

A generic approach to explicit simulation of uncertainty in the NEMO ocean model

Jean-Michel Brankart
Florent Garnier, Pierre Brasseur

Institut des Geosciences de l'Environnement
Equipe de Modélisation des Ecoulements Océaniques Multi-échelles

Grenoble, 20-21 April 2017



**Since important decisions
must rely on simulations,
it is essential that its validity be tested,
and that its advocates be able to describe
the level of authentic representation
which they achieved.**

Summer Computer Simulation Conference (1975),
cited by Richard Hamming (1997)

Motivations for a probabilistic approach

The deterministic approach is not always sufficient to describe the dynamical behaviour of the system

Comparison between simulations and observations is easier with the probabilistic approach

A good knowledge of model accuracy is necessary to solve data assimilation problems

Outline

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Introduction

2

Explicit simulation of uncertainties

3

Stochastic circulation model

4

Stochastic biogeochemical model

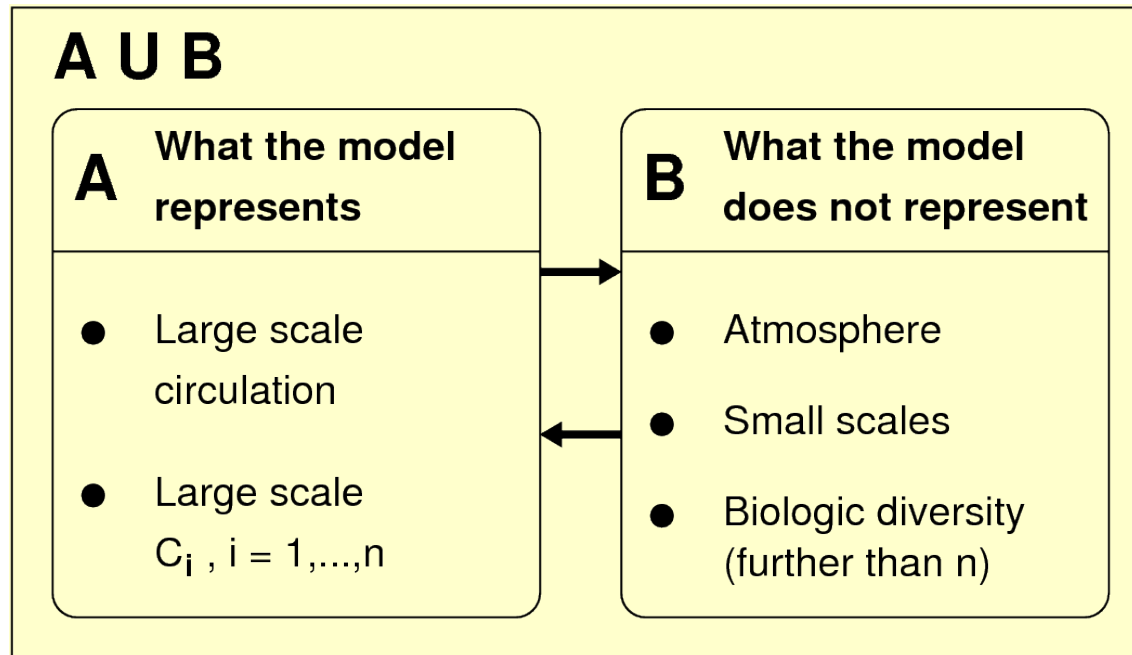
5

Conclusions

1

Introduction

Sources of uncertainties in ocean models



- Even if the dynamics of **U** can be assumed deterministic, the system **A** alone **cannot be assumed deterministic**.
- To obtain a deterministic model for **A**, one must assume, either that **B** is known (\rightarrow atmospheric forcing), or that the effect of **B** can be parameterized (\rightarrow paramétrisation of unresolved scales or unresolved biologic diversity).
 - \rightarrow **B is the main source of uncertainty in the model.**

Uncertainty, as a key component of our systems

**What are the uncertain components
of our systems ?**

How to describe uncertainties ?

**How does it participate
to the solution of inverse problems ?**

2

Explicit simulation of uncertainties

A first simple implementation based on autoregressive processes (1)

Method: explicitly simulate uncertainties in the model using *random numbers*

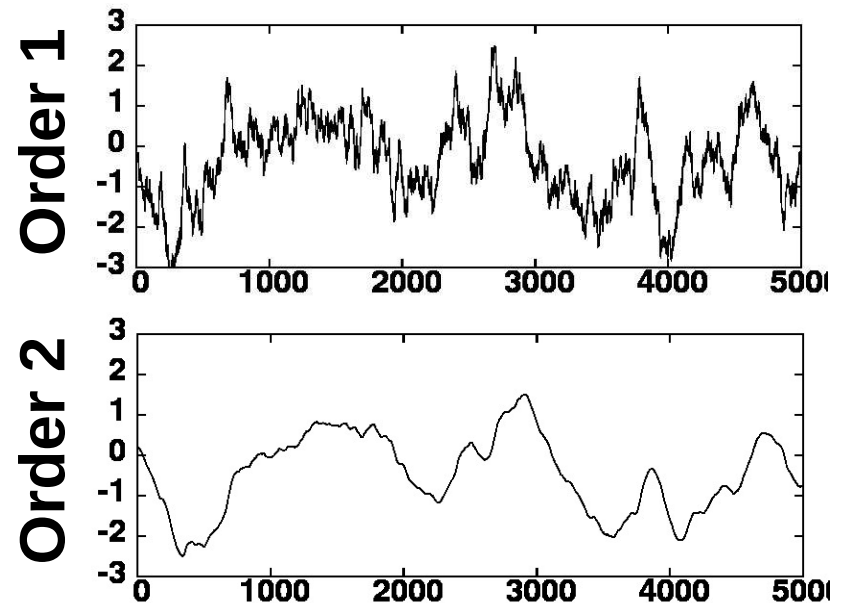
At every model grid point (in 2D or 3D), generate a set of independent **Gaussian autoregressive processes:**

$$\xi(t_k) = a \xi(t_{k-1}) + b w + c$$

where w is a Gaussian white noise (\rightarrow order 1 process)
or an autoregressive process of order $n-1$ (\rightarrow order n process)

