Bridging the Scale Hierarchy Problem in Biogeochemical Models

Francesco Paparella
Division of Sciences, New York University Abu Dhabi, UAE
`francesco.paparella@nyu.edu`

جامعة نيويورك أبوظبي
NYU | ABU DHABI

The problem

Models of ocean biogeochemistry are expressed as advection–diffusion–reaction equations.

$$\frac{\partial c_1}{\partial t} + \boldsymbol{u} \cdot \nabla c_1 = D_1 \nabla^2 c_1 + f_1(c_1, \ldots, c_n)$$
$$\vdots$$
$$\frac{\partial c_n}{\partial t} + \boldsymbol{u} \cdot \nabla c_n = D_n \nabla^2 c_n + f_n(c_1, \ldots, c_n)$$

Where $c_1, \ldots, c_n$ are scalar fields representing plankton species, nutrients, etc.; $\boldsymbol{u}$ is the velocity field of the ocean (assumed known); $f_1, \ldots, f_n$ specify the reaction kinetics.

The Péclet numbers

$$Pe_l = \frac{UL}{D_l} \gg 1; \qquad l = 1, \ldots, n$$

are enormous even when the diffusion coefficients $D_1, \ldots, D_n$ are intended as "eddy diffusivities". Therefore **the scalar fields have structure at scales so small that they cannot possibly be resolved** with today's supercomputers (nor tomorrow's...).

Eulerian numerical schemes use spurious fluxes to cope with the problem, and **the concentrations at a node represent averages over the mesh.** Ok without reactions, bad with them:

$$\overline{f_l(\mathbf{c})} \neq f_l(\overline{\mathbf{c}})$$

The average reaction is not the reaction of the averages!

Lagrangians to the rescue?

With no diffusion use the "method of characteristics":

1. Advect uniformly seeded Lagrangian particles;

2. Solve the reaction ODEs on each particle.

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

The concentrations carried by each particle are a pointwise rather than locally averaged representation of the scalar fields. This is still underresolved, but the chemistry is unaffected.

But some diffusion is crucial, especially in the presence of barriers to transport (e.g. steady vortex full of nutrients and no plankton, surrounded by plankton–rich, nutrient–poor waters).

Diffusively coupling the Lagrangians

With the method of characteristics each particle is independent of the others. To represent diffusion one needs to couple nearby particles. An acceptable coupling should have these properties:

- **Conserve mass;**
- **Respect the maximum principle;**
- **Be free of numerical fluxes, thus recover the method of characteristics in the limit $D_l \to 0$.**

Split–step approach: alternate advection–reaction and diffusion over time intervals of length τ. The solution of the diffusion equation is a convolution with a kernel. This suggests to couple the particles as in the following scheme:

$$\begin{cases} \dot{\boldsymbol{x}}_i &= \boldsymbol{u}(\boldsymbol{x}_i(t), t) \\ \dot{c}_{l;i} &= f_l(c_{1;i}, \ldots, c_{n;i}) \\ c_{l;i}(t+\tau) = c_{l;i}(t) - \sum_j q_{j;i} c_{l;i}(t) + \sum_j q_{l;ij} c_{l;j}(t) \end{cases}$$

evolve from t to $t+\tau$

exchange mass
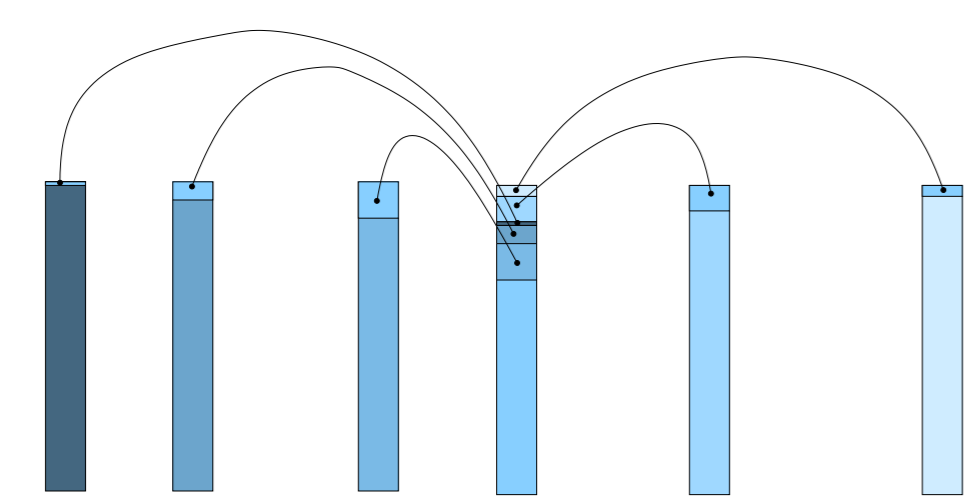
Properties satisfied if:
$$q_{ij} = q_{ji} \geq 0; \qquad 0 \leq \sum_j q_{ij} < 1$$

