A fast algorithm for neutrally-buoyant Lagrangian particles in numerical ocean modeling

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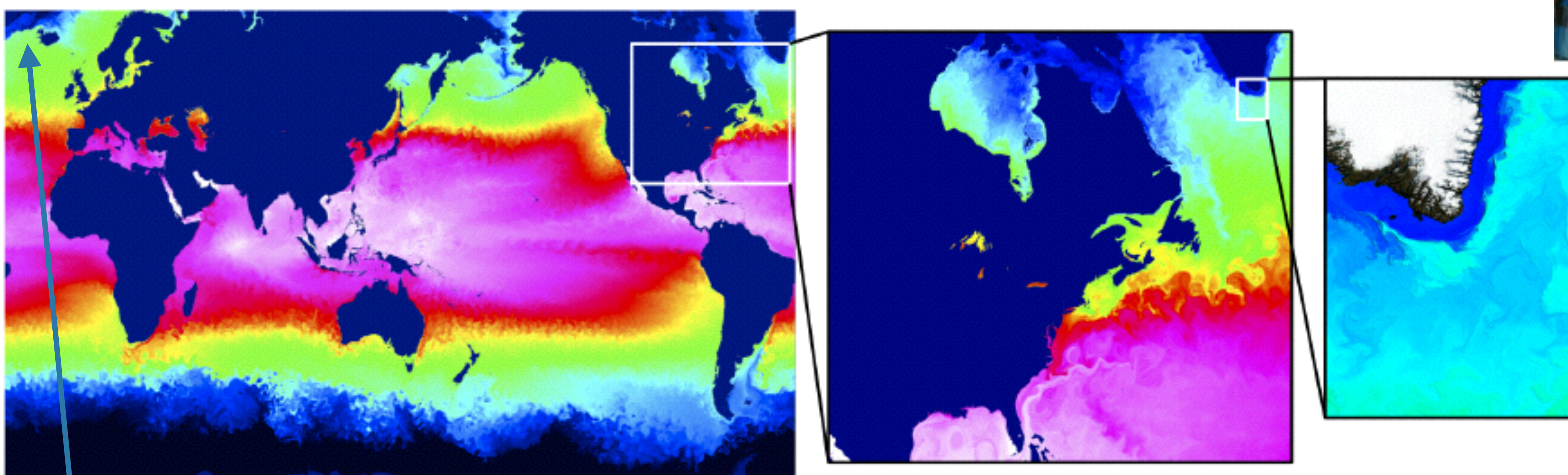
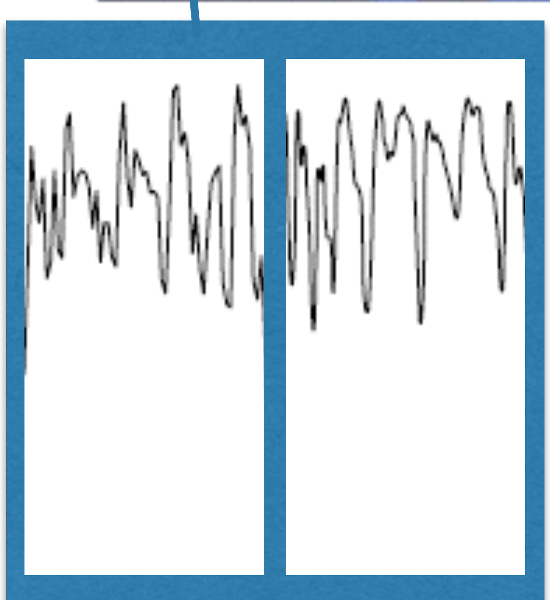
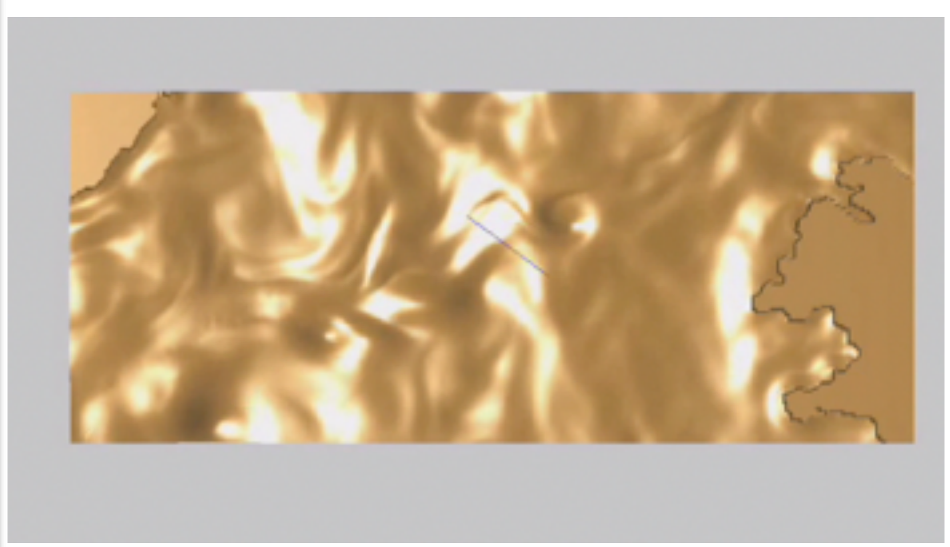
eScience, Baltimore, 26 October 2016

Ultra-high-res. ocean models are now highly realistic, revealing,





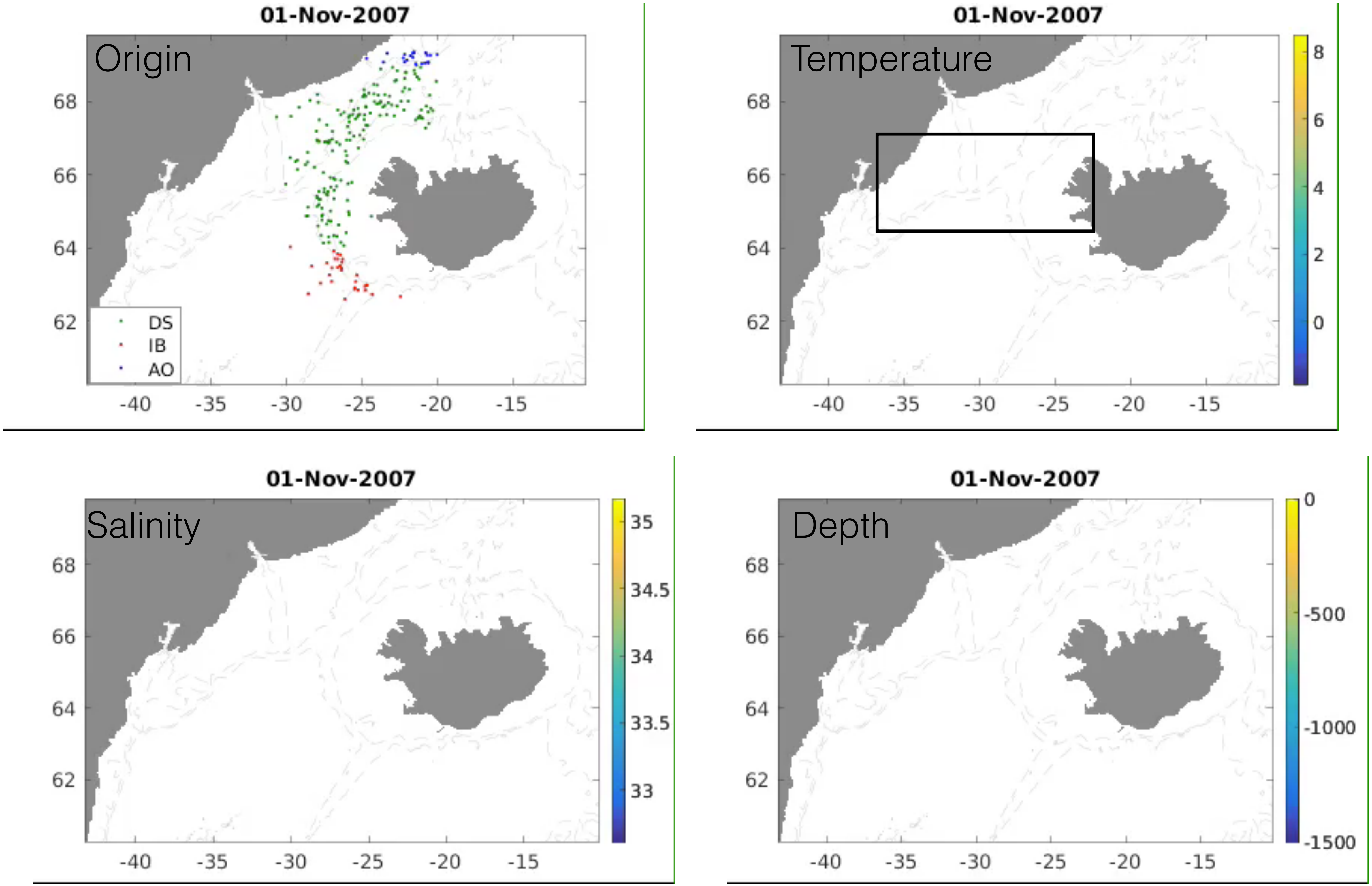


About 10^{10-11} numbers per snapshot
10^{3-6} snapshots stored per run
$= 10^{13-17}$ nos. per run

Source: Chris Hill, MIT, http://mitgcm.org, Haine, 2010.

and need good tools for post processing

Gelderloos et al., 2016b



Lagrangian particle models

$$\begin{aligned} \frac{d\mathbf{x}_i(t)}{dt} &= \mathbf{u}(\mathbf{x}_i, t) \\ T_i(t) &= T(\mathbf{x}_i, t) \end{aligned}$$

Two types of offline Lagrangian particle-tracking models available:

1. **Analytical models**: Very fast, but assume stationarity between model samples —> inaccurate

2. **Numerical model**: CMS most widely used example, needs Unix and unphysical solid boundary conditions

Our code is numerical with correct boundary-sliding conditions, but very slow —> needs speeding up

