General Assembly
#vEGU21
19-30 April 2021

Stochastic analysis of time-series related to ocean acidification

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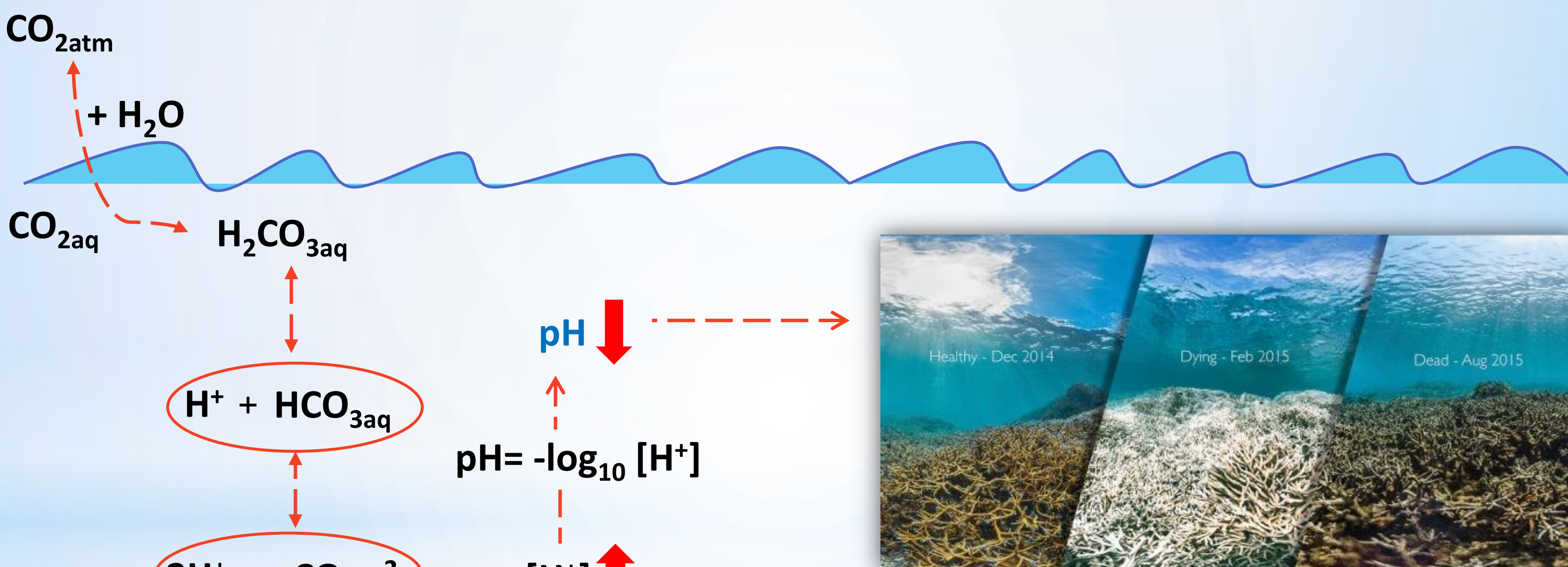
European Geosciences Union
General Assembly
(April -2021)

“Ocean acidification (OA): The other CO_2 problem” [1]

The phenomenon: OA is described as the constant increase of atmospheric carbon dioxide (CO_{2atm}) which reduces ocean pH and causes wholesale shifts in seawater carbonate chemistry[1].



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Objective: We perform time-series analysis focused on temporal changes in month and annual time lag, in order to detect the interaction between each variable element along with the seasonality effect.

Methodology (1)

Data (Time-series) specifications:

Variables

1) Aquatic measurements: Hawaii Ocean Time series (HOT) [2]

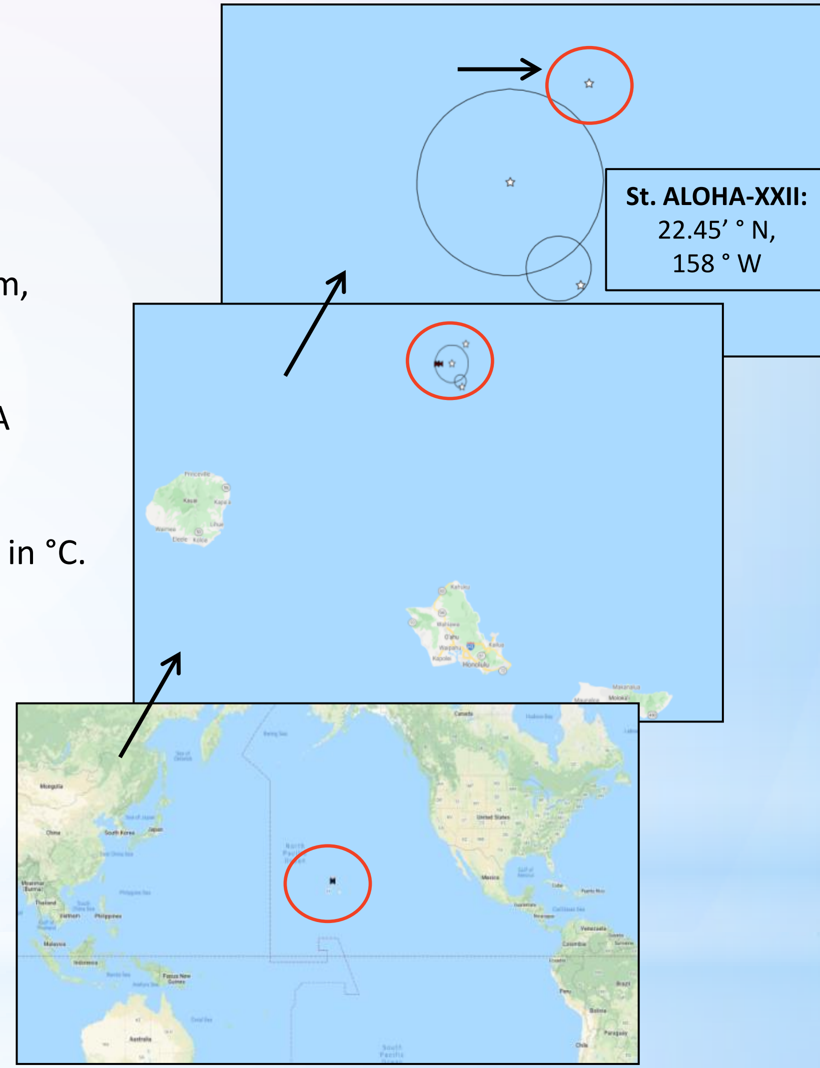
   CO_{2aq}: The mean surface seawater CO_2 partial pressure, in µatm, calculated from DIC* and TA** at in situ temperature.

   PH: The mean surface seawater pH, calculated from DIC and TA at in situ temperature, on the total scale.

   Temperature: The mean surface in situ seawater temperature, in °C.

2) Atmospheric measurements: (Mauna Loa, Hawaii) [3]

   CO_{2atm}: Surface CO_2 in-situ measurements (ppm)



Location: North Pacific Ocean (Hawaiian Archipelago)

Year Range

October 1988 – October 2018 (30 years)

Time-step (Δt)

Monthly measurements

*Dissolved Inorganic Carbon
**Total Alkalinity

Methodology (2)

Time series procedures-functions (Analysis steps):

1) <u>Linear Interpolation</u>

Step standardization at y (NA value), at a given x, was operated with the use of the following formula[4]:

$$y(x) = y_i + (y_{i+1} - y_i)\frac{x - x_i}{x_{i+1} - x_i} \quad , \quad x_i < x < x_{i+1}$$

2) <u>Cross- correlation function (CCF)</u>

CCF (r_{xy}) at a discrete time k was calculated according to the formula of[5,6]:

$$r^{x,y}{}_k = \frac{\sum_{s=max(1,-t)}^{min(n-t,n)} (x_i(s+t) - \overline{x_i})(x_j(s) - \overline{x_j})}{\sqrt{SD_x SD_y}}$$

X_i=predictor variable (x)
X_j=response variable (y)
$\overline{x_j}$=expected value of x
$\overline{x_i}$=expected value of y

$c_{i,j}$ =CCF function
n=sample size
t=time lag
SD=st. deviation

The statistical significance of the CCF was approximately approached with the 95% confidence intervals ($CI_{95\%}$) of the CCF, estimated as follows[6]:

$$\mathrm{CI}_{95\%} = -\frac{1}{n} \pm \frac{2}{\sqrt{n}}$$

where n is the number of data points used in the calculation of the CCF, and the $CI_{95\%}$ equations which are depicted as dashed blue lines in the CCF plots. We utilized the simplified tool of CCF since it represent one of the most informative indicators in terms of directionality[7]. In cases where significant time dependence was observed, Monte-Carlo simulation (MCS) was applied to determine the 95% confidence intervals through the fundamental stochastic Markovian process AR(1) depicted as purple dot-dashed lines.

