DNS Modeling and Upscaling

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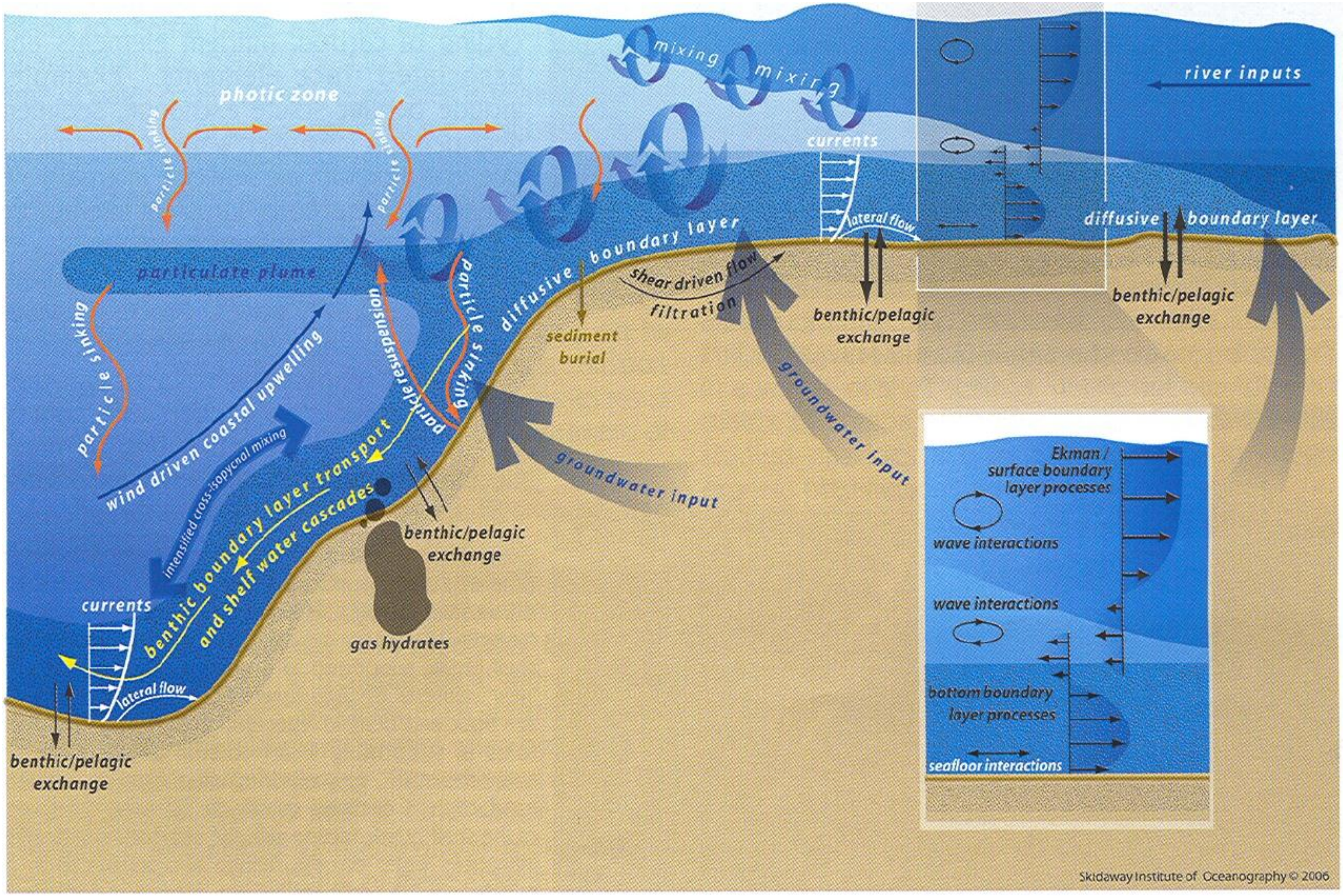
- *Motivation*
- *Governing equations for Direct Numerical Simulations (DNS)*
  - *dimensionless parameters*
  - *computational effort*
- *Need for turbulence modeling*
  - *Reynolds-averaged Navier-Stokes (RANS) simulations*
  - *Large-eddy simulations (LES)*
- *Other aspects of upscaling*
- *Summary and outlook*

