Analyzing lakes in the time frequency domain

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Summary

The central aim of this thesis is to demonstrate the benefits of innovative frequency-based methods to better explain the variability observed in lake ecosystems. Freshwater ecosystems may be the most threatened part of the hydrosphere. Lake ecosystems are particularly sensitive to changes in climate and land use because they integrate disturbances across their entire catchment. This makes understanding the dynamics of lake ecosystems an intriguing and important research priority. This thesis adds new findings to the baseline knowledge regarding variability in lake ecosystems. It provides a literature-based, data-driven and methodological framework for the investigation of variability and patterns in environmental parameters in the time frequency domain.

Observational data often show considerable variability in the environmental parameters of lake ecosystems. This variability is mostly driven by a plethora of periodic and stochastic processes inside and outside the ecosystems. These run in parallel and may operate at vastly different time scales, ranging from seconds to decades. In measured data, all of these signals are superimposed, and dominant processes may obscure the signals of other processes, particularly when analyzing mean values over long time scales. Dominant signals are often caused by phenomena at long time scales like seasonal cycles, and most of these are well understood in the limnological literature. The variability injected by biological, chemical and physical processes operating at smaller time scales is less well understood. However, variability affects the state and health of lake ecosystems at all time scales. Besides measuring time series at sufficiently high temporal resolution, the investigation of the full spectrum of variability requires innovative methods of analysis.

Analyzing observational data in the time frequency domain allows to identify variability at different time scales and facilitates their attribution to specific processes. The merit of this approach is subsequently demonstrated in three case studies. The first study uses a conceptual analysis to demonstrate the importance of time scales for the detection of ecosystem responses to climate change. These responses often occur during critical time windows in the year, may exhibit a time lag and can be driven by the exceedance of thresholds in their drivers. This can only be detected if the temporal resolution of the data is high enough. The second study applies Fast Fourier Transform spectral analysis to two decades of daily water temperature measurements to show how temporal and spatial scales of water temperature variability can serve as an indicator for mixing in a shallow, polymictic lake. The final study uses wavelet coherence as a diagnostic tool for limnology on a multivariate high-frequency data set recorded between the

onset of ice cover and a cyanobacteria summer bloom in the year 2009 in a polymictic lake. Synchronicities among limnological and meteorological time series in narrow frequency bands were used to identify and disentangle prevailing limnological processes.

Beyond the novel empirical findings reported in the three case studies, this thesis aims to more generally be of interest to researchers dealing with now increasingly available time series data at high temporal resolution. A set of innovative methods to attribute patterns to processes, their drivers and constraints is provided to help make more efficient use of this kind of data.

Zusammenfassung

See-Ökosysteme sind eine der bedrohtesten Ressourcen der Hydrosphäre. Sie reagieren besonders sensibel auf Veränderungen des Klimas und auf Einflüsse durch Landnutzung, da verschiedene Prozesse im gesamten Einzugsgebiet auf sie einwirken. Daher ist es von besonderer Dringlichkeit, die verschiedenen Prozess-Dynamiken in See-Ökosystemen besser zu verstehen. Die hier vorliegende Doktorarbeit hat zum Ziel, das bestehende Wissen bezüglich der verschiedenen einwirkenden Prozesse in See-Ökosystemen zu erweitern. Die Arbeit stellt ein Forschungsdesign zur Diskussion, das eine Literatur-basierte und auf empirischen Erhebungen beruhende Analyse von Variabilität und Mustern in großen Datensätzen verschiedener Umweltparameter im Zeit-Frequenz-Raum ermöglicht.

Umweltparameter sind häufig charakterisiert durch eine hohe zeitliche Dynamik. Diese Variabilität steht im Zentrum dieser Arbeit. Sie wird durch eine Fülle an periodischen und stochastischen Prozessen innerhalb und außerhalb des Ökosystems getrieben. Diese Prozesse können gleichzeitig und auf sehr unterschiedlichen Zeitskalen, von Sekunden bis hin zu Dekaden, ablaufen. In Messdaten überlagern sich alle diese Signale, und dominante Prozesse können die Signale anderer Prozesse verschleiern, insbesondere wenn Mittelwerte über längere Zeiträume analysiert werden. Dominante Signale werden oft durch Prozesse auf längeren Zeitskalen verursacht, wie z. B. saisonale Zyklen. Diese sind im Allgemeinen in der limnologischen Literatur gut dokumentiert. See-Ökosysteme werden allerdings von Prozessen auf allen Zeitskalen beeinflusst. Insbesondere biologische, chemische und physikalische Prozesse operieren in kürzeren Zeitrahmen. Die Variabilität, die über solche Prozesse in See-Ökosysteme eingebracht wird, ist bisher weit weniger gut erforscht. Neben der Notwendigkeit, Umweltparameter in hoher zeitlicher Auflösung zu messen, erfordert die Untersuchung der kompletten Bandbreite an Variabilität innovative Analysemethoden.

Die Berücksichtigung der Zeit-Frequenz-Domäne kann dabei helfen, Dynamiken auf verschiedenen Zeitskalen zu identifizieren und daraus bestimmte Prozesse abzuleiten. Diese Arbeit zeigt die Vorzüge dieser Herangehensweise anhand von drei Fallstudien auf. Die erste Studie zeigt die Bedeutung von Zeitskalen für die Erfassung von Ökosystem-Reaktionen auf klimatische Veränderungen. Diese ereignen sich oft während kritischer Zeitfenster im Jahresverlauf und können durch die Überschreitung von Schwellenwerten in den treibenden Variablen, unter Umständen zeitlich verzögert, verursacht sein. Solche Zusammenhänge können nur erfasst werden, wenn die zeitliche Auflösung der Daten hoch genug ist. In der zweiten Studie wird die Spektralanalyse, basierend auf der Fast Fourier Transformation, auf einen Datensatz

täglicher Messungen der Wassertemperatur über zwanzig Jahre hinweg angewendet. Es wird gezeigt, wie zeitliche und räumliche Skalen der Variabilität der Wassertemperatur als Indikator für Mischprozesse in einem polymiktischen See dienen können. In der dritten Studie wird die Wavelet Coherence als Diagnose-Werkzeug für einen multivariaten, hochfrequenten Datensatz genutzt. Dieser wurde zwischen dem Einsetzen einer Eisbedeckung und einer Sommerblüte von Cyanobakteriern in einem polymiktischen See im Jahr 2009 erhoben. Synchronizitäten zwischen limnologischen und meteorologischen Zeitreihen in schmalen Frequenz-Bändern wurden genutzt, um vorherrschende limnologische Prozesse zu identifizieren und analytisch zu trennen.

Neben den neuen empirischen Erkenntnissen, die in den drei Fallstudien präsentiert werden, zielt diese Doktorarbeit darauf ab, Forscher*innen, Behörden und politischen Entscheidungsträger*innen eine Grundlage zu liefern, die hohe zeitliche Auflösung der heute vielfach verfügbaren Monitoring-Datensätze effizienter zu nutzen. Innovative Methoden sollen dabei helfen, Muster in den Daten Prozessen zuzuordnen und die entsprechenden Treiber und Limitationen zu identifizieren.

Contents

1 Introduction

1.1 Variability, lakes and time scales

Variability is a fundamental property of our world. But what exactly is variability, and how can we quantify and characterize it? Although "variability" is among the most common words in the ecological literature, the term is often used rather vaguely (Kareiva and Bergelson 1997). Seasonal cycles of sunlight and temperature, for example, in temperate and polar regions are among the most striking variations that can be observed. They influence manifold processes in all aspects of human, animal, plant or microbial life. Changes on longer time scales, such as climate or land use changes, have received much attention, as their effects (e.g. heat waves, floods, droughts, shifts in phenology or changes in species composition) increasingly manifest (IPCC 2013) and are often accompanied by tremendous loss of life and/or economic assets (Easterling et al. 2000). On the other hand, shorter time scales are much more directly experienced by living beings, as the variability from week to week, from day to day, from hour to hour or on even shorter time scales forms an important part of their daily lives. However, changes on short time scales have received much less scientific attention, as they are often less obvious and harder to understand in observational data (Benedetti-Cecchi 2003; Guadayol et al. 2014). Variability can have periodic (i.e. composed of regular cycles on specific time scales) and stochastic (i.e. originating from random, unpredictable variations) components at all of these time scales, ranging from seconds to days to years to decades. Besides this temporal characterization, variability can also be described in terms of the "frequency", which gives information on the number of occurrences of a considered quantity in a given time interval. The variability components at all of these frequencies act simultaneously and, superimposed, constitute the variability observed in the world (Sabo and Post 2008; Franke et al. 2013). Aquatic ecosystems form no exception.

The availability of freshwater is one of the most vital factors for the livability on planet Earth. At the same time, freshwater ecosystems may be the most threatened part of the hydrosphere (Abell et al. 2007; Kernan et al. 2010) and face a disproportionately high risk of species extinction and decline in abundances compared to marine and terrestrial ecosystems (Young et al. 2016). Lakes are particularly vulnerable to changes in climate parameters, because variations in climate and land use in their entire catchment directly affect the entire lake ecosystem, and because freshwater fauna is spatially highly constrained (IPCC 2013; Young et al. 2016). For example, variations in air temperature, solar radiation, wind speed or precipitation affect water temperature, evaporation, water chemistry, rates of biological processes, intensity and duration of ice cover, thermal regime and mixing processes in lakes. Lakes react sensitively to variations in their entire catchment and are therefore particularly suitable as sensors for climatic changes (Adrian et al. 2009; Schindler 2009; Williamson et al. 2014). Lakes integrate over external drivers, i.e. related to climate, weather and land use, and internal physical, chemical or biological processes. Externally and internally driven processes in lake ecosystems occur from short to long time scales, or at high to low frequencies. Therefore, lakes provide very intriguing and fundamentally important examples for the investigation of patterns of variability and their ascription to processes.

One example of (low-frequency) variability is the fact that our world is warming (IPCC 2013), and with it the majority of lakes worldwide (O'Reilly et al. 2015; Sharma et al. 2015; Fig. 1.1). Water temperature is the major driver of almost all processes in lakes (Winder and

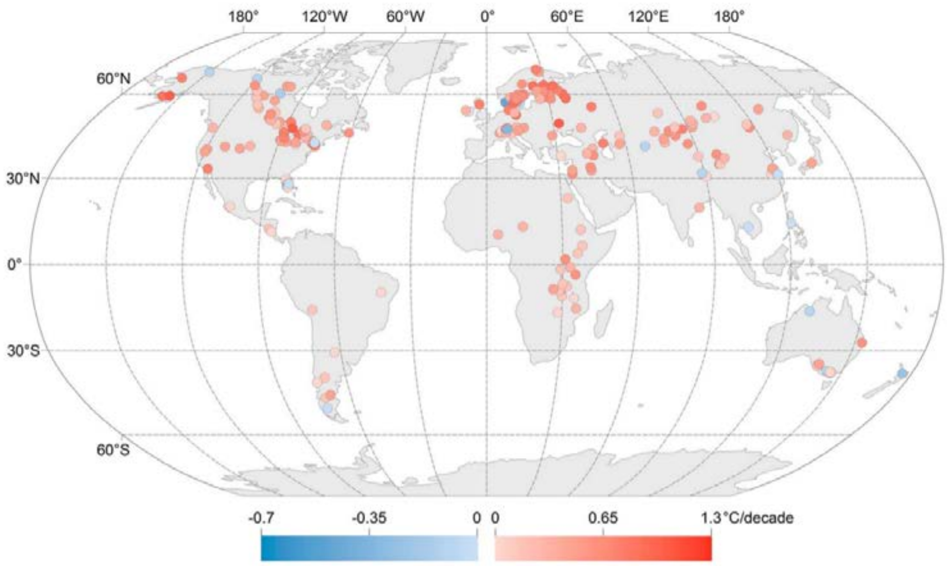

Fig. 1.1: Map of trends in lake summer surface water temperature from 1985 to 2009 (O'Reilly et al. 2015).

Schindler 2004; Hanson et al. 2006; Lampert and Sommer 2007), which makes it particularly important to capture and understand patterns and time scales of water temperature variability. How much lakes are warming is subject to substantial regional variation and is not per se explained by geographic location or morphologic features such as lake depth, water volume or lake surface area (O'Reilly et al. 2015). Furthermore, trends in lake water temperature may differ seasonally (Livingstone 2003) and between water depths (Kraemer et al. 2015). These examples illustrate that climate change is often addressed in terms of changes of the mean. However, there is evidence that, together with an overall increase in temperature, the variance may increase as well. This implies not only a shift, but also a broadening of the statistical distribution of temperature (Fig. 1.2). Recent increases in the variability of air temperature have been reported especially in Europe (Schär et al. 2004; Vidale et al. 2007; Huntingford et al. 2013; IPCC 2013) and have as well been suspected for lake water temperature (Nickus et al. 2010;

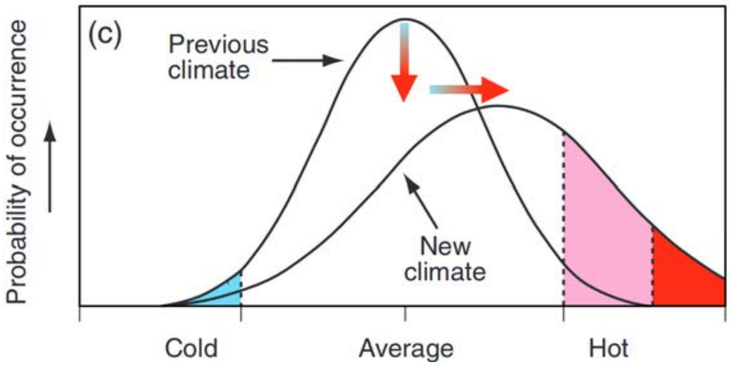

Fig. 1.2: Illustration of the effect of an increase in mean and variance on the probability density function of temperature; adapted from IPCC (2001, 2013).

Guadayol et al. 2014). This increased temperature variability is not captured in temperature means or changes of the mean.

Nevertheless, environmental variables are often communicated as mean values over longer periods of time (Benedetti-Cecchi 2003; Coble et al. 2016). Yet, looking at a mean value is similar to reading only the cover of a book – the reader may get a certain notion of the content, but the story that led to the title (or the mean value) will be obscured. When considering monthly mean values or discrete monthly measurements, for example, a seasonal variation may be revealed, which could be the most dominant time scale of variability. However, this would correspond to reading every tenth page of a book, enabling a broad understanding of the story. To really grasp the entire information would, however, require reading every single word of that book. Detecting the entire spectrum of variability in an ecosystem requires to consider long time scales at high temporal resolution. Mean values mask environmental variability, which is, however, fundamentally important for the structuring and functionality of (aquatic) ecosystems (Reynolds 1990; Benedetti-Cecchi 2003; Fraterrigo and Rusak 2008; Benincà et al. 2011; Guadayol et al. 2014). Yet, Platt and Denman (1975) as well as Coble et al. (2016), 40 years apart, observe that although researchers are aware that the climate is variable, they often fail to adequately address this variability in analytic, experimental or laboratory studies. Coble et al. (2016) go as far as to attest large parts of the literature a "concerning lack of baseline knowledge" of even understanding the role, characteristics and implications of variability in many ecosystems.

Addressing temporal variability is important for several reasons. For example, temperature time series with the same mean value can otherwise exhibit substantial differences, as a mean value can derive from a multitude of patterns. Such detailed characteristics of the temporal evolution of temperature can play a crucial role for ecology in general (e.g. Drake 2005; Wang et al. 2014), and for climatically driven aquatic processes and aquatic organisms in particular (Reynolds 1990; Müller-Navarra et al. 1997; Cloern and Jassby 2010; Shurin et al. 2010; Posch et al. 2012). Local populations can even be driven to extinction by environmental fluctuations, with the risk of extinction being determined by the amount of, and relationship between, short-term and long-term variation (Ripa and Lundberg 1996; Heino et al. 2000; Lögdberg and Wennergren 2012). There is evidence that aquatic organisms might be more affected by increased variability of physical driving forces (mainly water temperature) than by increases in the mean of drivers: Barbosa et al. (2014) showed that under increased temperature variability, *Daphnia magna*, a zooplankton species, was unable to respond appropriately to predation risk and had reduced growth rates and impaired development of morphological defenses. On the other hand, increased long-term growth rates in zooplankton were recorded under increased variation in temperature (Drake 2005). Lastly, Shurin et al. (2010) observed higher zooplankton species richness in lakes with greater water temperature variability at interannual, seasonal and residual time scales. While the effects of increased environmental variability may hence be beneficial or detrimental for organisms, their physiological stress appears to be enhanced overall (Sabo and Post 2008; Barbosa et al. 2014). It is therefore crucial to capture and characterize the temporal variability inherent in climate and weather observations in order to understand ecosystem responses to them.

Variability in aquatic ecosystems happens at time scales that reach from sub-seconds to decades, meaning from high to low frequencies (Fig. 1.3). Biochemical reactions happen at

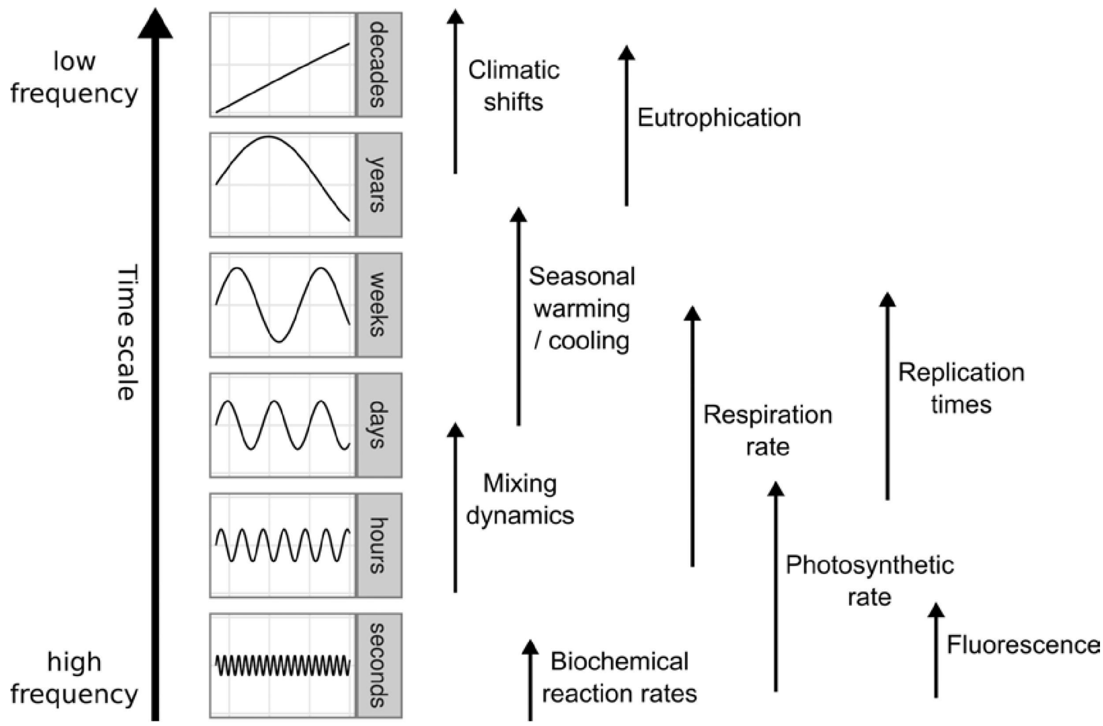

Fig. 1.3: Time scales of environmental variability; modified from Reynolds (1990).

high frequencies on time scales below seconds (Reynolds 1990). Photosynthetic reactions can span seconds to days, while population dynamics of planktonic species occur between hours and weeks (Reynolds 2006; Lampert and Sommer 2007). Depending mainly on the depth and climate zone of a lake, mixing processes occur at scales between minutes and days or weeks (Reynolds 1990; Behrendt et al. 1993; Read et al. 2011). Seasonal warming and cooling patterns determine the annual succession of plankton communities (Sommer et al. 1986, 2012). Longer time scales of eutrophication or climatic shifts span decades (George and Harris 1985; Anderson 1995; Climate Research Committee 1995). Short time scales are particularly relevant for planktonic organisms (Reynolds 1990) and other limnological processes (Marcé et al. 2016). Furthermore, small stochastic or periodic fluctuations in environmental forcing can induce strong resonance in species responses (Benincà et al. 2011). However, the longer-scale environmental variability, such as annual mean values, seasonal cycles or long-term trends, has received more attention than the variability at short time scales (Benedetti-Cecchi 2003; Guadayol et al. 2014). Yet, short-term and long-term temperature variability in environmental drivers might affect the ecosystem in different ways, and the physical and ecological impacts of climatic changes might be overlooked if the time scale of analysis is too coarse (Platt and Denman 1975; Fraterrigo and Rusak 2008; Marcé et al. 2016). To characterize the whole spectrum of variability experienced by organisms is therefore important, and focusing on smaller scale variability is particularly relevant. To that end it is crucial to account for the time scale of ecosystem variability (Harris 1980; Reynolds 1990).

To capture patterns of ecosystem variability, routine measurements of various parameters have been performed for many decades in lake ecosystems across the globe. Physical sensors recording limnological and meteorological variables such as water and air temperature, wind speed and humidity were among the first developed automated sensors, enabling researchers to gain quasi-continuous data (Meinson et al. 2016). The development of electrochemical sensors such as pH and oxygen electrodes then enabled the assessment of chemical dynamics, followed by sensors recording biological parameters such as chlorophyll *a* or phycocyanin (Dubelaar et al. 2004; Marcé et al. 2016; Meinson et al. 2016). However, high-frequency automated sensor systems that measure physical, chemical and biological state variables at high temporal resolution are still a relatively new technology. Research based on this kind of data is still just emerging, and the opportunities and pitfalls they offer are just now becoming evident (Porter et al. 2005; Dur et al. 2007; Porter et al. 2009; Hampton et al. 2013; Marcé et al. 2016; Meinson et al. 2016). Nevertheless, if in operation for a certain amount of time, high-frequency monitoring data allow to investigate the interplay between short-term and long-term variability.

There is the notion that physical, chemical and biological time series originating from these monitoring stations allow the retrieval of information about the system and the processes, constraints and time scales that generated them (Ghil 2002; Lischeid 2009; Gnauck et al. 2010). However, the usability of automated high-frequency measurements, their explanatory power for the assessment of lake ecosystem dynamics and the identification of the underlying processes is not straightforward. It is not necessarily clear how to interpret fluctuations in a specific parameter. Furthermore, one state variable may be controlled by various drivers operating at different time scales (Hanson et al. 2006; Müller et al. 2010). The interaction of meteorological and lake-internal drivers can make it difficult to disentangle processes that happen in parallel.

For example, variations in water temperature can originate from manifold drivers and processes at various time scales. While the seasonal variation may be the most dominant and obvious source of variability, longer-term fluctuations on time scales of multiple years, so-called atmospheric modes of variability such as the North Atlantic Oscillation, the Pacific Decadal Oscillation or the El Niño Southern Oscillation, have been shown to drive water temperature variability decisively (Arhonditsis et al. 2004a; Blenckner et al. 2007). On shorter time scales, short-and long-wave radiation, conduction and evaporation drive dynamics in water temperature, which in turn depend on meteorological drivers such as ambient air temperature, cloud cover and wind speed (Edinger et al. 1968). Additionally, lake-internal processes such as mixing dynamics during time periods of thermal stratification, acting on time scales between minutes and weeks, can have a strong impact on water temperature variability (Reynolds 1990; Behrendt et al. 1993).

Other commonly measured state variables in lakes are pH and dissolved oxygen, which can be driven by processes such as photosynthesis, respiration, chemical reactions such as calcite precipitation and dissolution, gas exchange with the atmosphere, mixing processes or input from the catchment (Hanson et al. 2006). These drivers act simultaneously, but on different time scales, and their importance differs according to the productivity, alkalinity and mixing type of a lake and according to the time of year.

While understanding phytoplankton dynamics is crucially important, as they form the base of most aquatic food webs (Wetzel 2001; Thackeray et al. 2013) and their potential to form toxic blooms can cause mass mortalities (Castle and Rodgers 2009; Lürling and De Senerpont Domis 2013), their assessment remains challenging (Dubelaar et al. 2004). Phytoplankton abundance is commonly approximated by the fluorescence of chlorophyll *a*, the main pigment responsible for the absorption of light for photosynthesis (Lorenzen 1966; Proctor and Roesler 2010; Escoffier et al. 2015). Fluorometers are optical sensors which quantify chlorophyll *a* fluorescence and allow the assessment of phytoplankton dynamics at high temporal resolution. Potential drivers of phytoplankton dynamics are e.g. water temperature, light availability, nutrient availability, water column mixing and herbivory (Arhonditsis et al. 2004b; Reynolds 2006). These can have varying importance over the course of a year and in different lake types (Sommer et al. 1986, 2012) and act at different time scales (Harris 1980; Reynolds 1990).

The examples above illustrate that the ascription of variability in parameters to processes is not straightforward. Furthermore, processes are often difficult to identify and disentangle and require the consideration of the time scale of variability. Making use of multivariate data at high temporal resolution and an appropriate methodological approach seem promising to identify and disentangle processes, their drivers and constraints (Lischeid and Bittersohl 2008; Lischeid 2009; Langman et al. 2010; Recknagel et al. 2013).

Taking into account time scales of variability requires methods that are capable of separating, e.g., hourly from daily, weekly, monthly, seasonal or yearly time scales. Many commonly used methods to quantify variability, such as the standard deviation, are not per se able to accomplish this. In geophysical variables, low frequencies often dominate over high frequencies. As a result, e.g., a standard deviation calculated over a year of a seasonally changing variable measured at daily resolution will most probably be dominated by this seasonality. The standard deviation will therefore describe the deviation of a daily value from the annual mean rather than the daily variability. This could be partly overcome if data were deseasonalized beforehand. However, short-term variations can also be masked by longer-term non-seasonal oscillations. Also, short-term variability such as diurnal variations can affect the variability at longer time scales. Hence, long-term (or low-frequency) variability can mask short-term (or high-frequency) variability, and, conversely, high-frequency variability can blur low-frequency variability. For this reason, an appropriate way to separate time scales of variability from each other is needed. This task can be accomplished by analyzing time series in the time frequency domain (Kestin et al. 1998; Ghil 2002; Schaefli et al. 2007; Cazelles et al. 2008; Gnauck et al. 2010).

1.2 Analyzing in the time frequency domain

The frequency information inherent in every time series can be used to identify characteristic time scales and the corresponding variability components that contribute to the dynamics in the time series. Spectral methods, such as the Fourier transform or the wavelet analysis, make use of this frequency information. The Fourier transform provides a representation of a time series in the frequency domain (Bloomfield 2000), informing about how much of the variability in the data results from processes with certain frequencies. The wavelet analysis transforms a time series from the time domain to the frequency domain (Torrence and Compo 1998), giving the additional information of how the frequency-dependent signal changes with time. The wavelet coherence allows for the analysis of two time series together to detect their joint dynamics in time frequency space (Grinsted et al. 2004). These methods were applied in this thesis and are presented in more detail in the following.

The spectral analysis based on the Fourier transform decomposes a time series into a superposition of sine and cosine waves of varying frequencies, and hereby transforms the times series from the time domain to the frequency domain (Platt and Denman 1975; Bloomfield 2000). The discrete Fourier transform X_k is defined as:

$$X_k = \frac{1}{N} \sum_{t=0}^{N-1} x_t e^{i2\pi k \frac{t}{N}} \tag{1.1}$$

where k is a frequency and x is the value of a time series of length N at time t (Cooley and Tukey 1965; Singleton 1969). The spectral density is given by $|X_k|^2$. It provides a measure of the magnitude of periodic variability at specific frequencies. The Fourier transform is a fully invertible procedure and hence an exact representation of the signal in frequency space. The measurement resolution defines the highest frequency that can be assessed, which is half the measurement resolution (Nyquist frequency). The spectral analysis can furthermore be used as a band-pass filter by averaging over adjacent frequencies (Platt and Denman 1975; Ghil 2002).

An example of a spectrum of water temperature, measured hourly over the time span of year in Müggelsee, a polymictic lake in Northern Germany, is given in Fig. 1.4. The frequency is

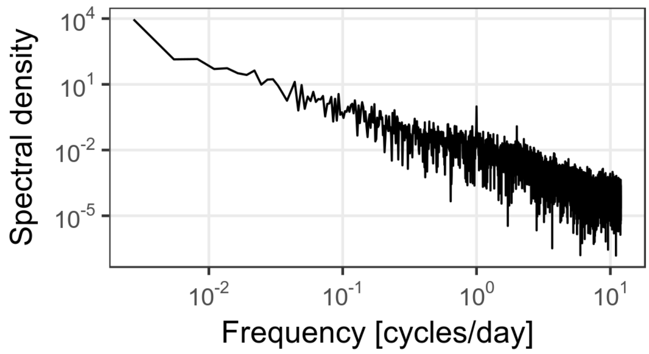

Fig. 1.4: Frequency spectrum of water temperature measured hourly in 1.5 m depth in Müggelsee in 2009. Note logarithmic scales on x- and y-axes.

given on the x-axis, while the y-axis shows the intensity of periodic variability at the respective frequencies. Here, the spectral density decreases from low frequencies (long-term variability) to high frequencies (short-term variability). This means that long-term dynamics, such as seasonal cycles, dominate the variability, while shorter-term dynamics, such as daily variations, contribute less to the total variability. The peak at a frequency of one cycle per day indicates pronounced diurnal cycles. This scaling behavior from low to high frequencies can be quantified as the slope of a spectrum, calculated by simple linear regression of the $\log_{10}$-transformed spectral density on the $\log_{10}$-transformed frequency. It gives a rough characterization of the dependence of water temperature variability on frequency, commonly termed the noise color (Vasseur and Yodzis 2004; Sabo and Post 2008). In this case, the decrease from low to high frequencies corresponds to a red noise spectrum, which is common in geophysical variables (Pelletier 1997; Cuddington and Yodzis 1999; Cyr and Cyr 2003; Vasseur and Yodzis 2004).

