1	Supporting	Inform	ation
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- 2 Accompanying Manuscript: A multi-scale approach to timescale analysis: Isolating diel signals
- 3 from solute concentration time series

# 4 Authors:

- 5 Cathy Chamberlin
- 6 Duke University
- 7 9 Circuit Drive, Durham, NC 27709
- 8 <u>catherine.chamberlin@duke.edu</u>
- 9 (now at <u>chamberlin.catherine@epa.gov</u>)
- 10
- 11 Gaby Katul
- 12 Duke University
- 13 9 Circuit Drive, Durham, NC 27709
- 14 <u>gaby@duke.edu</u>
- 15
- 16Jim Heffernan
- 17 Duke University
- 18 9 Circuit Drive, Durham, NC 27709
- 19 james.heffernan@duke.edu
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## **30 Video Captions:**

*Video S1:* A demonstration of the IMFs derived from the Ichetucknee year-long timeseries 31 32 through EEMD. The timeseries is shown in black, data gaps are highlighted in grey, and 33 successive IMFs are displayed overlain on each other in blue, beginning from the highest frequency IMF and ending with the overall trend in the data. 34 35 Video S2: A demonstration of the IMFs derived from the Potomac year-long timeseries through EEMD. The timeseries is shown in black, data gaps are highlighted in grey, and successive IMFs 36 are displayed overlain on each other in blue, beginning from the highest frequency IMF and 37 ending with the overall trend in the data. 38 39 Video S3: A demonstration of the IMFs derived from the Connecticut year-long timeseries 40 through EEMD. The timeseries is shown in black, data gaps are highlighted in grey, and successive IMFs are displayed overlain on each other in blue, beginning from the highest 41 frequency IMF and ending with the overall trend in the data. 42

43

## 45 Appendix S1: A model for the background variability - White versus colored noise

To illustrate why the background concentration time series may follow a Lorentzian spectrum
('brown noise' instead of 'white noise'), the following argument and simplified model is offered.
If the concentration dynamics underlying the chemical constituent C are given by a simplified
balance

50 
$$\frac{dC}{dt} = -\tau C + I_c(t),$$

where  $\tau$  is the inverse reaction or transformation time scale, and  $I_c(t)$  is a time series of sources or sinks of C (due to stochastic hydrological additions or biological activities or both), then it can be shown that the Fourier power spectrum of C, defined as  $E_c(f)$ , is given as

54 
$$E_c(f) = \frac{E_I(f)}{\tau^2 + f^{2'}}$$

where  $E_I(f)$  is the Fourier spectrum of the sources and sinks  $I_c(t)$ , and f is the frequency (i.e. 55 inverse timescale)<sup>1</sup>. In this reduced dynamical system featuring a balance between changes in 56 storage (dC/dt), a first-order reaction or transformation loss ( $-\tau C$ ), and time-dependent sources 57 and sinks  $I_c(t)$  for C, diel patterns can arise when  $E_I(f)$  itself exhibits diurnal variations (e.g., 58 due to photochemical activities driven by variability in incident shortwave radiation with 59 60 stochasticity originating from clouds and water level/turbidity changes). At high frequencies  $(f/\tau >> 1)$  and for an  $I_c(t)$  exhibiting uncorrelated (white-noise) structure, the simplified model 61 here predicts  $E_c(f) \sim 1/f^2$  (brown noise)<sup>2</sup>. Likewise, at low frequencies  $(f/\tau << 1), E_c(f) \approx$ 62  $\tau^{-2}E_I(f)$  and the concentration spectrum scales as the 'input' or  $E_I(f)$  spectrum with no 63 frequency modulations. White noise structure is characterized by  $\alpha = 0$ , where  $\alpha$  is the slope of 64 the power spectrum, meaning that  $E_I(f)$  is a constant independent of f. Brown noise structure, 65

often produced by random walks, has  $1/f^2$  scaling and shows a decreasing slope with frequency 66 in the power spectra. When  $E_I(f)$  maintains white noise properties ( $\alpha = 0$ ) across all 67 frequencies,  $E_c(f)$  reduces to the so-called 'Lorentzian' spectrum (flat at low frequency and 68  $1/f^2$  at higher frequencies). In the analysis here,  $E_I(f)$  is rarely described by 'white-noise' and 69 at short times or high frequencies, it may exhibit its own statistical structure so that  $E_I(f) \sim f^{-\beta}$ . 70 This noise structure for  $E_I(f)$  leads to a concentration spectrum given by  $E_c(f) \sim f^{-2-\beta}$  for 71  $f/\tau >> 1$ . That is, concentration spectra here resemble 'black-noise' when  $\beta > 0$ . 72 The goal of the work here is to detect and isolate diel modes superimposed on a concentration 73 spectrum given as  $E_c(f) \sim f^{-2-\beta}$ . In summary, the conjecture here is that at  $f/\tau >>1$  (high 74 frequency range),  $E_I(f)$  can be decomposed into a background 'noise' characterized by 75  $E_I(f) \sim f^{-\beta}$  (where  $\beta \ge 0$ ) and other *deterministic modes* of variability (i.e. single spike at a 76 fixed frequency) due to biological activity. It is these deterministic modes that we seek to detect 77 from measured  $E_c(f)$  using Empirical Mode Decomposition analysis. 78 79 In the Lorentzian synthetic timeseries models we produced, we introduced the diel, seasonal, and tidal signals as a timeseries of sources and sinks  $I_c(t)$ . We chose the decay rate  $\tau$  to be one 80 month so that the diel frequency  $f_{diel}$  would be in the realm of  $f/\tau >>1$  (high frequency range) 81 where  $E_I(f) \sim f^{-\beta}$ . Choosing a  $\tau$  of this magnitude produces timeseries power spectra similar to 82 many signals reported in the literature<sup>3,4</sup>, and to signals of the measured timeseries in this work 83

84 (Appendix S2, Figures S3, S4).