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

p, D are free parameters that determine the diffusivity of the method; m is a cut-off parameter; $d = 1, 2, 3$ is the dimensionality of the space.
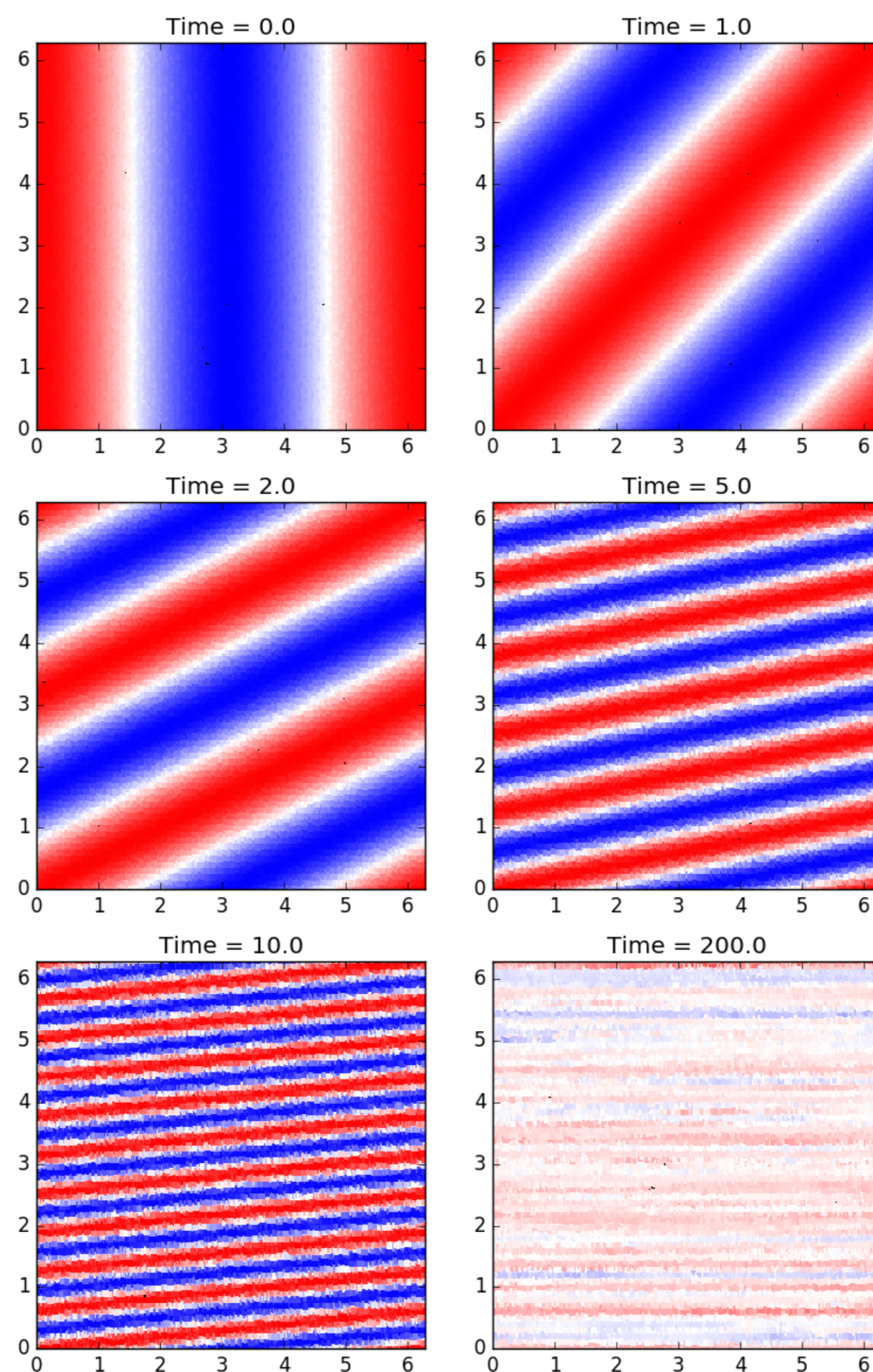
Test case: the Rhines & Young flow

Advection by a constant shear and diffusion, in an unbounded domain.

