

A flexible processing system for the calculation of air-sea gas fluxes: a dynamic tool for the community

Jamie Shutler, Jean-Francois Piollé, Peter Land, David Woolf, Lonneke Goddijn-Murphy, Frederic Paul, Fanny Girard-Ardhuin, Craig Donlon, Bertrand Chapron



OceanFlux GHG is funded by:



and affiliated to:



Introduction

- Keen for Earth observation data to be exploited for SOLAS studies
- Issues:
 - Simplifying access to these data (e.g. standard file types and tools)
 - Ability to handle large data sets
- Flexible system needed for project uncertainty and scientific analyses
- Simple to provide community access.
 - Greater transparency and traceability for publications
- Users can create own climatologies, generate net fluxes and re-grid data
- Data can be ingested into standard software packages and tools (e.g. Matlab, IDL, Excel).

Cloud computing

Cloud computing: inter-connected computing resources that can be easily scaled up (grown) or down (shrunk) while maintaining its capability or function (rather like a 'cloud' in the atmosphere).

Features:

- Redundancy
 - Servers can be removed or upgraded without users noticing
- Scale-able
 - Uses standard hardware and software
- Simple backup and restoration
- No specific skills required by user
- Speed
 - Processing is close to data (no bottleneck)
- System is tailored
 - No reliance on physical hardware e.g. use of virtual servers
- Maximises use of resources
 - Dynamic re-allocation of resources as and when needed

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Nephelae

600 processing nodes.
1.5 Peta bytes of storage

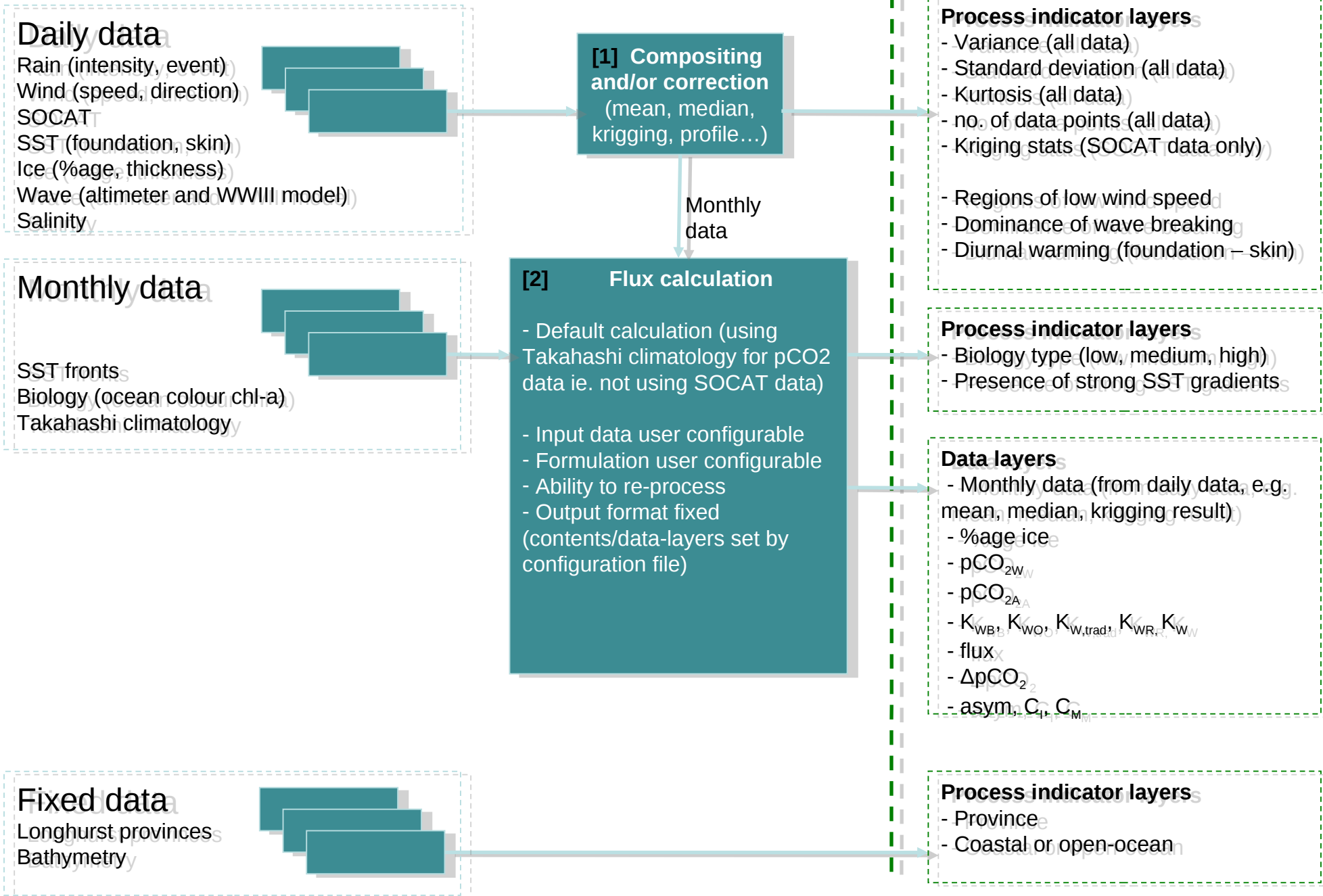
Available input data

- All input data are 1° x 1° global monthly composites.

Parameter	Dataset (current number of datasets)	Uncertainty	Years
SST	NOAA AVHRR, ESA CCI, GHRSSST datasets (4)	yes	1992-2010
U10	ESA GlobWave archive (2+)	yes	1992-2010
Hs	ESA GlobWave archive (1+)	yes	1992-2010
pCO ₂ /fCO ₂	LDEO Takahashi 2002, LDEO Takahashi 2009, OceanFlux/SOCATv1.5, OceanFlux/SOCATv2 (4)	majority	2000 2010
Rain	GPCP, TRMM, SSMI (4)	yes	1992-2012
Chl-a	ESA GlobColour, ESA Ocean Colour CCI (2)	yes	1997-2011

