

5. Conclusions

We draw several key conclusions:

- 1) There is a rapid increase in the accuracy and significance of modeled trends as time series lengths extend from 10 to 20 yr. This improvement slows from 20 to 30 yr, and as time series approach 40 yr in length the accuracy of models becomes nearly exact. Modeled trends from time series at or under 25 yr in length should be interpreted with extreme caution.
- 2) For our variable coastal seawater, a time series of 520 months in length is required to detect a decadal trend in line with the global average (i.e., near 0.1° C decade⁻¹) with perfect accuracy; however, an additional 120 months of data is often required for the detected trend to be considered significant ($p \le 0.05$).
- 3) The length of a time series required to detect a decadal trend at 0.1°C decade⁻¹ may rapidly exceed 100 yr when a large amount of variance is present.
- 4) The larger the decadal trend within a time series, the more accurately it will be modeled regardless of the amount of variance in the time series.
- 5) There is a complicated relationship between the accuracy of a trend fitted to a time series and the %NA of that time series. As the %NA increases, so too does the chance of committing type-1 (with gentle trends) or type-2 errors (with steeper trends).
- 6) A measurement precision finer than 0.5°C is not required to confidently detect the long-term trend in a time series; however, precisions at or finer than 0.1°C may reduce the length of time required to accurately detect a long-term trend, if one does exist, by as much as 2 yr.
- 7) Improving the precision of measurements finer than 0.1°C has almost no appreciable effect on a models ability to detect a long-term trend, provided that the reported effect size matches the level of precision by the instruments.

We understand that time series of >30 yr may be exceedingly rare. Therefore, as we move forward as a scientific community investigating the issues of climate change, the continuity of any current time series of sufficient length must be ensured as these commodities are practically irreplaceable.

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Conclusion

In the process of analysing and quantifying the changes caused by certain variables within the SACTN dataset we were able to determine that these data are very useful for climate change science within South Africa. Over half of the time series are recorded with a precision coarser than the recommended minimum of 0.5 °C, but we found that due to the length of these time series they were more useful than the shorter more precise time series created through more modern means. This was an important finding because as much as two thirds of the SACTN dataset consists of these longer coarser time series, and were they found to be unusable for the detection of climate trends it would have been a massive blow to coastal investigations in South Africa.

Another important conclusion from this first study in the PhD was that one may not 'trust' a decadal signal found within a time series that is shorter than 30 years. With this knowledge, and having determined the most effective linear model to use for extracting decadal trend signals from the SACTN data, we were able to also determine the decadal trend (climate change) signals found along the coast of South Africa in areas that have been sampled for at least 30 years. This information is publicly available for academic use as meta-data for the SACTN dataset.

After having further validated the SACTN data, it was now possible to use these data for a more focussed application. The initial proposal for this thesis was to quantify the impact that extreme thermal events may have on kelp forest ecosystems. The problem with this proposal was that no one had yet recorded the history of these extreme events in South Africa. So any possible comparisons of damage were not possible to be drawn. It was at this moment that the thesis pivoted away from coastal ecology towards coastal oceanography.



Appendix

Contribution

The idea to switch from a power analysis to a control series of experiments on the components of the time series was provided by AS, as was the initial iteration of the generalised least squares model (GLS) used for detecting the decadal trends. RS managed the SACTN data and produced the dataframes upon which the controlled experiments were based. RS considered the extent to which the controlled experiments could be expanded to, and wrote the code accordingly. RS then integrated the GLS supplied by AS into the iterative controlled experiment code. The interpretation of the results and the write up of both the first and final drafts was performed by RS. With extensive edits on both versions provided by AS. Most figures were created by RS. RS handled all correspondence with the journal as well as between the journal and UWC. RS attended to all of the reviewer comments and AS addressed many of them as well. RS collated all of the comments and made all of the edits to the text. RS is also the corresponding author on the final article as well as the maintainer of the publicly available code¹.

Written consent

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¹https://github.com/robwschlegel/Trend_Analysis



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Reviewer #2

General

RC: Sea surface temperature (SST) is an essential climate variable and is central to the understanding of climate change (cf., GCOS, 2011). Given the growing use of satellite SST products for long-term monitoring of climate (temperature) changes, the paper is interesting and topical - as it starts by highlighting the weaknesses in using satellite data for coastal applications (a known and expected issue). The title of the paper says: "Effects of a set of parameters on the ability to detect temperature trends". Therefore, I do not expect much of conclusive statements about the trends itself but on the analyses of suitability of data to detect trends - fair enough. (Also, my expertise is in satellite/in situ measurements and long-term monitoring of global products, not climate, that makes the paper suitable for me to comment upon).

RC: I have no substantive methodological comments. The methodology (STL, Power analyses) is well-known, available in published literature, can be applied using standard functions of Matlab/R and other s/w packages and is applied correctly to 127 time-series of data (I assume that the implementation is correct and did not check the GitHub link). The simple and known concepts of statistics, significance, effect of outliers etc. are neatly applied and the authors have put good care to carefully avoid misuse or misinterpretation of data that I appreciate.

RC: Thinking from a larger perspective, I feel that the authors can possibly discuss with the wider SST community to further bring this issue up, share or generate a set-up for the data for coastal validation of SST and provide feedback to see if satellite SST can be improved in coastal regions - if at all possible given the spatial resolution, shallow depth and diurnal warming specifics. But some thinking and initiative along these lines will be helpful to users in general (I understand that one of the authors has published a paper about this). This is indeed something we are working on accomplishing. We have presented our findings at the GHRSST meeting in Cape Town in 2015 and have been in talks with people at NOAA and NASA responsible for the curation of SST data from those sources. The post-doc in our lab has been working on a better Bayesian based Optimal Interpolation (OI) algorithm to correct satellite SST for coastal use.

AR: This is indeed something we are working on accomplishing. We have presented our findings at the GHRSST meeting in Cape Town in 2015 and have been in talks with people at NOAA and NASA responsible for the curation of SST data from those sources. The post-doc in our lab has been working on a better Bayesian based Optimal Interpolation (OI) algorithm to correct satellite SST for coastal use.

RC: The paper is generally well-written, despite a handful of typographical errors, and possibly some missing references. After addressing those concerns and removing typo that I will write below, I recommend the paper to be accepted after a minor revision and look forward to seeing further progress.

Suggestions and questions

Question

- RC: An important concern for analyzing the suitability of any instrument for climate studies (be it satellite sensor, thermometer or drifter) is 'the stability of the instrument/s itself' over a long period of time. It is important to ensure that the stability is sufficient to detect temperature trends and the trend is not attenuated by instrumental drifts. If instruments are changed/updated at a location, they must also be characterized to the same standards (SI traceability etc.). This provides the basis for a long-term foundation of change detection. Such requirements have been set up by international bodies, e.g., www.bipm.org. This aspect of 'temporal stability' should be discussed and if it is not important or relevant in your case, explain why. Or if it not addressed, then it should be a mentioned as a limitation of this particular study.
- AR: A very unfortunate reality of long-term data in South Africa is that much of the meta-data for instruments/ collection methods etc. is either not kept or is routinely 'misplaced' as governmental departments are juggled around whenever it suites the body politic to perform a bit of 're-branding'. We have therefore had to use the data 'as is' because when these various monitoring 'programmes' were set up, they were done without anyone conceiving that it would be used for climate research, never mind merging it into one national database (SACTN). So we are using the data with their inherent limitations. The important thing is that we are now (as the SACTN) aware of this, and are ensuring that SI traceability is factored into the continuation of the programme when new instruments are being installed. The reality is that many networks such as this one will initially start with whatever is available, and that it gradually morphs into a system designed for climate research. But old data are useful nevertheless, and using it is what we do here. We acknowledge these limitations in the text on Ln-371-389.

Suggestion

- RC: In your list of conclusions, you may want to add that when instruments are replaced (or in your case updated), it is necessary to have some overlap time, possibly for a year or more, to ensure that the data characteristics can be matched or related for a given location.
- AR: Ln-382-385: That we do this when updating our instruments is now mentioned.

Corrections, or minor questions and suggestions

- RC: Ln-18: manipulated -> possibly use another word (I leave it to your discretion, though). Basically, you are referring to a controlled experiment.
- AR: Ln-15-16: Changed manipulated to systematically varied.
- RC: Ln-24-27: Yes, but put simply, it just means that 'long-term' datasets with certain minimum precision are more useful than 'short-term' ones. If UTR were long-term, they would be more useful. Rephrase or add, 'if we were to choose between the two'.
- AR: Ln-26-29: Changed the way in which this relationship is discussed..

- RC: Ln-35-38: I have some concerns about the way it is presented. To what I understand, the producers of satellite/model SST provide some suggestions on where to use the data, along with quality level indicators. If this is the case, then the users ignoring the suggestions are vulnerable to errors.
- AR: Ln-51-57: Yes, true. But people are nevertheless using satellite derived SST along the coast in the absence of anything better. Biologists are not oceanographers and seldom get into the technicalities of various data products, which cause them to open themselves up to various problems. This is discussed in Smit et al. 2013, and three papers that erroneously use SST data at the coast are referenced as well.
- RC: Please make sure that the suggestions are not violated by the referred uses (papers) or rephrase somehow to reflect that the coastal data are sub-optimal and are acknowledged by the producers. Simply put, please do justice to both the producers and the users.
- AR: Ln-48-51: Three papers are referenced that have looked into and discuss the usability of certain satellite-derived gridded SST products in coastal waters.
- RC: Ln-46-47: '..., whereas the software systems...'. I am really unsure what you intend to say here. The global network and related software are quite mature. Or are you referring to the local bodies?
- AR: Ln-60-66 We were referring to local bodies but realised that this part of the sentence was unnecessary and so deleted it. Combined the following sentence and drew attention to the fact that this issue refers to local data specifically.
- RC: Ln-52: '... together in lieu of the SST data...' -> '... together in lieu of the satellite-based SST data...'
- AR: Ln-72: Changed to "...together in lieu of remotely-sensed SST data..."
- RC: Ln-65: '... ii) variability, and iii) precision have on the 'quality' of the time series.' -> '... ii) variability, iii) precision, and iv) data gaps have on the 'quality' of the time series.' Then modify the last sentence in the paragraph, accordingly.
- AR: Ln-78-86: The enumerated list of aims was removed in favour of a written paragraph. The effect of gaps in the time series is addressed specifically in Ln-87-90.
- RC: Also, why the word quality is in quotes?
- AR: *Ln-82-83: The word 'quality' meant the accuracy and significance of the results. The word has been removed and the meaning stated explicitly.*
- RC: Ln-67: '... precision...' -> '... instrument precision...' to separate it from quality
- AR: Ln-78-79: 'precision' changed to 'data precision'. Pains were taken to use correct nomenclature throughout the document in regards to the word 'precision'. 'Instrument precision', 'measurement precision' or 'data precision' are used where appropriate.
- RC: Ln-79: remove 'of these'.
- AR: Ln-92: Removed
- RC: Ln-81: began on
- AR: *Ln-94: Changed accordingly*
- RC: Ln-88: Data at other localities ...
- AR: Ln-104: Changed accordingly

- RC: Ln-110: 'parties' = 'bodies'?, as you have already defined earlier.
- AR: Ln-116: Changed accordingly
- RC: Ln-113: remove dash use ';' ..., however, as of this ...'
- AR: Ln-120: Changed accordingly
- RC: Ln-114: All may not be familiar with the acronym '.csv' comma separated values ...
- AR: Ln-121-122: Changed accordingly
- RC: Ln-116: 'src', 'temp' -> expand
- AR: Ln-122: Sentence containing this issue was altered via Reviewer#4. Specific names of column headers no longer provided as they are not relevant to the methodology.
- RC: Ln-189-193: a bit confusing; please improve clarity.
- AR: Ln-165-170: The range of results for different sub-groupings of the time series are no longer investigated so the paragraph referred to here has been removed. The outcome of the models, and not the ranges of stats in the sub-groupings, is more in line with the aims of this paper. This is writen in the line numbers I have provided here.
- RC: Ln-205: 'confidant'?
- AR: The sentence containing this comment has been removed and not replaced with anything comparable.
- RC: Ln-223-226: was it a moving window or plain increment?
- AR: Ln-155-164: The method through which length is manipulated has been updated and is discussed in the line numbers provided.
- RC: Ln-246-248: What's the physical explanation?
- AR: Ln-37-46: The paragraph this comment refers to has been removed however, the physical basis for differences in thermal properties due to coastal location is discussed in the line numbers provided.
- RC: Ln-298: 'One can see ...': unreadable font size
- AR: This sentence and the figure it was referring to have been removed however, pains have been taken to ensure that font sizes are large enough in the figures. Currently, the figures provided in this draft article are slightly smaller than they will be in press as the 'jcl' draft formatting settings performed by LaTeX puts the figures on individual pages at the end of the document with double spaced captions, preventing them being displayed at full size. They are fully vector based and so one may 'zoom-in' on them without loosing any resolution to read them more easily. When they are displayed at full size in the final article format they are legible.
- RC: Ln-320: '... for these data show...' -> '... for these data (in gray ribbon) show ...'
- AR: The figure referred to here has been removed and no comparable figure exists.
- RC: *Ln-387: '... as evinced...'?*
- AR: The sentence in which this issue was found was removed and no comparable sentence exists.
- RC: Ln-392: 'to have better R2' -> did you mean to say 'higher'
- AR: Yes. R2 however no longer features as an important statistic throughout this paper and so this issue is no longer a concern as any mention of 'better' R2 has been removed entirely.

- RC: *Ln-412: 'tough'?*
- AR: The sentence containing this comment was removed and no comparable one exists.
- RC: Ln-427: '... see in 5 ...'?
- AR: This sentence was removed, though pains were taken to ensure that this error was not committed throughout the paper. The problem arose when we moved from using an automatic referencing package in LaTeX to the manual one that JCL requires, which changed the automatic naming conventions in the compiled text.
- RC: Ln-439: 'We we...'
- AR: The sentence containing this comment was removed and no comparable one exists.
- RC: Ln-466-468: Will orthogonal regression instead of a simple linear fit be more helpful here?
- AR: Generalised Least Squares (GLS) models are used throughout this paper in favour of orthogonal regression as the assumption is made that the independent variable used here (date) does not have measurement error. Orthogonal regression is best used for determining linear trends between two variables in which measurement error exists for both. Furthermore, our GLS model allows us to infer linear decadal trend values in the same manner as the IPCC (2014 Synthesis Report, pg2).
- RC: Ln-477-478: I have some concerns about the way it is presented here and elsewhere in the paper regarding the findings that certain precision is adequate or certain length is required. While these statements are true, previous statements/definitions by bodies responsible for climate reports should be referred. Its sounds as if the authors are the first ones to report this.
- RC: For example: US NRC definition of CDR: "A climate data record is a time series of measurements of sufficient length, consistency, and continuity to determine climate variability and change".
- RC: Also, some well-established studies have provided accuracy and stability requirements of SST for climate applications. For example, Table 1 of Ohring et al. (2005), Bulletin of the AmericanMeteorological Society 86:1303-1313
- RC: These are just examples and may not be the only ones or best ones. Please make some additional research to refer to such work and definitions, possibly by NRC, IPCC, WMO, ESA CCI etc. I do not remember at the top of my head, but bringing statements in perspective is needed to make progress.
- AR: Ln-342-345: We refer here to "Guidelines on climate metadata and homogenization (Aguilar et al. 2003)" and "Guide to meteorological instruments and methods of observation (Jarraud 2008)" to highlight the requirements established for the use of data in studies on climate change.
- RC: Ln-487: Unsure if it's a novel methodology standard known methods have been applied in a sound way.
- AR: The conclusion has been shortened substantially and the sentence referred to in the comment has been removed and not replaced.
- RC: Ln-525: '... with a precision 1.0 ...': not relevant. Such a precision is anyway useless for climate use.
- AR: The use of precision 1.0°C has been removed from this paper.

Tables

- RC: The font size is too small and barely readable in all the tables for figures inside the table and headers (at least on the print out that I have). Please increase the font-size; I actually skipped reading most part because of this issue.
- AR: All tables have been removed from the paper. The problem of small text in the figures persists but has been addressed in a previous comment.
- RC: Table A1: too lengthy header very uncommon. Please consider shortening it significantly. Lines 667-674 can easily be moved to the main text or elsewhere.
- AR: As the meta-data of the individual sites is no longer of interest in this study, the massive table in question has been removed.
- RC: Too high R2 values are a real concern, e.g., 0.81. The authors have discussed about it in the text, but still I would double check that the results are derived appropriately.
- AR: These results have been removed due to changes in the methodology.

Figures

- RC: Fig. 1 and 2.:
- RC: Reduce figure size
- RC: Increase font size
- RC: Add the names of the Oceans.
- AR: Fig 2 has been removed as the information it showed is no longer relevant to the methodology.
- AR: Fig 1 size has been reduced.
- AR: The font size was increased by 25%.
- AR: Ocean names and labelled arrows showing currents have been added.
- AR: Added an inset map of the African continent in the left hand corner, a scale bar in the right hand corner and international borders on the main map for better clarity of global location.
- **RC:** Fig.4 and 5:
- RC: Add start year
- RC: Increase font size significantly
- RC: Vertically expand all the 7 plots
- RC: The color-scale for p-values is not helpful to discern values on the plot. Somehow increase the contrast if you are not using a colored scale bar.
- AR: Fig 4 and Fig 5 have been removed but many of these comments still apply and so are addressed here.
- AR: The starting year of the time series cannot be added to the figures as each time series potentially starts at a different date, which prevents comparing the effect of changes in statistics over time if the same x-axis cannot be used.
- AR: Furthermore, the actual date at which the time series begins is not of interest in this study, only the length of the time series itself. The potential issue of comparing all time series based on

their length, and not the actual date in which they start is ameliorated in the length extending portion of the study by shaving off the first X months of each time series so that they all begin in January, providing for an equitable start point for the seasonal signals within the time series. This is discussed on Ln-155-164.

AR: Font sizes were increased throughout.

AR: A beautiful rainbow colour palette is now being used that more clearly delineates the range in the featured statistics.

Reviewer #3

General

- RC: I read this MS with some interest but also consternation. It is potentially of considerable use in analysing inshore temperature time series for studies of trends and even climate change. However, I am not a time series statistician and hesitate to comment on the validity of the methods used. I would have thought that wavelet analysis and other such modern techniques would also have been employed to detect cycles in such time series.
- AR: We have improved upon our methodology as per comments from Reviewer#4 and the analysis performed here is more in line with methods used to analyse time series employed by the IPCC. The approach we have taken in preparing our data is outlined in Ln-138-170 and how it more readily reflects methods used by the IPCC is discussed on Ln-173-195. We avoid using the term 'time series analysis' specifically as the definition for that term does not apply exactly to our methodology here. Furthermore, we are not interested in cycles but in trend detection (their frequency, amplitude, variance, etc.) and so have not employed wavelet analysis here.
- RC: The text is riddled with errors of grammar and style. The Discussion is far too long and wordy and the Conclusion is spoiled by the long paragraphs after the 8 key points enumerated. I believe the text should be reduced by 30% and needs thorough editing for lapses of style, grammar and spelling (e.g. "it's" for "its").
- AR: The main body of the text has been reduced by 6 pages, or roughly 25%. The conclusion has been shortened substantially to include the enumerated points and only a single concluding paragraph. The discussion has been largely re-written, parred down where possible and is now one page shorter in length. Pains have been taken to ensure consistent style and correct use of English grammar throughout.

Corrections, or minor questions and suggestions

RC: Ln-200: punctuation needed!

RC: Ln-205: confident is the verb and adverb

RC: Ln-229: its no apostrophe!

RC: Ln-230: These data...

AR: The sentences containing the above five comments have been removed and not replaced with anything comparable.

RC: Ln-250: Symbols indistinct in Fig 2

AR: Fig 2 has been removed as it no longer shows any information relevant to the study.

RC: Ln-276: Define NA in text and caption

AR: Ln-124-126: Meaning of NA first explained in the text.

AR: Fig 7 caption: NA explained as ...percentage of missing values (%NA)...

AR: All tables have been removed and so it is no longer necessary to explain NA for a table

RC: Ln-338: in length

RC: Ln-340: occurring

RC: *Ln-342: the*

RC: Ln-343: detected

RC: *Ln-346: term*

RC: Ln-349: in length

RC: Ln-351: in length

RC: Ln-355: "... necessity for longer time series..." not "of"

AR: The sentences containing the above eight comments have been removed and not replaced with-anything comparable.

RC: Ln-367: missing data in a time series analysis (not "for")

AR: *Ln-310-319: The paragraph containing this comment was changed to the line numbers given here and the issue was corrected.*

RC: Ln-381: of not "for"

RC: *Ln-383: its not "it's"*

RC: Ln-396: magnitudes ... are dubious ... not "magnitude"

RC: Ln-412: though not "tough"

RC: Ln-412: was

AR: The sentences containing the above five comments have been removed and not replaced with anything comparable.

WESTERN CAPE

VERSITY of the

RC: *Ln-427: Fig.? 5*

AR: This sentence was removed, though pains were taken to ensure that this error was not committed throughout the paper. The problem arose when we moved from using an automatic referencing package in LaTeX to the manual one that JCL requires, which changed the automatic naming conventions in the compiled text.

RC: Ln-448: are

AR: Ln-343-345: Corrected accordingly

Reviewer #4 – Round 1

General

RC: 1 - Does the paper identify a gap in scientific knowledge and add new knowledge to the overall body of scientific understanding, or repeat another study to verify its findings?

- RC: Yes. I think the idea is interesting.
- RC: 2 Is the paper free of errors in logic?
- RC: No. Something that worries me is that the Authors spend a lot of time looking within REAL data for factors that affect significance of climate-change signals. But this pre-supposes that there ARE climate-change signals in their data. Clearly, if there is no signal, no amount of precision, or length of time series will discover one (or, at least, not a real signal). Surely the more appropriate approach would be to find time series with trends that could be attributed to climate change, and then study those? Taking this a step further, it seems obvious to me that the influence of precision on power will depend on the rate of temperature change experienced. If the rate of change is large by comparison to the change in precision, then precision will have little effect...and vice versa. These issues need to be resolved before this paper could be accepted.
- AR: The first issue raised here, of accurately measuring long-term trends, has been addressed through a large improvement to the methodology of the paper. Rather than using STL to find the non-linear trend in a time series and then extrapolate from that the decadal trend signal and the attendant statistics as seen in the previous version of the paper, we are now taking the residuals of the detrended the time series we have and in a controlled manner adding a known decadal trend before fitting a Generalised Least Squares (GLS) linear model equipped with second-order autoregressive AR(2) correlation structure fitted using Restricted Maximum Likelihood (REML). A more thorough explanation of the detrending of the data may be found on Ln-138-170. The explanation of the fitted model may be found on Ln-172-194.
- AR: The power of the time series is no longer relevant to the aims of this paper, given the aforementioned changes to the methodology and so has been removed entirely.
- RC: 3 Do the conclusions follow from the evidence?
- RC: Yes, mostly.
- RC: 4 Are alternative explanations explored as appropriate?
- RC: Yes, generally.
- RC: 5 Are biases, limitations, and assumptions clearly stated, and uncertainty quantified?
- RC: I think the Authors do a reasonable job of covering biases and limitations, but miss some obvious assumptions (see Point 2 above, plus the annotated MS)

WESTERN CAPE

- AR: The issue of uncertainty in the decadal trends in the time series has been addressed by using detrended data, and adding our own decadal trend, which we are then able to be certain of a priori for our analyses.
- RC: 6 Is methodology explained in sufficient detail so that the paper's scientific conclusions could be tested by others?
- RC: No. The underlying approach seems a little arcane to me: extract seasonality, trend and noise, then analyse the trend. I would feel more confident if the Authors (in Supplementary Material, or even just by mentioning it) explored the efficacy of this approach using synthetic data constructed to cover a range of scenarios (i.e., is this method really doing what you think it's doing). It's possible that this was done, but it wasn't mentioned in the text. Even without this step, more explanation of the method is needed, I think.
- AR: The issues with the methodology outlined in this comment have been changed entirely. The data are now detrended by taking the residuals from a linear model fitted to a "real" time

series, these residuals are then treated as "semi-virtual" and manipulated in a series of steps to investigate the effects of the variables noted in the title of the paper. This is explained in greater detail on Ln-138-170.

- AR: More importantly, these changes allow us to track the efficacy of our methods as we know the decadal trend that the models should be detecting a priori. Therefore we may be confident in our findings as to what effect the myriad of variables studied here are indeed having on the ability to detect long-term trends.
- RC: 7 Is previous work and current understanding cited and represented correctly?
- RC: Yes.
- RC: 8 Is information conveyed clearly enough to be understood by the typical reader?
- RC: No. The writing really needs work. It needs to be concise and direct, but instead is convoluted, intricate, and in places, confusing. Moreover, both the Discussion (because Results are repeatedly restated) and the Conclusion (a précis of the entire paper) are far too long, and need to be shortened and tightened. I have annotated the MS liberally...but this work really needs a thorough revision.
- AR: The main body of the text has been reduced by 6 pages, or roughly 25%. The results that were repeated in the discussion have been removed. The discussion has been largely re-written, parred down where possible and is now one page shorter in length. The conclusion has been shortened substantially to include the enumerated points and only a single concluding paragraph. Pains have been taken to ensure consistent style and correct use of English grammar throughout.
- RC: 9 Are all figures and tables necessary, appropriate, legible, and annotated (as appropriate)?
- RC: Yes, although some figures could be clearer (see annotated MS).
- AR: All tables have been removed from this paper.
- AR: All of the figures used in the previous version of this paper, with the exception of Fig 1 have been removed.
- AR: The figures currently shown in this paper were created in accordance with the comments from all reviewers.
 - Corrections, or minor questions and suggestions
- RC: Ln-1: Natural Variability of Seawater Temperature
- AR: Ln-1: Changed accordingly
- RC: Ln-10: Avoid concatenating nouns. "...thermal characteristics of coastal seawater" reads better and makes sentence structure easier. Please resolve throughout.
- AR: Ln-11: Changed to "...thermal characteristics of coastal seawater". Pains have been taken throughout the paper to correct concatenated nouns and to not write them into any new text.
- RC: Ln-15: Concatenating again...
- AR: Ln-15: Concatenated words deleted
- RC: Ln-17: Power is associated with an effect size and a significance level, but you dont mention these here. Please clarify.

- AR: The power analyses were not necessary to the central aim of the paper, explaining the effect certain variables have on the detection of decadal trends and so were removed.
- RC: Ln-20: Awkward wording. Write directly. "We determined that low instrument precision has less effect on the ability of a time series to detect climate change than does..."
- AR: *Ln-17-20*: Reordered sentence to be more readily understood.
- RC: Ln-24: hyphenate compound modifiers
- AR: Ln-23-26: Sentence structure change, words no longer need hyphenating.
- RC: Ln-36: hyphenate compound
- AR: *Ln-53: Hyphenated*
- RC: Ln-41: SI units...abbreviate...
- AR: Ln-58: Abbreviated
- RC: Ln-46: Do you have a better word than "ingest"? Seems a little informal, although it is intuitive...
- AR: Ln-63-64: Sentence containing this word altered at Reviewer #2's request. "ingest" replaced with "collected and refined".
- RC: *Ln-52: set*
- AR: Ln-68: Changed "created" to "Set"
- RC: Ln-52: Insert comma
- AR: Ln-72: Inserted
- RC: Ln-54: Hyphenate compound modifiers
- AR: *Ln-73: Hyphenated*
- RC: Ln-55: Not clear what "these" are...
- AR: Ln-75: Changed "these" to "the in situ time series that comprise the SACTN."
- RC: Ln-56: You use undefined abbreviations in the figure caption. Figures should stand on their own, so please add brief explanation of UTR to the caption at first use. In fact, you haven't even defined UTR in the text, yet...
- AR: Ln-12-13: The UTR acronym is first mentioned in the abstract where it is defined
- AR: Ln-70: The UTR acronym is first used in the main body of the text where it is addressed
- AR: No use of UTRs is made in the figures and so it is no longer necessary to define it in any of the captions.
- RC: Ln-58: statistical characteristics of their temperatures... I'm not correcting any more of these concatenations. Please fix throughout.
- AR: The sentence containing this comment was removed and not replaced with anything comparable.
- RC: Ln-65: The fact that you have to use quotes around "quality" suggests that you really need to define what you are really interested in measuring/assessing...
- AR: Ln-82-83: The word 'quality' meant the accuracy and significance of the results. The word has been removed and the meaning stated explicitly.