UCSB

Coastal margin processes



Turbidity current

- Gravity-driven sediment flow down the continental slope
- Important element of global sediment cycle
- Often triggered by storms or earthquakes
- Can transport many km^3 of sediment
- Distances ~ O(1,000)km or more
- Front velocity ~ O(10m/s)
- Front height ~ O(100m)

Turbidity current.
http://www.clas.ufl.edu/

High-resolution modeling framework: Dilute flows

Assumptions:

- *volume fraction of grains < $O(10^{-2} - 10^{-3})$*
- *grain radius « grain separation*
- *small grains with negligible inertia*

Dynamics:

- *effects of grains on fluid continuity equation negligible*
- *coupling of fluid and grain motion primarily through momentum equation*
- *sediment loading modifies effective fluid density*
- *sediment follows fluid motion, with superimposed settling velocity*

Moderately dilute flows: Two-way coupling (cont'd)

Conservation of

a) mass:

$$\nabla \cdot \vec{u}_f = 0$$

b) momentum:

$$\frac{\partial \vec{u}_f}{\partial t} + \left(\vec{u}_f \cdot \nabla\right) \vec{u}_f = -\nabla p + \frac{1}{Re} \nabla^2 \vec{u}_f + c\,\vec{e}_g$$

effective density

c) sediment:

$$\frac{\partial c}{\partial t} + \left[\left(\vec{u}_f + \vec{U}_s\right) \nabla\right] c = \frac{1}{Sc\,Re} \nabla^2 c$$

settling velocity

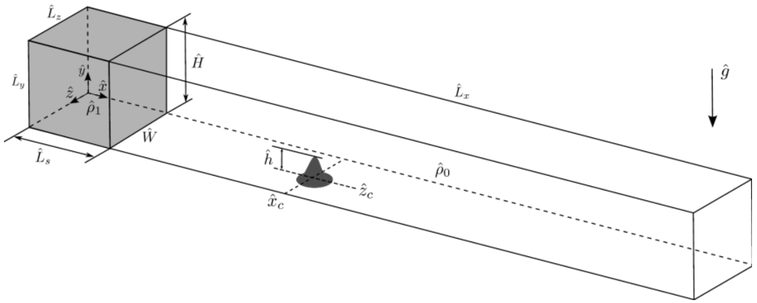
Dimensionless parameters: $Re = \frac{u_b\,L}{\nu}$, $Sc = \frac{\nu}{D}$, $U_s = \frac{u_s}{u_b}$

Field scale turbidity current:

$$u_b \approx 10m/s\ ,\ L \approx 100m\ ,\ \nu \approx 10^{-6} m^2/s \quad \rightarrow \quad Re_{field} \approx O(10^9)$$

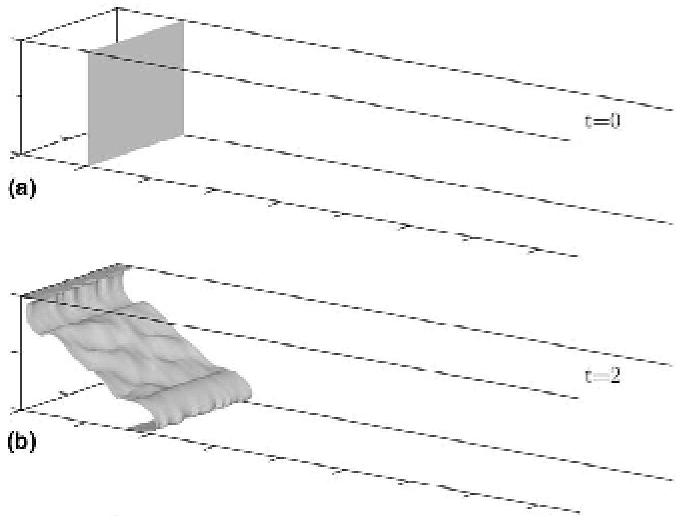
Model problem for DNS simulation (with M. Nasr-Azadani)