Methodology (2)

Time series procedures (Analysis steps):

3) <u>Moving Average (Rolling Monthly Average)</u>

A simple (unweighed) moving average (MA) was calculated successively for complete annual time series (Jan-Dec) for monthly (q=2 month) and annual (q=12 month) time step:

$$\mathrm{MA}_q(i) = \frac{\underline{X}_{n-k+1} + \underline{X}_{n-k+2} + \cdots + \underline{X}_n}{q} = \frac{1}{q}\sum_{i=n-q+1}^{n} \underline{x_i}$$

q=rolling grade (months)
n=sample size
X_i=x value
k=dynamic variable (initial k=0)
$\underline{x}$=random variable

4) <u>Annual differencing - Δ (Rolling Annual Difference)</u>

Annual differencing Δ ($\underline{\tilde{x}}$) was calculated successively for complete annual time series as follows in order to eliminate periodicity[7]:

v=time step differencing

$$\underline{\tilde{x}}_{k,v} \coloneqq \underline{x}_{k+v} - \underline{x}_v$$

5) <u>Seasonality effect (SE) at various time lags (q)</u>[7]

$$\mathrm{SE_q(i)} = X_t(\mathrm{i}) - \mathrm{MA}_q(\mathrm{i})$$

X_t=Time series

Methodology (2)

Time series procedures (Analysis steps):

6) <u>Empirical climacogram (Monthly & Annual) & Hurst parameter</u>

Climacogram (GR: *κλίμαξ~climax; EN: scale*) is defined as the variance of the averaged process at discrete time scale κ: [8]

$$\rho_\kappa \coloneqq \mathrm{var}\left[\frac{\underline{X}_\kappa}{\kappa\sigma}\right] = \frac{\gamma_\kappa}{\gamma_1}, \qquad \gamma_\kappa \coloneqq \mathrm{var}\left[\frac{\underline{X}_\kappa}{\kappa}\right] = \gamma_1 \rho_\kappa, \qquad \underline{X}_\kappa \coloneqq \underline{x}_1 + \cdots + \underline{x}_\kappa$$

$$\gamma_{(\kappa)} = \frac{\gamma_{(1)}}{\kappa^{2-2\mathrm{H}}}$$

γ =variance (var)
κ=time scale
H= Hurst parameter
$\gamma_{(\kappa)}$=climacogram
$\rho_{(\kappa)}$= dimensionless climacogram

The selection of climacogram for the estimation of the Hurst parameter was applied since it functions as the most statistical reliable tool towards the stochastic explanation of geophysical processes, compared to the widely-used auto-covariance and power spectrum[9].

<u>Classification of temporal phenonomenona based on Hurst</u>[8]

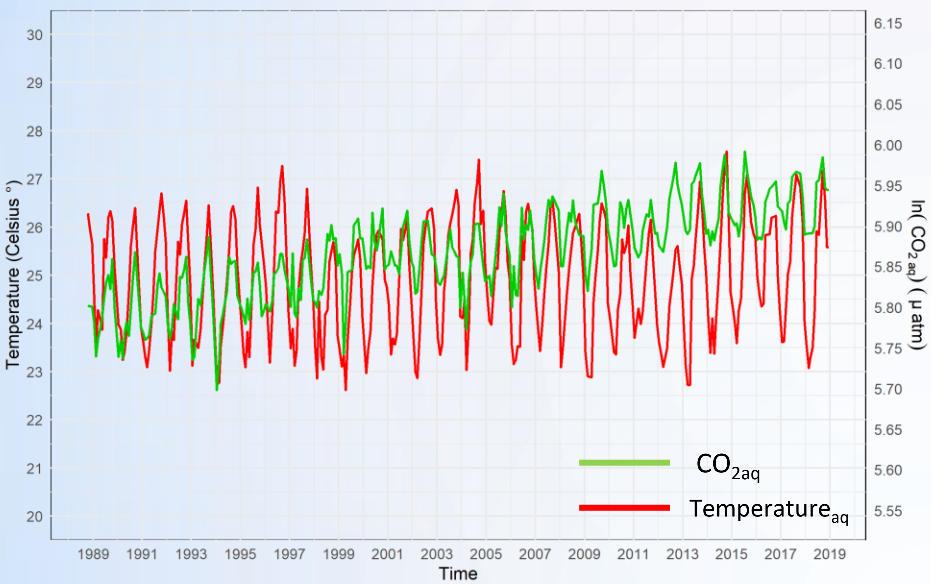
- $H > \frac{1}{2}$: $\boldsymbol{persistence}$

- $H = \frac{1}{2}$: $\boldsymbol{white\ noise}$ ($\boldsymbol{purely\ random\ process}$)

- $H < \frac{1}{2}$: $\boldsymbol{anti-persistence}$

CO_{2aq} ~ Temperature

Time series of aquatic $CO_{2\ aq(\mu atm)}$ and Temperature (HOT) measurements (1988-2018)

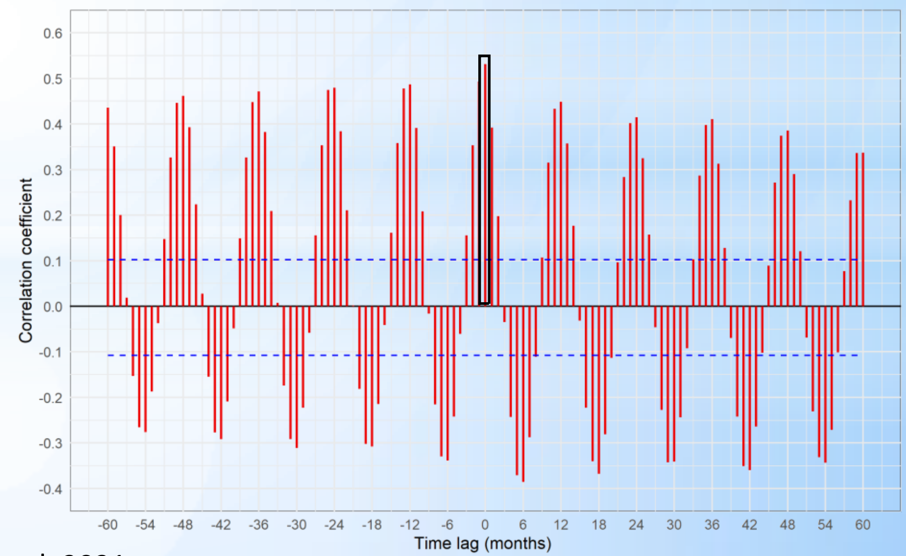


In the original time series of the ocean **carbon dioxide** (natural logarithm transformation[7]) and **temperature** measurements it is apparent that during the last 30 years there is a discrete increasing trend of CO_{2aq}, while temperature exhibits a more erratic behavior. Both processes appear to be under a strong seasonal effect, a behavior that will be further analyzed in the following sections.

In the CCF plot between the original observations of aquatic CO_{2aq} (x) and **temperature** (y) the highest positive value has been attained at lag zero (+0.53) and it keeps a decreasing periodic positive and negative peak in a sequence of 6 and 12 lag (months), respectively. There is a significant cross-symmetric behavior around lag zero and the periodic peaks indicate a seasonal phenomenon[5]. Additionally, causality cannot be explained through the above graphs[7].