The spectral analysis of nonstationary time series can only be done by Fourier analysis with some extra effort of, e.g., applying it successively to time windows (Kestin et al. 1998). The constraints of the Fourier analysis, i.e. the inability to detect changes in the frequency spectrum over time, are overcome by the wavelet analysis (Torrence and Compo 1998; Schaefli et al. 2007; Cazelles et al. 2008). Applying a wavelet analysis to a time series transforms it from the time domain to the time frequency domain. The wavelet transform of a time series x_t is defined as the convolution of x_t with a wavelet function, the so-called mother wavelet $\psi(t)$. A widely used example for a mother wavelet is the Morlet wavelet function, defined as:

$$\psi_0(t) = \pi^{-1/4} e^{i\omega_0 t} e^{-t^2/2} \tag{1.2}$$

where ω_0 is the central angular frequency. The continuous wavelet transform $W(f,\tau)$ at scale f and time τ is given by:

$$W(f,\tau) = \frac{1}{\sqrt{f}} \int_{-\infty}^{+\infty} x(t)\psi^* \left(\frac{t-\tau}{f}\right) dt = \int_{-\infty}^{+\infty} x(t)\psi^*_{f,\tau}(t)\, dt \tag{1.3}$$

where $(^*)$ indicates the complex conjugate form (Cazelles et al. 2008). The mother wavelet is dilated by scale f, connecting a time window to a particular frequency, and shifted by time position τ, which controls the location of the time window in the time domain (Kestin et al. 1998; Torrence and Compo 1998). This yields the amplitude at a particular scale (or frequency) and the variation of this amplitude with time. The wavelet transform can be thought as a cross-correlation of a time series x_t with a set of wavelets exhibiting different widths f at different time positions τ (Cazelles et al. 2008).

An example of the graphical representation of the wavelet transform of water temperature measured hourly in Müggelsee is shown in Fig. 1.5. The time domain is represented on the x-axis, while the frequency domain is represented as period length (the inverse of the frequency)

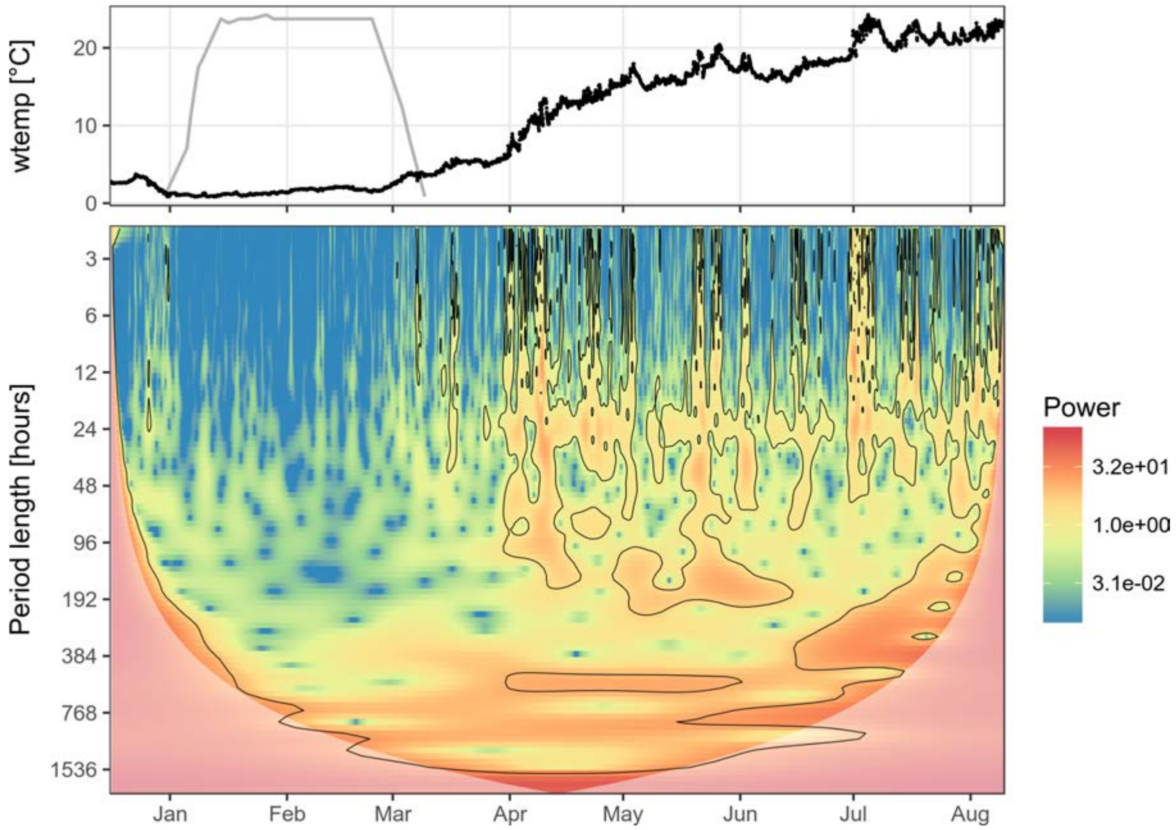

Fig. 1.5: *Upper panel*: time series of water temperature (wtemp) [°C] measured hourly in 1.5 m depth in Müggelsee in 2009; time window with an ice cover (grey line). *Bottom panel*: Continuous wavelet transform of water temperature; black contours around regions where the power is significant against red noise; the lighter shade denotes the cone of influence, where edge effects are present. The x-axis applies to both panels.

on the y-axis. The cone of influence, where edge effects are present, is shown in lighter shade. Colors indicate the strength of the signal at a particular period and during a particular time window. Regions surrounded by black lines indicate significance against red noise. For example, the variability of water temperature between January and March resembles red noise as the power of the signal is very low at high frequencies of hourly time scales (blue color). It increases to higher power at low frequencies of weekly time scales (red color). This time window was characterized by an ice cover on the lake, reducing substantially any meteorological influence on water temperature variability. On the other hand, from April onwards, there is a band of high power around period lengths of 24 hours that differs significantly from red noise, representing the diurnal variability of water temperature. High power from short to long time scales occurs during several time windows. There is furthermore a frequency band from April to June with high low-frequency power around period lengths of several weeks. In this way, time windows and frequencies in a time series can be identified that exhibit certain features in time frequency space.

Often, the statistical relationship between two time series is of interest. The wavelet analysis can be extended to the joint analysis of two time series via the cross wavelet transform and the wavelet coherence (Grinsted et al. 2004; Cazelles et al. 2008). The cross wavelet transform W^{XY} between two time series x_t and y_t is given by the product of the wavelet transformed time series x_t, $W^X_{f,\tau}$, with the complex conjugate of the wavelet transformed time series y_t, $W^Y_{f,\tau}$ as:

$$W^{XY}_{f,\tau} = W^X_{f,\tau}\, W^{Y*}_{f,\tau} \tag{1.4}$$

where $(^*)$ indicates the complex conjugate form. The cross wavelet transform detects areas in the time frequency space where two time series exhibit high common power (Grinsted et al. 2004; Maraun and Kurths 2004). The wavelet coherence on the other hand is a method that detects time windows and frequencies where two time series co-vary, but not necessarily exhibit high power. The wavelet coherence R^{XY} between two time series x_t and y_t is defined as the cross wavelet normalized by the individual power spectra of each time series (Torrence and Compo 1998; Grinsted et al. 2004; Maraun and Kurths 2004; Cazelles et al. 2008) as:

$$R^{XY}_{f,\tau} = \frac{|S(W^{XY}_{f,\tau})|}{|S(W^X_{f,\tau})|^{1/2} \cdot |S(W^Y_{f,\tau})|^{1/2}} \tag{1.5}$$

where S denotes a smoothing operator. It detects synchronicities between two time series and can be thought of as local cross-correlation in the time frequency space. In contrast to the cross wavelet transform, it can detect coherence between two signals even though their common power is low (Grinsted et al. 2004). It is superior to the cross wavelet transform for significance testing the relationship between two signals, as the cross wavelet transform can produce misleading peaks (Maraun and Kurths 2004). High wavelet coherence over extended regions in the time frequency space can point to a causal relationship between two time series. Thus, causes and effects of patterns and processes can be explored. The direction of causality can be assessed by calculating the phase difference between two time series, giving information about time lags in the synchronicities between two time series.

The wavelet coherence between time series of wind speed and water temperature is exemplified in Fig. 1.6. The time domain is represented on the x-axis, while the frequency domain

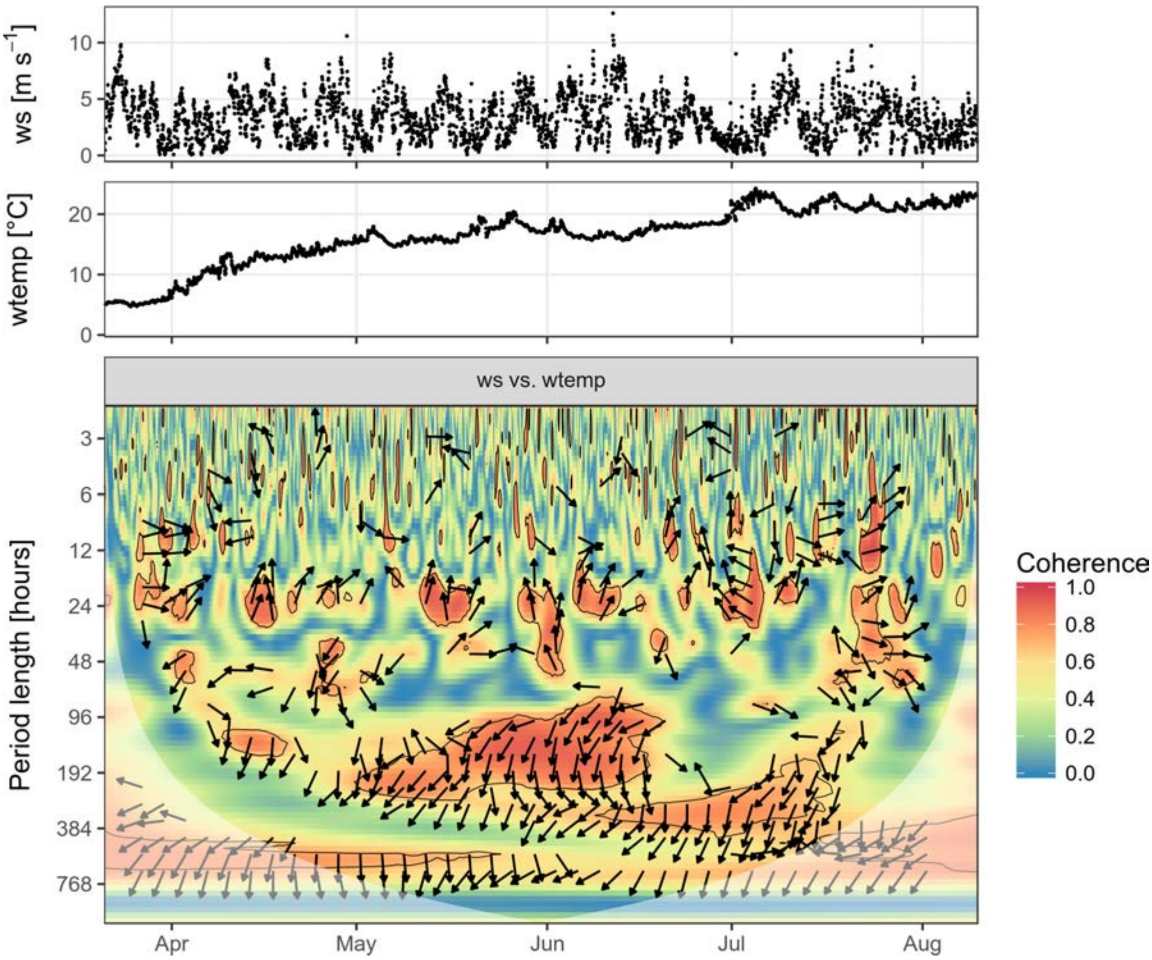

Fig. 1.6: *Upper panels*: time series of wind speed (ws) [m s^{-1}] measured hourly in 4 m height above Müggelsee and water temperature (wtemp) [°C] measured hourly in 1.5 m depth in Müggelsee in 2009. *Bottom panel*: wavelet coherence between ws and wtemp; black contours around regions where the coherence is significant against red noise, based on Monte Carlo AR (1) time series (significance level 0.95); black arrows indicate the relative phase relationship (in-phase pointing right; anti-phase pointing left; out of phase pointing up/down); the lighter shade denotes the cone of influence, where edge effects may distort patterns of coherence. The x-axis applies to all three panels.

is represented as period length on the y-axis. The color indicates the degree of coherence and can exhibit values between zero and one. The area in lighter shade denotes the cone of influence, where edge effects may distort the wavelet coherence. Regions in time frequency space bordered by a black line indicate significant coherence between the time series. The black arrows visualize their phase relationship. For example, the extended area in May and June around period lengths of one week exhibits high coherence, meaning that wind speed and water temperature were somehow related during this time window and around weekly time scales, but not for instance at sub-daily time scales. Their phase relationship is mostly out of phase, indicating a time lag in the response of water temperature dynamics to variations in wind speed.

The above examples illustrate how an analysis of lakes in the time frequency domain can be accomplished. The Fourier transform spectral analysis quantifies the periodic variability of a signal in the frequency space. The wavelet transform is particularly useful for the analysis of nonstationary time series and detects periodic or non-periodic variability in the time frequency space. The wavelet coherence quantifies the degree of synchronicity between two time series in the time frequency space. All of these methods can help to extract features in limnological and meteorological time series to identify processes, their time scales and constraints.

The tendency of ecosystems to oscillate in space and time means that they can be characterized by their spectral behavior – a research priority encouraged by Platt and Denman (1975) over 40 years ago. A review of the spatiotemporal scales of phytoplankton variability is presented by Harris (1980), who emphasize the importance of high-frequency as well as low-frequency variability and of considering the "correct algal scales of perturbation and response". Subsequent studies of lakes in the time frequency domain have proven promising to reveal patterns and processes and to identify their drivers and constraints. For example, Kimura et al. (2014) used spectral analysis to discriminate between rainstorm-induced and wind-induced vertical mixing and their impact on internal waves in a shallow subtropical lake. An extensive analysis of the noise color of temperature variability in terrestrial and aquatic ecosystems demonstrated that the slopes of air and water temperature spectra became steeper (more red) from land to river to lake to ocean ecosystems, revealing substantial differences according to the lake type (Cyr and Cyr 2003). Winder and Cloern (2010) assessed annual cycles of phytoplankton, proxied by chlorophyll *a* concentration, to reveal periodicities in phytoplankton patterns across lake, estuarine and ocean ecosystems via wavelet analysis. They found large site-specific differences, while acknowledging the limitation of their approach due to an only monthly sampling frequency. Changes in the periodicity of phytoplankton seasonal succession from year to year were highlighted by Carey et al. (2016). Physical and biological drivers of the variability in dissolved oxygen differed with respect to their time scale and among lakes, as revealed by wavelet analysis (Langman et al. 2010). Guyennon et al. (2014) used wavelet analysis and wavelet coherence to extract oscillation modes of internal waves and the exchange of water between two basins of a large deep lake from time series of water temperature and wind speed. Analyses in the time frequency domain using wavelet coherence revealed time lags in the response of phytoplankton biomass to environmental drivers (Recknagel et al. 2013; Li et al. 2015). These examples describe promising roads to an insightful analysis of lakes in the time frequency domain.

1.3 Research questions

Motivated by the above discussion on lake ecosystems, variability in the parameters that characterize them and the time scales governing this variability, the overarching research question of this thesis is:

> **How can the consideration of the time scale of variability and an analysis in the time frequency domain help to enhance our understanding of lake ecosystems and their responsiveness to the variability in climate and weather conditions?**

Specifically, I intend to answer the following three questions with this thesis:

1. What role does the time scale of analysis play in detecting the underlying mechanisms of ecosystem responses to climate variability?

2. What are the temporal and spatial scales of water temperature variability in a polymictic lake, and how can they be explained?

3. How can the joint dynamics of limnological and meteorological parameters be used to identify processes, their drivers, constraints and time scales?

These questions are addressed by a literature-based review of previous studies and thorough investigations of empirical data collected over the last twenty years in Müggelsee, a shallow polymictic lake in northeastern Germany. Data comprise both limnological and meteorological time series measured by automated sensor systems. This thesis adopts a frequency-based methodological approach with the aim to explore and explain patterns and processes in lake ecosystems. An overview of how the research questions are addressed is outlined in the following.

1.4 Outline of this thesis

The research questions of this cumulative thesis are addressed in the following three chapters. A conceptual analysis is presented in the second chapter: *Windows of change: temporal scale of analysis is decisive to detect ecosystem responses to climate change*. The content is based on an article by Rita Adrian, Dieter Gerten, Veronika Huber, Carola Wagner and Silke R. Schmidt and was published 2012 in *Marine Biology* (Adrian et al. 2012). Here, the role of the time scale of analysis regarding the detection of responses of limnic and marine ecosystems to climate change is addressed. It is demonstrated that average annual, seasonal or monthly climate data often fall short of characterizing the meteorological and ecosystem thermal dynamics that most organisms respond to. Potential time scales of ecosystem responses to meteorological forcing are summarized. It is emphasized that a profound understanding of the mechanisms underlying responses to climate warming requires that records of ecological processes are not only sufficiently long, but are also collected at an appropriate temporal resolution and time of year. It is documented that ecological responses are often triggered by changes in critical time windows and that the triggering mechanism often involves the exceedance of critical thresholds in the forcing variables. Moreover, responses tend to occur with a time lag. In an empirical analysis, two years sharing almost the same annual mean are compared regarding their variability at different time scales. The author of this thesis performed the quantitative analyses, contributed to interpreting the results and to drafting the manuscript.

A systematic, frequency-based investigation of patterns of variability in near-surface water temperature of Müggelsee is presented in the third chapter: *Temporal and spatial scales of water temperature variability as an indicator for mixing in a polymictic lake*. This chapter was submitted to *Inland Waters* by Silke R. Schmidt, Dieter Gerten, Thomas Hintze, Gunnar Lischeid, David M. Livingstone and Rita Adrian and is currently under review. Here, seasonal and spatial patterns of water temperature variability are compared to the variability in corresponding air temperature and related to mixing dynamics, stratification stability and the duration of ice cover to explore potential drivers of water temperature variability. An indicator of lake mixing is presented that helps to explain the observed temporal and spatial scales of water temperature variability. The author of this thesis designed the research, performed all analyses, interpreted the results and drafted the manuscript. Contributions to the study design, discussions of the results, commenting and proofreading of the draft by the co-authors is acknowledged.

The fourth chapter *Using wavelet coherence as a diagnostic tool in limnology* was submitted to *Limnology and Oceanography* by Silke R. Schmidt, Gunnar Lischeid, Thomas Hintze and Rita Adrian and is currently under review. It presents a methodological approach to investigate how wavelet coherence can be used to identify and disentangle physical, chemical and biological processes and to detect the time scales these processes operate on. It is tested whether processes such as algal growth, photosynthesis, respiration, biogenic calcite precipitation or wind-induced resuspension of particles can be detected analyzing synchronicities between limnological and meteorological parameters measured at a high temporal resolution in Müggelsee during a time span from the onset of an ice cover in winter until a summer cyanobacteria bloom in the year 2009. The author of this thesis designed the research, performed all analyses, interpreted the results and drafted the manuscript. Contributions by the co-authors to the design of the study approach, support in interpreting the results, commenting and proofreading of the draft is acknowledged.

The fifth chapter *Synthesis and outlook* concludes with a discussion of the answers to the research questions given in chapters 2 – 4 and the main findings of this thesis. It is a conclusion how this thesis contributes to a better understanding of the variability in lake ecosystems and the processes that generate it with a literature-based and a data-driven methodological approach.

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2 Windows of change: temporal scale of analysis is decisive to detect ecosystem responses to climate change *

Abstract

Long-term ecological research has become a cornerstone of the scientific endeavor to better understand ecosystem responses to environmental change. This paper provides a perspective on how such research could be advanced. It emphasizes that a profound understanding of the mechanisms underlying these responses requires that records of ecologic processes be not only sufficiently long, but also collected at an appropriate temporal resolution. We base our argument on an overview of studies of climate impacts in limnic and marine ecosystems, suggesting that lakes and oceans respond to (short-term) weather conditions during critical time windows in the year. The observed response patterns are often time-lagged or driven by the crossing of thresholds in weather-related variables (such as water temperature and thermal stratification intensity). It becomes clear from the previous studies that average annual, seasonal or monthly climate data often fall short of characterizing the thermal dynamics that most organisms respond to. To illustrate such literature-based evidence using a concrete example, we compare 2 years of water temperature data from Müggelsee (Berlin, Germany) at multiple temporal scales (from hours to years). This comparison underlines the pitfalls of analyzing data at resolutions not high enough to detect critical differences in environmental forcing. Current science initiatives that aim at improving the temporal resolution of long-term observatory data in aquatic systems will help to identify adequate timescales of analysis necessary for the understanding of ecosystem responses to climate change.

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2.1 Introduction

About 20 years ago, Magnuson (1990) published a land-mark paper which suggested that ecologists should move beyond a mere focus on present ecosystem dynamics and adopt longer-term perspectives. His main point was that our perception and understanding of the physical, chemical and biological processes acting over decades in limnic, marine and terrestrial ecosystems is necessarily limited by the length of the existing observational time series. If the availability of long-term time series enabled researchers to extend their temporal "window" of analysis, they might well discover new phenomena and possibly unexpected trends that might put the present "into a context that makes it more understandable and more interesting" (Magnuson 1990).

Two further decades of long-term ecological research have passed since. During this time, numerous studies have been published that shed light on the long-term dynamics of ecological processes, helped situating current observations in a longer-term context and also advanced the integration of statistical and modeling methods in ecological research. A substantial part of this research was and still is driven by the quest for evidence of climate change impacts on ecosystems and synchronization of such impacts over large distances (for overviews, see Drinkwater et al. 2003; Edwards and Richardson 2004 and Alheit et al. 2005 on marine ecosystems; Gerten and Adrian 2002a and Straile et al. 2003 on limnic ecosystems; and Mysterud et al. 2003 on terrestrial ecosystems) – so much so that one might characterize this development as a paradigm shift (Gerten 2008; Livingstone 2008). These studies certainly benefited from the fact that the length of observation records is increasing over time (as long as measurements are being continued) and that climate's signature on ecosystems tends to become stronger the further anthropogenic climate change proceeds.

In the present paper, we seek to further stimulate such research by presenting a complementary perspective. We argue that a thorough understanding of long-term dynamics of ecological processes – be it in limnic, marine or terrestrial systems – requires observation and data analysis at multiple timescales. As will be demonstrated in more detail below, evidence suggests that detection of trends, interpretation of single events in the context of their long-term dynamics and profound understanding of underlying mechanisms requires that records of ecological processes be not only sufficiently long but also be at an appropriate temporal resolution (Haury et al. 1978; Harris 1980; Anderson 1995). For instance, recent research on lake ecosystems clearly demonstrated that the detailed (high-frequency) seasonal evolution of water temperature and of correlated phenomena such as thermal stratification is crucial for habitat refuge, nutrient dynamics, plankton phenology and abundance, growth initiation, bloom formation, emergence from resting stages and responses to extreme events (Reid et al. 1998; Gerten and Adrian 2002b; Edwards and Richardson 2004; Jansen and Hesslein 2004; Mooij et al. 2005; Sommer and Lengfellner 2008; Wagner and Adrian 2009a; Huber et al. 2010, 2012).

Thus, information about whether the average climate in a season or month is changing may not be sufficient to detect and explain climate impacts on highly dynamic ecosystem processes that are controlled by meteorological conditions fluctuating at much shorter timescales. For example, monthly or even weekly averages of meteorological conditions are likely to mask the exceedance of ecologically critical temperature thresholds and responses of species to (short-term) meteorological changes that occurred immediately before, or time-lagged, substantially earlier in the year (Fig. 2.1).

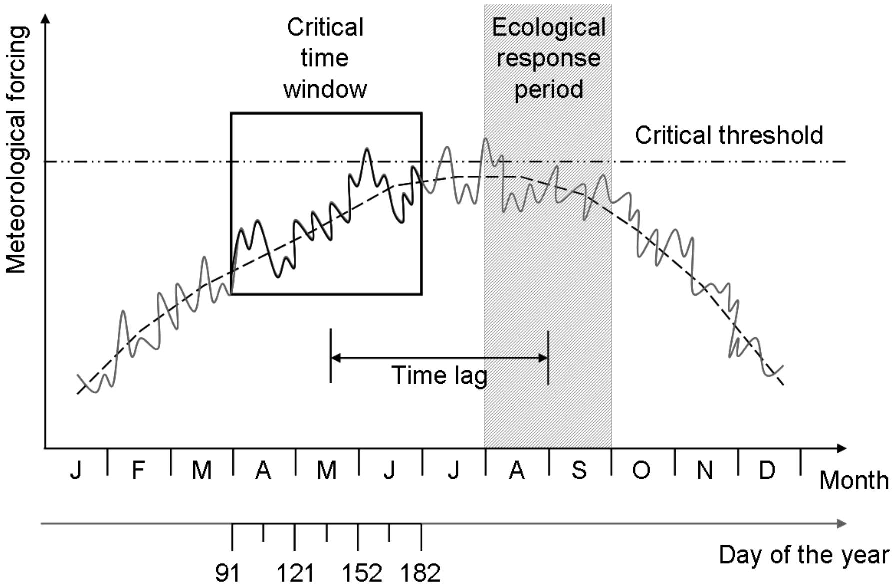

Fig. 2.1: Timescales of ecosystem responses to meteorological forcing. Ecological responses are often triggered by changes in critical time windows. The triggering mechanism frequently involves the crossing of critical thresholds in forcing variables (*dashed-dotted line*), and responses tend to occur with a time lag. The challenge lies in identifying the adequate timescale of analysis to detect relationships of this kind. In this conceptual sketch, analysis at the monthly timescale (*dashed line*) would not be sufficient to detect threshold exceedance, in contrast to analysis at the daily timescale (*solid line*).

Using examples from a suite of studies of climate impacts on foremost limnic and marine ecosystems, this paper demonstrates that average annual, seasonal or monthly climate data indeed often fall short of characterizing the meteorological and ecosystem thermal dynamics that most organisms respond to. It is not our intention to provide a comprehensive review and synthesis of previous studies, but we hope that our exemplary analyses – many of which are derived from the AQUASHIFT project – help to sharpen the focus of future statistical, modeling and experimental ecosystem studies on the adequate timescales of investigation. As such, it is meant as a thought-provoking perspective paper aimed at stimulating research in this direction. The paper concludes with a discussion of implications of our findings for experimental approaches and model-based climate impact projections that necessarily rely on coarse-resolution output from climate models.

2.2 Approach and data

We start out by illustrating typical variability in the pattern of meteorological forcing which aquatic ecosystems are exposed to at a range of temporal scales. By comparing different years, we also show how easily crucial differences in forcing can be missed if the temporal resolution of analysis is not sufficiently high. This illustrative example is based on observed *water temperature data* of a well-studied polymictic lake (Müggelsee; Berlin Germany). We investigated the differences in average water temperatures for one pair of years sharing almost the same annual mean at temporal scales of minutes, days, weeks, months and seasons. Years were also compared in terms of cumulative rates of change at these different temporal scales, which were computed according to Eq. (2.1):

$$\sum |x_{t+1} - x_t|, \tag{2.1}$$

with x being the water temperature at time $t+1$ and time t, respectively. All analyses were performed using R (R Core Team 2010) supported by the packages ggplot2 (Wickham 2009) and TSA (Chan 2010). For information on the lake, methodology of temperature recording and data processing, see Wilhelm et al. (2006).

The subsequent sections on published literature for the limnic and marine domains are organized as follows: we first address *critical time windows* of change in the course of organism's life cycles. Second, we present characteristic *time lags* in responses of organisms to anomalies in temperature. Third, we explore the role of *thresholds* in weather- or climate-related forcing that potentially cause regime shifts of ecosystems. The focus is on thresholds in water temperature, but we also address thresholds in variables that are independent of, or only indirectly dependent on, water temperature (e.g. thermal stratification, day length-specific water temperature). Although many of the cited studies investigated all of these three characteristics of ecological responses to meteorological forcing together (critical time windows, time-lagged responses, critical thresholds), we here discuss these three issues separately for reason of clarity.

2.3 Results and discussion

2.3.1 Small-scale variability in temperature forcing

Investigation of three decades of water temperature records in Müggelsee showed that there were several years that exhibited almost the same yearly average. We focus on the relatively warm years 1989 and 2009, characterized by almost the same annual temperature mean of 11.6 °C in 1989 and 11.3 °C in 2009 (Fig. 2.2a). When comparing the progression of water temperature in these 2 years at yearly, seasonal, monthly, weekly, daily and hourly timescales, we found a strong increase in the deviation in water temperature between the two time series, which becomes the greater the finer the temporal resolution is. Differences at the seasonal or

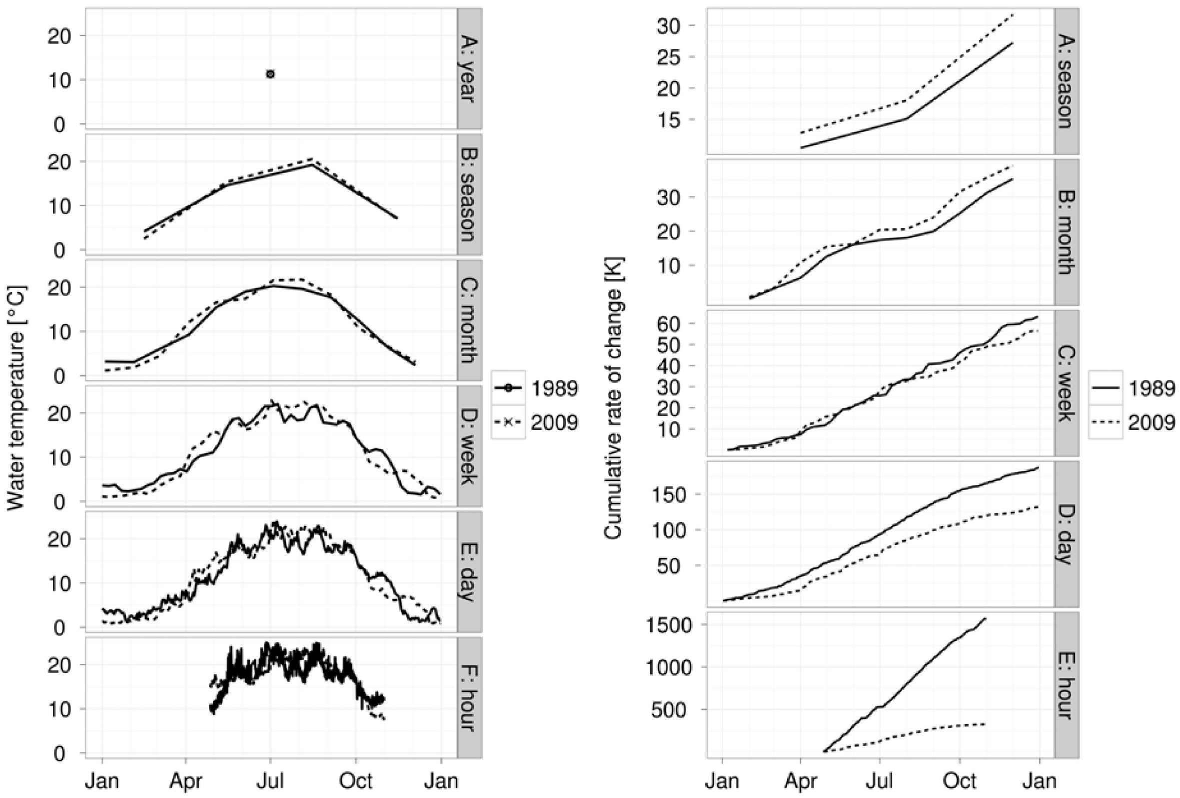

Fig. 2.2: *Left panel* Temporal evolution of water temperature in Müggelsee shown as yearly to hourly averages of 2 years sharing almost the same yearly average of 11.6 °C in 1989 (*solid line*) and of 11.3 °C in 2009 (*dashed line*). *Right panel* Cumulative absolute values of the rate of change of water temperature from seasonal to hourly temporal scales for the 2 years. Note the differences in scale of the y-axis.

monthly scale did not exceed 3 K (which, however, can be considered a large difference at this aggregation level), but reached up to 8 K at the hourly scale (data not shown). The difference between these years becomes even more obvious when looking at the rates of change. Whereas the two curves are still quite similar and almost parallel from the seasonal to the weekly scale, they drift apart quite extremely at the hourly scale, where the total absolute cumulative rate of change in 2009 was 326 and 1570 K in 1989, respectively (Fig. 2.2b). Thus, water temperatures in 1989 fluctuated a lot more on the finest timescale than in 2009. This fluctuation, however, leveled out at coarser timescales. It may be exactly this fine-scale variability that contributes to the large fraction of unexplained interannual variability of plankton community composition and succession that ecologists are still confronted with (for review, see Cottingham et al. 2001).