Lock exchange configuration



Dense front propagates along bottom wall

Light front propagates along top wall

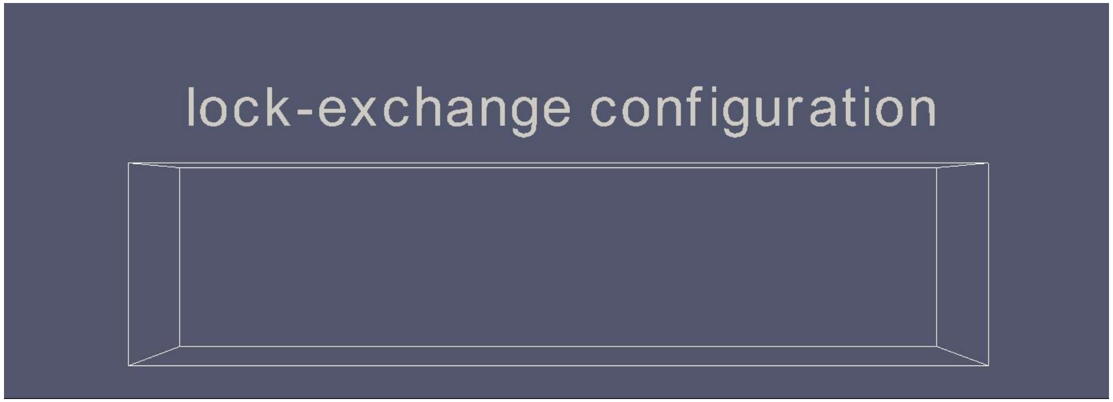


Numerical method

- *second order central differencing for viscous terms*
- *third order ENO scheme for convective terms*
- *third order TVD Runge-Kutta time stepping*
- *projection method to enforce incompressibility*
- *domain decomposition, MPI*
- *employ PETSc (developed by Argonne Nat'l Labs) package*
- *non-uniform grids*
- *immersed boundary method for complex bottom topography*

Example: 3D turbidity current over bottom topography

Direct Numerical Simulation (DNS): all scales are resolved



Nasr-Azadani, Callies and Meiburg (2011)

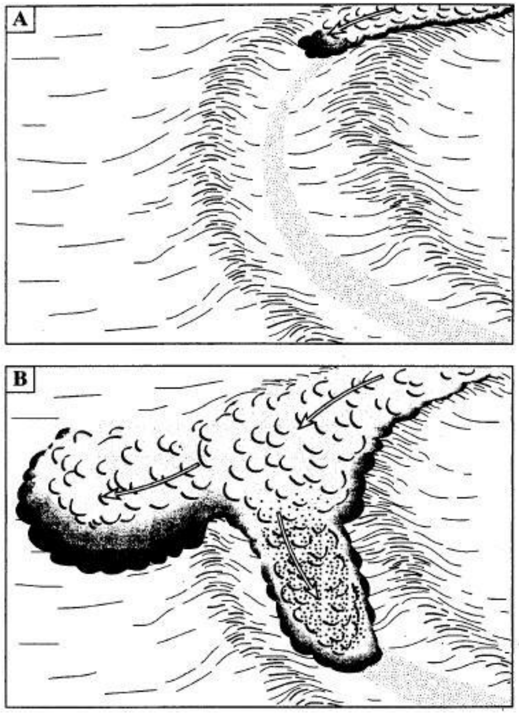
- *turbidity current develops lobe-and-cleft instability of the front*
- *current dynamics and depositional behavior are strongly affected by bottom topography*