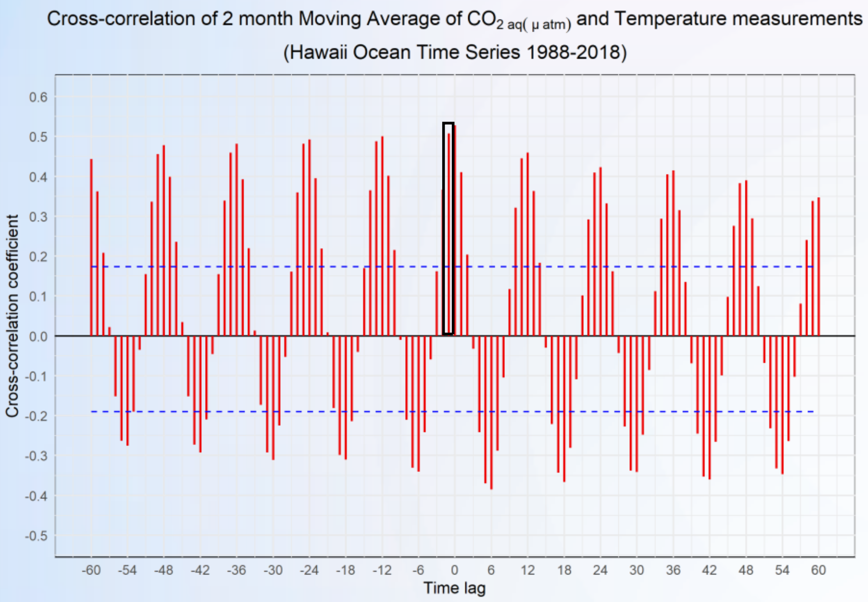
Cross-correlation of $CO_{2\ aq(\mu\ atm)}$ and Temperature measurements

(Hawaii Ocean Time Series 1988-2018)

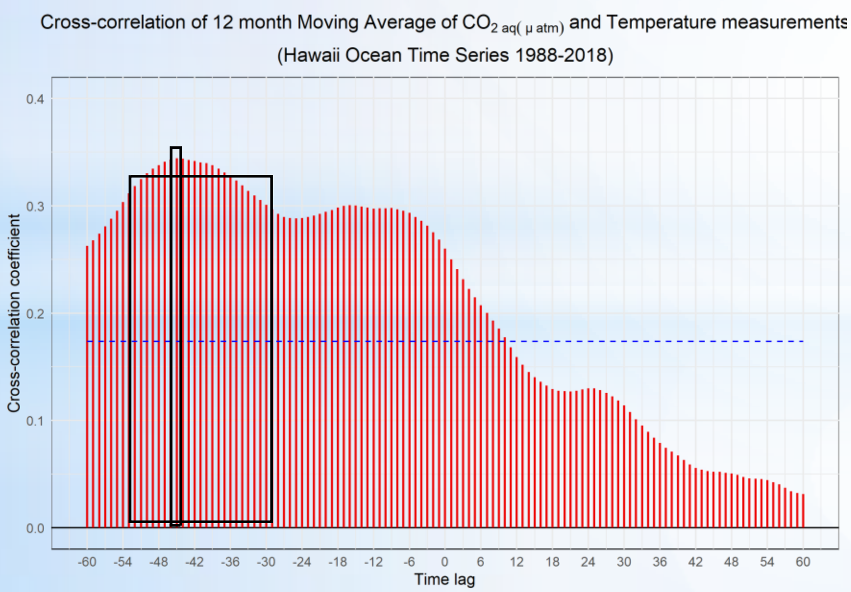


Time-series Analysis (1)

CO_{2aq} ~ Temperature



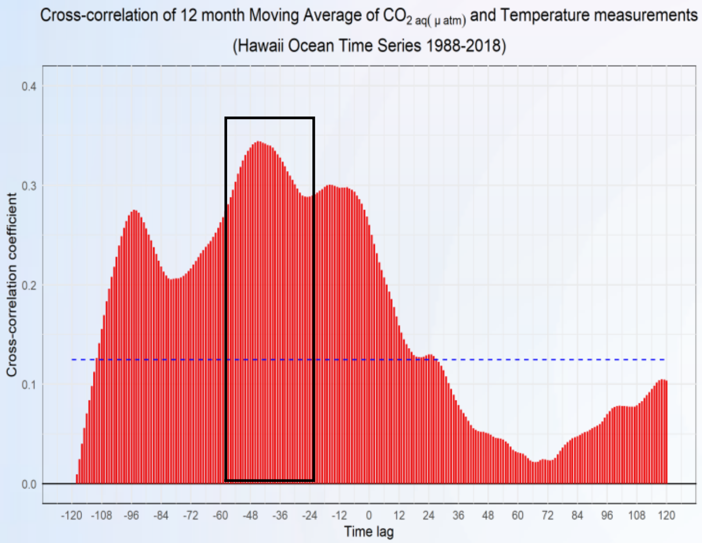
With the application of a 2-month moving average (2 month lag) on the aquatic **CO_{2aq}**(x) and **temperature** (y), the seasonal periodicity is still apparent with the highest positive value recorded at lag zero (+0.52).



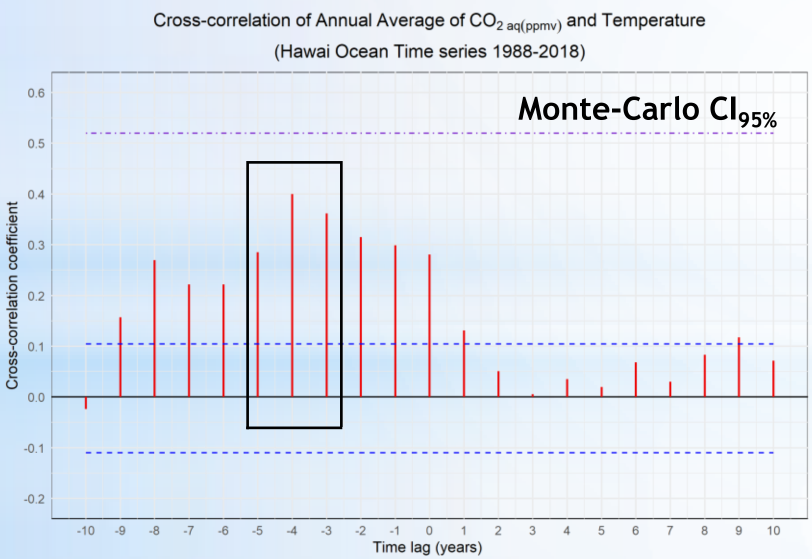
The annual (12-month) moving average showed an interesting behavior, with an increasing and exclusively significant CCF at negative lags, with the maximum observed at the lag -45 (~4 years) with a positive value of +0.34.