For those 2 years, for example cardinal events in plankton phenology differed quite substantially (Table 2.1). The timing of the spring phytoplankton bloom differed by 3 weeks. It occurred exceptionally early in 1989 – a year without any ice development (Table 2.1; Huber et al. 2008). On the contrary, daphnids developed their spring population maximum earlier in 2009 than observed in 1989 (Table 2.1). The timing of the *Daphnia* spring peak is more or less independent of the winter climate but determined by water temperatures during spring

Table 2.1: Timing of cardinal events in 1989 and 2009 exhibiting almost the same annual mean water temperature (see Fig. 2.2): ice-off date; maxima of total algal biomass (phytoplankton), and daphnid abundances in spring and summer

Year	Ice-off	Phytoplankton		Daphnids	
		Spring	Summer	Spring	Summer
1989	No ice	11	26	22	27
2009	11	14	34	19	35

The timing of the cardinal events is given in calendar weeks

(Gerten and Adrian 2000). Thus, the higher water temperatures during the critical time window of their development in the spring of 2009 (Fig. 2.2) caused the discrepancies in phenology in the 2 years. In contrast, the summer phenology of both phytoplankton and zooplankton was rather similar in both years (Table 2.1). During summer, indirect temperature effects such as the duration of stratification events are more important driving forces for the development of the phytoplankton (Wagner and Adrian 2009a, 2011), while complex interactions between meteorological conditions in spring and summer may determine the summer crustacean zooplankton development (Huber et al. 2010; see also below).

2.3.2 Critical time windows

Aquatic ecologists are just beginning to understand the importance of such temporal fluctuations of water temperature for ecosystem processes. Rather, few studies have considered system-specific time windows of change in temperature critical for ecosystem responses to climate change.

At the seasonal temporal scale, prominent examples of critical time windows are the well-known changes in phenology in marine (Edwards and Richardson 2004; Wiltshire and Manly 2004; Aberle et al. 2007; Martens and van Beusekom 2008) and freshwater ecosystems (Weyhenmeyer et al. 1999; Gerten and Adrian 2000; Straile 2002; Winder and Schindler 2004; Rusak et al. 2008). In lakes, critical time windows were, for example, ice-off dates affecting the timing of the spring phytoplankton bloom, day length-specific water temperature affecting emergence of resting stages or the timing of surpassed temperature thresholds initiating spawning (Adrian et al. 2006; Blenckner et al. 2007; Straile et al. 2007; Wilhelm and Adrian 2007). It was also observed that compared to more immediate responses in aquatic systems during the spring, phenological changes in summer were not as coherent and seem to have established only after a transition period of several years (Martens and van Beusekom 2008; Wagner and Adrian 2009b). In marine habitats, critical thermal windows for physiological mechanisms such as aerobic performance of fish have been studied in the context of future warming trends (Pörtner and Knust 2007; Pörtner and Farrell 2008). Warming-induced shifts in seasonal phenology may cause mistiming between such thermal windows and processes timed according to constant cues such as day length (freshwater: Adrian et al. 2006; marine: Pörtner and Farrell 2008).

Besides studies of climate-induced phenology shifts, Shatwell et al. (2008), for example, showed how short-term (in the order of weeks) windows of opportunity for population development can be opened for cyanobacteria in warm springs in an otherwise diatom-dominated season in Müggelsee (Germany). They argued that if cyanobacteria attain a critical biomass during that very time window, they may dominate the phytoplankton throughout the summer (see also Teubner et al. 1999). Another study showed that for lake summer crustacean zooplankton, differences in water temperatures in rather narrow time windows, either before (2.2 weeks) or after the typical clear-water phase (3.2 weeks), affected their start-up populations (Huber et al. 2010). These differences explained some of their contrasting success during three hot summers characterized by more or less the same average summer temperature (Huber et al. 2010). For species with complex life cycles such as copepods, critical time windows affected the survival rate of the juveniles, whereas the longer life time of the adults may have buffered the adults' population dynamics against seasonal variability in abiotic forces in lakes (Seebens et al. 2007, 2009; Winder et al. 2009).

Another example of critical time windows is that changes in a lake's thermal regime in response to water temperature changes during specific time windows within a year induce subsequent changes in oxygen and nutrient dynamics. Of particular importance is that the duration of stable thermal stratification may operate over a broad range of timescales related to lake morphometry: on monthly scales in monomictic or dimictic lakes (Gerten and Adrian 2000; Livingstone 2003; Mooij et al. 2005) and on sub-daily (Wilhelm and Adrian 2008) to weekly scales in polymictic lakes (Wagner and Adrian 2009a). Longer summer stratification in the range of one to several weeks has been shown to positively affect the magnitude of the autumnal algal bloom in productive dimictic lakes (Adrian et al. 1995; Huisman et al. 2004; Jöhnk et al. 2008) or during sufficiently long-time windows of stable stratification in the order of a few weeks during the summer in polymictic lakes (Wagner and Adrian 2009a) – mostly mediated by enhanced internal nutrient loading (Elliott et al. 2006; Mooij et al. 2005; Wilhelm and Adrian 2008) and/or species replacements (Winder and Hunter 2008; Wagner and Adrian 2009a).

Recent studies also provide an important insight into the definition of the timing of seasonal events. The widespread observed changes in phenology in marine and freshwater ecosystems during recent warming episodes indicate that the timing of seasonal events should not be defined based on fixed calendar dates, but according to cardinal events in the ecosystem itself. Important cardinal events that have been successfully used in the past to define phenology-adjusted temporal scales in lakes are, for example, ice-off dates, the timing of the clear-water phase or periods of stable thermal stratification (Rolinski et al. 2007; Wagner and Adrian 2009a; Huber et al. 2010).

2.3.3 Time lags in response

Most of the above-cited studies also demonstrate lags between the described (more or less short) forcing time window and the response time window in the range of weeks to months. For example, water temperature, early in the year, is decisive for the summer development of phyto- and zooplankton in lakes (Teubner et al. 1999; George and Hewitt 2006; Seebens et al. 2007; Wagner and Benndorf 2007; Huber et al. 2010) as well as of benthic species in marine habitats (Kirby et al. 2007). Temperature-driven changes in the timing of food availability and of predation by young-of-the-year fish during critical time windows in spring/early summer determined the mid-summer decline of daphnids in a reservoir in Germany (Benndorf et al. 2001). Regarding freshwater and marine copepods, the abundances of cyclopoid (Gerten and Adrian 2002b; Martens and van Beusekom 2008; Seebens et al. 2009) and calanoid copepods (Beaugrand et al. 2002; Seebens et al. 2007; Martens and van Beusekom 2008; Batten and Mackas 2009) in summer and autumn were found to be determined by weather in spring – likely related to temperature-induced changes in the emergence of resting stages (Adrian et al. 2006) or short-time windows of high food quantity for offspring survival (Seebens et al. 2009). Similarly, even in large-scale marine ecosystems, the intensity of the response of North Sea plankton phenology in summer was reported to be driven by sea surface temperature in spring (Edwards and Richardson 2004). Moreover, reproduction and survival of benthic species in summer were influenced by sea surface temperature in winter/spring (Kirby et al. 2007). Besides changes in population size, extensions of the growing season in summer/autumn have been found for both marine (Martens and van Beusekom 2008) and freshwater copepods in response to climatic changes in spring and summer that involved exceedance of temperature thresholds during specific, rather short-time windows (Gerten and Adrian 2002b).

Even time lags at the scale of several months to years are known for physical and biological system levels. It has been established that lake morphometry determines the memory of large-scale signals such as the NAO in water temperatures from weeks to several months (Gerten and Adrian 2001) to multiple years (Livingstone 2003). Species encompassing longer life cycles, such as fish, are also affected by such extensive time lags. For example, year-class strength of *Coregonus lavaretus* followed a 1-year time lag related to specific mixing dynamics in Lake Constance (Straile et al. 2007).

Overall, time lags between the time windows of the climatic forcing window and the biological response window (differences in center of time windows) lay between 1.5 months for phytoplankton, 2-3 months for parthenogenetically reproducing cladocerans, 3.3-3.5 months for copepods and 11 months for whitefish for the limnetic examples depicted in Fig. 2.3. In spring, the responses tend to be of a more immediate nature, because fast-growing species, adapted to spring-specific steep gradients in temperature and light conditions, prevail in lakes (Adrian et al. 2006). For slow-growing species with longer and more complex life cycles of months to years such as copepods or fish, discrepancies between climatic forcing and response windows

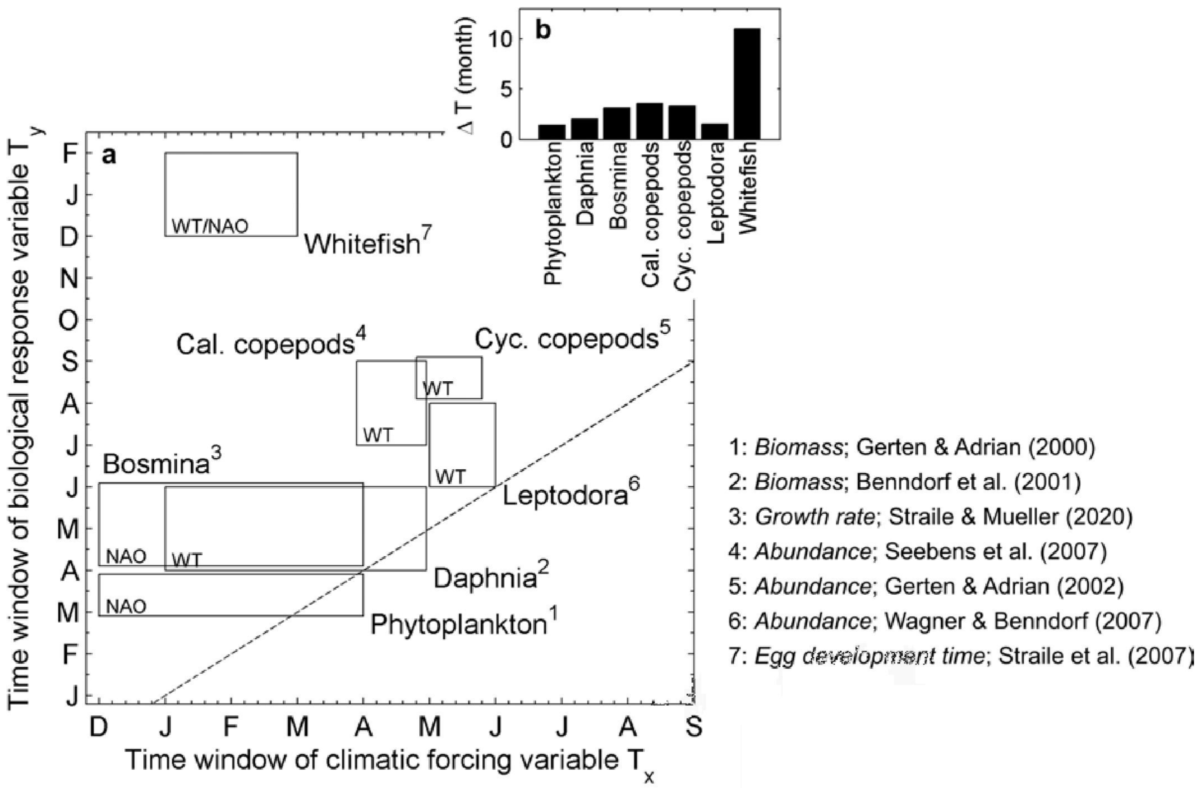

Fig. 2.3: Typical time lags between climate-related forcing and biological response in freshwater ecosystems. *Squares* in **a** indicate the seasonal timing of different species responses (*vertical lines*) with regard to the forcing time period (*horizontal lines*), as identified in the literature (exemplary studies 1-7). **b** Shows the corresponding mean time lags (differences in centers of time windows), which are also illustrated by the *vertical* offsets of *boxes* to the *dashed* concurrence line in **a**. Climate forcing considered in the selected studies were water temperature (*WT*) and/or the index of the North Atlantic oscillation (*NAO*), and the biological responses were mean or peak biomass/abundance, growth rates and egg development time as indicated in the legend. For example, study 4, based on a long-term record of Lake Constance, found that the abundances of *Eudiaptomus gracilis* (calanoid copepod) in July/August were positively correlated with mean WT in April (**a**). The mean time lag between forcing and response was approximately 3.5 months (**b**).

are usually longer (Adrian et al. 2006; Straile et al. 2007; Fig. 2.3). Warming may be required during decisive developmental stages such as emergence from diapause, egg and/or larval development within one year or on different developmental stages across years as shown for whitefish in Lake Constance. Here, the winter NAO affected larval growth of whitefish in spring, while their egg development time was affected with a time lag of 1 year (Straile et al. 2007). Time lags of 2 years were found between the NAO signal and cod recruitment in the Barents Sea (Dippner and Ottersen 2001). While it seems plausible that generation time and response windows are linked, the underlying mechanisms are complex. Besides temperature and prey resources, lake morphometry has been identified as an important driver for whitefish recruitment (Straile et al. 2007). In the marine realm spawning stock (Brander 2005), prey resources or water fluxes (Drinkwater et al. 2003) are known to affect cod recruitment, independent of generation time.

2.3.4 Critical thresholds

In addition to the determination of critical time windows, the quantification of critical thresholds has put another quality to recent climate impact studies. The surpassing of critical thresholds in abiotic and biotic drivers is an important force that manifests at all system levels. Pertinent examples are thermally limited oxygen delivery for marine fish (Pörtner and Knust 2007), the hatching of marine calanoid copepods (Holste and Peck 2006), surpassed temperature thresholds for the first spawning of freshwater mussel *Dreissena polymorpha* larvae (Wilhelm and Adrian 2007), surpassed thresholds of freshwater competitor and/or predator densities (Adrian 1997), thermal windows for growth and survival of larval and juvenile and adult fish (reviewed by Pörtner and Peck 2010), all the way to the susceptibility of freshwater fish species to diseases (Hari et al. 2006). Furthermore, the exceedance of direct and indirect temperature thresholds may trigger processes, such as the onset of cyanobacteria blooms in lakes (Wagner and Adrian 2009a; Huber et al. 2012), alterations in aquatic species composition (Holste and Peck 2006; Parmesan 2006; Helaouët and Beaugrand 2007; Wagner and Adrian 2009a) or habitat shifts (Jansen and Hesslein 2004; Hari et al. 2006; Wiedner et al. 2007). Peeters et al. (2007) quantified surpassed critical thresholds in spring for a number of meteorological variables acting in concert, such as air temperature, wind and light conditions and their relative importance in determining an early or late onset of phytoplankton growth in Lake Constance.

Temperature thresholds can play a critical role, not only at the scale of single species or processes, but also at ecosystem level, possibly causing a change into a different ecosystem state often referred to as regime shift (Scheffer and Carpenter 2003). Beaugrand et al. (2008) showed, for example, that regions in the North Atlantic, which were at the edge of the 9°-10° isotherm, had the highest sensitivity to small changes in temperature, with large impacts on all system levels as well as on biodiversity. The quantification of critical thresholds and related nonlinear ecosystem responses has been a big step forward as they help to improve ecosystem modeling approaches and thus enhance their predictive power.

During the last decades, several climate-induced regime shifts have been observed within marine and limnic ecosystems over the entire Northern Hemisphere, in particular around 1976/1977 in marine habitats (Hare and Mantua 2000; Alheit et al. 2005; Weijerman et al. 2005) and the late 1980s in freshwater habitats (Gerten and Adrian 2000; Straile et al. 2003; Blenckner et al. 2007). Such shifts have been attributed to large-scale climate modifications, in particular to changes in the Pacific Decadal Oscillation, (Hare and Mantua 2000; DeYoung et al. 2004) or the North Atlantic Oscillation (Gerten and Adrian 2000; Alheit et al. 2005; Blenckner et al. 2007; Möllmann et al. 2011). Regime shifts are inherently difficult to predict given the non-stationary relationship that often characterizes the links between climatic forces and ecological responses (Scheffer and Carpenter 2003) along with the complexity of overlapping forces (Wagner and Adrian 2009b). Theory developed already in the 1980s proposed that recovery rates from perturbation slow down when approaching a tipping point, which may be used as an early warning signal for upcoming regime shifts (Wissel 1984). Most recent studies indeed point to statistical signals that precede nonlinear transitions – and as such may serve as early warning signals for abrupt regime shifts. A critical slowingdown in fluctuations measured as an increase in autocorrelation has been detected in ancient climatic time series prior to abrupt regime shifts (Dakos et al. 2008). Limited empirical evidence for several statistical signals suitable as early warnings of aquatic regime shifts come from laboratory experiments (phyto- and zooplankton; Drake and Griffen 2010; Veraart et al. 2012) and whole-lake experimental studies (Carpenter et al. 2011). The slowdown in fluctuations does not point to any specific mechanism, but is more likely a universal property of a system moving towards a threshold (Wissel 1984; van Nes and Scheffer 2007). Given the inherent unpredictability of complex ecosystems, it remains to be tested whether statistical signals such as an increase in autocorrelation are indeed suitable to predict transitions in ecosystem states (Veraart et al. 2012).

2.3.5 Outlook

The above-described studies from the literature demonstrate that physical, chemical and biological processes in aquatic ecosystems often respond, potentially time-lagged, to meteorological conditions within very narrow time windows, for example, because specific temperature thresholds were surpassed during that period (see also Fig. 2.1). These observations are crucial in the light of global climate change, as changes in climatic conditions principally can manifest themselves during any time window within a year, while there may be pronounced differences among years with respect to the detailed seasonal pattern of change. The challenge lies in identifying the adequate timescale of analysis to detect climate-induced response pattern in aquatic ecosystems.

Current understanding of the importance of variability at multiple temporal scales for these response patterns – as documented in the reviewed literature – has implications for improving the design of experimental and model-based climate impact studies. So far, temperatures in experimental and modeling approaches have been typically manipulated by a continuous increase of, for example, 1-6 °C over an experimental period covering several months (de Senerpont Domis et al. 2007; Sommer and Lengfellner 2008; Elliott 2010; Gaedke et al. 2010; Moss 2010). For most modeling studies of ecosystem impacts of future climate change, projections of, for example, monthly or daily air temperature are constrained to output from general or regional circulation models (downscaled by statistical or dynamical methods) in an attempt to capture a range of potential trajectories. In addition, although current climate models operate at high temporal resolution already, they only represent a specific trajectory – while in reality, a change, for example, in mean annual or monthly temperature can be realized by myriad ways of temperature progression not accounted for by climate models. We do not question the value of such studies but suggest that future studies would profit from the incorporation of high-frequency fluctuations as documented in the above case study of Müggelsee (Fig. 2.2), as these might be decisive for the dynamics of specific species and other ecosystem processes (Langman et al. 2010; Sadro et al. 2011a,b).

A way forward might be the emulation of (sub)-daily temperature progressions in hundreds of simulations, comparable to how it is being done with the statistical climate model STAR (Orlowsky et al. 2008). STAR generates climate predictions based on observed historic time series of meteorological variables, which are permuted in segments based on a linear trend of a characteristic climatological variable. In general, such research needs to integrate analysis of effects operating at multiple temporal scales, ranging from descriptive illustrations as proposed in the present paper to more analytical methods of multivariate statistics (taking into account the data time series at different temporal resolutions) and of time series analysis (for example autoregressive conditional heteroscedasticity models) that jointly account for time-lagged dependencies and autocorrelations of time series (Engle 1982).

In conclusion, our overview strongly supports science initiatives that aim at improving the temporal resolution of long-term observatory data in aquatic systems (such as the Global Lake Ecological Observatory Network GLEON; Hanson 2007). Most of these initiatives employ modern in situ sensor techniques (Staehr et al. 2010; Pierson et al. 2011) generating data at sub-daily temporal scales with a global coverage. These data will help to identify adequate timescales of analysis for a large range of different ecosystems necessary for the understanding of ecosystem responses to climate change.

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3 Temporal and spatial scales of water temperature variability as an indicator for mixing in a polymictic lake *

Abstract

Applying coarse spectral analysis to over two decades of daily near-surface water temperature (WT) measurements from Müggelsee, a shallow, polymictic lake in Germany, allowed us to systematically characterize patterns in WT variability from daily to yearly temporal scales. Comparison of WT with local air temperature indicates that the patterns found in WT variability are likely attributable to both meteorological forcing and internal lake dynamics. We identify seasonal patterns of WT variability and show that WT variability increases with increasing Schmidt stability, decreasing Lake number and decreasing ice cover duration, and is higher near the shore than in the open water. We introduce the slope of WT spectra as an indicator for the degree of lake mixing that helps to explain the identified temporal and spatial scales of WT variability. The explanatory power of this indicator in other lakes with different mixing regimes remains to be established.

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3.1 Introduction

Water temperature (WT) variability is a fundamental driving force of almost all processes in lake ecosystems at temporal scales extending from biochemical reaction rates to life histories (Reynolds 1990). The detailed characteristics of the temporal evolution of WT and scale-dependent changes in its variability can play a crucial role for aquatic organisms. The importance of variability has been shown on many levels, from individual species (Drake 2005; Barbosa et al. 2014) to community composition (Benedetti-Cecchi 2003; Benincà et al. 2011; Thompson et al. 2013) and biodiversity (Shurin et al. 2010). Yet, despite this, the majority of studies investigating climate change and its impacts are focused only on changes in mean temperature. This is also the case in freshwater sciences, where significant increases in mean WT have been observed in lakes over the past few decades (Adrian et al. 2009; George 2010; Kernan et al. 2010; IPCC 2013; O'Reilly et al. 2015). There is, however, evidence that climate change also involves changes in the overall temperature probability distribution that imply an increase in variability on at least the regional level, especially in Europe (Schär et al. 2004; Salinger 2005; Vidale et al. 2007; Hansen et al. 2012; Huntingford et al. 2013 (regionally); IPCC 2013). These examples focus on meteorological variables, and up to now the effect of an increase in air temperature variability on aquatic ecosystems has been merely the subject of speculation. Such a "concerning lack of baseline knowledge" together with the "inescapable reality of climate variability on multiple scales" (Coble et al. 2016) calls for advances to be made in aquatic research that will focus not only on changes in the mean, but on comprehensively assessing the multiple facets of climate variability in experimental and observational studies.

Variability in water temperature is generated by various external and internal processes acting on different temporal and spatial scales. In temperate regions, the most important driver of WT variability is the seasonality of the weather. The main weather-related drivers of WT variability are air temperature (AT), wind speed, relative humidity, solar (short-wave) radiation, atmospheric (long-wave) radiation and, in some cases, precipitation (Edinger et al. 1968; Wilhelm et al. 2006). Oscillatory climate modes, such as the North Atlantic Oscillation, act on longer time scales (Gerten and Adrian 2000; Straile and Adrian 2000; George et al. 2010). Despite the strong coupling between AT and WT, especially in shallow lakes (Gerten and Adrian 2001), the unique physical properties of water (e.g., its high heat storage capacity), coupled with specific internal lake processes, shape patterns of lake WT variability decisively (MacKay et al. 2009). For instance, polymictic lakes can stratify at high ambient AT, but stratification periods are often interrupted by events of turbulence and vertical mixing induced by short-term changes in the weather (Lampert and Sommer 2007). The duration and intensity of summer stratification in lakes has been on the increase and is expected to increase further as global warming progresses (Elo et al. 1998; Livingstone 2003; Wagner and Adrian 2011), possibly causing a transition between different mixing regimes (Livingstone 2008; Kirillin 2010). Internal waves, which can occur throughout the year (Lorke 1998), even under ice (Kirillin et al. 2012), also induce fluctuations in WT (Wetzel 2001) and thus affect WT variability. Finally, the presence or absence of ice cover during winter, which is also strongly affected by global warming (Livingstone and Adrian 2009), may significantly change the physical and biotic conditions of lakes in general (Adrian et al. 1999), as well as WT variability in particular (Kirillin et al. 2009). However, the effect of changes in the most important internal driving forces of WT variability in shallow lakes – seasonality, mixing dynamics and ice cover – has not yet been systematically quantified.

Lakes are often spatially heterogeneous. This has been observed for dissolved substances and planktonic organisms, which can be distributed in patches (Wiens 1989; Lampert and Sommer 2007). Furthermore, water temperature can exhibit horizontal differences. The shallower water near the shore of a lake warms and cools more rapidly than the deeper regions, leading to differential warming and cooling of pelagic and littoral regions and distinct horizontal and vertical circulation patterns (Imberger and Patterson 1990; Farrow and Patterson 1993; Peeters et al. 2003). Despite a growing interest in the spatial variability of substances and processes within lakes (Yurista and Kelly 2007; Van de Bogert et al. 2012), studies of spatial variability that also incorporate temporal scales of variability are still rare (but see Akyuz et al. 2014; Guadayol et al. 2014).

Among the reasons why the variability of lake WT is often neglected, despite the fact that it is a fundamental property of lakes and plays a crucial role for lake biota, are its inherent multi-faceted nature and the fact that the quantification of variability is far less straightforward than the quantification of average conditions (Coble et al. 2016). A wide variety of statistical descriptors are commonly used to quantify the variability of a time series: e.g., the second and higher moments of the probability density function; range; coefficient of variation; median absolute deviation; and interquartile range (for an overview see Heath 2006; Fraterrigo and Rusak 2008). However, all of these descriptors have one major disadvantage: they are unable to account for any dependence on temporal scale, as they fail to distinguish between short-term (high-frequency) and long-term (low-frequency) variability. Thus, they are all dominated by the variability of the underlying (long-term) temporal scales. Yet, short-term temperature variability and long-term temperature variability are likely to affect the (aquatic) ecosystem in different ways (Litaker et al. 1993; Steele et al. 1994; Fischer and Schär 2009; Benincà et al. 2011; Adrian et al. 2012; Foster et al. 2014). Therefore, a method capable of resolving the total variance of a time series into its frequency components, or at the very least, partitioning it into coarse frequency bins, is required to adequately address the variability of a time series on different temporal scales. Spectral analysis based on the Fourier Transform (e.g., Bloomfield 2000) is an appropriate method for accomplishing this.

Here, we document patterns in the WT variability of a shallow, polymictic lake, a lake type in the transition zone likely to switch from polymixis to dimixis under future climate scenarios (Kirillin 2010; Shatwell et al. 2016). Specifically, we ask what are the temporal and spatial scales of water temperature variability, and what impact do the most important drivers of WT variability – air temperature variability, seasonality, ice cover, stratification stability and mixing dynamics – have? We base our study on a unique 22-year-long data set of daily near-surface WT measured at the shore and in the open water in Müggelsee, applying Fast Fourier Transform (FFT) spectral analysis over time windows of years, seasons and months and analyzing temporal scales from days to years. The results of our study contribute to a better understanding of the specific characteristics of lake WT variability on different temporal and spatial scales and at different times during the course of a year.

3.2 Methods

3.2.1 Study site

Our study site, Müggelsee, is a well-studied, shallow, polymictic lake in Berlin, Germany, with a surface area of 7.3 km^2, a mean depth of 4.9 m and a maximum depth of 7.9 m (Fig. 3.1; Driescher et al. 1993). The River Spree flows through the lake, resulting in a theoretical

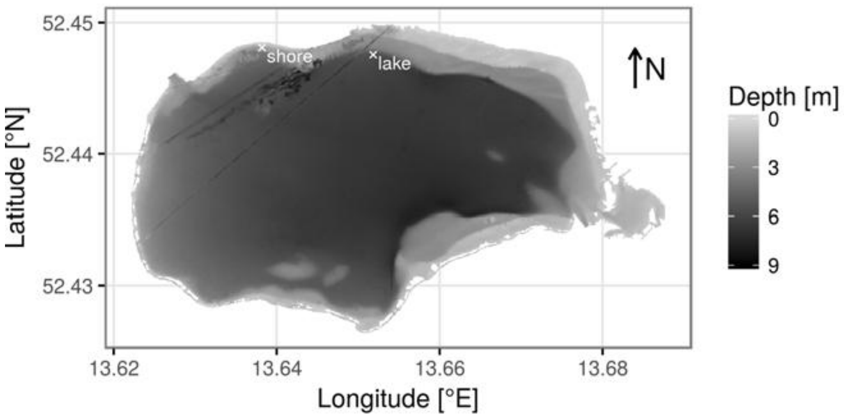

Fig. 3.1: Bathymetric map of Müggelsee with sampling locations.

retention time of about 6-8 weeks (Köhler et al. 2005). Because of its mainly east-west orientation and the dominance of westerly winds in the region, the lake is very much exposed to wind. Wind speeds are highest from November to April and lowest in August and September (Fig. S3.1; Driescher et al. 1993). Müggelsee is situated in a geographic region where the severity of winter is highly variable. Thus, depending on the winter, ice cover on the lake can be either continuous, intermittent or completely absent (Adrian and Hintze 2000). In the long term, however, the overall duration of annual ice cover exhibits a decreasing trend (Livingstone and Adrian 2009). As a polymictic lake, Müggelsee is characterized by irregular shifts between mixed and stratified conditions. These shifts occur mainly during the growing season (April to September). Most stratification events last less than 24 hours (Wilhelm and Adrian 2008), but longer stratification events can last from 1-2 weeks up to a maximum of 8 weeks (Wagner and Adrian 2009). Müggelsee is eutrophic, with intense algal blooms occurring in spring and summer that may affect the thermal structure and mixing dynamics of the lake, and hence the variability of its WT (Shatwell et al. 2016). Internal seiches are present throughout the year (Lorke 1998; Wüest and Lorke 2003) and occur even in winter under ice (Kirillin et al. 2012).