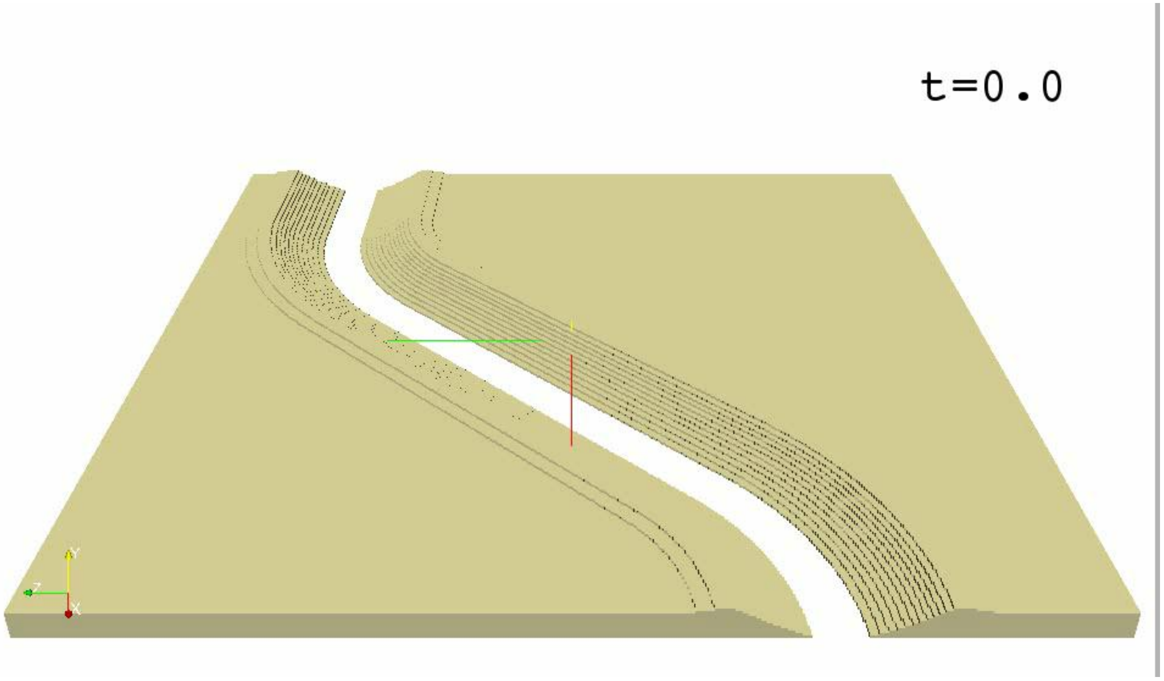
$$Re_{sim} = 2,000 : \; u_b \approx 2cm/s \; , \; L \approx 10cm \; , \; \nu \approx 10^{-6} m^2/s$$

→ *simulation corresponds to a laboratory scale current, not field scale!*

Turbidity current/sediment bed interaction

'Flow stripping' in channel turns: lateral overflows





DNS simulations

Advantages:

- *accurately reproduce physics*
- *provide very detailed information*
- *require a minimum of empirical modeling assumptions*

Disadvantages:

- *computationally very expensive*
- *limited to small Reynolds numbers*

Why can we not do a DNS simulation at Re=10^9?

- *Re is a measure of the ratio of the largest ("integral") length scale L of the flow to the smallest ("Kolmogorov") length scale η, at which kinetic energy is dissipated into heat*
- *turbulence theory shows that* $\frac{L}{\eta} = Re^{3/4}$
- *DNS, which resolves all scales, needs to have grid spacing $\Delta x \sim \eta$, and computational domain size ~ L $\rightarrow$ number of grid points in each direction $N \sim Re^{3/4}$. For 3D simulation $N_x \cdot N_y \cdot N_z \sim Re^{9/4}$. Time step $\Delta t \sim \Delta x \rightarrow$*

Computational effort $E \sim N_x \cdot N_y \cdot N_z \cdot \Delta t^{-1} \sim Re^3$!!

- *field scale simulation would require 10^{18} times effort of lab scale simulation*

How can we perform simulations at field scale?

Key idea:

- *While the large scale flow features are unique for every flow, the smallest scale flow features are similar for all turbulent flows → we may not have to resolve them, but instead may be able to model their main effect (energy extraction from large scales) by means of a* ***turbulence model***

- *Two different approaches:*
  - *temporal averaging of governing equations →* ***Reynolds-averaged Navier-Stokes (RANS) simulations***
  - *spatial averaging of governing equations →* ***Large-eddy simulations (LES)***

Reynolds-averaged Navier-Stokes (RANS) simulations

Split all variables (velocity, pressure, sediment concentration…)
into time-averaged value and fluctuation

$$\phi(x,y,z,t) = \bar{\phi}(x,y,z,t) + \phi'(x,y,z,t)$$

time-averaged value, can still depend on time — *fluctuation*

Take time average of the governing equations

$$\bar{c}_t + \overline{(uc)}_x + \overline{(vc)}_y + \overline{(wc)}_z = \ldots$$

Problem: nonlinear terms

$$\overline{(uc)} = \overline{(\bar{u}+u')(\bar{c}+c')} = \bar{u}\,\bar{c} + \overline{u'c'}$$

$$\overline{u'c'} \neq 0$$

cannot be calculated from time-averaged quantities

(closure problem)

→ need for RANS turbulence models!