RC: Ln-71: You need to pick a better word here...

AR: Ln-86: Changed "employee" to "technician"

RC: Ln-73: Insert comma here.

AR: Ln-87: Word order changed, comma no longer necessary.

RC: Ln-79: of these

AR: Ln-92: Removed

RC: Ln-79: Hyphenate compound modifiers

AR: Ln-93: Hyphenated

RC: *Ln-84*: *using*

AR: Ln-96: Changed "via" to "using"

RC: Ln-89: Number_SPACE_units

AR: *ln-103*: Corrected spacing between number and unit here and throughout the paper.

RC: Ln-90: Hyphenate compound modifiers

AR: Ln-104: Hyphenated "low-water" but not "spring tide"

RC: Ln-93: and to those

AR: Ln-371-372: Sentence has been moved and restructured

RC: Ln-95: Would this point not be better made in the Discussion?

AR: Ln-371-389: Yes. The sentence has been moved to the end of the discussion and expanded into a paragraph discussing the inherent weaknesses in the dataset and validating their use in the face of these limitations. UNIVERSITY of the

RC: *Ln-97: is the*

AR: Ln-107: Changed "are" to "is the"

RC: Ln-97: s

AR: Ln-107: Deleted

RC: Ln-97: These devices have

AR: Ln-107-109: Changed accordingly

Ln-110: I don't see the need to report this. RC:

AR: Ln-116: Deleted "Currently we still receive all data via e-mail or memory stick from the relevant parties."

RC: Ln-113: Insert semi-colon here.

AR: Ln-120: Inserted before "however"

RC: Ln-113: Insert comma here.

AR: Ln-120: Inserted

RC: Ln-114: Hyphenate compound modifiers

AR: Ln-121: Hyphenated

RC: Ln-116: Too much irrelevant detail. Just say that the data were written to a standard data format and layout.

AR: Ln-121-124: Deleted "The data were all given the following standard column headers: site, src, date, temp, depth and type." and added "with consistent column headers" to the previous sentence.

RC: Ln-126: Hyphenate compound modifiers

AR: Ln-109-112: Words needing hyphenation removed

RC: Ln-128: How? Mean? Median? Clarify.

AR: Ln-130: Changed "binned" to "averaged"

RC: Ln-133: Taken together...

RC: Ln-139: Insert comma here.

RC: Ln-139: Insert comma here.Ln-139: This seems piecemeal and awkward, and really needs a better justification...

RC: Ln-141: Insert comma here.

RC: Ln-141: shorter

AR: The paragraph containing the above six corrections has been removed and not replaced with anything comparable. The paragraph in question discussed our reasoning for which statistics (e.g. min/ max or 5 th / 95 th percentile) we chose to use to display the range of values within certain sub- groupings of time series. Because these sub-groupings have been removed, as they are no longer relevant to the methodology, it is no longer necessary to display the ranges.

RC: Ln-144: Insert comma here.

RC: Ln-150: Insert comma here.

RC: Ln-158: warmest and coolest

RC: Ln-163: SI units...abbreviate...

RC: Ln-165: a

AR: The two paragraphs containing the above five corrections were removed as the methodology no longer requires coastal groupings to be determined by hierarchical cluster analysis.

RC: Ln-177: I am not overly familiar with the method used here, but "trend" usually refers to a rate...so are you calculating the rate of a rate here, similar to acceleration? Perhaps clarify by rewording?

AR: The sentence in question failed to mention that the "trend" being referred to was actually a "non-linear trend" and that by fitting a liner model to this non-linear trend signal we were effectively quantifying the linearity and thereby the mean decadal rate of change, which is otherwise not possible for a non-linear trend. As STL is no longer used in this paper, in favour of a GLS model, the section in which this sentence is found has been removed and the methodology that refers to the new creation and measuring of slopes may be found on Ln-147-151 and Ln-185-189.

RC: Ln-179: quantifying

RC: Ln-180: was

- AR: The sentences containing the above two comments were removed and not replaced with anything comparable.
- RC: Ln-182: Brackets are incorrect here...
- AR: Ln-173-174: Changed sentence structure so that brackets were appropriate.
- RC: Ln-184: suggesting
- The sentence containing this comment was removed and not replaced with anything comparable.
- RC: Ln-185: we?
- AR: All uses of "the authors" have been changed to "we" throughout the paper. The sentence containing this specific comment has been removed.
- RC: Ln-190: Insert comma here.
- Ln-192: This again needs more rationale/a better explanation...its just not clear to me... RC:
- The necessity of displaying ranges of values in this manner is no longer necessary, as explained previously, and so the paragraph that contained the above two comments has been removed.
- RC: Ln-195: among
- Ln-195: A correlation coefficient tells you about the strength of the linear relationship of RC: temperature vs time, but not about temperature change over time. Clean up the language here...
- RC: Ln-197: To detect significant trend? And what do you consider "significant". More information needed here.
- RC: Ln-200: Break the sentence here.
- RC: Ln-201: s
- UNIVERSITY of the Ln-201: results of power analyses RC:
- Ln-202: This last sentence is awkward and needs some thought... RC:
- AR: The power analysis has been removed from this paper as it is no longer relevant to the aims or objectives. Because we are now artificially manipulating the decadal trend directly it is no longer necessary to perform a power analysis to test a posteriori how many months of data are necessary to reach a certain power given a certain effect size. Therefore the paragraph that contained the above seven comments has been removed.
- RC: Ln-207: Awkward wording...revise entire sentence.
- This sentence has been removed as it is no longer necessary to relate the analysis of the time series to the non-existent power analysis.
- RC: Ln-208: Insert comma here.
- RC: Ln-209: of
- RC: *Ln-209: have*
- AR: Ln-165-170: The sentence containing the above three comments has been removed. The comparable sentence may be found on the lines provided.
- RC: Ln-209: Awkward wording...revise...

- AR: Ln-142-144: The sentence has been largely re-worded.
- RC: Ln-214: Insert comma here.
- RC: Ln-215: Insert comma here.
- RC: Ln-216: subjected to
- AR: The two sentences containing the above three comments were removed as they relate to the power analysis and sub-groupings of data which no longer exist in the papers present form.
- RC: Ln-220: Insert comma here.
- AR: Ln-155-157: Sentence restructured, comma used appropriately
- RC: Ln-222: Awkward. Write actively and directly. There are far too many convoluted sentences here.
- AR: *Ln-157-160*: *Sentence split into two and written more actively and directly.*
- RC: Ln-227: Insert comma here.
- RC: Ln-229: its
- AR: The two sentences containing the above two comments were removed and not replaced with anything comparable because we are no longer affecting the variance of the time series directly.
- RC: Ln-230: This assumes that the "noise" component was random. Did you explore this unstated assumption. Clarify.
- AR: Ln-185-192: As we are no longer adding randomly generated data to the time series to simulate noise, checking this assumption is no longer necessary. In the new methodology seen in this paper, we control for autocorrelation in the time series using an AR(2) autoregressive correlation structure and is explained further on the line numbers provided here.
- RC: Ln-241: determine the point at which precision...
- AR: Ln-151-153: This sentence has been largely restructured.
- RC: Ln-245: statistical
- RC: Ln-252: further
- RC: Ln-252: further
- AR: The paragraph containing the above three comments has been removed as the coastal classification is no longer being performed.
- RC: Ln-262: SI units. Abbreviate.
- AR: The paragraph containing this comment has been remove however, pains have been taken to ensure appropriate abbreviation of all SI units throughout the paper.
- RC: Ln-263: I'm sorry, but I don't understand how a squared number can be negative...?
- AR: These slightly negative R2 values are artefacts of the Adjusted R2 values produced by the programming language R. The changes to the methodology have seen the removal of all R2 values and so they are no longer present in this paper.
- RC: Ln-264: responsible
- AR: The sentence containing this comment was removed and not replaced with anything comparable.

- RC: Ln-273: Could you tell us whether the slope of this relationship is positive or negative?
- AR: The sentence containing this comment was removed and not replaced with anything comparable. Pains have been taken to ensure that any mention of relationships in the text are explained to be either negative or positive when such a clear relationship exists.
- RC: Ln-276: Proportion of missing values? Write in terms the naive reader can understand unambiguously...
- AR: Ln-125: The use and definition of "NA" is first given here.
- RC: Ln-274: Insert comma here.
- RC: Ln-278: those from
- RC: *Ln-279: coasts*
- AR: The paragraph containing the above three comments was removed as the groupings outlined therein are no longer used.
- RC: Ln-285: You could always simply list the 95th percentile numerically to the right of each bar...
- AR: The figure in question has been removed due to the changes to the methodology however, before removing it the 95 th percentiles were added, as suggested here, and it worked very well.
- RC: *Ln-290: months*
- RC: Ln-292: Insert comma here.
- AR: The paragraph containing the above two comments was removed as the power analysis is no longer being performed.
- RC: Ln-294: Fig. 4 really needs to be expanded vertically, so that patterns can be more easily inspected.
- AR: The original Fig 4 has been removed. Pains have been taken to ensure that the new figures are tall enough for the patterns therein to be inspected with ease.
- RC: Ln-294: These are wasted words. Simply tell the reader what the point is, and then reference the figure.
- AR: The figure and sentence this comment refers to have been removed. Reference to figures in the results section is now done with less wordiness.
- RC: Ln-297: The shading in Figs 4 & 5 doesnt really allow the reader to ascertain when thresholds in p values are crossed. It might well be better to use a binned palette than a continuous one...
- AR: Fig 4 & 5 have been removed, but before they were the shaded colour range was replaced with a discrete scale showing values under 0.05, 0.01 and everything above 0.01 as black, grey and whiterespectively and it worked very nicely. The new figures used in this paper use a beautiful rainbow colour palette instead of grey scale.
- RC: Ln-312: I think you need to tell us what the range of "noise" SD was in your data...
- AR: Ln-223-224: Reference to the effect of SD on the time series is first made in the results but the range is not given as the specific range is not relevant.
- AR: Fig 5: The range of SD present in the study is shown

- AR: Ln-324-327: Mention of specific SD is made.
- RC: Ln-316: This is not self-evident. Why would the mean temperature influence the effect of SD? Explain.
- AR: The sentence was deleted as this portion of the methodology has since been removed. The reasoning behind this statement is that SD is a measure of variance around a mean, and if that mean value is larger, the SD value is likely to be larger as well. So a set of data with a smaller mean than another set of data will also likely have a smaller SD, all things considered. To accurately compare variance between two sets of data with different sized means a better statistic to use is standard error (SE) as this is the SD divided by the mean, effectively controlling for the differences in mean and SD between datasets.
- RC: Ln-315: Did R2 decrease TO this value or BY this value? Not clear from what is written here...
- RC: Ln-317: Hyphenate compound modifiers
- RC: Ln-317: affected
- RC: Ln-320: greatest
- AR: The four sentences containing the four comments above were removed due to changes in methodology and were not replaced with anything comparable.
- RC: Ln-320: percentile?
- AR: Percentiles are no longer measured in this paper and so all mention of either "quartiles", "quantiles" or "percentiles" has been removed.

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- RC: Ln-327: There
- AR: This sentence has been removed however, pains have been taken to ensure the correct use of "there", "their" "they're".

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- RC: Ln-340: Hyphenate compound modifiers
- RC: Ln-341: in
- AR: The sentence containing the above two comments has been removed and not replaced with anything comparable.
- RC: Ln-350: Im not sure that this is the word you should use here.
- RC: Ln-351: Insert comma here.
- **RC**: *Ln-352: those for*
- AR: The sentence containing the above three comments has been removed and not replaced with anything comparable.
- RC: Ln-355: You need to justify why you think this is impossible. Certainly, I'd agree that rates of ocean warming of this magnitude are unlikely, but this doesnt make their measurement impossible...I can think of several ways (including simple instrument failure) that such values could be achieved.
- AR: The methodology has changed so that we now control the decadal trends directly, which no longer allows extreme results like those commented on in the sentence in question. This sentence has been removed and not replaced with anything comparable.
- RC: Ln-358: Insert comma here.

- AR: Ln-227-240: The paragraph containing the comment has been largely changed.
- RC: Ln-359: This is a MAJOR issue that needs to be highlighted in the Methods. I dont remember seeing it there at all!
- AR: Ln-131-134: The exclusion of time series based on %NA is first mentioned. As linear interpolation is no longer used to fill gaps any mention of it has been removed from the paper.
- AR: Ln-227-240: The results of the effect of %NA are discussed here.
- AR: Ln-310-319: Further discussion on %NA takes place here.
- RC: Ln-365: We again have a negative square...?
- AR: This has been addressed previously.
- RC: Ln-366: suggests
- AR: *Ln-233-243: The information discussed in the sentence in question has been expanded upon and may be found at these lines.*
- RC: *Ln-372: small*
- RC: Ln-373: It is NOT nonsensical. The problem is that you have the unstated assumption that all of your temperature series are responding to changing climate, which is not necessarily the case. And for those series that are responding, there will be a range of rates of response.
- RC: Ln-381: In what sense misleading?
- RC: Ln-383: its
- RC: Ln-385: A REASON is not attributed...a TREND or response is attributed.
- RC: Ln-389: Insert comma here.
- AR: The section containing the above six comments has been removed entirely as a power analysis is no longer performed. The above comments that address problems in substance have been addressed previously.
- RC: Ln-396: Surely this depends on when the time series was initiated relative to decadal cycles in temperature?
- AR: If the time series was initiated a few years before the turn around of a decadal pattern and the first ten years has a roughly even split of increasing and decreasing directionality in the non-linear trend then the relevant statistics in the first ten years will be relatively low, but the results show that this was almost never the case. This is however what happens to all of the time series after 20 years, and then starts to even out after 30 years. The use on non-linear trends has however been removed from this paper and so the sentence referred to here has been removed.
- RC: Ln-401: This is a truly horrible word...
- AR: True. But it somehow worked it's way into my heart at some point. The sentence in which this word was found has since been removed and not been replaced with anything comparable.
- RC: Ln-403: It is a statistical principle that to estimate a statistic with any confidence, independent replicates are needed. So if you want to know the annual trend, you can use a sample of annual temperatures...but if you want to know the decadal trend, you need a sample of decadal temperatures...
- AR: Ln-297-298: This tautology has been removed and is mentioned more clearly on these lines.

RC: Ln-406: Does this really pertain to ANY time series, or only to the timing of the initiation of time series studied here? The wording suggests that this is a general principle, but I dont think there is any convincing evidence that it is...

AR: The statement in the sentence in question was supported by the findings within the dataset used forthis study, so it that sense yes, these findings are correct generally in as far as we were able to include given the data we had access to. Perhaps data from Chile, for example, would show different results. Regardless, this sentence and the results it discusses have been removed from the paper.

RC: *Ln-412: were*

AR: This sentence has been removed and not replaced with anything comparable.

RC: Ln-427: ???

AR: This sentence was removed, though pains were taken to ensure that this error was not committed throughout the paper. The problem arose when we moved from using an automatic referencing package in LaTeX to the manual one that JCL requires, which changed the automatic naming conventions in the compiled text.

RC: Ln-427: It isnt necessary to repeat the Results in the Discussion... Use the Results to point to the patterns/phenomena that you want to explore in the Discussion, and leave the Discussion for that exploration...

AR: As discussed in item 8 above, redundant mention of results has been expunged from the Discussion section.

RC: Ln-432: Insert comma here.

RC: Ln-432: Insert comma here.

RC: Ln-434: Insert comma here.

RC: Ln-434: Insert comma here.

AR: Ln-282-296: The paragraph containing these comments has been largely rewritten and may be found at these lines.

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RC: Ln-437: I don't remember seeing units for SD in the Results/Methods. Please check.

AR: This has been corrected for where missing.

RC: Ln-451: Hyphenate compound modifiers

RC: Ln-452: Insert comma here.

AR: Ln-336-338: The sentence containing these two comments has been largely rewritten.

RC: Ln-464: Your sentence loses its parallel structure here....

AR: *Ln-395-396: The sentence has been split into two separate sentences.*

RC: Ln-467: Is this really a conclusion. Is this not true by definition?

RC: Ln-469: It's not the trend lines that increase or decrease, but some feature of the trend lines. Be clear what you mean.

RC: Ln-470: Insert semi-colon here.

AR: These two concluding points containing the above three comments have been removed as non-linear trends are no longer used.

- RC: Ln-472: Sentence structure throughout these bullet points is confusing. Rewrite.
- AR: Concluding points have been rewritten so as to be stand alone factoids.
- RC: Ln-477: Assuming that the trend moves the temperature by more than 0.1°C...You could have a perfectly linear increase with a gentler slope and never detect it.
- AR: Ln-356-358: This issue is addressed in more depth here.
- RC: Ln-479: Read this highlighted part of the sentence and imagine you have little context for the paper...write so that the reader doesnt have the read the sentence three times to be sure they understand what you really mean...
- AR: The confusing wording of appropriately describing the improvement of a value by decreasing it has been largely addressed throughout the paper by simply providing the values to and from which the increase or decreases are occurring. An example may be seen on Ln-355.

Reviewer #4 – Round 2

General

- RC: The writing is improved, but is still somewhat problematic throughout. Although editorial issues are minor, there are places where poor sentence construction leads to ambiguity, and these need to be corrected. I have included some minor suggestions below, but will leave final sign off on copy editing to the Journal's Editor.
- AR: All suggested changes have been made and both authors have once more proof read the manuscript and made changes to sentence structure and ambiguity where appropriate.

Corrections, or minor questions and suggestions

- RC: Line 25: Break sentence.
- AR: Line 25: Sentence split in two: "There is no appreciable effect on model accuracy between measurement precision of 0.1 °C to 0.001 °C. Measurement precisions of 0.5 °C require longer time series to give equally accurate model results."

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- RC: Lines 34-36: Awkward sentence. Is SST the main determinant of several physical variables, or is it just one of the most-used physical variables. Ambiguous.
- AR: Lines 34-36: Sentence changed to: "A thorough understanding of these coastal processes is provided by several physical variables, with temperature being one of the main determinants."
- RC: Line 41: The first few phrases are parallel, but this falls apart toward the end. Maybe just delete "tending towards"?
- AR: Line 40-42: Sentence changed to: "Based on these thermal properties, the coastline has been classified into a cool temperate west coast, a warm temperate south coast and a sub-tropical east coast."
- RC: Line 45: "cooled at"?
- AR: Line 45: The phrase "cooled at" could not be found in the manuscript. But this likely refers to the wording for the decadal rate of change in the Benguela. This is now written as "decreased by" in the manuscript.
- RC: Line 55: Break the sentence to avoid complex sentence structure in the second half.

- AR: Line 51-56: Sentence split in two: "Nevertheless, a widespread approach in coastal ecological research is to use satellite and/or model-generated temperature data as a representation of SST along coastlines (e.g. Blanchette et al. 2008; Broitman et al. 2008; Tyberghein et al. 2012). Either the dangers of applying gridded SSTs to the coast are not widely known or in many places in the world there simply are no suitable in situ coastal temperature time series available."
- RC: Line 58: "...of the shoreline..."
- AR: Line 57: Changed accordingly
- RC: Line 70: "...(UTRs), which have an..."
- AR: Line 69: Changed accordingly
- RC: Line 79: "...and this forms the core..."
- AR: Line 78: Changed accordingly
- RC: Line 87: "...characteristics of a time series..."
- AR: Line 86: Changed accordingly
- RC: Line 88: Second use of "time series" in the same sentence is a bit awkward.
- AR: Line 87: "... temperature time series" changed to "...temperatures."
- RC: Line 130: "...finer than..."
- AR: Line 129: Changed accordingly
- RC: Line 135: "binned"...do you mean averaged? Not clear?
- AR: Lines 133-135: Sentence changed to: "At the time of this analysis, this usable daily dataset consisted of 84 time series, consisting of 819,499 days of data; monthly averages were then made from these daily data to create the 26,924 temperature values available for use in this study."
- RC: Line 138: "composed of" or "comprising", but not "comprised of..."
- AR: Line 137: Changed to "composed of".
- RC: Line 190: "This approach is..."
- AR: Line 189: Changed accordingly
- RC: Lines 237-239: Confusing sentence structure resolve
- AR: Lines 236-239: Sentences changed to: "In other words, the more missing values (NA) there are in a time series with no discernible decadal trend, the more likely a model is to erroneously detect one. On the other hand, model results from time series that do have detectable decadal trends tend to produce fits that are not significantly different from 0°C dec⁻¹."
- RC: Line 275: "...length of data series."
- AR: Line 275: Changed to "...the length of the time series."
- RC: Lines 290-291: "coastal sections" ...clumsy wording
- AR: Lines 290-291: The term "coastal sections" is used first in the abstract on line 39 and also throughout the manuscript. The term "coastal regions" is not used instead as this implies to much ambiguity. The "coastal sections" of South Africa have well defined borders as seen in Smit et al. 2013 and so the term is used in this manuscript as well.
- RC: Line 297: "requires"

- AR: Line 297: Changed accordingly
- RC: Line 309: "...needs..."
- AR: Line 309: Changed accordingly
- RC: Lines 323-324: It's not impossible, it just didn't happen in your study.
- AR: Lines 323-324: Sentence changed to: "No trends with a slope < 0.05 °C dec⁻¹ were found to be significant in this study."
- RC: Line 325: "...an SD..."
- AR: Line 325: Changed accordingly
- RC: Line 355: "...a time series's ability..."
- AR: Lines 353-356: Sentence changed to: "Extending time series in this way will serve to make themmore dependable as length is the primary criterion through which one should initially assess the potential to accurately detect a decadal trend before refining ones assumptions with any statistical analyses."
- RC: Lines 356-357: Use finer/coarser when referring to resolution; greater/less introduces ambiguity.
- AR: Lines 356-357: Corrected here and throughout the manuscript.
- RC: Lines 366-370: I think this argument needs to be more carefully phrased. Quoted out of context, a statement like this might easily be used to misrepresent the authors' point.
- AR: Lines 366-370: I find this sentence to accurately reflect the point the authors are making. That the statistical significance of a trend is not as important as the real world application of the trend for applied research. One of the most important conclusions made in this manuscript is that a model may accurately detect a trend more than a decade before the variance in the time series allows that trend to be shown as significantly different from 0. Given that data must be collected for decades before they may be used, shaving a decade or two off of this process is a very useful consideration; therefore, it is important to note that one must not focus exclusively on the significance of a detected trend.
- RC: Some specific and generic epithets remain unitalicised in the reference list. Please check references carefully.
- AR: Italics and other minor issues corrected for: Bolton et al. 2012, Chao et al. 2009, Cliff et al. 1988, Grant et al. 2010, Kennedy et al. 2011, Roberts 2005, Smit et al. 2013, Stocker et al. 2013 and Vazquez-Cuervo 2013.
- RC: Fig. 2...and goes to Methods, also. Many of the detrended series have a slight preponderance of negative residuals. Given that these will be a consequence of the fit to the data (the removed trend was likely not as linear as suggested by the model)...is it worth considering centring them to zero before adding a trend back in?
- AR: It was deemed appropriate to keep the detrended time series as is, even with their preponderance of slightly negative residuals, so as to allow them to better represent the natural variability found in the raw data. That negative residuals are so widespread throughout all of our anomaly time series shows that this is perhaps a universal property of coastal seawater data sets. The higher number of time series with more negative anomalies is caused by more warm outliers than cold, as seen in Figure 2. If the time series were centred to zero this would change the variance present in the data and reduce the fidelity of this analysis to the central research

question of "How capable are models at detecting decadal trends in coastal seawater temperature time series?" These time series are infamous for the greater variance they show over their meso-scale+ counterparts, so allowing this natural variability to remain is crucial. Furthermore, after detrending all 84 time series the anomalies were fitted again with a simple linear model to ensure that the slope of each anomaly time series was indeed 0.





C H A P T E R

SECOND STUDY

Introduction

was now possible to use these data for a more direct application. The initial proposal of this thesis was to use these SACTN data for investigations into the effect of extreme temperature events on kelp forests. Upon beginning this second study I discovered very quickly that so little was known about said events as to prevent any such research. For this reason I then chose to focus my thesis more on the detection of these events than on the impacts they may have.

The detection of extreme thermal events along the coastline of South Africa had not yet been performed. Offshore trends in remotely-sensed temperatures were the closest thing in the literature (*e.g.* Rouault et al., 2009), but this was not the mode of climate change I was interested in addressing. To simply document and record the events did not contribute enough to our collective knowledge to be worthy of a publication. More was required. And so I began to look for what the potential causes of these coastal MHWs may be.

It has been assumed that nearshore phenomena must normally be forced by offshore phenomena. For this reason I chose to look for rates of co-occurrence between MHWs happening in the SACTN data, and MHWs happening offshore. I determined offshore here by taking shore-normal transects from each SACTN time series that was at least 10 years long, and then determining what the remotely-sensed temperatures over the continental shelf along that transect were. By affording certain periods of lag around these events it allowed me to quantify the rates of co-occurrences over certain periods of time as well as how often the offshore MHWs preceded the nearshore ones and *vice versa*. This study served the dual purpose of further testing the strength of the relationship between nearshore and offshore temperatures. Because of this, I also decided to look for the rates of co-occurrence between what I called 'marine cold-spells' (MCSs). The idea here was that these would serve as a sort of proxy for upwelling events and that the rates of co-occurrence for these events would be lower for the MHWs due to a different relationship in their forcing.

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Nearshore and offshore co-occurrence of marine heatwaves and cold-spells



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ABSTRACT

A changing global climate places shallow water ecosystems at more risk than those in the open ocean as their temperatures may change more rapidly and dramatically. To this end, it is necessary to identify the occurrence of extreme ocean temperature events - marine heatwaves (MHWs) and marine cold-spells (MCSs) - in the nearshore (<400 m from the coastline) environment as they can have lasting ecological effects. The occurrence of MHWs have been investigated regionally, but no investigations of MCSs have yet to be carried out. A recently developed framework that defines these events in a novel way was applied to ocean temperature time series from (i) a nearshore in situ dataset and (ii) $\frac{1}{4}$ ° NOAA Optimally Interpolated sea surface temperatures. Regional drivers due to nearshore influences (localscale) and the forcing of two offshore ocean currents (broad-scale) on MHWs and MCSs were taken into account when the events detected in these two datasets were used to infer the links between offshore and nearshore temperatures in time and space. We show that MHWs and MCSs occur at least once a year on average but that proportions of co-occurrence of events between the broad- and local scales are low (0.20-0.50), with MHWs having greater proportions of co-occurrence than MCSs. The low rates of cooccurrence between the nearshore and offshore datasets show that drivers other than mesoscale ocean temperatures play a role in the occurrence of at least half of nearshore events. Significant differences in the duration and intensity of events between different coastal sections may be attributed to the effects of the interaction of oceanographic processes offshore, as well as with local features of the coast. The decadal trends in the occurrence of MHWs and MCSs in the offshore dataset show that generally MHWs are increasing there while MCSs are decreasing. This study represents an important first step in the analysis of the dynamics of events in nearshore environments, and their relationship with broad-scale influences. © 2017 Elsevier Ltd. All rights reserved.