85

#### 87 Appendix S2: Fast Fourier Transform and Wavelet Transform

#### 88 Fourier Analysis

89 Fourier Transform in general and Fast Fourier Transforms (FFT) in particular are common 90 methods for converting data from the time domain (e.g. a time-series of a water quality 91 constituent) into the "power" of different frequencies<sup>1</sup>. This method can efficiently decompose a 92 time series into a summation of sinusoidal waves, with each wave representing the 'energy' (also 93 'activity', 'variability' or 'variance') of a frequency in the series ranging from half the sampling 94 frequency (or the "Nyquist Frequency") to the inverse of the record duration<sup>5</sup>. The energy of a certain frequency is determined by the squared amplitude of the associated wave. Fourier 95 96 transforms are energy preserving in that the sum of the squared amplitudes of all frequencies recovers the energy of the original time series. Practically for the scientist, the precise definition 97 of the sampling interval n and the normalization of the series of length N are incorporated 98 differently in different software packages, necessitating caution when comparing activity across 99 100 methods.

One major drawback to Fourier analysis is its inability to sense locality of events in time. For
example, a time series characterized by a single 'spike' in time affects all the amplitudes
describing the Fourier decomposition. All FFT methods assume linearity (i.e. all time-series are a
linear combination of sine waves with different amplitudes, frequencies and periods) and
stationarity (i.e. the median value does not change with time) of the time series.

106 To illustrate the use of Fast Fourier Transformation (FFT) compared to the method developed in

this manuscript, we performed FFT on the synthetic and measured time series using the base R

108 `spectrum()` and `fft()` functions. Gaps in the timeseries were filled with a linear spline. We

109 identified peaks in the power spectra using the pracma package in R, then filtering peaks by 110 comparing them to  $1/f^2$  ( $\alpha = 2$ ) scaling. The  $1/f^2$  scaling is representative of chemical 111 constituents in channels with more catchment filtering, usually rivers of higher Strahler stream 112 orders<sup>4</sup>.

113 The resulting power spectra from the spectrum() R function show that the synthetic data sets initially all had scaling significantly steeper than 1/f or  $1/f^2$ , and converged on  $1/f^2$  scaling when 114 environmental variability was added to the series. The component frequencies for the linear 115 116 timeseries were correctly identified (Figure S3a,d), however the non-linear series created by a pulse and exponential decay signal produced a large number of high harmonics in the power 117 spectra (Figure S3g). This is consistent with spurious frequencies attributed to windowing and 118 finite-size effects acting on low frequency trends<sup>6</sup>. The diel frequency had an energy in the range 119 of 1.3-4.4 for the synthetic series, with the lower energies associated with the signals that had 120 observational error (i.e. gaps) introduced, and signals resulting from the pulse-decay function. 121 The spectrum() function applies various normalization and smoothing functions, such that the 122 total energy of the transformed signal differs from the total energy of the original timeseries, in 123 124 violation of Parseval's theorem. To estimate the recovery of signal strength through FFT, we therefore used the fft() R function instead. The amplitudes of the recovered diel signals were 125 closest to original (0.102 mg/l) for the clean S&D Sin and S,D&T Sin signals. FFT of the clean 126 127 Pulse-Decay signal returned signal of amplitude 0.074 mg/l. Introduction of environmental 128 variability and observational energy reduced the amplitude of the recovered diel signal to 0.067 129 mg/l for the S&D Sin and S,D&T Sin signals, and to 0.047 mg/l for the Pulse-Decay signal. 130 The concentration power spectra of the three measured data series using the spectrum() function

131 showed an approximate  $1/f^2$  scaling, consistent with catchment and hillslope filtering of

environmental variability<sup>3, 4, 7</sup> (Figure S4). Superimposed on this power-law behavior, the 132 Ichetucknee showed a strong peak at daily frequencies, as well as a number of harmonics. 133 134 Though only the largest of these harmonics was detected with our peak detection algorithm, 4 other higher harmonics can be seen visually. The Connecticut had tidal peaks strong enough to 135 be detected by our peak detection criteria, a peak at the diel frequency could still be seen visually 136 137 but was not strong enough to pass the peak detection criteria. The Potomac had no peaks strong enough for detection through our algorithm, however a small peak near the diel frequency can be 138 139 seen. All three spectra flattened into white noise at frequencies commensurate to 5000/year or about a 2-hour period commensurate with the Nyquist frequency (defined as twice the sampling 140 frequency). Diel signal amplitude extracted using the fft() function indicated a diel amplitude of 141 0.012 mg/l for the Ichetucknee, 0.001 mg/l for the Connecticut, and 0.004 mg/l for the Potomac. 142

## 143 Wavelet Transforms

Wavelet transforms have some 'time-frequency' localization capabilities that circumvent the 144 limitations of Fourier analysis in this regard. Full properties of wavelets are reviewed elsewhere<sup>8</sup> 145 and are not repeated here. In wavelet analysis, a kernel of a given shape, amplitude and 146 147 frequency is compared to the data at different time steps and the wavelet power of that frequency at that time is related to the goodness of fit. Unlike Fourier analysis, the wavelet kernel is not 148 unique and numerous kernels or basis functions are allowed provided they satisfy a number of 149 150 normalizing properties not discussed here. Like FFT, normalization methods differ amongst software packages, and the shapes of the kernels can impact the results under certain 151 circumstances (e.g. symmetric versus asymmetric wavelets, degree of localization in frequency 152 153 versus time, etc.) though wavelets under certain conditions (especially in detection of powerlaws) are insensitive to kernel shape as demonstrated elsewhere<sup>9</sup>. A review article by Torrence 154

and Compo<sup>10</sup> presents a clear explanation of how to use wavelets and how to link frequencies in
Fourier and wavelet analyses depending on choices made about the wavelet basis function.