3.2.2 Data sets

Near-surface water temperatures have been measured near the northern shore of Müggelsee since 1994. These measurements were made daily, between 08:00 h and 09:00 h local time, at a mean depth of 0.8 m, using a YSI multi-parameter probe (6600 V2 sonde, with a resolution of 0.01 K and an accuracy of ±0.15 K. The measurement location changed once during the measurement period. From 1994 until 2002, the probe was deployed at a jetty 30 m from the shore (52°26′48.1″N; 13°38′10.9″E), where the lake is about 2 m deep (henceforth termed the "shore" location). In the year 2002, a measuring station was put into operation 300 m from the shore (52°26′46.1″N; 13°39′0.2″E), where the lake is 5.3 m deep (henceforth termed the "lake" location). In winter, measurements were continued under the ice cover at a depth of about 1.5 m. In 2002, when the measurement location was changed, simultaneous measurements were made at both locations on 98 days between June and September. Aside from this overlap, the shore measurements (1994-2002) and the lake measurements (2002-2015) were performed during consecutive time periods. During the period of simultaneous WT measurements, WT was found to be on average 0.1 K higher at the lake station than at the shore station. This difference was therefore added to the shore measurements. No macrophytes were present at either location.

To determine whether any patterns found in WT were generated by internal lake processes or by local weather, we compared WT at the two locations with AT measured at Schönefeld Airport, located approximately 10 km from Müggelsee. This enabled us to attribute differences between the time series from the shore and lake locations to either a location effect or a time effect, which would otherwise have confounded each other.

3.2.3 Data preparation

The analysis of the data sets was conducted separately for three time windows: annual, seasonal and monthly scales (Fig. 3.2a). To guarantee uniformity for each time window, each year was defined as consisting of 365 consecutive days (discarding 31 December in leap years). The year was divided into four seasons of 92 days each, with a one-day overlap between consecutive seasons, as follows: winter, Julian days 1-92 (1 January – 3 April in non-leap years); spring, Julian days 92-183 (3 April – 2 July in non-leap years); summer, Julian days 183-274 (2 July – 1 October in non-leap years); and fall, Julian days 274-365 (1 October – 31 December in non-leap years). Lastly, the year was divided into 12 months of 31 days each, also with a one-day overlap between consecutive months. January was defined as Julian days 1-31; February as Julian days 31-61 (31 January – 2 March in non-leap years); March as Julian days 61-91 (2 March – 1 April in non-leap years); etc.

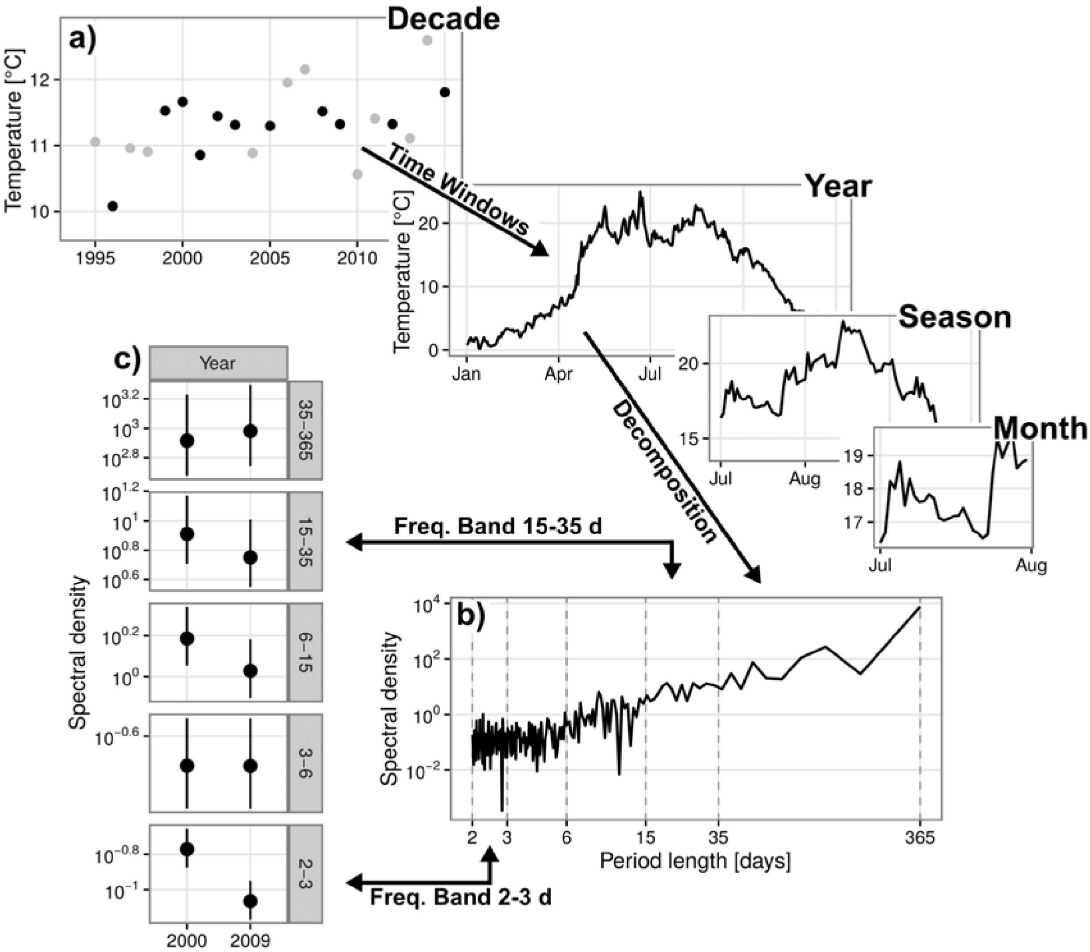

Fig. 3.2: Illustration of the study approach. **(a)** Annual mean near-surface water temperature (*black*, complete years; *gray*, years containing gaps) with examples of annual, seasonal (summer) and monthly (July) time series for the year 2000. **(b)** Fourier spectrum of Müggelsee near-surface water temperatures from the year 2000; the five frequency bands used for frequency-band averaging, corresponding to period lengths of 2-3, 3-6, 6-15, 15-35 and 35-365 days, are shown as *dashed vertical lines*. **(c)** Spectral means over these five frequency bands with 95 % confidence intervals for the years 2000 and 2009.

There were 212 gaps in the WT time series, ranging from 1 to 100 days in duration and accounting for 10 % of the total number of days in the time series. Gaps of 3 days or less accounted for 78 % of the total number of gaps. As spectral analysis by FFT requires regularly spaced data, interpolation was necessary to increase the sample size. Recognizing that interpolation may distort the variability structure of the data, and hence the spectrum, we developed a decision procedure to define which gaps to interpolate over and which data to exclude from the analyses, as follows. To estimate the influence of interpolating missing values on the calculation of monthly means, all months in the WT data set that contained no gaps were used to calculate “true” monthly means. Then, gaps of increasing duration from 1 day up to a maximum of 29 days were created within this data set; these gaps were furthermore shifted to all possible positions within each month. The gaps were then filled by linear interpolation and a new “artificial” mean value was calculated. For each month, the deviation of the artificial from the true mean was calculated. This deviation was found to vary during the course of a year, being greatest during summer and least during winter. The criterion for interpolating over a gap was based on the mean absolute deviation. This was calculated separately for each gap length (1-29 days) and for each month of the year (January – December) as the mean of all absolute deviations for all possible positions of a gap of the given length within the given month. The maximum acceptable mean absolute deviation for interpolating over a gap was set at 0.15 K. Application of this criterion to each month of the year separately resulted in maximum gap lengths acceptable for interpolation that varied seasonally, being shorter in summer than in winter (Table 3.1). At the end of this procedure, a total of 457 gap days had been filled by interpolation, corresponding to 56 % of all gap days and 6 % of all days over the whole 22-year time series from 1994 to 2015. To make sure that the linear interpolation did not overly bias the WT variability patterns by damping the signals from the interpolated sections, the analyses were additionally run over those sections of the original data set that were without gaps. This resulted in the same overall patterns as the results gained from the interpolated data set.

Table 3.1: Outcomes of the gap filling procedure. *Mean dev*: Absolute mean deviation of "artificial" monthly mean water temperature (WT) (after linear interpolation of artificially created gaps) from "true" monthly mean WT (before the creation of artificial gaps) [K]. *Max dev*: Maximum deviation of "artificial" monthly mean WT from "true" monthly mean WT [K]. *Length*: Maximum duration of created gaps [days].

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Mean dev	0.13	0.15	0.14	0.14	0.13	0.14	0.12	0.13	0.15	0.14	0.15	0.15
Max dev	0.58	0.56	0.50	0.86	0.46	0.73	0.48	0.47	0.60	0.60	0.54	0.67
Length	14	16	12	8	7	7	6	8	11	10	12	13

3.2.4 Statistical approach

To analyze the frequency dependence of the variability within the WT time series we calculated FFT power spectra over time windows of years, seasons and months of the 22-year data set using

$$X_k = \frac{1}{N} \sum_{t=0}^{N-1} x_t e^{i2\pi k \frac{t}{N}} \tag{3.1}$$

where X_k = discrete Fourier Transform at frequency $k = 0, \ldots, N-1$ of the time series x of length N at time t (Cooley and Tukey 1965; Singleton 1969). This gives the power spectral density S_k at frequency k as

$$S_k = |X_k|^2 \tag{3.2}$$

The mean was subtracted and the trend removed from each time window prior to analysis, and no zero-padding was applied. The power attributed to a specific frequency (i.e., the spectral density at that frequency) gives a measure of the magnitude of the variability at that frequency. A high spectral density thus implies a strong ("highly variable") signal at that frequency. In the present context, high frequencies (i.e., short periods) represent "short-term" (daily to weekly) variability, medium frequencies represent "medium-term" (weekly to monthly) variability, and low frequencies represent "long-term" (monthly to yearly) variability. To improve the statistical robustness of the spectra obtained, frequency-band averaging was used to increase the number of degrees of freedom, yielding coarse, low-resolution spectra well-suited to the purpose of this study. Five frequency bands were defined corresponding to periods $1/k < 3$ days; 3 days $\leq 1/k < 6$ days; 6 days $\leq 1/k < 15$ days; 15 days $\leq 1/k < 35$ days; and $1/k \geq 35$ days. All five were used for the annual windows (up to 365 days) and the seasonal windows (up to 92 days), and the first four of these for the monthly windows (Fig. 3.2b). As an example, the mean spectral estimates for these five frequency bands are illustrated in Fig. 3.2c for the years 2000 and 2009.

For each location (shore or lake), the resulting estimates for each spectral band and time window were averaged to yield one annual spectrum, four seasonal spectra and twelve monthly spectra per location and spectral band. For each aggregation, 95 % confidence intervals were calculated based on the distribution df/χ^2_{df}, with df = number of degrees of freedom. As spectra were calculated without tapering or smoothing, there are two degrees of freedom associated with each initial spectral estimate. Averaging across i neighboring frequencies and j spectra increases df by the factor ij. No overlap in confidence intervals implies a statistically significant difference between estimates at the 95 % level, which is a very conservative approach (Payton et al. 2003). Hereafter, all references to statistical significance imply non-overlapping 95 % confidence intervals (Fig. 3.2c). A potential source of error in spectral analysis is the aliasing of power at frequencies greater than the Nyquist frequency (0.5 cycles per day). However, a comparison of daily and hourly WT data from 2009 showed this to be unlikely (Fig. S3.2), as the spectrum of the daily data (with a Nyquist frequency of 0.5 c/d) differed only slightly from the spectrum of the hourly data (with a Nyquist frequency of 12 c/d).

The scaling behavior of WT variability from low to high frequencies was characterized as the slope of the non-aggregated power spectrum, calculated by simple linear regression of the $\log_{10}$-transformed spectral density on the $\log_{10}$-transformed frequency. The slope of the spectrum, sometimes described in terms of "noise color" (e.g., Vasseur and Yodzis 2004), gives a rough characterization of the dependence of WT variability on frequency. A (steep) negative slope implies a red-noise or brown-noise spectrum, in which low-frequency variability exceeds high-frequency variability; a (steep) positive slope implies a blue-noise or violet-noise spectrum, in which high-frequency variability exceeds low-frequency variability; and an approximately flat slope implies a white-noise spectrum, in which low-frequency variability and high-frequency variability are similar.

3.2.5 Drivers of WT variability

The AT data were subjected to a similar procedure to that used for the WT data to allow direct comparison between the two. To ensure consistency with the WT data, only those AT measurements recorded on days on which WT was also measured were included in the analysis. The AT spectra were averaged over the time windows during which the corresponding WT was measured at the same location (shore or lake). As AT was always measured at the same nearby location, differences in the statistical properties of WT measured at the two locations (the early data from the shore station and the later data from the lake station) could be attributed either to a time effect (if AT showed similar differences in variability between the early and later years), or to a location effect (if AT variability did not change over the entire time period). Seasonality in WT and AT was accounted for by calculating monthly means.

Internal lake processes that we related to monthly WT spectra were taken into account as follows. The intensity of thermal stratification was determined from hourly WT profiles by calculating the monthly mean Schmidt stability, which quantifies the overall resistance of a water body to mechanical mixing (Schmidt 1928; Idso 1973). The Wedderburn number, which describes the potential for upwelling events in lakes (Imberger and Patterson 1990), was calculated from hourly WT profiles and local hourly wind speed measurements. The Lake number (Imberger and Patterson 1990) was also calculated from hourly WT profiles and local hourly wind speed measurements to quantify the degree of internal mixing due to internal waves induced by wind stress during stratified conditions. To relate hourly calculations of the Wedderburn number and Lake number to monthly WT spectra, we tested different percentiles of the $\log_{10}$-transformed Wedderburn and Lake numbers for monthly time windows, and their ability to explain identified patterns. As WT profiles were available only at the lake location, the Schmidt stability, Wedderburn number and Lake number could be calculated only for this location. The duration of ice cover was defined as the percentage of days per month during which more than 80 % of the lake surface was covered with ice (Adrian and Hintze 2000). Trends were calculated from simple least squares regression and considered significant if p-values were < 0.05.

A comparison of the variability derived from the FFT power spectra with the standard deviation as a more traditional variability metric is given in the supporting information.

All analyses were performed using R (R Core Team 2015). Power spectra were calculated using the function spec.pgram of the R package stats (R Core Team 2015), Schmidt stability and Lake number were calculated using the R package rLakeAnalyzer (Read et al. 2011; Winslow et al. 2014), and graphics were created using the R package ggplot2 (Wickham 2009).

3.3 Results

We analyzed the variability in WT, quantified as spectral density, in 22 years of daily near-surface water temperature from Müggelsee (1994-2015) at different temporal scales (days to years) and spatial scales (open water, near shore). Measurement location, air temperature variability, seasonality, stratification stability, mixing dynamics and ice cover were tested as potential drivers of WT variability.

3.3.1 Slopes of spectra

For the majority of time windows, the spectral densities in the spectra of the WT time series increased from high frequencies (short-term variability, with a minimum period of 2 days) to low frequencies (long-term variability, up to a period of 365 days) (Fig. 3.2b), corresponding to a red-noise spectrum. The slopes of the spectra characterize this scaling behavior. In order to investigate the explanatory power of the slopes of the spectra of WT, we tested their relationship to the limnological indicators Schmidt stability, Wedderburn number and Lake number. The slopes of the monthly WT spectra were found to decrease significantly with an increase in the 1st percentile of the $\log_{10}$-transformed Lake number ($p < 0.0001, r^2 = 0.2$; Fig. 3.3). Monthly spectra with steep negative slopes were associated with high values of the 1st per-

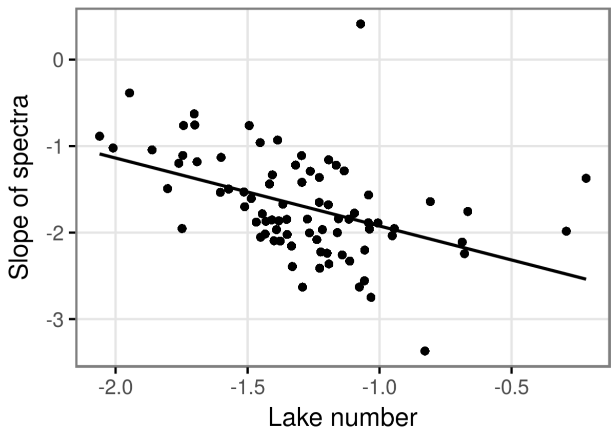

Fig. 3.3: Slopes of monthly spectra of near-surface water temperature measured at the Müggelsee lake station as a function of the 1st percentile of the $\log_{10}$-transformed Lake number.

centile of the $\log_{10}$-transformed Lake number, implying a strong, stable thermal stratification with little potential for vertical mixing through the action of wind-induced nonlinear internal waves. On the other hand, monthly spectra with flat slopes were associated with low values of the 1st percentile of the $\log_{10}$-transformed Lake number, implying a high potential for mixing by wind-induced nonlinear internal waves. The relationship was also highly significant with other, especially low, percentiles and the mean of the Lake number. Furthermore, different percentiles of the $\log_{10}$-transformed Wedderburn number also exhibited a significant relationship with the slopes of the WT spectra, but the Schmidt stability, for instance, did not. The relationship with the 1st percentile of the $\log_{10}$-transformed Lake number had the lowest p-value and explained most of the variance, and is therefore the one shown here. Low percentiles of the Lake number characterized the probability of incipient occurrence of internal waves during stratified conditions better than higher percentiles, and better than any other of the limnological indicators tested.

3.3.2 Differences in WT variability between shore and lake locations

In almost all years, seasons and months, WT variability was higher at the shore station than at the lake station at all temporal scales investigated (Fig. 3.4). In the annual time windows,

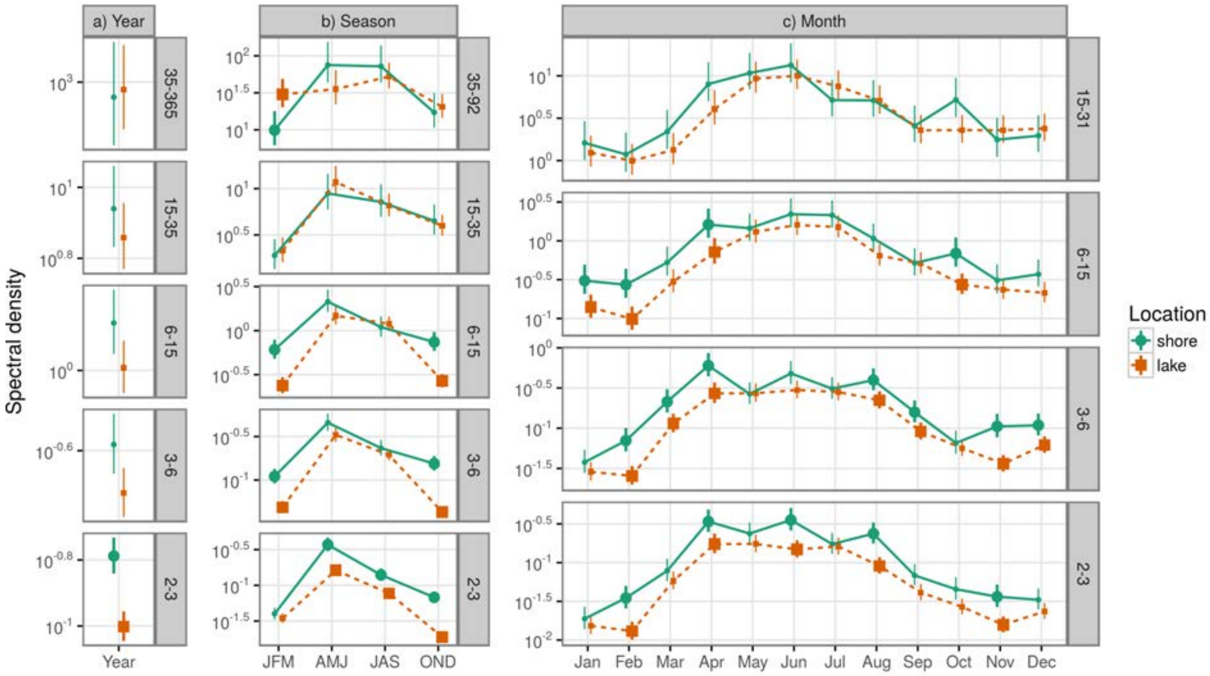

Fig. 3.4: Spectral density (with 95 % confidence intervals) of near-surface water temperature measured at the Müggelsee shore station and lake station, averaged over five frequency bands for time windows of **(a)** years, **(b)** seasons and **(c)** months. *Large dots* represent estimates of spectral density with non-overlapping confidence intervals within one frequency band and time window (significant difference between locations); *small dots* represent estimates with overlapping confidence intervals. Note logarithmic scale on y-axes.

this was found for daily to monthly variability, although only the daily variability differed significantly between the two stations (Fig. 3.4a). In 7 seasonal time windows (Fig. 3.4b) and 16 monthly time windows (Fig. 3.4c), distributed over the whole year for daily to biweekly variabilities, differences were significant. The only exception to this, with variability at the shore station significantly lower than at the lake station, was the long-term variability in the winter season (Fig. 3.4b). In 2002, when parallel measurements were conducted at the shore and lake stations, we also found short-term variability to be higher at the shore station (results not shown). The slopes of the mean annual, seasonal and monthly spectra of the WT measured at the shore location were generally flatter than the slopes of the corresponding spectra of the WT measured at the lake location (Fig. 3.5).

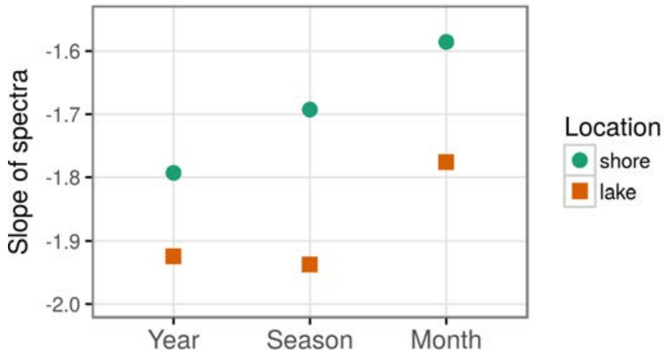

Fig. 3.5: Slopes of the mean annual, seasonal and monthly spectra of near-surface water temperature measurements at the Müggelsee shore station and lake station.

In some cases, AT showed higher variability during the time windows when WT measurements were available from the shore station than during the time windows when WT was measured at the lake station (Fig. S3.3a-c). However, for daily to weekly AT variability, significant differences between the shore station and lake station time windows were found only in three seasons (spring, summer and fall) and three months (April, September and November). In fact, the daily variability of AT showed a significant decreasing trend over time during the 22 years investigated, but trends in AT variability at temporal scales longer than one day were not significant (results not shown).

3.3.3 Seasonality

Within the seasonal cycle, the WT variability in the monthly time windows increased significantly with increasing WT from winter to summer and decreased significantly with decreasing WT from summer to winter over all frequency bands (Fig. 3.6a). This relationship depended on the month of the year: variability was lowest in January and February and highest between April and July. Seasonality in WT variability was, however, not dependent solely on mean WT: variability was much higher in spring months (March to May) than in fall months (September to November), despite the similarity in monthly mean WT in these two seasons. These differences between spring months and fall months were greatest for short-term variability and decreased with increasing temporal scale (Fig. 3.6a).

No differences between spring and fall were present in AT variability, which showed very little change during the course of the year, despite a slight, but significant, decrease in variability with increasing mean AT (Fig. 3.6b).

To further investigate the most prominent differences in WT variability detected within the seasonal cycle – i.e., those between spring and fall – we compared the slopes of the spring and

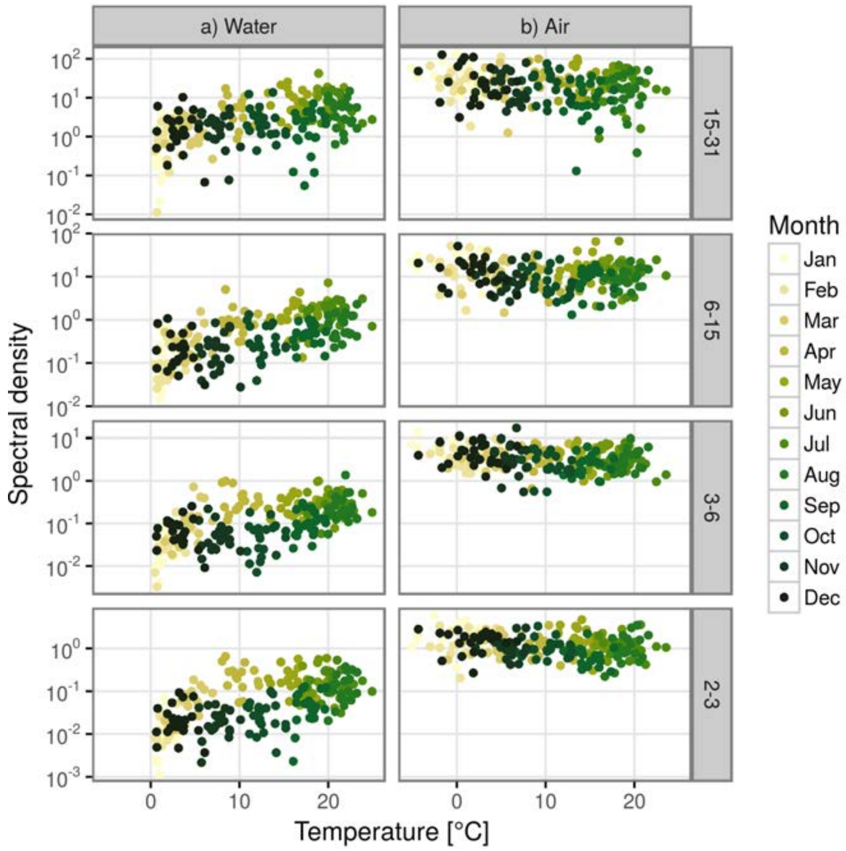

Fig. 3.6: **(a)** Spectral density of near-surface water temperature (WT) in Müggelsee in each of four frequency bands as a function of monthly mean WT, grouped by month of the year. **(b)** Spectral density of air temperature (AT) measured at Schönefeld airport as a function of monthly mean AT, grouped by month of the year. Note logarithmic scale on y-axes.

fall WT spectra. The slopes of the monthly spectra of WT measured in spring (March to May) were significantly less steep (i.e., flatter) than the slopes of the monthly spectra of WT measured in fall (September to November; Wilcoxon rank sum test, $p < 0.001$; Fig. 3.7).

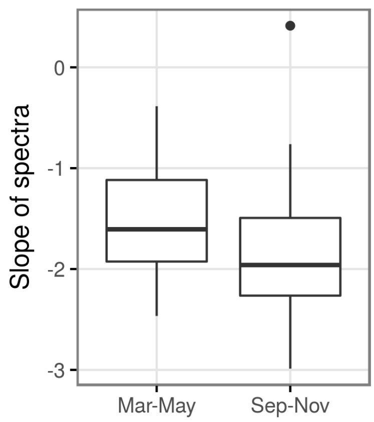

Fig. 3.7: Box plots of slopes of monthly spectra of near-surface water temperature in Müggelsee measured in spring (March to May) and fall (September to November).

3.3.4 Stratification stability, wind-induced mixing and ice cover

WT variability increased significantly with increasing Schmidt stability (*St*) in all frequency bands for values of monthly mean *St* up to ~20 J m^{-2} (Fig. 3.8a). From November to March the lake was mixed in all years and *St* was therefore very close to zero. In spring (March to May), WT variability was higher than in fall (September to November), although *St* was similar. Furthermore, WT variability decreased significantly with increasing 1st percentile of the $\log_{10}$-transformed Lake number for daily to weekly variabilities, but not for longer timescales (Fig. 3.8b). In months with potential ice cover (December – March), the WT variability decreased with increasing ice-cover duration (Fig. 3.8c). This decrease was significant for the shore station at all frequency bands (with higher significance levels for short-term variability) and for the lake station at all frequency bands except daily variability.

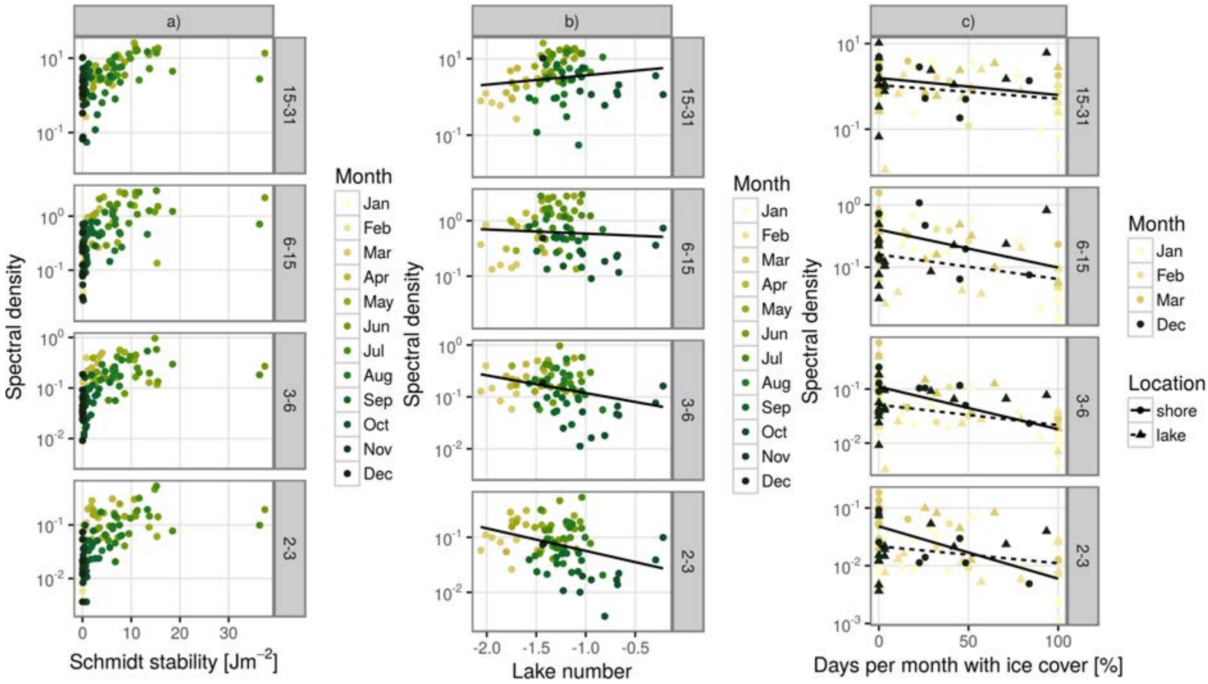

Fig. 3.8: **(a)** Spectral density of near-surface water temperature (WT) measured at the Müggelsee lake station in each of four frequency bands as a function of the monthly mean Schmidt stability. **(b)** Spectral density of near-surface WT measured at the Müggelsee lake station in each of four frequency bands as a function of the 1st percentile of the $\log_{10}$-transformed Lake number. *Black lines* represent the linear regression fits to the data. **(c)** Spectral density of near-surface WT measured at the Müggelsee shore station and lake station, averaged over four frequency bands, as a function of the percentage of days per month during which the lake was ice-covered. *Black lines* represent linear regression fits to the data. Note logarithmic scale on y-axes.