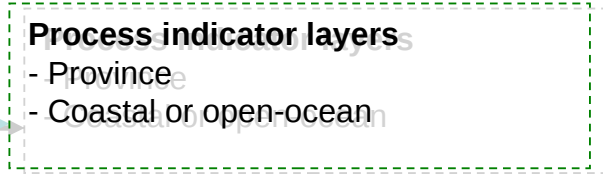
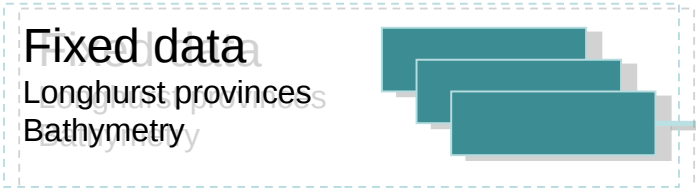
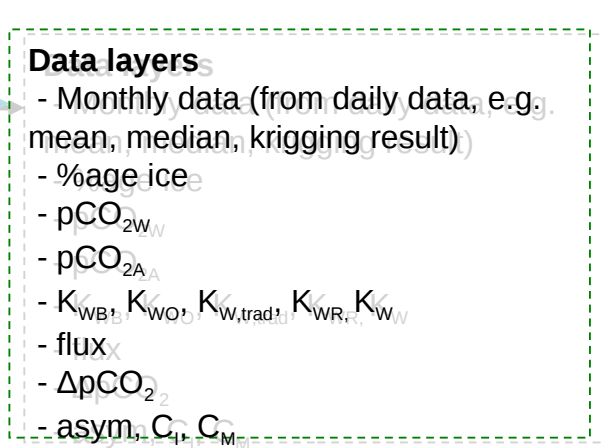
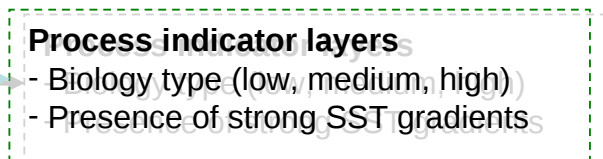
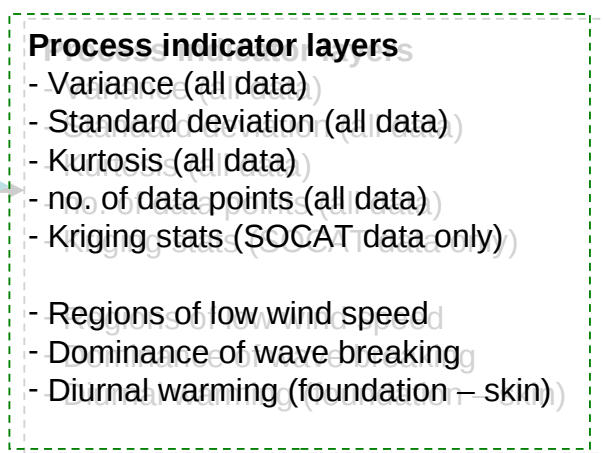
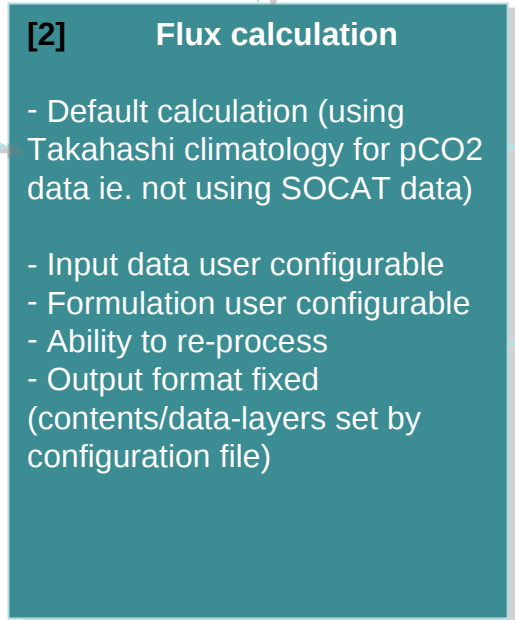
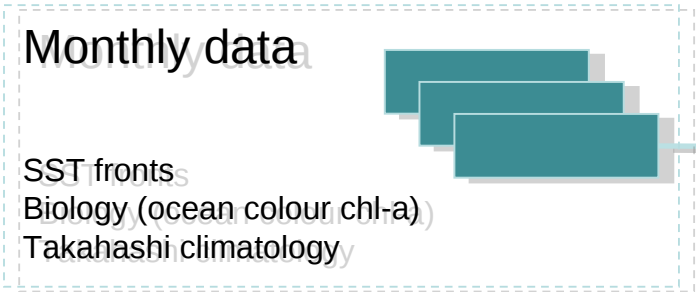
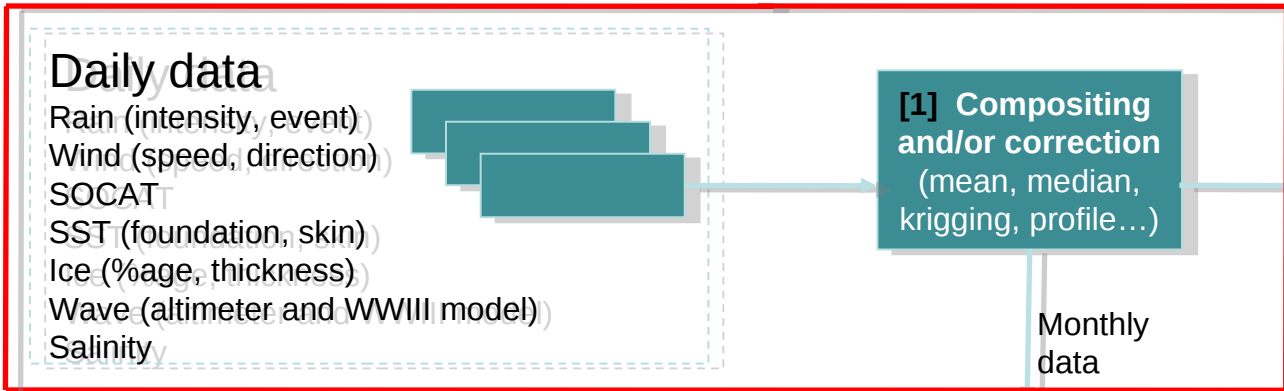
Basic climatology processing system

Climatology (monthly NetCDF)



Basic climatology processing system

Climatology (monthly NetCDF)



Basic climatology processing system

Climatology (monthly NetCDF)

Daily data

Rain (intensity, event)
Wind (speed, direction)
SOCAT
SST (foundation, skin)
Ice (%age, thickness)
Wave (altimeter and WWIII model)
Salinity

[1] Compositing
and/or correction
(mean, median,
kriging, profile...)

Monthly
data

Monthly data

SST fronts
Biology (ocean colour chl-a)
Takahashi climatology

[2] Flux calculation

- Default calculation (using Takahashi climatology for pCO₂ data ie. not using SOCAT data)
- Input data user configurable
- Formulation user configurable
- Ability to re-process
- Output format fixed (contents/data-layers set by configuration file)

Fixed data

Longhurst provinces
Bathymetry

Process indicator layers

- Variance (all data)
- Standard deviation (all data)
- Kurtosis (all data)
- no. of data points (all data)
- Kriging stats (SOCAT data only)

- Regions of low wind speed
- Dominance of wave breaking
- Diurnal warming (foundation – skin)

Process indicator layers

- Biology type (low, medium, high)
- Presence of strong SST gradients

Data layers

- Monthly data (from daily data, e.g. mean, median, kriging result)
- %age ice
- pCO_{2W}
- pCO_{2A}
- K_{WB} , K_{WO} , $K_{W,trad}$, K_{WR} , K_{WW}
- flux_X
- ΔpCO_2
- asym, C₁, C_M