1. Introduction

Over the past three decades, anthropogenically mediated warming has negatively affected marine and terrestrial ecosystems with far reaching consequences for humanity and natural ecological functioning. Although climate change is generally understood as a gradual long-term rise in global mean surface temperature (Stocker et al., 2013), which will continue for decades or centuries, it is generally the associated increase in frequency and severity of extreme events that affects humans and ecosystems in the short-term (Easterling et al., 2000). Impacts of extreme events such as floods, wind storms, tropical cyclones, heatwaves and cold-spells

are often sudden with catastrophic consequences. The recognition to focus more on the extremes and less on the background mean state has emerged as a critical direction of climate change research (Jentsch et al., 2007).

'Heatwaves' usually refer to atmospheric phenomena where vague definitions such as "a period of abnormally and uncomfortably hot [...] weather" are invoked (Glickman, 2000), but there are also precise definitions based on statistical properties and other metrics of the temperature record that are relative to location and time of year (e.g. Meehl, 2004; Alexander et al., 2006; Fischer and Schär, 2010; Fischer et al., 2011; Perkins and Alexander, 2013). As the definitions for heatwaves have increased, so too have the investigations of heatwaves in the ocean (e.g. Mackenzie and Schiedek, 2007; Selig et al., 2010; Sura, 2011; Lima and Wethey, 2012; DeCastro et al., 2014). Well-known marine heatwaves (MHWs) have occurred in the Mediterranean in

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2003 (Black et al., 2004; Olita et al., 2007; Garrabou et al., 2009), off the coast of Western Australia in 2011 (Feng et al., 2013; Pearce and Feng, 2013; Wernberg et al., 2013), in the north west Atlantic Ocean in 2012 (Mills et al., 2012; Chen et al., 2014, 2015) and more recently the "Blob" in the north east Pacific Ocean (Bond et al., 2015). The extreme temperatures from these events have had negative impacts on the local ecology of the regions in which they occur. For example, the 2003 Mediterranean heatwave may have affected up to 80% of the gorgonian fan colonies in some areas (Garrabou et al., 2009), and the 2011 event off the west coast of Australia is now known to have caused a 100 km range contraction of temperate kelp forests in favor of seaweed turfs and a tropicalisation of reef fishes (Wernberg et al., 2016).

Although the consequences of these anomalously warm events have been widely publicized, the events themselves have until recently not been objectively characterized. In part, this has been due to the lack of a consistent definition and metrics. In response to this need, Hobday et al. (2016) developed a definition of a MHW as "a prolonged discrete anomalously warm water event that can be described by its duration, intensity, rate of evolution, and spatial extent," and in doing so have derived statistical metrics that quantify these properties. For example, the count of MHWs within a time series and their maximum and cumulative intensity are quantifiable parameters that can be calculated in an objective and consistent manner irrespective of geographical location. The focus of this paper is on marine thermal events that are anomalous with respect to the seasonal climatology as per the Hobday et al. (2016) definition. They may be anomalously warm events, or anomalously cold (marine cold-spells, MCSs; introduced here). While MHWs are becoming reasonably well known by virtue of their increasing count and intensity, MCSs have received less recognition. Whereas extreme hot events may be demonstrably damaging to organisms and ecosystems, extreme cold events also have the potential to negatively impact organisms and ecosystems (Lirman et al., 2011). In both cases their drivers and dynamics, offshore as well as in the nearshore (<400 m from the coastline), remain poorly understood.

MCSs are projected to become less frequent under future climatic scenarios, but there are also examples of them becoming more frequent in some localities (e.g. Gershunov and Douville, 2008; Matthes et al., 2015). They are frequently lethal to marine organisms (Woodward, 1987) and are known to have caused mass fish (Gunter, 1941, 1951; Holt and Holt, 1983) and invertebrate (Gunter, 1951; Crisp, 1964) kills, the death of juvenile and subadult manatees (O'Shea et al., 1985; Marsh et al., 1986) and coral bleaching (Lirman et al., 2011). Cold temperatures are very important in setting species population distribution limits, particularly limiting their range north- or southwards towards higher latitudes (Firth et al., 2011), and the timing of the onset of growing seasons (Jentsch et al., 2007). It is easy to imagine how population-level consequences might aggregate to drive whole ecosystem responses (e.g. Kreyling et al., 2008; Rehage et al., 2016). Indeed, the range contractions of ecosystem engineer species such as mussels have been shown to relate to MCSs (Firth et al., 2011, 2015).

Although we understand that the sea surface temperature (SST) of the upper mixed layer is influenced by oceanic and atmospheric processes (see Eq. (1) of Deser et al., 2010), there is by no means a good understanding of how these processes are modulated by local- vs. broad-scale influences, thus resulting in nearshore MHWs and MCSs. Some of the MCSs known to have impacted populations were caused by atmospheric cold-spells affecting the intertidal and coastal biota locally (Gunter, 1941; Firth et al., 2011). We hypothesise that these localized events are manifestations of extreme atmospheric cold weather phenomena situated over the coast resulting in rapid heat loss from coastal waters. On the other hand, we also hypothesize that broader-scale teleconnections may also

affect the thermal properties and dynamics of coastal systems. For example, large-scale atmospheric-oceanographic coupling is being affected by global warming, which is projected to cause the intensification of upwelling favorable winds and consequently the intensification and increasing count of upwelling events (see García-Reyes et al., 2015 for a review of this and alternative hypotheses). It is therefore possible that the development of some nearshore MCSs may be attributed to an intensification of upwelling. MHWs at any scale likely originate directly from atmosphere-ocean heat transfer as in the Mediterranean Sea (e.g. Garrabou et al., 2009) or from advection, i.e., the transport of warm water due to currents such as what happened off Western Australia in 2011 (Feng et al., 2013; Benthuysen et al., 2014), the NW Atlantic in 2012 (Mills et al., 2012; Chen et al., 2014, 2015) and potentially off SE Australia in 2016. Because MHWs and MCSs are both able to effect ecosystem change, a mechanistic understanding of their drivers may be useful for conservation and management purposes. To this end our study serves as a constructive first step to understand the prevalence of anomalous thermal events with respect to forcing mechanisms at different scales.

Hobday et al. (2016) applied their MHW framework to the $\frac{1}{4}$ ° NOAA Optimally Interpolated SST dataset (hereafter referred to as OISST; Reynolds et al., 2007), but warned users to be cognizant that different data sets would provide different kinds of information pertaining to heatwaves. Our study applied this MHW (MCS) definition to datasets of nearshore in situ (local-scale) and offshore gridded OISST (broad-scale) temperature time series collected at different locations along coastlines influenced by contrasting ocean currents - the Benguela Current, an eastern boundary upwelling system, and the Agulhas Current, a western boundary current and locally modified by regional aspects of the coastal bathymetry, geomorphology and other smaller scale coastal features. Having assessed these systems within a framework that coupled localand broad-scale features permitted us to assess how MHWs (MCSs) developed in coastal regions. Specifically, we aimed to assess the significance of MHWs (MCSs) within the context of the datasets inherent differences, and examine the various dynamical properties that then emerged out of the regional oceanographic context and out of the local-scale modifications of the regional ocean features as they approached the coast. In doing so, the aim was to provide some insights into possible mechanisms that determine the nature and origin of MHWs (MCSs) within regionally distinct ocean/coastal sections. We hypothesized that (i) nearshore localscale MHW events are coupled with offshore broad-scale thermal patterns; (ii) MCSs originate at the local-scale in the nearshore in situ dataset as isolated incidents decoupled from broader-scale patterns; (iii) different coastal sections, each variously influenced by interactions between local- and broad-scale processes, display different dynamics (timing, count, duration and intensity) of MHWs (MCSs); and (iv) the count of warm (cold) events increases (decreases) with time under a regime of climate change. The effect of atmospheric forcing on nearshore events was considered but not assessed within the scope of this study.

2. Methods

2.1. Study region

The variety of oceanographic features around the ca. 3100 km long South African coast provides a natural laboratory for the potential effects of different ocean forcing mechanisms on the occurrence of MHWs and MCSs. Annual mean (\pm standard deviation; SD) coastal seawater temperatures range from 12.3 ± 1.2 °C at the western limit near the Namibian border (Site 1) to 24.4 ± 2.0 °C in the east near the Mozambican border (Site 21).

Our study sites covered this full range (Fig. 1). We classified the coast into three sections based on their major oceanographic features, their temperature characteristics, and aspects of the underlying continental shelf. The west coast section is dominated by the Benguela Current, which forms an Eastern Boundary Upwelling System (EBUS) (Hutchings et al., 2009). Seasonal upwelling is maintained by prevailing south-easterly trade winds and low temperatures are especially noticeable at upwelling cells over a relatively narrow continental shelf in the region from the Cape Peninsula to Cape Columbine. The west coast represents a cool temperate regime, with a range of monthly mean temperatures at generally intermediate between cold temperate and warm temperate (Lüning et al., 1990). The warm temperate east coast section is strongly influenced by the warm south-westerly flowing Agulhas Current, which hugs tightly along the narrow continental shelf (except for the Natal Bight) (Lüning et al., 1990). This stretch of coast is spatially homogeneous with respect to temperature and characterized by a moderate amount of seasonal variation. Although the Agulhas Current retroflects back into the southern Indian Ocean (Hutchings et al., 2009) just south of the much wider and cooler Agulhas Bank (Roberts, 2005), its influence regularly extends as far west as False Bay (Sites 5-21; Fig. 1). Between the west and east coasts is the south coast section overlying the Agulhas Bank. Although also warm temperate, the south coast is fundamentally different from the other coastal sections in that it is dominated by not one strong current, but rather consists of a broad continental shelf on which the interplay of the Agulhas and Benguela Currents form a 'mixing-pot' between two oceans, as well as hosting an attendant array of complex coastal processes that modify the already thermally variable waters overlying the Agulhas Bank (Lutjeharms et al., 2003; Roberts, 2005; Hutchings et al., 2009). It experiences a much larger range in annual temperature and variability compared to the west and east coast sections, which is in part influenced by the retention and cooling of Agulhas Current water on the bank, the presence of some current-driven upwelling cells along this coastal section (Sites 15–17) (Roberts, 2005), and from the effects of capes and embayments throughout the region. A more detailed description of these three coastal sections may be found in Smit et al. (2013).

2.2. Temperature data

The *in situ* seawater temperature dataset used in this study was comprised of 127 records of daily measurements of up to 40 years with a mean duration of ca. 19 years. These in situ time series are generally shorter than the recommended 30 year minimum for the characterization of MHWs (Hobday et al., 2016) and have occasional gaps of missing data. However, there is a clear benefit of using in situ data over satellite data as they provide a more accurate representation of the thermal characteristics near the coast where satellite measurements do not capture maximum and minimum temperatures well (e.g. Smale and Wernberg, 2009; Castillo and Lima, 2010). For example, satellite SST data along the coast of South Africa have shown warm biases as high as 6 °C over in situ temperatures in the nearshore environment Smit et al. (2013). All time series from the in situ dataset under 10 years in duration were excluded from this study to ensure at least one decade of data was used to estimate the climatology required for the identification of MHWs (MCSs). Time series missing more than 10% of their daily temperature measurements were also excluded, leaving a total of 21 time series. These were then classified into the three coastal sections detailed above. Metadata for the selected time series, including location, duration, and the coastal sections they were aggregated into can be found in Table S1.

The remotely sensed temperature dataset used in this study were the daily $\frac{1}{4}$ ° NOAA Optimally Interpolated SST (OISST; Reynolds et al., 2007) derived from the Advanced Very High Resolution Radiometer (AVHRR). To create time series from these OISST

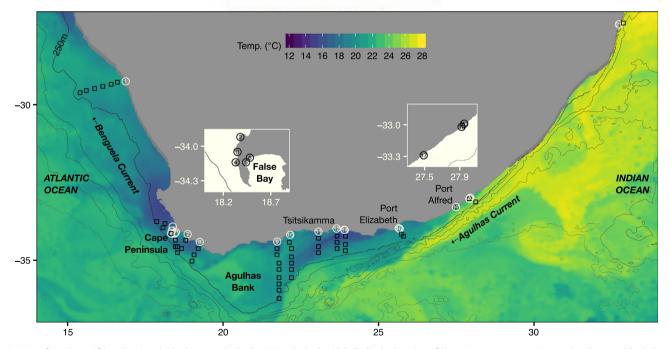


Fig. 1. Map of southern Africa showing the bathymetry (only the 250 m isobath is labelled), the location of thein situ temperature time series shown with circles and approximations of the pixels used along the shore-normal transects from the daily $\frac{1}{4}$ ° NOAA OISST (Reynolds et al., 2007) shown with black boxes. The JPL G1SST 1 km blended SST field shows the state of the ocean on 2016-02-14; this image was selected as it clearly shows the full range of ocean processes around southern Africa. The Agulhas Current along the east coast of the country (Sites 18–21) is visualized here in a yellowish color as a jet of relatively warmer water projecting in a south-westerly direction, and hugging the continental shelf. The blueish patches north of the Cape Peninsula along the west coast (Sites 1–4) represent upwelled water. Some upwelled water on the south coast (Sites 5–17) may also be present around Sites 14 (Tsitsikamma) and 15–16 (Port Elizabeth). The inset maps show detail of the Cape Peninsula/False Bay area and the Port Alfred region where site labels are obscured due to overplotting of symbols. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

data representing offshore mesoscale temperatures and also comparable against the *in situ* time series, shore-normal transects extending to the 200 m isobath were drawn from each of the 21 sites where in situ time series were available. Temperature values from the OISST data were then extracted at each of the roughly 25×25 km pixels along these transects, shown as black boxes in Fig. 1. Where the shelf was less than 25 km wide (Sites 17–21) the nearest 'ocean pixel' to the in situ time series coordinate was used. The daily temperatures for each pixel from the OISST dataset within each of the 21 shore-normal transects were meaned to create offshore time series that could be compared against the nearshore in situ time series from which each transect was drawn. Offshore transects were used to generate the time series this way as they better represent the mesoscale temperatures we were interested in comparing against the coastal events. Had we simply used the nearest OISST pixel to generate time series to compare against the in situ data this would only draw a comparison between the two different data types at the coast, and not the mesoscale activity in the ocean. These 21 OISST time series could then be analyzed for MHWs (MCSs) in the same way as the in situ data (see below). Note that the OISST time series had valid data covering 1982-2015 which did not match exactly with the individual in situ sites. The full lengths of the OISST time series were used to create the climatology against which their MHWs (MCSs) could be calculated, rather than matching the shorter lengths of the in situ time series, so as to better follow the methodology found in Hobday et al. (2016).

2.3. Defining and calculating MHWs and MCSs

MHWs are defined here following Hobday et al. (2016) as 'discrete prolonged anomalously warm water events in a particular location.' MCS are defined in the same manner as MHWs with the exception of being 'anomalously cold water events'.

The algorithm developed by Hobday et al. (2016) does so by finding the occasions that SST exceeds a threshold in the probability distribution of the data (i.e. relative to the 10th or 90th percentiles) calculated based on an 11-day wide moving mean smoother centered on each Julian day at each site (or pixel in the case of gridded data). These events are atypical relative to the normal climatology by definition, and various metrics that define their properties may be calculated, including, but not limited to, the number of events per year, their duration, and the mean, maximum and cumulative intensity above (below) the threshold (Hobday et al., 2016). The 90th (10th) percentile was used in our study for the threshold of events, rather than the 95th (5th) or 99th (1st) so as to allow for the detection of a greater number of anomalous events. This is an important consideration as it is not only the very largest events that may pose a threat to local ecosystems. Starting from the 3 day minimum duration set for atmospheric heatwaves in Perkins and Alexander (2013), different minimum lengths for the definition of marine events were tested for by Hobday et al. (2016). They found that a minimum length of 5 days allowed for more uniform global results in event detection; therefore, we have used this 5 day minimum length in our study, too. Because our in situ time series were of differing durations, with many under the proscribed 30 years, we calculated the climatology over all available years; in the case of the OISST data, climatologies were calculated over a fixed 33-year base period (1982–2015). Furthermore, discrete events with well-defined start and end dates but with 'breaks' between events lasting ≤2 days followed by subsequent ≥5 day events were considered as continuous events (Hobday et al., 2016). After the events were defined, a set of metrics (Table 1) were calculated including maximum and mean intensity (measured as anomalies relative to the climatological mean, in °C), duration (time from start to end dates, in days), and cumulative intensity (the integrated intensity over the duration of the event, analogous to degree-heating-days; °C·days). MCS intensities are calculated as negative values (i.e. anomalies) and are reported in the text as such. When comparing MHW and MCS intensities the absolute values of these metrics were used.

A Python script (https://github.com/ecjoliver/marineHeatWaves; see Hobday et al., 2016) was used to calculate the individual MHWs (MCSs) for both the *in situ* and OISST time series. After the individual events were recorded, mean annual values for the metrics seen in Table 1 were calculated for each year of each times series. This provided two different sets of measurements for the extreme events that will be referred to specifically throughout this paper. 'Annual' data refer to the annual means of events for each year of each time series whereas 'event' data refer to the individually calculated events within each time series.

Because MHWs (MCSs) were calculated relative to percentile exceedances, rather than absolute definitions such as periods with temperatures above an arbitrary fixed temperature threshold, any time of year could have experienced a MHW (MCS). This is an important and necessary consideration to make as, for example, unusually warm waters that occur during the winter months of a year, the time when many species need cold water for effective spawning/spore release, can have a negative effect on the recruitment success of that population for the year (Wernberg et al., 2011).

2.4. Detecting co-occurrence of coastal and offshore events

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In order to better understand the potential impact offshore mesoscale phenomena had on local coastal events, the proportion of MHWs (MCSs) that co-occurred between the two datasets was calculated for each matched time series. This was initially done by taking each event (warm and cold) within an in situ time series and looking for an event in the matched OISST time series that occurred within a certain period of time before the *in situ* date. These co-occurrence proportions were used to describe how often the mesoscale oceanography off the coast may have led to extreme events that occurred locally along the coast. All events that occurred outside of the dates shared between the matched time series were removed from this calculation. The sum of OISST events found to occur within the shared date window was then divided by the sum of events in the in situ time series that occurred during that same period to produce a co-occurrence proportion. The proportions of cooccurrence were then recalculated controlling for the size of the lag window used when comparing the two different datasets for concurrent events, as well as the directionality used for this comparison. In other words, a range of window sizes from 2 to 14 days were used for each site to see how far apart events generally occurred and the lag period used was also

Table 1Metrics of MHWs and their descriptions as proposed by Hobday et al. (2016). In the case of MCSs, values were calculated with respect to the 10th percentile.

Name [unit]	Definition
Count [No. events per year]	n: number of MHWs per year
Duration [days]	<i>D</i> : Consecutive period of time that temperature exceeds the threshold
Maximum intensity [°C]	i_{max} : highest temperature anomaly value during the MHW
Mean intensity [°C] Cumulative intensity [°C·days]	i_{mean} : mean temperature anomaly during the MHW i_{cum} : sum of daily intensity anomalies over the duration of the event

applied after the *in situ* events, allowing us to see how often coastal events led the offshore events.

In addition to controlling for the duration and direction of lag, the sizes of the individual events were factored into the calculations of co-occurrence proportion. This was accomplished by ranking the events within each time series in steps of 10th percentiles by cumulative intensity. Comparisons were then made between matched sites with smaller events progressively removed until only the largest events were being compared. This allowed us to isolate the proportion of co-occurrence found within each site that was caused by smaller events that occurred at similar times as large events, which were more likely to have co-occurred randomly, and not an indication of a teleconnection between the datasets.

The top three MHWs (MCSs) for each *in situ* and OISST time series as defined by cumulative intensity were also noted in order to visually compare the co-occurrence of events in detail, both within and between the different datasets.

2.5. Decadal trends in MHWs and MCSs

Given that the anthropogenic forcing of climate change has increased mean ocean temperatures over the past few decades (Stocker et al., 2013), it stands to reason that, as a function of the 90th and 10th percentiles, the larger MHWs would likely be near the end of the time series and the larger MCSs near the beginning. This can be tracked visually by looking at the top three warm and cold events for each time series. Given that the OISST time series are greater than 30 years in duration it is possible to discern the long term trends within the data apart from the noise of any inter-decadal patterns (Schlegel and Smit, 2016). Using generalized linear models (Poisson with log-link), the decadal trend in the annual count of MHWs (MCSs) were calculated for all OISST time series as well as the in situ time series over 30 years in duration. The 17 in situ time series under 30 years were cut in half and the sum of the annual count of both warm and cold events for each half was calculated. Using a series of general linear hypotheses (Hothorn et al., 2008) we tested the significant differences between the count data in the first and second halves of the time series for the overall count of MHWs (MCSs) as well as each coastal section. The sum of MHWs (MCSs) in the second half of each time series was divided by the sum of those in the first to produce proportional values of event occurrence that could be used to compare the different coastal sections.

3. Results

3.1. Event metrics

Using series of general linear hypotheses (Hothorn et al., 2008) to look for differences in the metrics of MHWs (MCSs) between datasets and between coastal sections (Table 2) revealed significant differences in the count of MHWs (MCSs) between the *in situ* and OISST datasets, with the OISST dataset displaying more events of both kinds (MHWs: t = -5.37, p < 0.01; MCSs: t = -5.28, p < 0.01). There were no differences in the number of warm or cool events within either of the datasets, nor in the number of MHWs (MCSs) between coasts.

MHWs (MCSs) in the OISST dataset were of greater duration than in the *in situ* dataset (MHWs: t = -2.34, p < 0.05; MCSs: t = -3.31, p < 0.01). Comparing events between coasts within the in situ dataset, MCSs along the east coast were shorter than along the south (t = 5.41, p < 0.01) or west coasts (t = 2.06, p < 0.05); MHWs showed the same response, with the duration along the east coast less than along the south (t = 3.79, p < 0.01) or west coasts (t = 2.67, p < 0.01). In the OISST dataset, MCSs along the east coast were only significantly shorter than those on south coast (t = 2.83, p < 0.01); MHWs on the east coast were shorter than those on the south (t = 6.01, p < 0.01) and west coasts (t = 3.79, p < 0.01). A comparison of the duration of MHWs against MCSs within coast and dataset showed that the durations of the two event types were identical. The one exception being along the east coast within the OISST dataset where MCSs were longer than MHWs (t = -2.70, p < 0.01).

The *in situ* dataset yielded more intense MHWs (t = 19.80, p < 0.01) and MCSs (t = 14.19, p < 0.01) than the OISST dataset. Looking at the difference in intensity of events within the dataset, MCSs were more intense than MHWs in the OISST dataset (t = -4.10, p < 0.01). There were also differences in the intensity of MHWs and MCSs between coasts within a dataset. Within the in situ dataset, the intensity of event types was greater along the south coast for both MHWs (south vs. east: t = -2.58, p < 0.01; south vs. west: t = 3.28, p < 0.01) and MCSs (south vs. east: t = 5.48, p < 0.01; south vs. west: t = -6.66, p < 0.01). More intense MCSs were present in the OISST dataset on the south coast compared to the east (t = -2.15, p < 0.05), whereas MHWs were less intense along the east compared to the south (t = 3.01, p < 0.01) or west coasts (t = 2.18, p < 0.05). Focusing on differences between coasts and within datasets, MHWs in the in situ dataset were more intense than MCSs along the west (t = 4.48, p < 0.01) and east

Table 2
The mean (±SD) values for event count, duration and mean intensity from the annual data for MHWs and MCSs for each coastal section as calculated from the *in situ* (A) and OISST (B) time series. The aforementioned annual data were averaged across all years for all time series within each respective coast to produce the mean values shown. Lower case letters indicate if any of the coastal sections differ within the same dataset and event type, with metrics sharing the same letter being statistically indistinguishable from one-another. For example, the duration of MHWs on the east coast in the *in situ* data were significantly less than MHWs on the west and south coasts, which were not significantly different. The upper case letters indicate if the coastal sections differ between the datasets, but within coast and event type. For example, the count of MCSs on the west and east coasts were not significantly different whereas the count of MCSs on the south coast in the OISST dataset was significantly greater than in the *in situ* dataset.

Coast	MHW			MCS		
	Count [n]	Duration [days]	Mean intensity [°C]	Count [n]	Duration [days]	Mean intensity [°C days]
A – in situ						
All	1.6 ± 1.8^{-A}	9.3 ± 5.1^{-A}	2.65 ± 0.79^{-A}	1.5 ± 1.7^{-A}	9.0 ± 5.1^{-A}	-2.79 ± 1.09^{-A}
West	1.8 ± 1.9 ^{aA}	9.1 ± 3.9 ^{aA}	2.86 ± 0.90^{aA}	1.5 ± 1.9 ^{aA}	8.5 ± 5.2^{aA}	-2.32 ± 0.58^{aA}
South	1.5 ± 1.8 ^{aA}	9.8 ± 6.1^{aA}	2.50 ± 0.65^{bA}	1.5 ± 1.6^{aA}	9.7 ± 5.5 ^{aA}	-3.08 ± 1.22^{bA}
East	1.5 ± 1.7^{aA}	7.7 ± 2.2^{bA}	2.85 ± 0.89^{aA}	1.6 ± 1.6^{aA}	7.1 ± 1.9^{bA}	-2.37 ± 0.67^{aA}
B – OISST						
All	2.2 ± 2.1^{-B}	10.2 ± 5.4^{-A}	1.72 ± 0.33^{-B}	2.2 ± 2.6^{-B}	10.2 ± 5.1^{-B}	-1.83 ± 0.52^{-B}
West	2.1 ± 1.8^{aA}	10.9 ± 6.7^{aA}	1.75 ± 0.41 ^{aB}	2.3 ± 2.7^{aA}	$9.8 \pm 6.6^{\text{adA}}$	-1.87 ± 0.61^{adB}
South	2.2 ± 2.1^{aB}	10.6 ± 5.5^{aA}	1.74 ± 0.29^{aB}	2.1 ± 2.7^{aB}	10.7 ± 5.0^{aA}	-1.79 ± 0.45^{aB}
East	2.5 ± 2.3^{aA}	8.3 ± 2.4^{bA}	1.64 ± 0.33^{bB}	2.2 ± 2.2^{aA}	9.4 ± 3.4^{dA}	-1.93 ± 0.61^{dB}

coasts (t = 3.06, p < 0.01), whereas MCS were more intense than MHWs along the south coast (t = -5.66, p < 0.01). A coastal difference in intensity of MHWs and MCSs in the OISST dataset was only seen along the east coast (t = -4.36, p < 0.01), with MCSs being greater.

The mean annual statistics shown in Table 2 give a broad overview of the events that occurred along the coasts; however, an examination of the largest MHWs and MCSs provided a clearer picture as to which coastal sections showed the most intense events. The ranking of these events was based on the cumulative intensity metric as explained in Table 1. To calculate the mean cumulative intensity of all events it was necessary to use the individual event data, and not the annual mean data used for Table 2. Doing so for MHWs from both datasets showed a significant difference (t = 7.68, p < 0.01) in the mean (±SD) cumulative intensities with the *in situ* dataset (26.11 ± 24.37 °C·days) having greater cumulative intensities than in the OISST dataset (18.65 ± 15.10 °C·days). The mean (±SD) cumulative intensities for MCSs between the two datasets were also significantly different (t = 2.99, p < 0.01) with the in situ events (26.45 ± 24.25 °C·days) being greater than the OISST events (23.17 ± 23.49 °C·days).