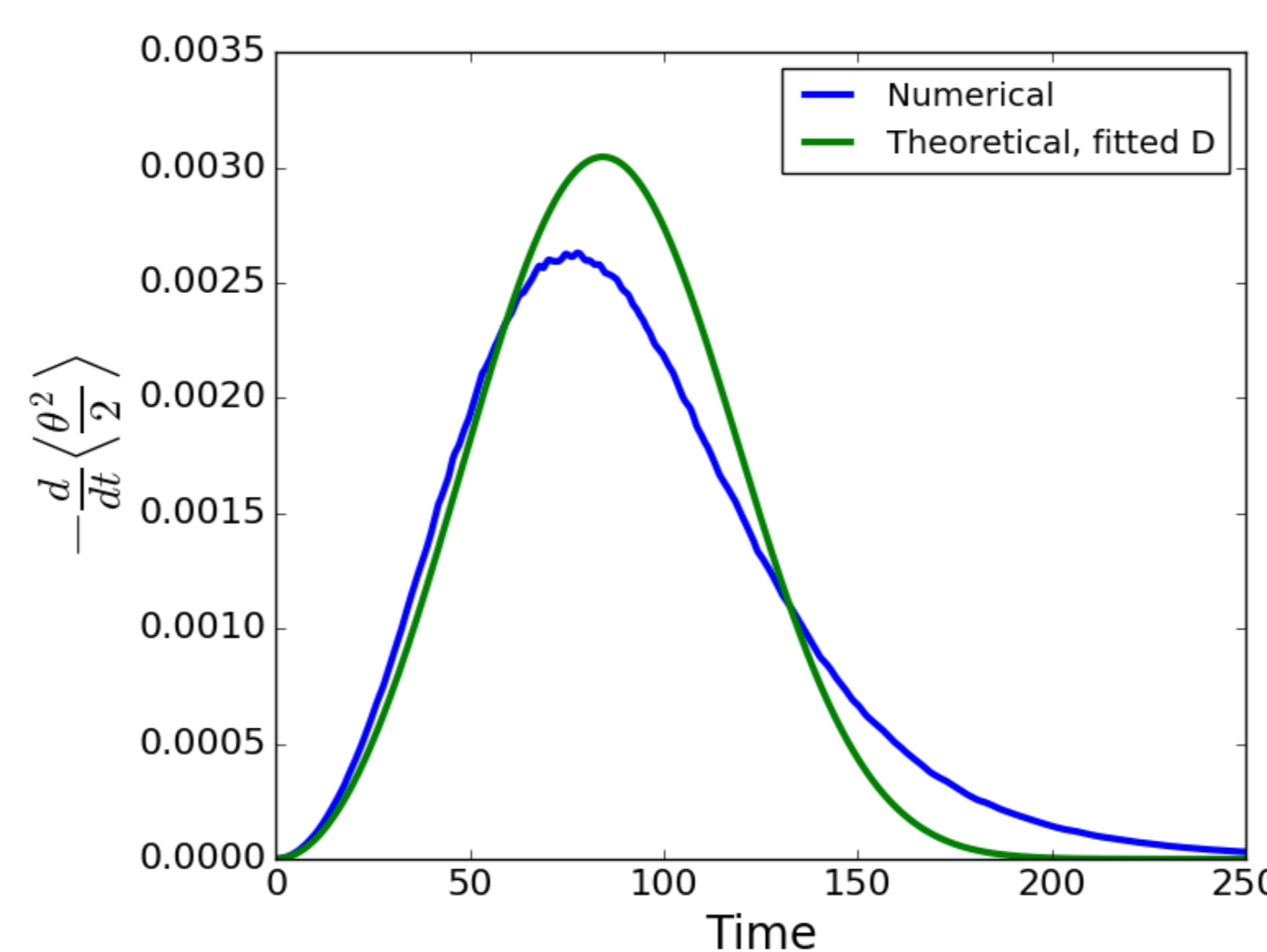$$\frac{\partial c}{\partial t} + y \frac{\partial c}{\partial x} = D\nabla^2 c$$

with initial condition

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

Rhines & Young flow with an effective (fitted) diffusion coefficient $D \approx 10^{-6}$; 40000 particles.