To further investigate the differences identified in the winter WT spectra (December to March), we compared the slopes of the spectra in "warm" winter months (mean monthly temperature above the median) to those in "cold" winter months (mean monthly temperature below the median). The slopes of the spectra of WT measured at the shore location were significantly flatter in warm winter months than in cold winter months (Wilcoxon rank sum test, $p < 0.001$; Fig. 3.9). The slopes of the spectra of WT measured at the lake location were slightly steeper in warm winter months than in cold winter months (Wilcoxon rank sum test, $p < 0.05$; Fig. 3.9).

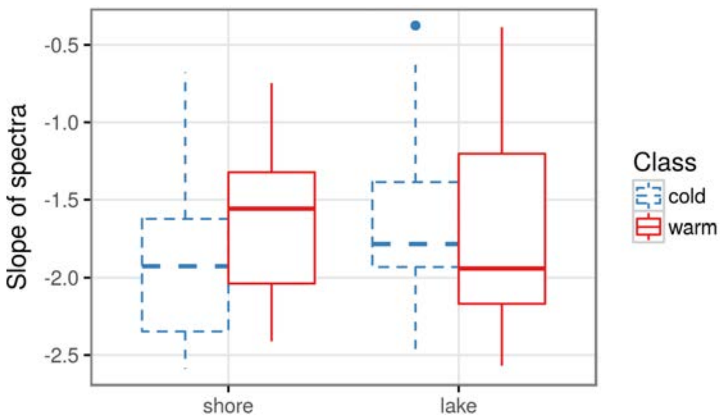

Fig. 3.9: Box plots of slopes of monthly spectra of near-surface water temperature in Müggelsee measured in "cold" (mean annual, seasonal or monthly temperature below the median) and "warm" (the same above the median) winter months (December to March).

3.4 Discussion

To elucidate patterns of WT variability and their drivers, we analyzed short-term to long-term WT variability at temporal scales ranging from days to years. Overall, we found: higher WT variability at the shore station than at the lake station; seasonally specific differences in WT variability although mean WTs were similar (spring / fall); increasing WT variability with increasing stratification stability; decreasing short-term WT variability with increasing probability of occurrence of wind-induced internal waves; and decreasing WT variability with increasing ice-cover duration. Patterns of variability in AT differed from those in WT. The slope of the WT spectra turned out to be a good indicator for identifying patterns of WT variability. In the following, we discuss the temporal and spatial scales of WT variability and their potential drivers.

3.4.1 Spatial variability

On all time-scales, WT variability was higher at the shore station than at the lake station (Fig. 3.4). However, as most WT measurements at the two stations were not conducted simultaneously, this difference could not immediately be attributed solely to the difference in measurement location. Short-term variability in AT exhibited a significant decreasing trend with time, implying that the lake was exposed to a higher short-term variability in AT during the earlier years, when WT was measured at the shore station, than during the later years, when WT was measured at the lake station (Fig. S3.3). However, the differences in AT variability between the earlier and later years were significant in only a few months and seasons, and were undetectable at longer temporal scales (weeks to years). The parallel measurements conducted at both locations in 2002 also showed WT variability to be substantially higher at the shore station than at the lake station. This suggests that the observed differences can be attributed at least in part to the difference in measurement location. Hence, for WT, a trend toward decreasing short-term variability with time, induced by external climatic forcing, would seem to be superimposed on a location effect.

The flatter slopes of the spectra of WT measured at the shore station (Fig. 3.5) indicate higher short-term variability and a higher potential for vertical mixing by nonlinear internal waves at the shore (Fig. 3.3). At the lake station, on the other hand, the slopes of the spectra were steeper, indicating that the influence of internal waves was weaker. The shallower water at the shore station likely responds more directly to meteorological forcing than does the deeper water at the lake station due to the limited heat capacity of the smaller water volume near shore (Farrow and Patterson 1993; Benincà et al. 2011). This so-called differential warming and cooling between the shore and the open water, which can result in horizontal temperature differences between the pelagic and littoral regions of lakes (Imberger and Patterson 1990; Farrow and Patterson 1993; Peeters et al. 2003), might also result in WT variability close to the shore being higher than in the open water.

Assuming that inflowing water from the River Spree, the main inflow to Müggelsee, mixes rapidly into the lake (Barthelmes 1962), any influence of Spree water on the variability of the lake WT at the distant lake station is likely to be slight. Moreover, the potential impact of groundwater flowing into the lake can most likely be neglected. At the lake station, located ~300 m offshore, where the lake is 5.5 m deep, the influence of groundwater on the lake is insignificant (Driescher et al. 1993). At the shallower shore station, where the lake depth is only 2 m, continuous groundwater withdrawal along the shore is likely to reduce any influence of groundwater on the lake water.

Overall, although the potentially confounding factors of location and time are difficult to disentangle, the higher reactivity of the smaller water volume and the higher probability of occurrence of wind-induced internal waves at the shore location would seem to be the most important drivers of the greater degree of short-term variability observed there. This agrees with Guadayol et al. (2014), who found – albeit in a very different system – all analyzed WT variance components, ranging from hourly to weekly time scales, to decrease with distance from the shore along a transect in a shallow coastal coral reef. On the other hand, Lorke et al. (2006) found WT variability at a nearshore station in Lake Constance to be only slightly higher than at an offshore station for timescales between 10 and 15 min, and no difference at longer timescales up to several days. However, the nearshore location used in their study was 75 m offshore at a depth of 19 m and hence represented a substantially larger water volume than the shore location used in our study.

3.4.2 Seasonal variability

In all frequency bands, WT variability was lowest in fall and winter, highest in spring and summer and higher in spring than in fall at similar mean WT (Fig. 3.6a). This was not the case for ambient AT, which exhibited no such seasonal differences in variability (Fig. 3.6b). Thus, there seem to be seasonally dependent physical processes at work which modify the link between AT and WT variability (MacKay et al. 2009). To our knowledge, a dependence of the seasonality of WT variability on frequency has not yet been discussed in the limnological literature.

The seasonal differences were reflected in the apparent dependence of WT variability on thermal stratification and mixing dynamics. WT variability increased with increasing intensity of thermal stratification (Fig. 3.8a) and decreased with decreasing potential for vertical mixing through the action of wind-induced internal waves (Fig. 3.8b). Although the mean WT was similar in spring and fall, the WT variability was higher in spring than in fall (Fig. 3.6a) and the slopes of the spectra were flatter (Fig. 3.7). This indicates a higher potential for high-frequency internal waves in spring than in fall (Figs. 3.3, 3.8b), leading to the observed higher WT variability, especially on short temporal scales. This higher variability in spring and summer WT is in line with the findings of Woolway et al. (2016), who describe substantially larger diel temperature ranges in summer than in winter in 100 temperate and boreal lakes. The seasonal pattern of Schmidt stability (Read et al. 2011; Sadro et al. 2011) suggests that from spring to summer, an epilimnion of varying thickness is often present in this polymictic lake. Such an epilimnion will respond more sensitively to climatic forcing than would a completely mixed larger water body (Lampert and Sommer 2007), leading to higher WT variability in the epilimnion than during periods when the lake is well-mixed. In summer the external input of heat to the lake reaches a maximum, resulting in increased thermal stratification (Fig. 3.8a), while mean wind speeds are lowest (Fig. S3.1). The reduced wind stress hence had less effect on the thicker epilimnion, leading to higher Lake numbers (Fig. 3.8b) and only slightly higher WT variability in summer than in spring. In fall on the other hand, the water column was already almost completely mixed (Fig. 3.8a) and wind-induced internal waves were less likely (Fig. 3.8b). This resulted in reduced WT variability.

It might be anticipated that the observed warming of Müggelsee during the past few decades (O'Reilly et al. 2015) will lead to more frequent and longer periods of thermal stratification, and possibly to a thermal regime shift (Livingstone 2003, 2008; Kirillin 2010; Shatwell et al. 2016). This would result in a generally thicker epilimnion with lower WT variability. This hypothesis is supported by the two months in the data set (June and July 2006) that exhibited exceptionally long stratification periods and relatively high monthly mean Schmidt stabilities of over $30\,\mathrm{J\,m^{-2}}$ (with daily values up to $80\,\mathrm{J\,m^{-2}}$), but only medium levels of WT variability (Fig. 3.8a). If this hypothesis is correct, such changes in thermal regime may tend to counteract the increases in lake water temperature variability that might otherwise be expected to occur as a result of global warming (Wilhelm and Adrian 2008; Nickus et al. 2010; Guadayol et al. 2014; Coble et al. 2016).

Ice formation in winter reduces the external energy input to the lake and imposes a lower limit (0 °C) on the WT. WT variability in winter was related to the duration of ice cover and tended to be low in months when the lake was ice-covered most of the time; i.e., in colder months (Fig. 3.8c). This was also reflected in the steeper slopes of the WT spectra at the shore location in cold winter months as compared to warm winter months. These steeper slopes resulted from the lower short-term variability in cold winter months, during which the lake was often ice-covered (Fig. 3.9). Obviously, the presence of ice on a lake drastically reduces the influence of meteorological forcing on the lake, which will likely result in a reduced WT variability under ice. Kirillin et al. (2012) have shown that internal seiches also occur under ice, albeit with lower amplitudes and lower current speeds than during ice-free periods. Such internal seiches may well occur in Müggelsee at the measurement depths considered here (Kirillin et al. 2009). At the lake location, ice cover did not have much effect on the already very low WT variability, which may indicate that direct heating of littoral sediment by solar radiation adds to the WT variability at the shore location in winter, but not at the lake location. Furthermore, the ice may be thinner toward the center of the lake, enabling a greater influence of solar radiation there.

Overall, the observed high degree of heterogeneity in WT variability patterns may stem from the high degree of variation in two major internal drivers of variability – ice cover and mixing dynamics during thermal stratification. Both of these drivers are themselves characterized by strong alterations within shallow lakes in this geographical area as a consequence of natural climate variability and global warming. Müggelsee, for example, experiences either no ice cover, intermittent ice cover, or continuous ice cover depending on the severity of winter (Livingstone and Adrian 2009). Although the thermal stratification in Müggelsee in summer is undergoing a general long-term increase as mean WT increases (Wagner and Adrian 2011), it is also characterized by short-term alternations between mixed and stratified periods of different duration depending on the weather, especially wind stress. These propagating and overlapping effects of internal physical and biological drivers of WT variability modify the direct link between AT and WT variability. Thus, the weak link between AT and WT variability found in our study is not surprising. This is in line with the counterintuitive result that regional consistency in observed lake WT warming trends on a global scale is the exception rather than the rule (O'Reilly et al. 2015). All in all, a warmer climate may have pronounced effects on WT variability in polymictic lakes. Climate warming, associated with shorter periods of ice cover in winter and longer periods of stratification in summer, will increase WT variability in these seasons in the medium term, but may in the long term decrease WT variability in summer as a result of a decrease in the frequency of mixing events.

3.4.3 The slope of a spectrum as an indicator for mixing dynamics

The relationship between the slope of a spectrum of near-surface WT and a low percentile of the Lake number (Fig. 3.3) indicated that WT spectra scale according to the potential for wind-induced vertical mixing. White-noise spectra, in which short-term and long-term variability components exhibit similar intensity, were associated with a high potential for vertical mixing, while red-noise spectra, in which the intensity of long-term variability exceeds that of short-term variability, were associated with more stable thermal stratification and little potential for vertical mixing. The ecological relevance of internal waves and mixing dynamics is well established in the limnological literature, and its effect has been shown, for example, on phytoplankton distribution and productivity (Spigel and Imberger 1987), spatial patterns of zooplankton (Pernica et al. 2013) and changes in oxygen concentration (Robertson and Imberger 1994; Hanson et al. 2006). In Müggelsee, short-term vertical mixing has been shown to be responsible for the vertical transport of algae, influencing primary production (Nixdorf et al. 1992), and for variations in oxygen concentration and the release of phosphorus from the sediment (Behrendt et al. 1993).

Here, the slope of WT spectra turned out to be a good indicator for identifying patterns of WT variability. Spatial differences were related to the slope of WT spectra such that the probability of occurrence of wind-induced internal waves and vertical mixing was higher at the shore station, where WT exhibited higher variability than at the lake station. Similarly, the slope of the WT spectra explained the fact that WT variability was higher in spring months than in fall months. Lastly, it showed that the variability of WT measured close to the shore in winter is significantly reduced if the lake is covered with ice. This is not the case in pelagic regions, however, where the influence of the sediment is smaller due to the greater water depth and the ice may be thinner. These examples highlight the potential usefulness of the slope of WT spectra as an indicator for lake mixing. This is especially the case when a lack of WT depth profiles or wind speed measurements precludes the calculation of other indicators of mixing dynamics such as the Lake number. In the present study, this was the case for measurements at the shore location, and also for measurements at the lake location when the lake was ice-covered. The slope of WT spectra would therefore seem to be a promising indicator for assessing WT dynamics. However, the generality of its usefulness beyond polymictic lakes remains to be tested in lakes exhibiting different mixing regimes.

3.4.4 Conclusions

To reveal timescale-dependent differences in lake water temperature variability, both high-resolution data and an adequate method of analysis that is capable of separating short-term from long-term variability are required. Here, a coarse spectral analysis was demonstrated to be a suitable method of accomplishing this granular analysis. It was found that WT variability depended not only on the temporal scale, but also on the measurement location (littoral or pelagic).

We also showed that the occurrence of seasonal events such as ice cover and stratification, which are both strongly coupled to climate warming, played a crucial role in determining WT variability. We identified differences in WT variability especially in short-term cycles. Hence, when studying environmental variability, we consider it crucial to take into account higher-frequency (sub-monthly) variability. The use of the slope of the spectra of WT as an indicator for lake mixing proved to be promising for assessing WT variability. It may be especially useful when measurements of wind speed and/or depth profiles of WT are not available for the calculation of more usual indicators of mixing dynamics, such as the Lake number. The specific scaling of WT variability with respect to frequency – the slope of the spectrum – can resonate in biological communities, inducing large oscillations in species abundances (Benincà et al. 2011). This may contribute to the unexplained day-to-day and interannual temporal dynamics of aquatic communities, which represents an ongoing challenge in plankton ecology. The resolution of variability into different frequencies might help to explain short-term and long-term ecological patterns that are linked to temperature.

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SI Supporting information

SI.1 Supplementary figures

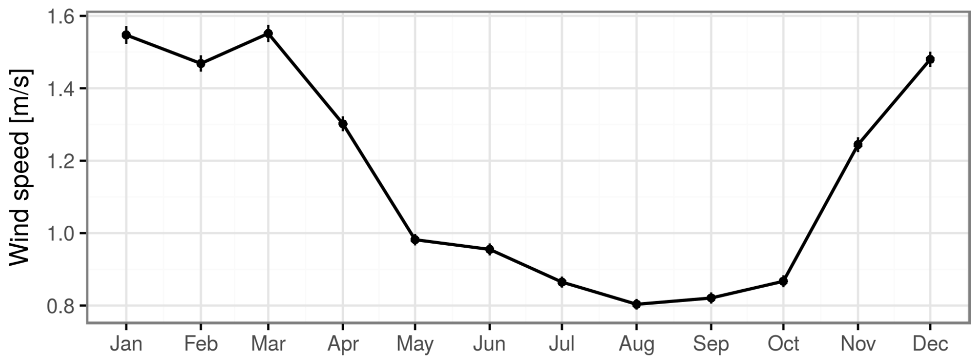

Fig. S3.1: Monthly mean wind speed (with 95 % confidence intervals) measured 15 m above ground level at the shore of Müggelsee, based on data from 2002 to 2015.

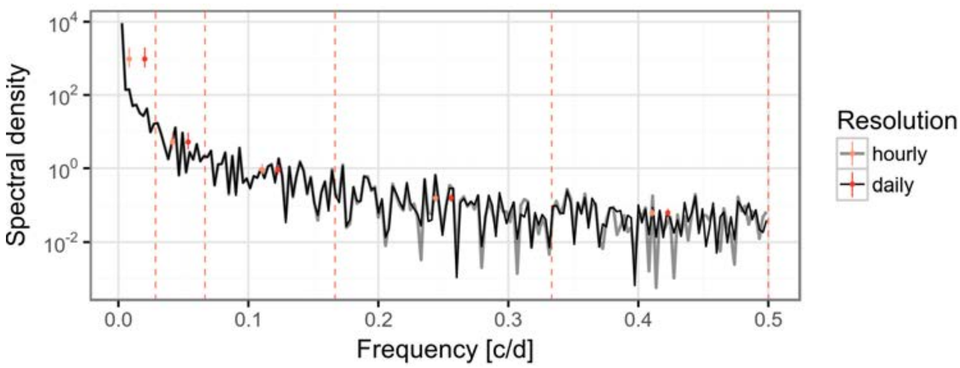

Fig. S3.2: Spectra of near-surface water temperature measured at the Müggelsee lake station in 2009, based on hourly data (*gray*) and daily data (*black*). The same spectra after frequency-band averaging and binning into five frequency bands are shown in *orange* and *red*, respectively (mean and 95 % confidence intervals).

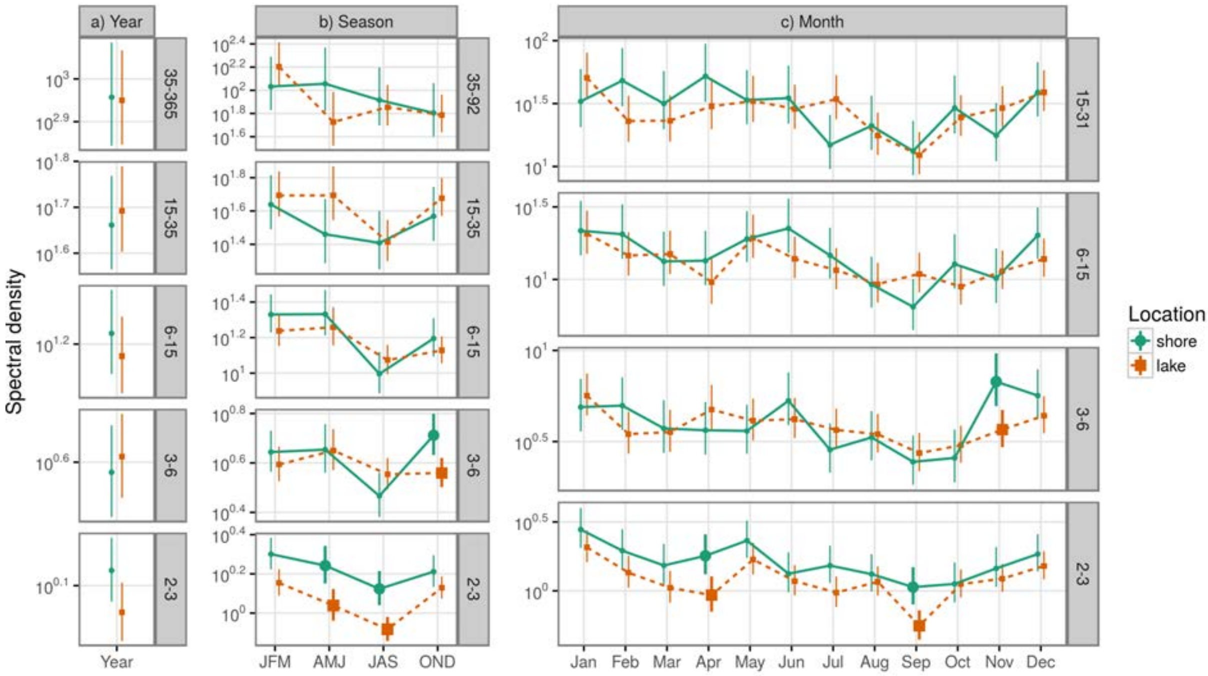

Fig. S3.3: Spectral density (with 95 % confidence intervals) of air temperature measured at Schönefeld airport during the same time windows when water temperature was measured at the shore station and at the lake station, averaged over the same frequency bands for time windows of **(a)** years, **(b)** seasons and **(c)** months. *Large dots* represent estimates of spectral density with non-overlapping confidence intervals within one frequency band and time window (significant difference between locations); *small dots* represent estimates with overlapping confidence intervals. Note logarithmic scale on y-axes.

SI.2 Comparison with the standard deviation as a measure of variability

To compare the variability derived by the FFT power spectra with a more traditional method, we calculated standard deviations of the same yearly, seasonal and monthly water temperature (WT) time windows and averaged them over years, seasons and months measured at the same location (shore or lake). The standard deviation (*sd*), as a more traditional measure of the total variance in the WT time series (the integral over the entire spectrum), showed to some extent similar patterns to the long-term variability estimated by spectral analysis (Fig. S3.4). However, because *sd* was dominated by the WT seasonality, the seasonal time windows in Fig. S3.4b) largely reflected the range of the data (steep increase in spring and steep decrease in fall) rather than the shorter-period (e.g., daily) variability. As *sd* always includes the underlying lower-frequency temporal scales, it is not able to resolve scale dependence; e.g., it cannot separate daily, weekly or monthly variability. This could be partly avoided by deseasonalizing the data beforehand, which is essentially what we did by frequency-band averaging the spectrum. However, even then, using the standard deviation does not allow variability at short, medium and long temporal scales to be analysed separately, which is a main focus of this study.

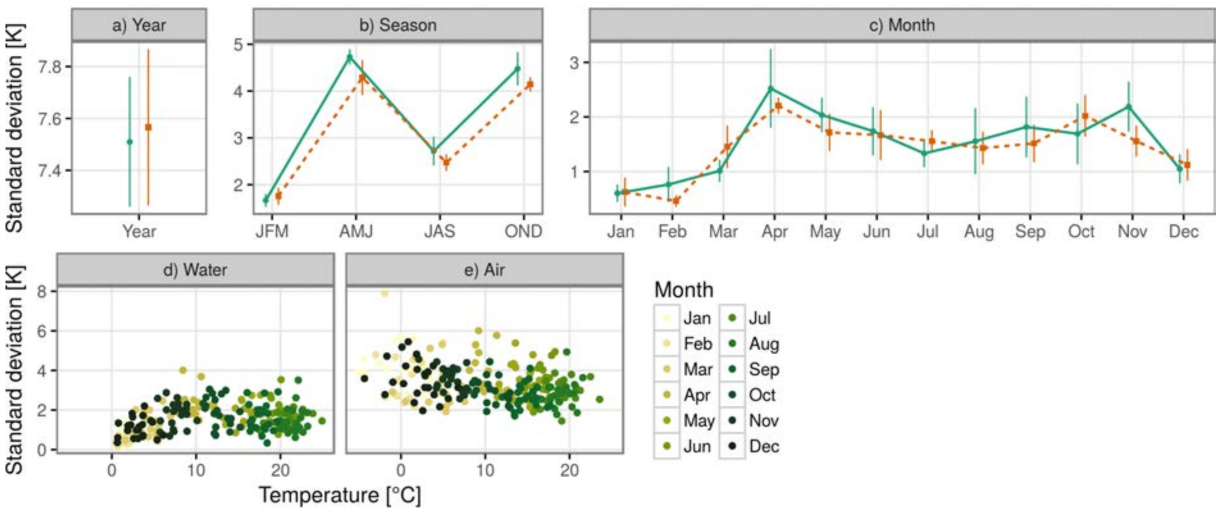

Fig. S3.4: Standard deviation (with 95 % confidence intervals) of near-surface water temperature (WT) measured at the Müggelsee shore and lake stations for time windows of **(a)** years, **(b)** seasons and **(c)** months. *Large dots* represent estimates of standard deviation with non-overlapping confidence intervals (significant difference between shore and lake location); *small dots* represent estimates with overlapping confidence intervals. **(d)** Standard deviation of near-surface WT in Müggelsee as a function of monthly mean WT, grouped by month of the year. **(e)** Corresponding standard deviation of air temperature (AT) at Schönefeld airport. Mean standard deviation and monthly mean WT and AT over all months (*squares*) are connected chronologically (*black line*).

4 Using wavelet coherence as a diagnostic tool in limnology *

Abstract

State variables in lake ecosystems are subject to processes that act at different time scales. The importance of these processes changes over time, e.g., due to varying constraints of physical, biological and biogeochemical processes. Correspondingly, continuous automatic measurements at high temporal resolution often reveal intriguing patterns that can hardly be directly ascribed to single processes. More powerful methods are required than applied hitherto to disentangle an often rather complex interplay. To that end we tested the potential of wavelet coherence, based on the assumption that different processes result in correlation between different variables, at different time scales and during different time windows. The approach was tested on a set of multivariate hourly data measured between the onset of an ice cover and a cyanobacterial summer bloom in the year 2009 in a polymictic eutrophic lake. We found that processes such as photosynthesis and respiration, the build-up and decay of phytoplankton biomass, dynamics in the CO_2-carbonate system, wind-induced resuspension of particles and vertical mixing were alternating dominant drivers of the variability in our data. We conclude that high-resolution data and a method capable of analyzing time series in both the time and the frequency domain can help to enhance our understanding of the time scales and processes responsible for the high variability in driver and response variables, setting the ground for mechanistic analyses.

*in revision for *Limnology and Oceanography* as: Schmidt SR, Lischeid G, Hintze T and Adrian R. Using wavelet coherence as a diagnostic tool in limnology.

4.1 Introduction

Since long, limnologists seek to understand the processes causing temporal variability in physical, chemical or biological state variables. Dynamics in these variables can be caused by changes in the prevailing constraints of the dominant limnological processes. For example, the potentially exponential growth of phytoplankton populations is constrained alternately by light availability, supply of nutrients and grazing pressure of zooplankton (Sommer et al. 1986, 2012). Calcite precipitation often occurs during spring and summer in productive, carbonate-rich water bodies when photosynthetic uptake of carbon dioxide increases pH levels (Heine et al. 2017), while a decrease in pH can lead to calcite dissolution (Lampert and Sommer 2007). On the other hand, calcite precipitation can, through co-precipitation of phosphate, limit eutrophication and thereby phytoplankton growth (Hamilton et al. 2009). Finally, the replenishment with oxygen in oxygen-depleted lake bottoms is constrained to periods of vertical mixing at high wind speeds (Lampert and Sommer 2007; Read et al. 2011). In this regard research now focuses more and more on episodic events and how for instance storms affect a lake ecosystem or certain processes in it (Jennings et al. 2012; Klug et al. 2012; Kasprzak et al. 2017). These examples illustrate that the type of prevailing constraint of a limnological process may change over time and can happen at different time scales ranging from fractions of seconds ((bio-)chemical reaction rates), seconds to days (photosynthesis), minutes to days or weeks (mixing processes), hours to weeks (population dynamics) to several months (seasonal dynamics) (Reynolds 1990; Behrendt et al. 1993; Hanson et al. 2006). Yet, understanding and identifying the huge intra-annual variability of various state variables, their interactions and time scales remains challenging.

Analyzing limnological processes, their time scales and constraints requires a high amount of multivariate data, which are now increasingly measured in lakes worldwide (Meinson et al. 2016). With automated high-frequency measurements, the temporal resolution has become almost unlimitedly high. Improvements in the development of automated sensors have increased the number and quality of measured variables (Cushing 2013; Marcé et al. 2016). These data allow us to capture patterns of variability in space and time in the first place. Yet, the interpretability of these variables and the implications for the state of a lake are not always straightforward, as different variables or processes operate on different time scales. The inherent complexity of internal and external forces structuring lake ecosystems adds to that variability. There is, however, an understanding that the measured variables are indicative of certain processes. For example, oxygen concentration and pH values are strongly affected by photosynthesis, while chlorophyll *a* indicates the build-up and decay of phytoplankton biomass. However, how the variation in a variable, or the covariation of two variables, can pinpoint a process is not necessarily clear, as many processes likely affect more than just one single variable, and each of them in a different way during different times of the year. Methods are hence needed that can grasp patterns of covariation between variables at a range of time scales the processes they reveal operate on. There is now a number of studies which separate e.g. hourly variability from daily, monthly, seasonal or yearly variability (Benincà et al. 2011; Blauw et al. 2012; Kara et al. 2012; Adrian et al. 2012; Guadayol et al. 2014). Yet, the benefit of using high-frequency compared to lower-frequency measurements and the role of different time scales of variability still lack sufficient consideration (Adrian et al. 2012; Coble et al. 2016). To that end, methods are required that are able to differentiate between processes, time scales, and particular time windows. Once we have identified the temporal patterns and time scales of covariation, subsequent analytical or modeling steps may allow us to further our understanding of the mechanisms driving overall temporal variability in lakes.

Wavelet coherence (Torrence and Compo 1998; Grinsted et al. 2004; Cazelles et al. 2008) is a method by which the direction and strength of coherence of two time series across different time scales can be analyzed, which can point to a causal relationship between the respective two variables. Other than correlation analyses, wavelet coherence differentiates time scales, as the variability of the coherence between two variables is partitioned into frequencies. These range from twice the measurement resolution up to the length of the time span under investigation. Importantly, wavelet coherence can track periods of synchronicity even when they are limited to rather short time spans. Thus, the analysis of synchronicity of temporal patterns of different variables at different time scales is a first step in disentangling different processes that occur in parallel.

This study aims at testing how wavelet coherence can be used to identify plausible temporal synchronicities between physical, chemical and biological variables in a eutrophic polymictic lake spanning time scales between hours and several months. We intend to identify the most prominent time scales these synchronicities operate on across different seasons and water depths. We base our study on a dataset of hourly automated measurements of water temperature, chlorophyll *a* as an indicator for algal biomass, phycocyanin as a proxy for cyanobacterial biomass, oxygen concentration, pH, turbidity, electrical conductivity quantifying ionic substances, wind speed as an important meteorological driver of turbulence in the water column, and manually measured ice development. We selected five examples out of a set of many possible combinations of variables where we expected to find a causal relationship that could indicate processes such as photosynthesis, build-up of phytoplankton biomass, particle resuspension, calcite precipitation and lake mixing. However, sound proofs of causality would require more elaborate examinations of each single case and were beyond the scope of this study. We show how the coherence between variables in time-frequency space and of a single variable between different measurement depths can help to identify processes that occurred during limited time windows and at certain frequencies.

