

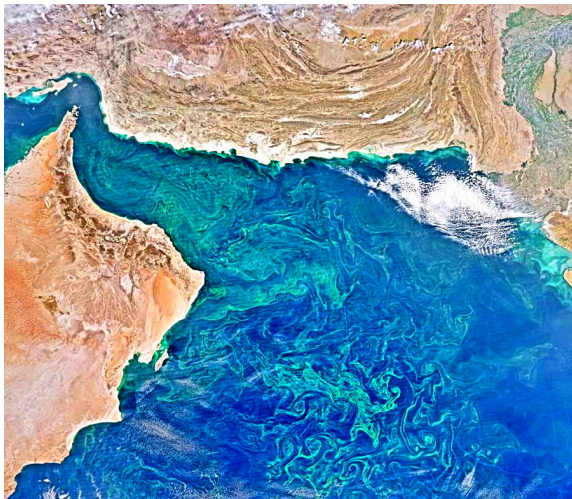
The Mutual Interplay of Stirring, Mixing, Growing (and what it means for biogeochemical modeling)

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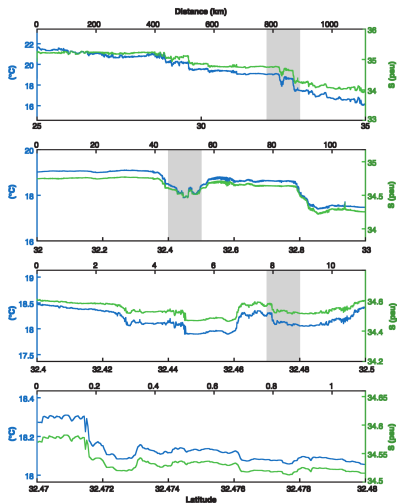
MIT/WHOI Joint Program Summer Reading Group
The Internet, August 14th, 2020

Chlorophyll from Space



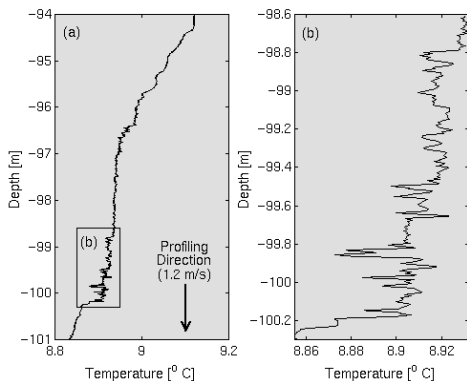
NASA - Modis

Zooming In...



Rudnick & Ferrari - Science (1999)

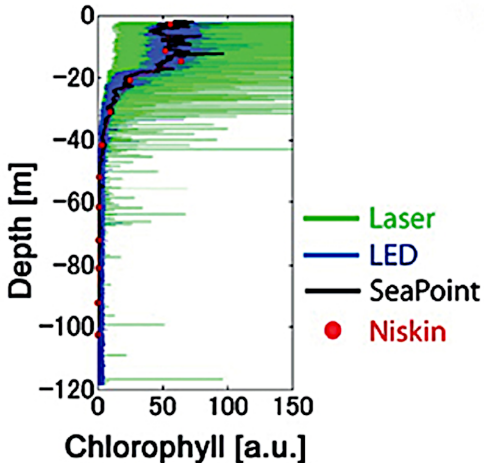
More Zooming...



Nash, Caldwell, Zelman & Moum - J. Atmos Ocean. Tech. (1999)

Assuming a perpetual Moore's law...
...when you'll be able to explicitly resolve all those scales in your
computer model?

Microstructure of Chlorophyll



Mandal et al. - Frontiers in Marine Sciences (2019)

Yamazaki's high-resolution fluorescence profilers show amazing microscale fluctuations.

Does it matter?

Not so much for a passive scalar.