Time-series Analysis (1)

CO_{2aq} ~ Temperature



In order to verify whether if the CCF values occur at larger lags, we investigated the behavior in a larger lag-window (+120,-120) and **we concluded that, indeed, the time lag range (months) from -37 to 47 (3y-4y) had the highest CCF observations in both processes.**

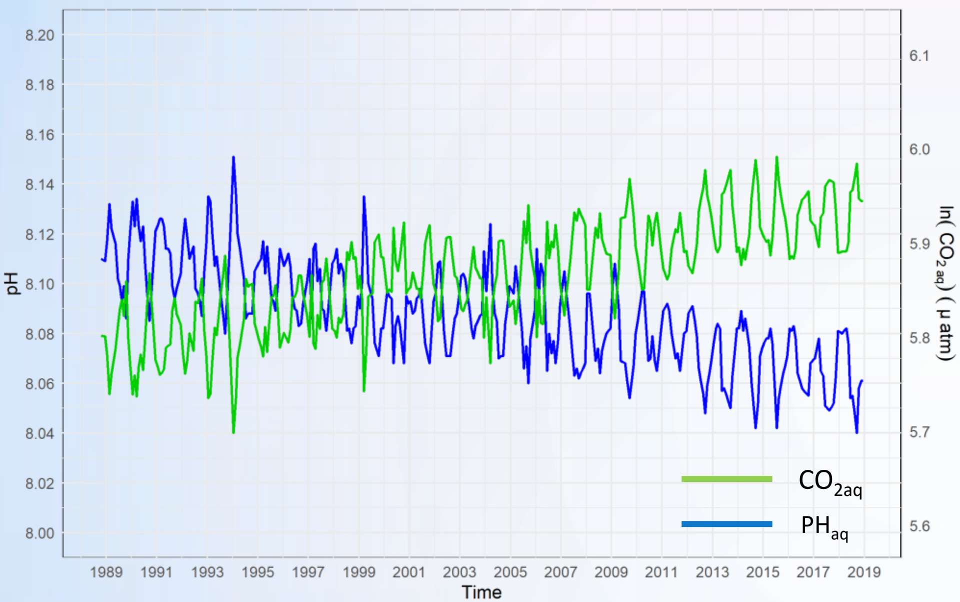


Apparently, with the application of a MSC in a AR(1) model based on the statistical characteristics of annual CO_{2aq} and **temperature**, the observed directionality **was not statistical significant** at 95% of confidence intervals.

Time-series Analysis (1)

PH~CO_{2aq}

Time series of aquatic $CO_{2\,aq(\mu atm)}$ and PH (HOT) measurements (1988-2018)

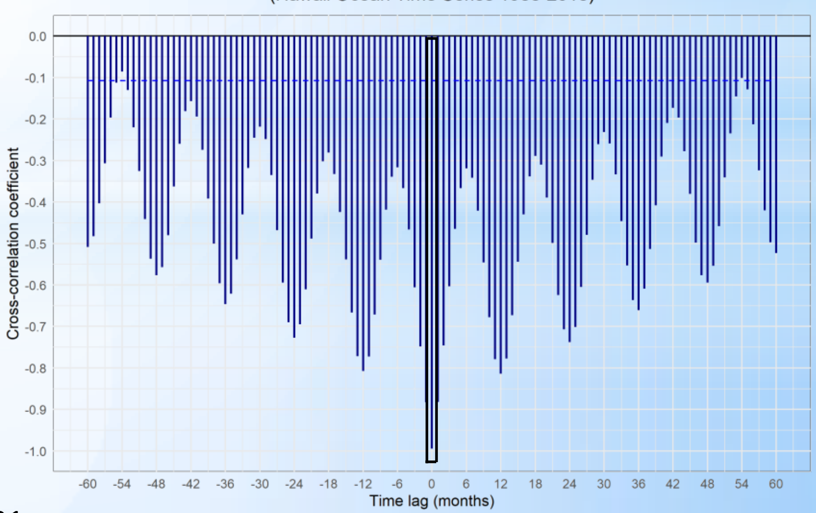


In the original time series of the ocean **carbon dioxide** (natural logarithm transformation [7]) and **pH** measurements there is a clear reflecting mirroring effect between the interaction of both variables.

In the CCF between the original observations of aquatic **pH** (x) and **carbon dioxide** (y) the highest negative value has been attained at lag zero (-0.99) and it keeps a decreasing negative periodic peak in a standard sequence of 12 lag (months). There is a significant symmetric behavior around lag zero and the periodic peaks indicate a synchronous seasonal interaction of processes.

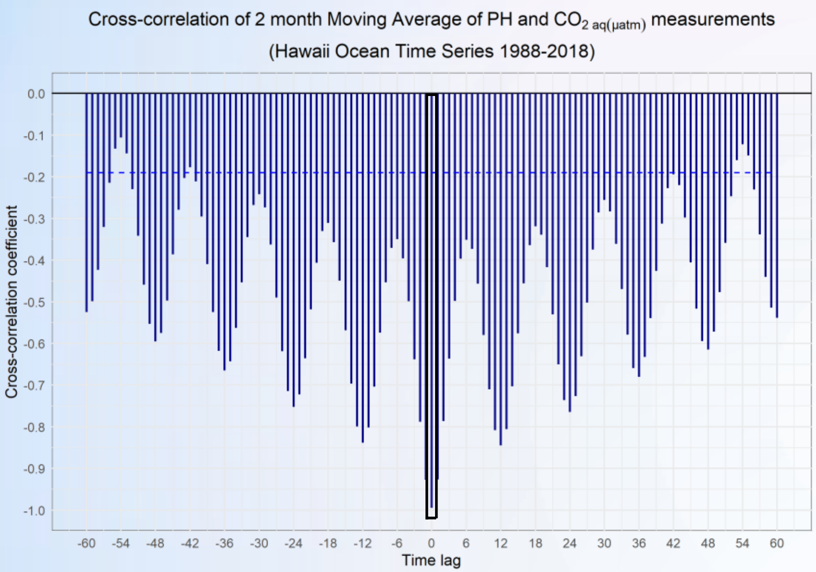
Cross-correlation of PH and $CO_{2\,aq(\mu\,atm)}$ measurements

(Hawaii Ocean Time Series 1988-2018)

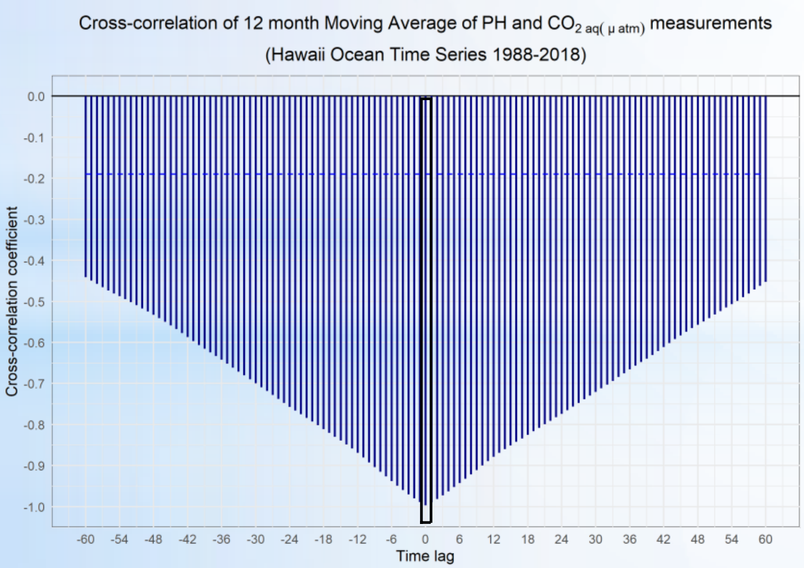


Time-series Analysis (1)

PH ~ CO_{2aq}



At a next phase, the 2-month moving average on the aquatic **pH** (x) and **carbon dioxide** (y) resulted in significant negative correlations with the maximum CCF value recorded at lag zero (-0.99). Additionally, there is a seasonal periodic cycle with subsequent decreasing negative peaks towards larger positive and negative lags.