4.2 Methods

4.2.1 Study site

Müggelsee is a shallow (mean depth 4.9 m, maximum depth 7.9 m), polymictic, eutrophic lake in North-Eastern Germany with a surface area of 7.3 km^2 and a mean retention time of 6-8 weeks (Köhler et al. 2005). The river Spree flows through Müggelsee and rapidly mixes with the lake water (Barthelmes 1962). Müggelsee is a highly wind-exposed lake. This, together with its shallowness, leads to frequent events of complete mixing that interrupt time windows of thermal stratification (Driescher et al. 1993). Events of stable thermal stratification during summer were to 79.3 % shorter than one day (Wilhelm and Adrian 2008) but can occasionally last up to several weeks. The catchment area is 7000 km^2 and dominated by agriculture and forestry (Driescher et al. 1993). Müggelsee is a calcium-rich hard water lake with high levels of alkalinity (Driescher et al. 1993). The river Spree has a large influence on its water quality (Köhler and Nixdorf 1994), while groundwater withdrawal from wells around the lake reduces any influence of the adjacent groundwater on the water quality of Müggelsee. Due to high nutrient levels, Müggelsee is eutrophic and experiences substantial algal blooms during spring and summer. Summer blooms are often dominated by cyanobacteria (Wagner and Adrian 2009).

4.2.2 Automated sensor measurements

Limnological data were collected by automated measurements with a multi-parameter probe (YSI 6600 V2-4) at a platform 300 m from the northern shore of Müggelsee (52°26′46.1″N; 13°39′0.2″E). The probe measured water temperature, chlorophyll *a*, phycocyanin, turbidity, oxygen, pH and electrical conductivity at 1.5 m depth below surface. Water temperature and electrical conductivity were measured with a combined physical sensor. A pH electrode determined hydrogen ion concentrations. Chlorophyll *a*, phycocyanin, turbidity and oxygen were measured with optical sensors, equipped with integrated anti-fouling wipers for self-cleaning. Once per hour, depth profiles were measured between 0.5 m and 5 m depth at increments of 0.5 m. The multi-parameter probe has a sampling frequency of twice per second. Each measurement was derived from a mean over 20 single measurements recorded over a time period of 10 seconds every hour. The measurements in different depths were performed with an offset of a few minutes. Therefore, we only interpreted time scales exceeding 3 hours. During winter, measurements with the same probe were performed hourly below the ice cover at a fixed depth of 1.5 m at the same location. Hence, measurements in depths other than 1.5 m were only available after ice-off in March. We used measurements in 1.5 m depth to analyze the coherence between different variables, and measurements in 1.5 and 5 m depths to analyze the coherence of a single variable between these depths. The thickness of the ice cover was measured circa daily at several locations. Wind speed was measured after ice-off at the same location in 4 m height above the water surface with a cup anemometer (Thies GmbH).

4.2.3 Data preprocessing

We selected a time span between December 2008 and August 2009 that was almost free of data gaps. As the focus of the study was to capture patterns of natural short- to long-term variability, any kind of gap filling would result in major artifacts. However, even within the selected time span there were a few short gaps in the dataset. Due to fouling of the optical turbidity sensor, 31 hours of turbidity measurements in April were excluded from the analyses. The fouling was indicated by a steep increase of turbidity values before the sensor was cleaned manually. One extreme outlier in chlorophyll *a* measurements in April was excluded as well. There was furthermore a gap of 24 hours in all variables in March, when the measurement protocol changed from winter measurements to regular measurements that included depth profiles. A 19-hour gap in July, a 5-hour gap in February, a 2-hour gap in August and 4 one-hour gaps in June and July occurred due to probe malfunction. All gaps were filled by linear interpolation and marked in red in all figures. The wavelet coherence especially at sub-daily frequencies should be interpreted with caution at these instances, as the low variability of the linearly interpolated gaps can lead to spurious results. However, apart from the one gap in turbidity of 31 hours, gaps were no longer than 24 hours and the coherence at longer time scales can hence be interpreted with sufficient confidence. All variables were normalized to zero mean and unit variance prior to analyses.

As some variables were not normally distributed, we repeated all analyses on log-transformed data. Most log-transformed variables exhibited a reduced skewness, but this resulted only for some variables in a normal distribution. We therefore additionally repeated all analyses on the rate of change of the log-transformed data, calculated as the difference between data values of adjacent time steps. This resulted in normal distributions of all variables. The analyses of original data, log-transformed data and the rate of change of log-transformed data all resulted in very similar patterns. We therefore only show the results of the original, untransformed data.

4.2.4 Wavelet coherence

We applied wavelet coherence (Torrence and Compo 1998; Grinsted et al. 2004; Maraun and Kurths 2004) to detect synchronous fluctuations between two time series. For this purpose, both time series are decomposed via the continuous wavelet transform, defined as the convolution of the time series with a wavelet, i.e. a basis function localized in both time and frequency. This wavelet is continuously scaled and shifted in time and thus exhibits specific information on frequency and time localization. The wavelet coherence is given by the square of the product of the first time series wavelet transform with the complex conjugation of the second, normalized by the individual power spectra of each time series. It exhibits values between zero and one and identifies phases of local cross-correlation between two time series as a function of frequency. The phase difference between the time series, indicated by arrows in the figures of wavelet coherence, gives information about a possible time lag in the relationships between two variables, and thus points to the direction of potential causality.

All analyses were performed with R (R Core Team 2016). The wavelet coherence and phase relationships were calculated with the R package biwavelet (Gouhier et al. 2016), whose code is based on the Matlab package WTC (Grinsted et al. 2004). We chose the Morlet wavelet as the basis function, because it represents a good compromise between time and frequency resolution (Torrence and Compo 1998). No zero-padding was applied. The significance of the wavelet coherence was calculated as significant deviation from red noise generated by an AR1 model with 100 Monte Carlo randomizations. Significance was tested using a χ^2 test at a significance level of 0.95. To quantify the intensity of thermal stratification, we calculated the Schmidt stability (Schmidt 1928; Idso 1973) from hourly water temperature profiles using the R package rLakeAnalyzer (Winslow et al. 2016). All figures were created with the R package ggplot2 (Wickham 2009).

In the following, "period length" always refers to the regarded period length as $1/\text{frequency}$. In contrast, references to certain time intervals are termed "time span" if referred to the whole available time interval and termed "time window" if shorter.

4.2.5 Analyzing patterns for processes

Here we focus on the following patterns that we related to specific processes. We chose five examples where we expected plausible relationships between two variables or between one variable measured at different depths. Some of these patterns are restricted to lakes with circum-neutral pH values where hydrogencarbonate (HCO_3^-) is the prevailing form of dissolved inorganic carbon (Lampert and Sommer 2007), like in the lake studied here.

- Synchronous fluctuations of pH and oxygen (O_2) are ascribed to photosynthesis, where uptake of CO_2 reduces HCO_3^- concentration and thus increases pH, and release of O_2 increases oxygen saturation. The inverse pattern holds for respiration. This is likely to occur at all time scales. In contrast, phases of pronounced decay of algal and cyanobacteria biomass will likely occur at period lengths $\gg 1$ day.

- Synchronous increase of water temperature, chlorophyll *a* and phycocyanin points to the build-up of algal and cyanobacteria biomass at a time scale of several hours to days. This can be regarded as a measure of potential photosynthesis of the existent phytoplankton biomass, whereas synchronous fluctuations of pH and O_2 are related to the actual productivity of the existent phytoplankton biomass.

- Synchronous changes of turbidity and chlorophyll *a* or phycocyanin at time scales $\gg$ 1 day are indicative of a causal relationship between chlorophyll *a* or phycocyanin and turbidity, respectively. In contrast, changes of turbidity that are not reflected by those of chlorophyll *a* or phycocyanin point to, e.g., input of turbid water via streams during heavy rain storms or resuspension from the bottom layer of the lake, e.g., during heavy wind storms.

- A decrease of electrical conductivity in parallel with an increase of pH points to calcite precipitation, and the inverse pattern to calcite dissolution. This process is not restricted to specific time scales.
- Changes of single variables at different depths that occur with inverse sign (indicating a phase shift of half a period length) are interpreted as an indicator of mixing of shallow and deep water. This phenomenon will likely affect different variables in parallel, but might not necessarily be visible for all of them, because not all variables might exhibit a clear depth gradient during that phase. Mixing is not restricted to specific time scales.

4.3 Results

From December 31, 2008 until March 9, 2009 the lake was covered with ice (Fig. 4.1). A phytoplankton bloom started already underneath the ice and lasted until the onset of the clear water phase around May 2, 2009. In June, the weather was mostly stormy, as indicated by low air pressure, high wind speeds, frequent precipitation, cool air and water temperature and low Schmidt stability, i.e., favoring mixing (Fig. 4.1). In July, the weather was more settled and a stable thermal stratification developed in the lake as indicated by relatively high Schmidt stabilities (Fig. 4.1), followed by a cyanobacteria bloom.

Wavelet coherence between two time series is visualized in Figs. 4.2 – 4.10. The time domain is shown on the x-axis with the same scaling as for the time series given above, while the respective period length is given on the y-axis. Colors indicate the degree of coherence. For example, a red area in the time-frequency space bordered by a black line would mark a range of period lengths and a time window during which two variables fluctuate in a highly coherent way and differ significantly from red noise. The black arrows indicate the phase relationship between two variables at the indicated period length and time window. Arrows pointing right mean that the two variables are in phase, i.e. they oscillate synchronously at that period length. Arrows pointing left mean that the synchronicity is in anti-phase, hence an increase in one variable is accompanied by a decrease in the other variable and vice versa. Arrows pointing upward mean the variables are out-of-phase with a lead of the first variable, while arrows pointing downward reflect an out-of-phase relationship with a lead of the second variable. Both hint to a time lag between the variables of a quarter of a period length. If significant coherence and phase relationships are consistent over a certain extent of the time-frequency space, causality between the leading and the following variable can be assumed (Grinsted et al. 2004; Maraun et al. 2007). In the “cone of influence”, marked in lighter shade, edge effects due to the limited length of the respective time series may distort the wavelet coherence and should be interpreted with caution.

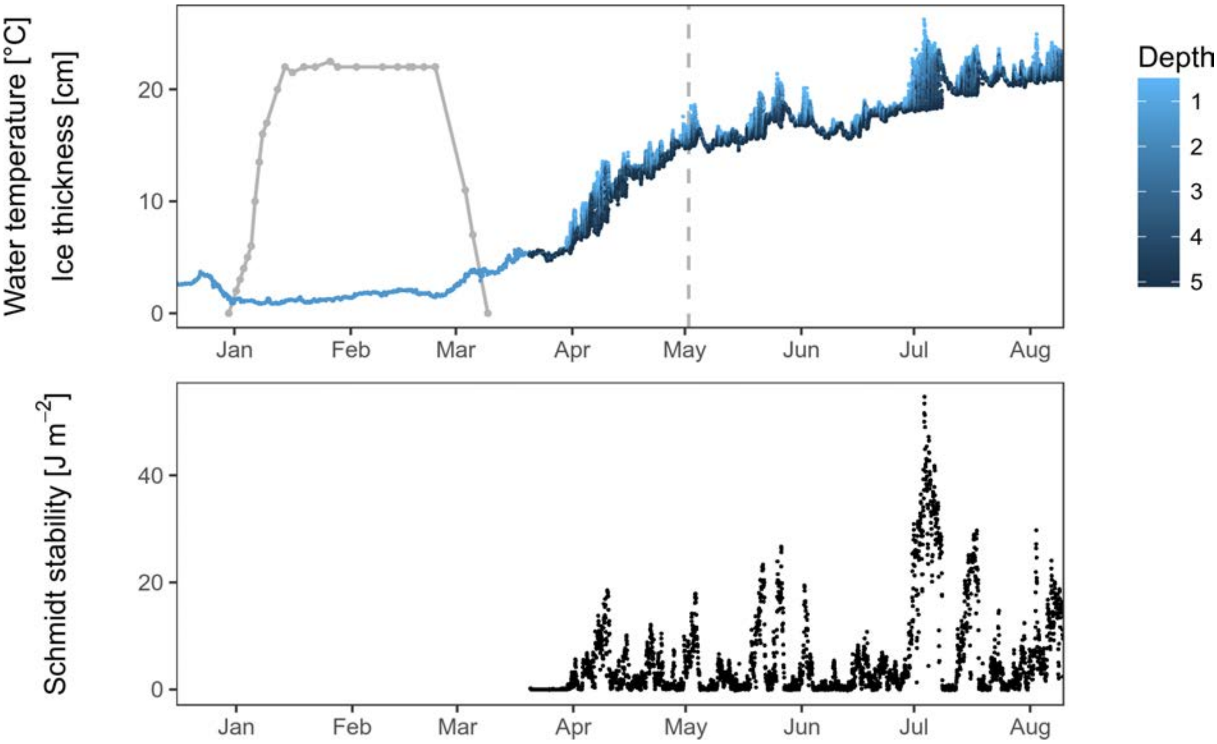

Fig. 4.1: *Upper panel*: Time series of water temperature [°C] in Müggelsee with blue color gradient according to measurement depth; ice thickness [cm] (grey dots and line); vertical dashed line: peak of zooplankton abundance as indicator of the clear water phase, calculated as local maximum of the fit of a Weibull function to weekly cladocera abundance data (Rolinski et al. 2007). *Bottom panel*: Time series of Schmidt stability [$\mathrm{J\,m^{-2}}$], calculated from vertical water temperature profiles.

Over the course of the considered time span from December 2008 until August 2009 patterns of coherence between most variables changed frequently, resulting in rather patchy patterns in Figs. 4.2 – 4.10. These were often restricted within the time-frequency space, and especially at short period lengths of a few hours, coherent and non-coherent phases were usually quite short-lived.

Photosynthesis and respiration: High in-phase coherence between oxygen concentration and pH would indicate photosynthetic processes if both increased synchronously or respiratory processes if both decreased synchronously. We found high coherence in phase between O_2 and pH at all time scales throughout until the end of the studied time span, except for sub-daily patterns during the first month (Fig. 4.2). Time series of oxygen concentrations and pH values showed a synchronous abrupt and substantial decline in mid-January, pointing to a dominance of respiration over photosynthesis. O_2 and pH increased synchronously in early February and even more after ice-off, which coincided with the begin of the phytoplankton spring bloom, indicating an increase of photosynthesis. This was followed by a substantial decrease toward the clear water phase, signalling that respiration exceeded photosynthesis. Another two-month cycle occurred in May and June and several much shorter cycles thereafter.

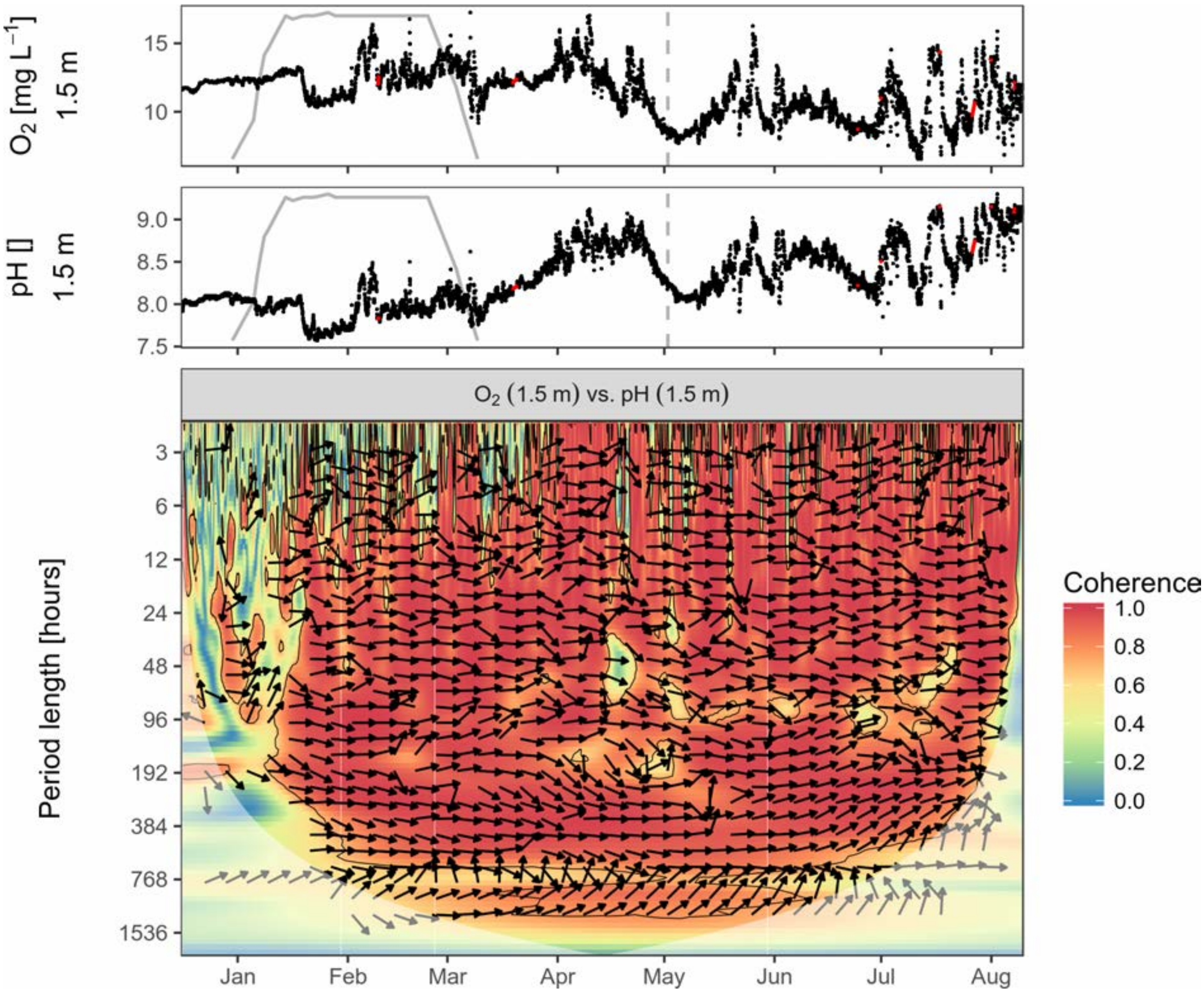

Fig. 4.2: *Upper panels*: time series of oxygen concentration (O_2) [$mg\,L^{-1}$] and pH [] measured hourly in 1.5 m depth in Müggelsee; time window with an ice cover (grey line); vertical dashed line: onset of the clear water phase. *Bottom panel*: wavelet coherence between O_2 and pH; black contours around regions where the coherence is significant against red noise, based on Monte Carlo AR (1) time series (significance level 0.95); black arrows indicate the relative phase relationship (in-phase pointing right; anti-phase pointing left; out of phase pointing up/down); the lighter shade denotes the cone of influence, where edge effects may distort patterns of coherence. The x-axis applies to all three panels.

Build-up of algae and cyanobacteria populations: High in-phase coherence between water temperature and chlorophyll *a* or phycocyanin would indicate the build-up of a phytoplankton population driven by water temperature, while high in-phase coherence between chlorophyll *a* and phycocyanin would indicate similar drivers of the dynamics of algae and cyanobacteria populations. Water temperature and chlorophyll *a* were for rather short time windows of one to three weeks between January and August coherently in phase (Fig. 4.3). Their strongest and longest coherence was observed during the intensified phytoplankton spring bloom in April after ice-off and covered period lengths from hours up to a week. This indicates that water temperature drove the build-up of phytoplankton populations during this time window. In summer the coherence between chlorophyll *a* and water temperature was generally lower and more short-lived and restricted to small ranges of period lengths. This suggests that water temperature did not play a major role in the build-up of phytoplankton populations in summer. Chlorophyll *a* and phycocyanin were coherently in phase in the first 4.5 months of 2009 for period lengths exceeding 12 hours, indicating similar drivers of algae and cyanobacteria populations during this time window. This synchronicity was interrupted during the clear water phase (Fig. 4.4). Coherence between chlorophyll *a* and phycocyanin was to a lesser degree re-established shortly after the clear water phase at period lengths greater than 12 h. In July, after time windows of intense and long-lasting thermal stratification as indicated by high Schmidt stabilities (Fig. 4.1), cyanobacteria developed a bloom that was not captured by chlorophyll *a*, and their coherence was low.

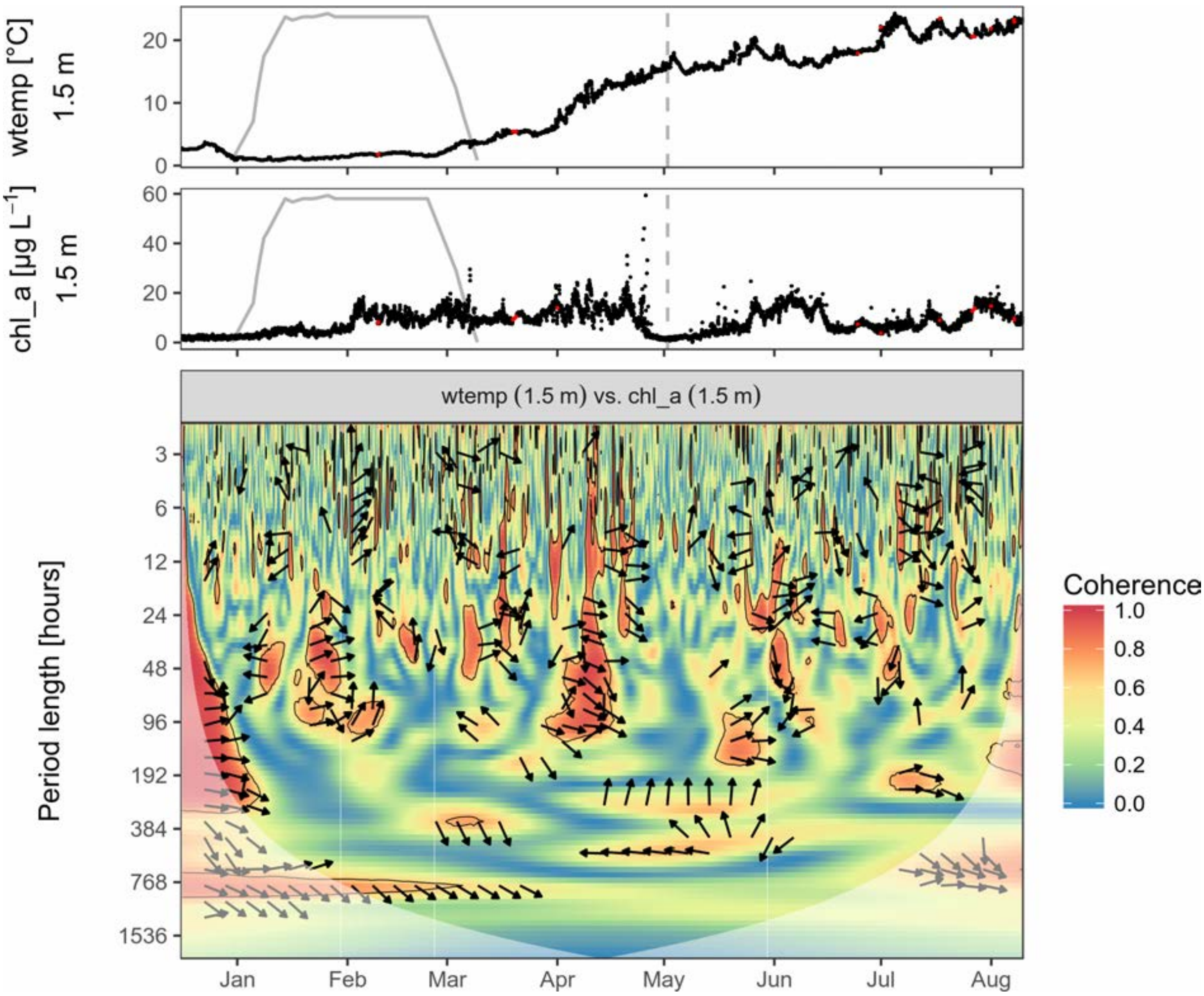

Fig. 4.3: *Upper panels*: time series of water temperature (wtemp) [°C] and chlorophyll *a* (chl_a) [$\mu g\,L^{-1}$] measured hourly in 1.5 m depth in Müggelsee; time window with an ice cover (grey line); vertical dashed line: onset of the clear water phase. *Bottom panel*: wavelet coherence between wtemp and chl_a; black lines, arrows and lighter shade as in Fig. 4.2. The x-axis applies to all three panels.

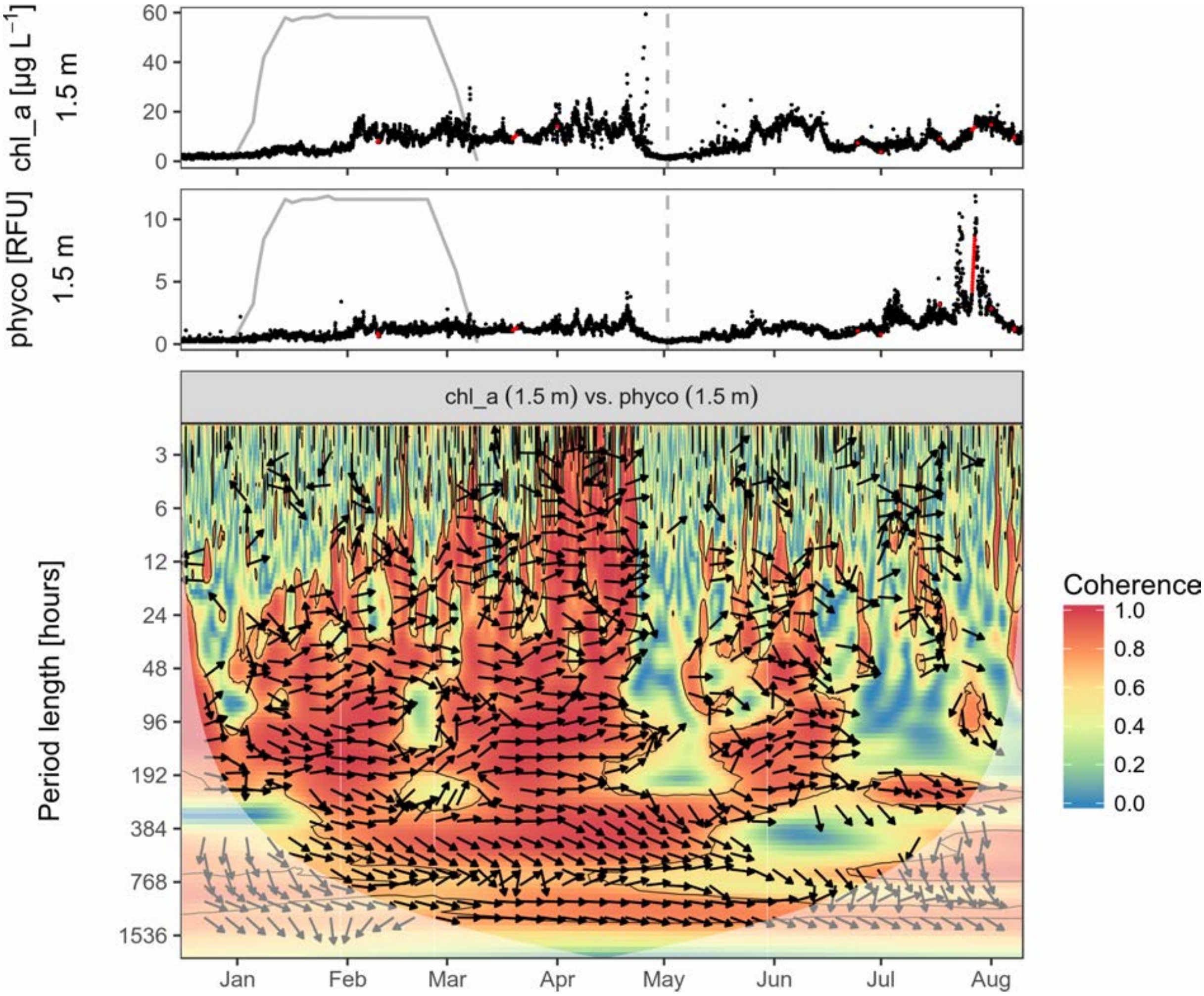

Fig. 4.4: *Upper panels*: time series of chlorophyll *a* (chl_a) [µg L^{-1}] and phycocyanin (phyco) [relative fluorescence units (RFU)] measured hourly in 1.5 m depth in Müggelsee; time window with an ice cover (grey line); vertical dashed line: onset of the clear water phase. *Bottom panel*: wavelet coherence between chl_a and phyco; black lines, arrows and lighter shade as in Fig. 4.2. The x-axis applies to all three panels.

Turbidity: High in-phase coherence between turbidity and either phytoplankton, electrical conductivity or wind speed would indicate that either biological, chemical or physical processes were responsible for dynamics in turbidity. The coherence between phycocyanin and turbidity was most of the time rather low and short-lived (Fig. 4.5). Only in July during several weeks of the cyanobacteria bloom, coherence was high and in phase at period lengths from hours to weeks, indicating a biological driver of turbid conditions during this time window. Coherence between chlorophyll *a* and turbidity exhibited mostly similar patterns due to the high coherence between chlorophyll *a* and phycocyanin (Fig. 4.4), but was low and short-lived during the cyanobacteria bloom (not shown). One time window in January below the ice cover exhibited coherent in-phase variations between electrical conductivity and turbidity at period lengths between one day and a week, indicating a chemical driver of turbidity in January (Fig. 4.6). Fluctuations of wind speed and turbidity were coherently in phase in May and June at scales of several days up to two weeks while the weather was stormy (Fig. 4.7). This indicated a physical driver of turbidity in May and June, possibly the settling and resuspension of particles from the lake bottom.