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = D \nabla^2 c$$

under the low-pass filter $^{-\ell}$ the equation becomes

$$\frac{\partial \bar{c}^\ell}{\partial t} + \bar{\mathbf{u}}^\ell \cdot \nabla \bar{c}^\ell = \underbrace{\mathcal{D}(\bar{c}^\ell)}$$

diffusion-like

operator

*that represents the
unresolved dynamics*

Biogeochemical models

$$\frac{\partial c_1}{\partial t} + \mathbf{u} \cdot \nabla c_1 = f_1(c_1, c_2, \dots, c_n) + D_1 \nabla^2 c_1$$

⋮

$$\frac{\partial c_n}{\partial t} + \underbrace{\mathbf{u} \cdot \nabla c_n}_{\text{advection}} = \underbrace{f_n(c_1, c_2, \dots, c_n)}_{\text{reaction}} + \underbrace{D_n \nabla^2 c_n}_{\text{diffusion}}$$

But the trouble is

$$\overbrace{f(c_1, c_2, \dots, c_n)^l} \neq \overbrace{f(\bar{c}_1^l, \bar{c}_2^l, \dots, \bar{c}_n^l)}$$

*what we would
like to know*

*what we can
compute with an
Eulerian code*

A simple example

From Paparella, Popolizio - J. Comp. Phys. (2018)

$$\mathbf{u} = (-\partial_y \psi, \partial_x \psi); \quad \psi = \sin(x) \sin(y)$$

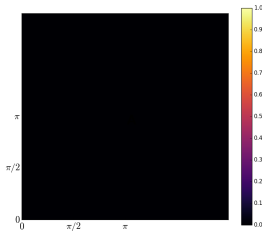
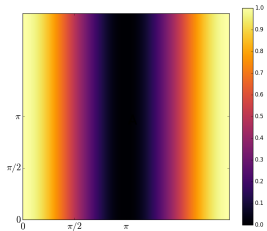
$$\frac{\partial c_1}{\partial t} + \mathbf{u} \cdot \nabla c_1 = -\frac{1}{5} c_1 c_2 + D \nabla^2 c_1$$

$$\frac{\partial c_2}{\partial t} + \mathbf{u} \cdot \nabla c_2 = +\frac{1}{5} c_1 c_2 + D \nabla^2 c_2$$

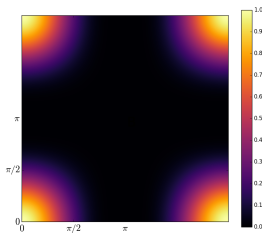
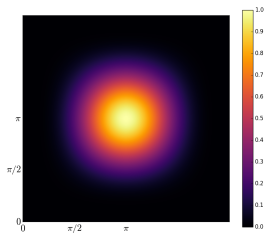
Two distinct initial conditions

Resource

Consumer



Initial Condition A



Initial Condition B

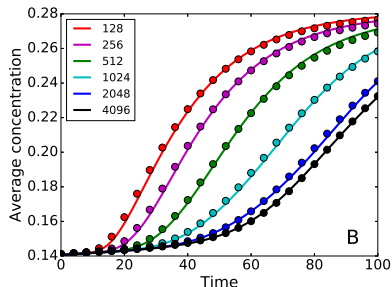
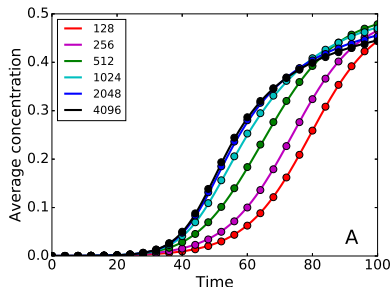
Average consumer as a function of time

Pseudo-spectral simulations on grids:

$$(128 \cdot 2^k) \times (128 \cdot 2^k), \quad k = 0, 1, \dots, 5$$

Diffusivities:

$$D = 10^{-3} \cdot 2^{-2k}$$



Let's talk about iron...

A Trivially Simple Iron Model

$$\begin{cases} \dot{C} &= rC \\ \dot{F} &= -\phi rC \end{cases}$$

C - carbon concentration (mg/m^3)

F - iron concentration ($\mu\text{mol}/\text{m}^3$)

r - growth rate

ϕ - iron quota

Initial concentrations C_0 and F_0 .

Model applies until $F = 0$.

At that point you have the following carbon concentration:

$$C_{end} = C_0 + \frac{F_0}{\phi}$$

Trivially, the initial F_0 amount of iron has turned into a F_0/ϕ amount of carbon.