157 Wavelet transforms are beneficial in decomposing signals in both space and time, however there 158 are several circumstances under which empirical methods may be preferred. Tradeoffs exist, where better locality in one domain (say time) can be achieved if appropriate wavelet analyzing 159 160 functions are selected, but this gain comes at a loss of resolution in the other domain (say frequency) and vice-a-versa. No wavelet transform can be fully accurate in both time and 161 frequency domains simultaneously. Practically, this can mean a loss of timeseries properties such 162 as phases of oscillations. Another drawback is redundancy – a time series of length N results in 163  $N^2$  wavelet coefficients (N coefficients required for all frequencies at every time instant for 164 165 continuous wavelet transforms) - a huge redundancy in information content that is 'manufactured' by the transform, not the process under consideration<sup>11, 12</sup>. This manufacturing of 166 information can produce bands of energy that are not descriptive of the underlying timeseries. 167 Orthonormal wavelet transforms may be used to preserve the precise information content of a 168 series without redundancy, but the arrangements of the wavelet coefficients require a courser 169 170 resolution of the frequency-time wavelet half-plane making detection of some patterns more difficult <sup>13, 14</sup>. 171

To demonstrate the use of wavelets, we used the WaveletComp package in R to compute
continuous wavelets of our synthetic (Figure S5) and measured timeseries (Figure S6). Wavelet
analysis of the synthetic timeseries were constant throughout time, and showed the same
frequencies as the Fourier transform, including the first harmonics from the pulsed decay signal.
The resolution of frequency in the Wavelet analysis is courser than Fourier, with wide bands
appearing around the 24 hr periodicity rather than narrow and discrete horizontal bands (Figure

178 S5). The diel and tidal frequencies became more difficult to identify once environmental 179 variability was added to the timeseries. The wavelet of the Potomac and Connecticut had very low power at most frequencies, with short durations (1-5 days) of slight power increases at the 180 181 diel (Potomac & Connecticut) and tidal (Connecticut only) frequencies that are difficult to visually identify. The Ichetucknee showed consistent power at the diel frequency that was 182 interrupted only by gaps in the data. All wavelet analyses showed significant distortion at the 183 ends of the timeseries – an artifact of windowing and mathematical assumptions made about the 184 form of the signal extrapolated past the ends of the measured or simulated timeseries. 185

#### **Appendix S3:** Estimation of N-uptake and Gross Primary Productivity

The N uptake predicted by the diel IMFs were calculated using a procedure described 188 189 elsewhere<sup>15</sup>, where the nighttime peaks of the timeseries were assumed to represent no 190 autotrophic uptake, and the concentration differences between the diel trace and a linear spline 191 that connected concentration peaks represented concentration deficits due to autotrophic 192 biological uptake. We calculated this concentration deficit for each timestep and converted to a 193 mass deficit though multiplication with the absolute value of simultaneous high-resolution sampled flowrate. Using the absolute value of discharge was necessary because of flow reversals 194 in the Connecticut River on 160 of the days in the time series. After converting to mass deficits 195 at each timestep, we summed the deficits at each timestep to a daily value. The conversion from 196 197 concentration to mass allows for a consistent, biologically meaningful, interpretation of values 198 across flow conditions. The same concentration deficit on a high flow day would indicate more N-uptake than the same concentration deficit on a low flow day, and by converting to mass 199 200 uptake, this difference is more readily apparent.

201 The GPP estimates for the Potomac and Connecticut rivers were determined earlier using the 202 StreamMetabolizer R package, which partitions changes in dissolved oxygen to GPP, ecosystem respiration and air-water gas exchange<sup>16</sup>, and we accessed them through the StreamPulse data 203 204 portal (data.streampulse.org). As the Connecticut River experiences flow reversals, and as these 205 days were excluded from the published data set, we used the available oxygen data for the Connecticut River to remodel GPP using the StreamMetabolizer package<sup>17</sup>. Though flow 206 reversals result in suboptimal metabolism estimates, given the high number of flow reversal days 207 208 and the nature of our study, we decided that an increased number of less precise GPP estimates 209 was preferable to fewer precise estimates. The GPP estimates derived here closely matched

published estimates for overlapping days. As these published estimates represent an ensemble of
model fits, we used the mean and standard deviation of daily values in our calculations. GPP was
estimated for the Ichetucknee using a 2 station approach, with the upstream O<sub>2</sub> concentration
treated as a constant arising from the flow-weighted concentrations of the Ichetucknee's
contributing springs<sup>15</sup>, and gas evasion estimated from correlations among discharge, velocity,
and gas exchange (as measured from floating domes).

All GPP estimates were provided as areal mass oxygen production, and were converted to 216 estimates of N-uptake using a C:O<sub>2</sub> molar productivity ratio of  $0.52 \pm 0.15$  for the Potomac and 217 Connecticut which reflects a distribution of autotrophic respiration quotients<sup>18-20</sup>, and a C:O<sub>2</sub> 218 molar productivity ratio of 0.5 for the Ichetucknee to be consistent with previous work<sup>15</sup>. A C:N 219 biomass molar ratio of 25:1<sup>15, 21</sup> was used for the Ichetucknee and  $16.1 \pm 5.46$  :1<sup>22</sup> for the 220 Potomac and Connecticut. Estimates of autotrophic N-uptake from these two methods were 221 compared to assess how well the EEMD method isolated the diel signal from complex data 222 series. These two metrics are nearly identical for previous work on the Ichetucknee River<sup>15</sup>. 223

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#### 226 Appendix S4: Solute footprint estimation

We estimated the areal concentration footprint of a diel nitrate excursion using the width of a river and a one-dimensional advection-dispersion equation<sup>23</sup> rearranged to solve for longitudinal distance travelled by the excursion<sup>24</sup>:

230
$$x = \frac{u\left(\frac{1}{4D}\left(\frac{uT}{\operatorname{erfc}^{-1}\left(1-2\frac{C_{\tau}}{C_{0}}\right)}\right)^{2}+T\right)}{1000}$$