Parameters a , b , c
to specify:

mean, standard deviation
and correlation timescale



A first simple implementation based on autoregressive processes (2)

Introduce a spatial correlation structure

by applying a spatial filter
to the map of
autoregressive processes:

$$\tilde{\xi} = \mathcal{F}[\xi] \quad (\text{filtering operator})$$

$$\mathcal{L}[\tilde{\xi}] = \xi \quad (\text{elliptic equation})$$

which can easily be made
flow dependent if needed

Modify the marginal probability distributions

by applying anamorphosis
transformation to every
individual Gaussian variable:

$$\tilde{\xi} = \mathcal{T}[\xi] \quad (\text{nonlinear function})$$

for instance to transform the
Gaussian variables into
lognormal or gamma
variables if positive noise is
needed

→ This provides a generic technical way of implementing
a wide range of stochastic parameterizations

Technological approach: a stochastic module in NEMO

These processes are generated using a **new module in NEMO**, and **can be used in any component** of the model (Brankart et al., 2015):
circulation model, ecosystem model, sea ice model

Algorithm 1 sto_par

```
for all (map  $i = 1, \dots, m$  of autoregressive processes) do
  Save map from previous time step:  $\xi_{-} \leftarrow \xi_i$ 
  if (process order is equal to 1) then
    Draw new map of random numbers  $w$  from  $\mathcal{N}(0, 1)$ :
     $\xi_i \leftarrow w$ 
    Apply spatial filtering operator  $\mathcal{F}_i$  to  $\xi_i$ :  $\xi_i \leftarrow \mathcal{F}_i[\xi_i]$ 
    Apply precomputed factor  $f_i$  to keep SD equal to 1:
     $\xi_i \leftarrow f_i \times \xi_i$ 
  else
    Use previous process (one order lower) instead of white
    noise:  $\xi_i \leftarrow \xi_{i-1}$ 
  end if
  Multiply by parameter  $b_i$  and add parameter  $c_i$ :  $\xi_i \leftarrow b_i \times$ 
   $\xi_i + c_i$ 
  Update map of autoregressive processes:  $\xi_i \leftarrow a_i \times \xi_{-} + \xi_i$ 
end for
```

- Generic and flexible technological approach
 - Model independent implementation
- Possible to simulate many kinds of uncertainty

Algorithm 2 sto_par_init

```
Initialize number of maps of autoregressive processes to 0:
 $m \leftarrow 0$ 
for all (stochastic parameterization  $k = 1, \dots, p$ ) do
  Set  $m_k$ , the number of maps of autoregressive processes re-
  quired for this parameterization
  Increase  $m$  by  $m_k$  times the process order  $o_k$ :  $m \leftarrow m +$ 
   $m_k \times o_k$ 
end for
for all (map  $i = 1, \dots, m$  of autoregressive processes) do
  Set order of autoregressive processes
  Set mean ( $\mu_i$ ), standard deviation ( $\sigma_i$ ) and correlation
  timescale ( $\tau_i$ ) of autoregressive processes
  Compute parameters  $a_i, b_i, c_i$  as a function of  $\mu_i, \sigma_i, \tau_i$ 
  Define filtering operator  $\mathcal{F}_i$ 
  Compute factor  $f_i$  as a function of  $\mathcal{F}_i$ 
end for
Initialize seeds for random number generator
for all (map  $i = 1, \dots, m$  of autoregressive processes) do
  Draw new map of random numbers  $w$  from  $\mathcal{N}(0, 1)$ :  $\xi_i \leftarrow$ 
   $w$ 
  Apply spatial filtering operator  $\mathcal{F}_i$  to  $\xi_i$ :  $\xi_i \leftarrow \mathcal{F}_i[\xi_i]$ 
  Apply precomputed factor  $f_i$  to keep standard deviation
  equal to 1:  $\xi_i \leftarrow f_i \times \xi_i$ 
  Initialize autoregressive processes to  $\mu + \sigma \times w$ :  $\xi_i \leftarrow \mu +$ 
   $\sigma \xi_i$ 
end for
if (restart file) then
  Read maps of autoregressive processes and seeds for the ran-
  dom number generator from restart file (thus overriding the
  initial seed)
end if
```

List of uncertainties that have been implemented in NEMO using this generic stochastic module

In the circulation model

- Effect of unresolved scales in the equation of state
- Uncertainties in the parameterized tendencies (SPPT scheme)
- Uncertainties in the horizontal momentum diffusion
- Uncertainties in vertical diffusion (lognormal distribution)
- Uncertainties in bulk parameters C_D , C_E , C_H (gamma distribution)

In the ecosystem model

- Effect of unresolved scales in the SMS terms of the equations
- Uncertainties in model parameters (primary production and grazing)