Let's add some mortality/respiration losses

$$\begin{cases} \dot{C} &= rC - mC \\ \dot{F} &= -\phi rC \end{cases}$$

C - carbon concentration (mg/m^3)

F - iron concentration ($\mu\text{mol}/\text{m}^3$)

r - growth rate

m - mortality / respiration rate

ϕ - iron quota

Initial concentrations C_0 and F_0 .

Model applies until $F = 0$.

At that point you have the following carbon concentration:

$$C_{\text{end}} = C_0 + \underbrace{\frac{(r - m)}{r}}_{\text{efficiency}} \frac{F_0}{\phi}$$

Ah! Now the efficiency of the conversion of F into C depends on the growth and mortality rates...

What happens if the efficiency depends on the iron concentration?

Three fish tanks

(But no fish, just phytoplankton and iron)

- ▶ Let's say that the growth rate is r_1 if $F > F_t$, and r_2 otherwise. Take $0 < m < r_2 < r_1$.
- ▶ Tank A starts with $F_0^{(A)} = 3/2 F_T$
- ▶ Tank B starts with $F_0^{(B)} = 1/2 F_T$
- ▶ Tank C starts with $F_0^{(C)} = F_T = (F_0^{(A)} + F_0^{(B)}) / 2$
- ▶ In all tanks the initial carbon is C_0

End carbon of the three tanks

Average end carbon of tank A and tank B:

$$\frac{1}{2} \left(C_{end}^{(A)} + C_{end}^{(B)} \right) = C_0 + \left(\frac{1}{4} \underbrace{\frac{r_1 - m}{r_1}}_{\text{high efficiency}} + \frac{3}{4} \underbrace{\frac{r_2 - m}{r_2}}_{\text{low efficiency}} \right) \frac{F_T}{\Phi}$$

End carbon of tank C:

$$C_{end}^{(M)} = C_0 + \underbrace{\frac{r_2 - m}{r_2}}_{\text{low efficiency}} \frac{F_T}{\Phi}$$

Difference:

$$\frac{1}{2} \left(C_{end}^{(A)} + C_{end}^{(B)} \right) - C_{end}^{(M)} = \frac{1}{4} \frac{(r_1 - r_2)m}{r_1 r_2} \frac{F_T}{\Phi}$$

Taking r_2, m really small, and r_1 really big, this can be made as big as you wish!

If tank A and tank B were connected, the difference with tank C would be smaller...

The largest the fluxes between A and B the closest their average end carbon would be to that of tank C

Something a little more realistic

$$\dot{C} = r \underbrace{\frac{F}{F + F_h} f^E C}_{\text{growth}} - \underbrace{bC}_{\text{respiration}} - \underbrace{\frac{aC^2}{C_h + C}}_{\text{crowding}}$$

$$\dot{F} = - \underbrace{\phi r \frac{F}{F + F_h} f^E C}_{\text{growth}} + \underbrace{\Lambda_f R}_{\text{remineralization}}$$

$$\dot{R} = \phi \underbrace{\frac{aC^2}{C_h + C}}_{\text{crowding}} - \underbrace{\Lambda_f R}_{\text{remineralization}}$$

R is detritus iron

$f^E = 1 - e^{-\frac{E_{par}}{E_0(t)}}$ light availability, $E_0(t)$ depends on season and ml depth.

Measured Michaelis-Menten iron-limited growth

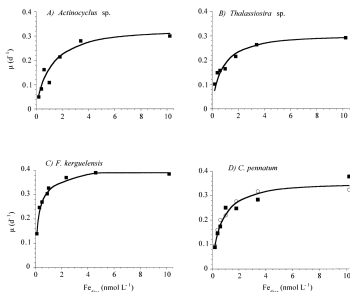


Fig. 1. Growth rates (d⁻¹) and nonlinear Monod fit (line) in cultures of (A) *Actinocyclus* sp., (B) *Thalassiosira* sp., (C) *F. kerguelensis*, and (D) *C. pennatum* in relation to Fe_{ext} concentrations (nmol L⁻¹). For cultures of *C. pennatum*, results of duplicate incubations are given with different symbols.