231 where x is the longitudinal distance travelled by the excursion (in km), u is water velocity (in m s<sup>-1</sup>), T is the time duration of the excursion (in s), D is the dispersion rate (in  $m^2 s^{-1}$ ), erfc() is the 232 complementary error function,  $C_{\tau}$  is the concentration downstream at location x and time  $\tau$  (in 233 mg  $l^{-1}$ ), and  $C_0$  is the magnitude of the concentration perturbation (in mg  $l^{-1}$ ). We calculated this 234 235 value for each river assuming a stream with no nitrate gets a 12-hour pulse (T = 43,200 s) of magnitude equal to the diel nitrate range exhibited by the measured timeseries ( $C_0$  = diel range 236 on each day). The  $C_{\tau}$  was defined as  $C_0/2$ , or complete mixing of the water. We parameterized 237  $D = \alpha u^* h$  where  $\alpha$  is specified as a distribution derived from published work<sup>25</sup>, h is the gage 238 height (in m) and  $u^*$  was parameterized as the slope of the relation between u and  $(1/\kappa) \log(h)$ 239 240 from USGS site visits where  $\kappa \approx 0.41$  is the van Karman's constant. For each site, we used data reported by the USGS from site visits to relate u to discharge (in m<sup>3</sup> s<sup>-1</sup>), and to relate depth of 241 flow (h) and channel width (w) to u. For each day in the timeseries, average discharge was 242 converted to u, h, and w times using these relations, and footprints were computed as the product 243 244 of distance x (in km) and width w (in km) of the river reach. This computation was performed 10,000 times for each day sampling the distributions of u, h, w, and  $\alpha$ . The mean and standard 245

error of the resulting concentration footprints were used in creating the vertical error bars in Figure S7 and are reported in the text. This approach may over-estimate the areal footprint because of 3 implicit assumptions: (i) lateral dispersion is ignored in the estimation of x, (ii) bulk estimates of u and D are used, which overestimate the local advection and dispersion in the vicinity of the biological sink (i.e. river bed and sides), and (iii) the flow field is assumed to be uniform along x (channel section irregularities act as 'retardation' factors due to the presence of bends and dead-zones).





Figure S1: Synthetic time series used for illustrating detection and separation of diel patterns from other modes of variability. a) seasonal and diel sinewaves superimposed on each other b) seasonal, diel and tidal sinewaves superimposed on each other and c) seasonal sinewave and diel pulse-decay patterns superimposed on each other. Subsections i) show the simple time series, ii) show the time series with environmental variability included, and iii) show the time series with environmental and sensor induced variability and gaps included. In all plots, time periods highlighted with shaded boxes are amplified in the insets to illustrate fine-scale variability.



Figure S2: Measured nitrate concentration time series sampled at 15-minute intervals from the
a) Ichetucknee River in 2010 b) Potomac River in 2015 and c) Connecticut River in 2014.
Subsections i) show the whole series, and time periods highlighted with shaded boxes are
amplified in subsections ii) for visualization of diel features.



Figure S3: Power spectra of the three synthetic data series; Seasonal & Diel Sine: a-c; Seasonal, Diel & Tidal Sine: d-f; Pulse-Decay g-i; Blank with just the environmental structure j-l). Power spectra are shown of the simple signal (a, d, g & j), the signals with environmental variability (b, e, h & k) and the signals with variability from environmental and detection processes (c, f, I & l). The dashed line shows  $1/f^2$  scaling ( $\alpha = 2$ ), and blue dots show peaks with power at least 50x  $1/f^2$ scaling.

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- 280



**Figure S4:** Power spectra of the example three measured data series Power spectra are shown for

the a) Ichetucknee River, b) Connecticut River, and c) Potomac River. The dashed line shows

284  $1/f^2$  scaling ( $\alpha = 2$ ), and blue dots show peaks with power at least 50x  $1/f^2$  scaling.



Figure S5: Wavelet analysis of the three synthetic data series; Seasonal & Diel Sine: a-c;
Seasonal, Diel & Tidal Sine: d-f; Pulse-Decay g-i; Blank with just the environmental structure jl). Wavelet heatmaps are shown of the simple signal (a, d, g & j), the signals with environmental
variability (b, e, h & k) and the signals with variability from environmental and detection
processes (c, f, I & l). The color maps on all panels correspond to the quantiles of energy within
each measured timeseries. Thus, colors within panels are comparable, but colors are not
comparable across panels.



**Figure S6:** Wavelet heatmaps of the example three measured data series. Wavelets are shown

- for the a) Ichetucknee River, b) Connecticut River, and c) Potomac River. The color maps on all
- 298 panels correspond to the quantiles of energy within each measured timeseries. Thus, colors
- within panels are comparable, but colors are not comparable across panels.

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Figure S7: Areal daily N-uptake estimated from concentration deficit in the diel IMF (y-axis; 303 UN03, NO3) plotted against areal daily N-uptake estimated from GPP (x-axis; UN03, GPP) with 304 305 accompanying error in a) the Ichetucknee River, b) the Connecticut River, c) the Potomac River, 306 and d) the Potomac River minus 3 outliers that correlated with storm events. Error bars represent the 95% confidence interval ( $\pm 2$  standard error). Error for U<sub>NO3, GPP</sub> stems from uncertainty 307 around estimates of GPP, autotrophic respiration quotients, and C:N stoichiometry of 308 photoautotrophs. Error for U<sub>N03, N03</sub> derives from uncertainty around the size of the chemical 309 signature footprint. The black dotted line shows the 1:1 line. Grey triangles in a) denote 310 311 estimates from days that had flow reversals and are therefore less reliable than days shown in black circles. They are maintained because of their prevalence in the time series. In all panels, 312

only days on which signal was extracted from the timeseries are shown. Though theoretically,
negative uptake values are impossible, published model results of GPP are occasionally
negative<sup>16</sup>, and are kept for consistency in describing uncertainty. Error bars in the Ichetucknee
River do not account for error associated with GPP, as it was computed arithmetically and not
statistically.

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MetadataS1	
·· Data S1	
All Compiled Data and Code	
thor(s) [of the material provided in DataS1.zip]	
Catherine Chamberlin	
Duke University	
9 Circuit Drive Durham NC 27709	
catherine chamberlin@duke.edu	
catherine.enamberini@duke.edu	
Jim Heffernan	
Duke University	
9 Circuit Drive, Durham, NC 27709	
james.heffernan@duke.edu	
Gabriel Katul	
Duke University	
9 Circuit Drive, Durham, NC 27709	
gaby@duke.edu	
e list (files found within DataS1.zip)	
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EMDComputation.Rmd	
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     ./Nuptake Connecticut.Rmd
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     ././EEMDIch pl.png ... EEMDIch pl6.png
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     ././EEMDPot pl.png ... EEMDPot pl6.png
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```

# 437 **Description**

This compilation should run on most systems provided the folder structure and file organization
is left intact.