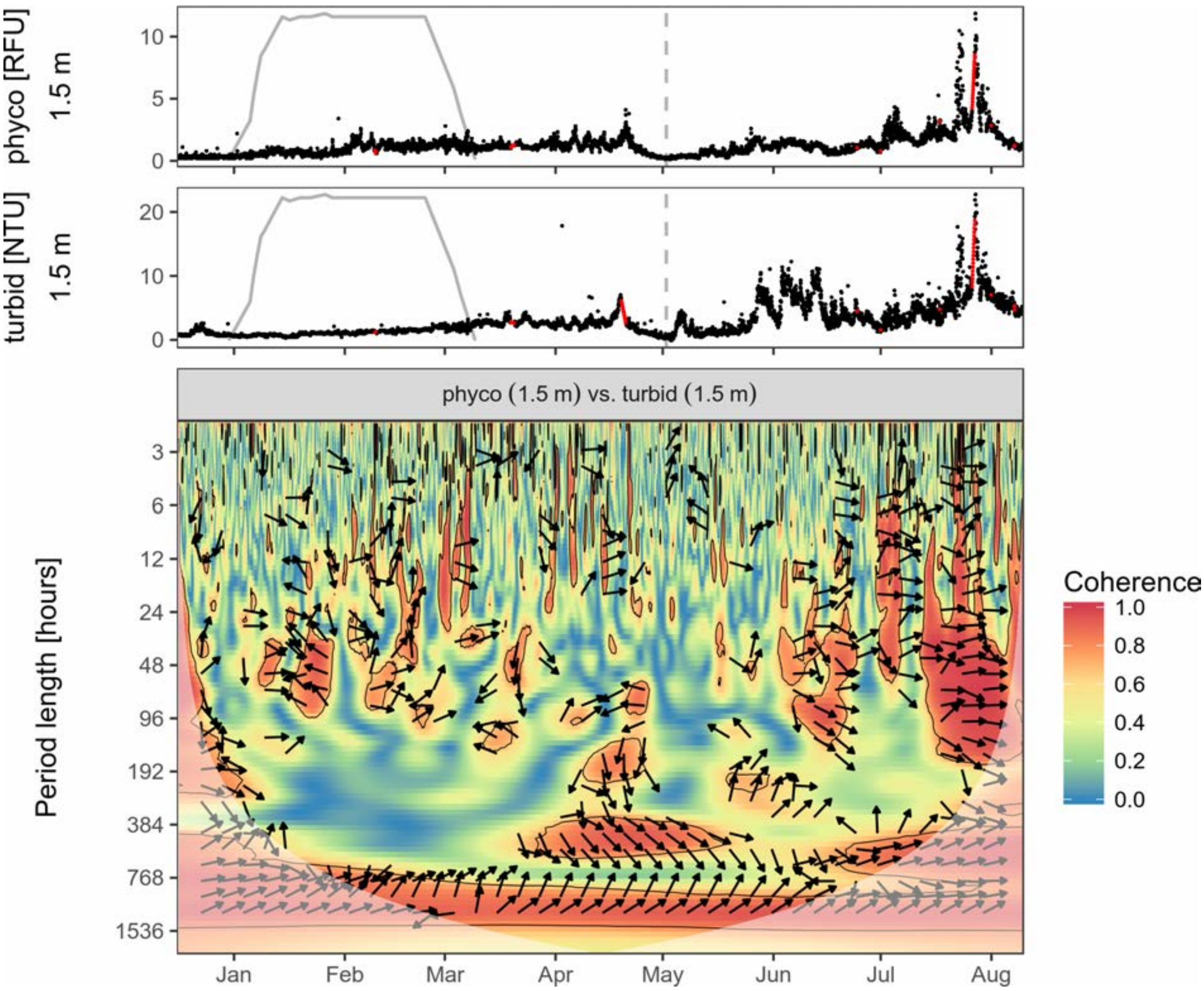

Fig. 4.5: *Upper panels*: time series of phycocyanin (phyco) [relative fluorescence units (RFU)] and turbidity (turbid) [nephelometric turbidity units (NTU)] measured hourly in 1.5 m depth in Müggelsee; time window with an ice cover (grey line); vertical dashed line: onset of the clear water phase. *Bottom panel*: wavelet coherence between phyco and turbid; black lines, arrows and lighter shade as in Fig. 4.2. The x-axis applies to all three panels.

Calcite precipitation and dissolution: High anti-phase coherence between pH and electrical conductivity would indicate either calcite precipitation if pH increased while electrical conductivity decreased or calcite dissolution if pH decreased while electrical conductivity increased. Coherence between pH and electrical conductivity was in anti-phase during several time windows in winter under ice between daily and weekly scales, during the phytoplankton spring bloom in April at similar scales, and to a lesser extent in summer at sub-daily scales (Fig. 4.8). The overall increase in electrical conductivity in January, accompanied by a synchronous decrease in pH, hints to calcite dissolution. In contrast, calcite precipitation was probably confined to short time windows under the ice, as to be concluded from the small diametrical spikes in the

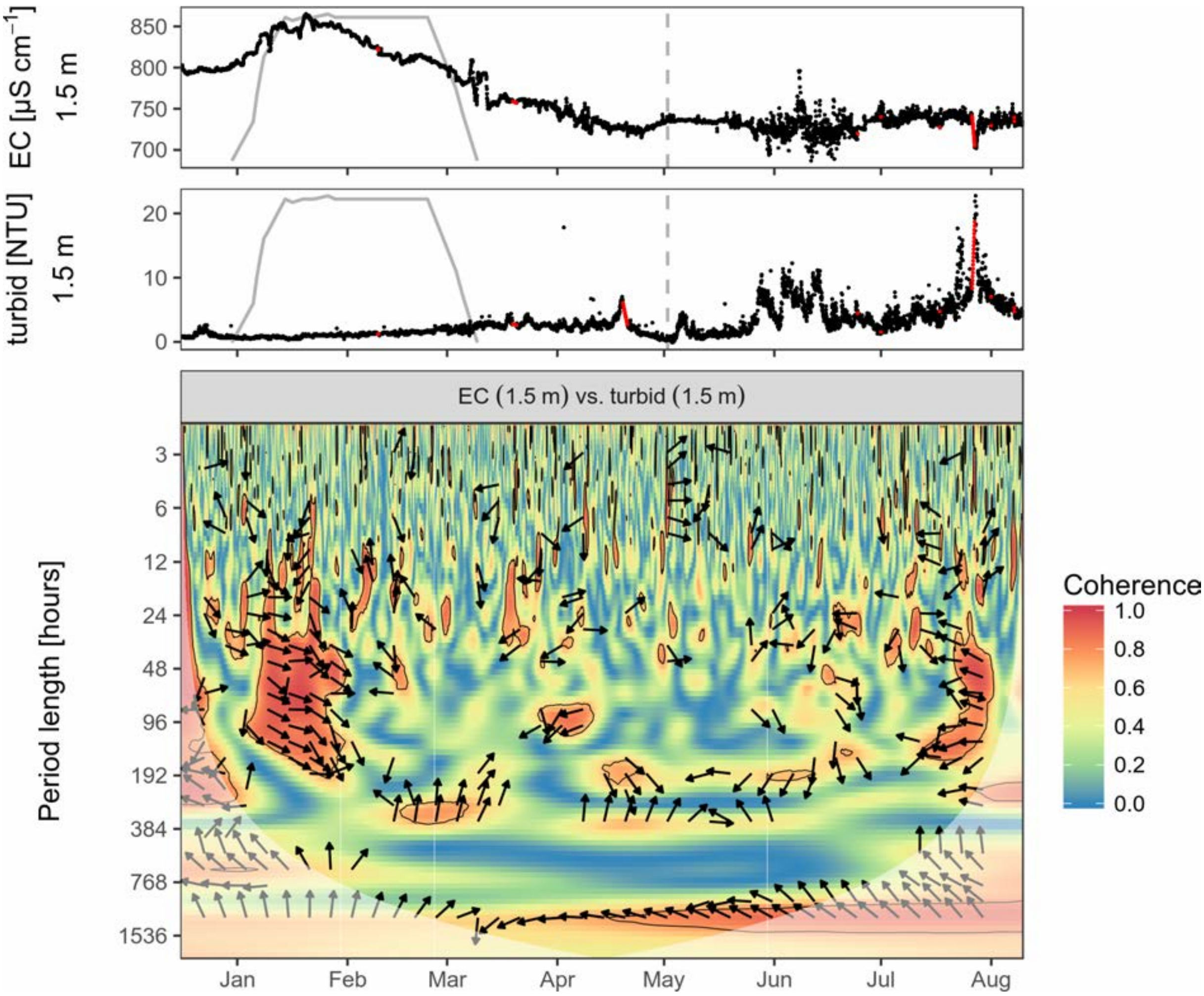

Fig. 4.6: *Upper panels*: time series of electrical conductivity (EC) [µS cm^{-1}] and turbidity (turbid) [nephelometric turbidity units (NTU)] measured hourly in 1.5 m depth in Müggelsee; time window with an ice cover (grey line); vertical dashed line: onset of the clear water phase. *Bottom panel*: wavelet coherence between EC and turbid; black lines, arrows and lighter shade as in Fig. 4.2. The x-axis applies to all three panels.

time series of pH and electrical conductivity. The increase in pH accompanied by a decrease in electrical conductivity during the phytoplankton spring bloom and during short time windows in summer, on the other hand, indicated calcite precipitation.

Vertical mixing: High anti-phase coherence of a single variable between different measurement depths would indicate mixing of shallow and deep waters. The coherence in pH between measurements in 1.5 and 5 m depths was high and in anti-phase at period lengths between four days and one week in May and between one and over two weeks in June and July, indicating mixing between the two layers (Fig. 4.9). At shorter period lengths, the coherence was sometimes in phase for short time windows. Patterns of coherence of O_2 between the same depths were very similar to those of pH (Fig. 4.10). Fluctuations in O_2 and pH were very large and happened often abruptly. Especially the steady decline down to oxygen depletion and minimum pH values in the hypolimnion during the second week of July was interrupted almost instantly

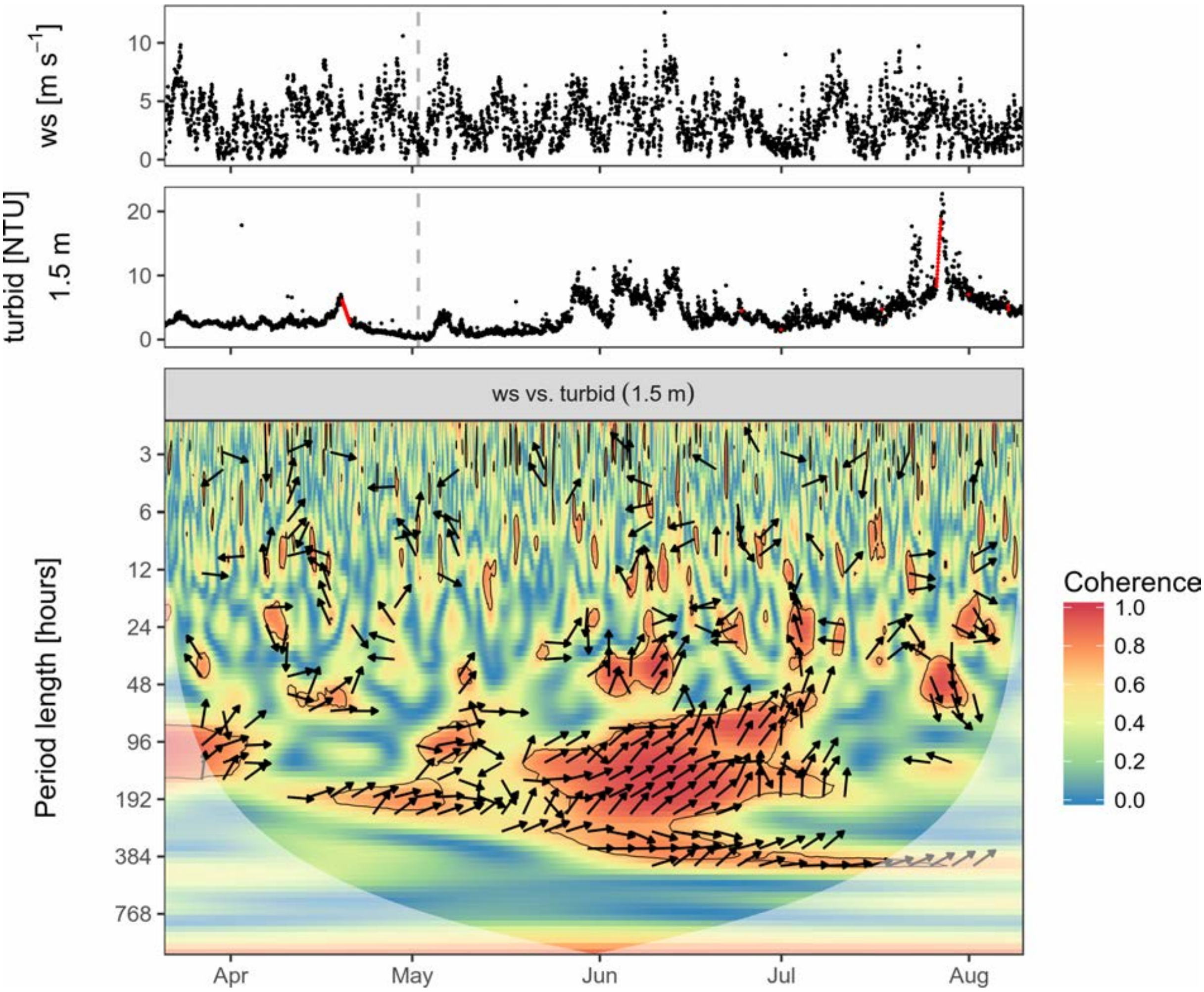

Fig. 4.7: *Upper panels*: time series of wind speed (ws) [$\mathrm{m\,s^{-1}}$] measured hourly in 4 m height above Müggelsee and turbidity (turbid) [nephelometric turbidity units (NTU)] measured hourly in 1.5 m depth in Müggelsee; time window with an ice cover (grey line); vertical dashed line: onset of the clear water phase. *Bottom panel*: wavelet coherence between ws and turbid; black lines, arrows and lighter shade as in Fig. 4.2. The x-axis applies to all three panels.

with increases of about 1.5 pH units and 10 $\mathrm{mg\,L^{-1}}$ O_2 within a few hours. Mixing events, as indicated by a Schmidt stability near zero (Fig. 4.1), coincided with high wind speed (Fig. 4.7) and decreases of near-surface O_2 and pH and increases of bottom O_2 and pH, balancing their levels in the whole water column. High coherence was observed for other variables (water temperature, chlorophyll *a*, phycocyanin, turbidity and electrical conductivity), comparing measurements in 1.5 and 5 m depths, during limited time windows and for certain period lengths (not shown). However, they were in phase and thus could not be related to vertical mixing events.

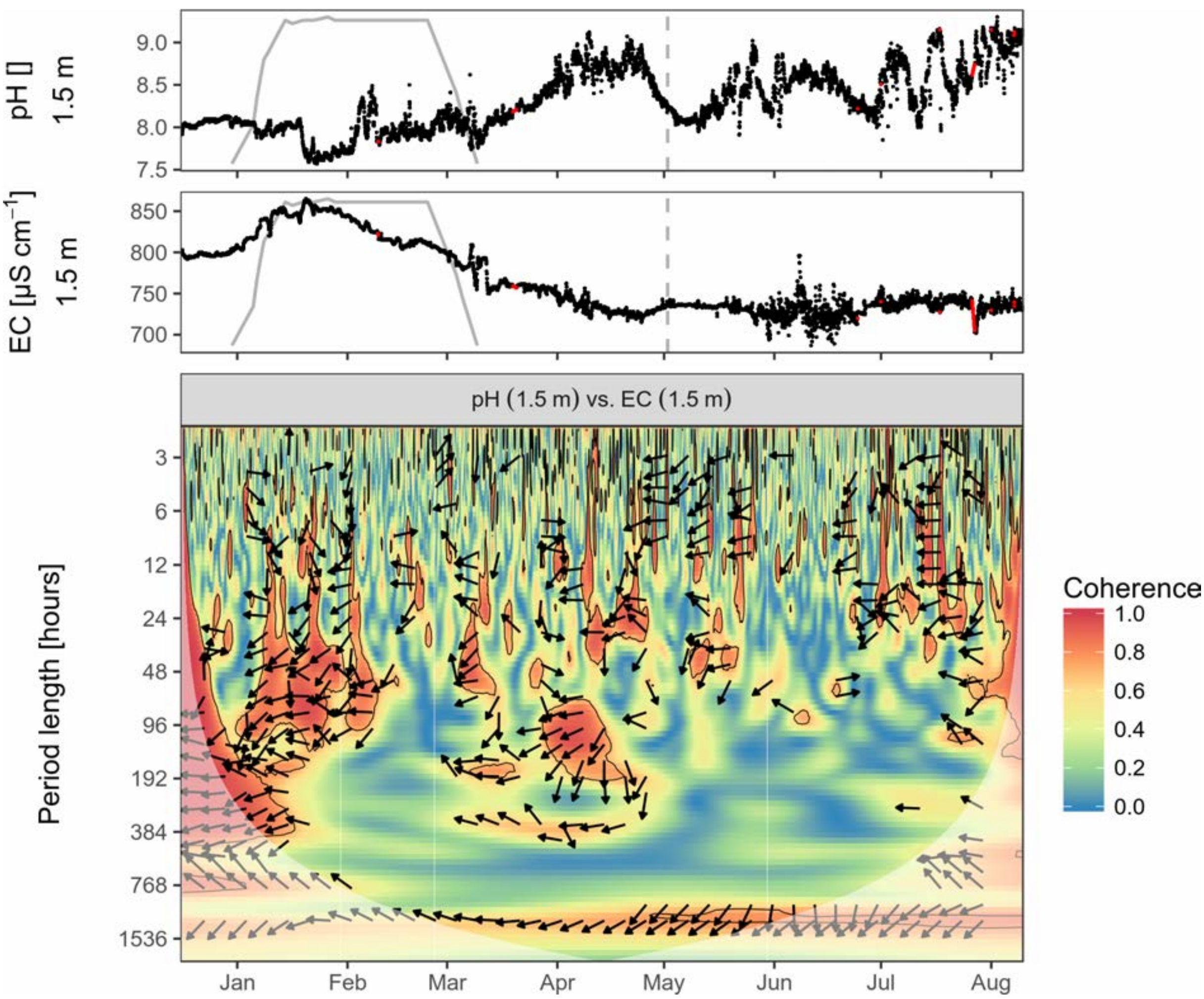

Fig. 4.8: *Upper panels*: time series of pH [] and electrical conductivity (EC) [µS cm^{-1}] measured hourly in 1.5 m depth in Müggelsee; time window with an ice cover (grey line); vertical dashed line: onset of the clear water phase. *Bottom panel*: wavelet coherence between pH and EC; black lines, arrows and lighter shade as in Fig. 4.2. The x-axis applies to all three panels.

4.4 Discussion

We investigated in what way wavelet coherence may serve as a diagnostic tool to identify and disentangle limnological processes in polymictic eutrophic Müggelsee. Coherent dynamics among limnological and meteorological variables were detected during limited time windows and at specific time scales. These suggested reversible processes such as photosynthesis and respiration, the build-up of phytoplankton biomass, calcite precipitation and dissolution, wind-induced resuspension of sedimented particles and vertical mixing of water masses. The plausibility of the ascription of synchronicities between state variables to certain processes and the characteristics of the identified time scales of these synchronicities are discussed in the following.

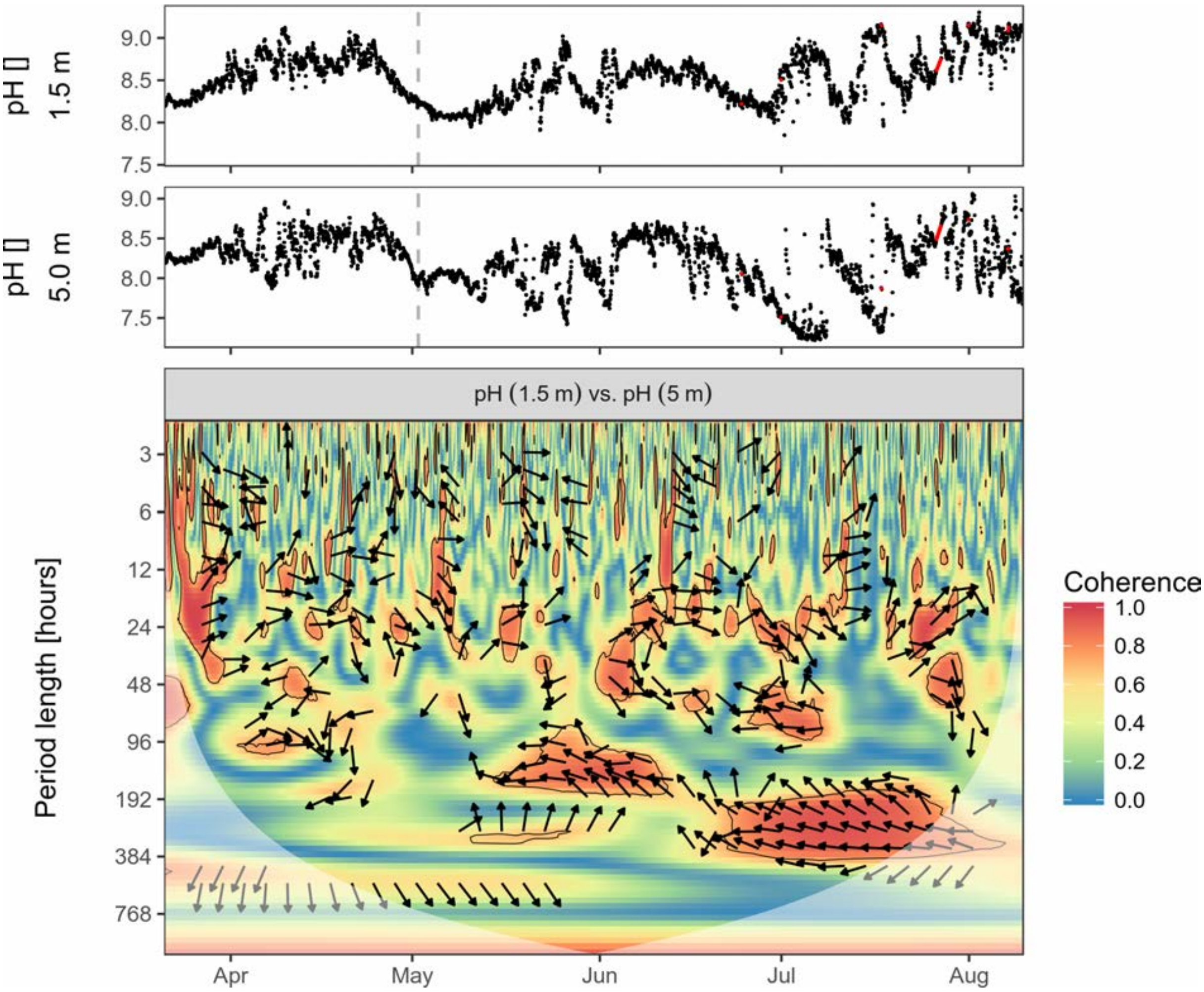

Fig. 4.9: *Upper panels*: time series of pH measured in 1.5 m depth and in 5 m depth in Müggelsee; time window with an ice cover (grey line); vertical dashed line: onset of the clear water phase. *Bottom panel*: wavelet coherence between pH measured in 1.5 m depth and pH measured in 5 m depth; black lines, arrows and lighter shade as in Fig. 4.2. The x-axis applies to all three panels.

4.4.1 Plausibility of ascription to processes

Under the ice cover of Müggelsee in mid-January, we observed a synchronous decrease of O_2 and pH, which we ascribed to a dominance of respiration over photosynthesis. This was substantiated by low levels of algal biomass, quantified as chlorophyll *a* and phycocyanin, until February. Similar patterns of O_2 and pH decreases have been observed under the ice cover of several lakes and were attributed to respiration processes (Kratz et al. 1987; Wetzel 2001; Baehr and Degrandpre 2002; Hanson et al. 2006). According to Bertilsson et al. (2013), rates of oxygen depletion and concurrent increases of the partial pressure of CO_2 are fastest after the onset of ice cover, when the ratio of photosynthesis to respiration changes in favour of respiration. The observed decrease of pH under ice can hence be assumed to be caused by increases in pCO_2, which can lead to strong undersaturation with calcite and consequential calcite dissolution (Ohlendorf and Sturm 2001). This may have led to the observed high anti-phase coherence

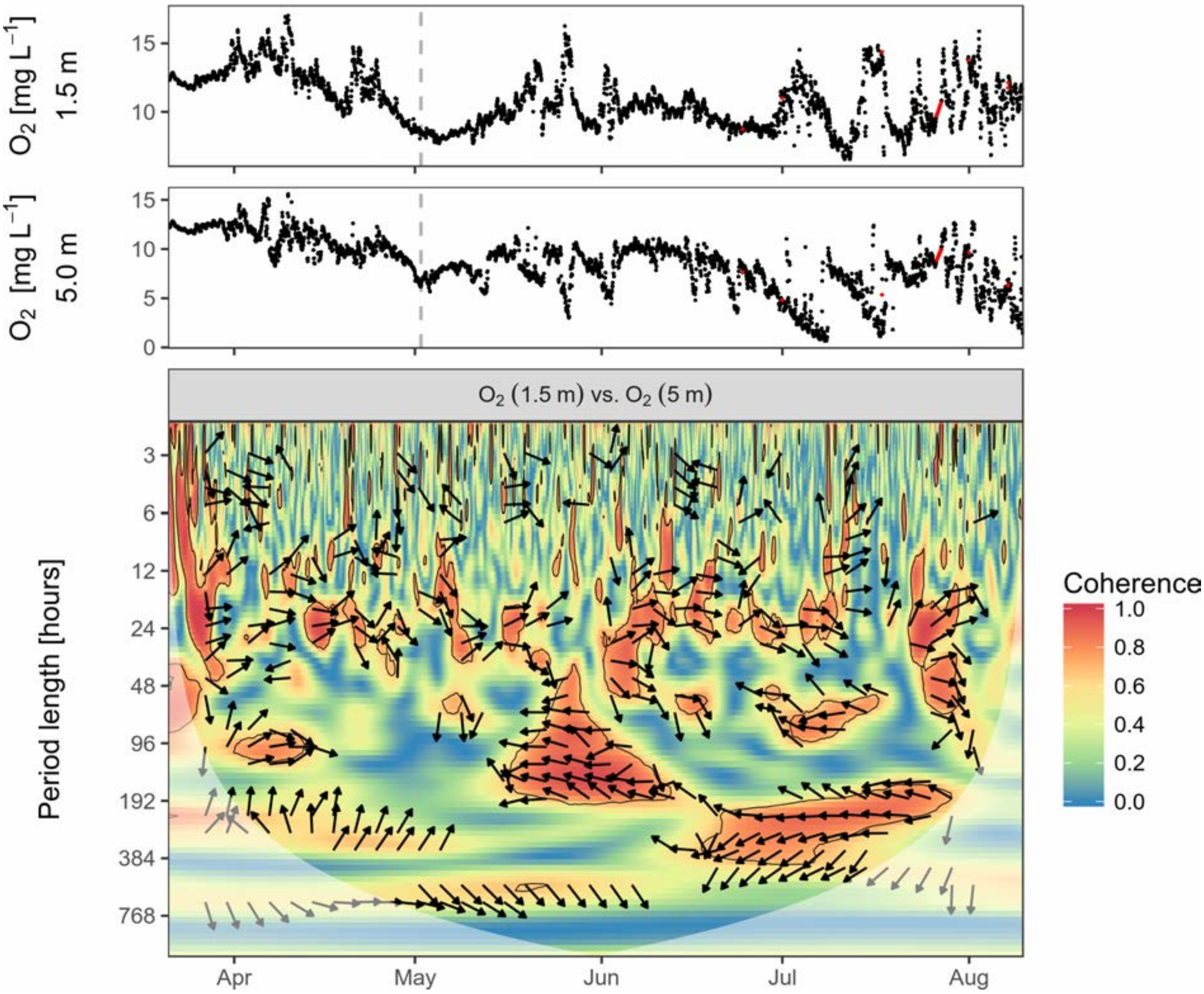

Fig. 4.10: *Upper panels*: time series of oxygen concentration measured in 1.5 m depth (O_2) [mg L^{-1}] and in 5 m depth in Müggelsee; time window with an ice cover (grey line); vertical dashed line: onset of the clear water phase. *Bottom panel*: wavelet coherence between O_2 measured in 1.5 m depth and O_2 measured in 5 m depth; black lines, arrows and lighter shade as in Fig. 4.2. The x-axis applies to all three panels.

between pH and electrical conductivity at daily to weekly scales in January, indicating calcite dissolution. It might furthermore have driven the dynamics of turbidity as indicated by the high in-phase coherence between electrical conductivity and turbidity during the same time window and at the same time scales. On the other hand, photosynthesis can be substantial under ice if light availability is sufficient (Wetzel 2001; Sommer et al. 2012; Hampton et al. 2017). This can account for the observed increase in O_2 and pH in February. Their increase coincided with rising levels of chlorophyll *a* and phycocyanin, implying that it was most likely caused by under-ice photosynthesis. The lack of persistent coherence between water temperature and chlorophyll *a* below the ice indicates that the initiation of the phytoplankton spring bloom was not caused by increasing water temperatures, but probably by enhanced light conditions (Adrian et al. 1999). Oxygen concentrations and pH were coherently in phase throughout the time window of ice cover and thereafter at time scales of hours to months. The only exception were the first four weeks in late December and early January, when only small and non-coherent fluctuations of O_2 and pH were observed that have to be ascribed to minor random disturbances.

After ice breakup, the time window in April exhibiting the steepest increase in water temperature was the only time window showing high in-phase coherence between water temperature and chlorophyll *a* over a broad range of time scales. In light-saturated conditions, water temperature is assumed to drive photosynthesis (Lampert and Sommer 2007). A positive feedback of spring water temperature on phytoplankton development has been shown for Müggelsee (Gerten and Adrian 2000) and other lakes for certain phytoplankton species (Reynolds 1990; Adrian et al. 1995; Feuchtmayr et al. 2012; Talling 2012). Li et al. (2015) found high synchronicity, estimated by wavelet coherence, between chlorophyll *a* and water temperature in certain regions in the time-frequency space, although based on monthly data only. The detected high in-phase coherence between chlorophyll *a* and water temperature during the phytoplankton spring bloom in Müggelsee indicated that only during this time window of a few weeks, water temperature and phytoplankton growth were characterized by a causal relationship. Water temperature may have driven phytoplankton growth directly by affecting replication rates or indirectly, e.g., through the control of stratification intensity in turn improving light availability, as deep mixing of algal cells is prevented. The high anti-phase coherence between electrical conductivity and pH at daily to weekly time scales during the phytoplankton spring bloom indicates that the phytoplankton growth was accompanied by biogenic calcite precipitation during this time window. In Müggelsee, sediment dredging has indicated the precipitation of calcite due to high photosynthetic activity (Kozerski and Kleeberg 1998). This is commonly observed in productive hard water lakes such as Müggelsee where calcium is the main cation (Dudel and Kohl 1992; Driescher et al. 1993), when photosynthetic uptake of CO_2 increases the pH, leading to oversaturation with calcite (Lampert and Sommer 2007; Heine et al. 2017). The high coherence between pH and electrical conductivity around a period length of 24 hours matches with diurnal variations in CO_2 due to metabolic day-night cycles (Morales-Pineda et al. 2014). The collapse of most synchronicities, most strikingly the coherence between chlorophyll *a* and water temperature and between chlorophyll *a* and phycocyanin, marked the clear water phase and was accompanied by substantial decreases in chlorophyll *a*, phycocyanin, O_2 and pH. The coherences between water temperature and chlorophyll *a* and between chlorophyll *a* and phycocyanin were high before, completely absent during, and low and more short-lived after the clear water phase. Only the coherence between O_2 and pH remained high at all time scales, while their synchronous decrease signalled that respiration exceeded photosynthesis. This indicates that zooplankton grazing broke the formerly synchronous relationships (Sommer et al. 2012). This has been shown to be one important explanation of the collapse of phytoplankton spring blooms in Müggelsee during the past two decades (Huber et al. 2008). The clear water phase hence represented a cardinal event that clearly marked a time window of altered interactions between variables and processes, thus a change of the prevailing constraints.