The parameters r , F_h of the growth term

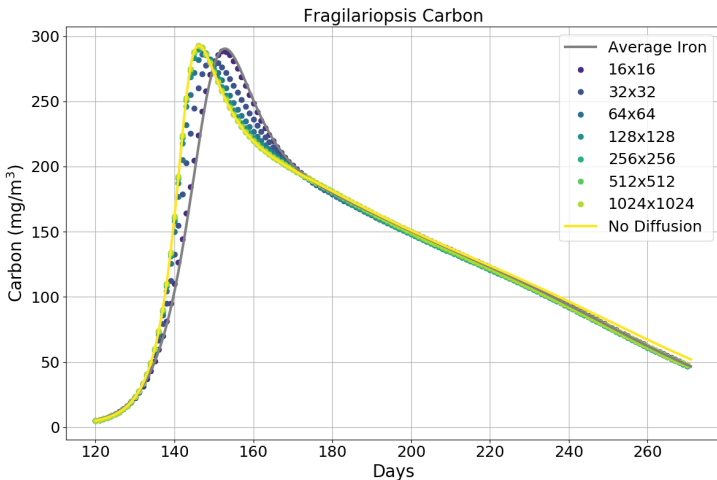
$$r \frac{F}{F + F_h}$$

are taken from laboratory measurements of different diatom genera.

From Timmermans et al., *Limnol. Oceanogr.* (2004)

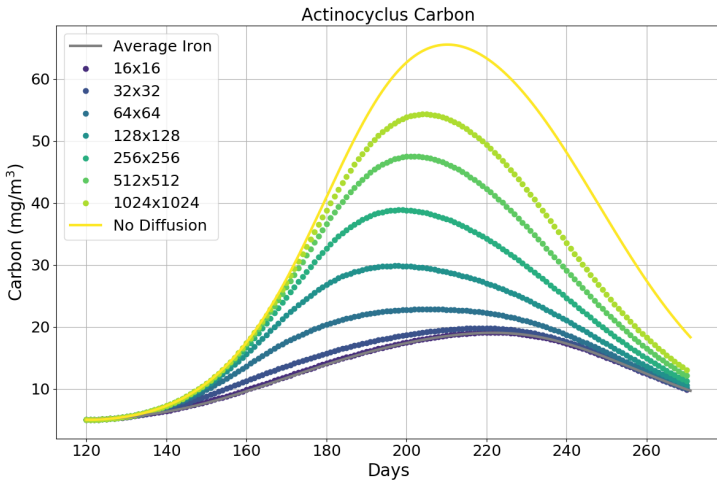
Fragilariopsis kerguelensis

Oops... not much of a difference! $F_h = 0.19 \mu\text{mol}/\text{m}^3$



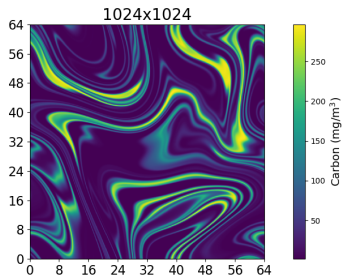
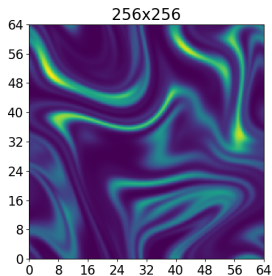
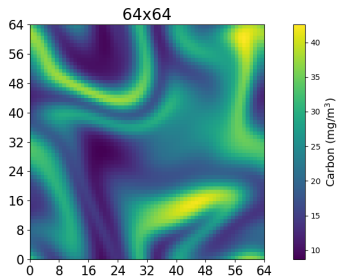
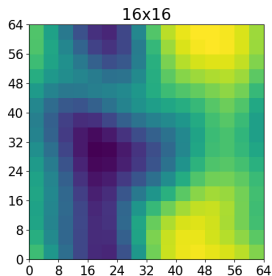
Actinocyclus sp.

Staggering! $F_h = 0.34 \mu\text{mol}/\text{m}^3$



Actinocyclus sp.

Look at the colorbar scale



Conclusions

For strongly limited critters, the productivity obtained with the average nutrient will be horribly different than the average productivity of a patchy nutrient distribution.