In the sea-ice model

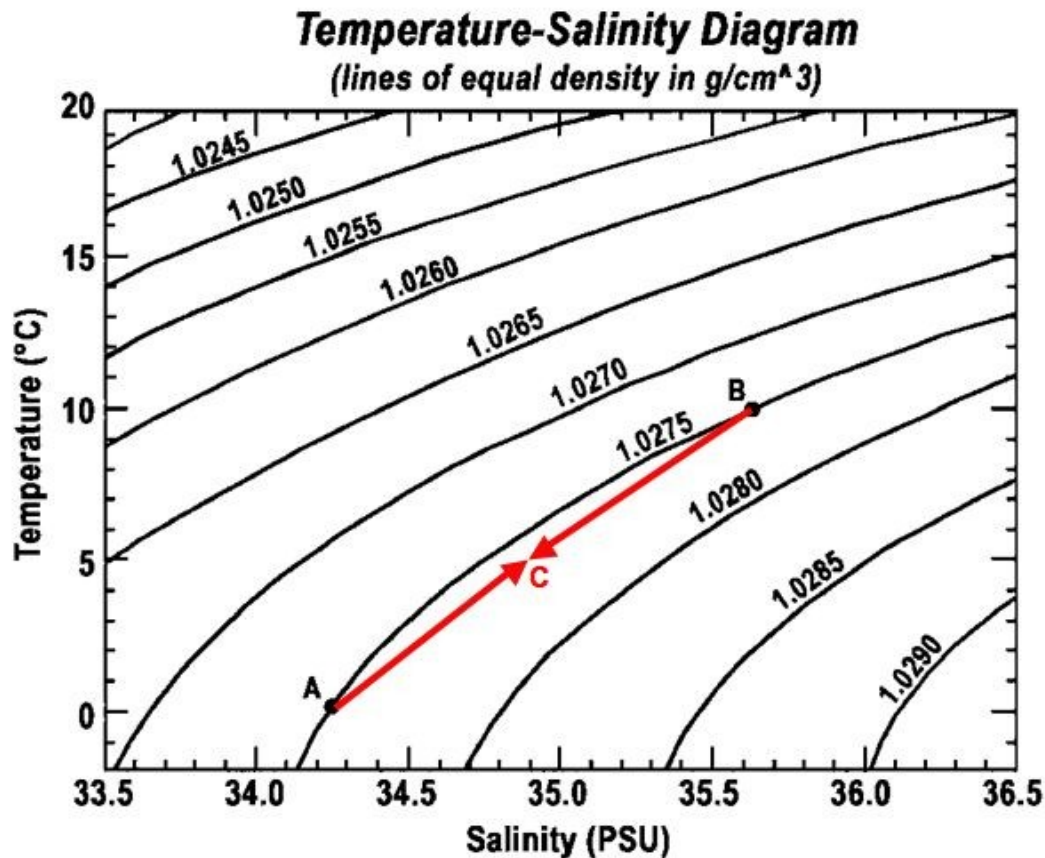
- Uncertainties in ice strength (gamma distribution)
- Uncertainties in ice/atmosphere drag (gamma distribution)
- Uncertainties in ice/ocean drag (gamma distribution)
- Uncertainties in ice albedo (beta distribution)

3

Stochastic circulation model

Uncertainties in the computation of density

In the model, the large-scale density is computed from large-scale temperature and salinity, using the sea-water equation of state.



(a)

Mixing waters of equal density but different T&S systematically increases density (cabbeling)

(b)

Averaging T&S equations systematically overestimates density (in a fluctuating, non-deterministic way)

Because of the nonlinearity of the equation of state, unresolved scales produce an average effect on density.

Stochastic equation of state for the large scales

Stochastic parameterization (Brankart, 2015)

using a set of random T&S fluctuations

$$\Delta T_i \text{ et } \Delta S_i, i=1, \dots, p$$

to simulate unresolved T&S fluctuations

$$\rho = \frac{1}{p} \sum_{i=1}^p \rho [T + \Delta T_i, S + \Delta S_i, p_0(z)] \quad \text{with} \quad \sum_{i=1}^p \delta T^{(i)} = 0, \quad \sum_{i=1}^p \delta S^{(i)} = 0$$

No effect if the equation of state is linear.

Proportional to the square of unresolved fluctuations.

Correction $\Delta\rho$ applied in the thermal wind equation, as in the semi-prognostic method of Greatbatch et al. (2004)

No direct modification of T&S; no enhanced diapycnal mixing.

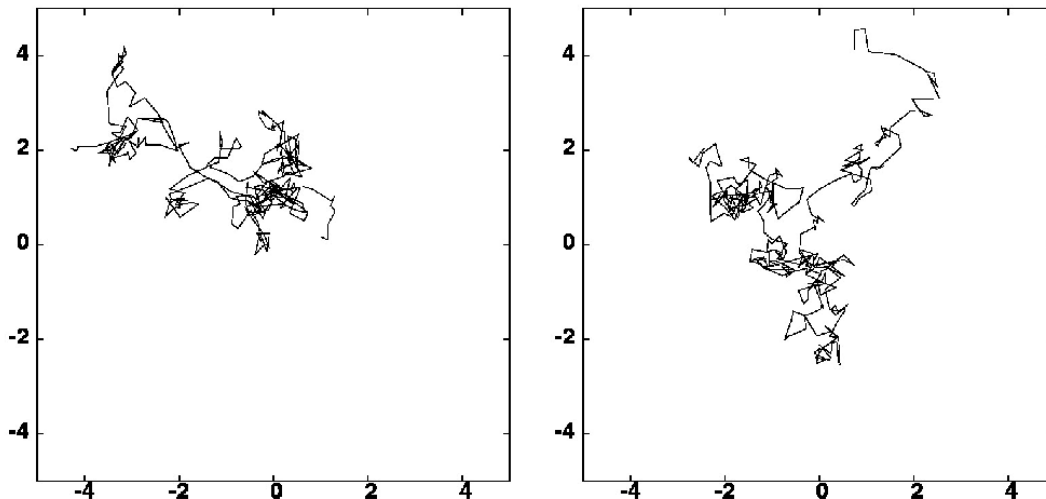
T&S only modified indirectly through a modification
of the main currents

Random walks to simulate unresolved temperature and salinity fluctuations

Computation of the random fluctuations ΔT_i et ΔS_i
as a scalar product of the local gradient with random
walks ξ_i

$$\Delta T_i = \xi_i \cdot \nabla T \quad \text{and} \quad \Delta S_i = \xi_i \cdot \nabla S$$