The rate of dissipation of scalar variance can be computed analytically, and compared with the numerical results.

Rate of dissipation variance (Lagrangian code: blue, analytical formula: green). The fitted diffusion coefficient is $D \approx 10^{-6}$; 40000 particles.

Albeit the matching is imperfect, it is remarkable that the qualitative behavior is roughly correct, even at diffusivities this low.
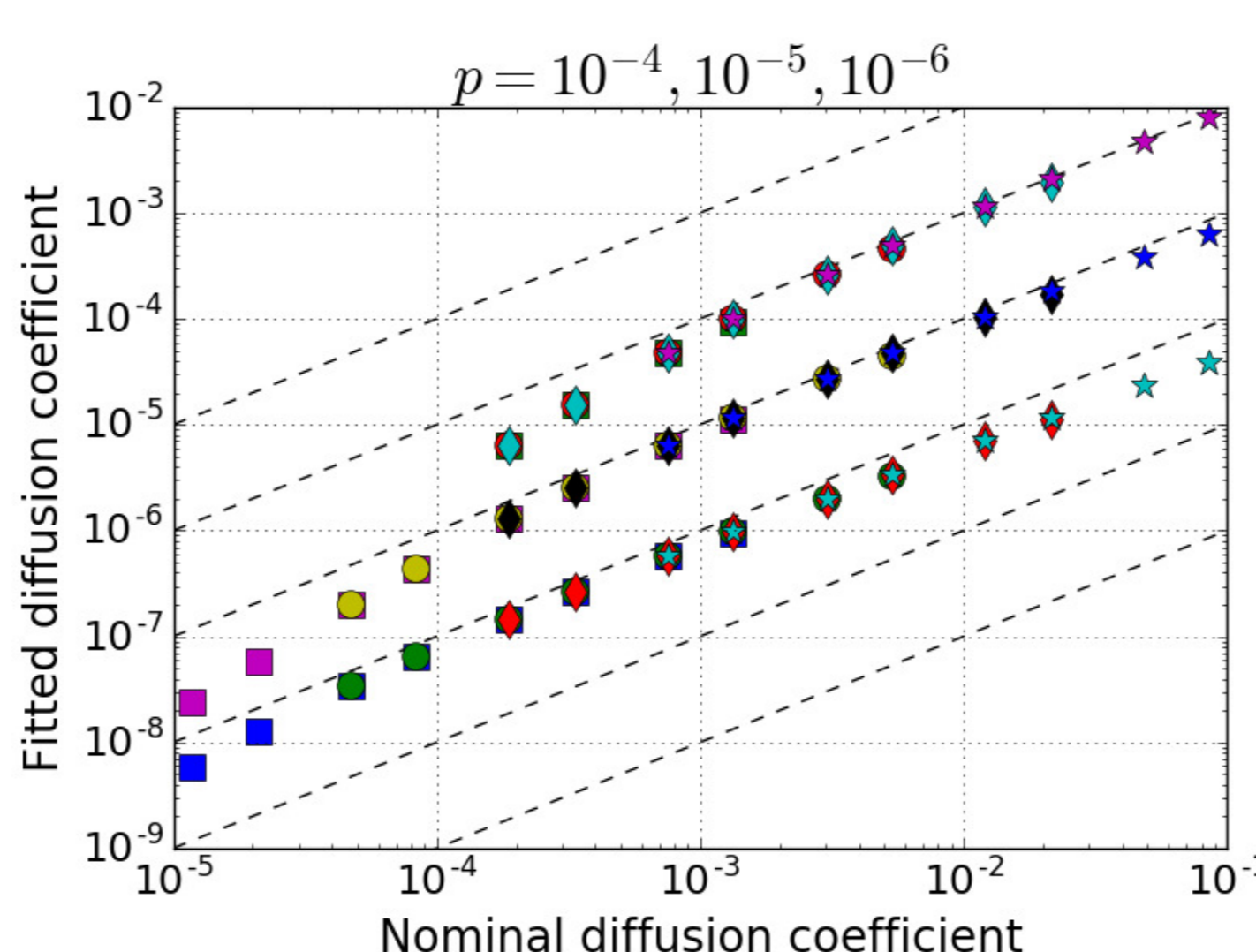