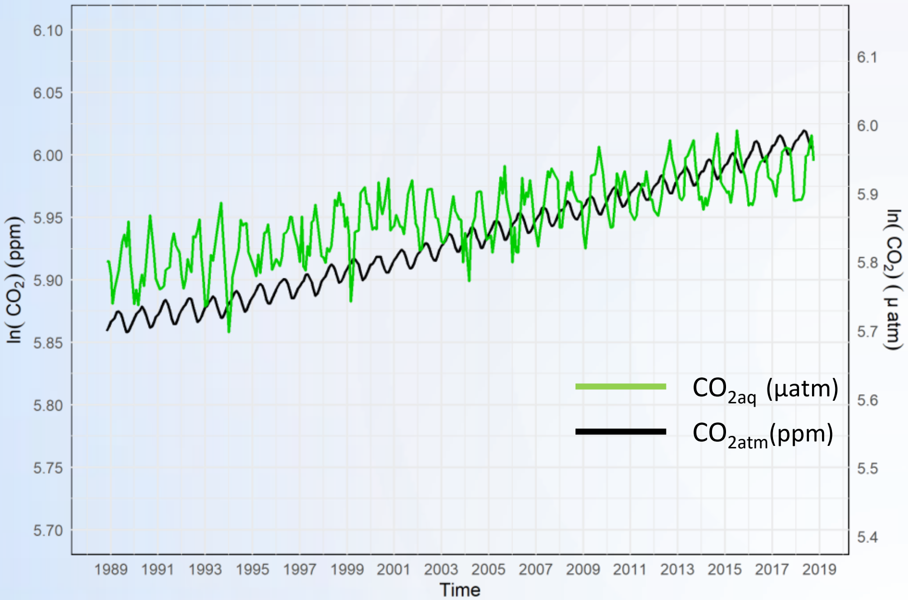


The annual (12-month) moving average sustained the symmetric negative correlation at lag zero (-0.99), a consistent behavior with the previous analyses.

Time-series Analysis (1)

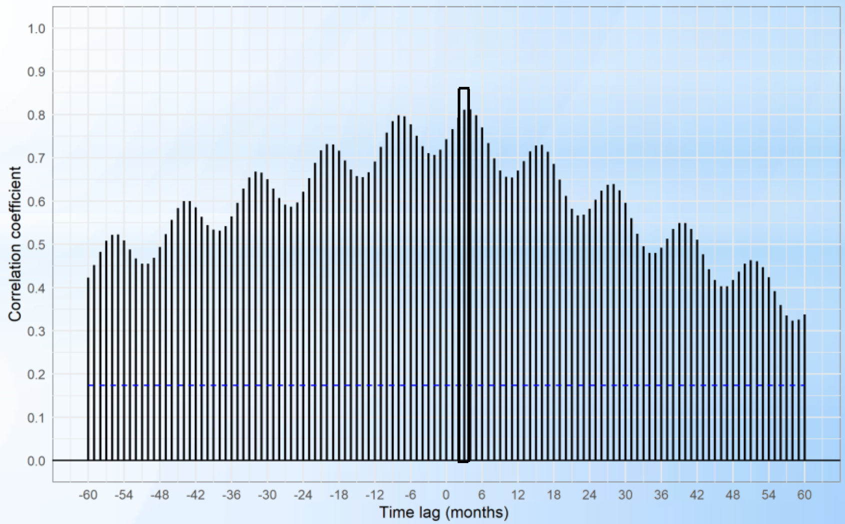
$CO_{2aq} \sim CO_{2atm}$

Time series of atmospheric $CO_{2\ atm(ppm)}$ (NOAA) and aquatic $CO_{2\ aq(\mu atm)}$ (HOT) measurements (1988-2018)



Based on the of the **aquatic** and **atmospheric** carbon dioxide (natural logarithm transformation[7]) measurements, a common increasing process occurs. Atmospheric observations demonstrated a steady positive escalation while aquatic carbon dioxide time series exhibited a similar, though variant, behavior.

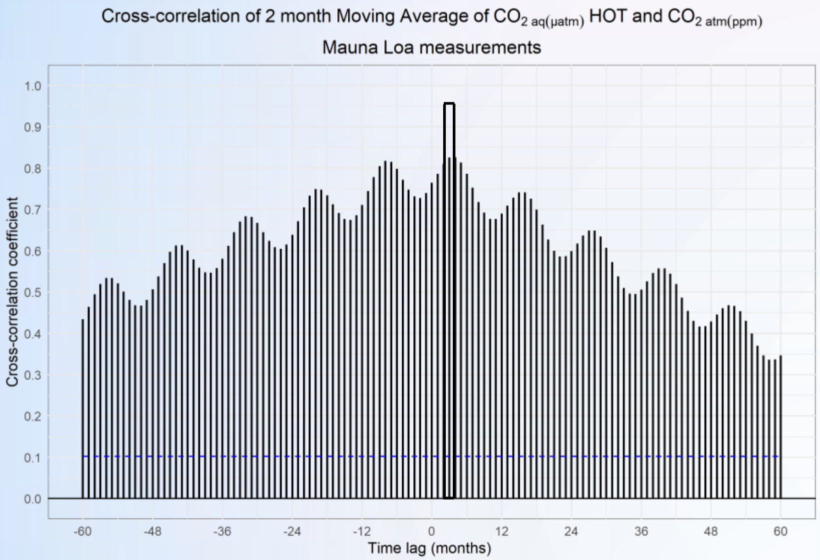
Cross-correlation of $CO_{2\ aq(\mu atm)}$ HOT and $CO_{2\ atm(ppm)}$ Mauna Loa measurements



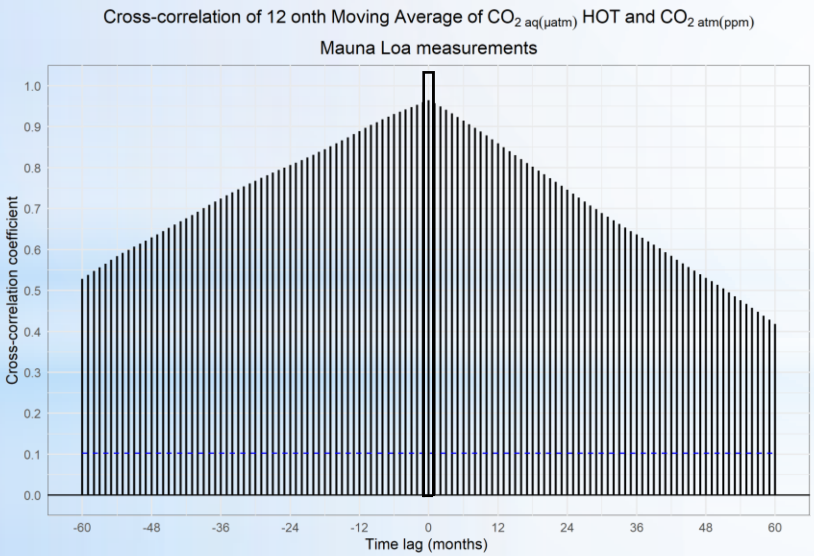
The highest positive value n the CCF analysis between the original observations of **aquatic** (x) and **atmospheric** (y) carbon dioxide, was recorded at the 4th lag (+0.81) and therefore, there is a positive periodic peak in a sequence of an annual lag (12 months). Regarding larger time lags, the interaction is characterized as significant symmetric behavior around the fourth lag and once more, the periodic peaks indicate the presence of a seasonal phenomenon[5].

Time-series Analysis (1)

$CO_{2aq} \sim CO_{2atm}$



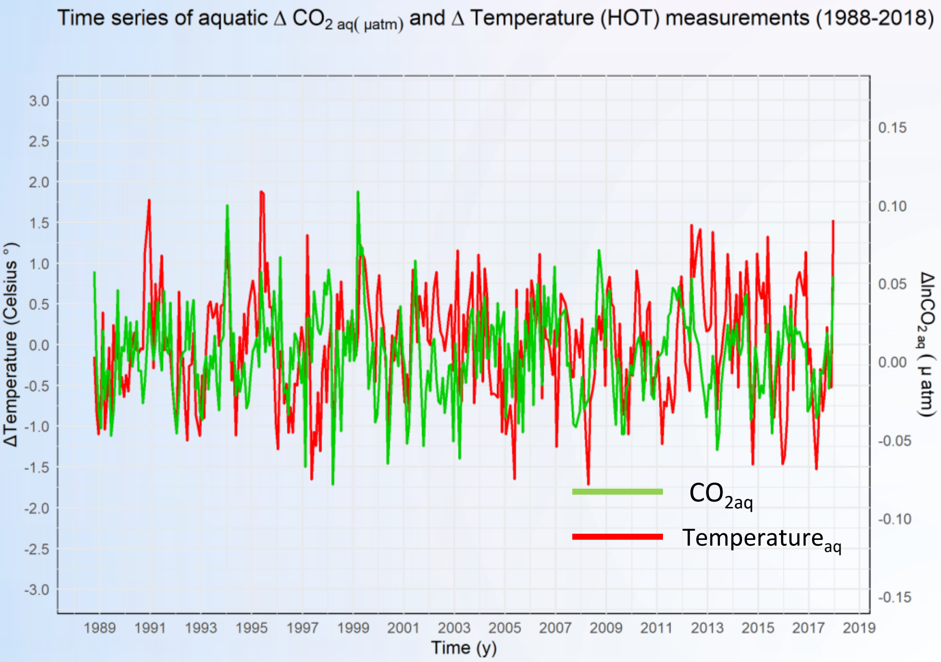
Similarly, the 2-month moving average (2 month lag) on the aquatic (x) and **atmospheric** (y) carbon dioxide exhibited significant seasonal periodicity around the 4th lag, with the CCF calculated the maximum CCF value (+0.81).