Random walks



Assumptions

AR1 random processes

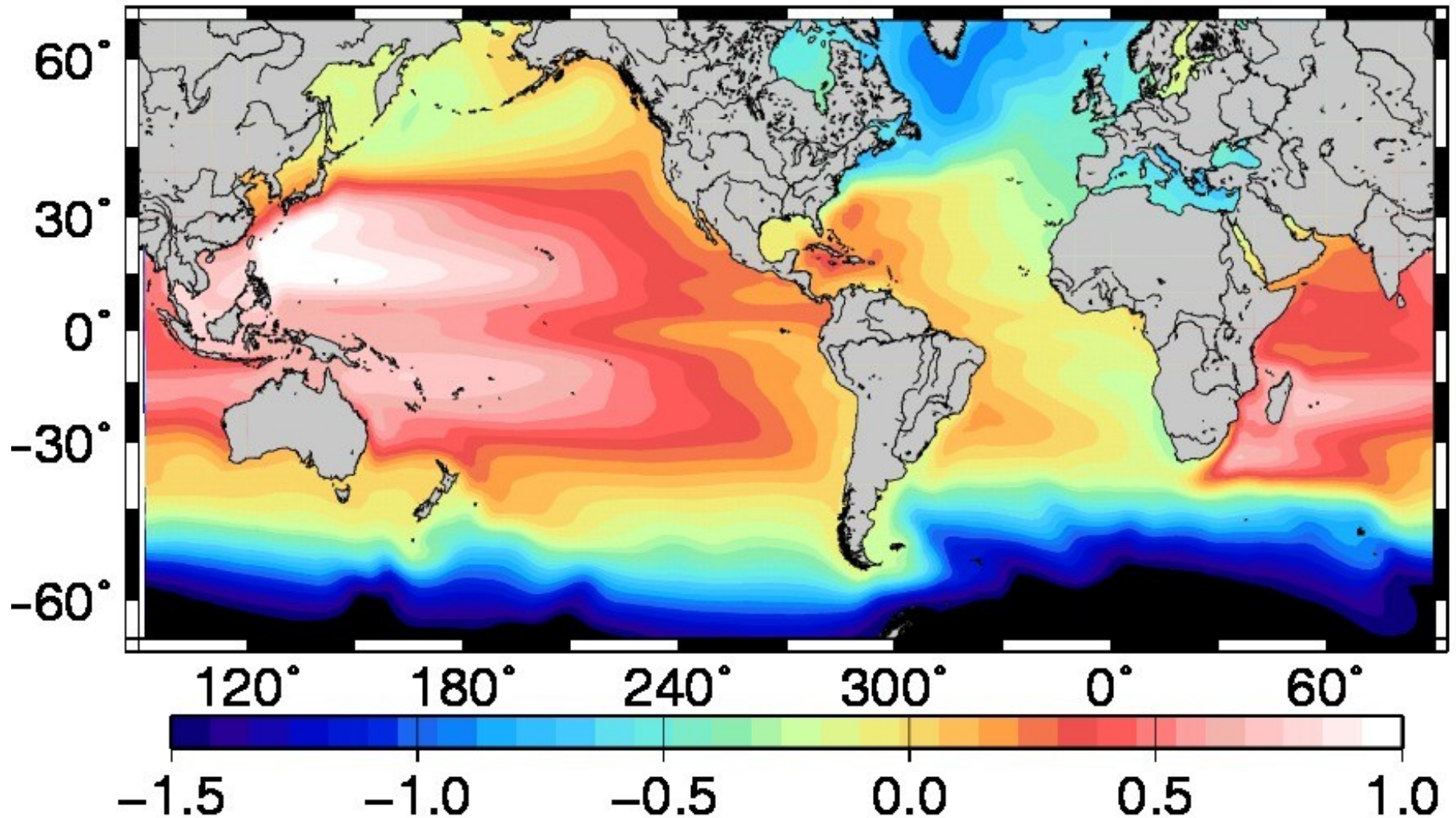
uncorrelated on the horizontal

fully correlated
along the vertical

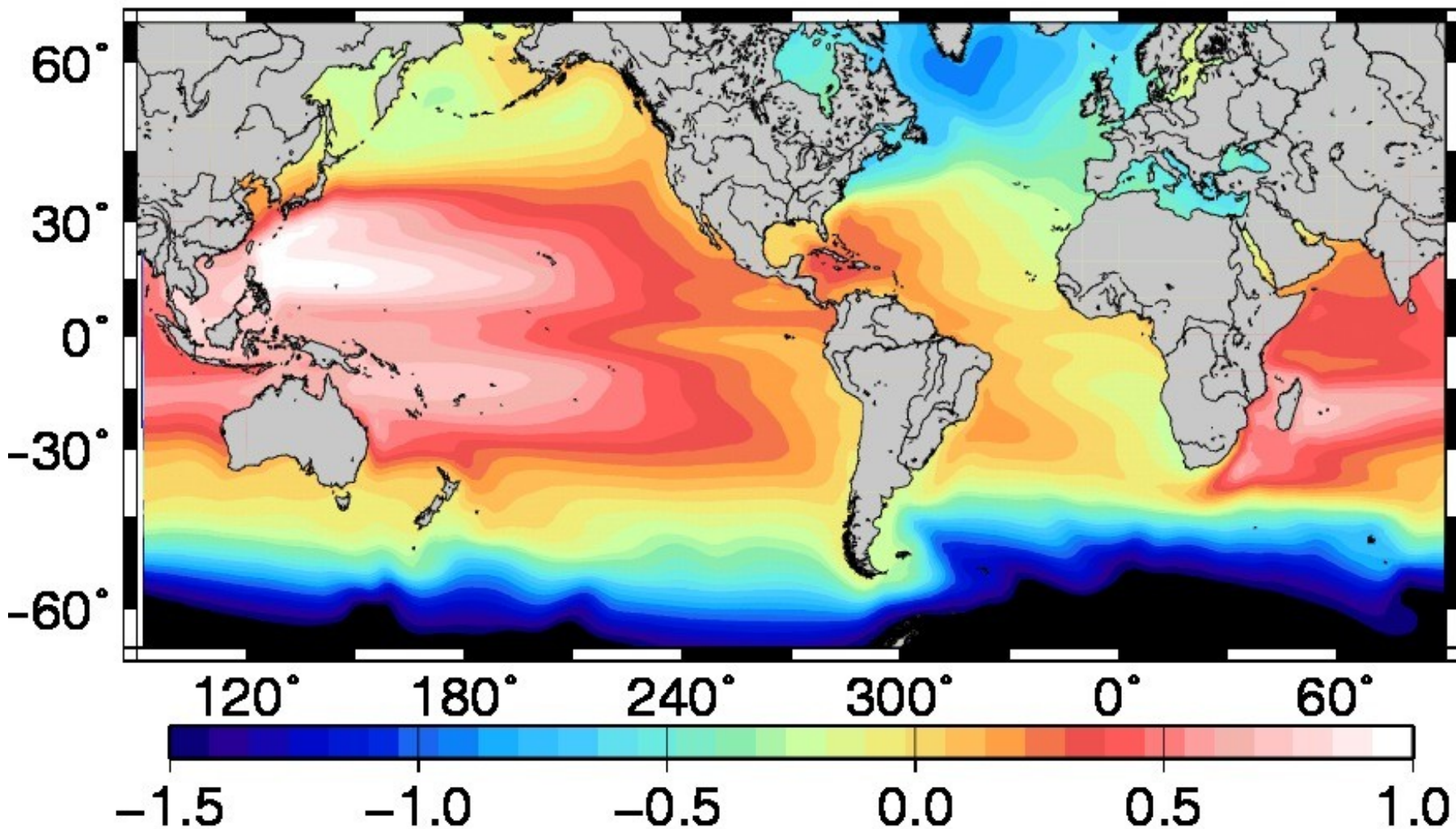