Process indicator layers

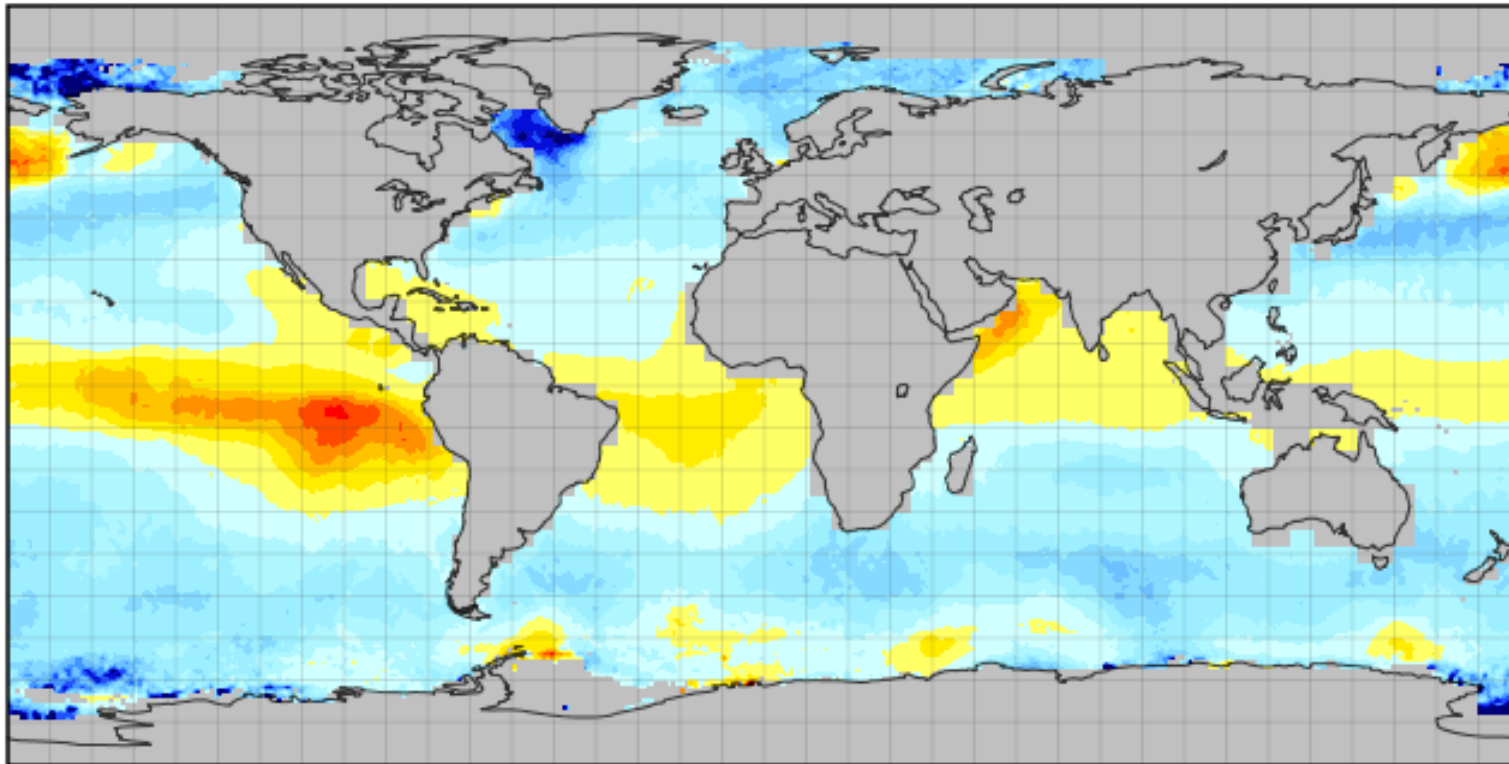
- Province
- Coastal or open-ocean

Features of climatology processing system

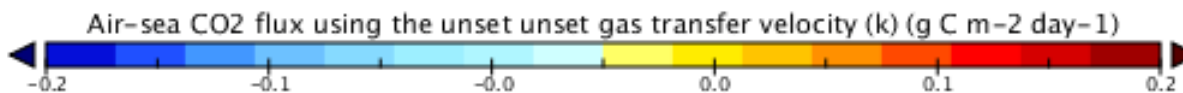
- All datasets are online and pre-processed into monthly composites.
- Monthly composites include mean, median, σ^2 and 2nd - 4th order moments.
- 1 Year global climatology takes 40 mins to generate.
- Ability to disable process indicator layers for speed increase
 - 1 year takes ~20 mins to generate
 - 10 year global run = 3.5 hours.
- Flux calculation is user configurable.
 - e.g user configurable wind based k relationships, optional handling of vertical thermal and haline gradients.
- Ability to inject noise or biases into input datasets
 - e.g. inject random noise based on known uncertainties of individual input data.
- Additional tools:
 - Net flux tool
 - Takahashi style grid re-sampling tool
- Python and Perl using standard libraries. ie no licenses are required and portable (>4000 lines of code !)

Example output

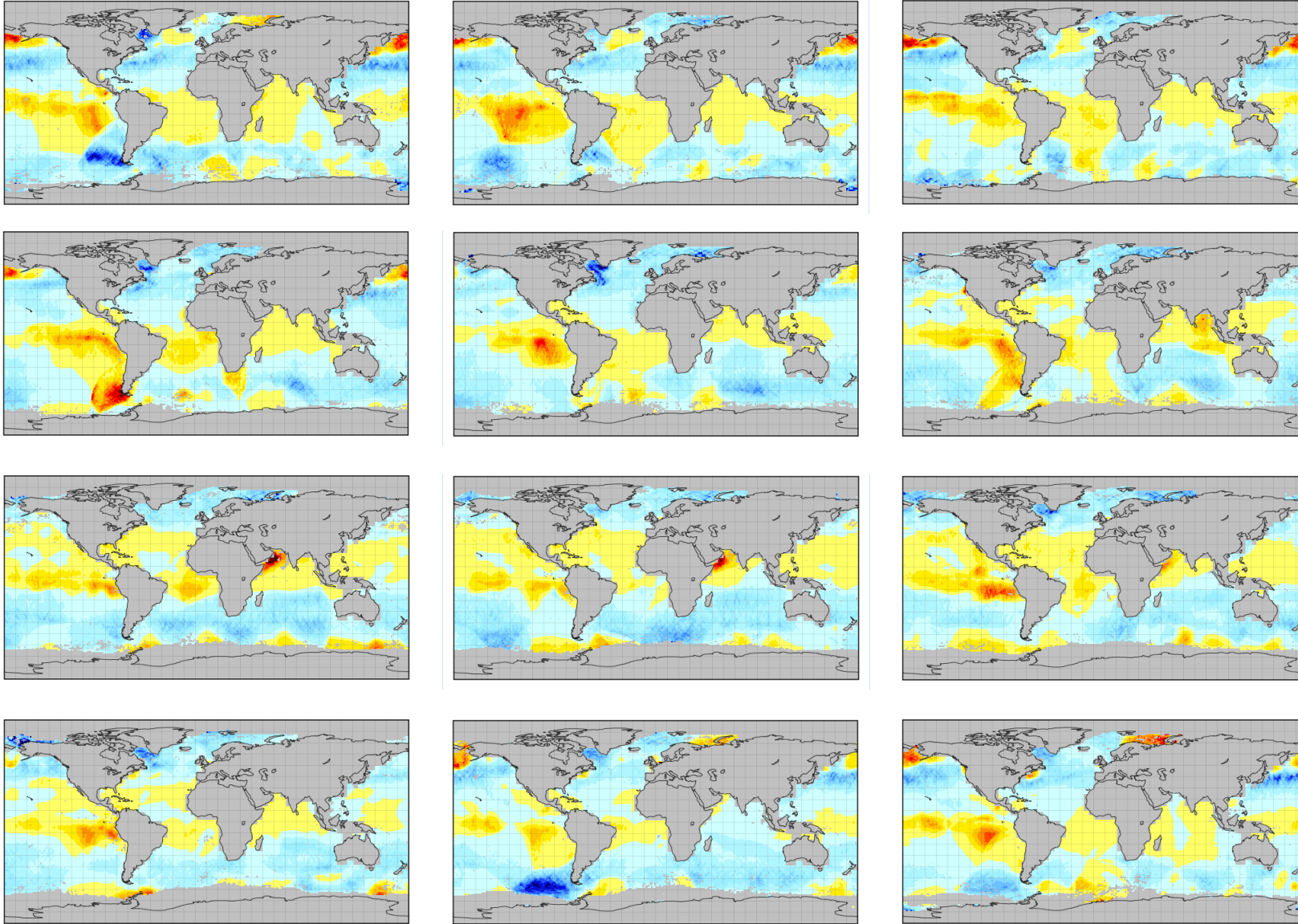
Global regular grid 1° x 1° NetCDF 3.0, CF 1.6