Many such models have been developed, e.g. mixing length models, k,ε-models, Reynolds stress models etc.

Problems:

- *each model involves several empirical constants*
- *these constants depend on flow geometry, flow physics etc.*
- *especially difficult to determine these empirical constants for complex multiphase flows, e.g. sediment-laden flows with erosion and deposition*

→ large amount of uncertainty associated with RANS simulations of complex multiphase flows

Alternative approach: Large-eddy simulations (LES)

Employ spatial filtering, resolve only the large scales, model the effects of the small scales

$$\bar{u}(x,t) = \int G(x,x')\, u(x',t)dx'$$

filtered velocity

filter kernel, has length scale Δ associated with it

Problem: nonlinear terms still lead to closure problem

$$\overline{uc} \neq \overline{u}\,\overline{c}$$

→ *have to model 'subgrid scale' stresses and transport*

→ *need for LES turbulence models!*

Several models have been developed, e.g. Smagorinsky model

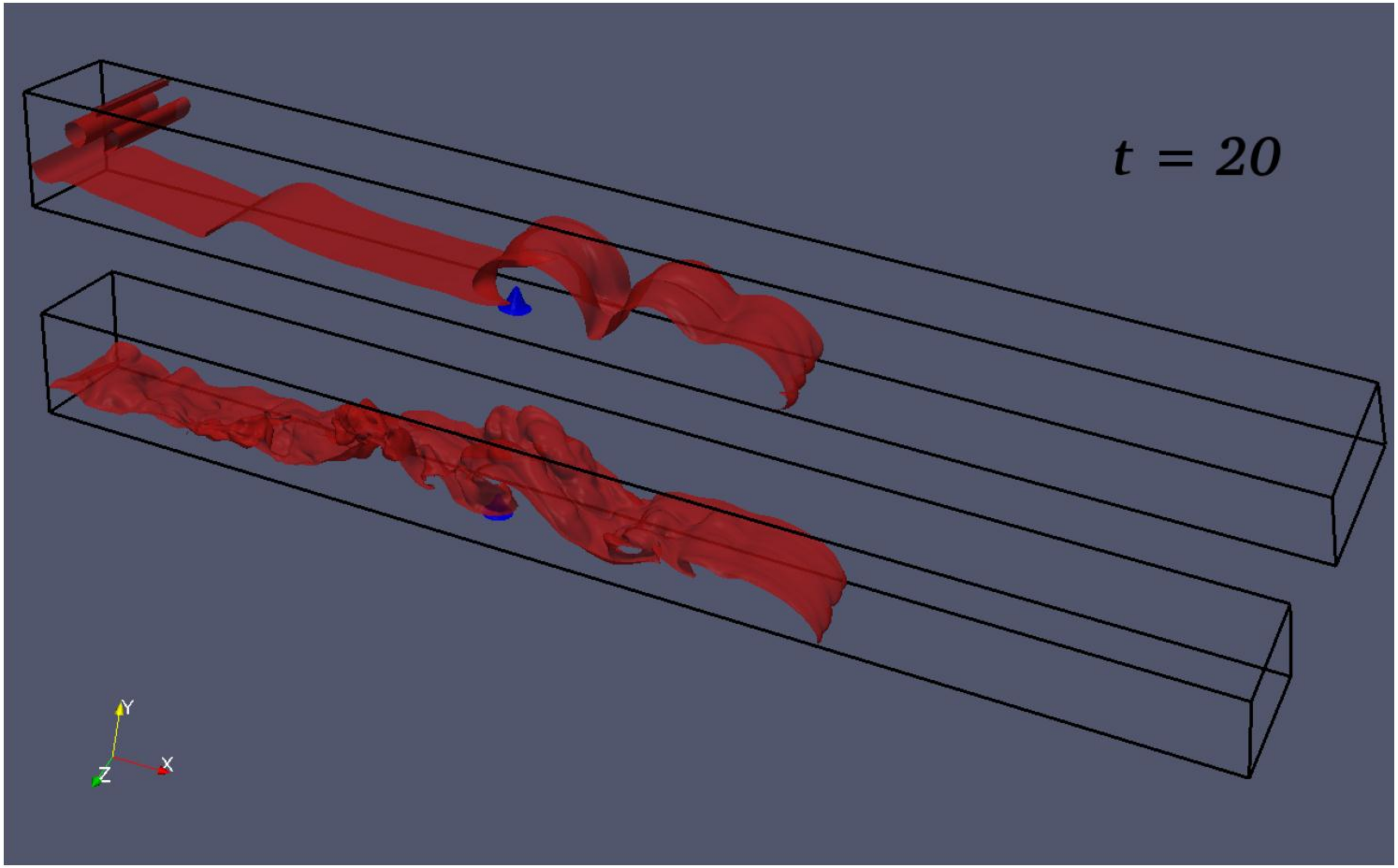
Problems:

- *each model involves several empirical constants*
- *'dynamic' models have been developed that determine these constants automatically during the simulation by applying two filters of different sizes*
- *LES generally more accurate than RANS, but also more expensive computationally*
- *still, there is some uncertainty associated with these models for complex multiphase flows*

→ *more research needed on turbulence modeling*

LES example: Lock-exchange gravity currents (with S. Radhakrishnan)

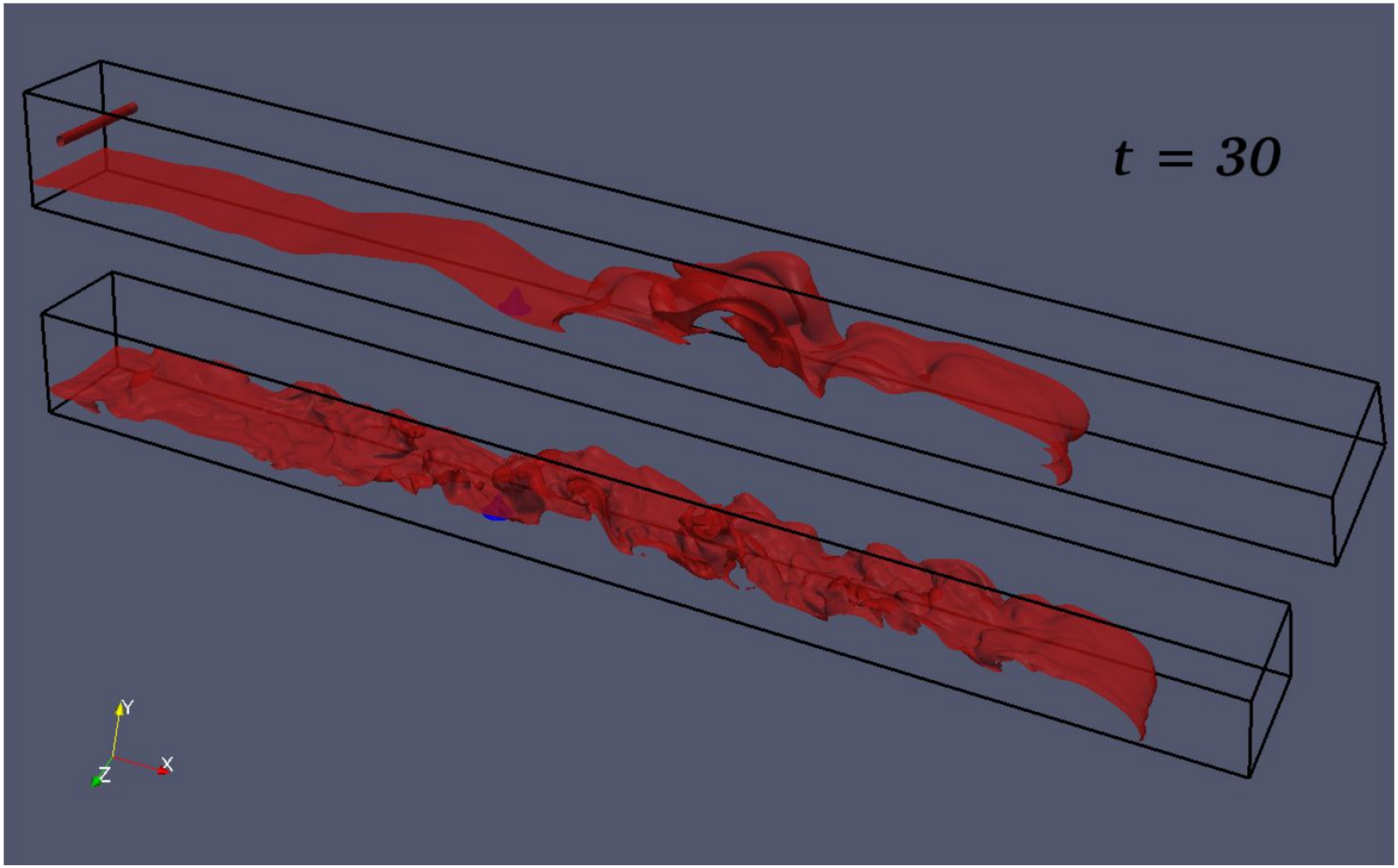
- *Re=1,000 (DNS)*
- *Re=200,000 (LES)*