3.2. Patterns in mean cumulative intensity

The three largest (greatest cumulative intensity) MHWs within the *in situ* dataset were all recorded along the south coast (Table 3). The cumulative intensity of the three largest events along the west coast were less than the greatest three south coast events, but greater than the largest three MHWs from the east coast. This is due in part to the events on the south coast having had greater durations than the other two coastal sections, which influenced the cumulative intensity metric. As with the MHWs, the largest three MCSs from the *in situ* data were also on the south coast (Table 3). The west coast had the next largest three events and the east coast the smallest. The south coast MCSs had greater durations than the MCSs from the other coastal sections, but were less pronounced than the MHWs.

The pattern seen in the *in situ* dataset of the largest MHWs and MCSs having occurred on the south, west and east coasts respectively was not repeated with the OISST dataset. Whereas the single largest MHW occurred on the south coast in the OISST data, the three largest MHWs from the west coast were larger than the second and third largest events from the south coast (Table 3). The

Table 3
The three largest MHWs and MCS per coast from the *in situ* (A, B) and OISST (C, D) data. The coast column shows in which coastal section the event occurred. The site column gives the name of the site, as seen in Table S1, which gives the index number necessary to find its location along the coast in Fig. 1. The start date column gives the day on which the event began and the duration [days] column shows how many days the event lasted for. The mean intensity and cumulative intensity columns are explained in Table 1.

Coast	Site	Start date	Duration [days]	Mean intensity [°C]	Cumulative intensity [°C·days]
		TI	in situ		
A – MHW			111 111 111		
West	Sea Point	1996-01-04	40	3.08	123.20
West	Sea Point	2005-05-21	39	2.56	99.66
West	Sea Point	1975-12-30	38	2.62	99.41
South	Muizenberg	1999-12-01	98	3.17	310.30
South	Mossel Bay	1993-06-25	97	1.77	171.30
South	Muizenberg	1999-10-20	35	4.47	156.40
East	Nahoon Beach	1995-10-14	18	5.18	93.31
East	Eastern Beach	1985-12-27	19	3.33	63.18
East	Orient Beach	1990-06-25	STEPN (3.80	45.59
B – MCS		AA T	SIERN	ACAL EL	
West	Sea Point	1990-06-23	44	-2.88	-126.60
West	Sea Point	1983-06-10	39	-2.84	-110.90
West	Sea Point	2000-11-28	23	-3.70	-85.04
South	Muizenberg	1984-07-14	63	-2.92	-183.70
South	Muizenberg	1992-03-24	56	-2.78	-155.60
South	Ystervarkpunt	2000-05-11	51	-2.94	-150.10
East	Sodwana	2004-02-12	17	-3.25	-55.20
East	Orient Beach	1984-03-31	13	-3.73	-48.44
East	Orient Beach	1995-12-6	15	-3.01	-45.13
			OISST		
C – MHW					
West	Sea Point	1992-01-21	39	2.96	115.60
West	Hout Bay	1992-01-20	36	3.15	113.50
West	Kommetjie	2004-10-29	53	2.03	107.40
South	Knysna	1992-05-3	50	2.41	120.40
South	Fish Hoek	2004-10-30	53	1.92	101.60
South	Pollock Beach	1994-03-27	31	3.19	99.05
East	Nahoon Beach	2006-10-21	25	1.81	45.34
East	Eastern Beach	2000-06-24	26	1.58	41.12
East	Orient Beach	2000-06-24	26	1.58	41.12
D - MCS					
West	Kommetjie	2010-12-13	54	-3.92	-211.90
West	Hout Bay	2010-12-25	41	-4.06	-166.30
West	Sea Point	2010-12-25	41	-3.78	-154.90
South	Hamburg	1984-02-5	65	-3.91	-254.20
South	Storms River Mouth	1982-03-13	60	-2.79	-167.30
South	Tsitsikamma East	1982-03-13	60	-2.79	-167.30
East	Eastern Beach	2010-12-26	32	-2.90	-92.85
East	Orient Beach	2010-12-26	32	-2.90	-92.85
East	Eastern Beach	1984-02-24	22	-3.97	-87.26

three largest MHWs from the east coast were again smaller than those from the other coasts. Assigning the largest MCSs from the OISST dataset to either the south or west coasts was not possible due to an inconsistent pattern here. The east coast MCSs from the OISST dataset were however consistently the smallest three events. All of the coastal sections in the OISST dataset had at least two of their largest MCSs occurring at similar times at different sites. This is a level of co-occurrence that the *in situ* data did not show.

As well as having had significantly different cumulative intensities, Fig. 2 shows that the three largest events within each time series in the OISST dataset often occurred at different times from those seen in the *in situ* dataset. In addition, the OISST events showed a greater amount of co-occurrence with events detected at neighboring coastal stations than the corresponding *in situ* time series did.

The daily temperatures on the dates of the largest MHW (MCS) from the west and south coasts in the *in situ* dataset are shown concurrently with the daily temperatures from the OISST time series on matching dates in Fig. 3. When these largest events were occurring in the *in situ* data, the temperatures in the OISST data did not show similarly intense events.

3.3. Co-occurrence proportions

The proportion of co-occurrence found for MHWs (MCSs) between the datasets for each site can be seen in Figs. 4 and 5 respectively. When using the lag windows both before and after the occurrence of an *in situ* event to compare the *in situ* and OISST events, increasing the width of the lag window from 2 to 14 days caused the mean proportion of co-occurrence for all sites to

increase linearly for MHWs (0.09–0.38) and MCSs (0.10–0.30). Using these same constraints, the south coast sites had the largest mean increase in co-occurrence for MHWs (0.10–0.45) and MCSs (0.11–0.34), whereas the west coast sites showed the smallest increase for MHWs (0.07–0.28) and MCSs (0.08–0.19). With all variables controlled for in the same manner, the co-occurrence proportions between the different coastal sections were not significantly different for MHWs or MCSs at 2 day nor 14 day lags ($p \ge 0.12$).

The directionality of the lag window affected the proportion of co-occurring events. Comparing all events within a 14 day lag window before the in situ event gave higher mean (±SD) proportions of co-occurrence for MHWs (0.22 ± 0.13) than for the same lag window after the in situ event (0.18 \pm 0.10). This same comparison for MCSs showed that the lag window before the in situ event (0.16 ± 0.09) had a slightly lower proportion of co-occurrence than the lag window after the in situ event (0.17 ± 0.08) . When the smaller events were screened from comparison and only the largest half of the events used (50th perdifference in mean (±SD) co-occurrence centile), the proportions for MHWs lessened to 0.16 ± 0.11 before the in situ event and 0.15 ± 0.12 after. The mean ($\pm SD$) co-occurrence proportion of MCSs at this level was less when using a lag window before the in situ event at 0.05 ± 0.08 than for a lag window after at 0.08 ± 0.08.

There was no co-occurrence in the paired time series for the largest MCSs, whereas four of the 21 paired time series showed co-occurrence for their largest MHWs (Fig. 4). Interestingly, these four paired time series were on the south coast and three of the four showed co-occurrence for their largest MHW when the *in situ* event preceded the OISST event.

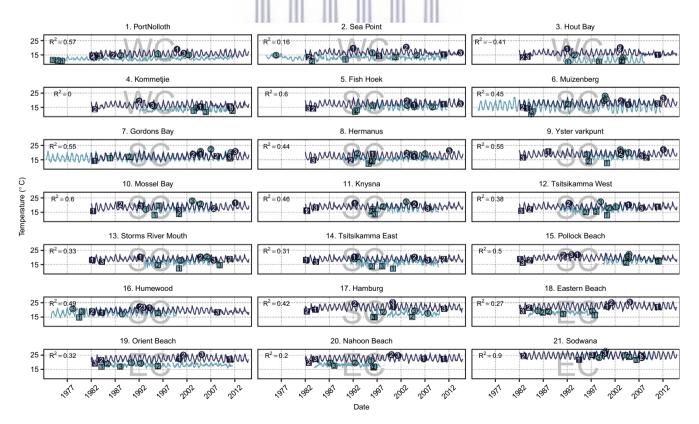


Fig. 2. The daily temperature values for each *in situ* time series (light blue) used in this study and the corresponding OISST time series (dark blue) extracted for comparison as seen in Fig. 1. The top three MHWs are indicated by circles (with the rank inside) for each site as judged by greatest cumulative intensity. The top three MCSs for each site are indicated by squares (with the rank inside). Sites 1-4 represent the west coast (WC), sites 5-17 represent the south coast (SC) and sites 18-21 represent the east coast (EC). The coefficient of determination (R^2) values for the daily temperatures between each paired set of time series are displayed in the upper left corner of each panel. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

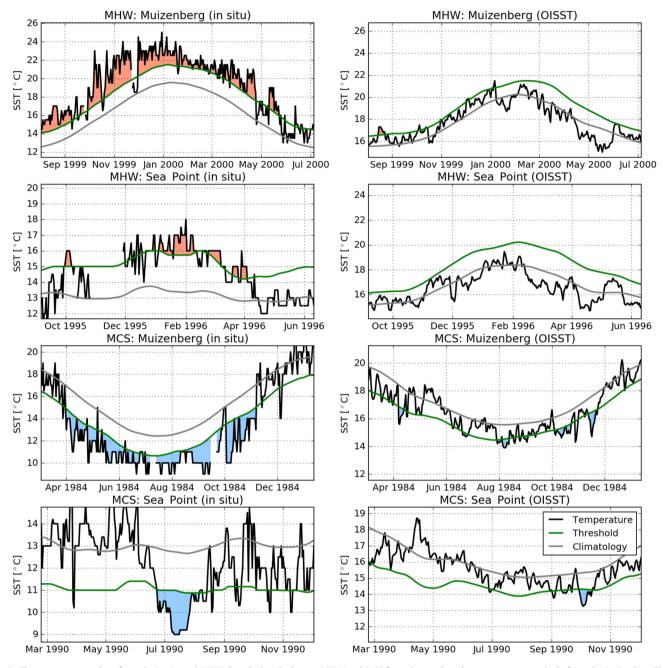


Fig. 3. The temperature values from the *in situ* and OISST data during the largest MHW and MCS from the south and west coasts respectively from the *in situ* data. The left column shows the *in situ* temperature values during the event while the right column shows the OISST temperature values occurring on the same dates. The top row shows the largest MHW that occurred on the south coast while the second row shows the largest MHW that occurred on the west coast. The bottom two rows show the largest *in situ* MCS that occurred on the south and west coasts respectively.

3.4. Decadal trends in MHWs and MCSs

The decadal trends in MHWs (MCSs) calculated for each OISST time series are given in Table 4. The mean (\pm SD) decadal trend for MHW occurrence in the OISST dataset is $0.2\pm0.1~\rm dec^{-1}$ across all sites and $-0.3\pm0.3~\rm dec^{-1}$ for MCSs. The decadal trends in MHW occurrence were less in the colder Benguela-fed west coast than the warmer Agulhas-driven east coast with the mean (\pm SD) decadal MHW trend on the west coast being $0.1\pm0.1~\rm dec^{-1}$, the south coast being $0.2\pm0.2~\rm dec^{-1}$ and the east coast being $0.3\pm0.1~\rm dec^{-1}$. Just as MHWs occurred more frequently per decade on the east coast than the west, the count of MCSs decreased more on the east coast than the west.

The decadal trend of MCSs on the west coast is $0.0\pm0.2~dec^{-1}$, $-0.4\pm0.2~dec^{-1}$ on the south coast and $-0.5\pm0.2~dec^{-1}$ on the east coast.

Of the four *in situ* time series that reached the 30 year minimum length, the mean (\pm SD) decadal trend for MHWs is 0.2 ± 0.4 dec⁻¹ and -0.1 ± 0.3 dec⁻¹ for MCSs. There were two sites from the west coast and two from the south, excluding the east coast from a possible calculation of decadal change for *in situ* MHWs (MCSs). The mean (\pm SD) decadal trend for MHWs (MCSs) on the west coast is 0.0 ± 0.3 dec⁻¹ (-0.2 ± 0.5 dec⁻¹) and 0.4 ± 0.4 dec⁻¹ (0.0 ± 0.3 dec⁻¹) on the south. Note that none of the decadal trends for MCSs from the > 30 year *in situ* time series from the west coast were significant.

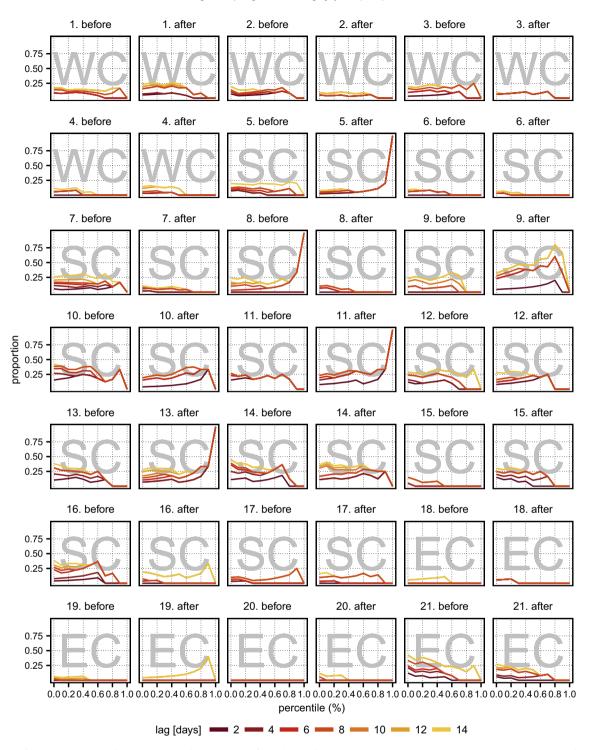


Fig. 4. Proportion of MHW co-occurrence between *in situ* and OISST datasets for each site where sites 1–4 represent the west coast (WC), sites 5–17 the south coast (SC) and 18–21 the east coast(EC). Columns denoted with "before" show the proportion of co-occurrence when events in the OISST data occurred on or before the dates of the *in situ* events. The columns denoted with "after" show the proportion of co-occurrence when OISST events occurred after the *in situ* event dates. The x-axis indicates the size of the events, based on percentiles, used for calculating the co-occurrence proportions. The days of lag used, from 2 to 14, are shown here in diminishing shades of red. The numbers above each panel show th ID number for each site. The names of the sites that relate to these ID numbers may be found in Figs. 2 and Table S1. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

The mean (\pm SD) proportion of MHWs that occurred during the second half of the shorter time series was $1.7\pm1.3~(p=0.37)$ and that of MCSs was $0.8\pm0.6(p=0.39)$, neither being significantly different. The counts for both MHWs and MCSs between the first and second halves of the time series for the west and south coasts were significantly different. Showing agreement with the longer time series, the short west coast time series had significantly more

MHWs in their second half at 1.5 ± 0.6 (p = 0.03), but differed from the longer time series by having more MCSs in the second half at 1.8 ± 0.6 (p < 0.01). The short south coast time series showed agreement with the longer time series in that the proportion of MHWs in the second half of time series was greater at 2.1 ± 1.4 (p < 0.01) and the proportion of MCSs in the second half was lesser at 0.5 ± 0.3 (p < 0.01). The short east coast time series however,

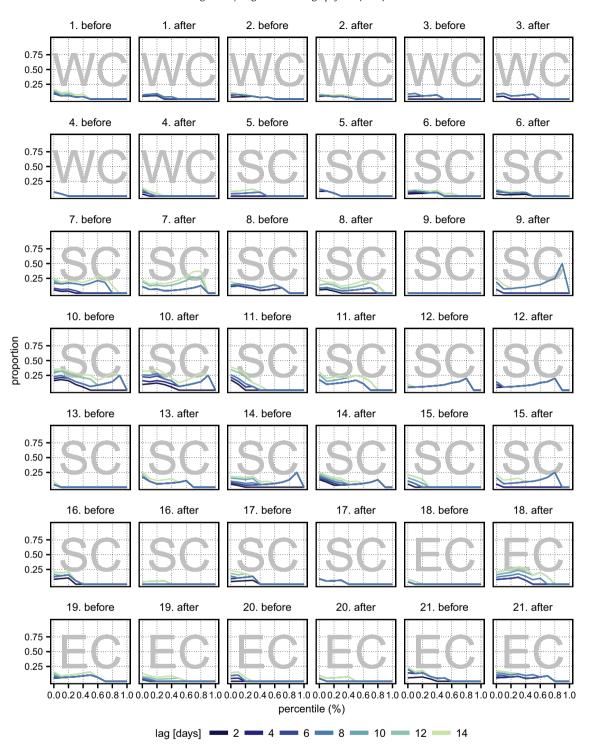


Fig. 5. Proportion of MCS co-occurrence between *in situ* and OISST datasets for each site as seen for MHWs in Fig. 4. The days of lag are shown here in diminishing shades of blue. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

showed no agreement with their longer counterparts. The proportion of MHWs in the second half of these short time series was 0.7 ± 0.4 (p = 0.10) and the proportion of MCSs was 1.0 ± 0.8 (p = 0.57).

3.5. Offshore MHWs and MCSs

As seen in Fig. 6, the pixels with the highest annual counts of MHWs occurred well south of the tip of the continent whereas some of the most frequent MCS activity was found

directly against the west coast and some small regions of the south coast. As for the duration of events, it is clear from Fig. 6 that the MHWs (MCSs) detected in the Agulhas current are relatively short-lived compared to those in the open ocean with almost all pixels that showed events in the upper range of duration detected well away from the coast. The offshore events along the west and south coasts have centers of intensity very near the shore whereas the east coast generally does not. The most intense events detected in the OISST data are found along or south of the south coast.

Table 4The results of generalized linear models fitted to the MHW and MCS annual event data of each time series >30 years from the *in situ* (A) and OISST (B) datasets showing the change in extreme events over time. The ID column gives the ID number necessary to locate the site in Fig. 1 and may also be used to find the site name given in Table S1. The coast column shows within which coastal section the time series may be found. The trend columns show the decadal trends of increasing or decreasing extreme events. The R^2 columns shows the coefficients of determination for each general linear model and the p columns show the significance of the trend.

ID	Coast		MHW			MCS		
		Trend	R^2	p	Trend	R^2	р	
A – in situ								
1	West	0.2	0.03	0.04	-0.5	0.09	0.00	
2	West	-0.2	0.01	0.15	0.2	0.02	0.13	
6	South	0.1	0.00	0.68	0.2	0.03	0.06	
7	South	0.7	0.18	0.00	-0.2	0.02	0.13	
B – OISST								
1	West	0.3	0.05	0.01	-0.2	0.03	0.05	
2	West	0.1	0.00	0.55	0.1	0.00	0.57	
3	West	0.0	0.00	0.91	0.2	0.02	0.05	
4	West	0.1	0.01	0.37	-0.2	0.02	0.06	
5	South	0.3	0.04	0.02	-0.6	0.14	0.00	
6	South	0.5	0.09	0.00	-0.7	0.17	0.00	
7	South	0.3	0.04	0.03	-0.6	0.12	0.00	
8	South	0.4	0.07	0.00	-0.6	0.13	0.00	
9	South	0.4	0.08	0.00	-0.7	0.19	0.00	
10	South	0.3	0.05	0.01	-0.6	0.13	0.00	
11	South	0.3	0.03	0.04	-0.4	0.07	0.00	
12	South	0.2	0.03	0.05	-0.3	0.03	0.03	
13	South	0.2	0.02	0.13	-0.2	0.02	0.08	
14	South	0.2	0.02	0.13	-0.2	0.02	0.08	
15	South	-0.0	0.00	0.75	0.0	0.00	0.71	
16	South	-0.1	0.00	0.61	0.0	0.00	0.80	
17	South	0.1	0.00	0.45	-0.4	0.04	0.01	
18	East	0.3	0.05	0.01	-0.4	0.08	0.00	
19	East	0.3	0.05	0.01	-0.4	0.08	0.00	
20	East	0.2	0.02	0.06	-0.3	0.04	0.02	
21	East	0.2	0.02	0.15	-0.7	0.16	0.00	

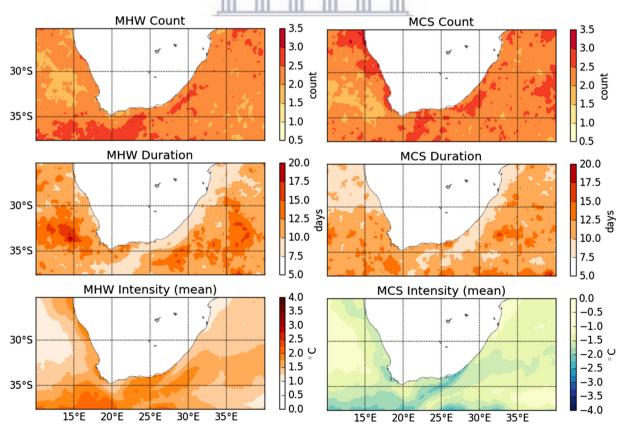


Fig. 6. Mean values from the annual data of each pixel from the OISST dataset around southern Africa. The first second and third rows show the mean count [n], duration [days] and intensity [°C] respectively of MHWs in the first column and MCSs in the second. The annual event values within each pixel were averaged to create one final value with which each pixel is populated.

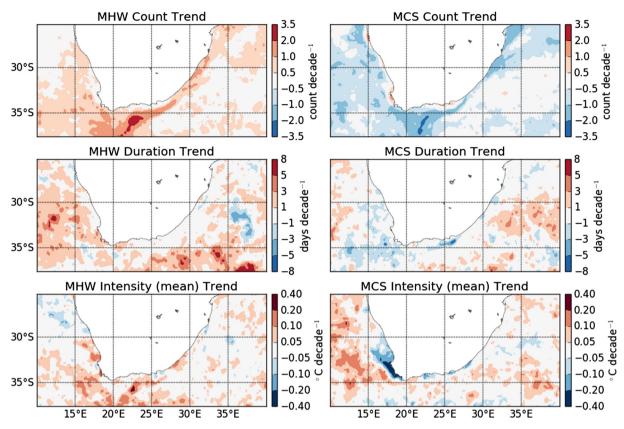


Fig. 7. Decadal trend values calculated from the annual OISST data around southern Africa. The decadal trends were calculated by fitting a linear model to the annual data of each pixel for the relevant metrics and multiplying the slope of the line by 10. The panels are in the same position as Fig. 6.

Whereas the mean count, duration and intensity of MHWs and MCSs offshore are telling, the picture is not complete without also considering the trend in these metrics, too. Fig. 7 shows that the count, duration and intensity of MHWs increased almost exclusively throughout the studied regions of the Indian and Atlantic Oceans. The count of MCSs decreased most rapidly along the coast of southern Africa with a couple of notable exceptions near Port Elizabeth and north of the Cape Peninsula where the count of MCSs increased very near to the coast. The duration of MCSs is seen to have generally increased further offshore with most of the near-shore region having changed little or decreased. The intensity of MCSs either changed little near the coast or increased dramatically, as seen in the dark blue spot north of the Cape Peninsula in the "MCS Intensity (mean) Trend" panel in Fig. 7.

4. Discussion

Our results clearly show that MHWs (MCSs) detected in two different ocean temperature datasets displayed markedly different counts, durations, intensities and timing in their occurrence. These differences appear to be related to the nature and variability of physical oceanographic processes at broad- and local-scales, and the coupling of the processes across these scales. These finding illustrate how a study of the properties of anomalous events can provide novel insights into drivers of the thermal regime along coastlines, and can be used to arrive at some mechanistic insights into the nature and origin of MHWs (MCSs).

4.1. Relation between local- and broad-scale MHWs and MCSs

The difference between the *in situ* and OISST datasets was striking. We anticipated a large degree of coupling between MHWs manifesting in datasets that encapsulate local- and broad-scale

patterns, as represented by the *in situ* and OISST datasets, respectively. We found instead that the broad-scale dataset yielded heatwaves that were more frequent and longer in duration, but less intense than their local-scale counterparts. Cold-spells, for which we expected a greater deal of decoupling between local- and broad-scale manifestations, showed more evidence of such than MHWs. MCSs were more frequent and lasted longer in the OISST data; however, the mean intensity of MCSs at the broad-scale was less than at the local-scale. The significantly larger intensities of both MHWs and MCSs from the *in situ* data may be an artifact of the inability of remotely sensed data to record the maximum and minimum temperatures that *in situ* instruments are capable of detecting (Smale and Wernberg, 2009).

Such a deterioration of the offshore thermal signal in coastal waters is known to occur due to the local modifications of nearshore circulation patterns by headlands, embayments, influences of the bathymetry and other such perturbations that introduce eddies and fronts and a shoaling of the thermocline (Okubo, 1973; Pingree and Maddock, 1979; Wolanski and Hamner, 1988; Black et al., 1990; Grundlingh and Largier, 1991; Graham and Largier, 1997). These processes are not yet fully understood, and what understanding we do have of physical oceanographic process remains weighted toward the mesoscale, as was noted by Graham and Largier (1997) in their study on upwelling shadows, another process responsible for the local modification of a phenomenon that is generally studied at the broad-scale. These local-scale deviations are known to affect coastal ecological processes, such as the transport, dispersal and settlement of larvae (Pineda, 1994; McCulloch and Shanks, 2003; Narváez et al., 2004) and the dynamics of phytoplankton and nutrient delivery (Graham and Largier, 1997; Pineda, 1994), and it is likely that thermal patterns over similar scales will also have local significance for nearshore biology.

4.2. MHWs and MCSs in different coastal sections

There was no difference in the annual count of events between coasts within each dataset (Table 1) but the duration and intensity metrics between coasts did differ. An important thing to note from Table 1 is that the MHWs and MCSs at both the local- and broadscale on the east coast were significantly shorter in duration than other two coastal sections; however, comparing the event duration between events, we see that on this coast the cold-spells lasted longer than heatwaves in the OISST data. Furthermore, the east coast also displayed the least intense MHWs but most intense MCSs of any coastal section in the OISST dataset. This stretch of coastline is heavily influenced by the warm Agulhas Current, separated from the coast only by a very narrow and steep continental shelf, which abruptly expands into the >200 km wide Agulhas Bank south of Port Alfred (Fig. 1). This narrow continental slope margin allows upwelling on the shoreward side of the Agulhas Current to occur along the entire length of the east coast, independent of local atmospheric conditions (Lutjeharms et al., 2000). It is therefore possible that this constant forcing of the Agulhas Current on the east coast would cause the nearshore events arising their to be advected southwards, returning the local temperatures to 'normal' before other factors may have ended the event. This seems to be a plausible explanation for why the largest events, both hot and cold, recorded on the east coast are so much smaller than those along the other two coastal sections. We suggest that the hydrodynamic properties of the Agulhas Current have prevented any prolonged thermal events that originated locally from persisting. Contrary to this conclusion it is clear from the literature that some of the largest documented heatwaves have been caused by anomalously high heat content of ocean currents, such as the Leeuwin Current in the case of the Western Australia MHW (Feng et al., 2013; Pearce and Feng, 2013; Wernberg et al., 2013). Conversely, large MHWs such as that documented in the north west Atlantic Ocean in 2012 have been shown to be coupled strongly with atmospheric phenomena (Mills et al., 2012; Chen et al., 2014, 2015). Therefore, while no MHWs or MCSs with cumulative intensities rivaling those of the largest events seen on the other two coasts have vet occurred on the east coast, the potential exists for some furtherafield phenomenon to cause such an event there.

Some of the in situ time series collected along the south coast are recorded in relatively shallow embayments, allowing for atmospheric heating to have a marked effect there - as is indeed seen in the cumulative intensities for MHWs in False Bay - and further offshore sheer-edge forcing creates eddies resulting from the departure of the Agulhas Current from the Agulhas Bank that may then be projected across the shelf (Lutjeharms et al., 2003). Such high temperature events last longer, and even if their mean intensities are lower, this contributes towards their high cumulative intensities. The significantly more intense nearshore MCSs on the south coast are attributed to the much greater mean intensity of events around Tsitsikamma (Sites 12-14). Without these three sites the nearshore MCSs on the south coast are not significantly greater than those along the other two coastal sections. Roberts (2005) hypothesized that a wind forced upwelling cell occurs near Tsitsikamma and the mean intensity of the events recorded here may support this.