5-day time correlation

horizontal std: 2-3 grid points
vertical std: <1 grid point

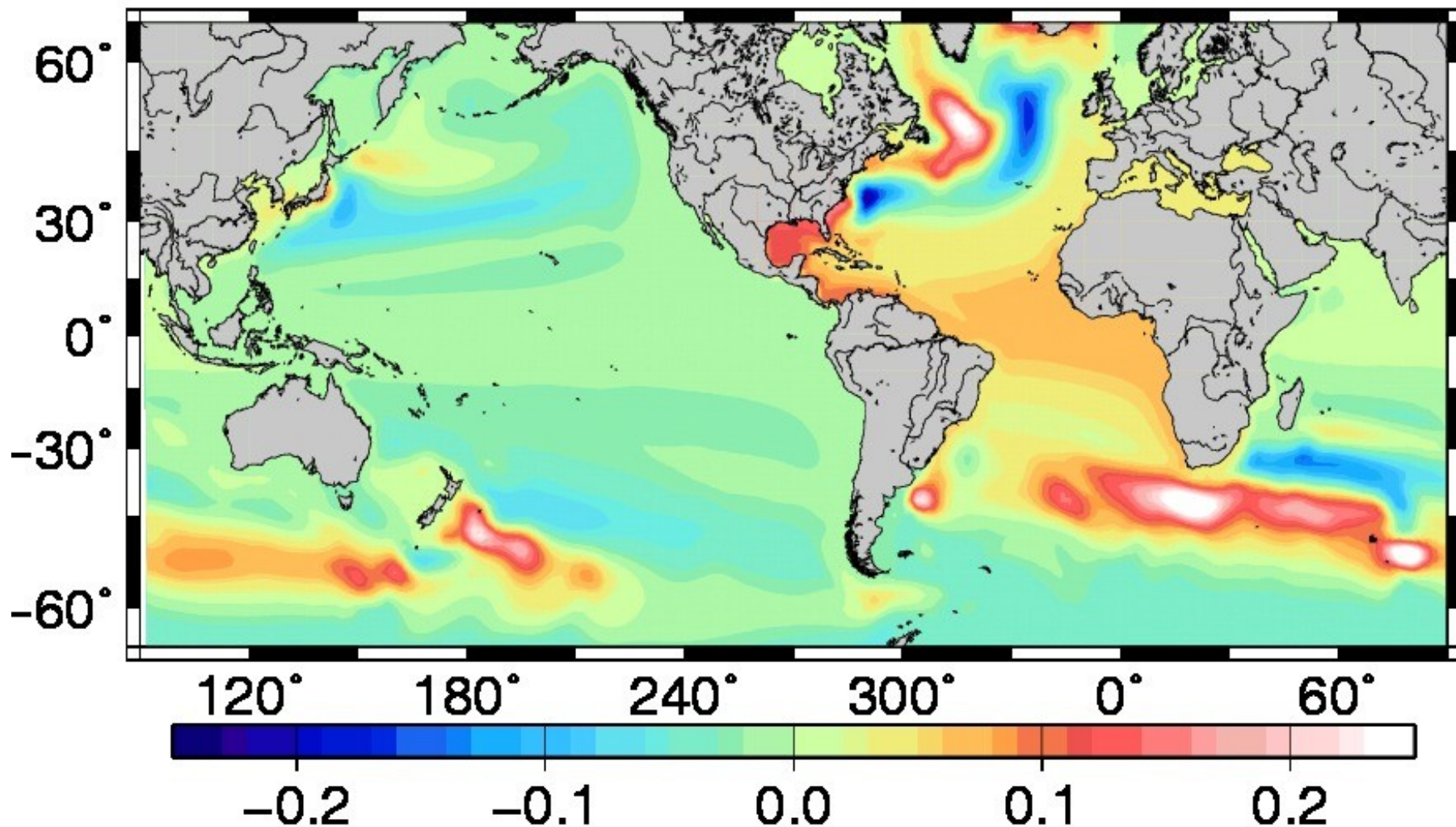
Mean sea surface elevation (standard)