All code was developed using R 4.0.2. The following packages must be installed to run the code:

```
streamMetabolizer_0.11.4
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      StreamPULSE 0.0.0.9043
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      Cairo_1.5-12.2
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      shiny_1.5.0
446
      padr_0.5.2
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448
      dataRetrieval_2.7.6
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      xts_0.12.1
      dygraphs_1.1.1.6
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451
      pracma 2.2.9
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      gridExtra 2.3
453
      lubridate_1.7.9
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      hht 2.1.3
      zoo_1.8-8
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461
      readr_1.3.1
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466
      tidyverse_1.3.0
      foreach 1.5.0
467
      WaveletComp_1.1
468
469
      README.txt - This file includes a brief description of the purpose of the zip folder
470
      DataS1.zip.
471
472
      AnalyzeConnecticutIMFs.Rmd - This file accesses files Conn USGSdata.RData
473
      and Connecticut compiled.RData. This file analyzes the compiled EEMD results of
474
      the decomposition of the measured timeseries from the Connecticut River. This R Markdown file
475
      can be knitted or run chunk by chunk. Code provided first views all of the IMFs, examines their
476
477
      periods, isolates the Diel IMF using functions sourced from the HelperFunctions.R file,
478
      and calculates statistics on the extent, magnitude and seasonality of diel signal.
479
      AnalyzeIchetuckneeIMFs.Rmd - This file accesses files Ich data.RData and
480
      Ichetucknee compiled.RData. This file analyzes the compiled EEMD results of the
481
      decomposition of the measured timeseries from the Ichetucknee River. This R Markdown file
482
      can be knitted or run chunk by chunk. Code provided first views all of the IMFs, examines their
483
      periods, isolates the Diel IMF using functions sourced from the HelperFunctions.R file,
484
485
      and calculates statistics on the extent, magnitude and seasonality of diel signal.
```

487 AnalyzeLorentzianIMFs.Rmd - This file accesses files

488 SyntheticSeries.RData, ts.blank.c compiled.RData,

489 ts.blank\_compiled.RData, ts1.b\_compiled.RData,

490 tsl.c\_compiled.RData, tsl\_compiled.RData, ts2.b\_compiled.RData,

491 ts2.c\_compiled.RData, ts2\_compiled.RData, ts3.b\_compiled.RData,

492 ts3.c\_compiled.RData and ts3\_compiled.RData. This file analyzes the compiled

EEMD results of the decomposition of the Lorentzian timeseries. This R Markdown file can be

knitted or run chunk by chunk for one timeseries at a time. Code provided first views displays all

- of names of the Lorentzian timeseries, and requires user input to choose which series to view forthe remainder of the file. Once a timeseries is selected, the code displays all IMFs, examines
- 497 their periods, isolates the Diel IMF using functions sourced from the HelperFunctions. R
- file, and calculates statistics on the extent, magnitude, and percent signal recovery.
- 499

500 AnalyzePotomacIMFs.Rmd - This file accesses files Pot\_USGSdata.RData and

501 Potomac compiled.RData. This file analyzes the compiled EEMD results of the

502 decomposition of the measured timeseries from the Potomac River. This R Markdown file can be

knitted or run chunk by chunk. Code provided first views all of the IMFs, examines their periods,

- isolates the Diel IMF using functions sourced from the HelperFunctions.R file, and
- 505 calculates statistics on the extent, magnitude and seasonality of diel signal.
- 506

507 CreateSyntheticSeries.Rmd - This file creates the Lorentzian timeseries following 508 the mathematical description in the Supplemental Information. A base timeseries of either 509 sinusoidal or exponential decay shape is successively contaminated with brown noise (i.e. a random walk) of a certain magnitude representing environmental variability, and then with white 510 511 noise and gaps representing measurement error or observational variability. The power spectra for each timeseries is available for viewing. "Blank" timeseries of just background variability are 512 513 also produced that do not have any structure as their base. Produces output 514 SyntheticSeries.RData.

515

516 Download+Save\_MetabolismEstimates.Rmd - This file accesses the metabolism 517 estimates for the Potomac and Connecticut rivers that were available in the literature<sup>16</sup>, and 518 accessible through the StreamPulse data portal (data.streampulse.org). As the metabolism of the 519 Connecticut River was also estimated locally, several graphical comparisons of the two 520 estimations are provided in this file. Produces output CT\_nwis-01193050\_metab.RData 521 and MD nwis-01646500 metab.RData.

522

523 EEMDComputation.Rmd - This file accesses files Conn\_USGSdata.RData,

524 Pot\_USGSdata.RData, Ich\_data.RData and SyntheticSeries.RData. It

uses the hht package to compute 200 trial decompositions of each timeseries, then compiles them

and resifts them according to the method described by the authors of the package<sup>26</sup>. Outputs of