Old implementation

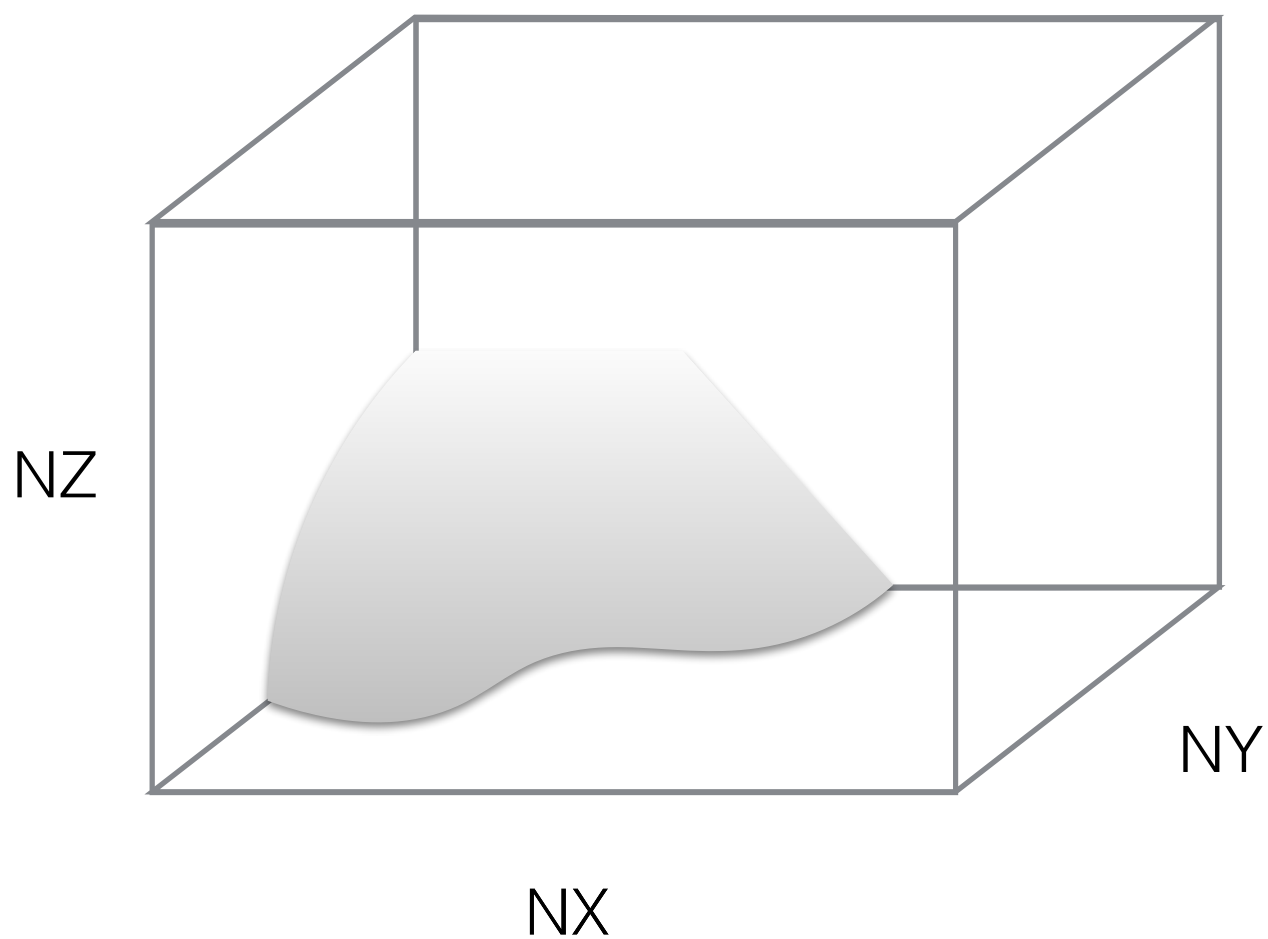
Koszalka et al., 2013

Old implementation

Four stages:

1. **Initialization**: model domain, grid, bathymetry and initial particle positions

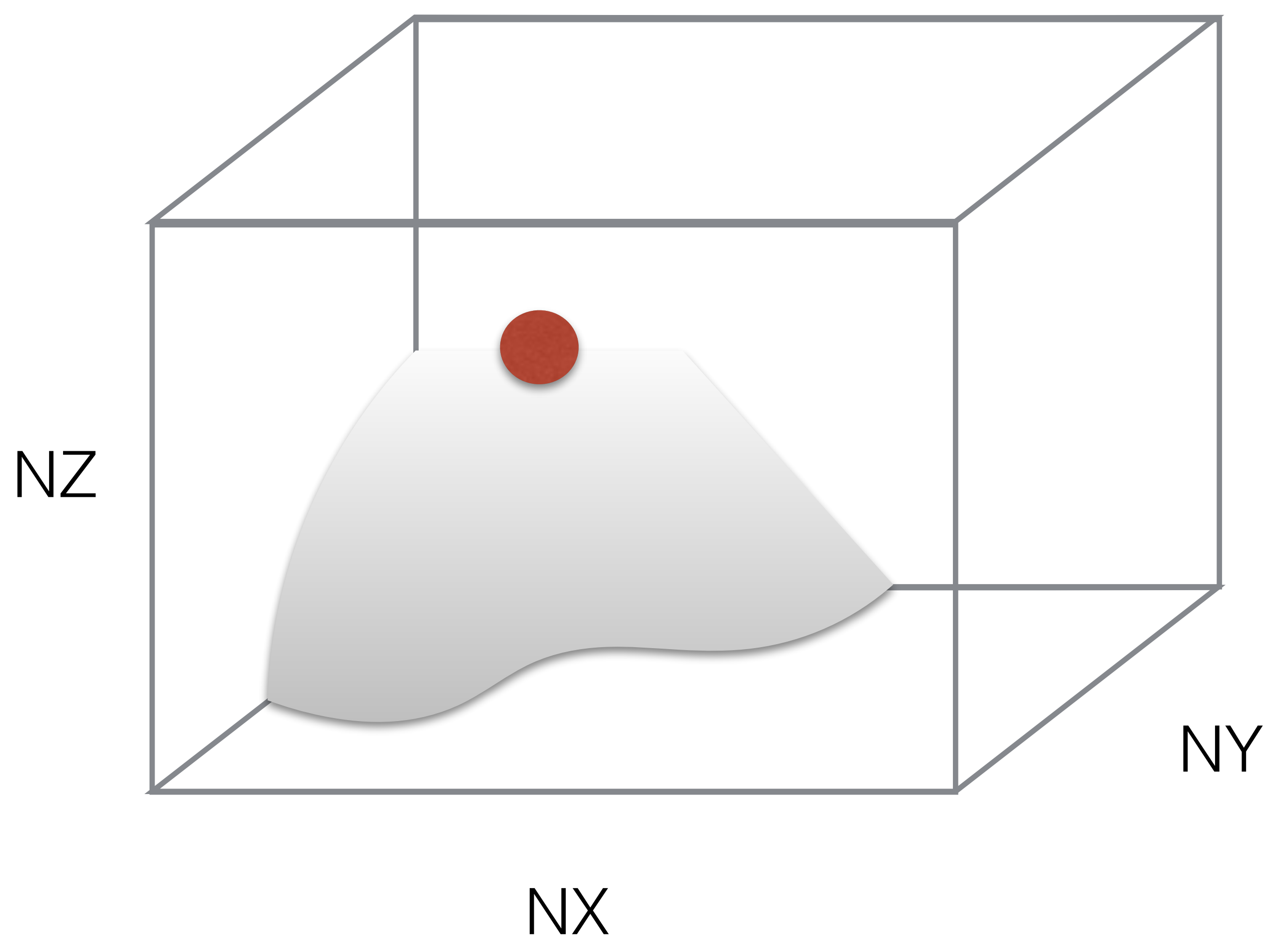
Old implementation: Step 1



Load grid and bathymetry info

$$H(\mathbf{x})$$

Old implementation: Step 1



Load grid and bathymetry info

Seed particles in the domain

$$\mathbf{x}_i(t=0)$$

Old implementation

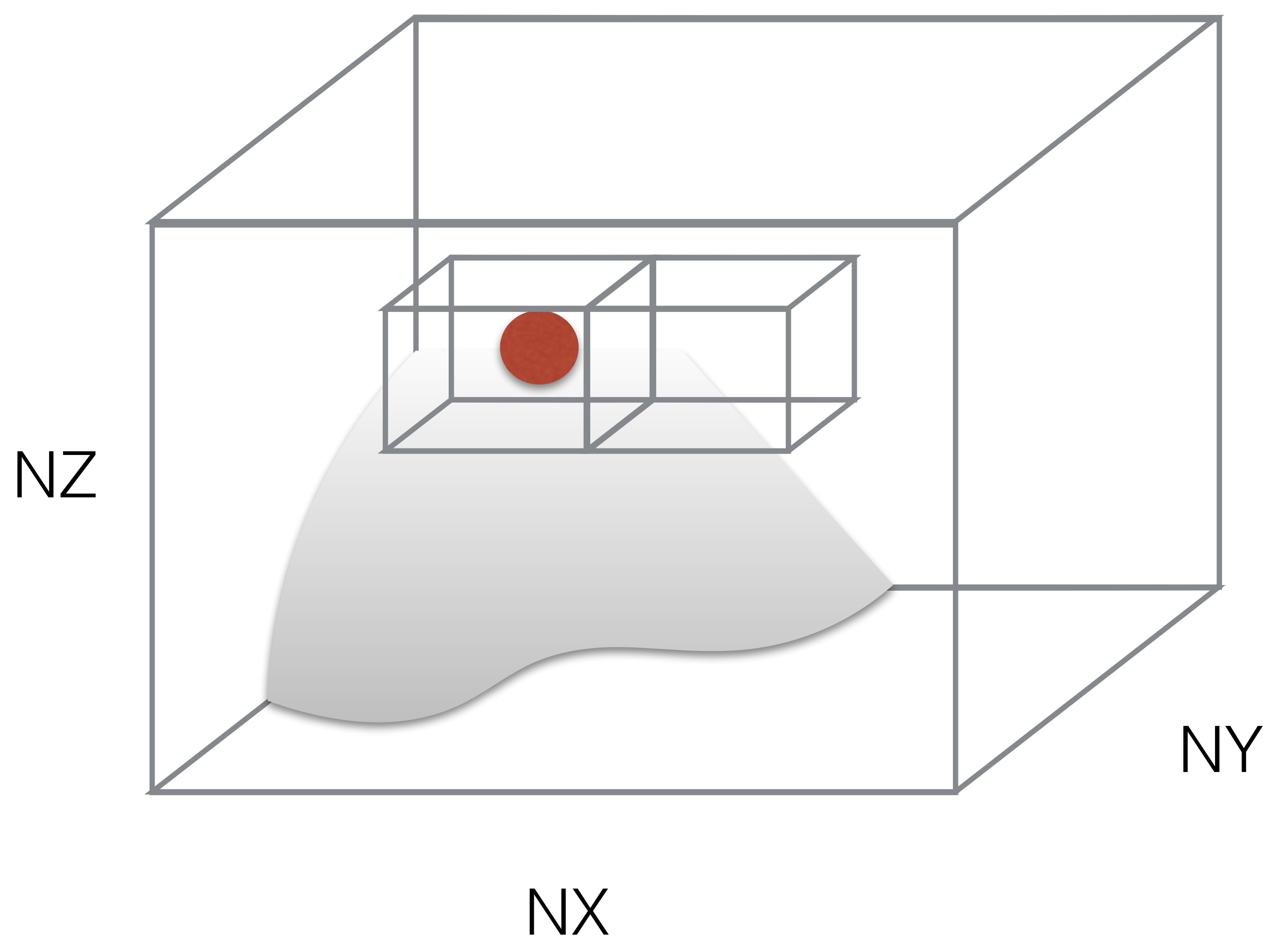
Four stages:

1. **Initialization**: model domain, grid, bathymetry and initial particle positions

2. Calculate **particle trajectories**: for predetermined length of time, trajectory is calculated based on ocean model velocity fields

$$\frac{d\mathbf{x}_i(t)}{dt} = \mathbf{u}(\mathbf{x}_i, t)$$

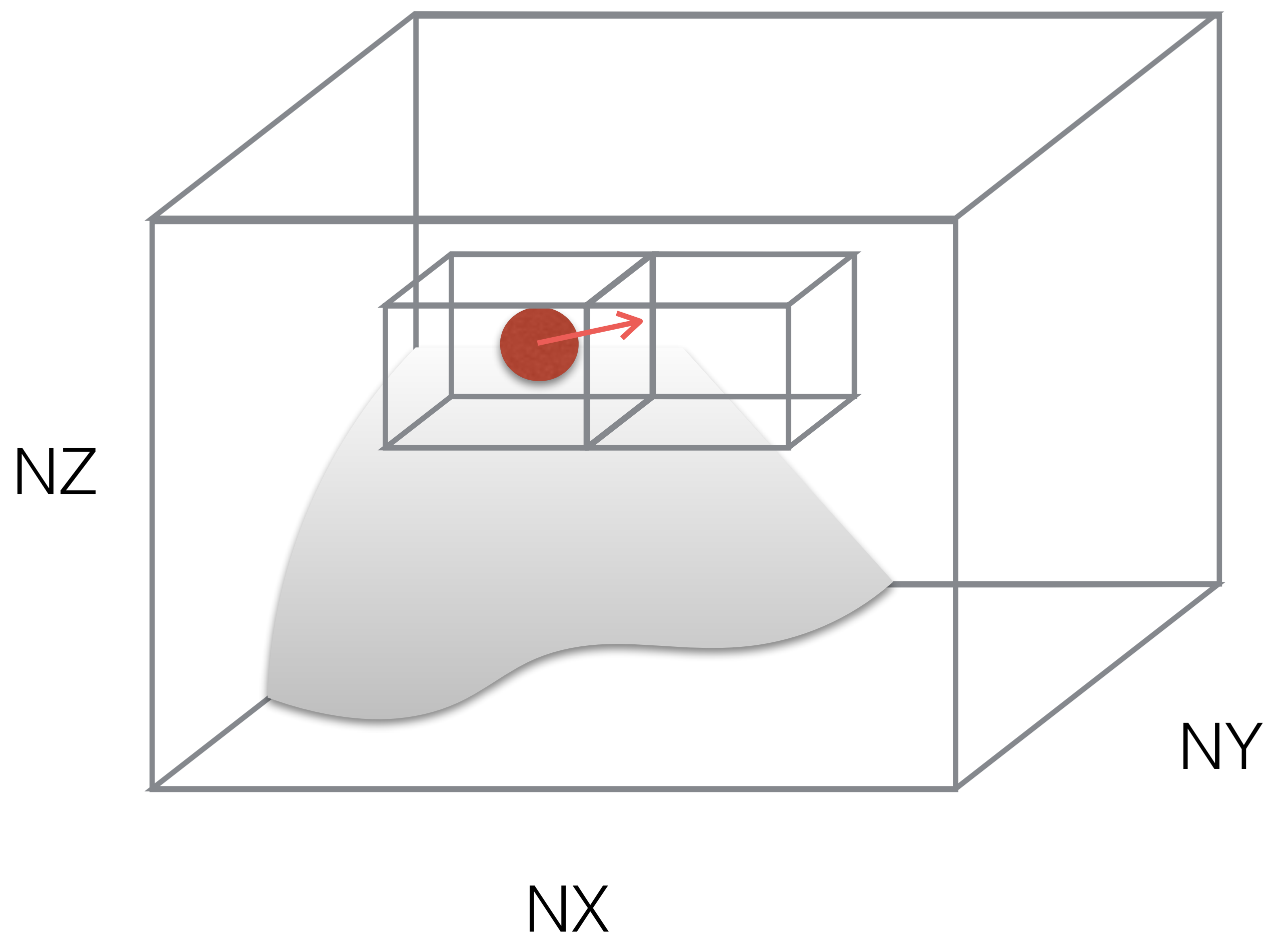
Old implementation: Step 2



Load 2 sequential 3D velocity fields

Create a local environment around the particle (necessary for old `interpn` function)