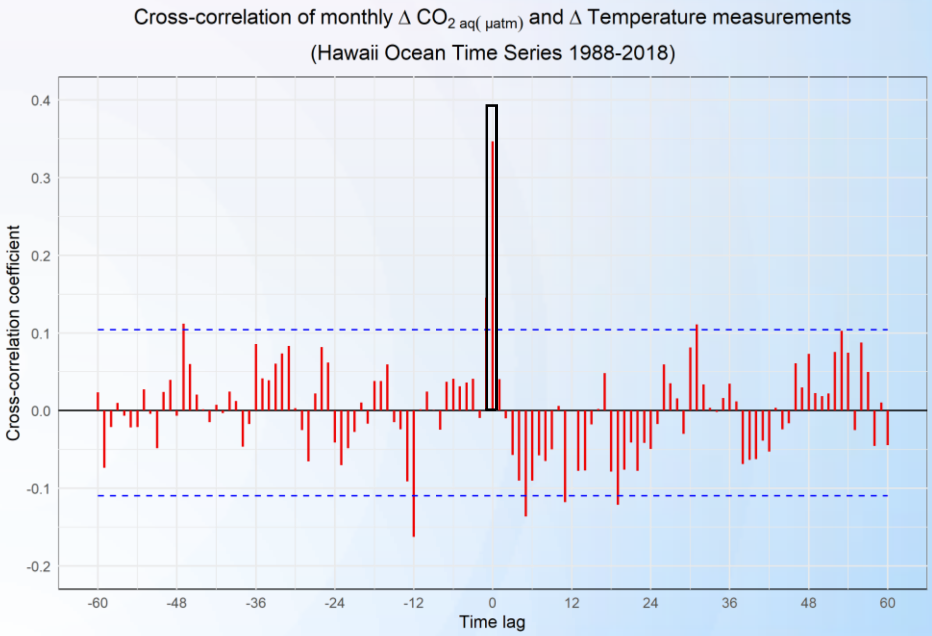


The annual (12-month) moving average between both processes showed a typical symmetric positively correlated interaction at zero lag (+0.96). Hence, the annual correlation is slightly greater than the effect of the monthly observations.

Time-series Analysis (2)

ΔCO_{2aq} ~ ΔTemperature

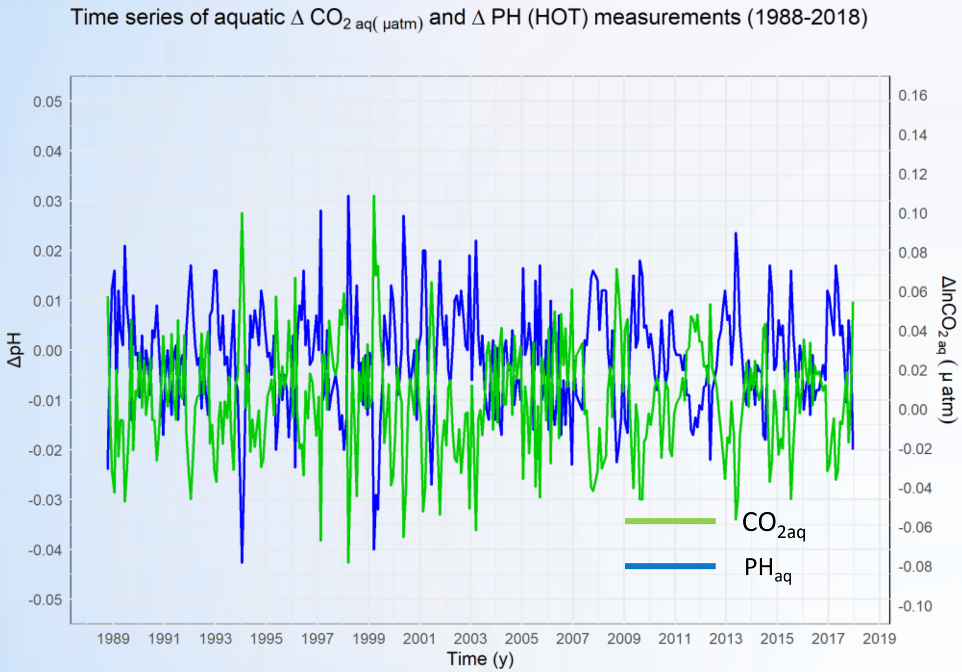


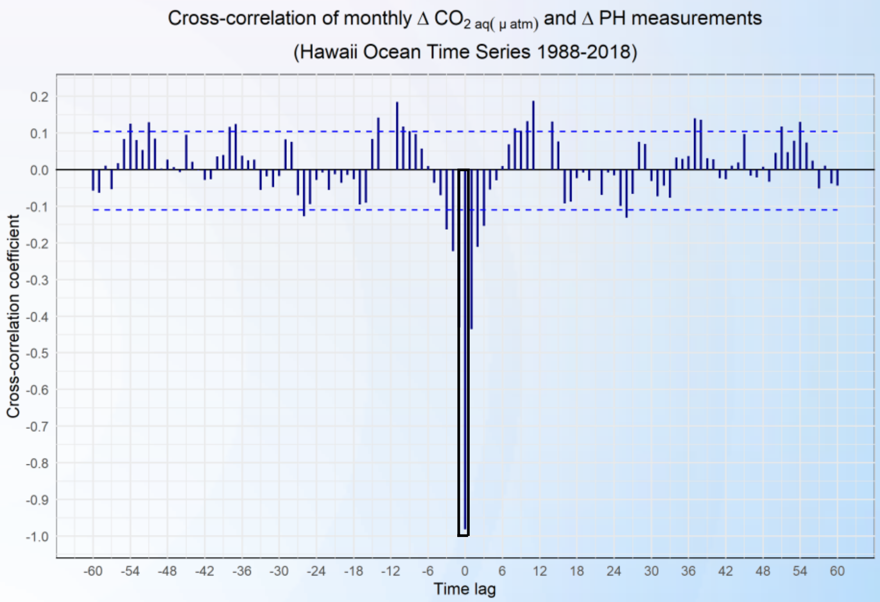


With the elimination of the periodicity effect on the processes, the annual difference (f.e. 1st PH value: PH_Oct_{1989}-PH_Oct_{1988}), ocean **carbon dioxide** and **temperature** measurements showed that there is not a clear pattern in the succession of events. This can be validated with the CCF plot, indicating that the highest value recorded at lag zero (+0.34) with a **non significant pattern** alongside the zero point, thus highlighting the erratic behavior of temperature in the original time series.