The west coast does not show exceptional patterns in MHW and MCS metrics. At first glance, we were surprised to find that the mean intensity of west coast (an EBUS) coastal MCSs is lower than those on the south coast. Upwelling systems are defined by periodic occurrences of cold water of deep origin near the coast (Lutjeharms et al., 2000; Hutchings et al., 2009) and it seems intuitive to associate these with the cold-spells. But cold upwelled water *defines* the climatology for the region, and for a cold-spell to manifest in an upwelling region the temperature of that water

would have to be colder than the 90th percentile based on a 30year climatological baseline period and would have to last for five or more days. Accordingly, upwelling events that occur within a seasonally predictable cycle are not anomalous in nature, and are therefore not flagged as MCSs. An upwelling event would need to be particularly cold or a-seasonal in its occurrence to be recorded as a MCS. This is certainly possible; however, the very nature of the required a-seasonality of MCSs obfuscates which phenomena may potentially be driving the extreme cold temperatures. This consideration casts doubt on our thoughts to use MCSs as a means to detect the intensification of upwelling, which is a plausible prediction in an age when Earth's climate gradually warms (García-Reves et al., 2015). Results show that offshore MCS are, on average, lasting significantly longer, occurring significantly more often and the largest events are more intense. As upwelling is known to occur along the coast here (Hutchings et al., 2009), that the offshore MCSs occur more often and last longer is strong evidence that the MCS algorithm does not provide a good means for upwelling detection and that the coastal cold events detected here are likely due to other factors. Upwelling events should have notable properties, such as rate of onset and duration of peak intensity, which set them apart from other events that may cause colder water to occur at the surface. Further work on the definition of the characteristics of upwelling events could be coupled with the MCS algorithm for accurate use in upwelling detection in temperature time series.

4.3. Patterns in mean cumulative intensity

The pattern of mean cumulative intensity within the local-scale data was very clear in that warm and cold events on the south coast were much more extreme than those along the west and east coasts. The OISST data were less conclusive on whether the south or west coast experienced the most extreme events, but it is apparent from all of the analyses from both datasets that the east coast experienced very few extreme MHWs or MCSs. These findings suggest that the east coast is the most thermally stable of the three coastal sections, and that MHWs or MCSs with mean cumulative intensities that could potentially damage ecosystems are least prone to develop there. It is the south coast section, however, where coastal ecosystems are most at risk due to excessively warm events.

Within the south coast (Sites 5-17), the sites within False Bay (Sites 5-7) have greater cumulative intensities for MHWs and MCSs than the sites over the Agulhas Bank (Sites 8-17). Whereas the Agulhas Bank experiences more thermal variation than the other two coastal sections, False Bay, which is ~50 km across, is situated within the transition zone between the Benguela and Agulhas Currents (Smit et al., 2013) and contains the most variable time series in the entire in situ dataset. Lower resolution satellite temperature products, such as Pathfinder version 5.0, have been shown to inadequately resolve the SST within the relatively small body of water that is False Bay (Dufois and Rouault, 2012). Embayments such as this often display thermal ranges (both temporally and spatially) large enough to effect species ranges (Ling et al., 2009) and are of great ecological (Klumb et al., 2003) and economic importance (Lugendo et al., 2005). We think that such regions are also more prone to MHWs (and perhaps MCSs) due to an even stronger decoupling from broad-scale thermal patterns and drivers: indeed, two of the three largest MHWs and MCSs detected in the local-scale dataset were recorded within False Bay, whereas only one large MHW and no MCSs were detected there within the OISST dataset. This illustrates the problem of using satellite temperature data for coastal ecological applications, and emphasizes the need for more comprehensive coverage of nearshore ecosystems in long-term in situ seawater temperature monitoring programmes.

Although Hobday et al. (2016) provide caveats regarding the use of event metrics across datasets, we nevertheless feel that it would be informative to bring the heatwave metrics measured along the South African coast into context by comparing them with MHWs from other regions. Within the two coastal time series that experienced the most extreme events, Muizenberg and Mossel Bay, heatwaves had on average cumulative intensities ranging from 156.4 to 310.30 °C·days, mean intensities from 1.77 to 4.47 °C and lasted from 35 to 98 days. The lengths of these two time series were 40 and 29 years respectively, ensuring that enough data were used to create the climatologies against which these events were calculated. Of the three MHWs from other regions now known to have had major ecological consequences (see introduction), the 2003 Mediterranean MHW had a cumulative intensity of 122 °-C·days, a mean intensity of 4.06 °C and a duration of 30 days; the 2011 Western Australia MHW had a cumulative intensity of 192 °-C-days, a mean intensity of 3.21 and a duration of 60 days; the 2012 MHW in the north west Atlantic had a cumulative intensity of 145 °C·days, a mean intensity of 2.59 °C and a duration of 56 days (Hobday et al., 2016). Even though the metrics of these three events are comparable to those found in South Africa, no investigations have yet been done to see if similar negative effects have taken place at the sites where we have recorded intense heatwaves locally. It seems unlikely that any wide spread ecological changes occurred as evidence for such do not appear amongst the fisheries survey data collected annually, but a more detailed investigation is warranted to see if some of the ecological changes known for the south coast section (Bolton et al., 2012) can be linked to such events. Nevertheless, considering that the south coast is a 'hot-spot' for heatwaves, the fact that these events are increasing in count and knowledge that events already experienced in this section are already on par with the intensity and duration of similar events known to have had ecological effects elsewhere in the world, it is a matter of time before South Africa experiences a similar marine environmental 'natural' disaster.

4.4. Co-occurrence proportions

We found that the majority of the events in the paired time series between the two datasets were unrelated and that some other influence(s) could have had a more pronounced effect on the nearshore events than offshore temperatures. This finding is important in light of the very strong mismatch in temperatures recorded by thermal loggers installed *in situ* at the coast (i.e. local-scale) compared to measurements of the ocean's temperature from space (i.e. broad-scale) (Smit et al., 2013).

When isolating co-occurrence proportions between the datasets to OISST events preceding *in situ* events, we see that the proportions of co-occurrence for MCSs were much lower than for MHWs (Figs. 4 and 5). This shows that if co-occurring events are indeed related, more MHWs are being caused by mesoscale activity than MCSs, as was expected. Additionally, more MCSs from the OISST data were shown to occur after *in situ* MCSs for all coastal sections. This may suggest some local heat loss process, perhaps related to atmospheric cold events, cooling the waters near the coast, which then spread to waters further offshore. The co-occurrence proportions of OISST MHWs before and after *in situ* MHWs are similar, implying that MHWs may be just as likely to propagate onshore from offshore mesoscale activity as MHWs originating near the coast may seep offshore and affect the thermal regime there.

We also infer from the proportions of co-occurrence for time series on the south coast, which are generally much higher than the other two coasts, that the broad continental shelf of the Agulhas Bank is allowing greater levels of influence between the near-shore and offshore. We also see that there is a higher proportion of co-occurrence for the larger MHWs and MCSs on the south coast

when a lag window after the *in situ* event is applied. This supports the argument that events originating in the nearshore are propagating out onto the Agulhas Bank and affecting the oceanography there more often than offshore events originating on the Agulhas Bank are affecting the nearshore environment. However, the overall low rate of co-occurrence for all three coastal sections reinforces the argument that it is not the mesoscale phenomena of the open ocean abutting the southern African landmass that are driving the majority of events in the nearshore, nor are locally forced events propagating from the nearshore the main driver for offshore events.

The decline in the proportions of co-occurrence between datasets as the smaller events are screened out is strong evidence against the hypothesis that mesoscale activity, both warm and cold, is related to nearshore thermal events. The small increases in co-occurrence for some sites as only larger events were compared does imply that there is some relationship between the nearshore and offshore at some localities, but that some other variable (e.g. atmospheric forcing) may be having a greater effect on nearshore events.

Another important consideration is the co-occurrence of the events with the highest mean cumulative intensity within and between datasets. None of the dates for the top three MHWs or MCSs for any of the coastal sections from the *in situ* dataset are the same (Table 3). They are all individually different events occurring at different times. The OISST dataset tells an entirely different story in that all but one of the coastal sections, for both MHWs and MCSs, have at least two of their three top events occurring at the same time. This means that the largest events detected in the OISST dataset occur over a broad area at the same time, whereas the *in situ* events are isolated temporally and spatially. This further reinforces our conclusion that the events detected by the different datasets are often intrinsically different from one another.

A final consideration to address for the apparent lack of relation between these datasets is that the OISST temperatures are remotely sensed representations of the surface and though they are converted from a "skin" temperature (roughly a micron deep) to a "bulk" temperature (roughly half a meter deep) (Reynolds et al., 2007), 7 of the 21 time series from the in situ dataset were recorded deeper than this with 2 of them recorded deeper than 10 m. However, these deeper in situ data are still comparable to the "bulk" upper mixed layer the OISST data are calibrated to measure as there is little vertical layering within the nearshore environment. Furthermore, the OISST temperatures are averaged across the width of the continental shelf at each site, and not simply to the nearest available pixel, largely addressing any inconsistencies in temperature caused by mismatches in depth as the mixed layer of the mesoscale temperature patterns of the open ocean should be comparable in depth to the nearshore water column. It is then worth noting that water temperatures being measured in the in situ dataset represent the area where the nearshore biota are living, and is better able to reflect what temperature patterns/exposure these flora and fauna experience. Therefore two datasets are necessary: one for the coast; one for the ocean. The aim is not to compare the accuracy of the two datasets to detect the same events, rather this study aims to show that fundamentally different outcomes exist, and that in order to show the vulnerability of nearshore ecosystems to climate change, an appropriate dataset must be used.

4.5. Climate change

Although all but four of the *in situ* time series used in this investigation are too short to draw adequate conclusions on the decadal trends seen in MHWs and MCSs, the OISST time series are long enough. As hypothesized, these data show positive decadal trends

for the annual occurrence MHWs and negative trends for MCSs. This means that over the past 33 years of satellite observation, more MHWs have been occurring every decade for each coastal section while the occurrence of MCSs has been decreasing. Whereas the literature surrounding the potential increase (decrease) of MHWs (MCSs) in the ocean is still in its infancy, atmospheric scientists have been investigating the shift in the occurrence of extreme events for over a decade. Both historic and modelled research shows that climate change is leading to an increase of extreme hot events in the atmosphere (Easterling et al., 2000; Perkins and Alexander, 2013), and decreasing extreme cold events (Meehl, 2004). It is not surprising to find the same pattern in the ocean as seen Fig. 7.

Though less conclusive than the trends calculated from the longer time series, similar patterns were found in the shorter *in situ* time series as well. As the algorithm used to calculate these events is based on percentiles, it stands to reason that as the mean temperature of the oceans has been increasing by roughly 0.1 °C per decade on average over the past several decades (Stocker et al., 2013), there will be an increase in the occurrence of MHWs and a decrease in MCSs. The gradual mean increase in temperature will cause the algorithm used here to be biased in its detection of MHWs as time progresses because temperatures are generally warmer in the later half of the time series. It is then important to note that the usefulness of the MHW (MCS) algorithm is not limited to the detection of the increase or decrease of the occurrence of events, but also to measuring the duration a region spends in an extremely warm (cold) state and how that may change over time.

5. Conclusion

It is our experience with these data that every time series used from both datasets experienced, on average, at least one MHW and MCS per year. Within each dataset, but not between, the count of events is similar for each coastal section, regardless of the local oceanographic and geographic properties. Instead, it is the duration, mean intensity and also the derived cumulative intensity of the events occurring on the different coastal sections that most clearly define spatial differences – so much so, that this will almost certainly translate to different rates of vulnerabilities of coastal sections, both the ecosystems and the humans that derive benefit from them, to the ravages of climate change. As the proportion of co-occurrence of events between the local- and broad-scale dataset are generally low, and the magnitude of events within the different datasets differ significantly from one another, we infer that some other force outside of mesoscale temperature phenomena is contributing to nearshore events. We think that direct atmospheric forcing of coastal thermal heating is one such driver that needs immediate research attention in order to better understand what is driving the occurrence and intensity of these events.

Of the metrics presented in this paper, cumulative intensity is perhaps the most important ecologically. As a product of the intensity and duration of an event, we propose that cumulative intensity may be used as an index to measure the threat of thermal events to coastal ecosystems. Future research conducted on damaging MHWs and MCSs will be able to record the cumulative temperature above the seasonal average experienced by the ecosystem in question. As the body of research on extreme events increases, the aggregated cumulative intensity values may be used to establish a global index of the thresholds for different ecosystems at which ecological perturbations, impairment or destruction have occurred. Combined with near real time monitoring, this metric may then be used to improve the decision making process on how when and how best to respond to unusually warm or cold bodies of water. Furthermore, we found in this study that the

cumulative intensity of events at the coast were not only greater than the corresponding OISST events, but that the upper range was much greater.

We have provided a cursory look at an oceanographic basis for explaining these differences, but we think that there is an urgent need to consider more carefully the complex local-scale modifications of broader-scale patterns seen further afield in order to fully appreciate the drivers of coastal thermal variability in space and time. That such studies are still lacking in an age when the pulse of the global ocean is measured with exquisite precision is a reflection on the oceanographic community's ongoing preoccupation with mainly broad-scale open ocean patterns and processes. Globally comprehensive ocean temperatures are made available almost in real time, but to the best of our knowledge the top coastal temperature databases are all comprised of records retrieved from delayed-mode instruments. In the latter case, near-real-time warnings of the onset and intensity of MHWs (or MCSs) are not yet feasible, whereas it is already possible to develop and implement such warning systems using currently-available gridded satellite SST products. Researchers in the tropics, on coral reefs specifically, are already doing just this as they implement (near) real-time satellite data for the monitoring of coral bleaching (e.g. http://coralreefwatch.noaa.gov/satellite/index.php). Other coastal communities should learn from the work of tropical communities in implementing monitoring systems for extreme temperatures, which is now becoming relevant as climate change is threatening previously (relatively) stable ecosystems, such as temperate kelp forests (Wernberg et al., 2016). We therefore feel that there is a need to begin implementing near-real-time monitoring systems so that we may track the benefits of these systems in terms of prediction, detection and mitigation of the potential damage caused by extreme events. Furthermore, we propose that the focus of this implementation be on nearshore ecosystems as these are disproportionately more important to human livelihoods as well as being at greater risk generally than other marine ecosystems.

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Appendix A. Supplementary material

Further meta-data for each time series and source listed in geographic order along the South African coast from the border of Namibia to the border of Mozambique may be found in Table S1. Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.pocean.2017.01.004.

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Conclusion

The results of this second study were rather surprising. I had assumed that the rates of co-occurrences would not be perfect, but I had not thought they would be so low. It was however determined that the rates of co-occurrence for MCSs were less than MHWs, as predicted. With co-occurrence proportions for MHWs ranging from 0.2 to 0.5, this meant that either there was some fundamental difference between the datasets being compared, or that some force other than offshore temperature was responsible for the forcing of extreme events in the nearshore.

It was already known that remotely-sensed data show a warm bias over their *in situ* counterparts, but I also found that there were significant differences in the length and size of the events detected between the SACTN and remotely-sensed data. The events in the remotely-sensed data were shorter and less intense. This is an artefact of the method in which remotely-sensed data are smoothed out. The take-away message from this discovery was that direct comparisons of these different datasets would no longer do. They were different in too many ways.

The problem now, however, was that I was not much closer to discovering what forces were driving extreme thermal events in the nearshore. I had shown that direct comparison of nearshore and offshore temperatures was not particularly fruitful, so that could now be ruled out. I also here decided to stop focusing on MCSs. The scope of the thesis was beginning to broaden too much and I wanted to redouble my efforts on determining the cause of MHWs, as these are documented as being a greater threat than MCSs. Consulting the literature I determined that far more MHWs had been recorded as being the result of atmospheric forcing than I had first thought. It was for this reason that for the final study in this PhD thesis by publication I decided to look for synoptic scale patterns in the atmosphere as well as the ocean during coastal MHWs. So rather than looking only at very proximate thermal causes I wanted to look broadly to allow for any teleconnections or large features that may be driving coastal MHWs.

WESTERN CAPE

Appendix

Contribution

The MHW algorithm on which this work was built was created by Hobday et al. (2016). The detection algorithm for MHWs and MCSs used in this paper was written in Python by EO. An R version was latter written by AS. TW organised the authors for the paper. The concept for calculating co-occurrence was developed by RS, as was the code to perform said calculations. The results were interpreted by RS, who also wrote the first and final drafts of the manuscript. The production of the figures was split roughly in half between RS and EO. Two rounds of edits on the manuscript were provided by AS, EO, and TW, with RS incorporating all of the changes. The correspondence between the reviewers and the authors was facilitated by RS. All correspondence with the journal was performed by RS. The publicly available code ¹ for this publication is maintained by RS.

Written consent

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¹https://github.com/robwschlegel/MHW

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Correspondence

Nearshore and offshore co-occurrence of marine heatwaves and cold-spells

Robert W. Schlegel, Eric C.J. Oliver, Thomas Wernberg, Albertus J. Smit *P*rogress in Oceanography, doi: 10.1016/j.pocean.2017.01.004

RC: Reviewer Comment, AR: Author Response, ☐ Manuscript text

Reviewer #1

Comments

RC: I read this with interest but some difficulty.

AR: We have endeavoured to improve the readability of this manuscript as well as address all comments made by the reviewer. All changes in response to each individual point are outlined below.

RC: 1. Why were moving 11-day windows chosen for the climatology?

AR: The 11-day window (and 31-day moving average) was chosen to ensure a large enough sample size to obtain robust estimates of the climatological mean and percentile threshold (Hobday et al. 2016). We have not found a strong sensitivity to reasonable other choices for these window sizes.

AR: p. 6 lines 167-111: This explanation was inserted into the text.

RC: 2. Why the 90th and 10th percentiles?

AR: The 90th (and by extension in this paper the 10th) percentile was chosen as a rather liberal estimate for defining the thermal threshold for marine heatwaves (Hobday et al. 2016). That is to say we are detecting all relatively warm periods (5 days or longer), including what you might consider (for lack of better terms...) "somewhat warm", "very warm" and "extremely warm". The kind of MHWs that are highlighted in the literature with significant ecological impacts tend to be the "extremely warm" ones, but there are many reasons to be interested in the weaker events also, and similar physical mechanisms may be at play across all events. By including moderate as well as extreme marine heatwaves we are not restricting our analysis to the most extreme, but leaving enough data to look at all events. This also gives us the freedom to later restrict to the most extreme events, as we have done in this manuscript in Figs. 4 and 5.

AR: p. 6 lines 174-177: This explanation was inserted into the text.

RC: 3. Why was a 5-day or longer period chosen?

AR: This choice was mainly motivated around extending a common atmospheric heatwave definition, based on a 3-day cutoff, to the ocean where it is assumed that the ocean variability was "slower" and so deserved a longer cutoff (Hobday et al. 2016). This choice was also motivated by some concerns of the ecologists around impacts, whereby marine ecosystems were likely resilient on longer time scales than terrestrial ones. Additionally, it was found that a 5 day minimum length in event detection produced more globally consistent results, with events distributed relatively uniformly over the globe (Hobday et al. 2016).

- AR: P 6-7 lines 177-181: This explanation was inserted into the text.
- RC: The 2nd and 3rd choices are based on Hobday et al. but it would help readers if the rationales for these choices were summarised in the methods section.
- RC: I'm a little uncomfortable with 10th and 90th percentiles being used to define "extreme events".
- AR: This has been done (see points above, including indications as to where new text has been inserted).
- RC: Another difficulty for me is the style of writing that I found dense and scattered with grammatical errors and stylistic problems. For example a lot of the text is written in the present continuous tense: "are acting", "are increasing", ... etc. assuming that the trends will continue after the time series. This may happen, but one cannot be sure so it would be safer to write in the present tense: "act", "increase" ... etc. (not the present continuous).
- AR: Almost all instances of present continuous tense have been removed from the paper, generally in favour of past perfect, e.g. "had acted", "were increased"
- AR: The only consistent use of present tense was reserved for reference to decadal trends, e.g. "the decadal trend of MHWs on the west coast is 0.1C"
- RC: The methods appear to be sound and are based on Hobday's statistical work, and extended to apply to Marine Cold Spells (MCSs) as well as to heatwaves (MHWs). The results compare inshore and offshore observations on very different spatial scales and the 30-year time series are a minimum for the climate-change linked objectives. It is interesting that the offshore results show increasing trends in MHWs and decreasing trends in MCSs, as hypothesised under a simple global warming scenario, with a most intense decreasing trend off the Cape Peninsula coastal upwelling region (suggesting increased upwelling favourable local winds). The inshore and offshore time series show little correlation, but there are links between larger offshore and inshore events with a lag suggesting some propagation from inshore to offshore on the south coast, but surprisingly little evidence for the reverse. Events detected by in situ inshore measurements seem to be intrinsically different from those detected by remote sensing over a broader area.
- RC: Figures are generally clear and necessary, some rather busy. The tables are clear and useful.
- RC: The Discussion is very wordy and could be shortened considerably, especially the first two sections 4.1 and 4.2.
- AR: Section 4.1 shortened ~60% by moving the second paragraph to the conclusion section and deleting some of the last paragraph. The rest was either deleted or assimilated piecemeal throughout the manuscript where appropriate.
- AR: Section 4.2 shortened ~25%. One paragraph was moved to the introduction section however, much of the text in this section was considered necessary to explain the effects the physical geography/ oceanography of the three different coastal sections may have had on the MHWs/ MCSs found there.
- AR: Section 4.3 shortened ~25% by deleting the last paragraph but adding one from section 4.5.
- AR: Section 4.4 shortened ~ 10% through editing.
- AR: Section 4.5 shortened ~50% by deleting the second paragraph and moving the last paragraph to section 4.3.

- AR: These reductions total over one full page of text removed from the manuscript.
- RC: The Conclusion is concise and well argued.
- AR: One paragraph was added to the conclusion from section 4.1.
 - Some detailed comments
- RC: p. 2 line 22: ... ecology of not "for" the regions...
- AR: p.2 line 22: Corrected
- RC: p. 4 line 94: ... increases (decreases) ... not "decrease"
- AR: p.4 line 93: Corrected
- RC: p.4 lines 94-95: "The possibility... was considered a very likely possibility ... " poor style, omit second possibility.
- AR: p.4 lines 93-94: Corrected to: "The effect of atmospheric forcing on nearshore events was considered but not assessed within the scope of this study."
- RC: p. 5 line 117: Lying ... not "laying" ...
- AR: p. 4 line 116: Corrected to "overlying"
- RC: p. 6 lines 125-126: ... 127 records of daily temperature measurements omit second "records of"
- AR: p.5 lines 129-130: Corrected to: "The in situ seawater temperature dataset used in this study was comprised of 127 records of daily measurements of up to 40 years with a mean duration of ca. 19 years."
- RC: p. 7 line 172: ... values of (not "for" these metrics...)
- AR: p. 7 lines 168-192: The paragraph containing this error was largely re-written so as to address the concerns expressed in the main comments above that not enough of the Hobday methodology was covered in the methods section of this manuscript.
- RC: p. 8 lines 202-203: ... the sizes of ... were compared (not "...size ... was compared")
- AR: p. 8 lines 221-222: Corrected to: "In addition to controlling for the duration and direction of lag, the sizes of the individual events were factored into the calculations of co-occurrence proportion."
- RC: p. 17 lines 328-329: "are occurring ... is decreasing" replace by <u>occur</u> and <u>decrease</u>, respectively.. (many other examples follow see main comments)
- AR: p. 17 lines 348-349: Corrected to: "Just as MHWs occurred more frequently per decade on the east coast than the west, the count of MCSs decreased more on the east coast than the west."
- RC: p. 18 line 346: ...show (not "shows") no agreement with their counterparts...
- AR: p. 18 line 366: Corrected to: "...showed no agreement with their..."
- RC: p. 25 line 529: ... argued by Roberts... (not "argued for")
- AR: The paragraph containing this error was removed to shorten the discussion section.
- RC: p. 25 Line 551-552: ...events appear (not "appears" ...)
- AR: The paragraph containing this error was rewritten while shortening the discussion section.

RC: p. 25 line 554: co-occurrence of (not "for") ...

AR: p. 25 line 559: Corrected

RC: p. 26 line 595: ... appropriate would be better than "correct" dataset.

AR: p. 25 line 583: Corrected



THIRD STUDY

Introduction

In this final study for the PhD thesis by publication I was determined to come closer to an answer for the question of what was forcing coastal marine heatwaves (MHWs). After the second study showed the rates of co-occurrence between nearshore and offshore events to be much lower than anticipated, I decided to broaden my scope to the entire region surrounding southern Africa. This included not only SST, but also air temperature, wind, and surface current data. Initially this was to be done by utilising the same methodology as in study two, but looking at the rates of co-occurrence over a larger area. After much deliberation with my co-authors, and several months of experimentation, it was decided to make a radical change.

One of my co-authors, Eric C. J. Oliver had recently completed an atlas of MHWs for Tasmania and was in the process of working out how to use self-organising maps (SOMs) to then find common patterns in the atmosphere and ocean during these events. I was very fond of this idea and so decided to change the focus of the study and write the necessary code to perform this task in R. This also allowed me the time to focus on creating an atlas ¹ for the MHWs of South Africa. With the atlas figures created, and the code written, it was then possible to pull out the potential patterns that were present during the coastal events.

A SOM is a type of clustering and so does not provide any statistical result that will inform the user about the patterns that may or may not be present. This requires that the user knows what to look for. Therefore the writing of the code and the creation of the atlas was only the first step. It was also necessary to thoroughly refer to the rather scarce literature on MHWs to see what patterns had been determined in the past. There have been several well documented MHWs around the world and so some knowledge on what the most likely drivers may be was able to be obtained beforehand. After knowing what patterns had been found in the past, I then needed to determine what patterns were known to exist in the atmosphere and ocean around South Africa. I was already familiar with such oceanographic patterns due to my background in marine science, but the atmospheric patterns I intended to interrogate

¹https://github.com/robwschlegel/AHW/tree/master/graph/synoptic

were largely unknown. This was a very large and possibly over-ambitious step to take, but I was determined that it was necessary to include atmospheric variables in the study and so I made a plan.







Predominant Atmospheric and Oceanic Patterns during Coastal Marine Heatwayes

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Schlegel RW, Oliver ECJ, Perkins-Kirkpatrick S, Kruger A and Smit AJ (2017) Predominant Atmospheric and Oceanic Patterns during Coastal Marine Heatwaves. Front. Mar. Sci. 4:323. doi: 10.3389/fmars.2017.00323 As the mean temperatures of the worlds oceans increase, it is predicted that marine heatwaves (MHWs) will occur more frequently and with increased severity. However, it has been shown that variables other than increases in sea water temperature have been responsible for MHWs. To better understand these mechanisms driving MHWs we have utilized atmospheric (ERA-Interim) and oceanic (OISST, AVISO) data to examine the patterns around southern Africa during coastal (<400 m from the low water mark; measured in situ) MHWs. Nonmetric multidimensional scaling (NMDS) was first used to determine that the atmospheric and oceanic states during MHW are different from daily climatological states. Self-organizing maps (SOMs) were then used to cluster the MHW states into one of nine nodes to determine the predominant atmospheric and oceanic patterns present during these events. It was found that warm water forced onto the coast via anomalous ocean circulation was the predominant oceanic pattern during MHWs. Warm atmospheric temperatures over the subcontinent during onshore or alongshore winds were the most prominent atmospheric patterns. Roughly one third of the MHWs were clustered into a node with no clear patterns, which implied that they were not forced by a recurring atmospheric or oceanic state that could be described by the SOM analysis. Because warm atmospheric and/or oceanic temperature anomalies were not the only pattern associated with MHWs, the current trend of a warming earth does not necessarily mean that MHWs will increase apace; however, aseasonal variability in wind and current patterns was shown to be central to the formation of coastal MHWs, meaning that where climate systems shift from historic records, increases in MHWs will likely occur.