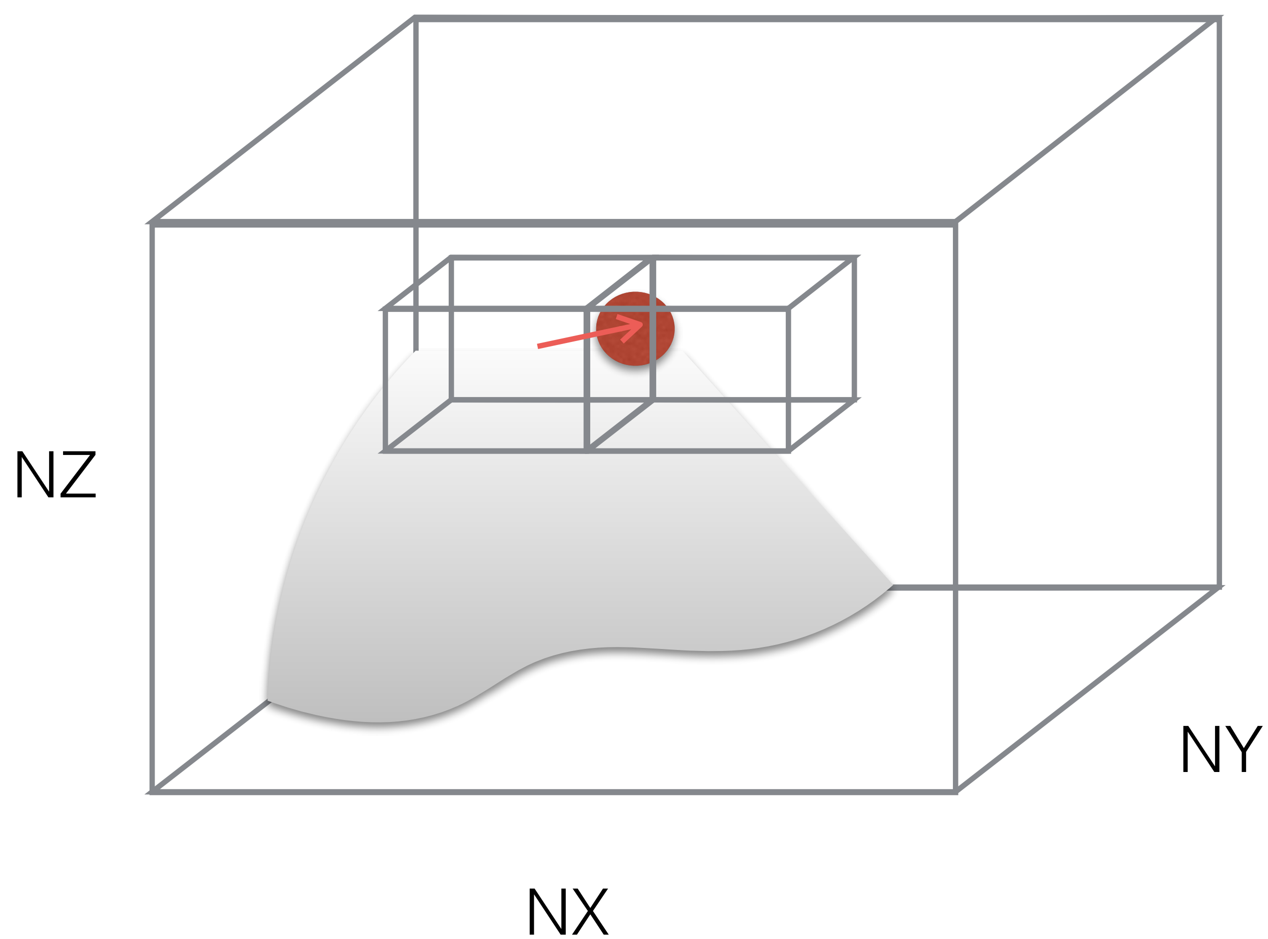
Old implementation: Step 2



Calculate next piece of the trajectory

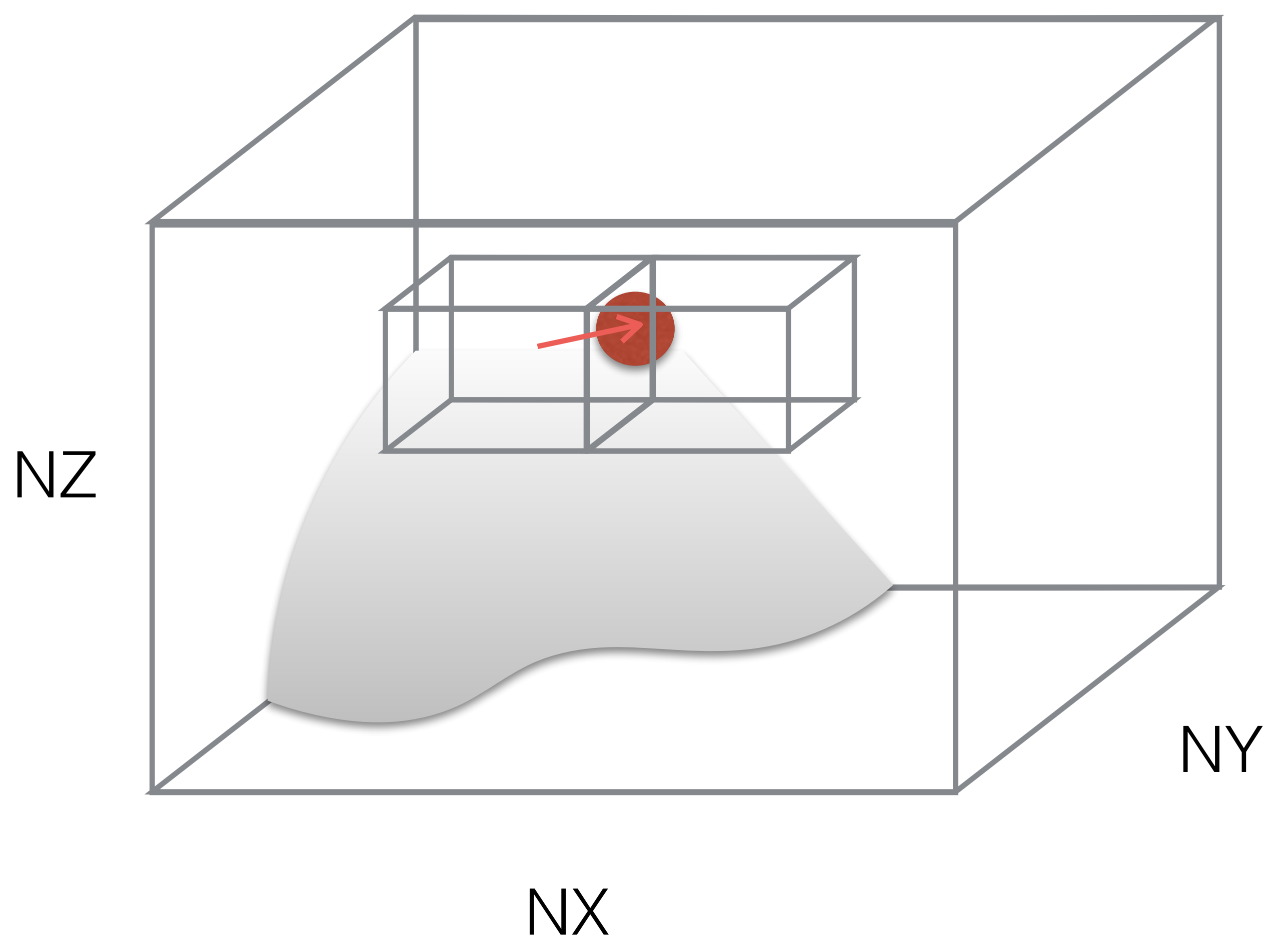
Explicit Runge-Kutta (2,3)-pair ODE solver for moderately stiff problems

Old implementation: Step 2



Step forward

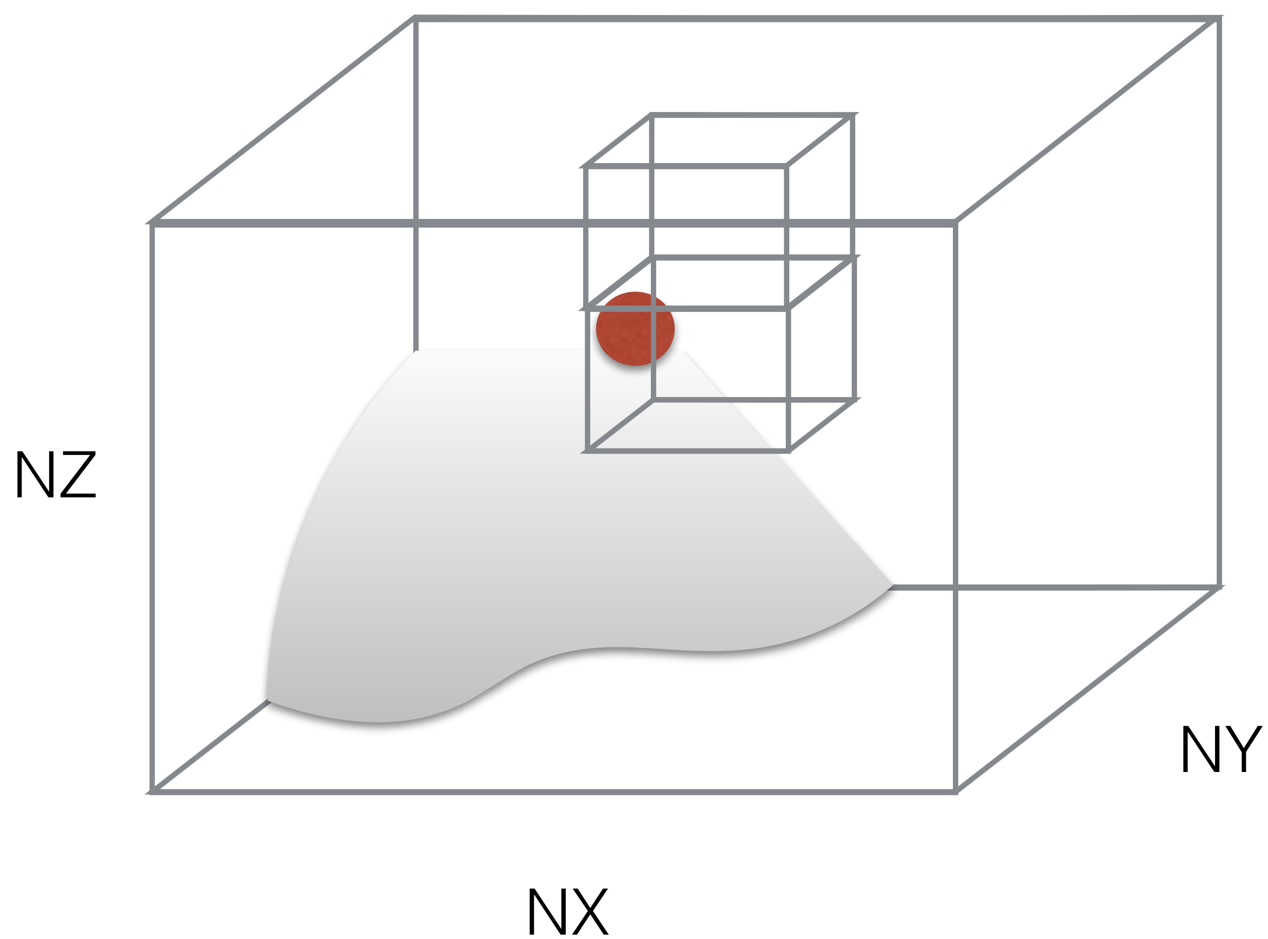
Old implementation: Step 2



Interrupt if:

1) particle moves to another cell
2) particle hits the bathymetry

Old implementation: Step 2

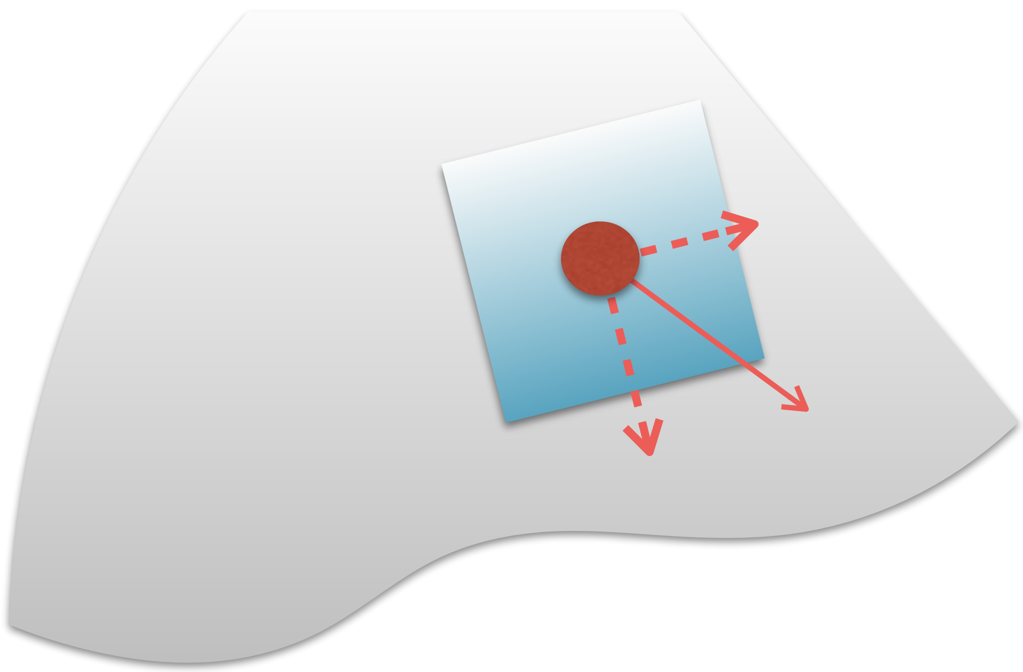


Interrupt if:

1) particle moves to another cell

Get new local neighborhood

Old implementation: Step 2



Interrupt if:
2) particle hits the bathymetry

Switch to along-bathymetry sliding mode

Old implementation: Step 2

Sequential implementation because:

- Required to handle small neighborhoods (because `interpn` used to be very sensitive to cutout size)

- Timings of interrupts are unknown *a priori*

Old implementation

Four stages:

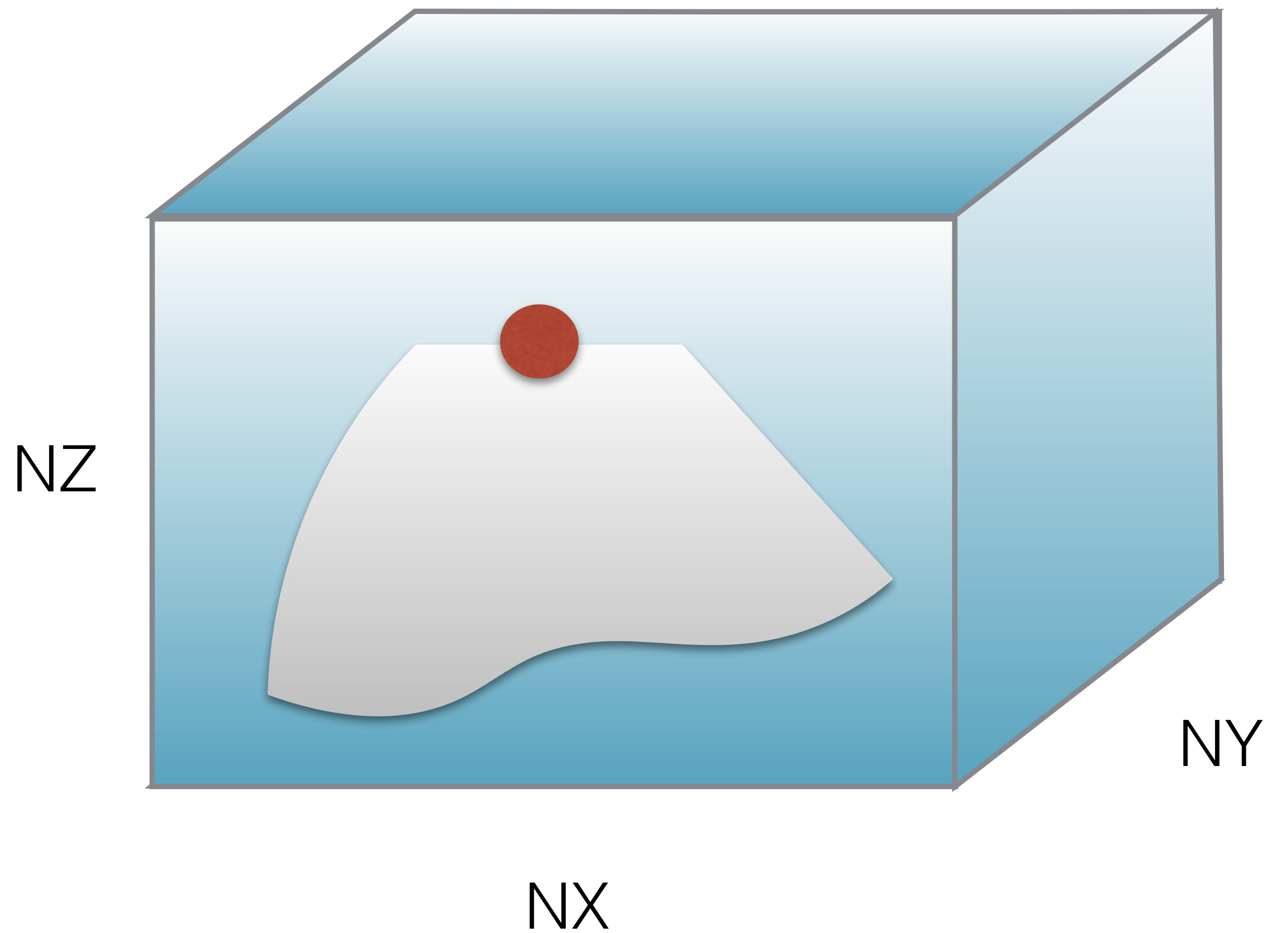
1. **Initialization**: model domain, grid, bathymetry and initial particle positions

2. Calculate **particle trajectories**: for predetermined length of time, trajectory is calculated based on ocean model velocity fields

3. Particle **property extraction**: Temperature/salinity along trajectory are found by interpolation of model T/S fields

$$T_i(t) \quad = \quad T(\mathbf{x}_i, t)$$

Old implementation: Step 3



Load sequential property fields and interpolate

Old implementation

Four stages:

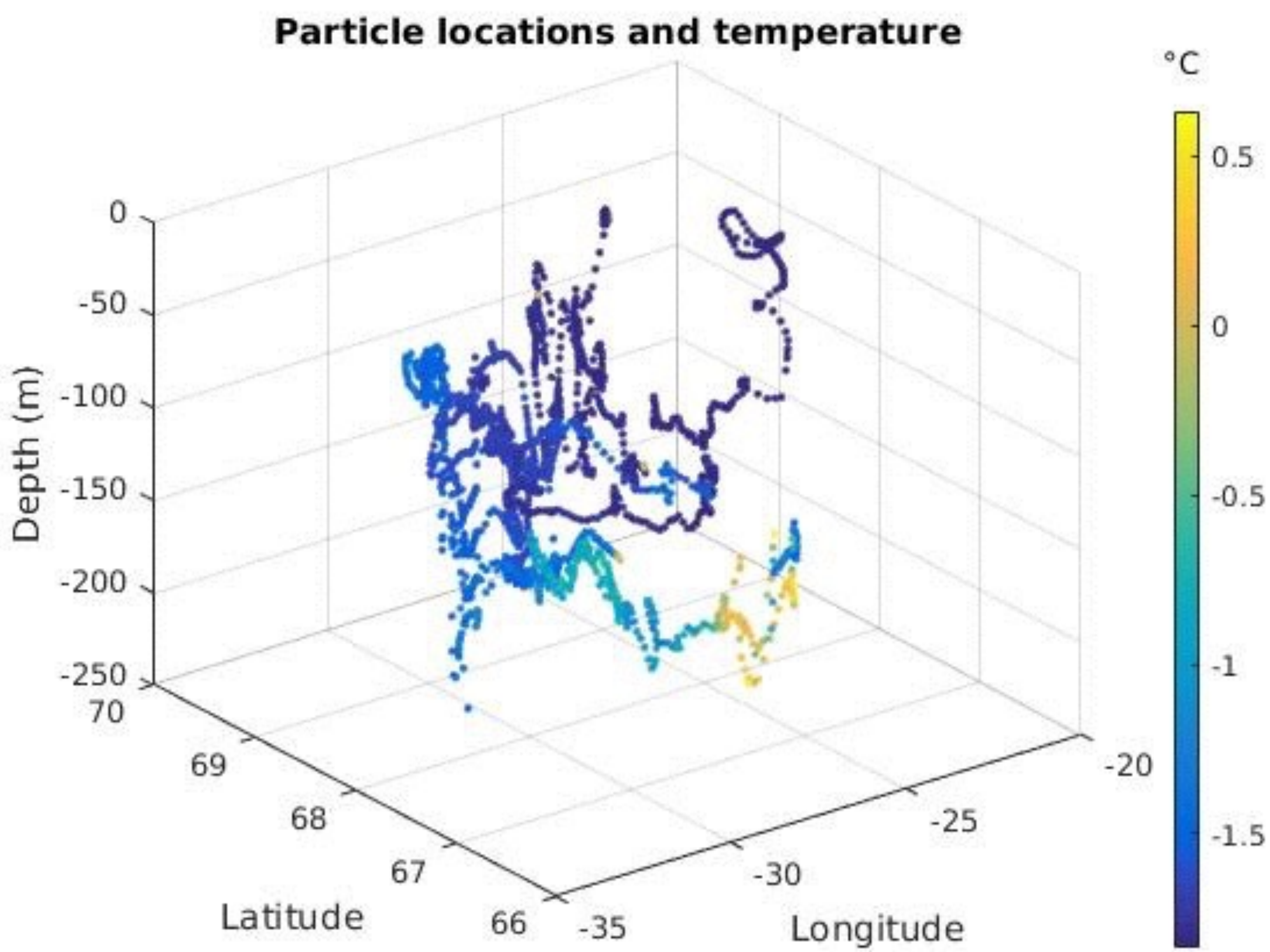
1. **Initialization**: model domain, grid, bathymetry and initial particle positions

2. Calculate **particle trajectories**: for predetermined length of time, trajectory is calculated based on ocean model velocity fields

3. Particle **property extraction**: Temperature/salinity along trajectory are found by interpolation of model T/S fields

4. Particles positions and T/S info **saved** for further analysis

Old implementation: Step 4



Save time series of particle locations and properties

Old implementation

Four stages:

1. **Initialization**: model domain, grid, bathymetry and initial particle positions

2. Calculate **particle trajectories**: for predetermined length of time, trajectory is calculated based on ocean model velocity fields

3. Particle **property extraction**: Temperature/salinity along trajectory are found by interpolation of model T/S fields