After the clear water phase, the rather low and short-lived coherence between water temperature and chlorophyll *a* indicated other drivers of the dynamics of the summer phytoplankton population than water temperature, indicating a change in the prevailing constraints of phytoplankton growth. Indeed, nitrogen limitation, in contrast to water temperature, was shown to play a role for the summer phytoplankton development in Müggelsee (Köhler et al. 2005). Cyanobacteria, on the other hand, thrive under increased water temperature and concomitant intense and long-lasting stratification stability (Huber et al. 2012; Merel et al. 2013). This may explain the observed low coherence between chlorophyll *a* and phycocyanin in summer. Furthermore, cyanobacteria blooms increase the turbidity of water bodies (Paerl and Huisman 2008). This seems to be responsible for the high in-phase coherence between phycocyanin and turbidity observed during the cyanobacteria summer bloom in Müggelsee in July at time scales of hours to weeks. In contrast, the high in-phase coherence between turbidity and wind speed at time scales of several days to two weeks in June indicated wind-induced resuspension of particles. Rising wind speeds were accompanied by an increase in turbidity, indicating the resuspension of particles from the lake bottom, while calm time windows enabled their settling, coinciding with low turbidity. Wind-induced resuspension is common in shallow, polymictic lakes (Kristensen et al. 1992; Kozerski and Kleeberg 1998; Eleveld 2012). Correspondingly, we found high anti-phase coherence of pH and O_2 between near-surface and near-bottom measurements from May to July at similar time scales. This was accompanied by large synchronous fluctuations of pH and O_2 diametrically in surface and bottom waters with substantial drops in surface water oxygen concentration, while bottom waters were re-oxygenated (Fig. 4.10). Similar patterns have been observed in other lakes and were correlated with wind events, suggesting vertical mixing (Robertson and Imberger 1994; Hanson et al. 2006; Langman et al. 2010), and in Müggelsee from May onwards in all years analyzed by Behrendt et al. (1993). The latter were related to a decoupling of production and consumption processes in surface and bottom waters, which were interrupted by irregular wind-induced changes of mixed and stratified conditions at time scales of hours to weeks (Behrendt et al. 1993). The period lengths of four days to one week in May and one to two weeks in June and July, which revealed the strong anti-phase coherence between near-surface and near-bottom water layers in our study, lay within the range of durations of general weather situations over Germany. These lasted three to five days in May, up to eight days in June, and up to ten days in July (Deutscher Wetterdienst 2017). Hence, the ascription of high anti-phase coherence between single variables measured in different depths to vertical mixing can be substantiated, and the characteristic time scale at which vertical mixing is observed might reflect the periodicity of the general weather situation. All in all, our hypothesized relationships between patterns of coherence of various state variables and certain limnological processes proved plausible.

4.4.2 Measuring synchronicity – advantages of analyzing at high resolution in both the time and the frequency domain

There is a large amount of literature concerned with temporal coherence of various state variables: Magnuson et al. (1990) and various studies thereafter (Wynne et al. 1996; Kratz et al. 1998; Rusak et al. 1999; Baines et al. 2000; Pace and Cole 2002; Chrzanowski and Grover 2005; Salmaso et al. 2014) define coherence as synchronous dynamics of time series of single variables between different lakes. These studies have in common that their measure of coherence is simple correlation analysis. They hence lack the ability to detect transient and frequency-specific relationships, as correlations between variables may go undetected if they occur only at a certain frequency or during limited time windows. For example, Arhonditsis et al. (2004) found no correlation between water temperature and chlorophyll *a* measured during 25 years in Lake Washington. However, their connection may have been masked by the weekly resolution of the data and the methodological approach of correlation analysis and linear regression, which lacked the ability to detect transient and potentially frequency-dependent correlations as revealed by our study. Other studies inferred causality from detected correlations or linear regression between numerous state variables in lake ecosystems (Gerten and Adrian 2000; Blenckner et al. 2007; Gaiser et al. 2009; Eleveld 2012), which could gain in accuracy and significance if a more advanced method like wavelet coherence would be applied.

In this respect, the high resolution in the time and the frequency domain applied in our study helped to identify the respective prevailing constraints during specific time windows. For example, phytoplankton growth was related to water temperature only during short time windows (Fig. 4.3), pointing to other constraints or drivers of its dynamics during the rest of the observation period. Furthermore, wavelet coherence helped to disentangle different processes that affected the same variable but to a different extent during different time windows. For example, according to our analysis, the observed dynamics of pH were related to photosynthesis and respiration (Fig. 4.2) during most of the study period as well as to calcite dissolution and precipitation (Fig. 4.8) and vertical mixing (Fig. 4.9) during rather short time windows. Similarly, the dynamics of turbidity were related to chemical (electrical conductivity, Fig. 4.6), biological (phycocyanin, Fig. 4.5) as well as physical (wind speed, Fig. 4.7) drivers during different time windows. Hence, process identification cannot necessarily be derived only from the dynamics of the variables themselves, but from their joint dynamics with other variables and a time- and frequency-resolved methodology. Lastly, wavelet coherence has proven the potential to identify reversible processes that do not necessarily result in observable net effects like calcite dissolution observed during a rather short time window in January and re-precipitation in early April (Fig. 4.8).

4.4.3 Conclusion

Applying wavelet coherence to multivariate limnological high-frequency data proved suitable to identify and disentangle reversible processes that affected the same variable, to detect their characteristic time scales, and to identify the prevailing constraints of processes that happened during limited time windows and often in parallel. This could not have been achieved using simpler methods, such as correlation or regression analysis, as the coherence between variables was found to be frequency-specific and to depend on the time window. This stresses the importance of considering process-specific time scales. A high temporal resolution of the data was necessary to detect characteristic time scales of variability and time windows in which processes occurred, as both were often rather short. Our results imply that wavelet coherence has a high potential to serve as a diagnostic tool in limnology, and potentially also in other types of ecosystems, especially non-stationary ones. For example, Schaefli et al. (2007) applied wavelet coherence to 20-year long time series of precipitation, temperature and discharge in an Alpine catchment. They detected potentially flood triggering situations, while identifying the prevailing critical hydrometeorological constraints of different flood types. A possible limitation of our approach is that wavelet coherence, as a statistical method, does not reveal the true underlying ecological mechanisms that cause periodicities or associations between variables (Cazelles et al. 2008). Causality can only be assumed from the phase relationship of extended regions of local cross-correlation in time-frequency space. To reveal mechanisms behind coherent regions, experimental or modelling studies and more elaborate examinations of each case, possibly comprising further variables, would be necessary. These could for instance include the Granger causality (Granger 1969) or convergent cross mapping (Sugihara et al. 2012) calculated over time windows and frequency ranges where high coherence has been identified beforehand, which may distinguish causality from correlation and hence result in a higher confidence on causal mechanisms. To this end, comparing wavelet coherence of the same set of state variables measured in different lakes over a range of mixing types, trophic states and chemical compositions would give insight into the general applicability of the approach and may reveal interesting connections and differences between lake types and their characteristic time scales of major processes. These might be promising next steps in diagnosing and understanding the processes behind temporal variability in limnological state variables.

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5 Synthesis and outlook

The aim of this thesis is to contribute to a better baseline knowledge concerning variability in patterns and processes in lake ecosystems. A literature-based and a data-driven approach were combined with an analysis in the time frequency domain to investigate patterns of variability, to identify processes and to enhance the overall understanding of the structure and functioning of lake ecosystems. In the following, the results presented in the previous chapters are discussed and synthesized.

5.1 Automated high-frequency data: opportunities and pitfalls

5.1.1 The role of the time scale of measurements and analysis

Environmental policies aiming to improve the water quality status of aquatic ecosystems (e.g., the EU Water Framework Directive or the US Clean Water Act), rely on a thorough understanding of the dynamics of various parameters measured in aquatic ecosystems and the underlying processes. Automated high frequency measurements can provide substantial benefits in determining the water quality status of aquatic ecosystems over traditional routine monitoring programs, where measurements often take place in bi-weekly cycles at most (Marcé et al. 2016). This is problematic if there is a mismatch between the time scale at which data are recorded and the time scale at which processes operate (Fraterrigo and Rusak 2008). For example, the build-up and decay of cyanobacteria blooms can easily be missed by a bi-weekly monitoring (Pomati et al. 2011). Studies reviewed in chapter 2 of this thesis also demonstrated the importance of short time windows of opportunity for cyanobacteria development in warm springs. Similarly, a comparison of sampling regimes between hourly and monthly sampling frequencies revealed that assessments of water quality in an urbanized river system were sensitive to the season, time of day and frequency of sampling. The Water Framework Directive status of dissolved oxygen ranged from a “good” status under monthly sampling to a “bad” status under hourly sampling during the same time period (Halliday et al. 2015). In this respect, the explanatory power of pattern recognition techniques in particular of biological parameters and in polymictic lakes can depend dramatically on the sampling resolution (Aguilera et al. 2016). Chapter 2 of this thesis also demonstrated that mistiming between thermal time windows and processes that depend on thermal cues can only be detected and understood if the sampling frequency is adequate. It was shown empirically that the variability of water temperature at high frequencies can differ substantially between years sharing similar low-frequency dynamics.

Many biological phenomena are driven by the detailed high-frequency evolution of water temperature as illustrated in the conceptual sketch in Fig. 2.1. The exceedance of ecologically critical thresholds and associated ecological responses can go undetected with a coarse sampling resolution. The role of critical thresholds has been shown at the scale of single species (Pörtner and Knust 2007; Wilhelm and Adrian 2007; Pörtner and Peck 2010), processes such as temperature-driven cyanobacteria blooms (Wagner and Adrian 2009; Huber et al. 2012) and habitat shifts (Hari et al. 2006; Wiedner et al. 2007), up to the ecosystem level, at which thresholds can trigger regime shifts (Scheffer and Carpenter 2003; Beaugrand et al. 2008) (see chapter 2). Often, these processes are driven by meteorological conditions within narrow time windows. For example, biological, chemical and physical processes are often limited to short time windows of days or weeks as shown in chapter 4 of this thesis. For example, a phytoplankton bloom was driven by water temperature only during a short time window of two weeks during spring. This is in line with Feuchtmayr et al. (2012) and Talling (2012), who detected season-specific, species-specific and lake-specific responses of phytoplankton to water temperature forcing. Also, processes of calcite precipitation and calcite dissolution, as described in chapter 4, happened during short time windows of weeks. Calcite precipitation often accompanies phytoplankton blooms in nutrient-rich hard water lakes (Lampert and Sommer 2007; Heine et al. 2017) and is thus as well limited to the respective time windows. The data analyzed in chapters 2 – 4 of this thesis, as well as the literature referenced in chapter 2, showed that especially in polymictic lakes, such as Müggelsee, short time scales are of particular importance regarding critical time windows, because thermal stratification periods are often very short in this type of lakes. It is thus easy to miss these time windows if the sampling regime is too coarse.

However, it is not enough to monitor environmental parameters at adequate temporal resolution. All three studies performed in the context of this thesis show that the time scale of analysis and the specific methods applied are equally crucial to detect and analyze the ecological responses of interest. The variability in water temperature was found to differ particularly at short time scales (see chapters 2 and 3), which underlines the importance of taking into account high-frequency variability and applying a frequency-based approach. This was also advocated by Platt and Denman (1975), Sabo and Post (2008), and Guadayol et al. (2014). On the other hand, long-term data are needed to form the framework in which short-term observations can be interpreted (Magnuson 1990; Müller et al. 2010). The available long-term dataset used in chapter 3 enabled to investigate general rules of identified patterns and enhanced the explanatory power of the applied methods. Generally, the long tradition of limnological research in Müggelsee and the availability of a unique long-term dataset at high temporal resolution highly supported the interpretation of results derived from all three studies presented in this thesis.

The "resonance effect" describes that the time scale of variability of environmental forcing, relative to intrinsic oscillations of organisms at characteristic time scales, can induce large oscillations in the response variables such as plankton populations, and hence underpins the importance of characterizing time scales of environmental forcing and ecological responses (Benincà et al. 2011). The resonance of biological populations to environmental noise can affect population sizes and ultimately lead to population extinctions, with the risk of extinction likely depending on the noise color (Cuddington and Yodzis 1999; Sabo and Post 2008). The slopes of the water temperature spectra found in the study presented in chapter 3 agree with those found for polymictic lakes by Cyr and Cyr (2003). They are indicative of only moderately reddened noise, which, according to Cuddington and Yodzis (1999), is associated with intermediate unpredictability and extinction risk. However, these and other studies of the power spectra of temperature, especially water temperature, are based on a monthly resolution at most, and are therefore not entirely comparable with the study presented in chapter 3.

The time scale of analysis was as well crucial for detecting synchronous dynamics between different time series in chapter 4. The separation of time scales performed by the wavelet analysis enabled the detection of temporal coherence in the first place. The characteristic time scales of coherent dynamics, on the other hand, were used to derive processes from them and facilitated their interpretation. Time scales of variability were found to be process-specific and to change over the course of the 8-month time period. For example, time windows of vertical upwelling occurred at time scales of days in May, but at time scales of weeks in June and July. Furthermore, ecological responses can occur with a time lag with respect to the forcing time windows, as demonstrated in the studies reviewed in chapter 2. The detection of time lags between driver and response parameters is possible using wavelet coherence. While this was not the primary focus in chapter 4, several recent studies successfully applied wavelet coherence to determine time-delayed responses of ecological parameters to different drivers (Recknagel et al. 2013; Guyennon et al. 2014; Morales-Pineda et al. 2014; Li et al. 2015). In chapter 4, the time scale of analysis, in particular the high resolution in both the time and the frequency domain, was necessary for inferring processes from synchronous dynamics of time series.

5.1.2 The role of spatial scales

The spatial scale of measurements impacts the analysis of ecosystem parameters in a similar way as discussed for the temporal scale above. In the same way as sampling (and method of analysis) in time should capture the relevant temporal dynamics of underlying processes, sampling (and method of analysis) in space must be adequate to capture the spatial dynamics of underlying processes. For example, if measurements are only taken at one specific location in a lake, as is often the case, these measurements are likely neither transferable to other parts of the lake, nor necessarily representative for the whole lake (Steele 1978; Van de Bogert et al. 2012; Akyuz et al. 2014; Marcé et al. 2016).

In chapter 3, spatial scales of water temperature variability were assessed. Consistently higher water temperature variability was detected at a measurement location at the shore of

Müggelsee than in the open water. The slopes of water temperature spectra were generally flatter at the shore, implying less difference between high- and low-frequency variability, than in the open water, where the steeper slopes indicated lower high-frequency variability. This was related to the higher probability of wind-induced internal waves at the shore. While two measurement locations within one lake are certainly not enough to capture the whole degree of spatial heterogeneity, the results are still valuable to add to the existent knowledge on spatial patterns in lakes. Although studies are rare that explicitly investigate frequency-dependent spatial differences in the variability of water temperature within lakes, some existent studies confirm a higher water temperature variability at littoral locations than at pelagic locations (Lorke et al. 2006; Guadayol et al. 2014).

Shallow lakes and coastal waters were found to exhibit more rapid temperature fluctuations than deep lakes or the open ocean (Benincà et al. 2011). Similarly, the slopes of water temperature spectra were flatter in shallow polymictic lakes and became steeper in larger lakes (Cyr and Cyr 2003). Phytoplankton and zooplankton species are sensitive to temperature fluctuations due to the above mentioned resonance effect (Benincà et al. 2011), explaining why plankton communities may differ between shore and open water locations. For similar reasons, there is also evidence that metabolic rates, which are strongly driven by ambient temperature (Brown et al. 2004), can differ substantially in terms of variability and absolute level between littoral and pelagic habitats within lakes (Lauster et al. 2006; Van de Bogert et al. 2007; Sadro et al. 2011). These studies lacked sufficient quantification of differential mixing dynamics according to locations within the investigated lakes, which could have explained at least part of the observed spatial patterns of metabolism. This calls for more comprehensive assessments of physical as well as biological differences between littoral and pelagic regions of lakes.

5.1.3 Pitfalls of automated monitoring data

Automated high-frequency data offer opportunities as well as pitfalls (Porter et al. 2005; Marcé et al. 2016). Time series derived from this type of data often possess a sometimes substantial amount of data gaps due to malfunction of the sensor or transmittance, routine maintenance or removal of biofouling (Dur et al. 2007; Meinson et al. 2016). Moreover, recorded data may require additional preprocessing, e.g. if biofouling has not been detected and measurements are deficient (Manov et al. 2004; Blauw et al. 2012; Xu et al. 2014). The use of automated monitoring data hence requires quality assessment and preprocessing. As missing data in time series can hamper the deduction of processes from them and lead to misinterpretation of their dynamics, it is necessary to adopt a strategy on how to handle missing data that is consistent with the specific requirements of the investigation (Müller et al. 2010). Especially if researchers want to make use of the full temporal resolution of automated high-frequency data and not risk to loose information, averaging or down-sampling the data is not an option (Dur et al. 2007).

Steps undertaken for this thesis in this respect differed between the Fourier transform approach of chapter 3 and the wavelet-based approach of chapter 4. The methods applied here strongly depend on the least possible amount of data gaps, as both the Fourier transform and the wavelet analysis in their classical forms require equidistant and uninterrupted time series (Dur et al. 2007).

The investigation of patterns over a long time period with a large sample size in chapter 3 required the interpolation of at least a certain amount of gaps present in the data. Water temperature, the main parameter investigated in this study, is highly autocorrelated. Thus, filling parts of the gaps in the data could be done successfully via linear interpolation. Linear interpolation is often well suited for this purpose and has the advantage that the time series itself is used to fill the gaps, instead of, e.g., approximating time series by a single fixed function (Gnauck 2004). As interpolation can distort a frequency spectrum, the robustness of the interpolation against a potential distortion of the spectra had to be tested. For this purpose, spectra of time series containing interpolated artificial gaps were compared to the spectra of original, continuous data to determine the length of gaps that could be interpolated without distorting the spectrum. Conversely, due to the rapid fluctuations of biological and chemical parameters, interpolation would have led to major artifacts in the analysis of short time windows and high-frequency variability in chapter 4. Instead, a time period of recorded data with minimal gaps was selected to not unduly compromise the interpretability of wavelet coherence results. As one purpose of this chapter was to test the suitability of using wavelet coherence as a diagnostic tool, uncertainties in the data basis due to missing values would have complicated the interpretation of results.

Both approaches to overcome the limitations of using automated sensor data stress the great importance of minimizing gaps in the measurement of environmental data, e.g. through self-cleaning systems with wipers or pressure (Rinke et al. 2013; Meinson et al. 2016) or copper-based antifouling systems (Manov et al. 2004). A thorough analysis of the consequences of interpolating data gaps is otherwise necessary. Introducing artificial gaps to test the robustness of interpolation procedures can help in the latter respect (see chapter 3). For example, (Aguilera et al. 2016) introduced gaps into weekly available time series of water temperature, water chemistry and algal biomass measured in Müggelsee to test the ability of a dimension-reduction technique to recognize patterns. Various studies explicitly approached time series containing gaps. For example, Keitt and Fischer (2006) applied wavelet analysis to irregularly sampled limnological data, adapting the shape of the wavelets near sampling gaps and boundaries. Dur et al. (2007) adapted spectral analysis to time series from the Seine estuary that contained a high percentage of missing values. Irregularly sampled data can be analyzed using kernel-based methods and the frequency-based Lomb-Scargle technique, which were shown to outperform linear interpolation in the analysis of correlation functions and persistence time in paleo data (Rehfeld et al. 2011).

5.2 From patterns to processes – diagnosing lake ecosystems

Automated high-frequency monitoring data provide the basis for detecting spatial and temporal scales of environmental processes. The parameters obtained through this type of monitoring are efficient proxies for the assessment of the water quality status and to capture ecological patterns at a broad range of time scales (chapters 3 – 4; Marcé et al. 2016). To fully understand the observed dynamics of these parameters, their drivers and constraints, requires to infer their underlying processes. This implies an “urgent need” of methods that are able to identify processes at the appropriate time scale (Lischeid and Bittersohl 2008). Similarly, Sabo and Post (2008) criticize that environmental data are often used inefficiently in ecology and suggest a frequency-based approach to quantify environmental variability. Good visualization techniques of often complex data help to find structures in the data, as visualization is “the most powerful interface between computer and human brain” (Lischeid 2009).

5.2.1 Detecting patterns in the time frequency domain

Testing the slopes of water temperature spectra for their suitability as an indicator of mixing, as shown in chapter 3 in this thesis, illustrated how a relatively simple measure can help to explain observed patterns and to infer processes, in this case mixing, from time series data. The robustness of this indicator was tested using the relationship of water temperature spectra with low percentiles of the Lake number (Imberger and Patterson 1990), an indicator well established in the limnological literature describing the potential for wind-induced internal waves. The Lake number, however, requires depth profiles of water temperature and measurements of wind speed. When these are not available, using the slope of water temperature spectra seems promising. The windowed approach applied in this chapter was suitable to compare the scaling behavior of water temperature spectra between seasons, measurement locations and months with and without an ice cover. A windowed approach proved as well suitable to assess changes of the frequency spectrum of three El Niño Southern Oscillation indices with time (Kestin et al. 1998) and to evaluate an optimal monitoring setup of surface and groundwater levels (Fahle et al. 2015). On the other hand, more commonly used methods to quantify variability, such as the standard deviation, failed to detect the temporal and spatial scales of water temperature variability (chapter SI).

The analysis of ecological time series in the time frequency domain are encouraged by Cazelles et al. (2008), who consider this methodological shift from stationarity assumptions of the data to the recognition of non-stationarities critical for a better understanding of ecological processes in rapidly changing environments. Disentangling drivers of specific processes can be greatly facilitated by a frequency-based approach (Keitt and Fischer 2006). While Gnauck et al. (2010) advocated the application of the wavelet analysis for extracting long-term dynamics from ecological time series to identify processes, wavelet analysis can as well very efficiently be used to extract short-term dynamics for the identification of processes that occur during very short time windows, as shown in chapter 4 in this thesis. The time window of analysis is in this respect also important as was shown in chapters 2 and 4. The wavelet coherence analysis applied in chapter 4 in this thesis offers a powerful tool that can help to derive processes from time series, identify the time scales they operate on and the time windows of their occurrence. An advantage of wavelet analysis techniques is that prior assumptions of the dominant processes governing the data are not required, a benefit stressed by Lischeid (2009). Instead, processes can be identified that dominate oscillations in the data during particular time windows and at specific time scales. The visualization of the wavelet coherence as in Figs. 4.2 – 4.10 can help the human brain to grasp structures in the data at a glance. Chapter 4 showed that the variability and especially the frequency-resolved covariation of multivariate high-frequency data can serve as a diagnostic tool to identify processes dominating a system and to detect changes in the driving or limiting forces. The wavelet coherence is superior to more commonly used methods that address temporal coherence by applying simple correlation analysis (Magnuson et al. 1990; Wynne et al. 1996; Kratz et al. 1998; Pace and Cole 2002; Salmaso et al. 2014) or infer causality from linear regressions (Gaiser et al. 2009; Eleveld 2012). These lack the ability to detect transient behaviors and frequency-specific relationships. Thus, potentially frequency-dependent correlations or processes limited to specific time windows can go undetected. The potential of wavelet coherence is obviously not limited to lake ecosystems. Another successful application is the detection of flood triggering situations and the underlying hydrometeorological constraints (Schaefli et al. 2007).

The methods applied in this thesis hence proved superior to more commonly used measures of variability, such as the standard deviation, simple linear regression or correlation analysis, in detecting patterns and signatures of dominant processes from parameters measured in lake ecosystems. How these patterns could be attributed to specific environmental processes is discussed in the following.

5.2.2 Attributing patterns to processes in lake ecosystems

Water temperature is the most important driver of processes in lakes (Winder and Schindler 2004; Hanson et al. 2006; Lampert and Sommer 2007), which makes understanding its variability and how processes are driven by it an essential research focus. Chapter 3 focuses on the variability in water temperature per se. Temporal and spatial patterns of water temperature variability differed between measurement locations, between spring and fall at similar mean water temperatures, and were related to the stability of thermal stratification and the duration of ice cover. These patterns were found to be driven by the potential for vertical mixing through wind-induced internal waves as indicated by the slope of water temperature spectra, but not directly by the variability in ambient air temperature, which exhibited no such patterns. Mixing dynamics play a crucial role for biological dynamics, as they control e.g. the availability of light and nutrients for phytoplankton (Spigel and Imberger 1987), the composition of phytoplankton species (Huisman et al. 2004) and the spatial distribution of zooplankton (Pernica et al. 2013). Vertical mixing was also detected by high anti-phase coherence in measurements of oxygen concentrations and pH between near-surface and near-bottom measurement depths in chapter 4. This was associated with the replenishment of the lake bottom with oxygen, accompanied by oxygen and pH depressions at the lake surface. Similar phenomena caused by wind-induced mixing have been reported earlier from Müggelsee (Behrendt et al. 1993) and from other lakes (Robertson and Imberger 1994; Hanson et al. 2006; Langman et al. 2010). Furthermore, wind-induced resuspension of particles from the lake bottom was indicated through high in-phase coherence between wind speed and turbidity during summer (chapter 4). The resuspension of sediments can severely affect the water quality of lakes; on the one hand due to reduced light availability resulting from increased turbidity, and on the other hand due to the recycling of nutrients from the sediments to the water column (Kristensen et al. 1992; Eleveld 2012), potentially fueling eutrophication (Kozerski and Kleeberg 1998). Wind-induced resuspension is especially relevant in shallow, polymictic lakes such as Müggelsee, as less wind energy is required to cause complete vertical turnover than in deeper lakes that often exhibit more stable thermal stratification. Furthermore, phosphorus release from the sediment adds to the already nutrient-rich state of eutrophic lakes such as Müggelsee (Kristensen et al. 1992; Søndergaard et al. 1992; Kozerski and Kleeberg 1998). Vertical mixing can also be caused by severe rainstorms, which can have a larger effect than wind-induced mixing (Kimura et al. 2014).

In light of the projected warming of lakes worldwide (O'Reilly et al. 2015) and the resulting more frequent, more intense and longer time periods of thermal stratification (Wagner and Adrian 2011), the investigation of mixing dynamics becomes particularly relevant. Potential thermal regime shifts were projected for polymictic lakes, with profound impacts on the structure and functioning of these ecosystems (Kirillin 2010; Shatwell et al. 2016). Warmer water temperatures, associated with shorter periods of ice cover in winter and longer periods of thermal stratification in summer, may indirectly increase water temperature variability in these seasons (see chapter 3). However, there was also evidence that in the long term, water temperature variability may be decreased though longer and more stable thermal stratification.

Increases in water temperature may fuel phytoplankton growth only during specific time windows. This was shown in chapter 4, as the coherence between water temperature and chlorophyll *a* was only high and in phase during a short time window before the clear water phase. Afterwards, other drivers such as nitrogen limitation may have constrained phytoplankton growth (Köhler et al. 2005). On the other hand, cyanobacteria blooms are often triggered by warm water temperature and strong stratification stability (Huber et al. 2012; Merel et al. 2013) and can impair the water quality through increases in turbidity (chapter 4; Paerl and Huisman 2008). As cyanobacteria can form toxic blooms and are projected to become more abundant with climate warming (Castle and Rodgers 2009; Lürling and De Senerpont Domis

2013), powerful methods to detect their drivers and constraints, such as shown in this thesis by wavelet coherence, are needed.

Wavelet coherence also identified chemical processes such as calcite precipitation and calcite dissolution through anti-phase coherence between electrical conductivity an pH (chapter 4). While of general interest for the diagnosis of lake ecosystems (Lampert and Sommer 2007; Heine et al. 2017), calcite precipitation can also limit eutrophication and thereby phytoplankton growth through co-precipitation of phosphate (Hamilton et al. 2009). Yet, these reversible processes do not necessarily have permanent effects, as calcite dissolution in winter was followed by biogenic re-precipitation in spring. Furthermore, as shown above, wind-induced resuspension of sediments can release precipitated phosphorus from the sediment. These dynamics underline the importance of investigating lake-specific dynamics at adequate time scales and over longer time periods, as processes may occur only during short time windows or their characteristic time scale may change.

5.3 Conclusions and outlook

The frequency-based approaches applied in this thesis were found to be useful to indicate processes, their drivers and constraints occurring in lake ecosystems. Future risk assessment will depend on reliable diagnoses of the health and state of this fundamentally important and vulnerable resource. This requires advanced methods that make use of the high temporal resolution of now increasingly available automated monitoring data, while long-term data can form the framework for a deeper understanding. Integrating different data sources, such as remote sensing data, may provide additional insight. Indicators such as the slope of the spectra of parameters and powerful visual methods such as the coherence between time series will be needed to inform decision makers concerned with improving the water quality status of freshwater ecosystems. They could be integrated in decision support systems for lake risk assessment. While this thesis is based on tests of the suitability of these indicators only for one lake ecosystems, it presents a promising route towards successful, efficient analyses of other ecosystems worldwide. Lakes exhibiting different morphometry, mixing regimes, trophic states and chemical compositions, and potentially also other types of ecosystems, will provide interesting research objects in the future. Beyond the novel empirical findings reported in the three case studies, this thesis aims to help researchers to make more efficient use of time series data at high temporal resolution by providing them with a set of innovative, frequency-based methods to attribute patterns to processes, their drivers and constraints.

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Declaration of authorship

I, Silke R. Schmidt, declare that this dissertation titled "Analyzing lakes in the time frequency domain" and the work presented in it are my own. I prepared this dissertation without illegal assistance. I confirm that the work is original except where indicated by references in the text and no part of the dissertation has been submitted for any other degree.

This dissertation has not been presented to any other university for examination, neither in Germany nor in any other country.

Silke R. Schmidt