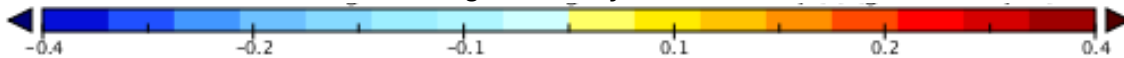
Example daily mean flux



Example 2010

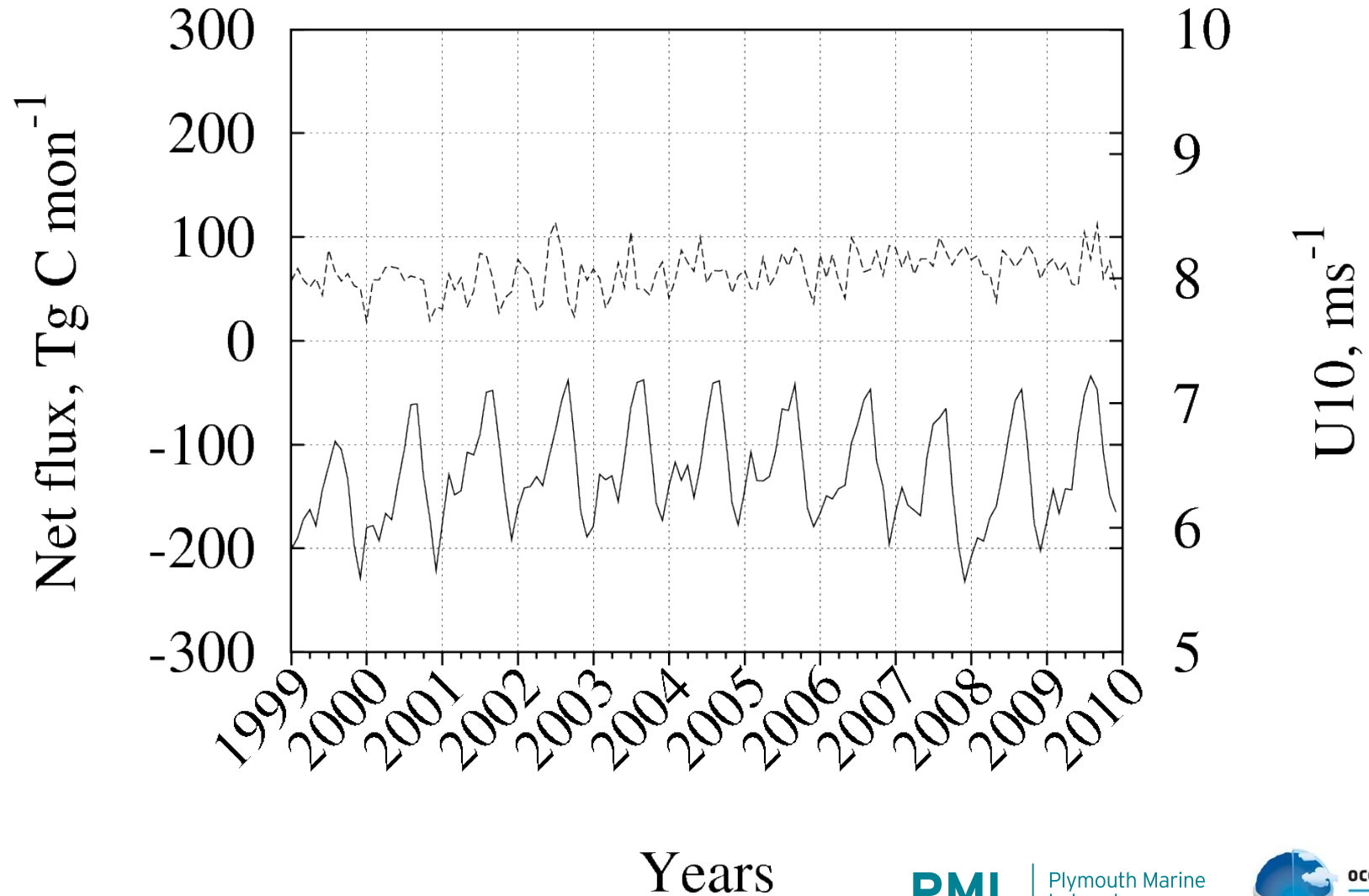


$\text{g C m}^{-2} \text{ day}^{-1}$



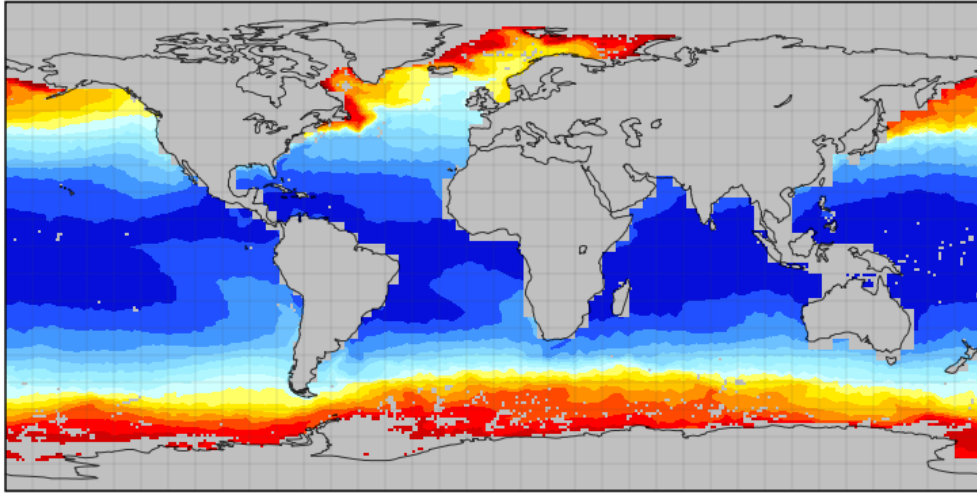
Example global time series

Global Monthly Net fluxes and U10



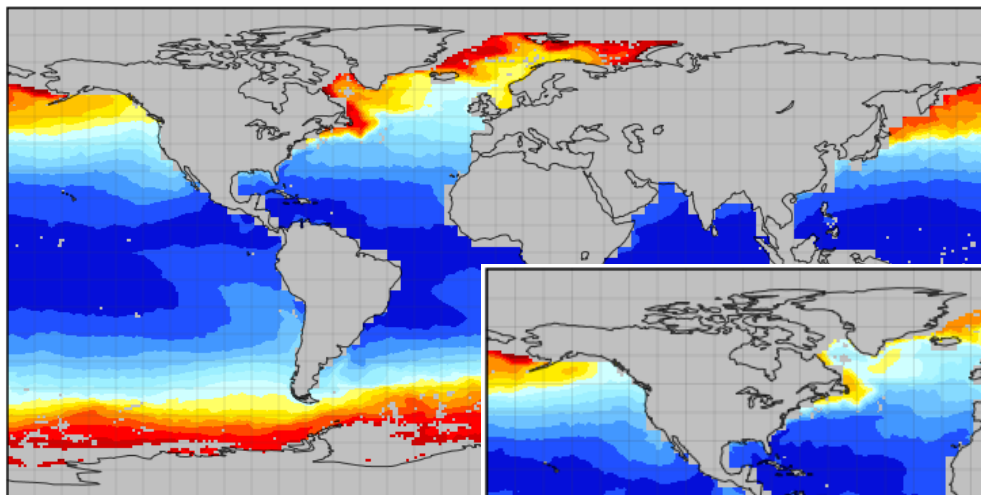
Years

Example output

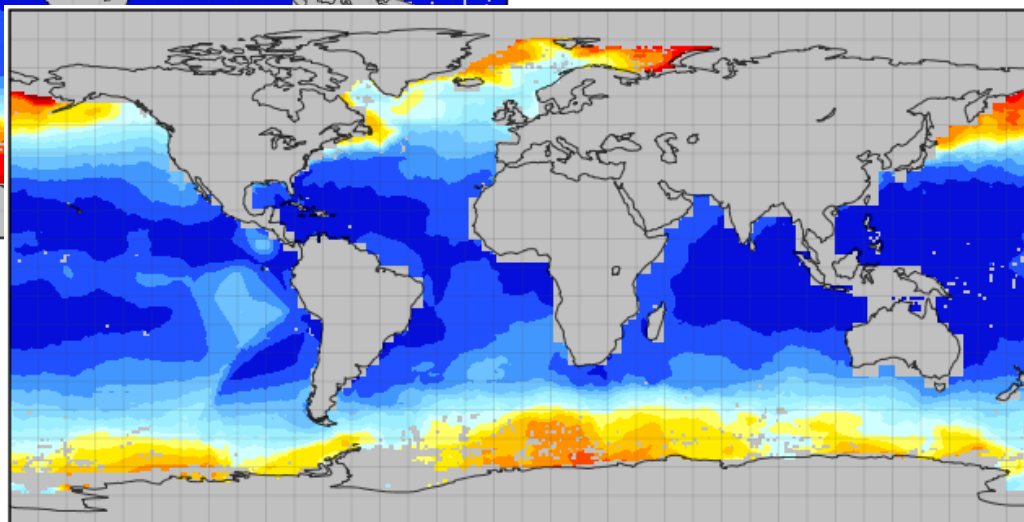


Concentration at the interface (C_i)

Example output

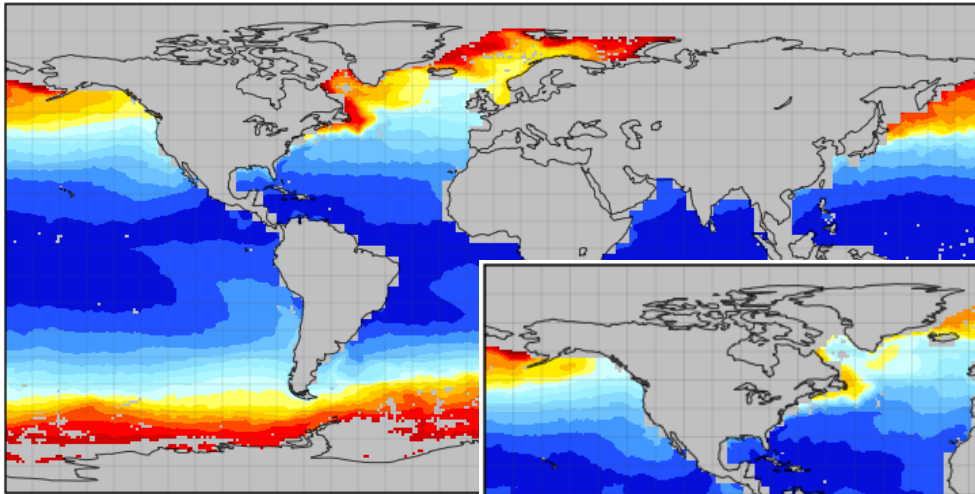


Concentration at the interface (C_i)