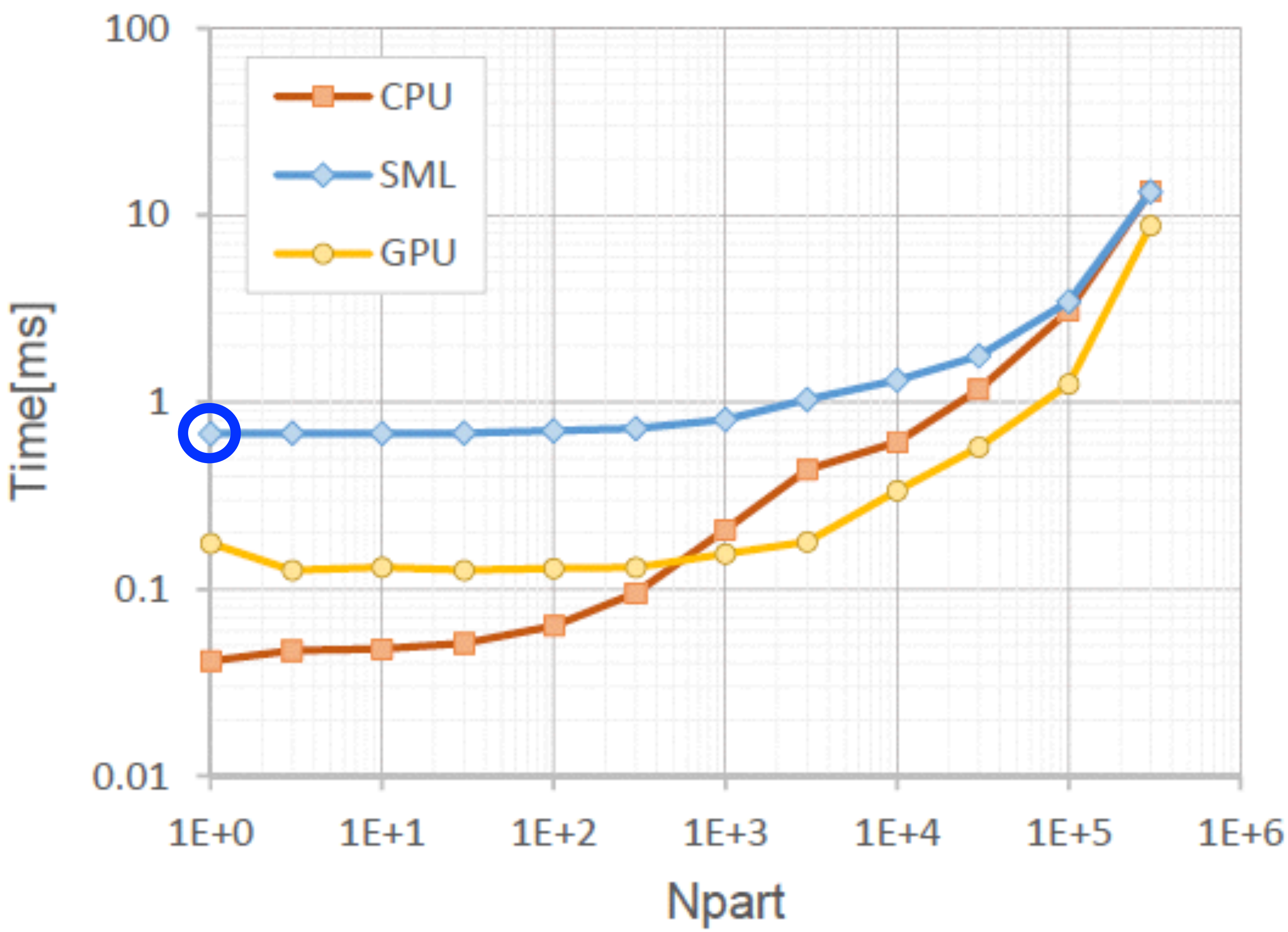
4. Particles positions and T/S info **saved** for further analysis

<u>Large potential gain by vectorization & parallelization of steps 2 and 3</u>

New implementation

Gelderloos et al., 2016a

Interpolation improvements (I)

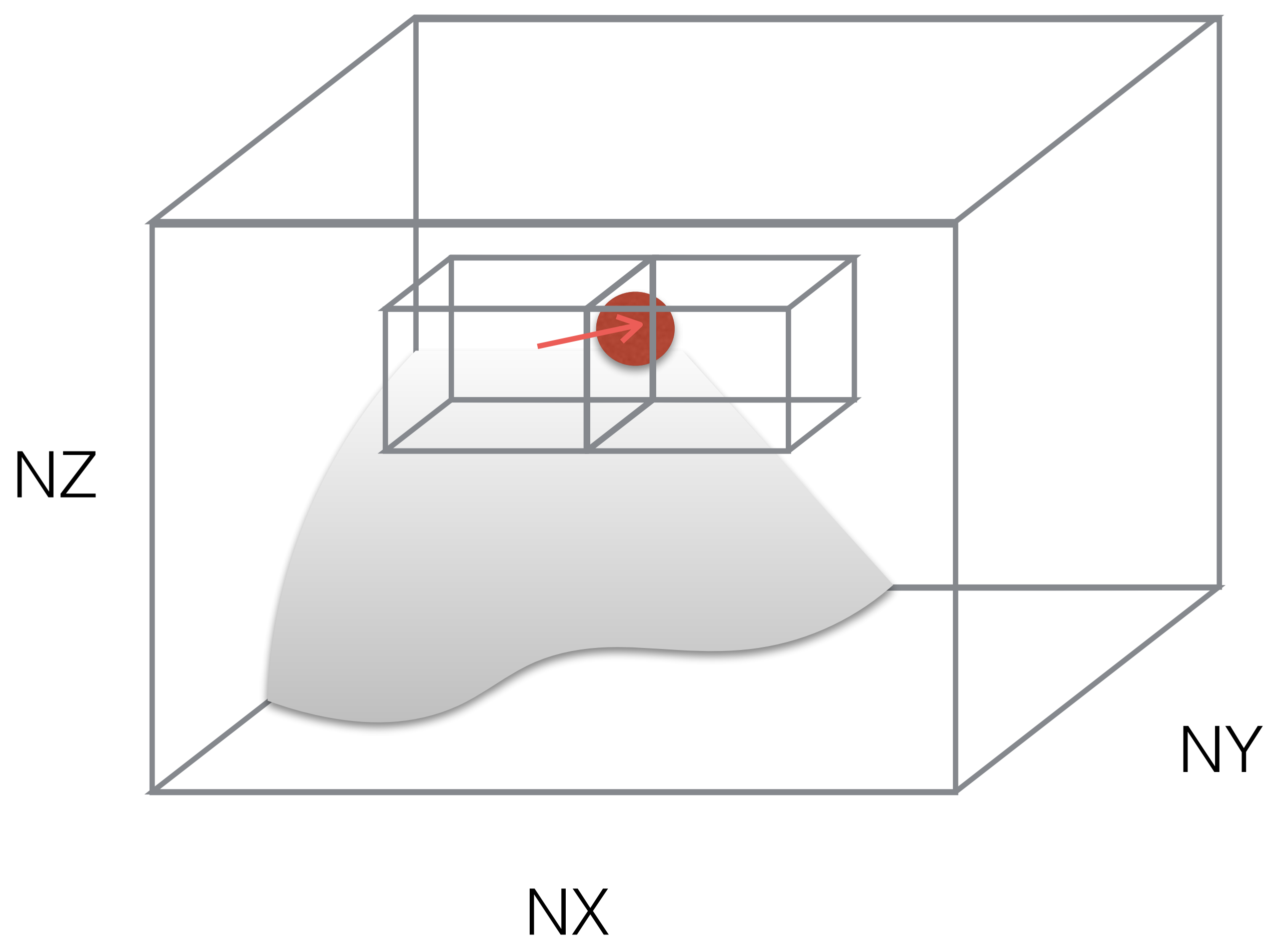


CPU: local small array no longer necessary

GPU: requires loading data into GPU memory —> faster for >1000 particles

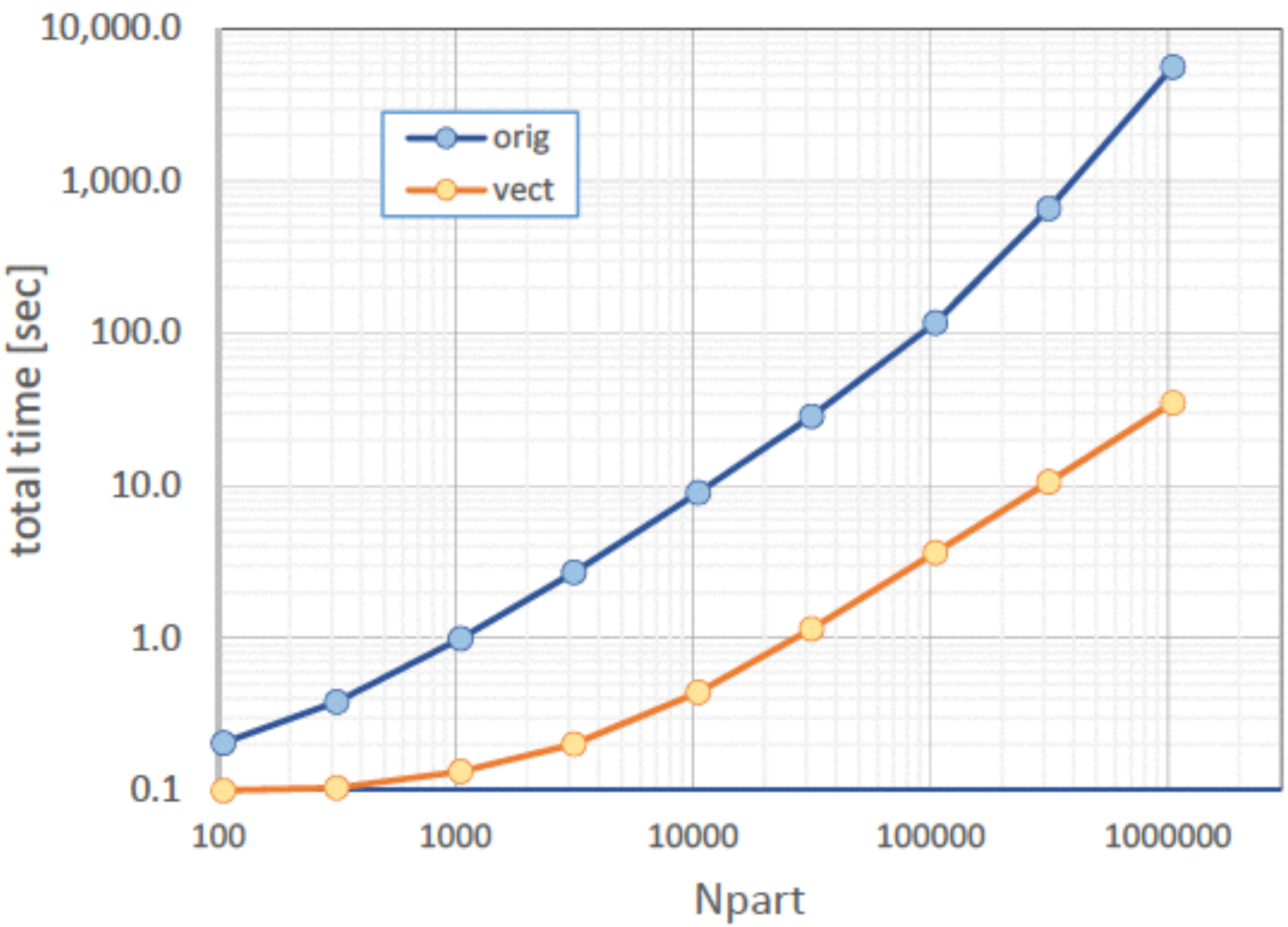
$$\frac{d\mathbf{x}_i(t)}{dt} = \mathbf{u}(\mathbf{x}_i, t)$$