High-Re LES shows much more fine-scale structure than low-Re DNS

LES example: Lock-exchange gravity currents (cont'd)

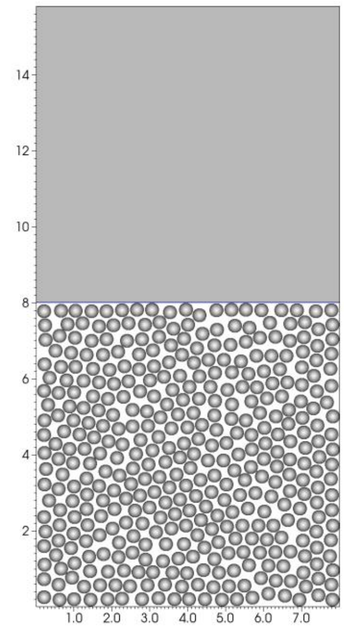
- *Re=1,000 (DNS)*
- *Re=200,000 (LES)*



Other aspects of upscaling (with Z. Borden)

Employ particle-based, microscopic approach to develop accurate macroscopic continuum models:

- *e.g., erosion models to date are mainly phenomenological, not based on first principles → research at the microscopic level is needed to develop improved macroscopic erosion models*



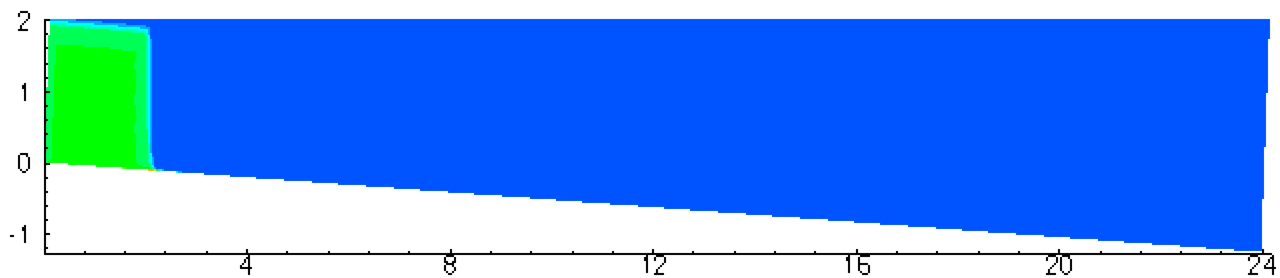
Borden and Meiburg (2011)