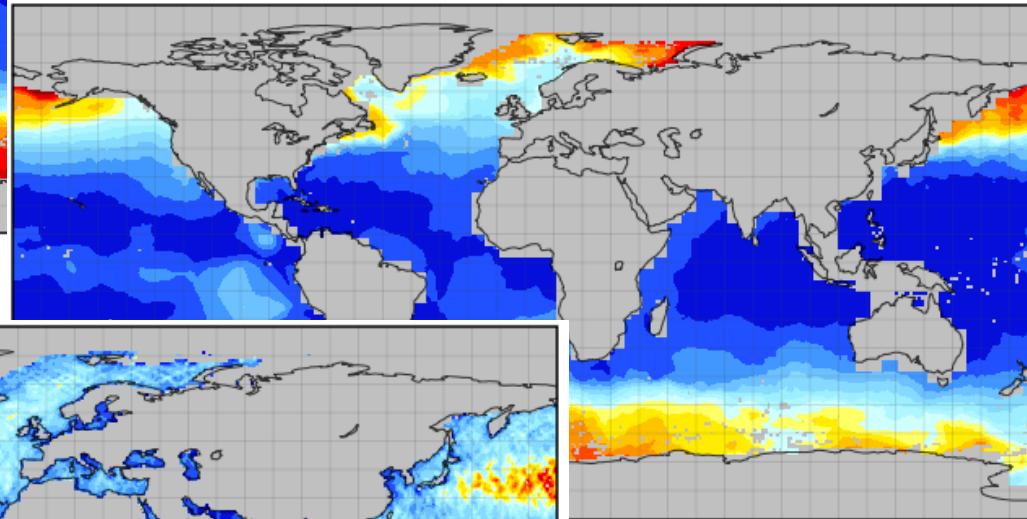


Concentration at the MBL (C_M)

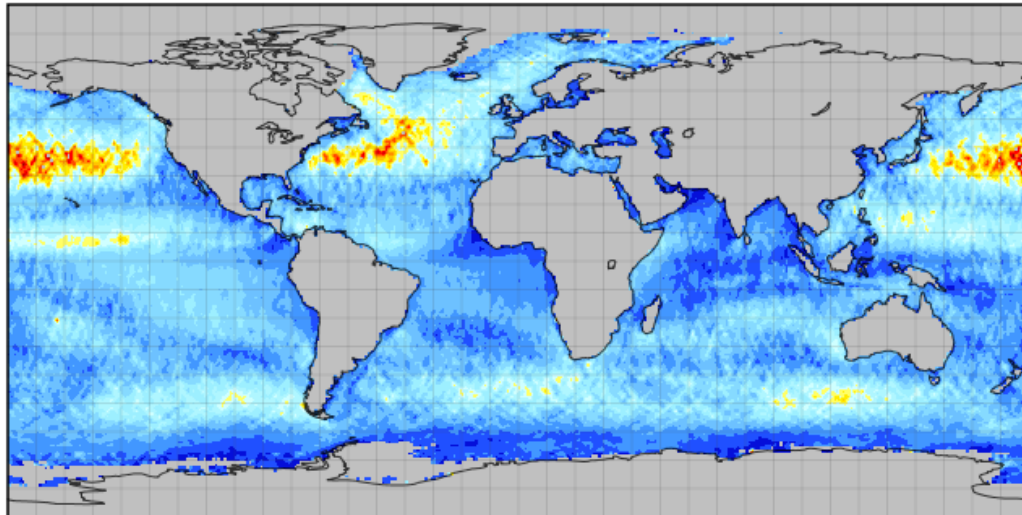
Example output



Concentration at the interface (C_i)

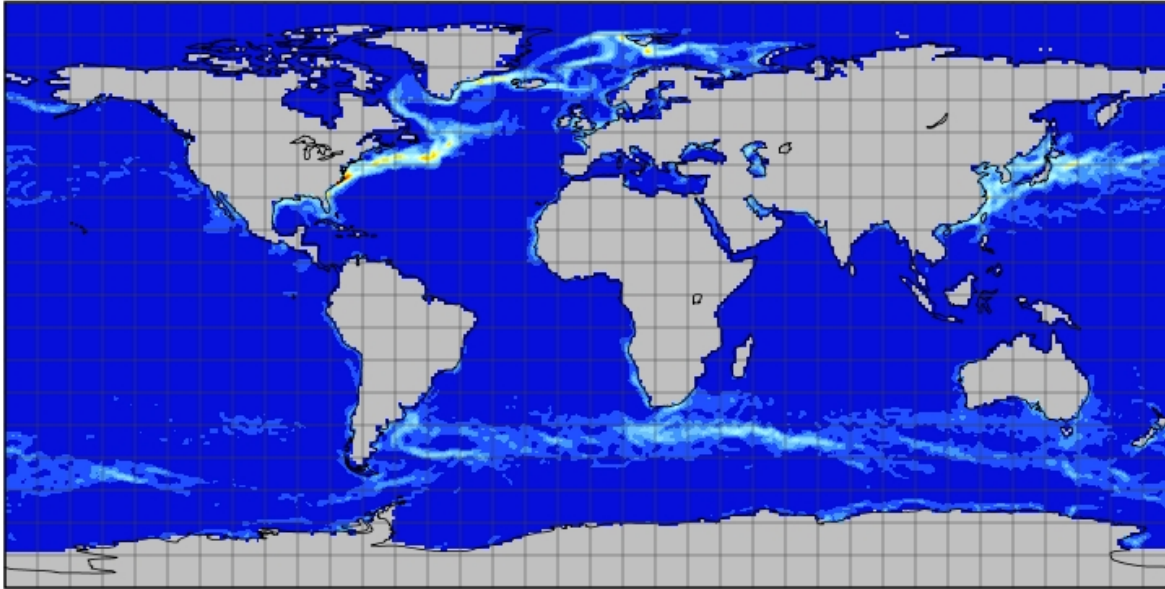


Concentration at the MBL (C_M)



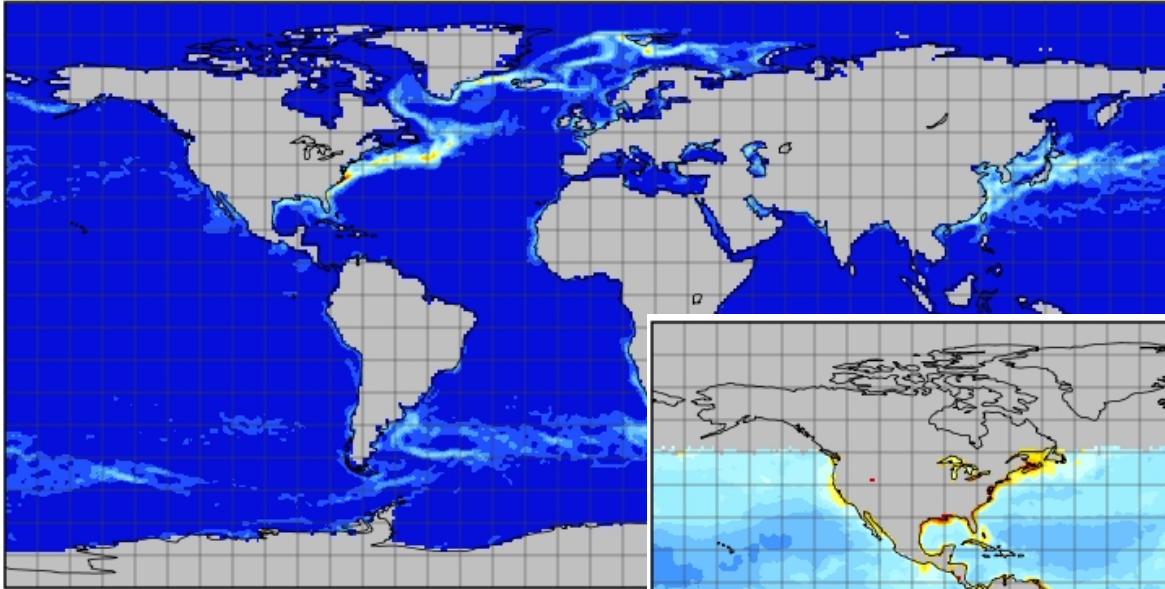
Gas transfer velocity (k)