Lagrangians for Advection-Reaction-Diffusion Equations

$$\frac{\partial c_1}{\partial t} + \mathbf{u} \cdot \nabla c_1 = f_1(c_1, c_2, \dots, c_n) + D_1 \nabla^2 c_1$$

⋮

$$\frac{\partial c_n}{\partial t} + \underbrace{\mathbf{u} \cdot \nabla c_n}_{\text{advection}} = \underbrace{f_n(c_1, c_2, \dots, c_n)}_{\text{reaction}} + \underbrace{D_n \nabla^2 c_n}_{\text{diffusion}}$$

If there were only advection and reaction, a Lagrangian method would be very appropriate

A Lagrangian Method Is Perfect for Advection + Reaction

Method of characteristics! Uniformly sample the domain with particles having position $\{\mathbf{x}_i(t)\}$ and concentration $\{\mathbf{c}_i(t)\}$, $i = 1, \dots, N$.

$$\begin{cases} \dot{\mathbf{x}}_i &= \mathbf{u}(\mathbf{x}_i, t) \\ \dot{c}_{1;i} &= f_1(c_{1;i}, \dots, c_{n;i}) \\ &\vdots \\ \dot{c}_{n;i} &= f_n(c_{1;i}, \dots, c_{n;i}) \end{cases}$$

...how do I add diffusion?

Split-Step Approach: Characteristics + Diffusive Coupler

Evolve from t to $t + \Delta t$ the o.d.e.:

$$\dot{\mathbf{x}}_i = \mathbf{u}(\mathbf{x}(t), t)$$

$$\dot{\mathbf{c}}_i = \mathbf{f}(\mathbf{c}_i)$$

then express the concentration of the i – th particle as a function \mathcal{D} (the diffusive coupler) of the concentrations of all the other particles

$$\tilde{\mathbf{c}}_i = \mathcal{D}(\mathbf{c}_1, \dots, \mathbf{c}_N)$$

Repeat using $\{\tilde{\mathbf{c}}_i\}$ as initial conditions for integrating the o.d.e.s from $t + \Delta t$ to $t + 2\Delta t$, etc.

What Do I Wish From My Diffusive Coupler?

- ▶ Conservation of mass.
- ▶ Respect the maximum principle (or at least positivity).
- ▶ Destroy variance at a tunable rate.

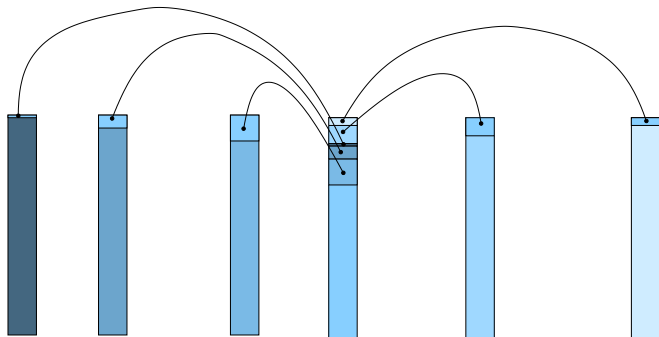
Please note: Accuracy is NOT in the list. The Laplacian is a (bad) parameterization, anyway.

A particle coupler

An attempt to discretize derivatives on an unstructured and time-changing mesh:

$$c_i(t + \Delta t) = c_i(t) - \sum_j q_{ji} c_i(t) + \sum_j q_{ij} c_j(t)$$

Properties satisfied if $q_{ij} = q_{ji} \geq 0$ and $0 < \sum_j q_{ij} < 1$.



A recipe for q_{ij}

$d = 1, 2, 3$ is the dimensionality of the space

$$q_{ij} = \begin{cases} \frac{p}{(4\pi D\Delta t)^{\frac{d}{2}}} \exp\left(-\frac{d^2(\mathbf{x}_i, \mathbf{x}_j)}{4D\Delta t}\right), & d(\mathbf{x}_i, \mathbf{x}_j) < m\sqrt{2D\Delta t} \\ 0, & d(\mathbf{x}_i, \mathbf{x}_j) \geq m\sqrt{2D\Delta t} \end{cases}$$

p , D are free parameters that determine the diffusivity of the method.