Interpolation improvements (II)



Removed cell boundary interrupts:
(1) Faster
(2) More accurate
(3) Simpler code

Interpolation improvements (III)

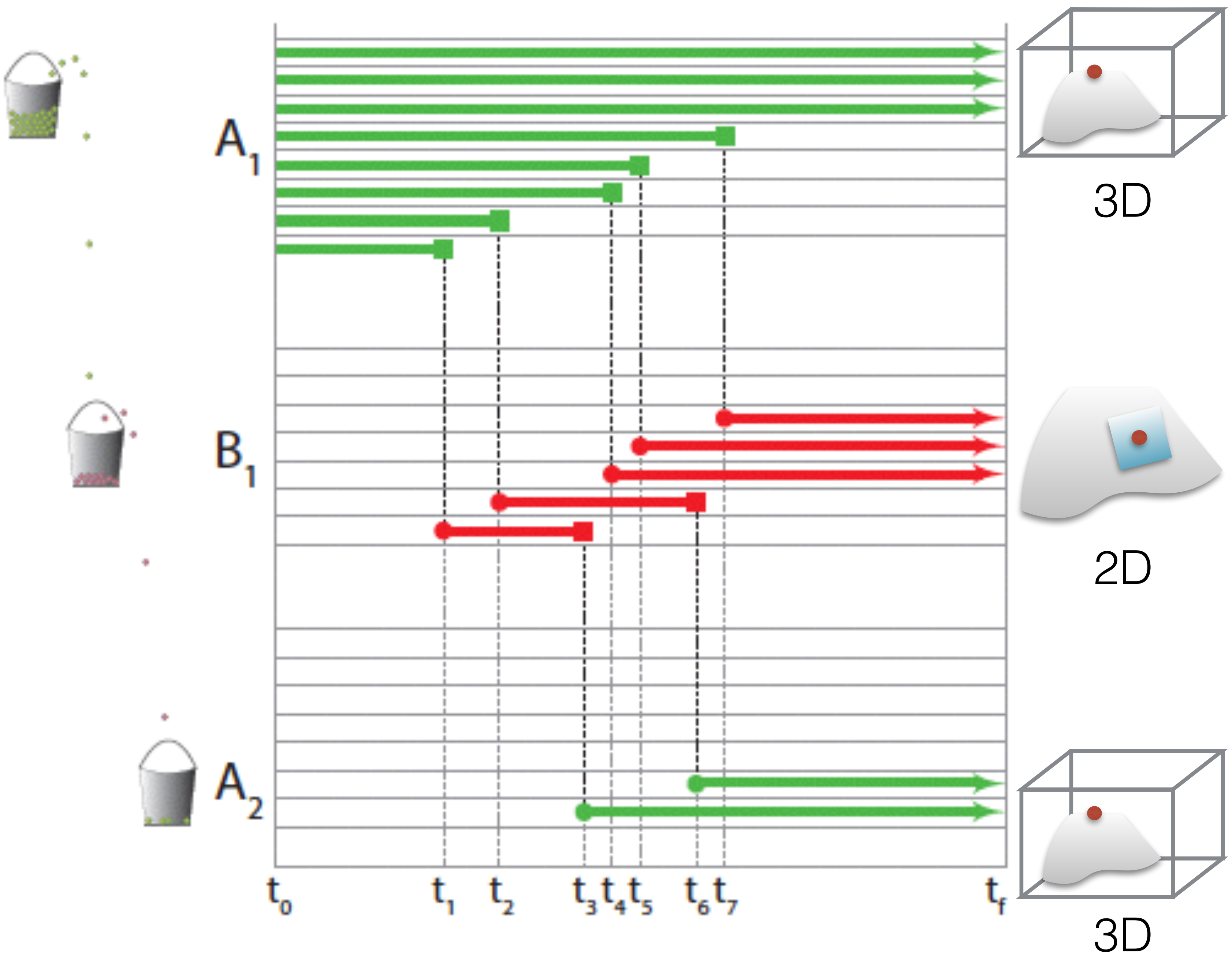


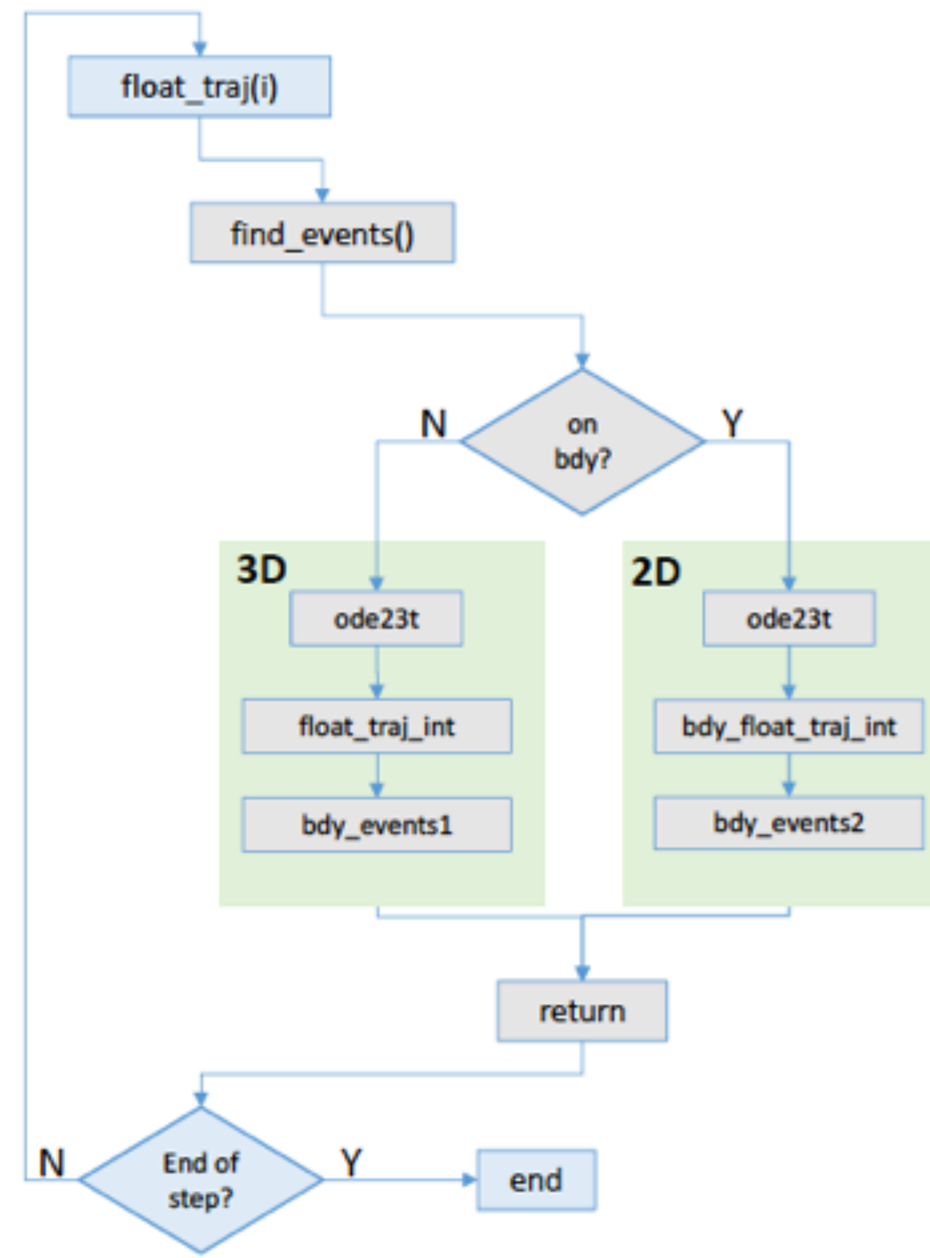
Vectorization of ocean-floor impingement interpolations yields a **160x** speedup for 10^6 particles