Fitted diffusion as a function of the parameters p and D ("nominal" diffusivity) for the Rhines & Young flow and 40000 particles. The different symbols correspond to different values of the cutoff m.
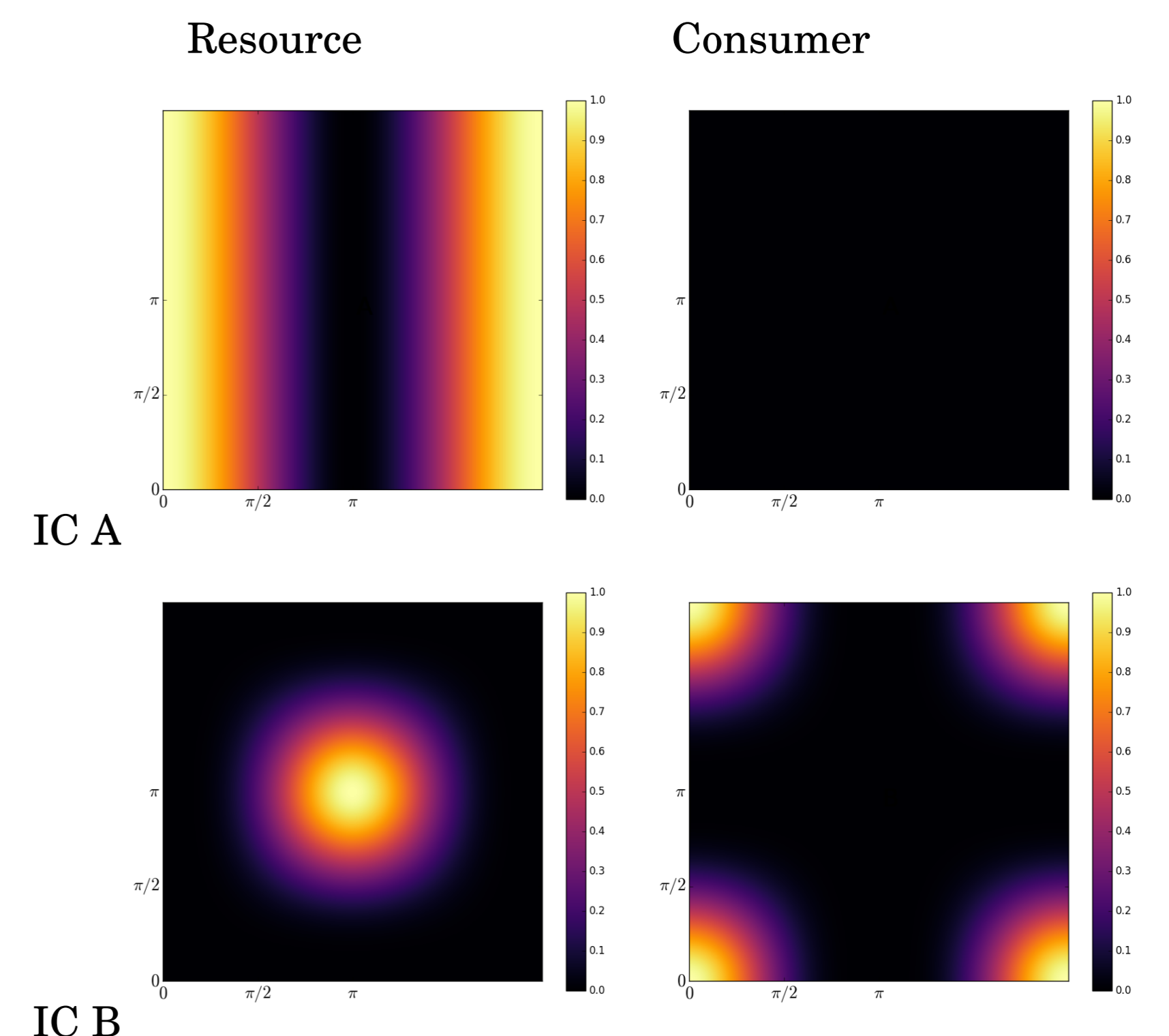
Test case: Mock Geochemistry

Next I consider the following toy model. Here c_1 behaves like a resource and c_2 like a consumer. The advecting field is a checkerboard of steady vortices.