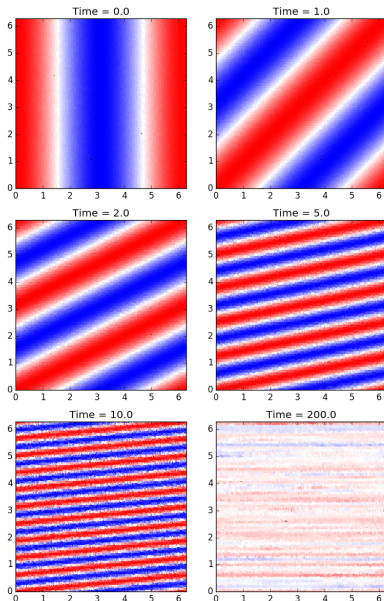
First test: dissipation of scalar variance in Rhines-Young flow

$$\frac{\partial c}{\partial t} + y \frac{\partial c}{\partial x} = D \nabla^2 c$$

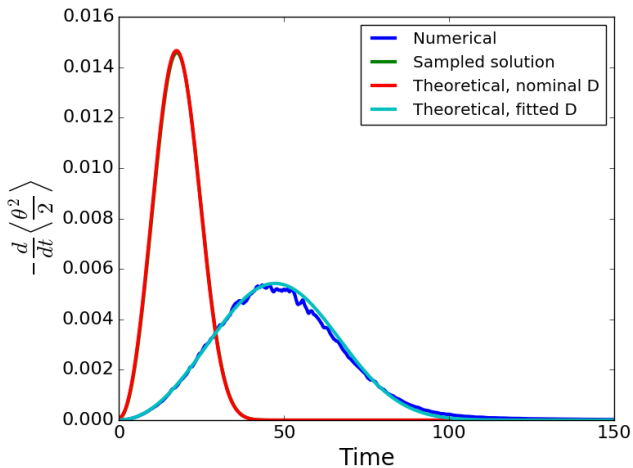
Initial condition

$$c(x, y, 0) = \cos(x)$$

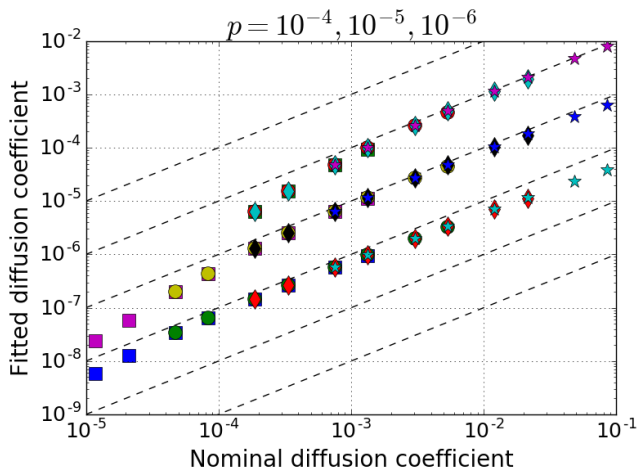
Has a simple analytical solution!



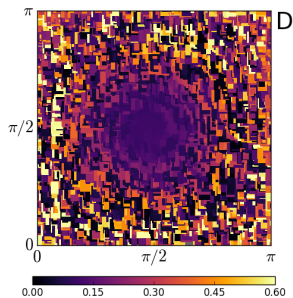
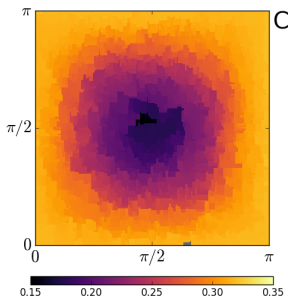
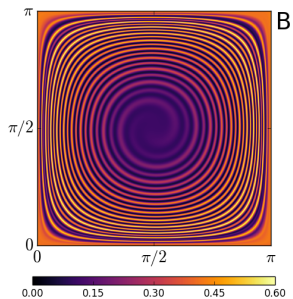
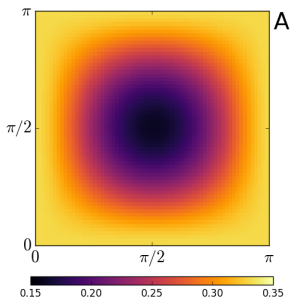
First test: dissipation of scalar variance in Rhines-Young flow



The Fitted Diffusion Coefficient



Back to Chemistry: 4096^2 pseudo-spectral vs 128^2 particles



Back to Chemistry: 4096^2 pseudo-spectral vs 128^2 particles

The dots are Lagrangian simulations with parameters tuned to match the diffusivity of the corresponding Eulerian simulation, but always using 128^2 particles.