527 this code file include Connecticut compiled.RData ,

```
528
      Ichetucknee compiled.RData, Potomac compiled.RData,
      ts.blank.c compiled.RData, ts.blank compiled.RData,
529
      ts1.b compiled.RData, ts1.c compiled.RData, ts1 compiled.RData,
530
      ts2.b compiled.RData, ts2.c compiled.RData, ts2 compiled.RData,
531
      ts3.b compiled.RData, ts3.c compiled.RData, and
532
533
      ts3 compiled.RData. Running the code also creates the folders
      Connecticut eemd/, Ichetucknee eemd/, Potomac eemd/,
534
      ts.blank.c eemd/, ts.blank eemd/, ts1.b eemd/, ts1.c eemd/,
535
      ts1 eemd/, ts2.b eemd/, ts2.c eemd/, ts2 eemd/, ts3.b eemd/,
536
537
      ts3.c eemd/, and ts3 eemd/, and 200 trials in each folder. For space reasons, these
538
      trial files are not included in the zipped folder. Please contact the authors if they are needed.
539
540
      FFTAnalysis.R contains code to perform Fourier analysis of the measured and synthetic
      timeseries and produce the power spectra plots in Fig S3 and Fig S4.
541
542
      HelperFunctions.R contains 5 functions that are called in many of the other code files.
543
      They are loaded when this script is sourced by the other RMarkdown files. The first function is
544
      auto.installer() which combines installation and loading libraries. Alternatively, experienced R
545
      users can install packages manually. The second is my PlotIMFs(), which is a very slight
546
      modification of PlotIMFs() from the hht package to allow for more descriptive plot titles.
547
      Investigate.IMF() creates an interactive graph of all of the selected IMFs overlain on each other.
548
      This is a helpful function for inspecting regions of a timeseries more closely.
549
      format_EEMD_result() and filter_imfs() are meant to be used in concert, where the input of
550
      filter_imfs() is the output of format_EEMD_result(). filter_imfs() will isolate the signal of a
551
      given period and phase from all of the IMFs. Phase is only supported for 24 hour periodicity at
552
553
      this point.
554
      MakeFigS1.Rmd contains code to create Fig S1 of the Lorentzian data series. This file loads
555
      SyntheticSeries.RData and writes FigS1.pdf and FigS1insets.pdf. The
556
557
      presented Fig S1 was created using these pdf files in Adobe Illustrator.
558
      MakeFigS2.Rmd contains code to create Fig S2 of the Measured data series. This file loads
559
      Ich data.RData, Conn USGSdata.RData, and Pot USGSdata.RData and
560
561
      writes FigS2.pdf. The presented Fig S2 was created using this pdf file in Adobe Illustrator.
562
      MakeFig1.Rmd contains code to create Fig 1. This file loads Conn USGSdata.RData
563
      and Connecticut compiled.RData and writes Figla.pdf, Figlb.pdf,
564
      Figlc.pdf and Figld.pdf. The presented Fig 1 was created using these pdf files in
565
      Adobe Illustrator.
566
567
568
      MakeFig2.Rmd contains code to create Fig 2. This file loads Ich data.RData,
```

569 Ichetuknee\_compiled.RData, Conn\_USGSdata.RData,

```
570
      Connecticut compiled.RData, Pot USGSdata and
      Potomac compiled.RData and writes Fig2.pdf.
571
572
      MakeVideo1.Rmd contains code to create the frames for Video S1. This file loads
573
      Ich data.RData, and Ichetucknee compiled.RData and writes
574
      EEMDIch p[1:16].png. The video was created using these images through Windows Video
575
      Editor.
576
577
      MakeVideo2.Rmd contains code to create the frames for Video S2. This file loads
578
      Pot USGSdata.RData, and Potomac compiled.RData and writes
579
      EEMDPot p[1:16].png. The video was created using these images through Windows Video
580
581
      Editor.
582
      MakeVideo3.Rmd contains code to create the frames for Video S3. This file loads
583
584
      Conn USGSdata.RData, and Connecticut compiled.RData and writes
585
      EEMDConn p[1:17].png. The video was created using these images through Windows
      Video Editor.
586
587
      ModelConnecticutMetabolism.R contains code to model metabolism using the
588
      streamMetabolizer package. Settings match those used in published literature<sup>16</sup> except for the
589
      decisions on which days to include in the model. This code produces the file
590
591
      CT Modelled metab.RData. As the model output file is large, the output is not included in
592
      this zipped folder. Please contact authors if the file is needed.
593
594
      Nuptake Connecticut.Rmd contains code to calculate the N-uptake for the Connecticut
595
      River predicted from the diel nitrate variability according to methods developed in the
596
      literature<sup>15</sup>. Independent estimates of N-uptake are also produced from GPP estimates. This file
597
      also calculates the theoretical concentration footprints based on literature methods<sup>24</sup>. All
598
      estimates are compared with each other, and error surrounding these estimates are provided. This
599
      file loads Conn USGSdata.RData, Connecticut compiled.RData,
      CT modelled metabolism.RData and Conn ratingcurve.RData, and writes
600
      Fig3b.pdf and FigS7b.pdf. AsCT modelled metabolism.RData is large, it is
601
      not included in this zipped folder. Please contact authors if the file is needed.
602
603
      Nuptake Ichetucknee.Rmd contains code to calculate the N-uptake for the Ichetucknee
604
      River predicted from the diel nitrate variability according to methods developed in the
605
      literature<sup>15</sup>. Independent estimates of N-uptake are also produced from GPP estimates. All
606
      estimates are compared with each other. This file loads Ich data.RData,
607
      Ichetucknee compiled.RData and Ichetucknee metabolism.csv, and
608
      writes Fig3a.pdf and FigS7b.pdf.
609
610
```

```
S28
```

Nuptake Potomac.Rmd contains code to calculate the N-uptake for the Potomac River 611 predicted from the diel nitrate variability according to methods developed in the literature<sup>15</sup>. 612 Independent estimates of N-uptake are also produced from GPP estimates. This file also 613 calculates the theoretical concentration footprints based on literature methods<sup>24</sup>. All estimates are 614 compared with each other, and error surrounding these estimates are provided. This file loads 615 616 Pot USGSdata.RData, Potomac compiled.RData, MD nwis-01646500 metab.RData and Pot ratingcurve.RData, and writes 617 Fig3c.pdf, Fig3d.pdf, FigS7b.pdf and FigS7c.pdf. 618 619 ProcessIchetuckneeData.Rmd contains code that formats the Ichetucknee nitrate data 620 to be consistent with data retrieved from the USGS NWIS site. The code loads 621 Ichetucknee 2010 parsed jbh.csv and writes Ich\_data.RData. 622 623 624 USGSDataDownload.Rmd contains code to access relevant data from the USGS NWIS site using the dataRetrieval R package. Continuous nitrate and discharge data are downloaded from 625 the Connecticut River (gage 01193050) and the Potomac River (gage 016456500). The data are 626 627 lightly processed to ensure a consistent sampling frequency, no duplicate measurements, and units of m3s for discharge. Rating curves for both sites are also downloaded and saved. This 628 629 script exports files Conn USGSdata.RData, Pot USGSdata.RData, Conn ratingcurve.RData and Pot ratingcurve.RData. 630 631 WaveletAnalysis.R contains code to compute and print the continuous wavelet analyses 632 of the measured and synthetic timeseries. The code saves the wavelet analyses in ./Output, and 633 due to their size, these output files are not included in the initial DataS1 zip file. The code also 634 creates .tif files to create Fig S5 and Fig S6. Fig S5 and S6 were compiled in Inkscape. 635 636 Ichetucknee 2010 parsed jbh.csv contains direct observations of NO<sub>3</sub> and other 637 water quality parameters as well as derived estimates of metabolism from O2 and nitrogen 638 uptake from diel NO<sub>3</sub><sup>-</sup> variability. NO<sub>3</sub><sup>-</sup> data were collected from Satlantic SUNA V1 sensors 639 640 and other water quality parameters collected by YSI sonde. Sensors were deployed ~5km downstream of the Ichetucknee Headspring at US Highway 27 near USGS gage 02322700, and 641 cleaned weekly concurrent with data download. Diel N uptake was estimated based on diel NO<sub>3</sub><sup>-</sup> 642 643 deviation from two different baselines: the prior nighttime maxima and the mean of the prior and subsequent nighttime maxima<sup>15</sup>. 644 645 Ichetucknee metabolism.csv contains estimates of metabolism (Gross Primary 646 647 Production and Ecosystem Respiration) derived from diel variation in O<sub>2</sub> concentrations and other physical and chemical parameters. Because the Ichetucknee's flow is derived from 5 648 distinct large springs, assumptions of longitudinal O<sub>2</sub> equilibrium required by single-station 649 methods were not applicable. Instead, metabolism was calculated using a 2-station approach 650 651 with the upstream boundary O<sub>2</sub> concentration estimated from the flow-weighted contributions of the hydrologically- and chemically-stable springs. Gas exchange was estimated from discharge 652