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

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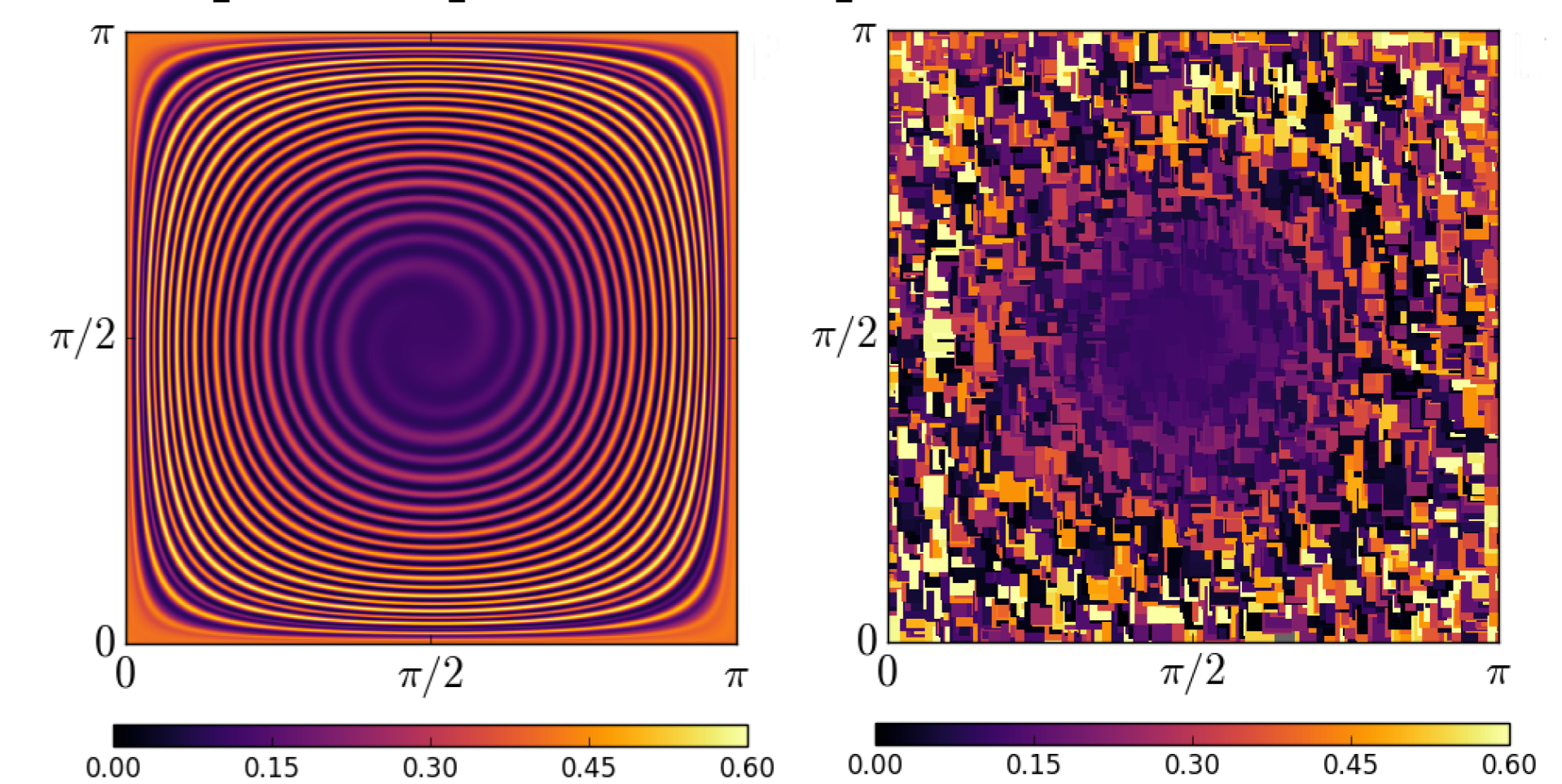
$$\frac{\partial c_2}{\partial t} + \boldsymbol{u} \cdot \nabla c_2 = +\frac{1}{5} c_1 c_2 + D\nabla^2 c_2$$