Time-series Analysis (2)

$\Delta PH \sim \Delta CO_{2aq}$



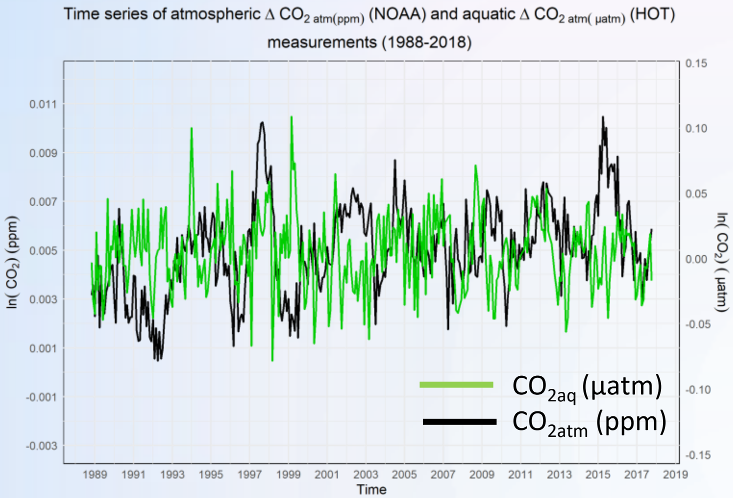


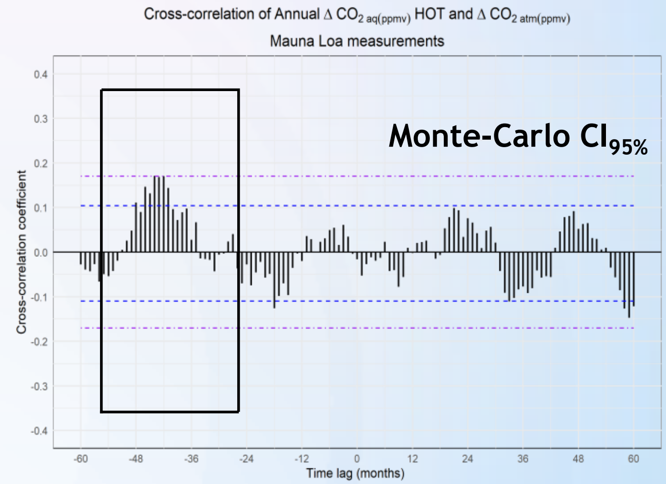
Contrarily, the Δ-transformed time-series of aquatic **pH** and **carbon dioxide** difference, resulted in the same reflected mirrored behavior of the time series. Furthermore, the cross-correlation of both variables strongly support the original time-series behavior with a clear **symmetric** pattern. The maximum value (lag zero) of the CCF was recorded at -0.98.

Time-series Analysis (2)

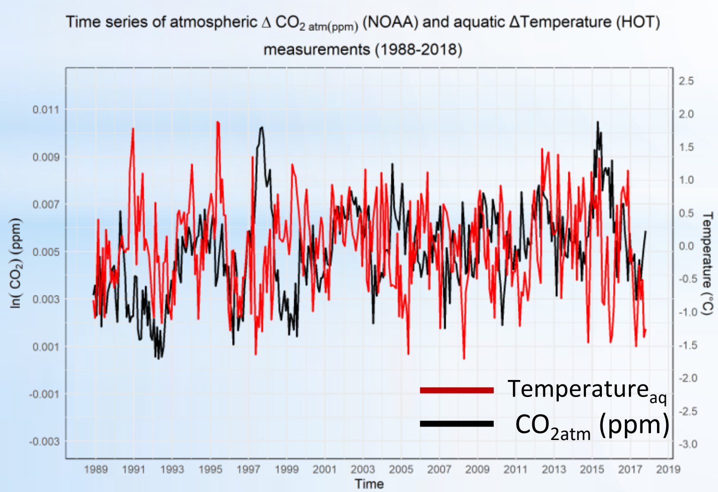
ΔCO_{2atm} ~ ΔTemperature

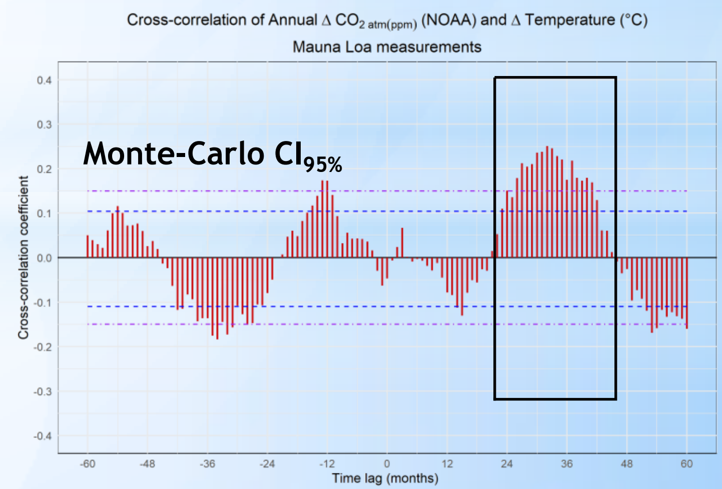
ΔCO_{2aq} ~ ΔCO_{2atm}



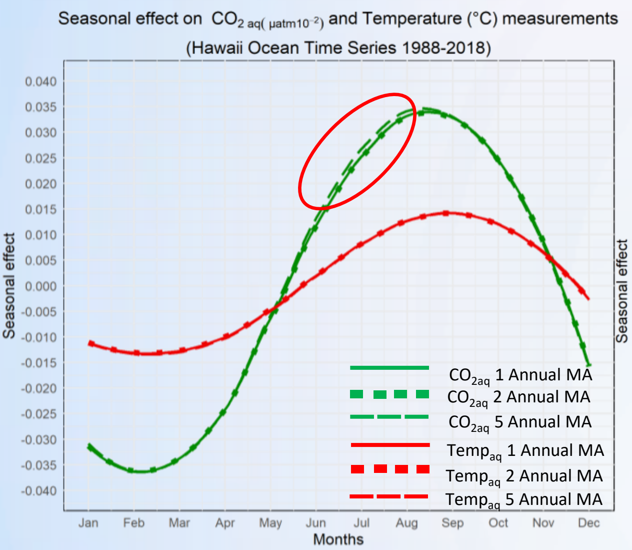


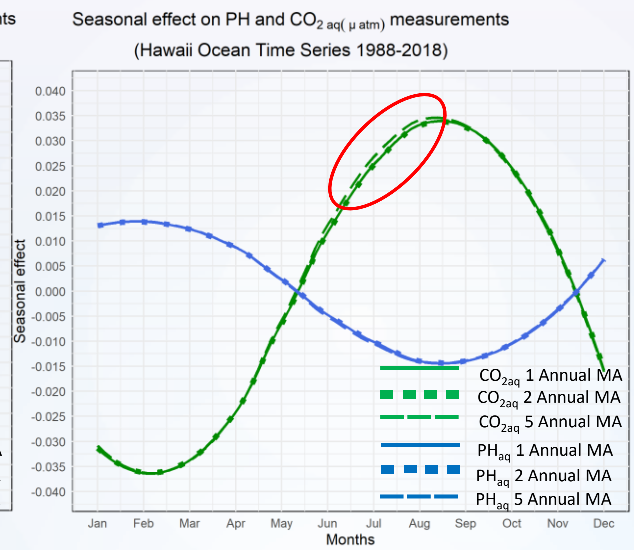
The differences between the CO_{2aq} and **CO_{2atm}**, demonstrated a clear pattern of a negligible statistical significance between the two processes, except an allocated time-lag grouping at -40 to -45 time lag (months) which was partially-rejected through the MSC $CI_{95\%}$ thresholds. Since temperature showed an interesting behavior in the previous section we tested its difference (Δ) related with the **ΔCO_{2atm}** and it appeared that there's **a validated and statistical significant directionality** of **T→CO_{2atm}** with a ~2.5 year lag.