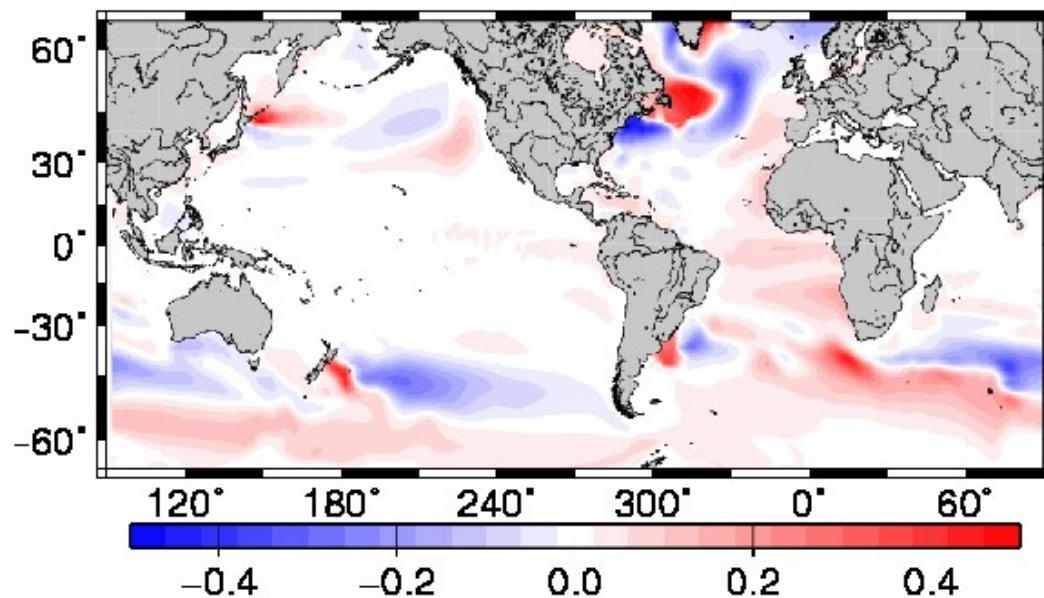
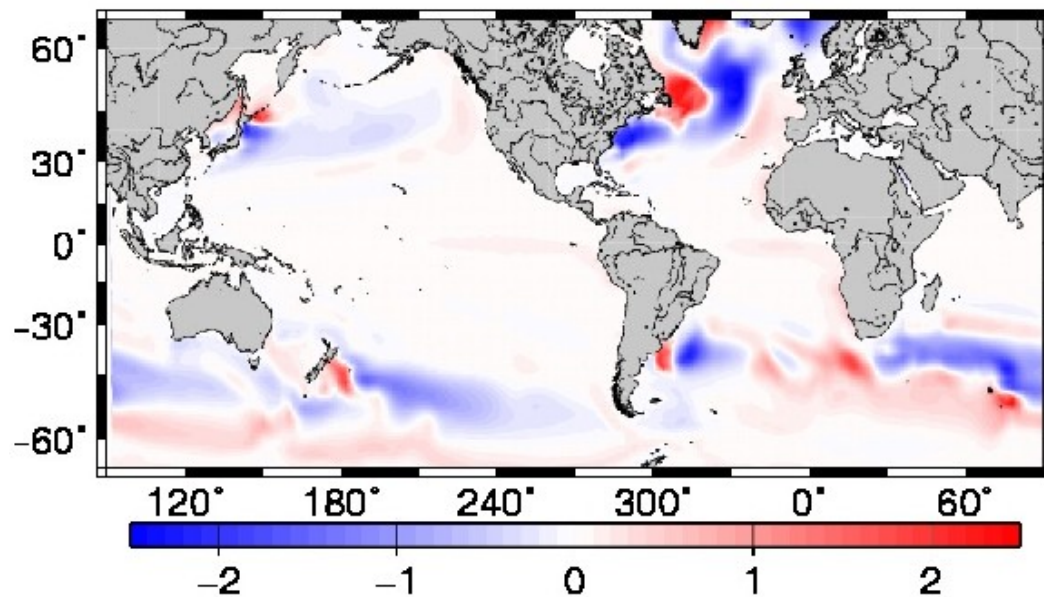
Mean sea surface elevation (stochastic)



Mean sea surface elevation difference



Averaged SST & SSS difference



**Modification
of the mean flow**



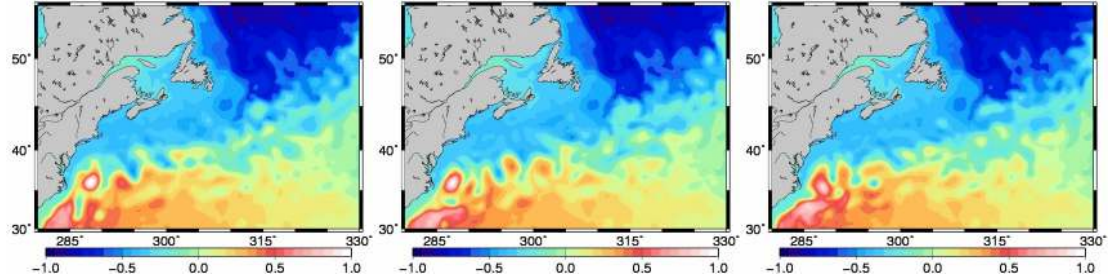
**Modification
of the mean
SST & SSS**



**Modification
of air/sea
interactions**

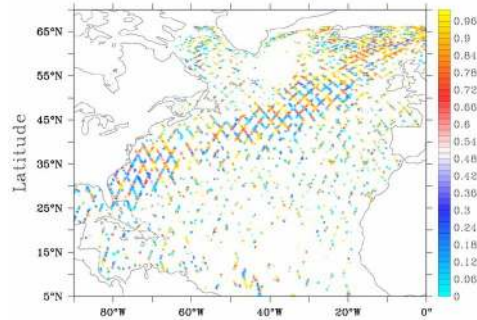
Ensemble of mesoscale flows

SSH pdf
ensemble NATL025:
3 members among 96

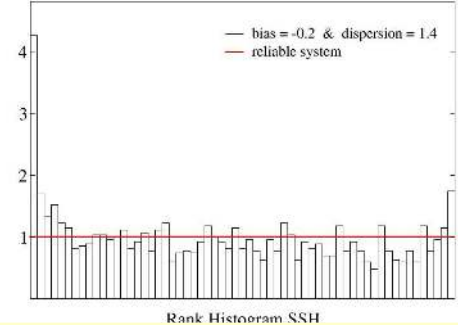


→ comparison to observation (rank histogram, CRPS score, etc.)