(Cubic interpolation only possible in CPU)

$$\mathrm{sgn}\left[H(\mathbf{x}_i) + z_i\right]$$

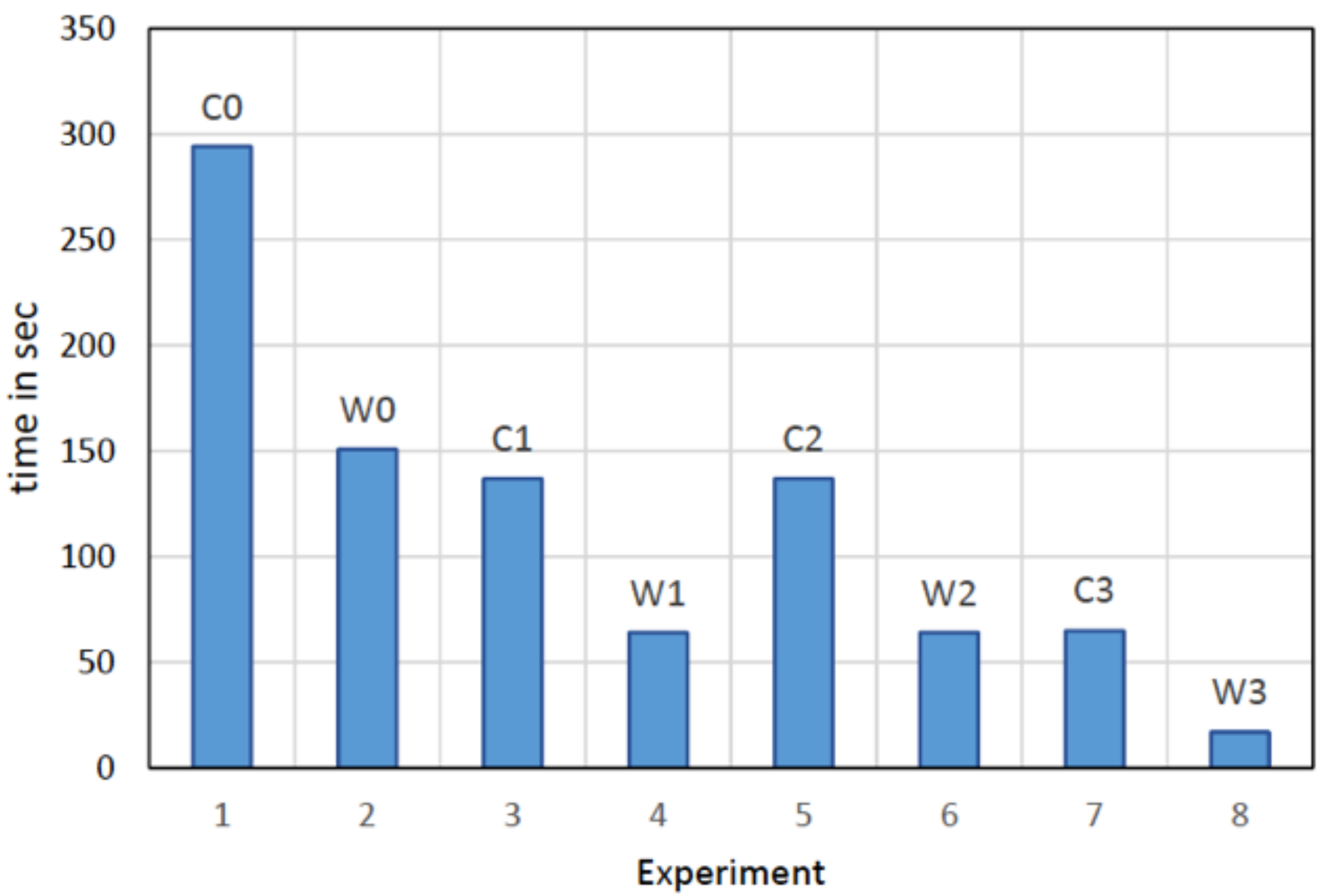
Bucket-List Algorithm





Parallelizing part 3

Vectorization *and* parallelization (with `parfor`)



$$T_i(t) \quad = \quad T(\mathbf{x}_i, t)$$

0: original
1: native little endian + `fread`
2: vectorized
3: parallelized

C/W: cold/warm cache

40 particles test case
yields **10x** speedup

Planned improvements

Speedup:

1. Implement Bucket-List algorithm
2. Use sparse array (disregard grid cells under the ocean floor)
3. Use databases and space-filling curves

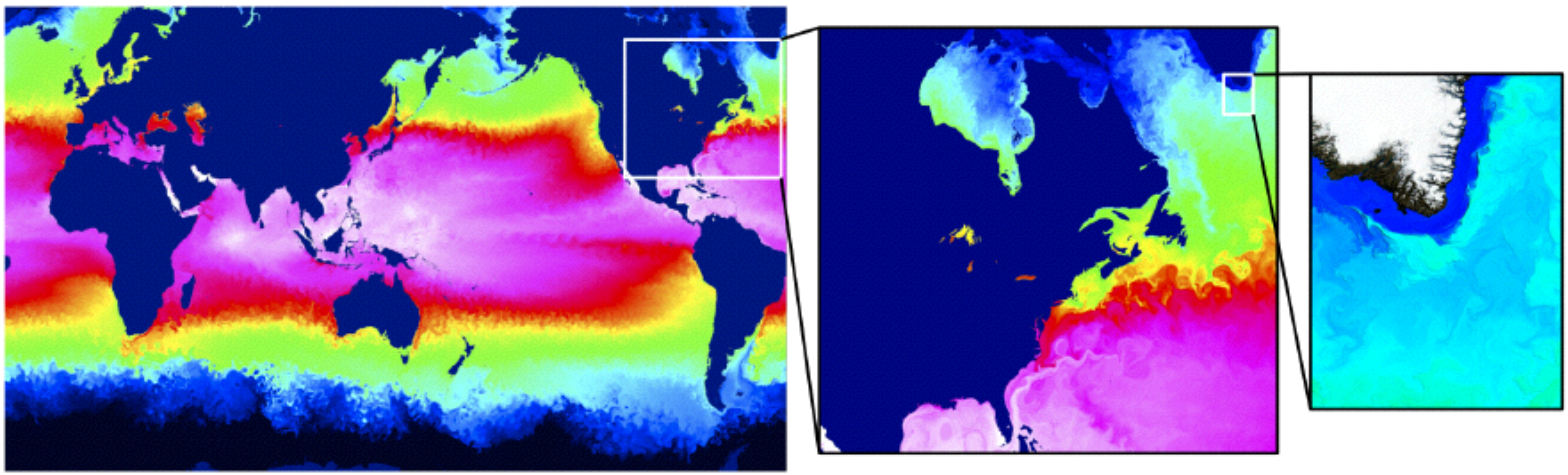
Accuracy:

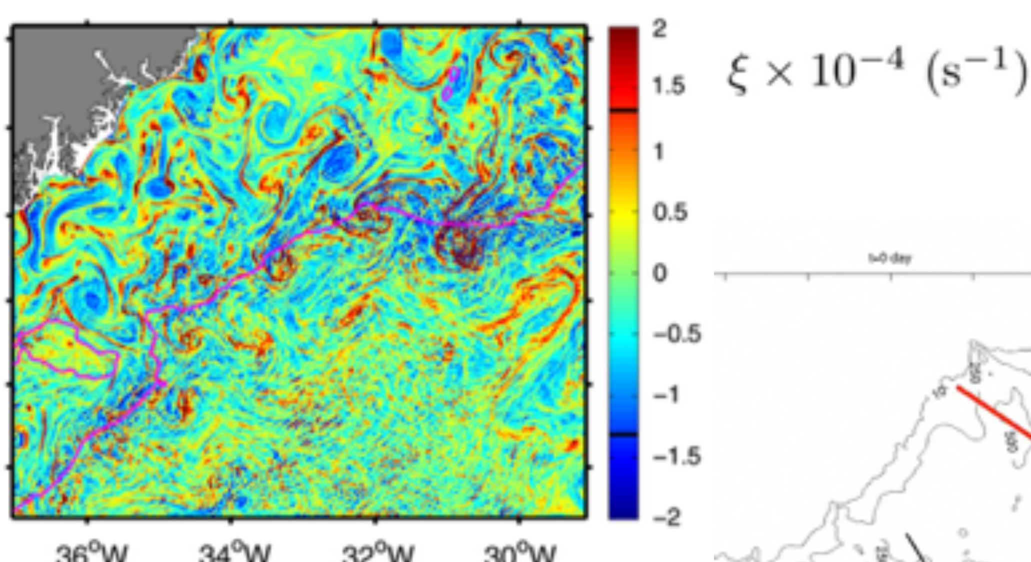
1. Use different ODE solver for interior and boundary-sliding particle trajectories (with different tolerance settings)

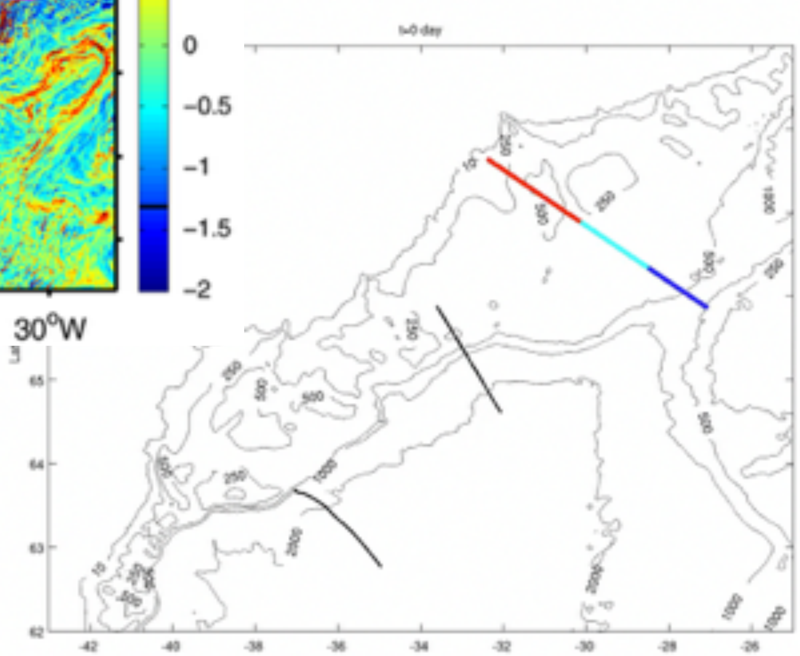
Conclusions

- We built a particle-tracking code with accurate boundary-sliding representation
- Vectorization of the particle-tracking part of the algorithm has yielded a 3500 times speedup for 10^3 particles (5000 for 10^6 particles)
- Vectorization of ocean-floor impingement has yielded an additional factor 6 for 10^3 particles (160 for 10^6 particles)
- Vectorization/parallelization of the property-extraction part of the algorithm has yielded a 10x speedup for 40 particles

Future Work







- Make the particle-tracking algorithm publicly available
- Improve the back-end database environment
- Enhance post-processing functionality
- Scale up to benchmark global ocean circulation solution

Koszalka et al., 2013; Magaldi & Haine, 2016