Two distinct initial conditions:

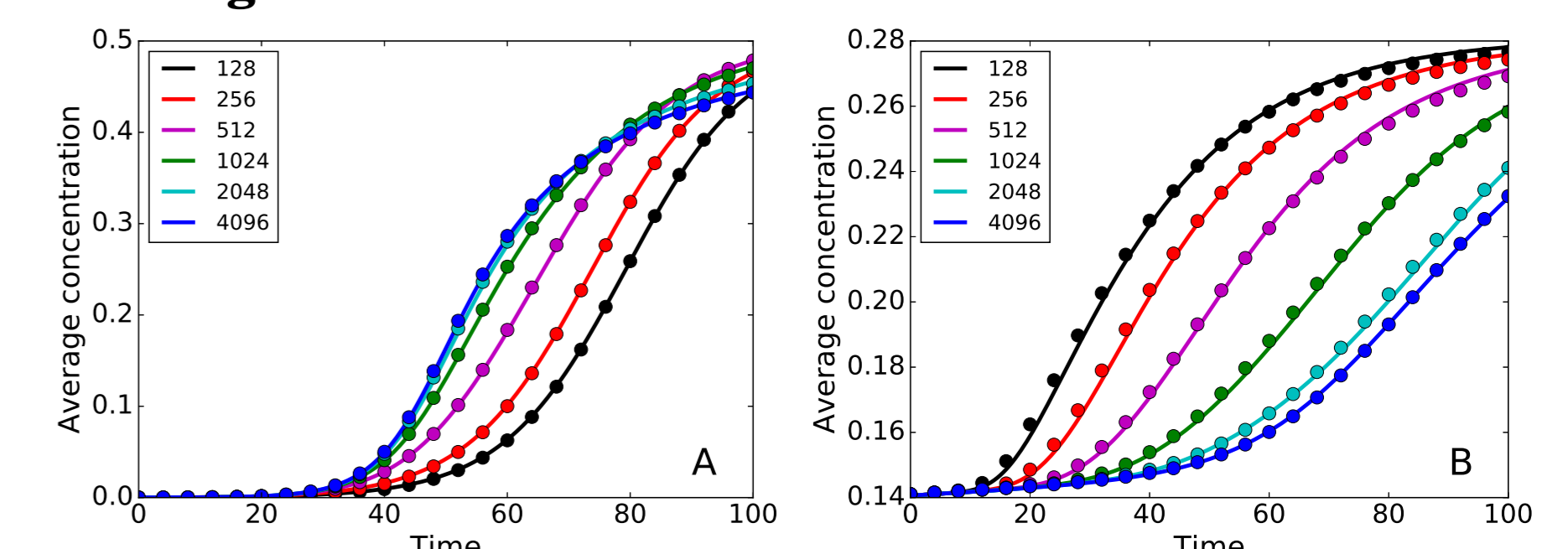Resource   Consumer

IC A

IC B

These equations with distinct initial conditions give different productivities of the consumer. Thus looking for effective reaction rates is not the solution.

4096^2 pseudo–spectral vs 128^2 particles:

Average consumer concentration as a function of time:

Solid lines: pseudo–spectral simulations with $(128 \cdot 2^k)^2$ grid points, $k = 0, \cdots, 5$ and diffusivity $D = 10^{-3} \cdot 2^{-2k}$. Dots: Lagrangian simulations with diffusivities matching that of the Eulerian one, but 128^2 particles.

Even tough the fine structures are not resolved by the Lagrangian simulations, the time evolution of the mean quantities is correct!

Perspectives

A numerical scheme that solves advection–reaction–diffusion equations by diffusively coupling Lagrangian particles may be superior to grid–based schemes when the diffusion term is much smaller than the other two.

The scheme has very nice properties (mass conservation, monotonicity, zero diffusion limit). The Laplacian operator is not accurately reproduced but that's irrelevant for biogeochemical applications: the Laplacian is a parameterization anyway.

The algorithm is fast: for uniformly random particle distributions, finding the nearest neighbors of N particles is an $O(N)$ task (grid the domain, and use countsort, and you'll do better than $O(N \log N)$. It's also parallel–friendly).