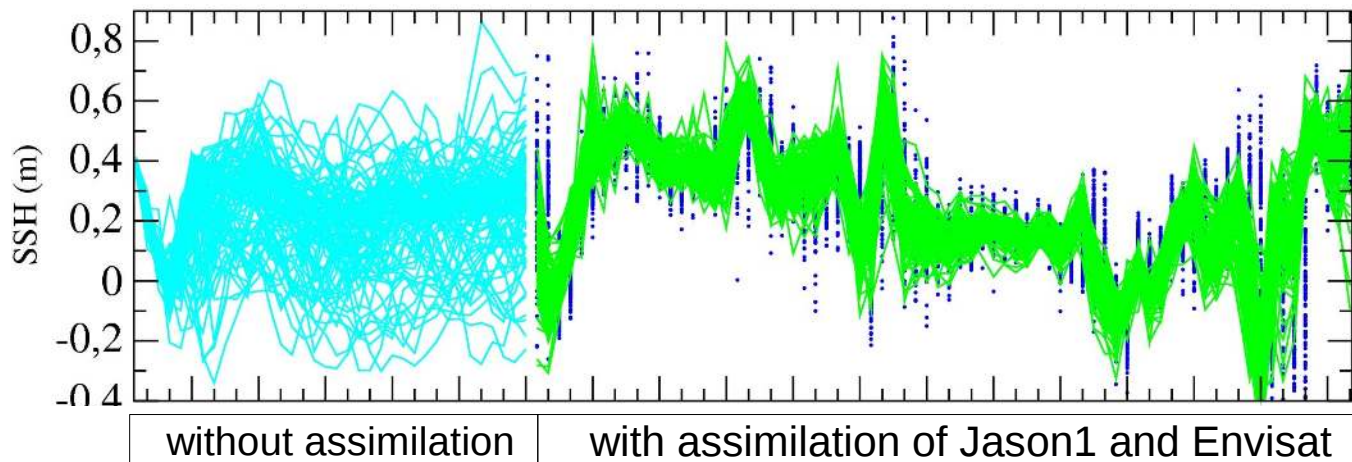
Map of ranks
of JASON
altimetric data



Rank histogram
to check
reliability



→ assimilation of altimetric data (Candille et al., 2015)



Time
evolution
of the pdf

from June 2005 to
December 2006

4

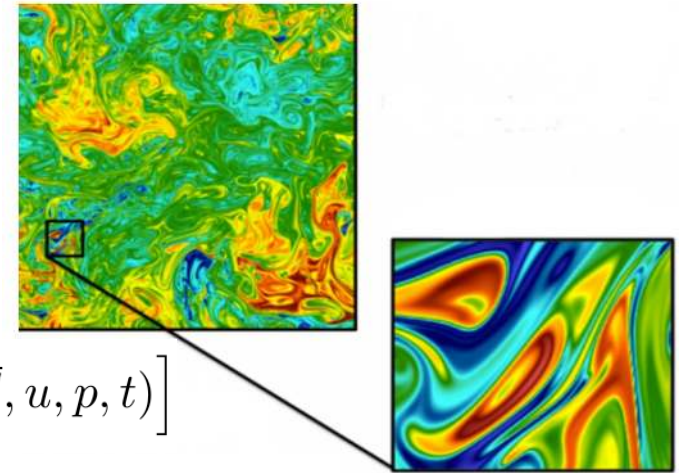
Stochastic biogeochemical model

Stochastic biogeochemical model

**Multiple sources of uncertainty in ecosystem model:
unresolved biological diversity, unresolved scales, etc.**

**Unresolved scales
stochastic processes
explicitly simulating
unresolved fluctuations of C_i**

$$\frac{\partial C}{\partial t}|_{bio} = \frac{1}{2} \left[SMS(\bar{C} + \delta\bar{C}, u, p, t) + SMS(\bar{C} - \delta\bar{C}, u, p, t) \right]$$
$$\delta\bar{C} = \xi(t)\bar{C}$$



**Unresolved diversity
multiplicative noise
in model parameters**

$$\frac{\partial C}{\partial t}|_{bio} = SMS(C, u, p', t) \quad \text{avec} \quad p' = \exp[\xi(t)]p$$

Assumptions

perturb 8 parameters governing
primary production and grazing

fully correlated
along the vertical

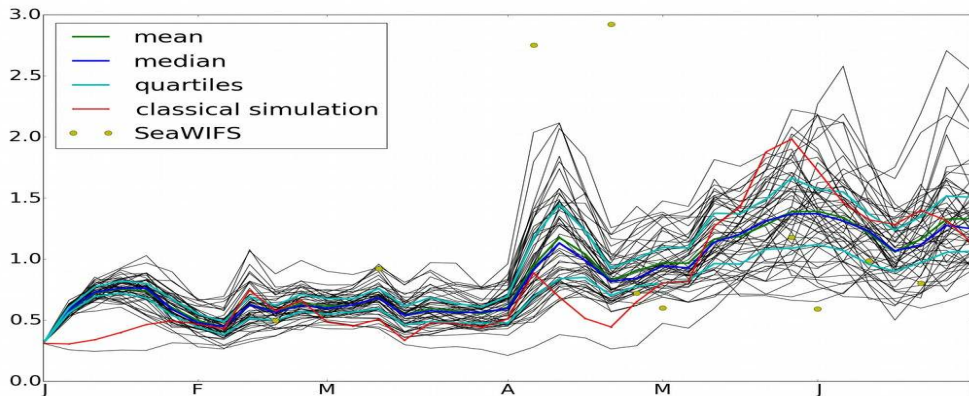
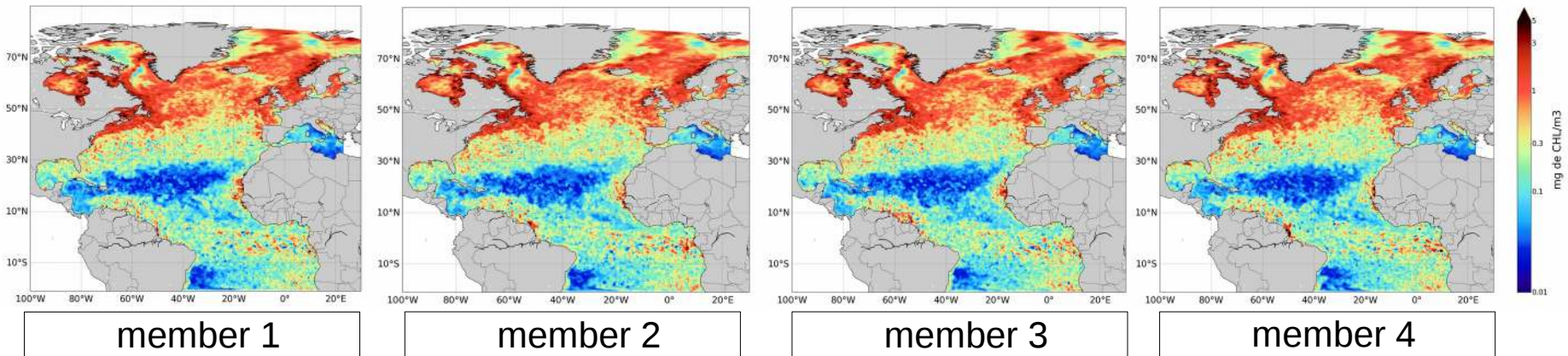
30-day time correlation