Keywords: marine heatwaves, code:R, coastal, atmosphere, ocean, in situ data, reanalysis data, climate change

1. INTRODUCTION

Extreme thermal events that occur in the ocean are classified here as "marine heatwaves" (MHWs) after Hobday et al. (2016). These events may occur suddenly, anywhere in the world, and at any time of the year. Several large MHWs, and their ecological impacts, have already been well documented. One of the first MHWs characterized occurred in 2003, and it negatively impacted as much as 80% of the Gorgonian fan colonies in the Mediterranean (Garrabou et al., 2009). A 2011 MHW is now known to have caused a permanent range contraction by roughly 100 km of the ecosystem forming-kelp species Ecklonia radiata in favor of the tropicalisation of reef fishes and seaweed turfs along the southern coast of Western Australia (Wernberg et al., 2016). The damage caused by MHWs is not only confined to demersal organisms or coastal ecosystems, e.g., a MHW in the North West Atlantic Ocean in 2012 indicated that these kinds of extreme events are also able to impact multiple commercial fisheries (Mills et al., 2013). When extreme enough, such as "The Blob" that persisted in the North West Pacific Ocean from 2014 to 2016, a MHW may negatively impact even marine mammals and seabirds (Cavole et al., 2016). Besides increases in mortality due to thermal stress, MHWs may also lead to outbreaks of disease in commercially viable species, such as that which occurred during the 2015/16 Tasman Sea event (Oliver et al., 2017a).

It is now possible to directly compare MHWs occurring anywhere on the globe during any time of year using a statistical methodology developed by Hobday et al. (2016) that defined these events as "a prolonged discrete anomalously warm water event that can be described by its duration, intensity, rate of evolution, and spatial extent." Whereas the metrics created for the measurement of MHWs allowed for the comparison of events, they did not directly reveal what may be causing them. Beyond common measurements, it is necessary to determine the predominant patterns that occur during MHWs in order to identify their physical drivers.

It has been assumed that coastal MHWs should either be caused by oceanic forcing, atmospheric forcing, or a combination of the two; however, the scale at which this forcing must occur in order to drive MHWs at the coast has yet to be determined. Recent research into the rates of co-occurrence between nearshore and offshore MHWs revealed that oceanic forcing from offshore (broad-scale) onto the nearshore (<400 m from the coast, i.e., also referred to as local-scale) was far less responsible for the formation of coastal MHWs than hypothesized (Schlegel et al., 2017). It is therefore necessary to consider broader meso-scale mechanisms that may be responsible for such events occurring at the local-scale. For example, the 2011 Western Australia MHW (Pearce and Feng, 2013) was caused by the aseasonal transport of warm water onto the coast due to a surge of the Leeuwin Current (Feng et al., 2013; Benthuysen et al., 2014). Oceanic forcing was also the main contributor of the anomalously warm water during the 2015/16 Tasman MHW when the southward flowing East Australian Current caused a convergence of heat there (Oliver et al., 2017a). Conversely, Garrabou et al. (2009) were able to show that atmospheric forcing played a clear role in formation of the 2003 Mediterranean MHW. While more complex, Chen et al. (2015) also showed that atmosphere-ocean heat flux could be attributed as the main forcing variable in the 2012 Atlantic MHW. The Blob, however, appears to have occurred due to the lack of advection of heat from surface waters into the atmosphere due to anomalously high sea level pressure (Bond et al., 2015). Outside of these few examples for these well documented events there has been little progress in developing a global understanding of the forcing of MHWs, nor has a methodology been developed with the capacity to determine the probable drivers of multiple MHWs simultaneously.

In order to develop a methodology that could be used to investigate the potential atmospheric and/or oceanic forcing of multiple coastal MHWs within a single framework, an index of the mean synoptic atmospheric and oceanic states around southern Africa during the occurrence of these events was created, similar to Oliver et al. (2017b) for Eastern Tasmania. The daily climatology for the atmosphere and ocean around southern Africa were also calculated to determine if the MHW states differed from the expected daily values. After determining this distinction, the MHW states were clustered with the use of a self-organizing map (SOM). The aim of the distinction and the clustering was to visualize meso-scale patterns in the atmosphere and/or ocean that occur during MHWs at coastal sites, and to be certain that these patterns were different from daily climatologies. We predicted that (i) atmospheric and oceanic states during MHWs would differ from daily climatology states; (ii) recurrent atmospheric and oceanic patterns would be revealed through clustering; and (iii) the clustered patterns would aid in the development of a broader mechanistic understanding of the physical drivers of coastal MHWs.

2. MATERIALS AND METHODS

2.1. Study Region

The ca. 3,100 km long South African coastline provides a natural laboratory for investigations into the forcing of nearshore phenomena as it may be divided into three distinct sections, allowing for a range of meso-scale oceanic influences to be considered within the same research framework (Figure 1); therefore, the extent of the study area was set at 10 to 40°E and 25 to 40°S. The range of sea surface temperatures experienced along all three coasts is large, and the gradient of increasing temperature from the border of Namibia (Site 1) to the border of Mozambique (Site 26) is nearly linear. The west coast of the country is distinct from the other two coasts as it is bordered by the Benguela Current, which forms an Eastern Boundary Upwelling System (EBUS) (Hutchings et al., 2009) against the coast. Conversely, the east coast is dominated by a western boundary current, the Agulhas Current (Lünning, 1990), a poleward flowing body of warm water. The south coast is also bordered by the Agulhas Current, but differs from the east coast in that it experiences both shear-forced and winddriven upwelling (Lutjeharms et al., 2000) in addition to having significantly more thermal variability than the other two coasts (Schlegel et al., 2017). The Agulhas and Benguela currents meet along the south coast of the subcontinent, and rather than having

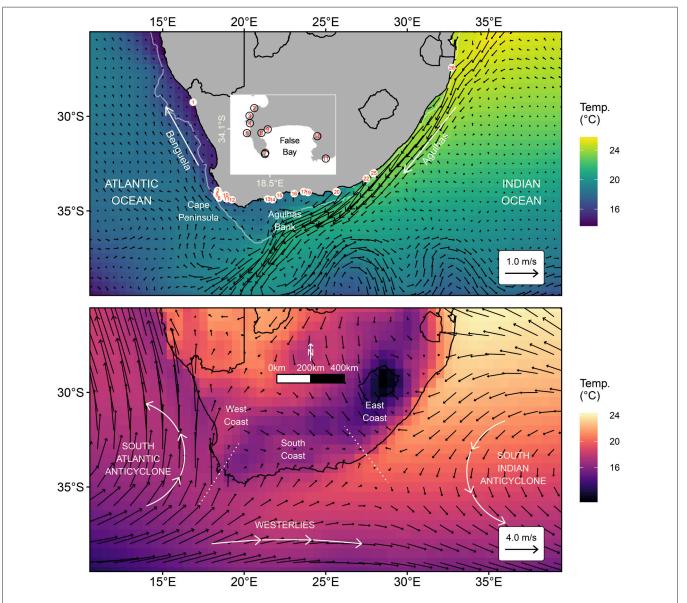


FIGURE 1 | Map of the study area where the **top panel** shows the mean annual sea surface temperature (SST) and surface currents from 1993 to 2016, as well as the locations referred to in the text. The sites of *in situ* collection are shown with red numerals over white circles. An inset map of the Cape Peninsula/False Bay area is shown where site labels are obscured due to overplotting. The **bottom panel** shows the mean surface atmospheric temperature and winds, and highlights the three coastal sections found within the study area as well as the three predominant wind patterns. Note that the temperature and vector scales differ between the two panels. The white vector arrows showing the predominant ocean and atmosphere circulation patterns are approximations and not exact values.

a fixed border, the two range from the Cape Peninsula in the west, to the western portion of the Agulhas Bank in the east. The Agulhas Current retroflects upon coming into contact with the Benguela (Hutchings et al., 2009); however, it will occasionally punch through into the South Atlantic. This event, known as Agulhas leakage, allows warm, saline eddies of Indian Ocean water to propagate into the Atlantic Ocean (Beal et al., 2011).

Atmospheric circulation over the study area is dominated by two quasi-stationary anticyclonic high pressure cells. The South Indian Ocean High (hereafter Indian high) is situated approximately on the eastern border of the study area and draws warm moist air toward the east coast, whereas the South Atlantic Ocean High (hereafter Atlantic high) is found to the west of the subcontinent and draws cool dry air onto the west coast (Van Heerden and Hurry, 1998). To the south of the subcontinent, prevailing westerly winds blow south of these two high pressure cells (Van Heerden and Hurry, 1998). From their annual mean mean wind patterns, these three atmospheric features can be discerned from **Figure 1**. Summer heating may lead to the development of heat lows within the subcontinent, which tend to be absent during winter (Tyson and Preston-Whyte, 2000), allowing for the Indian and Atlantic highs to link over land

(Van Heerden and Hurry, 1998). Additionally, the Indian and Atlantic highs, as well as the westerlies, move northwards during winter months, with the effect that the colder westerly winds influence the weather mostly along the southern parts of the sub-continent (Van Heerden and Hurry, 1998). Atmospheric temperatures along the coasts are largely influenced by the cold Benguela on the west coast and warm Agulhas Current along the east and south coasts (Van Heerden and Hurry, 1998).

2.2. Data

2.2.1. Atmospheric Data

To visualize a synoptic view of the atmospheric state around southern Africa during coastal MHWs (see sections "Marine heatwaves" and "Atmosphere-ocean state" below), we chose to use ERA-Interim to provide atmospheric temperatures (2 m above surface) and wind vectors (10 m above surface). ERA-Interim is a comprehensive global atmospheric model that assimilates a wide range of data to create short term forecasts for 60 vertical layers (Dee et al., 2011). These forecasts are then combined with the assimilated data again during each 12-hourly cycle (Dee et al., 2011). ERA-Interim is produced by the European Center for Medium-Range Weather Forecasts (ECMWF, http:// www.ecmwf.int/), and at the time of this writing the chosen variables were available for download from January 1st, 1979 to December 31st, 2016. The data used in this study were downloaded at a daily resolution on a 1/2° grid and within the latitude/longitude of the study region (Figure 1).

2.2.2. Oceanic Data

The in situ coastal seawater temperature data used in this study were acquired from the South African Coastal Temperature Network (SACTN)¹. These data are contributed by seven different organizations and are collected in situ with a mixture of hand-held alcohol or mercury thermometers as well as digital underwater temperature recorders (UTRs). This data set currently consists of 135 daily time series, with a mean duration of 19.7 years, meaning that many the time series in this dataset are shorter than the 30 year minimum proscribed for the characterisation of MHWs (see "Marine heatwaves" section below) (Hobday et al., 2016). It is however deemed necessary to use these data when investigating extreme events in the nearshore (<400 m from the low tide mark) as satellite derived sea surface temperature (SST) values along the coast have been shown to display large biases (Smit et al., 2013) or capture minimum and maximum temperatures poorly (Smale and Wernberg, 2009; Castillo and Lima, 2010). Whereas a 30+ year period is ideal for determining a climatology, 10 years may serve as an acceptable bottom limit (Schlegel et al., 2017). Following on from the methodology laid out in Schlegel et al. (2017), time series with more than 10% missing data or shorter than 10 years in length were excluded from this research. Accounting for these 10 year length and 10% missing data constraints, the total number of in situ time series used in this study was reduced to 26, with a mean length of 22.3 years.

Research on oceanic reanalysis data around southern Africa have shown that none of the products currently available model the complex Agulhas Current well (Cooper, 2014). It was therefore decided to use remotely sensed data to determine the SST and surface currents in the study area.

SST within the study region was determined with the AVHRR-Only Optimum Interpolated Sea Surface Temperature (OISST) dataset produced by NOAA. NOAA OISST is a global $1/4^{\circ}$ gridded daily SST product that assimilates both remotely sensed and *in situ* sources of data to create a level-4 gap free product (Banzon et al., 2016). These data were averaged to a $1/2^{\circ}$ grid to match the courser resolution of the ERA-Interim data. At the time of this writing these data were available for download from September 1st, 1981 to June 5th, 2017.

To determine ocean surface currents remotely on a daily global 1/4° grid, sea level anomaly (SLA) values are used to determine absolute geostrophic flows. The directional values of these flow vectors (U and V) were the values used in this study. These values were averaged to a 1/2° grid to maintain consistent spatial representation between the datasets. At the time of this writing these data were available from January 1st, 1993 to January 6th, 2017. These altimeter products were produced by Ssalto/Duacs and distributed by Aviso, with support from Cnes (http://www.aviso.altimetry.fr/duacs/).

2.3. Marine Heatwaves (MHWs)

We use here the definition as well as the methodology laid out in Hobday et al. (2016) for the analysis of MHWs in this research. The algorithm developed by Hobday et al. (2016) requires daily time series data and isolates MHWs by first establishing the daily climatologies for the given time series. This is accomplished by finding the range of temperatures for any given day of the year, and then pooling these daily values further with the use of an 11-day moving window, across all years. From this pool are calculated two statistics of interest: the first is the average climatology for each day, and the second the 90th percentile threshold for each day. When the observed temperatures within a time series exceed this threshold for a number of days it may be classified as a discrete event. Perkins and Alexander (2013) concluded that the minimum duration for the analysis of atmospheric heatwaves was 3 days whereas Hobday et al. (2016) found that a minimum length of 5 days allowed for more uniform global results. It was also determined that any MHW that had "breaks' below the 90th percentile threshold lasting ≤ 2 days followed by subsequent days above the threshold were considered as one continuous event (Hobday et al., 2016). Previous work by Schlegel et al. (2017) showed that the inclusion of these short five day MHWs may lead to spurious connections between events found across different datasets. Therefore we have limited the inclusion of MHWs within this study to those with a duration in the top 10th percentile of all events that occurred within the range of complete years of data available for all of the datasets used in this study (1994-2016). Thus, from the 976 total MHWs detected in the in situ dataset, only 86 were used here.

In order to calculate a MHW it is necessary to supply a climatology against which daily values may be compared. It is proscribed in Hobday et al. (2016) that this period be at

¹https://robert-schlegel.shinyapps.io/SACTN/

TABLE 1 | The descriptions for the metrics of MHWs as proposed by Hobday et al. (2016) and adapted from Schlegel et al. (2017).

Name [unit]	Definition			
Count [no. events per year]	n: number of MHWs per year			
Duration [days]	D: consecutive period of time that temperature exceeds the threshold			
Maximum intensity [°C]	$i_{\mbox{\scriptsize max}}$: highest temperature anomaly value during the MHW			
Mean intensity [°C]	$i_{\it mean}$: mean temperature anomaly during the MHW			
Cumulative intensity [°C·days]	$i_{\it Cum}$: sum of daily intensity anomalies over the duration of the event			
Onset rate [°C/day]	<i>r_{onset}</i> : daily increase from event onset to maximum intensity			
Decline rate [°C/day]	$r_{\it decline}$: daily decrease from maximum intensity to event end			

least 30 years. Because 20 of the 26 time series used here are below this threshold, we have opted to use the complete data period for each station as the climatological period. Using fewer than 30 years of data to determine a climatology prevents the accurate inclusion of any decadal scale variability (Schlegel and Smit, 2016); however, by using at least 10 years of data we are able to establish a baseline climatology to calculate MHWs (Schlegel et al., 2017). By calculating MHWs against the daily climatologies in this way, the amount they differ from their localities may be quantified and compared across time and space — the implication is that this allows researchers to examine events from different variability regimes (i.e., regions of the world, seasons) and compare them with a consistent set of MHW metrics. The definitions for the metrics that will be focused on in this paper may be found in **Table 1**.

The MHWs in the SACTN dataset were calculated via the R package "RmarineHeatWaves" (Smit et al., 2017). This package implements the methodology detailed above, as first proposed by Hobday et al. (2016). The original algorithm used in Hobday et al. (2016) is available for use via python².

It is worth emphasizing that MHWs as defined here exist against the daily climatologies of the time series in which they are found and not by exceeding an absolute threshold. Therefore, one may just as likely find a MHW during winter months as summer months. This is a valuable characteristic of this method of investigation because aseasonal warm winter waters may, for example, have deleterious effects on relatively thermophobic species (Wernberg et al., 2011), or aid the recruitment of invasive species (Stachowicz et al., 2002).

It must also be clarified that due to the irregular sampling effort in the SACTN dataset along the coastline of southern Africa, the spatial and temporal distributions of the 86 MHWs are not necessarily even, with some areas, specifically the south coast, having a much greater likelihood of MHWs that meet the selection criteria. Addressing this imbalance would require that the use of data from the south coast (seventeen time series) be

constrained to resemble that of the east coast (four time series) and west coast (five time series). This would reduce the number of time series used here roughly in half. Because the aim of this research was to determine the predominant atmospheric or oceanic states (see section "Atmosphere-Ocean States" below) during the longest events in the dataset, regardless of where or when they occurred, it was decided not to correct for this inequality in the data.

2.4. Atmosphere-Ocean States

In order to visualize meso-scale patterns in the atmosphere and ocean around southern Africa during a coastal MHW, it was necessary to first combine all of the daily values of these physical states for all days available across all of the datasets downloaded for this research (1994-2016). The oceanic states consisted of SST and surface currents while the atmospheric states were surface temperatures and surface winds. One mean atmosphereocean state was then created for each of the 86 MHWs in this study by taking the daily atmosphere-ocean states during each day during which the event occurred and averaging them together. For example, for a MHW that started on December 1st, 1999, and ended on March 7th, 2000, the 98 daily atmosphereocean states during that event were averaged to create a single atmosphere-ocean state that represented the overall pattern that was occurring during that one event. This example may be seen in the top row of panels in Figure 2.

The calculation of the anomalies that would be used for all subsequent stages of this research required that a daily climatology be created for the atmospheric and oceanic states. These 366 daily atmosphere-ocean climatologies were calculated using the same algorithm used to determine the average daily climatologies for the in situ time series, with the climatological period set from 1994 to 2016 as this was the widest period available across all of the gridded datasets. With the atmosphereocean climatology known for each calendar day of the year, it was then possible to subtract these daily climatologies from the daily atmosphere-ocean states during which a MHW was occurring before averaging each individual daily anomaly together to create one mean atmosphere-ocean anomaly state for each event. An example of the atmosphere-ocean anomaly states created in this way may be seen in the middle row of Figure 2. The daily climatology anomaly states to be used for comparison against the MHW anomaly states (see section "Nonmetric multidimensional scaling (NMDS)" below) were created by subtracting the annual mean climatology state from all of the daily climatology states.

2.5. Nonmetric Multidimensional Scaling (NMDS)

The goal of using Nonmetric multidimensional scaling (NMDS) to ordinate the MHW anomaly states (hereafter MHW states) and climatology anomaly states (hereafter climatology states) was not to perform a statistical analysis on the data; indeed no significance is tested, but rather to visualize how each state relates to every other state while simultaneously visualizing the effects of the categorical variables on the data. The resultant biplot generated by NMDS allows one to visually inspect the relationship between MHW and climatology states, in order

²https://github.com/ecjoliver/marineHeatWaves

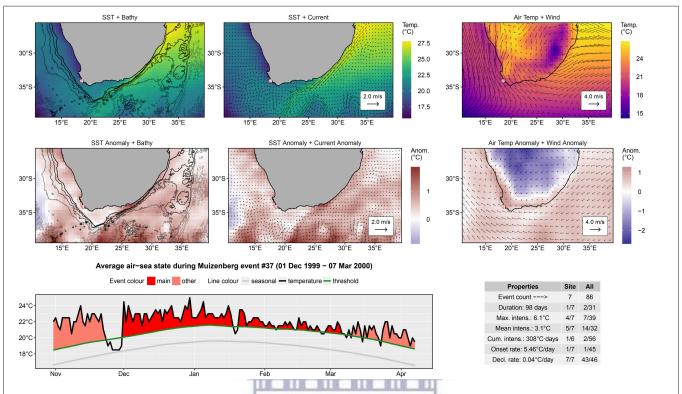


FIGURE 2 An atlas figure for a single coastal marine heatwave (MHW). The location of collection for the *in situ* coastal seawater temperature time series is shown in each of the top six panels as a white dot with a red border. The top row of panels shows the mean synoptic atmospheric and oceanic states during the MHW, created by averaging all daily synoptic atmosphere-ocean states during the event. The middle row shows anomalies for the mean atmospheric and oceanic states during the event. The left hand panel in the bottom row shows the period of the time series in which the MHW occurred. The table in the bottom right corner shows the values for the relevant metrics of the event as explained in **Table 1** as well as its ranking against other events at the same site and the entire study area. Similar figures for each of the 86 MHWs used in this study are available here.

to determine if they share a common pattern, or are indeed dissimilar from one another. This is done by reducing the dimensionality of the atmosphere-ocean states down to a twodimensional field that may be understood by mere humans. NMDS was chosen for this task over other ordination techniques, such as principal component analysis (PCA), as it may visualize all of the variance between the different states along only two axes, whereas PCA would only display part of that variance (Paliy and Shankar, 2016). NMDS is also one of the most robust unconstrained ordination methods available (Minchin, 1987). The use of this technique may not be wide-spread in climate science, but we found that it was effective for reducing the dimensionality of the atmosphere-ocean states used here. The temperature, U and V variables were first scaled to a mean of zero across the common variables within the same pixels for all MHW and climatology states. These scaled values were then converted into a Euclidean distance matrix before being fed into the NMDS algorithm. An additional benefit of NMDS is that it allows for the strength of the influence of the categorical variables within the data to be displayed on the resultant biplot as vectors, where the length of each vector represents the amount of influence that categorical variable has, and the direction of the vector shows where on the two-dimensional plain the ordinated data points are being influenced toward. The categorical variables considered

when ordinating the MHW and climatology states together were the season during which the day or event occurred/started, as well as if the value represented a MHW or a climatology. The steps outlined here were conducted with algorithms from the R package "vegan"; (Oksanen et al., 2017).

It is important to note with NMDS that the two dimensions (i.e., x and y axes) along which all data points are ordinated do not represent any specific variables or quantities within the dataset. Instead these axes represent the algorithm's best attempt at reducing the stress in the model when constraining a multi-dimensional dataset into a two-dimensional visualization (Kruskal, 1964). It therefore requires knowledge of the data being ordinated in order for the user to determine a best approximation for the variables most closely represented in the axes of ordination.

2.6. Self-organizing Maps (SOMs)

Several methods of clustering synoptic data have been employed in climate science. Of these K-means clustering is perhaps most often employed (e.g., Corte-Real et al., 1998; Burrough et al., 2001; Kumar et al., 2011), with hierarchical cluster analysis (HCA) less so (e.g., Unal et al., 2003). A newer technique, self-organizing maps (SOMs), has been gaining in popularity in climate studies (e.g., Cavazos, 2000; Hewitson and Crane, 2002;

Morioka et al., 2010). Here we have used a SOM to cluster the 86 MHW state anomalies.

The initialisation of a SOM is similar to more traditional clustering techniques (e.g., Jain, 2010) in that a given number of clusters (hereafter referred to as nodes) are declared by the user in order to instruct the SOM algorithm into how many nodes it should first randomly assign all of the data point (Hewitson and Crane, 2002). Each data point in this instance represents an atmosphere-ocean anomaly state during a MHW and consists of temperature, U and V anomalies, which reach a total 9774 variables each. Therefore, each SOM node is represented not by a single value, but by a 9774 value long reference vector. After all of the data points have been clustered into a node, the SOM then determines the most suitable reference vector for each node to represent the data therein (Hewitson and Crane, 2002). The data points are then reintroduced to the SOM and, based on Euclidean distance, each data point is then matched to the node of 'best fit' (Hewitson and Crane, 2002). During this process the reference vectors for each node are modified as the SOM algorithm "learns" how best to refine them to fit the data points, while also learning how best to fit the nodes in relation to one another (Hewitson and Crane, 2002). This means that not only does the SOM algorithm update the goodness of fit for each node during each run of the data, it also better orientates the nodes against one another and allows better clustering of higher densities of similar data points (MHW state anomalies) (Hewitson and Crane, 2002). This allows the user to see not only into which node a given data point (MHW state anomaly) best belongs in, but also what the relationship between the nodes may be and how prevalent certain MHW state anomalies are over others. Here we initially allowed the SOM algorithm to iterate this process 100 times. Analysis of the resultant SOM showed that little progress was made in the fitting of the data after 40 iterations, and so 100 iterations was deemed appropriate.

Because the SOM algorithm was not able to provide consistent results each time the analysis was run on these data, we opted out of using the default random initialisation (RI) method for the SOM in favor of principal component initialisation (PCI). PCI differs from RI in that it uses the two principal components of the dataset, as determined from a PCA to initialise the choice of node centers for the SOM (Akinduko et al., 2016). This allows the SOM model to recreate the same results when it is run on the same data. The SOM algorithm used in this study was taken from the R package 'yasomi' (Rossi, 2012).

The appropriate number of nodes to use in a cluster analysis is an important decision (Gibson et al., 2016). This is because it is necessary to include enough nodes to view a broad range of synoptic states, but not so many that the differences between the nodes become meaningless. Calculating the within group sum of squares (WGSS) as more nodes were included showed that four could be satisfactory, but that at least six would be better. Ultimately we settled on nine nodes as this allowed for a wider variety of different synoptic atmosphere-ocean states to be separated out from one another, allowing for a better understanding of the dominant patterns that exist during coastal MHWs. As proposed in Johnson (2013), the nodes that are output by a SOM should be significantly different from one another to

ensure that an excess of nodes has not been used. Running an analysis of similarity we found this to be true for the choice of nine nodes (p = 0.001).

Once each MHW state anomaly was clustered into a node a further mean atmosphere-ocean state anomaly for each node was calculated by taking the average of all of the MHW state anomalies clustered within each node. It was these final mean atmosphere-ocean state anomalies that were taken as the nine predominant atmosphere-ocean patterns during coastal MHWs.

3. RESULTS

3.1. Ordination of States

In order to determine any patterns in the differences between the MHW and climatology states, they were ordinated together using NMDS (stress = 0.14) and plotted on a biplot. Figure 3 shows that the climatology states were clustered together in a central position while the MHW states were scattered along the top and bottom. Furthermore, the climatology states have been ordinated by season in a very contiguous manner with little seasonal pattern existing for the MHW states. The vectors in Figure 3 showing the influence of the categorical variable "Season" very clearly relate to the occurrence of the climatology states, and not to the season of occurrence for the MHW states. The vectors indicating the direction of influence for the categorical variable "State" (i.e., MHW state or climatology state) show that the climatology states tend to center in the middle of the biplot, as we may see, but that the MHW states tend to be ordinated similarly toward states that occur during autumn months. It is important to remember that these results are in reality multi-dimensional, not two-dimensional as shown here. This is why Figure 3 shows MHW states both above and below the climatology states even though the vector for MHW states appears similar to the autumn vector. That the climatology states vary along the x axis in order of their occurrence throughout the year indicates that the variance this represents is the change in mean atmospheric and oceanic temperature throughout the seasonal cycle. The variance along the y axis is less clear, though it most likely represents differences in currents and winds. This inference is supported by the positioning of the spring and autumn climatology states, which are more variable than winter and summer, further up and down the y axis. There is also a significant (p = 0.002)relationship between the duration (days) of the MHW and its position along the y axis, with the shorter MHWs further from the center of the biplot. The MHW states are distributed either above the summer/spring climatology states or below the autumn climatology states. Furthermore, very few MHW states were near climatology states of the same season (e.g., winter MHW states may generally be found above the summer climatologies or below the autumn climatologies).