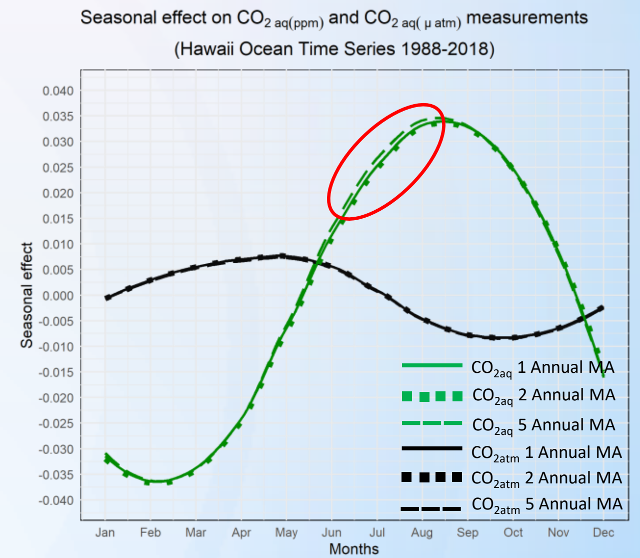




Seasonality effect







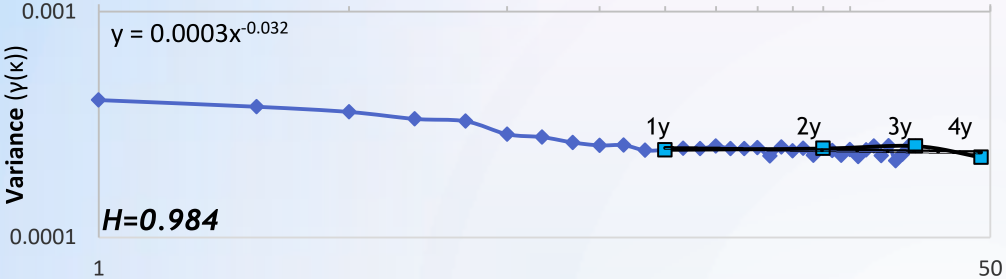
Since seasonality was highlighted as a crucial component in the behavior of the phenomenon, we extracted gradual increasing annual (1;2;5 years) moving averages (MA) from the original time-series, and we estimated the monthly average effect on the observations units. In the case of aquatic **temperature** and **CO_{2aq}**, both variables had a common phase with the highest positive peak between August-September and lowest in February. Correspondingly, **pH** had the exact opposite phase compared to the **CO_{2aq}** with the highest peak in February and lowest in September. The, exclusively seasonal effect, 4-month phase lag of the **air**-**ocean** CO_2 transferability was confirmed since the highest peak of **CO_{2atm}** appeared to be in May and the lowest between September-October.

It is worth mentioning that the different applied moving average (MA) extractions appeared to show equal behavior, with the 5th MA having a slight divergence during summer months (June-August).

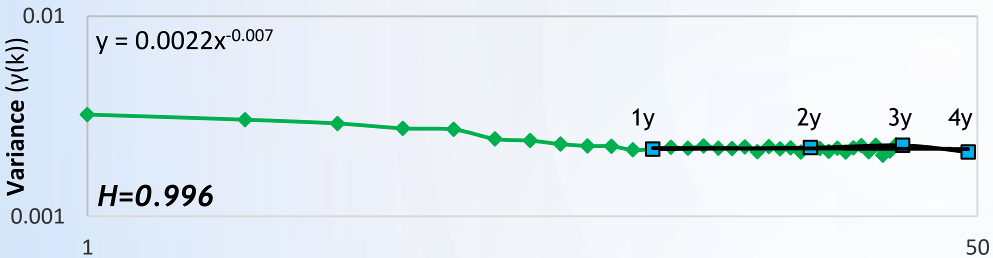
Time-series Analysis (4)

Climacograms

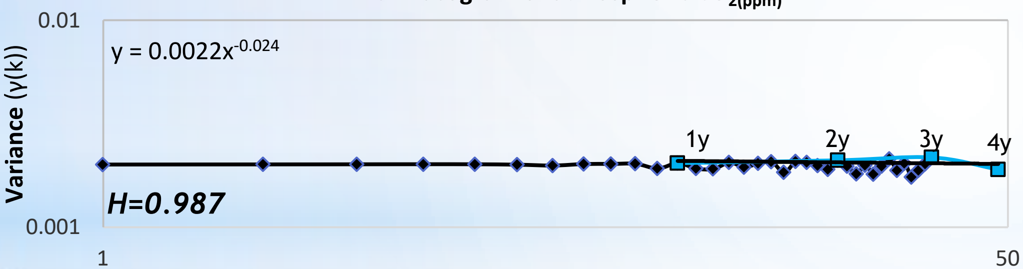
Climacogram of ocean surface PH



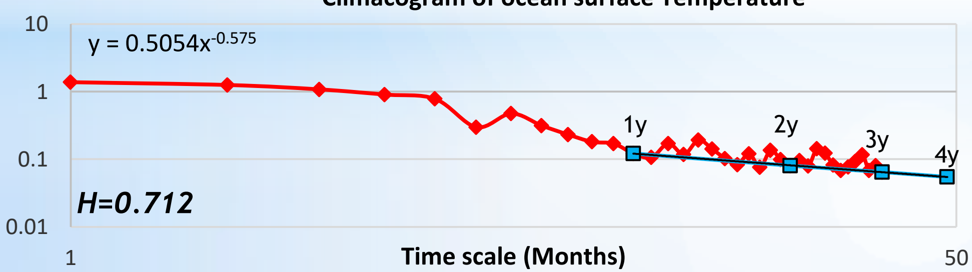
Climacogram of ocean surface $CO_{2(\mu atm)}$



Climacogram of atmospheric $CO_{2(ppm)}$



Climacogram of ocean surface Temperature



Finally, we implemented the empirical climacogram for all the variables during the examination of processes on the phenomenon of OA (log transformed γ_κ axis). Hurst parameter was estimated according to the power type slope of the annual scale (1-4 years) so as to exclude the non-desired effects of periodicity in monthly scale. **Overall, the 4 parameters showed H>1/2 which demonstrates temporal persistence**[7,10].

More specifically, the annual H parameter for aquatic **pH**, **CO_{2aq}**, **CO_{2atm}** obtained from the 30 year range time-series exhibited large values approximate to 1 (*H*>0.98). However, aquatic **temperature** presented a less similar behavior on annual scales as an irregular stochastic process.

Main findings –Conclusions

- Analyses of time-series related to OA concluded that the increase of **pCO_{2aq}** was similar to the **pCO_{2atm}**[11]. In the present analysis we discovered an interannual 4 month phase difference between both variables which was eliminated after the extraction of seasonality through appropriate procedures. The annual differences thereof exhibited a ~4 year lag with directionality **$CO_{2atm} \rightarrow CO_{2aq}$** which however is statistically non-significant (tested by MCS).
- An interesting observation was the detection of a statistically significant, assesed through stochastic simulation, **~2.5 year lag** in the annual differences (Δ), in the processes of T_{aq} **$\rightarrow CO_{2atm}$**. The directionality is consistent with the results of a previous study on atmospheric **$T_{atm} \rightarrow CO_{2atm}$** with a ~1 year lag **in an annual scale**[7].
- The relationship between **pH** and CO_{2aq} resulted in a reflecting-mirrored interaction, which is confirmed by previous studies [1,12]. Regarding the observed seasonality, **pH** seasonal variation appeared to be in agreement with previous analysis in the region[1].
- **Strong persistence (H>>1/2) was detected in all the examined variables,** which indicates strong clustering (grouping) of similar values, enhanced change and uncertainty, a quite common behavior in natural processes[7,10].
- A negative effect of OA is the **possibility that it can impact aquatic populations of shell-forming organisms**[1,14]. These ocean chemical alternations may cause progressive negative feedback response, starting from the population level to marine ecosystems as a whole.
- The present study was focused on a single site dataset. However, there exist site-specific differences on a global scale[11,12], along with a variability of biological responses and vulnerability to OA related with the latitude location of each case-study [1,13]. Except the geospatial variance, the interaction of impacts has been found to be diverging during the life-history (development) stages of an organism[14].
- Based on the findings of this work, it appears that there may exist an **interesting interdisciplinary research arena in the interaction between trends and seasonality effects on the response of marine biota.** This evolutionary concept of adaptivity, described as the "phenotypic plasticity" [15], may function towards the mitigation of the severe effects of environmental stressors related to OA.

References

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