Example output – process indicator layers



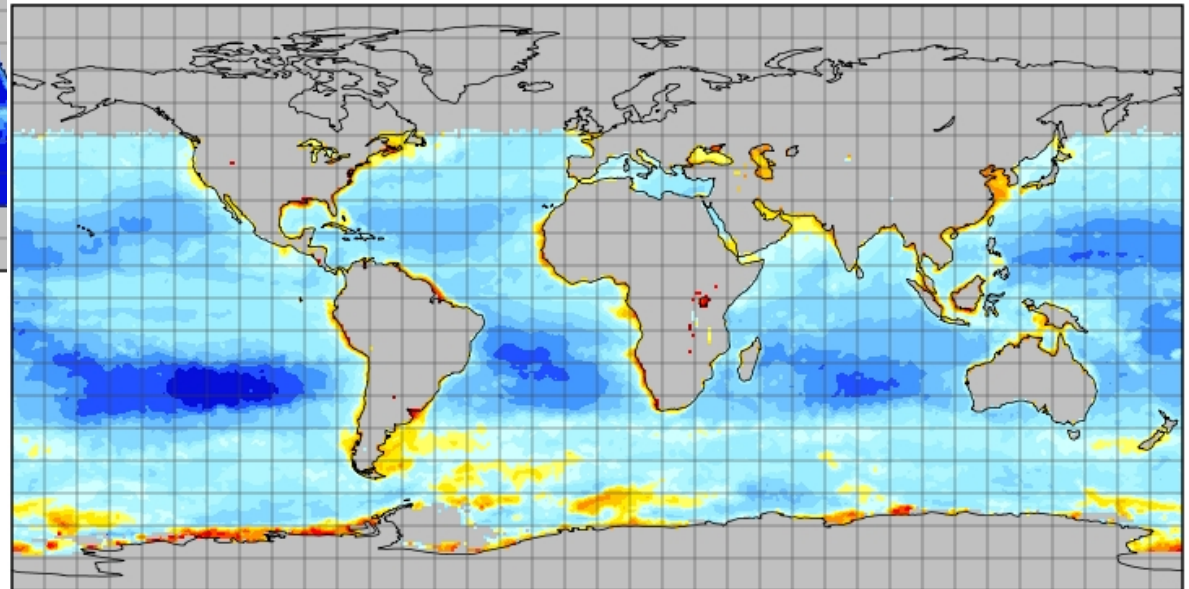
Persistent SST fronts (GHRSSST)

Example output – process indicator layers

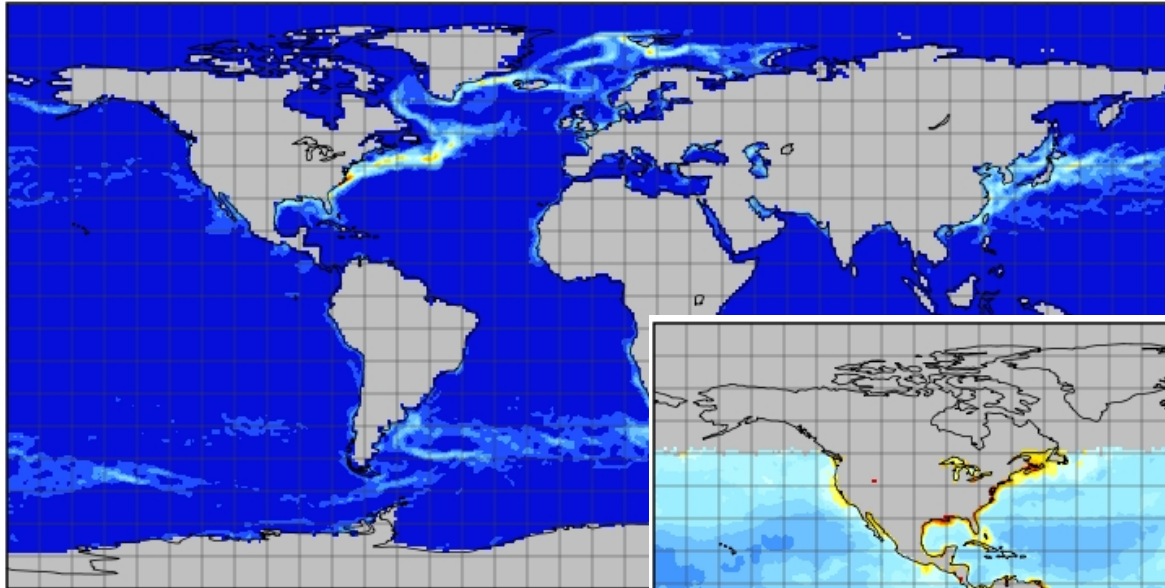


Persistent SST fronts (GHRSSST)

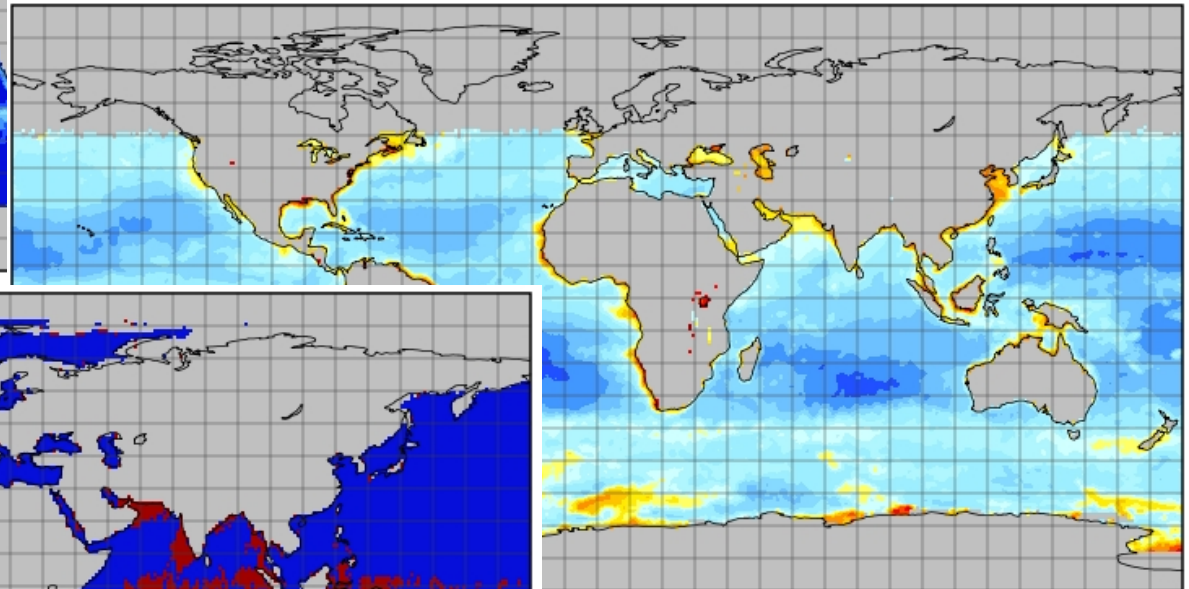
Surface chl-a (ESA CCI)