3.2. SOM Nodes

The nine predominant atmospheric and oceanic patterns around southern Africa during coastal MHWs may be seen in **Figure 4**. Note that while the oceanic and atmospheric patterns for each node are shown in separate panels, all atmosphere and ocean variables were fed through the SOM together, meaning

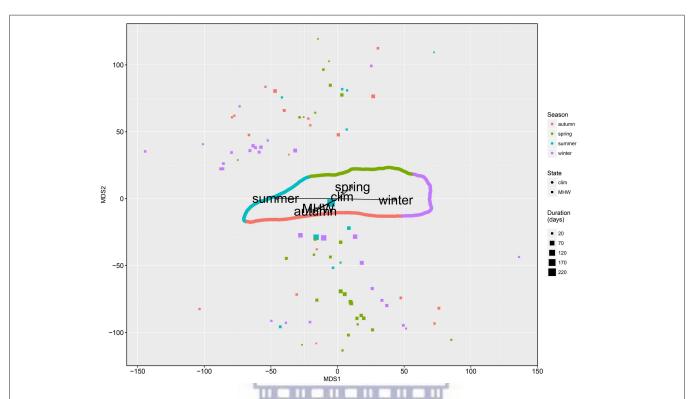


FIGURE 3 | Biplot (stress = 0.14) showing the ordination of climatology (clim) states (circles) and marine heatwave (MHW) states (squares). The *x* and *y* axes are not representative of any specific values of the states, rather the distance between each point shows the best fitting relationship of all states with one another based on the output of a nonmetric multidimensional scaling (NMDS) model. The season of the year during which the state occurred/started is shown in color. The influence of the two categorical variables, type of atmosphere-ocean state and season of occurrence, on the placement of each state in the two-dimensional space are shown as black labeled vectors. Note that the clim states (circles) are plotted so tightly together that they do not appear as individual points. The duration of the MHW states (not the clim states) are indicated by the size of the square points.

that the SOM had to consider both states when clustering them into nodes. The oceanic states appear to have been the most relevant criteria for clustering into the nodes in the top left corner, centered on Node 1, with nodes further away having less pronounced oceanic patterns. The nodes along the right edge, centered on Node 6, show that the primary influence for the clustering of MHW states there was the atmosphere. The further from Node 6 a node is placed, the less pronounced the atmospheric pattern becomes. The further from these two dominant points a node is, the less pronounced the patterns therein will become, as Node 7 shows.

MHWs that occurred during summer were the least common, only present in three nodes (Figure 5), with winter and spring events occurring more than twice as frequently (Table 2). Every node contained at least one spring event, and all but two nodes contained winter events. Three nodes lacked autumn events, but these were otherwise the most evenly distributed. Clustering of autumn, winter, and spring events that occurred over a range of years may be found in six of the nine nodes; however, the clustering of events that occurred within the same year is also consistent throughout the nodes. All but one of the nodes contained MHWs that were separated over large distances and by oceanographically dissimilar features. Additionally, only three

of the 86 MHWs in this study occurred on the east coast and were clustered into nodes that had events from all three coasts.

Table 2 shows that the largest values for duration (D), cumulative intensity (i_{cum}) and maximum intensity (i_{max}) were more than twice those of the smallest values. An individual description of each node may be found below, with a qualitative summary of the patterns given in **Table 3**. It is important to note that the wind and current anomalies shown in **Figure 4** do not show the absolute strength/direction of travel, but rather how these values deviated from the daily climatologies for the days during the MHWs in those nodes. The annual mean wind and current vectors may be seen in **Figure 1**.

3.2.1. Node 1

Node 1 showed the most striking oceanic pattern out of all of the nodes. The mean oceanic pattern from all of the MHW states clustered into this panel showed Agulhas Current leakage into the Atlantic as well as forcing onto the coastal region around the Cape Peninsula and potentially along the rest of the south coast. The SST anomalies along the coast, as well as in the open ocean were also the warmest of all the panels. The atmospheric temperature anomaly was mild relative to the other nodes but very strong north westerly wind anomalies were present to the west of the subcontinent and strong northerly wind anomalies

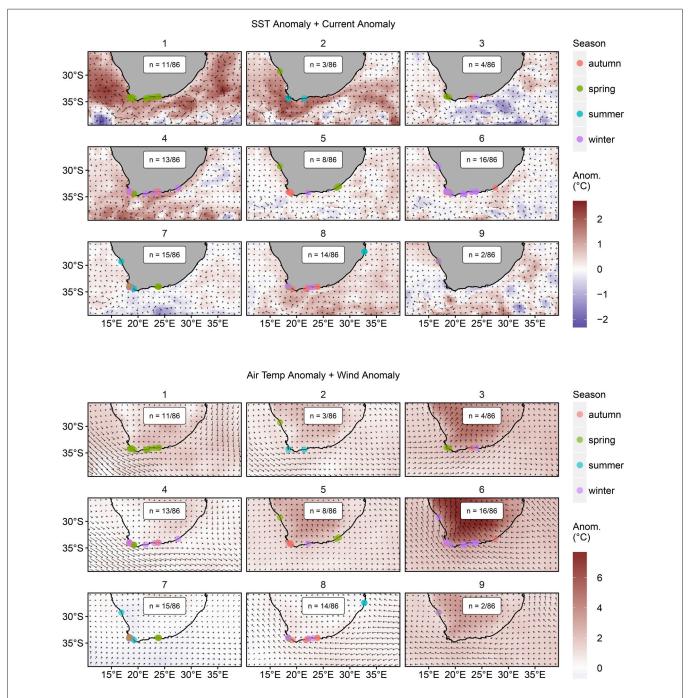


FIGURE 4 | Predominant anomalous atmospheric and oceanic patterns during coastal marine heatwaves (MHWs) as determined by a SOM. The top nine panels show the oceanic patterns while the bottom nine panels show the atmospheric patterns. The current and wind vectors are the same scale as those found in the respective atmospheric and oceanic panels of Figure 1. The number of events clustered into each node is shown within the white label in the middle of each panel. The location of each coastal MHW within each node is shown with a dot whose color denotes the season during which that event occurred/started. Note that the temperature anomaly scales differ for the top and bottom nine panels.

to the east. The north-westerly wind anomalies continued to the south of the subcontinent and along the south coast up to the location of the occurrence of the most eastward MHW before encountering the Indian high and abating. Neither of the high pressure cells showed any real influence on the overland

wind anomalies. Node 1 was unique in that all of the MHWs occurred during not only the same season (spring), but the same year (2004) as well. This also made it the node with highest concentration of spring events, as well as being one of only two nodes to have events that occurred on only one coast.

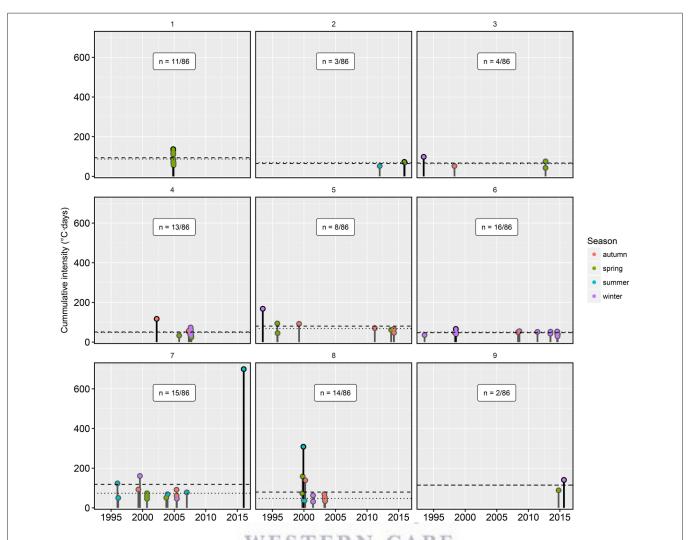


FIGURE 5 | Lolliplot showing the start date for each marine heatwave (MHW) within each node as seen in Figure 4, with the portion of total events per node shown within the white label in the middle of each panel. The height of each lolli shows the cumulative intensity of the event, as outlined in Table 1, while the lolli color denotes the season during which the event occurred/started.

3.2.2. Node 2

Node 2 showed similar warm SST anomalies in the nearshore along the west and south coasts as Node 1, with open ocean anomalies being cooler. There appeared to be some onshore forcing and leakage of the Agulhas Current but it was not as strong as in Node 1. The atmospheric temperature and wind anomalies in this panel were slightly less than Node 1 as well. The wind anomaly patterns were shifted slightly more to the south west with the westerly wind anomalies along the bottom of the panel reaching further east. The anomalous offshore wind circulation did not appear to move onshore. The average duration of the events in this node were the shortest of all the nodes.

3.2.3. Node 3

Node 3 showed the most negative SST anomalies of all the nodes, with some warm SST anomalies still present along much of the three coasts. There were atypical surface currents

occurring to the south west of the Cape Peninsula, similar to Nodes 1 and 2, but without clear onshore forcing. The overland atmospheric temperature anomalies were strong in this node with westerly wind anomalies pushing onshore along the west and south coasts from the south west and continuing overland. These onshore south-westerly anomalies were met on the eastern side of the subcontinent by neutral Indian high anomalies.

3.2.4. Node 4

Node 4 showed Agulhas leakage and onshore forcing with warm coastal SST anomalies along all three coasts, similar to Nodes 1 and 2. Warm open ocean SST and current anomalies were relatively even, with a large stretch of warmer SST anomalies and Agulhas retroflection along the bottom of the panel. Atmospheric temperature anomalies were relatively neutral, though slightly warmer over the subcontinent than the ocean. The wind

TABLE 2 | The count of MHWs clustered into each node, count of events for each season, count of events for each coast, and relevant metrics for those MHWs.

Node	Count	Summer	Autumn	Winter	Spring	West	South	East	D	i _{cum}	i _{max}
1	11	0	0	0	11	0	11	0	33.50	93.73	4.04
2	3	2	0	0	1	1	2	0	21.30	64.88	4.05
3	4	0	1	1	2	1	3	0	25.80	67.19	3.49
4	13	0	3	7	3	4	9	0	25.20	51.07	2.89
5	8	0	4	1	3	1	6	1	29.00	80.52	4.75
6	16	0	2	13	1	5	11	0	23.40	47.59	2.94
7	15	6	3	2	4	8	7	0	41.10	118.55	4.21
8	14	3	6	3	2	1	11	2	28.20	79.50	3.94
9	2	0	0	1	1	2	0	0	46.00	114.56	4.78
ALL	86	11	19	28	28	23	60	3	29.90	77.72	3.73

The mean duration of the events within each node are shown in column D with the i_{cum} and i_{max} columns showing the mean cumulative and maximum intensities respectively (**Table 1**). The bottom row of each column shows the sum or mean of the column as appropriate.

TABLE 3 | Qualitative descriptions and groupings of the predominant atmospheric or oceanic patterns present across the SOM nodes.

Node	Coast	Season	Pattern
(1,2,4)	West, South	All	Warm SSTs with onshore forcing, cool air with W/NW-erly wind anomalies
(3,5,6,9)	All	All	Cool or neutral offshore SSTs, warm air with mostly onshore wind anomalies
(8)	All	All	Warm SSTs with no onshore forcing, neutral air with E/SE-erly wind anomalies
(7)	West, South	All	Neutral

anomalies were similar to Nodes 1 and 2, but with the largest westerly wind anomalies of all of the nodes. Of the 13 MHWs clustered into Node 4, 11 of them occurred during the same aseasonally warm year (2007), over a span of several months. The events in this node had, on average, the second shortest durations, second lowest cumulative intensities, and the lowest maximum intensities. This node therefore serves as a good representations of atmospheric and oceanic states during the smaller events in this study.

3.2.5. Node 5

Node 5 showed some atypical currents to the south west of the Cape Peninsula, similar to most of the nodes. The SST anomalies during the events in this node were a mix of warm and cold, with very mild warm anomalies present along most of the coast. The atmospheric temperature anomalies, particularly overland, were strong during these events. Even though the wind anomalies were slight over the ocean during the events in this node, they were stronger overland where anomalous onshore wind movement occurred. This is also one of only two nodes that contain an event that occurred on the east coast. The average maximum intensity for the events in this node is very nearly the greatest.

3.2.6. Node 6

The surface current and SST anomalies in Node 6 were very similar to Node 5, with fewer warm SST anomalies along the coast. The atmospheric temperature anomalies overland during these events were in excess of $7^{\circ}C$ with strong south-easterly wind anomalies pushing not only onshore, but along the entire study area as well. The events clustered into this node had the greatest atmospheric temperature anomalies of all the nodes. Node 6 also shows a strong affinity for events from only one season, with 13 of the 16 MHW therein having occurred during winter, but were spread out from 1993 to 2014. This large concentration of winter events means that nearly half of all winter events were clustered into Node 6. The events in Node 4 battle those in Node 6 for the position of shortest and weakest, making this node another good example of the atmospheric and oceanic patterns during the smaller events used in this study. This node also has the greatest number of events clustered into it.

3.2.7. Node 7

Node 7 showed some atypical currents to the south west of the subcontinent but little in the way of onshore forcing or warm SST anomalies. The Southern Ocean appeared to be pushing up into the study area during these events as seen by the cold anomaly in the bottom middle of the panel. The atmospheric temperatures showed a very slight negative anomaly over much of the study area with very weak westerlies winds anomalies along the southern portion of the study area. That this node does not show any real patterns is not surprising given its position in relation to the nodes with stronger patterns. This node has the second greatest number of events clustered into it and contains half of all of the summer events in this study. These events also have the second longest average duration, the greatest average cumulative intensity, and the third greatest average maximum intensity. Because the node with the overall largest events only has two events clustered into it, Node 7 serves as the best representation of the atmospheric and oceanic patterns during very large events.

3.2.8. Node 8

Node 8 showed warm SST anomalies for all but the offshore portion of the Atlantic Ocean. There was some atypical vorticity along the south of the study area, but this was moving away from the coast and there appeared to be little leakage of the Agulhas Current. The atmospheric temperature anomalies during these

events were small with strong easterly wind anomalies moving across the entire study area. These wind anomalies wrapped around the subcontinent, and were not found overland. This node contained two of the three events that occurred on the east coast, and the third highest total of events clustered into a single node.

3.2.9. Node 9

The final node showed cold SST anomalies along much of the south and west coasts, with some warm anomalies further south of the subcontinent and atypical vorticity to the south east that did not appear to be reaching the coast. Easterly wind anomalies were found along the bottom of the study area with warm atmospheric temperature anomalies throughout. There are some slight onshore wind anomalies along the entire coastline. This is the only node that contains events from only one location (site 1; Figure 1). The two events clustered into this node have between them the greatest duration and maximum intensity, with the second greatest cumulative intensity. This makes the events in this node the overall largest however, the low number of events clustered here prevent this node from being a good indicator of a common atmospheric or oceanic pattern.

4. DISCUSSION

4.1. MHW States

The ordination of the MHW and climatology states has shown that they do differ in discernible ways. The clustering of the climatology states in the center of Figure 3 serves as a reference for better understanding the positioning of the MHW states. Because the proximity of points in an ordinated space shows their (dis)similarity to one another, the closer to the climatology states a MHW state may be found, the more it resembles it. This may seem contradictory at first given that all of the MHW states are ordinated most closely to climatology states that occurred during a different season. This means however that the states during all of the MHWs were aseasonal, and were more similar to climatology states during a different season of the year than the one in which they occurred. That none of the MHW states were ordinated near a winter climatology state is not surprising, as one would assume that MHWs should occur during warmer atmospheric or oceanic states. Following on this logic, a further assumption would be that the MHW states should most closely resemble the warmest time of year, summer. That the MHW states are instead ordinated more closely with autumn and spring climatology states means that high atmospheric or oceanic temperatures may be necessary for a MHW to occur, but are not the only driving force. During summer and winter months in southern Africa the Atlantic and Indian highs tend to stay in place latitudinally (Van Heerden and Hurry, 1998). It is during autumn and spring that, not always in a predictable manner, the synoptic atmospheric features around the subcontinent migrate north or south (Van Heerden and Hurry, 1998). As these systems shift they apparently create wind and/or current states that appear to be most similar to those that occurred during the coastal MHWs in this study. That high atmospheric and/or oceanic temperatures are not the only factor in the ordination of these MHW states

is good as, under a warming global climate (Pachauri et al., 2014), this would likely mean an increase in MHWs. Instead we have found that it is assasonality that is most consistently associated with MHW states. Therefore we may conclude that areas that experience increasingly divergent winds or currents from historical standards, without increasing temperatures, may also see an increase in MHWs.

Lastly, we have shown that in this ordinated space, the duration of the MHW around which each MHW state has been created, had a significant relationship with the proximity of the MHW state to climatology states. This is because the longer the event is, the more days of atmospheric and oceanic data are averaged together, creating a progressively smoother state, that will more closely resemble one of the climatology states. This is a potential, though unavoidable weakness in the methodology.

4.2. Agulhas Leakage

The most notable oceanic pattern from the clustering of these events into nodes with the use of a SOM has been Agulhas leakage. This phenomenon is when warm Indian Ocean water finds its way into the colder Atlantic Ocean (Beal et al., 2011). These warm eddies then typically spin up along the west coast. This transport of a large body of atypically warm water along a large stretch of coastline is a similar finding to the cause of the Western Australia MHW in 2011 where an unusual surge of the Leeuwin Current forced a large body of anomalously warm water onto the coast (Feng et al., 2013; Benthuysen et al., 2014). This onshore forcing of water is most apparent in Node 1 (Figure 4). However, Nodes 2 and 4 show a similar though less pronounced oceanic pattern, meaning that roughly one third of the events in this study occurred during Agulhas leakage. These three Agulhas leakage-dominated nodes also share the same anomalously warm atmospheric temperatures and north westerly to westerly wind anomaly patterns, to varying degrees. Therefore we may conclude that the predominant oceanic pattern during coastal MHWs is warm coastal SST anomalies occurring during Agulhas leakage while strong north-westerly wind anomalies exists along the west coast of the subcontinent, weak southeasterly wind anomalies along the east coast, and westerly wind anomalies that may be drawing aseasonally close to the south coast of the subcontinent. One of the primary causes of Agulhas leakage is when a weak Indian high does not provide enough of the positive wind stress curl the current needs to have enough inertia to retroflect upon meeting the Benguela current (Beal et al., 2011). The second feature that allows Agulhas leakage is when the latitude zero wind stress curl caused by the westerly wind belt has shifted further south of the subcontinent (Beal et al., 2011). We see in the Agulhas leakage panels that wind anomalies around the Indian high are much weaker than the Atlantic high. This could potentially be allowing for a loss in inertia of the Agulhas Current and an increased risk of leakage however, the westerlies appear to be shifted further north, which should inhibit leakage. These two diametric forces contributing to the atmospheric and oceanic states during the Agulhas leakage may be what is causing the Agulhas to move so close to the shore, leading to the large SST anomalies seen there.

Node 8 also shows some onshore forcing of the Agulhas Current, but with no large leakage into the Atlantic Ocean. Strong nearshore SST anomalies exist, but no ensuant leakage into the Atlantic due to the strong easterly wind anomalies over the Atlantic Ocean during the events in Node 8 that likely increased the inertia of the Agulhas Current enough that it retroflected upon meeting the Benguela current, while still forcing warm water onto the coast. Node 8 is also one of only two nodes that contain events from all three coasts, meaning that a strong Agulhas pushing onto the coast is a common pattern during MHW along the coastline of the entire study area.

Taken together with the events that occurred during Agulhas leakage, over half of the MHWs in this study occurred during some sort of anomalous Agulhas behavior coupled with warm nearshore SST anomalies. This is strong support for the relationship between the Agulhas Current and coastal MHWs. Beal et al. (2011) state, while difficult to say with certainty, Agulhas leakage is likely to increase under the continued regime of global anthropogenic warming. Biastoch et al. (2009) also found that Agulhas leakage is likely to increase, though due to the poleward shift of westerly winds. It is therefore likely that large MHWs like those seen in Nodes 1, 2, 4, and 8 will become more frequent.

4.3. Onshore Winds

With the exception of Nodes 7 and 8, all of the atmospheric states during coastal MHWs showed warm atmospheric temperature anomalies that were greater over the subcontinent than the ocean. The wind anomaly patterns during coastal MHWs were either strong north-westerly anomalies over the Atlantic with weak south-easterly anomalies over the Indian Ocean, or the inverse, but always showed some wind anomalies moving onshore. Furthermore, the nodes with the greatest overland atmospheric temperature anomalies (3, 5, 6, and 9) had comparable amounts of cold and warm SST anomalies as well as onshore wind anomalies. This implies that the MHWs in these nodes were forced by the onshore wind anomalies occurring during warm atmospheric anomalies and not by oceanic conditions. From this the conclusion may be drawn that MHWs forced by atmospheric variability will almost certainly occur during warm atmospheric anomalies with onshore wind anomalies. Three preferential mechanisms can be identified by which the pairing of atmospheric anomalies may cause MHWs. The first would be through direct atmospheric heating of the shallow nearshore water, as occurred over the Mediterranean in 2003 (Garrabou et al., 2009). The second could be that the anomalous onshore wind movement could have prevented seasonally regular wind forced upwelling from occurring, which would have then caused the coastal water at the location of the event to appear aseasonally warm. Lastly it is possible that the aseasonal wind anomalies could have acted upon the Agulhas Current, causing it to weaken and thereby broaden out over the Agulhas Bank and seeping warm water onto the cost. Taken together the events in these nodes (3, 5, 6, and 9) account for roughly one third of the events in this study.

4.4. Other Patterns

The lack of a strong atmospheric or oceanic pattern in Node 7 implies that the 15 events that were clustered there do not share any common pattern, meaning that there may still be many MHWs that occur not because of any recurrent or predominant atmospheric or oceanic pattern. This is an important finding as it shows that even though clear patterns in atmosphere and ocean may exist during most MHWs, these events may still occur during entirely novel conditions. A different interpretation of the lack of an apparent pattern in Node 7 is that because the events clustered into that event were the longest, on average, of all of the events in this study, creating a mean atmospheric and oceanic state for the entire duration of each event was impractical. That enough variation in atmosphere and ocean would have occurred over the lifespan of the event so as to "smooth out" any apparent signal. If this is so, it does not serve to address what may have caused such a large event. Upon closer inspection, the atlas figures for each event in Node 7 show that there are indeed patterns in the atmospheric and oceanic anomalies during these events, and that they do differ from the patterns in the other

The most seasonally predictable MHWs, those occurring during winter months and clustered into Node 6, were also the shortest and weakest. As these events were clearly a product of thermal heating, one could be led to assume that atmospheric forcing of MHWs causes less dramatic events than those forced by the ocean. This assumption would be incorrect as the MHWs clustered in Node 5, which also contain a clear atmospheric signal, have a greater cumulative intensity than most of the Agulhas leakage-dominated nodes. The largest events, those in Node 7, contain such disparate atmospheric and oceanic states that the mean atmospheric and oceanic patterns appear nearly blank. These factors prevent the drawing of a conclusion on whether the atmosphere or ocean may cause the largest MHWs.

A final note on the patterns visible in **Figure 4**. The south west corners of the oceanic states in Nodes 2, 3, 5, 6, 7, and 9, show an almost identical cyclonic (clockwise) anomaly on the exact same pixels. Upon more minute investigation it was determined that this cyclone, likely an Agulhas ring (Hutchings et al., 2009), occurred between roughly 12.5 to 14.5°E and 35.5 to 37.5°S. This eddy occurred during two thirds of all of the events in this study, making it the most common atmospheric or oceanic pattern found.

5. CONCLUSIONS

This research has shown that not only are the atmosphere and ocean states during coastal MHWs not closely related to the daily climatology states seen throughout the year, that what similarities do exist between MHW and climatology states are completely aseasonal. This means that the patterns that occur during MHW states are always more closely related to a different season than the one in which they occurred. Furthermore, the fewest MHWs occurred during summer months than any other season. These two facts taken together support the argument that MHWs are not simply a symptom of solar heating during the warm months

of the year, but that aseasonal winds and/or currents are also necessary for a coastal MHW to occur. It is also possible that MHWs are recorded less frequently during summer months because coastal waters will be warmer, and incursions of offshore water, or atmospheric heating will not cause a large enough difference in the expected daily temperatures to be flagged as a MHW.

The predominant oceanic pattern that emerged from the SOM clustering of the MHW states was the abnormal advection of warm water onto the coast in association with Agulhas Current leakage. The predominant atmospheric state was anomalously warm air centered over the subcontinent coinciding with strong onshore wind anomalies. The node containing the most lengthy, cumulatively intense events lacked any patterns, meaning that the majority of the MHWs in this study that had the potential to cause the most harm to nearshore ecosystems do not appear to have consistent or recurrent atmospheric or oceanic states. Rather, most of the largest events occurred during a novel atmospheric and/or oceanic state that was not repeated often enough to receive their own node. A third smaller scale pattern was found to occur more frequently than both the predominant atmospheric and oceanic patterns detailed here. This was a submeso-scale anticyclonic eddy, roughly two degrees wide, and centered at 13.5°E and 36.5°S. We did not investigate the ocean dynamics implied by the presence of this eddy as that was beyond the scope of this study.

The methodology utilized here has shown that it is possible to discern predominant atmospheric and oceanic patterns that occur during MHWs; however, one must have knowledge of the meso-scale oceanic and atmospheric properties of the study area in order to correctly interrogate the results. Even with this knowledge, many of the largest MHWs did not show any relationship to these potential meso-scale forces. One must therefore not assume that such broad patterns in either the atmosphere or ocean must be forcing any single MHW observed in nearshore environments. We have however shown that the likelihood of a large coastal MHW is greater during specific atmospheric and oceanic patterns. Given this consideration, it should be possible to apply this methodology to large-scale reanalysis products in an effort to forecast the occurrence of coastal MHWs at a fine-scale.

In order to determine potential patterns that may or may not exist during MHWs, this study utilized atmospheric and oceanic surface temperatures and velocity vectors. This was done because of the few large MHWs whose causes have been discerned

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(e.g., Garrabou et al., 2009; Feng et al., 2013; Pearce and Feng, 2013; Benthuysen et al., 2014; Chen et al., 2015; Oliver et al., 2017a), most were related to these variables. Having shown that temperature and surface vorticity patterns do exist during coastal MHWs, a follow up to this study should analyse surface pressure, which was the main driver of the The Blob (Bond et al., 2015), as well as eddy kinetic energy (EKE), which was a primary driver of the 2015/16 Tasman Sea MHW (Oliver et al., 2017a).

AUTHOR CONTRIBUTIONS

The central concept of developing a "Marine Heatwave Atlas" was first developed and implemented for Tasmania by EO with input from SP. RS then adapted this concept for use in South Africa. The idea to cluster recurrent atmospheric and oceanic states during marine heatwaves was also first implemented by EO with input from SP. The SACTN and ERA-Interim data were acquired by RS. The Aviso and OISST data were acquired by AS. All analyses, figures, and tables were performed or created by RS, with many of them adapted from earlier work performed by EO. All results were initially interpreted and drafted by RS, with EO, SP, AK, and AS providing two rounds of critical revisions on the developing manuscript. EO and AS provided additional insights into the oceanography of southern Africa while SP and AK provided additional insights into the meteorology. All authors give approval for the submission of this manuscript for review and agree to be accountable for all aspects of the work.