- **Considerable effect on the mean behaviour of the system**
- **Increase of patchiness (↔ ocean colour data)**

Ensemble simulation of the ecosystem

Probability distribution of chlorophyll concentration

as simulated here by ensemble NATL025/PISCES
with stochastic parameterization of uncertainty: 4 members among 50



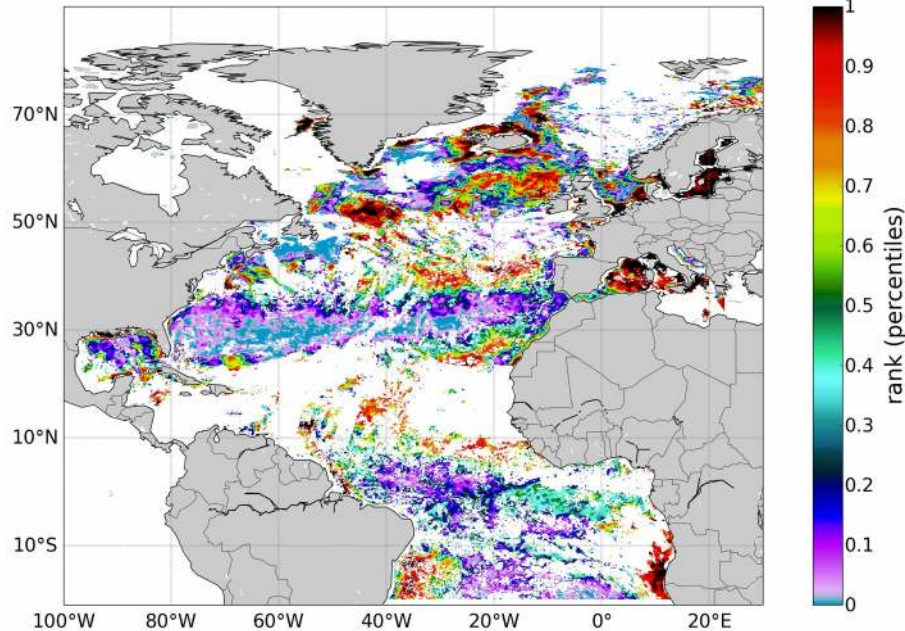
Time evolution
of the pdf
for phytoplankton

from January to June 2005

→ description of biogeochemical uncertainties (Garnier et al., 2016)

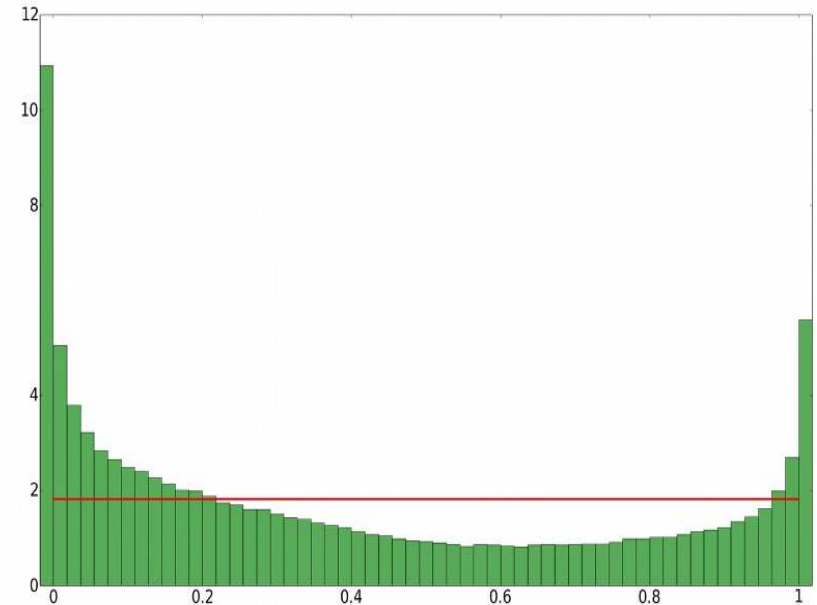
Comparison to ocean colour observations

Rank of SeaWifs observations in the ensemble simulation (May 2005)



The ensemble spread is already sufficient to include more than 80% of the observations (accounting for a 30% observation error)

Rank histogram for SeaWifs over the whole domain



The ensemble is not far from being reliable, even if still underdispersive (too many observations in the external ranges of the ensemble)

- objectively **test the consistency of simulations** as compared to observations
- prerequisite to ocean colour **data assimilation**

6

Conclusions

**The NEMO model becomes probabilistic;
it is seen as a complex system,
built up from uncertain components**

- The goal of ocean modelers is then to build a model as informative as possible at the lesser cost.

**This probabilistic description requires
ensemble simulations**

- Objective comparison between simulations and observations
- Deal with model uncertainty in ocean data assimilation systems

An appropriate simulation of uncertainty is necessary to make the link between model, observations, and data assimilation systems

Uncertainty is bound to become a key constituent of the systems that we are using in oceanography, not something that can be thought separately from the results

Properly dealing with uncertainty will require an integrated engineering approach at the interface between oceanography and applied mathematics

**Error is viewed therefore
not as an extraneous and
misdirected or misdirecting accident,
but as an essential part
of the process under consideration.**

John von Neuman (1956),
in « Probabilistic logics and the synthesis of
reliable organisms from unreliable components ».