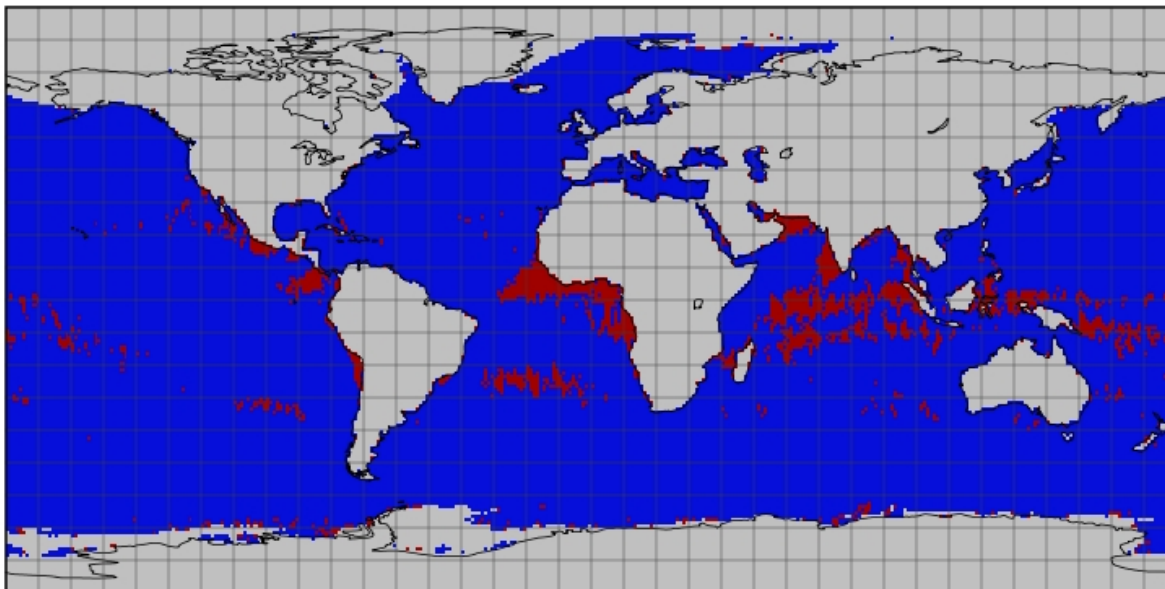
Example output – process indicator layers



Persistent SST fronts (GHRSSST)



Surface chl-a (ESA CCI)



Regions of low wind

Verification and testing

- Software extensively tested over a period of months.
- Quality layers highlight any regions which fail quality criteria as set out in the OceanFlux GHG Technical Specification (TS).
- Software verified using Takahashi climatology data (SST, XCO₂, U₁₀, pCO_{2w}, air pressure, ice) as input (at 1° × 1°):
 - kSW06 < 2 % difference
 - pCO_{2a} < 0.25 % difference
 - pH₂O < 1.4 % difference
 - K_o < 2 % difference
 - Annual global net flux 1.34 Gt C yr⁻¹ (ref: Takahashi 1.4 ± 0.7 Gt C yr⁻¹)
- Development version of software and output formats have been evaluated by an external independent third party company.
- NetCDF3 output follow CF 1.6 guidelines

Web based control

Cook your own climatology!

OceanFlux project offers to interested partners the ability to run their own climatology processing, selecting the parameterization and input data of their choices. This processing configuration can be defined online through a web interface. Users can then connect to the Nephelae processing platform of Ifremer/CERSAT and execute their climatology computation remotely.

This guidelines describes how you can cook your own climatology.

Parameter	Dataset	Bias	Random noise
Pressure	Select in catalogue NCEP/CFSR Global Monthly Pressure at Sea Level on a 1°x1° geographical grid by Oceanflux:	<input checked="" type="checkbox"/>	<input type="checkbox"/>
SST during pCO ₂ measure	Select in catalogue Global Monthly Carbon Dioxide on a 1°x1° geographical grid by OceanFlux: SST_1	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Significant wave height	Select in catalogue Atlimeter Global Monthly Significant Wave Height on a 1°x1° geographical grid by Oceanflux:	<input checked="" type="checkbox"/>	<input type="checkbox"/>
SST Skin	Select in catalogue ESA/AATSR Global Monthly Sea Surface Temperature Composite on a 1°x1° geographical grid by	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Salinity	Select in catalogue Global Monthly Carbon Dioxide on a 1°x1° geographical grid by OceanFlux: salinity	<input checked="" type="checkbox"/>	<input type="checkbox"/>
SST Foundation	Select in catalogue OSTIA Global Monthly Sea Surface Temperature Composite on a 1°x1° geographical grid by	<input checked="" type="checkbox"/>	<input type="checkbox"/>
CO ₂ concentration (Air)	Select in catalogue Global Monthly Carbon Dioxide on a 1°x1° geographical grid by OceanFlux: vCO ₂ _air	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Partial pressure of CO ₂ (Sea water)	Select in catalogue Global Monthly Carbon Dioxide on a 1°x1° geographical grid by OceanFlux: pCO ₂ _sw	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Rain	Select in catalogue TRMM Global Monthly Rain on a 1°x1° geographical grid by OceanFlux: pcp_mean	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Wind at 10m	Select in catalogue Atlimeter Global Monthly Wind Field on a 1°x1° geographical grid by Oceanflux: wind_speed_cor_mean	<input checked="" type="checkbox"/>	<input type="checkbox"/>
Sigma 0	Select in catalogue Atlimeter Global Monthly Ku-band sigma0 on a 1°x1° geographical grid by Oceanflux:	<input checked="" type="checkbox"/>	<input type="checkbox"/>

Configuration of processing inputs

You can select here a dataset for each input parameter to the climatology. Random noise and bias can be set for some of these parameters.

Missing a dataset? [Tell us!](#)

[Next](#)

Web based control

Experiment with OceanFlux data!

Parameterize your own greenhouse gas climatology with the [OceanFlux online configurator](#).

Current features include:

- Guided creation of a configuration to generate your climatology
- Upload of generated config files to your workspace on Ifremer cloud

Online processing will also be possible soon...

[What for?](#)

[Start now!](#)



For more information on how to get your account, run your climatology and analyze your results, please refer to our [online tutorial](#)



Web based control

OceanFlux [Home](#) [Configuration](#) [Saved files](#) [Process](#)

Experiment with OceanFlux data!

OceanFlux [Home](#) [Configuration](#) [Saved files](#) [Process](#)

[Introduction](#) [Input datasets](#) [Transfer velocity](#) [Traditional wind dependent transfer velocity](#) [Add correction to transfer velocity](#) [Schmidt Number of carbon dioxide](#) [Solubility of carbon dioxide](#) [Oceanic fugacity](#) [Interfacial fugacity](#)

[Flux calculation](#) [Additional layers](#) **Output settings**

Output settings

Output directory
Choose the directory that will be used to store the results.
The path should be relative to the user home directory (no leading slash).

Comments
Describe here the characteristics of this configuration. This will be useful later, when browsing your different configuration files.

[Previous](#) [Next](#)

Web based control

The screenshot displays the OceanFlux web interface. At the top, a navigation bar includes 'Oceanflux', 'Home', 'Configuration', 'Saved files', and 'Process'. Below this, a breadcrumb trail shows the current path: 'Introduction' > 'Input datasets' > 'Transfer velocity' > 'Traditional wind dependent transfer velocity' > 'Add correction to transfer velocity' > 'Schmidt Number of carbon dioxide' > 'Solubility of carbon dioxide' > 'Oceanic fugacity' > 'Interfacial fugacity'. The main content area is titled 'Experiment with OceanFlux data!' and features a small illustration of a hand holding a pen. Below the title, a secondary navigation bar highlights the current step: 'Flux calculation' > 'Additional layers' > 'Output settings'. The 'Additional layers' section lists several options: 'Whitecapping' (Godijn-Murphy et al., 2010) with a value of $W = 0.00159 U_{10}^2$; 'SST gradients' (=> choose gradient); 'Low wind indicator' (=> choose wind); 'Biological activity indicator' (=> choose biology); 'Diurnal warming ($\Delta T_{max} > \Delta T_{min}$)' (=> choose SST bins, SSTred); and 'Longhurst biogeographical provinces'. A 'Previous' button is visible at the bottom left, and a 'Next' button is at the bottom right.

Web based control

Experiment with OceanFlux data!