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- **Conflict of Interest Statement:** The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.
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Conclusion

This was by far the most ambitious study in the PhD thesis and the one that I think represents the greatest contribution to knowledge. I utilised a number of different statistical techniques in this paper, some in ways that had not yet, to my knowledge, been used in climate science. I accomplished this by taking all of the ecology statistics I had learned over my years in academia and applying them to climate data. It is known that this is valid to do with abiotic data, usually by using Euclidean distances rather than Bray-Curtis dissimilarities, but is not something that seems to be done often. The use of ordination with climate data may strike some as odd, but I found it to produce useful and intuitive results. I accomplished this by converting each synoptic state matrix into a one-dimensional vector. The vectors for the individual events were then combined into a matrix with each row representing an event and each column representing the same pixel from the synoptic states. This 'synoptic matrix' was then used for both the ordination and SOM algorithms.

The outcome of the novel application of these techniques is that we may now say that the most common oceanographic pattern that has occurred during coastal MHWs along South Africa was Agulhas Leakage, a well-known phenomenon. Likewise, the atmosphere has been shown to be anomalously warm overland during coastal MHWs when it is likely forcing these events.

Now that these patterns have been determined it is necessary to look into how well they serve as predictive variables, rather than simply finding that they co-occur. This will require another full study that builds on these findings. Had this thesis been longer, this would have been the next step. As it stands, this research will be performed outside of this body of work. One of the larger shortcomings that needs to be addressed in the detection of MHWs is that using the 90th percentile threshold to define events effectively makes them a statistical property of a time series, and not a discrete event in their own right. Future work on MHWs therefore needs to consider the calculation of events within a time series based on different baselines and/or climatologies. This may help to better classify discrete events as separate from the numerical structure of the time series in which they are found.

Appendix

Contribution

A detailed break-down of the authors contributions to this study may be seen on the second to last page of the publication.

Written consent

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Afrikaans abstract

I was invited to present at an Afrikaans science symposium at the end of November 2017 and had planned to attend before I realised that I had rather get serious about finishing up this thesis. Before coming to my senses I had translated the abstract for this third study. I have included it here for the enjoyment of the reader. Several of the terms used herein are likely new to Afrikaans.

Met die toename in die wêreld se gemiddelde oseaantemperature word daar voorspel dat mariene hittegolwe (MHGe) meer gereeld en met sterker intensiteit sal voorkom. Buiten die verhoging van oseaantemperature speel addisionele veranderlikes ook 'n rol in die ontwikkeling van MHGe. Om hierdie meganismes beter te verstaan, is atmosferiese (ERA-interim) en oseaniese (OISST, AVISO) data gebruik om patrone rondom Suider-Afrika gedurende kuslangse MHGe (< as 400 m van die laagwatermerk af) in situ te meet. Niemetrieke multidimensionele verskaling (NMDV) is eers gebruik om te bepaal of die atmosferiese en oseaniese toestande gedurende MHGe verskil van daaglikse klimatologiese toestande. Self-organiserende kaarte (SOKe) is verder gebruik om die MHGe toestande in een van nege bondels te groepeer om te bepaal watter oorheersende atmosferiese en oseaniese patrone tydens die gebeurtenisse teenwoordig was. Die bevindings toon dat die oorheersende oseaniese patrone teenwoordig gedurende MHGe die forsering van warm water na die kus is, veroorsaak deur onreëlmatige oseaansirkulasie. Warm atmosferiese temperature oor die subkontinent gedurende kus- of kuslangse winde was die mees prominente atmosferiese patrone. Ongeveer 'n derde van die MHGe is gegroepeer in 'n bondel met geen prominente patrone nie wat aandui dat hulle nie deur 'n herhalende atmosferiese of oseaniese toestand geforseer is nie, maar eerder deur die onvoorspelbare chaos van die klimaatsisteem veroorsaak is. Omdat warm atmosferiese en/of oseaniese temperatuuranomalieë nie die enigste patrone is wat met MHGe geassosieer word nie, beteken die huidige tendens van 'n aarde wat verwarm nie noodwendig dat MHGe se voorkoms sal toeneem nie. Die a-seisoenale variasie van wind- en waterpatrone speel egter 'n sentrale rol in die formasie van kuslangse MHGe wat daarop dui dat, wanneer klimaatsisteme van historiese tendense afskuif, die waarskynlikheid van MHGe toeneem.

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Correspondence

Climate Change in Coastal Waters: Time Series Properties Affecting Trend Estimation

Robert W. Schlegel, Eric C. J. Oliver, Sarah Perkins-Kirkpatrick, Andries Kruger and Albertus J. Smit

Frontiers in Marine Science, doi: 10.3389/fmars.2017.00323

RC: Reviewer Comment, AR: Author Response, \square Manuscript text

Reviewer #1

Abstract

RC: 1) line 4: Please split the sentence - "... and with increased severity. However, ..."

AR: line 4: Corrected

RC: 2) line 17: referring to the "unpredictable chaos of the climate system" is quite a strong statement. Please consider rephrasing into something like "they were not forced by a recurring atmospheric or oceanic state that could be described by the SOM analysis".

AR: line 17: Corrected as suggested here

RC: 3) line 20: if variability is the subject, please replace "were" with "was".

AR: line 20: Corrected

Introduction

RC: The Introduction provides a good summary of the scientific framework in which the article is positioned and a clear view on the rationale of the study. My only suggestion is to anticipate here a quantitative or semi-quantitative definition of MHW.

UNIVERSITY of the

AR: lines 38-44: The definition from the methodology section has been moved to the second paragraph of the intro: "It is now possible to directly compare MHWs occurring anywhere on the globe during any time of year using a statistical methodology developed by Hobday et al. (2016) that defined these events as "a prolonged discrete anomalously warm water event that can be described by its duration, intensity, rate of evolution, and spatial extent". Whereas the metrics created for the measurement of MHWs allowed for the comparison of events, they did not directly reveal what may be causing them. Beyond common measurements, it is necessary to determine the predominant patterns that occur during MHWs in order to identify their physical drivers."

Materials and Methods

RC: 1) Line 78: I guess the authors refer to sea surface temperatures? Please specify.

AR: line 80: Sea surface temperatures specified

RC: 2) Lines 237-238: "each all data point are ordinated" does not sound totally correct. Please rephrase.

AR: lines 245-246: Corrected to: "It is important to note with NMDS that the two dimensions (i.e. x and y axes) along which all data points are ordinated do not represent any specific variables or quantities within the dataset."

Results

- RC: The results are generally well explained and commented. I only have a few suggestions that may improve the overall clarity of the work, mostly for readers lacking a specific expertise in the statistical tools implemented.
- RC: 1) The interpretation of the bi-plot in Figure 3 may not be straightforward if one is not familiar with this representation. A few more comments could be most helpful.
- AR: Figure 3: The concept of the biplot is now covered in the figure caption: "The x and y axes are not representative of any specific values of the states, rather the distance between each point shows the best fitting relationship of all states with one another based on the output of a nonmetric multidimensional scaling (NMDS) model."
- RC: 2) Line 373: Since this seems to relate to some peculiar feature of that year, a further comment on that might be appropriate
- AR: lines 380-381: The years themselves were not of direct interest in this study, rather the individual events were the primary focus. I have however changed the sentence that introduces this peculiarity to also acknowledge the year in question. "Of the 13 MHWs clustered into Node 4, 11 of them occurred during the same aseasonally warm year (2007), over a span of several months."

Discussion

- RC: The discussion properly examines the results in the light of the scientific topic posed in the Introduction, ending in conclusions solidly supported by the data. Nevertheless, in my opinion the relevance of this study can be discussed also in the perspective of a deeper insight of the process underlying the occurrence of MHWs. Indeed, the classification resulting from this analysis paves the way for a detailed investigation of the metoceanic dynamics associated with MHWs particularly in terms of air-sea interactions, possibly benefiting from the opportunities provided by recent coupled modelling systems (e.g. COAWST, with a number of applications among others in the Atlantic Ocean and in the Mediterranean Sea).
- AR: lines 573-576: The potential for this future research has been stated in the conclusion. "We havehowever shown that the likelihood of a large coastal MHW is greater during specific atmospheric and oceanic patterns. Given this consideration, it should be possible to apply this methodology to large-scale reanalysis products in an effort to forecast the occurrence of coastal MHWs at a fine-scale."

Minor comments

RC: 1) Line 432: "all of thE MHWs"

AR: line 441: Corrected

RC: 2) Line 452: "a smoother and smoother state" sounds somewhat colloquial. Please consider rephrasing into "a progressively smoother"

AR: line 461: Corrected as suggested here

RC: 3) Lines 478-479: I guess this interruption is an oversight, please check

AR: line 486: The sentence fragment in question has been removed

RC: 4) Line 504: This is a most interesting message, but if a non-negligible fraction of the events is not accounted for by the nodes considered in the analysis, then the strength of this sentence should be slightly softened. I would suggest something like "Three preferential mechanisms can be identified by which the pairing of atmospheric anomalies may cause MHWs:"

AR: lines 511-512: The suggested sentence has been used

RC: 5) Line 527: "lead" should be replaced by "led"

AR: line 535: Corrected

Reviewer #2

General

RC: This paper studies the patterns of coastal marine heatwaves along South Africa's coast-line by analyzing the atmospheric (temperature and wind vectors) and oceanic data (sea surface temperature and ocean surface currents inferred from sea level anomaly). The authors utilized nonmetric multidimensional scaling to project data to two dimensions, then applied the self- organising maps method to cluster the data into nine modes. In order to visualize the meso-scale features during marine heatwaves events, they showed the nine predominant atmospheric and oceanic patterns. Their work demonstrated that the predominant oceanic pattern for MHW was the warm water coastward intrusion associated with Agulhas Current leakage; while the major atmospheric state was warm air coinciding with onshore wind. They also discovered a third smaller scale pattern which was a submeso-scale eddy. This paper relates directly to the topic of the journal, and presents a very interesting topic by the use of novel techniques. I would recommend it for publication. Minor comments are in the following.

RC: 1. In Line 4 and 461, there should be ". However,"

AR: line 4: Corrected

AR: line 470: Corrected

RC: 2. In line 10, MHW "are" different...

AR: line 10: Corrected

RC: 3. In line 12, "presented"

AR: line 12: I have left this as "present", rather than changing it to "presented", because my intention with this sentence was to communicate that the synoptic patterns in air and sea are existing during the event, and not that the events (MHWs) themselves are responsible for the synoptic patterns. I think that changing the word in question would make this less clear.

RC: 4. Line 20, "aspace" or "aspatial"?

AR: line 19: I think this is an appropriate word to convey the meaning of this sentence; the comparison of the development of two things that are not necessarily related.

- AR: Apace: adv. In such a way or at such a speed as to keep up the requisite momentum; abreast.
- RC: 5. In line 180, please give a brief explanation on how the R package works.
- AR: line 181: Clarification given: "This package implements the methodology detailed above, as first proposed by Hobday et. al (2016)."
- RC: 6. In line 191, how would you correct the inequality?
- AR: lines 189-197: This paragraph was re-written to address this issue more directly: "It must also be clarified that due to the irregular sampling effort in the SACTN dataset along the coastline of southern Africa, the spatial and temporal distributions of the 86 MHWs are not necessarily even. With some areas, specifically the south coast, having a much greater likelihood of MHWs that meet the selection criteria. Addressing this imbalance would require that the use of data from the south coast (seventeen time series) be constrained to resemble that of the east coast (4 time series) and west coast (5 time series). This would reduce the number of time series used here roughly in half. Because the aim of this research was to determine the predominant atmospheric or oceanic states (see section 'Atmosphere-ocean states' below) during the longest events in the dataset, regardless of where or when they occurred, it was decided not to correct for this inequality in the data."

RC: 7. In section 2.5, could you explain why not using the commonly-used Principle Component Analysis?

- AR: lines 229-232: This has been explained. "NMDS was chosen for this task over other ordination techniques, such as principal component analysis (PCA), as it may visualise all of the variance between the different states along only two axes, whereas PCA would only display part of that variance (Paliy and Shankar, 2016)."
- RC: 8. Line 348, "note" should be "not". Line 526, "where" should be "were". I would suggest a thorough proofreading because of typos like these.

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- AR: line 356: Corrected
- AR: line 534: Corrected
- AR: A thorough proofreading was performed and typos were corrected on lines:
- AR: line 247: Changed "algorithms" to "algorithms"
- AR: line 308: Added "figure" where it was missing
- AR: line 343: Added "figure" where it was missing
- AR: line 536: Removed "an"
- AR: line 542: Changed "anticyclonic" to "cyclonic"
- AR: line 543: Changed "anticyclone" to "cyclone"
- AR: Table 1: Changed "Consecutive period" to "consecutive period"



SYNTHESIS AND CONCLUSIONS

Brief recall

he intention behind the three research chapters in this thesis, which formed the basis of the three publications Schlegel and Smit (2016); Schlegel et al. (2017a,b), is briefly outlined under the next three subheadings.

Trend analysis

In the first study for this thesis, I used the South African Coastal Temperature Network (SACTN) dataset to test the ability of a generalised least squares (GLS) model to detect decadal trends that were known a priori — because they had been inserted experimentally — through a series of controlled experiments on the manipulation of several key variables within time series data a total of 1,344 times (84 base time series \times 4 decadal trends \times 4 levels of precision). This study served the dual purpose of demonstrating the use of the SACTN, first established in Smit et al. (2013), and for demonstrating the utility of this data set for long-term climate trend detection.

Event co-occurrence

After demonstrating the use of the SACTN dataset, and establishing confidence in its usability for climate science, my first attempt at identifying the forces responsible for coastal marine heatwaves (MHWs) was performed by looking at the co-occurrence between coastal and offshore events within similar time frames. This study also introduced the statistical definition for the concept of marine cold-spells (MCSs) into the literature.

Event states

Upon determining that the relationship between nearshore and offshore MHWs was weak, I decided to look at the potential effects of atmospheric forcing as well as oceanographic forcing. Synoptic atmospheric and oceanographic states during coastal MHWs were clustered using a SOM to determine the predominant patterns during these extreme events. The

methodology for this chapter was based largely on work begun by Oliver et al. (2017b). This study did not look into the forcing of MCSs as it was decided that focus should be given over to MHWs alone.

Contributions

My investigation into the properties of coastal seawater time series from the SACTN dataset yielded many useful results with regards to our understanding of how these data may be used for climate change science. I discovered that the ability of a model to detect a longterm trend in a time series increased rapidly from 10 to 20 years, slowing as it approached 30 years, with time series over 40 years in length not contributing much to the model's ability to detect the trend therein. That being said, given the large variance present in the SACTN data — as opposed to much smoother remotely-sensed data — I found that time series of 520 months (43.3 years) on average are required for highly accurate results. I also found that the proportion of missing data within a time series may increase the chances of both Type 1 ('false positive') and Type 2 ('false negative') errors and so I recommended that the use of time series with more than 5% missing data be avoided where possible. My most important finding from this paper, in terms of the focus of this PhD thesis, was that there was no significant effect of data precision on a model's ability to detect a decadal trend. A precision of 0.1°C or finer, as afforded by digital UTRs, is still preferable to that of hand-held thermometers, with a precision of 0.5°C, as it may reduce the necessary length of a time series by as much as 24 months (2 years) in order to be confident in the modeled trend results. The current standard in climate science is not to use data with precisions as coarse as 0.5°C (Ohring et al., 2005; Jarraud, 2008); however, I demonstrated that the most important factor in a time series is its length, so this criterion may be relaxed somewhat. This means that the longer, coarser thermometer time series in the SACTN dataset, which are in the majority, are more useful than the shorter finer UTR time series. Furthermore, I found no increase in ability of a time series for detecting decadal trends with precisions finer than 0.1 °C, meaning that it is only necessary to cultivate these very precise data when one is interested in detecting a trend with a precision finer than 0.01°C (e.g. Karl et al., 2015).

Of particular interest from the outcome of this first study was that a model was able to accurately detect a trend before it was able to say it was significant. This seeming paradox comes from the frequent misuse of the meaning of significance when referring to a linear model. A significant result here means literally that, given the variance in a time series, the underlying linear trend would only be reproduced randomly less than once in every 20 'throws'. Due to the large variance present in much of the time series in the SACTN as much as 640 months (53.3 years) of data are required before significant trends are reported. But we are not interested in significance, we are interested in model ability. It was conclusively shown that a model's ability to perform adequately outpaces the statistical detection of significance. This is not an issue that is discussed in the literature and so provides a very important argument for the usability of *in situ* collected seawater temperature data in the face of the overwhelming support for remotely-sensed data (*e.g.* Yang et al., 2013).

I then used the SACTN data to construct a complete historical record of all of the extreme events (i.e. MHWs and MCSs) along the coast of South Africa for all time series with at least 10 years of data (Schlegel et al., 2017a). The creation of this record was important, but tertiary to this study, with the primary reason for the creation being to establish rates of co-occurrence between the extreme coastal events and those found offshore within records of remotely-sensed data. I found that, on average, each time series had one MHW and MCS per

year. This was odd, but reading back over the paper in which the MHW detection algorithm was published (Hobday et al., 2016), I noticed that this was central to the reason why the algorithm was structured the way it is. By setting a minimum limit of five consecutive days of temperature above the 90th percentile threshold, one may expect to find one extreme event per year, on average, in any sea/ocean. That extreme events may be detected is a statistical property of any time series (Blender et al., 2008), so one must rather determine whether or not the extreme events are a consequence of the 'inertia' carried within the seawater, as seen by the time series' autoregressive properties (Trenberth, 1985), or whether the MHWs can be attributed to some anthropogenic forcing that influences the increasing frequency, intensity or duration of some of the MHW metrics (Trenberth, 2012). In this thesis I do not touch on any issues of attribution as I was fulfilling the basic inquiry of the detection and recording of these extreme events in order to first see what patterns may be deduced.

The secondary goal of the creation of the historical record of extreme events was to be able to determine differences between the three coastal sections of South Africa (e.g. Smit et al., 2013) based on the properties of the extreme events recorded there. I found that the duration and mean intensity of extreme events were ideally suited for this purpose, whereas the annual count of extreme events was not. The duration and intensity of extreme events were different enough for the coastal sections as to imply differing amounts of vulnerability to climate change. The impact of extreme events appeared largest on the west and south coasts, with significantly smaller extreme events on the east coast. The south coast (specifically False Bay) has had by far the largest extreme events on record. This means that the east coast is likely to be under less stress from climate change, with the south coast at greatest risk. This finding was an unexpected yet happy addition to the determination of the (dis)similarity between the extreme events detected in the SACTN and remotely-sensed data. Knowing that the different sections of coastline are more or less exposed to extreme events allows for the incorporation of this information into any future work on developing vulnerability assessments for coastal ecosystems in South Africa. This is an important and timeous field of research to embark on due to the importance of, and risk to, coastal ecosystems in this epoch of anthropogenic climate change (e.g. Addo, 2013; Arkema et al., 2013; Ellison, 2015).

The relatively low co-occurrence (20–50%) of extreme events between the *in situ* sampled SACTN and remotely-sensed data was surprising. Furthermore, the annual count and mean intensity of extreme events along all coastal sections were significantly different than those detected offshore. It was known that remotely-sensed data show a warm bias along the coast (Smit et al., 2013); however, the result of the second study showed that either these data differed dramatically in kind, or some other force was responsible for these extreme coastal events more frequently than offshore sea surface temperature. I hypothesised after this finding that atmospheric forcing must be playing a larger role in the formation of extreme coastal events than had originally been assumed.

In the process of determining the most likely forces causing coastal MHWs, I first discovered that the synoptic atmospheric and oceanic states around southern Africa during days without MHWs were very different from days during which an event was occurring (Schlegel et al., 2017a). I did so through an ordination technique (nonmetric multidimensional scaling; NMDS) so no statistic quantifying the difference was generated, but the pattern is striking. This finding was reassuring as it supported the central assumption to the third study that one could indeed find patterns during coastal MHWs because they were caused by exceptional circumstances in the ocean and/or atmosphere. I also found it interesting that of the largest (top 10%) MHWs analysed for the third study, summer was the season during which

the fewest extreme events occurred.

After showing that MHW sea/atmosphere states did differ from normal states, I used a self-organising map (SOM) to show what the most common patterns were. Roughly half of the MHWs were shown to have been forced by oceanographic properties and another third by atmospheric properties. The remainder displayed individual patterns that the SOM was not able to reconcile into any specific group, making these 'rogue' extreme events whose driving forces were not recurrent enough to be classified anywhere else.

Of the patterns that were identified, it was found that whenever the ocean was forcing a coastal MHW it was likely due to the Agulhas Current being warmer than usual while at least one of two phenomenon were occurring. The first of these is known as 'Agulhas leakage', when the current pushes though into the Atlantic Ocean rather than retroflecting south as normal. The second is known as Agulhas Current warm water intrusion and may be seen when the current moves up against the coastline (Roberts, 2010). More specifically, it appears that the retention of warm water in eddies from Agulhas Leakage move up the west coast, or Agulhas Current warm water intrusions push up against the south coast, is what is causing water temperatures recorded there to appear much warmer than expected, even though the Agulhas itself may not be. The frequency of the occurrence of these eddies has been found to be increasing (Backeberg et al., 2012), as well as Agulhas Leakage more broadly (Biastoch et al., 2009; Beal et al., 2011). Atmospheric forcing came about whenever air temperature over the interior of South Africa was roughly 3°C warmer than expected for a given day of the year while the predominant wind anomaly was moving onshore. That so few extreme events occurred during summer, and that central to the forcing of these extreme events was anomalous air and sea movement means that solar heating is not necessarily the central requirement for an event. Rather, it appears that it is when anomalous heat is combined with anomalous movement that extreme events occur most frequently along the coast. This was an important finding in the third study because it implies that even though the world is slowly heating up, that does not guarantee that we will start to see more extreme events. Instead, it shows that increases in extreme events may be more closely related to the departure from historic atmospheric and oceanographic circulation patterns.

A final anecdote on the contributions of the third study. A cyclonic eddy centred at 13.5°E and 36.5°S was found during two-thirds of all of the extreme events, making it the most predominant pattern of all. This is a rather curious finding whose implications I have not yet considered in depth as it was beyond the scope of the final study, but is certainly something that must be looked into further.

Lastly I would like to draw attention to the further aggregation of the SACTN performed throughout this thesis, and its incorporation into an online repository ¹ and online user interface ², allowing for ease of use for all interested parties. The user interface gives potential users all of the instruction necessary to not only understand how and why the SACTN dataset was established and maintained the way that it is, it also explains how one may extract and visualise any of the desired data. It is my intention that this will become a useful tool for improving the quality of coastal marine science in South Africa.

¹https://github.com/ajsmit/SACTN

²https://robert-schlegel.shinyapps.io/SACTN/

Limitations

All of the studies in this thesis were hampered by the number of multi-decadal time series available in the SACTN dataset. There are also large gaps in sampling along the west coast that prevent the documentation of extreme events there, even though this appears to be an area that is prone to such occurrences. Unfortunately there is little that may be done about this other than to ensure that sampling along these stretches of the coast continue into the future.

The first study in this thesis would have benefited from more complete SACTN meta-data records. Had these records been available, additional layers of inquiry could have been added to the analysis in an attempt to quantify the benefits of the meta-data. Regulations for the correct collection and maintenance of these records exist (Jarraud, 2008), but I think it would have been very interesting to have actually quantified their benefit. In the same way that the first study showed the lack of necessity for the collection of very fine precision measurements, perhaps the extent of the benefit of very meticulous meta-data recordings could have been demonstrated.

In retrospect, I would not have included MCSs in the second study in this thesis. It was assumed that their inclusion into a study on MHWs could be accomplished without detracting from the primary aim of comparing records of extreme events from *in situ* and remotely-sensed temperature data. Whereas the actual calculation and interpretation of the MCS results was accommodated by the workflow used to record MHWs without any undue difficulty, I think that the combined output being shoehorned into one publication detracted from the findings of the paper. I think that the study of MCSs is interesting, and that their relationship with upwelling still needs to be thoroughly investigated, but I do not think they should be included directly alongside MHWs as the outcome of the second study has highlighted that these two phenomena are not opposite sides of the same coin, as originally hypothesised. From an aesthetic point of view, I think that too much information was visualised in this study.

The final study in this thesis was by far the most ambitious of the three. It is also the first solid step on the path to unravelling the forces behind coastal MHWs. The real limitation with this study was that the methodology created only looked backwards in time. To produce a more thorough result, the patterns observed to potentially force coastal MHWs need to be tested against new data. That patterns were pulled out of the data is promising, but does not necessarily mean that the same patterns would hold in the future. A more complex methodology could have tested random time series for patterns and used other time series to validate the results; however, the methodology already implemented in the third study was massively complex and integrating these additional steps was beyond my coding capabilities at the time.

Though not a limitation in the sense intended within the framework of this dissertation, I think it is also necessary to comment on how the publication process itself impacted my thesis. Having had the opportunity to speak with academics, from post-grads to professors, about the merits of writing a PhD thesis by publication, I would like to weigh in on the matter by saying that I think I gained important insight into the publication process that I would not have acquired from the writing of a more traditional doctoral thesis. I understand the argument that a thesis by publication does not provide the prospective PhD candidate with the opportunity to organise their thoughts to the same extent that a classic thesis does. I would argue, however, that the publication process requires the PhD candidate to come to terms

with their thought process much earlier on in the writing the thesis, and that this benefits the candidate more than the organisation of the body of work at the end of however many years are spent on the dissertation. In addition to the developmental way markers in thought and practice that are ensured by the publication of the research chapters, is the benefit of publishing itself. Besides the early-career benefits that this entails, it also gives the candidate invaluable experience with the specifics of the publishing process itself. Through my own experiences in publishing my three research chapters I have been able to decide for myself what I think of the publishing process and how I would like to approach it if I am to continue in academia.

Further research

Of the many metrics that the MHW algorithm produces to quantify each event, it is my opinion that cumulative intensity is the most relevant ecologically as it can be used to quantify the risk that a MHW may pose on an ecosystem. In order to relate cumulative intensity of an event to actual damage will of course require that said damage be recorded whenever possible. This will then allow for the creation of an index of these extreme events, their cumulative intensity, and the impact that each event had. This is a massive, career-long project, but if embarked upon would be of paramount importance to the food and economic security of South Africa. As climate changes, these extreme events are becoming more frequent and more intense. Having a 'play book' to refer to when an event of a certain size occurs will prove necessary if coastal ecosystems are to truly be conserved. This body of work has already begun in other countries, most notably Australia (e.g. Wernberg et al., 2016). The work done in South Africa will therefore contribute to, and benefit from, this developing global body of knowledge.

More work must also be done on the improvement of the methodology for the detection of predominant atmospheric and oceanographic states during coastal MHWs. Specifically, it is of interest to me to develop the code I have written to allow it to be applied anywhere in the world by any user. This ensures not only reproducibility, but also usability. In addition to this it is necessary to incorporate the other atmospheric and oceanographic forces that may be driving these extreme events, which are surface pressure (Bond et al., 2015) and eddy kinetic energy (EKE) (Oliver et al., 2017a). This was not performed in the third study in this thesis due to the burgeoning complexity that it initially presented. This methodology must also be verified by applying the resultant patterns found to occur during MHWs to datasets from which the patterns where not generated.

Once the likely forcing of all of these different variables has been quantified and the code that summarises the predominant patterns is able to seamlessly induct them into its calculations, this knowledge must then be paired with reanalysis/forecast products to see how effective the identified states are as a predictive factor for coastal MHWs. This is a critically important goal as the main body of the work for this PhD thesis has not been predictive, but rather an investigation into the understanding of coastal MHWs and the extreme forces responsible for them. If the predictive capabilities of the methodology developed in this dissertation can be supported, it will allow for further investigations into the attribution of anthropogenic climate change to the formation of extreme coastal events and the threats they may represent to South Africa.

It must be noted that this bibliography contains all of the references for Chapters 1 and 5 only. This may mean that some sources cited in Chapters 2 through 4 are not found here. This has been done intentionally to maintain the distinction between the published work in this thesis and that of the introduction (Chapter 1) and the conclusion (Chapter 5) framing this published work.

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