based on prior studies of the relationship between dome-gas exchange and flow velocity and 653 applied to the river surface area upstream of the sensors. 654 655 Conn ratingcurve.RData is data accessed from the USGS describing their site visits to 656 gage 01193050. The file is written by USGSDataDownload. Rmd. 657 658 659 Conn USGSdata.RData is continuous monitoring data from USGS NWIS for site 660 01193050. The file is written by USGSDataDownload.Rmd. 661 662 CT nwis-01193050 metab.RData contains metabolism estimates for site 01193050 accessed through StreamPulse. The file is written by 663 Download+Save MetabolismEstimates.Rmd. 664 665 666 Ich data.RData contains the reformatted data from Ichetucknee 2010 parsed jbh.csv. The file is written by 667 ProcessIchetuckneeData.Rmd. 668 669 670 MD nwis-01646500 metab.RData contains metabolism estimates for site 016456500 accessed through StreamPulse. The file is written by 671 Download+Save MetabolismEstimates.Rmd. 672 673 Pot ratingcurve.RData is data accessed from the USGS describing their site visits to 674 gage 016456500. The file is written by USGSDataDownload. Rmd. 675 676 677 Pot USGSdata.RData is continuous monitoring data from USGS NWIS for site 016456500. 678 The file is written by USGSDataDownload.Rmd. 679 680 SyntheticSeries.RData contains the Lorentzian timeseries created by 681 CreateSyntheticSeries.Rmd. 682 FigS1.pdf is written by MakeFigS1.Rmd and contains segments of Figure S1. Figure S1 683 was created in Adobe Illustrator. 684 685 686 FigSlinsets.pdf is written by MakeFigSl.Rmd and contains segments of Figure S1. 687 Figure S1 was created in Adobe Illustrator. 688 FigS2.pdf is written by MakeFigS2.Rmd and contains segments of Figure S2. Figure S2 689 was created in Adobe Illustrator. 690 691 Figla.pdf is written by MakeFigl.Rmd and contains segments of Figure 1. Figure 1 was 692 created in Adobe Illustrator. 693 694

695	Figlb.pdf is written by MakeFigl.Rmd and contains segments of Figure 1. Figure 1 was
696	created in Adobe Illustrator.
697	
698	Figlc.pdf is written by MakeFigl.Rmd and contains segments of Figure 1. Figure 1 was
699	created in Adobe Illustrator.
700	
701	Figld.pdf is written by MakeFigl.Rmd and contains segments of Figure 1. Figure 1 was
702	created in Adobe Illustrator.
703	
704	Fig2.pdf is written by MakeFig2.Rmd and is the same as published Figure 2.
705	
706	Fig3a.pdf is written by Nuptake_Ichetucknee.Rmd and shows the correlation
707	between N-uptake estimates from GPP and from isolated diel oscillations of nitrate. Fig 3 in the
708	manuscript was created in Adobe Illustrator and Inkscape.
709	
710	Fig3b.pdf is written by Nuptake_Connecticut.Rmd and shows the correlation
711	between N-uptake estimates from GPP and from isolated diel oscillations of nitrate. Fig 3 in the
712	manuscript was created in Adobe Illustrator and Inkscape.
713	
714	Fig3c.pdf is written by Nuptake_Potomac.Rmd and shows the correlation between N-
715	uptake estimates from GPP and from isolated diel oscillations of nitrate. Fig 3 in the manuscript
716	was created in Adobe Illustrator and Inkscape.
717	
718	Fig3d.pdf is written by Nuptake_Potomac.Rmd and shows the correlation between N-
719	uptake estimates from GPP and from isolated diel oscillations of nitrate. Fig 3 in the manuscript
720	was created in Adobe Illustrator and Inkscape.
721	
722	FigS3.pdf is written by FFTAnalysis.R FigS3 in the manuscript was created in
723	Inkscape.
724	
725	FigS4.pdf is written by FFTAnalysis.R FigS4 in the manuscript was created in
726	Inkscape.
727	
728	FigS5a.tif is written by WaveletAnalysis.R FigS5 in the manuscript was created in
729	Inkscape.
730	
731	FigS5b.tif is written by WaveletAnalysis.R FigS5 in the manuscript was created in
732	Inkscape.
733	
734	FigS5c.tif is written by WaveletAnalysis.R FigS5 in the manuscript was created in
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737	FigS5d.tif is written by	WaveletAnalysis.R	Fig S5 in the manuscript was created in
738	Inkscape.		
739			
740	FigS5e.tif is written by	WaveletAnalysis.R	Fig S5 in the manuscript was created in
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743	FigS5f.tif is written by	WaveletAnalysis.R	Fig S5 in the manuscript was created in
744	Inkscape.		
745			
746	FigS5g.tif is written by	WaveletAnalysis.R	Fig S5 in the manuscript was created in
747	Inkscape.		
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749	FigS5h.tif is written by	WaveletAnalysis.R	Fig S5 in the manuscript was created in
750	Inkscape.		
751			
752	FigS5i.tif is written by	WaveletAnalysis.R	Fig S5 in the manuscript was created in
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754	-		
755	FigS5k.tif is written by	WaveletAnalysis.R	Fig S5 in the manuscript was created in
756	Inkscape.		
757	L L		
758	FigS51.tif is written by	WaveletAnalysis.R	Fig S5 in the manuscript was created in
759	Inkscape.		
760	L		
761	FigS6a.tif is written by	WaveletAnalysis.R	Fig S6 in the manuscript was created in
762	Inkscape.		
763			
764	FigS6b.tif is written by	WaveletAnalysis.R	Fig S6 in the manuscript was created in
765	Inkscape.		
766			
767	FigS6c.tif is written by	WaveletAnalysis.R	Fig S6 in the manuscript was created in
768	Inkscape.		
769	•		
770	FigS7a.pdf is written by	Nuptake Ichetuckne	ee.Rmd and shows the correlation
771	between N-uptake estimates	from GPP and from isolate	d diel oscillations of nitrate with error
772	bars for both methods. Fig S'	7 in the manuscript was cre	ated in Inkscape.
773	C	1	L
774	FigS7b.pdf is written by	Nuptake Connecticu	at.Rmd and shows the correlation
775	between N-uptake estimates	from GPP and from isolate	d diel oscillations of nitrate with error
776	bars for both methods. Fig S'	7 in the manuscript was cre	ated in Inkscape.
777	C	*	-