Oceanflux Home Configuration Saved files Process

Introduction Input datasets Transfer velocity Traditional wind dependent transfer velocity Add correction to transfer velocity Schmidt Number of carbon dioxide Solubility of carbon dioxide Oceanic fugacity Interfacial fugacity

Flux calculation Additional layers Output settings

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Flux calculation Additional layers

Additional layers

Whitecapping

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Flux calculation

Flux calculation

The concentration at the base of the mass boundary layer is assumed equal to the bulk concentration ("rapid model"). Each bulk concentration is calculated from the solubility of the water column for the specific month and grid square multiplied by the individual fugacity measurement corrected to the reference year. The full set of individual values are used to construct a climatological grid of concentrations for each calendar month of the reference year using geospatial optimal interpolation methods.

The concentration at the sea surface for each calendar month of the reference year and each grid square is calculated from the sea surface solubility and the interfacial solubilities

Mass boundary layer concentration (ie concentration in the water)

$$C_{water} = solubility_{ref} * pCO2_{water}$$

Interfacial concentration (ie at the interface between the ocean and the atmosphere)

$$C_{int} = solubility_{int} * pCO2_{air}$$

Flux formula

$$flux = k * (C_{water} - C_{int})$$

- Add flux component for wet deposition due to rain
◊ Komori et al., 2007

$$R_{wet} * solubility_{wet}(distilled water) * C_{atm}$$

where:

- R_{wet} is rain rate
- $solubility_{wet}(distilled water)$ is the solubility in zero salinity water

Previous

Previous

Previous

Next

Web based control

Experiment with OceanFlux data!



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Flux calculation Additional layers Output settings

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Flux calculation Additional layers

Additional layers

Whitewapping

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Flux calculation

Flux calculation

Oceanflux Home Configuration Saved files Process

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The concentration of water colour constant is

The concentration of mass bow

Interfacial

Flux forms

Previous

Previous

Previous

Previous

Next

Interfacial fugacity

For carbon dioxide, vertical gradients in its molar fraction of dry air are negligible. The molar fraction of the lower atmosphere (including regional, seasonal and secular variation) is known accurately (compared to oceanic values). The interfacial fugacity is calculated from the fraction of dry air, atmospheric pressure and the interfacial temperature and salinity. Gridded climatologies of each of these inputs is used to calculate the interfacial fugacity for each calendar month of the reference year and each grid square.

Fraction of CO₂ in dry air
GlobalView CO₂ database (see: http://www.esrl.noaa.gov/gmd/ccgg/bba/view/co2/co2_observations.html)
skin temperature
sea level pressure
salinity

air partial pressure pCO_{2a}
calculated as follows:
equation 26, Kettle et al. 2009, ACP

$$pCO_{2a} = xCO_{2a} (P - pH_2O)$$

where:

- P is the sea level pressure
- xCO_{2a} is the CO₂ molar fraction of the atmospheric air (in ppm) (Takahashi)
- p_{H₂O} is the water vapour pressure. For calculating atmospheric CO₂, we assume that the gas is at 100% humidity because it is the air just above the sea. The water vapour pressure must then be taken into account at sea surface temperature (SST in K) and salinity (S). It is given (in atmospheres) by the following formula (Webb and Price, 1980):

$$p_{H_2O} = 1013.25 \exp(24.4543 - 67.4509 / (100 + SST) - 4.8489 \ln(SST) / 100) - 0.000544 S$$

where:

- S is the salinity
- SST is the sea surface temperature in Kelvin

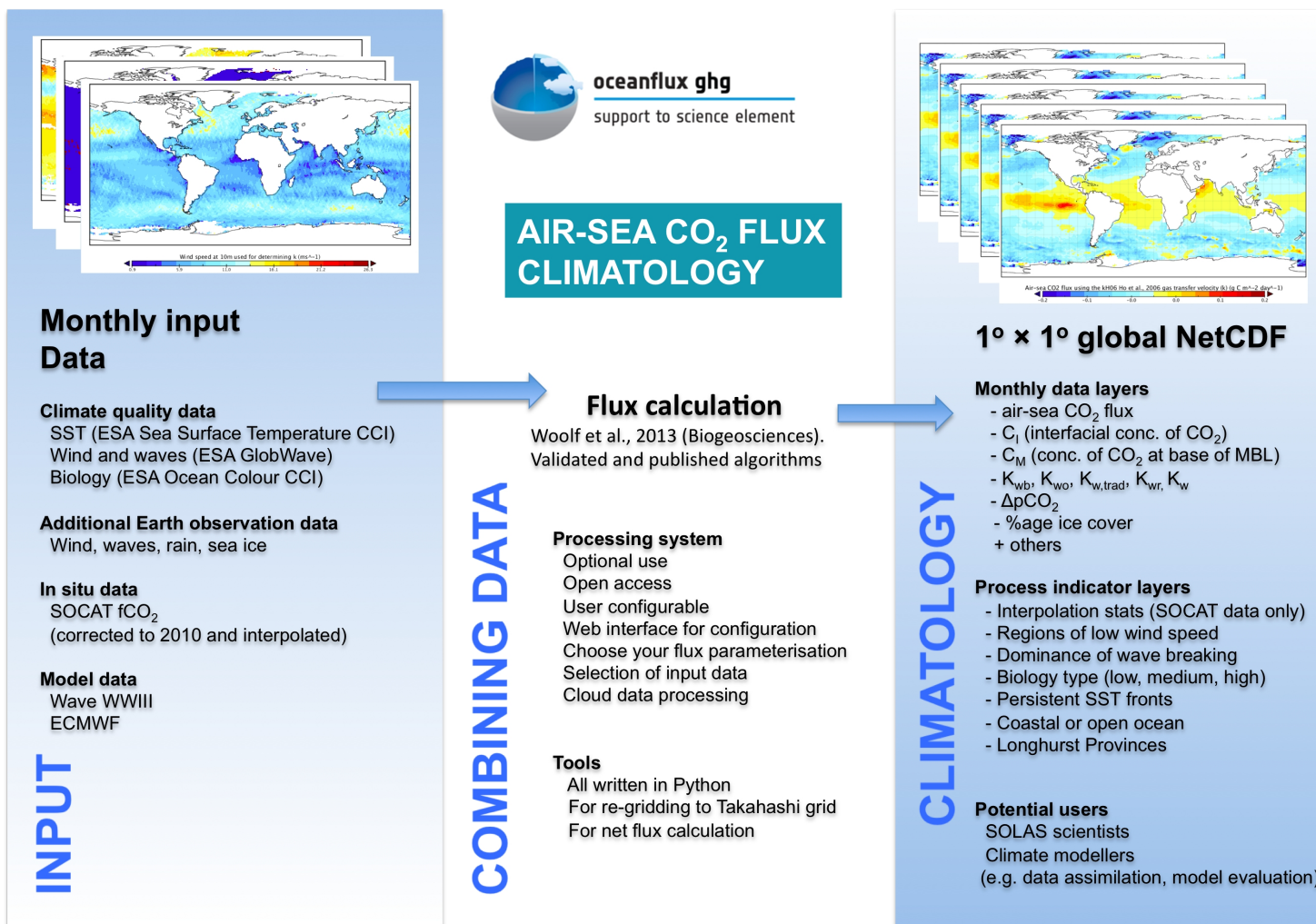
Corrections applied

- Long-term trend correction
Fugacity data is corrected to the reference year using an assumed long-term trend in fugacity (1.5 ppm/year) as defined by Takahashi et al. (2008). This assumption will inherit the uncertainties as described and calculated by

Takahashi et al., (2008): $pCO_{2a} = xCO_{2a} + (year - 1978) * 1.5$



And finally.... a brochure



PDF on project website

Conclusions

- Highly flexible community tool to calculate global air-sea CO₂ fluxes.
- Exploits Cloud based computing
- Large amount of *climate quality data* and processing capability available.
 - 8 Terra bytes available and/or has been pre-processed
 - 500 Terra bytes of EO data available
 - 600 processing cores
- Flexible solution
 - e.g. very simple to add additional datasets or run long time series.
- Output fluxes have been verified.
- System exploited for a number of OceanFlux GHG investigations and analyses.

Future:

Expand to handle other gases ?

Shutler, J. D., Piolle, J. F., Land, P. E., Woolf, D. K., Goddijn-Murphy, L., Paul, F., *et al.* (in-prep) Air-sea gas flux data processing system using Cloud computing: a flexible and dynamic tool for the community, *to be submitted to Journal of Atmospheric and Oceanic Technology.*