778	FigS7c.pdf is written by Nuptake_Potomac.Rmd and shows the correlation between N-
779	uptake estimates from GPP and from isolated diel oscillations of nitrate with error bars for both
780	methods. Fig S7 in the manuscript was created in Inkscape.
781	
782	FigS7d.pdf is written by Nuptake_Potomac.Rmd and shows the correlation between N-
783	uptake estimates from GPP and from isolated diel oscillations of nitrate with error bars for both
784	methods. Fig S7 in the manuscript was created in Inkscape.
785	
786	Connecticut_compiled.RData contains the compiled EEMD results from all 200 trials
787	for the Connecticut River. The results contain timeseries for each IMF. The file was produced by
788	EEMDComputation.Rmd.
789	
790	Ichetucknee_compiled.RData contains the compiled EEMD results from all 200 trials
791	for the Ichetucknee River. The results contain timeseries for each IMF. The file was produced by
792	EEMDComputation.Rmd.
793	
794	ts.blank.c_compiled.RData contains the compiled EEMD results from all 200 trials
795	for the blank Lorentzian timeseries with observational variation. The results contain timeseries
796	for each IMF. The file was produced by EEMDComputation.Rmd.
797	
798	ts.blank_compiled.RData contains the compiled EEMD results from all 200 trials for
799	the blank Lorentzian timeseries with environmental variation. The results contain timeseries for
800	each IMF. The file was produced by EEMDComputation.Rmd.
801	
802	ts1.b_compiled.RData contains the compiled EEMD results from all 200 trials for the
803	S&D Lorentzian timeseries with environmental variation. The results contain timeseries for each
804	IMF. The file was produced by EEMDComputation.Rmd.
805	
806	ts1.c_compiled.RData contains the compiled EEMD results from all 200 trials for the
807	S&D Lorentzian timeseries with observational variation. The results contain timeseries for each
808	IMF. The file was produced by EEMDComputation.Rmd.
809	
810	ts1_compiled.RData contains the compiled EEMD results from all 200 trials for the S&D
811	Lorentzian timeseries. The results contain timeseries for each IMF. The file was produced by
812	EEMDComputation.Rmd.
813	
814	ts2.b_compiled.RData contains the compiled EEMD results from all 200 trials for the
815	S,D&T Lorentzian timeseries with environmental variation. The results contain timeseries for
816	each INIF. The file was produced by EEMDComputation.Rmd.
81/	

ts2.c compiled.RData contains the compiled EEMD results from all 200 trials for the 818 S.D&T Lorentzian timeseries with observational variation. The results contain timeseries for 819 each IMF. The file was produced by EEMDComputation.Rmd. 820 821 ts2 compiled.RData contains the compiled EEMD results from all 200 trials for the 822 S,D&T Lorentzian timeseries. The results contain timeseries for each IMF. The file was 823 produced by EEMDComputation.Rmd. 824 825 826 ts3.b compiled.RData contains the compiled EEMD results from all 200 trials for the Pulse-Decay Lorentzian timeseries with environmental variation. The results contain timeseries 827 for each IMF. The file was produced by EEMDComputation.Rmd. 828 829 ts3.c compiled.RData contains the compiled EEMD results from all 200 trials for the 830 831 Pulse-Decay Lorentzian timeseries with observational variation. The results contain timeseries for each IMF. The file was produced by EEMDComputation.Rmd. 832 833 ts3 compiled.RData contains the compiled EEMD results from all 200 trials for the Pulse-834 Decay Lorentzian timeseries. The results contain timeseries for each IMF. The file was produced 835 836 by EEMDComputation.Rmd. 837 838 Potomac compiled.RData contains the compiled EEMD results from all 200 trials for the Potomac River. The results contain timeseries for each IMF. The file was produced by 839 840 EEMDComputation.Rmd. 841 842 EEMDConn pl.png ... EEMDConn pl7.png contain image frames to make Video S2. 843 Images are written by MakeVideo2.Rmd 844 EEMDIch pl.png ... EEMDIch pl6.png contain image frames to make Video S1. 845 Images are written by MakeVideo1.Rmd 846 847 EEMDPot pl.png ... EEMDPot pl6.png contain image frames to make Video S3. 848 849 Images are written by MakeVideo3.Rmd 850 851 852 853

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