- *Goal: Development of more accurate continuum erosion models*

Erosion, resuspension of particle bed by turbidity current

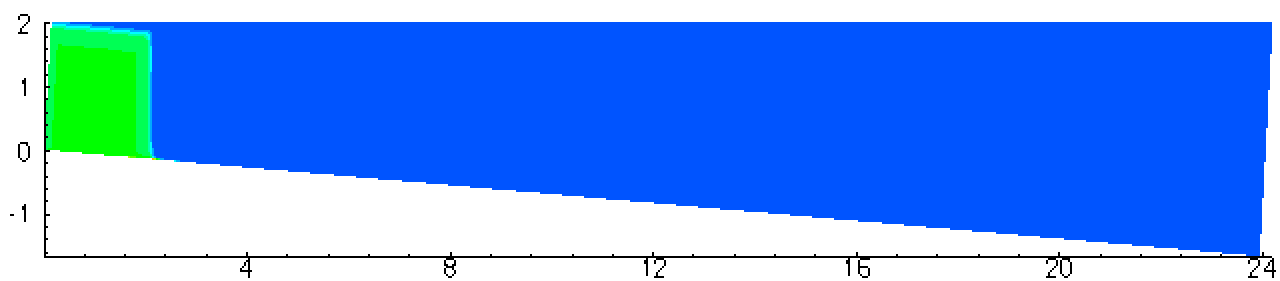
$\rho_p = 1.5g/cm^3$, $r_p = 50\mu m$, $\nu = 10^{-6} m^2/s$
current height $= 1.6m$
initial concentration $= 0.5\%$
Re $= 2,200$:

slope angle $= 3^o$:



deposition outweighs erosion: decaying turbidity current

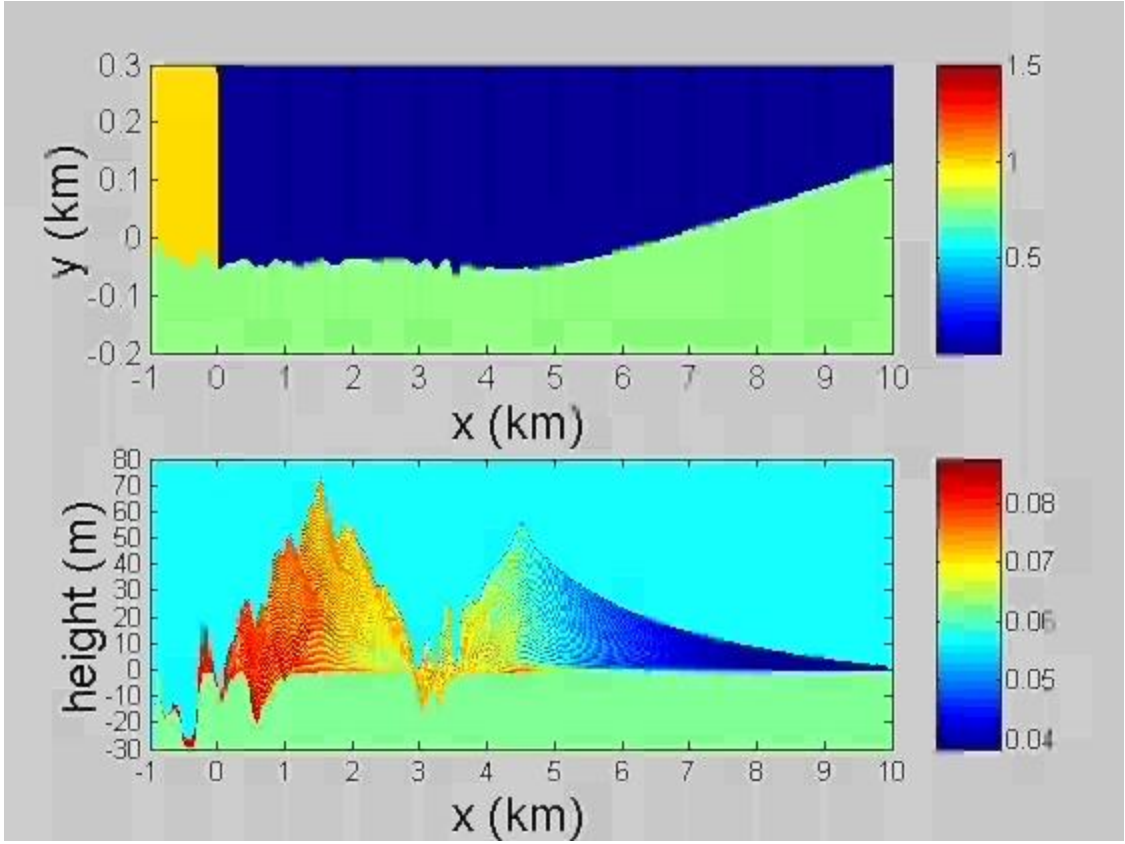
slope angle $= 4^o$:



erosion outweighs deposition: growing turbidity current

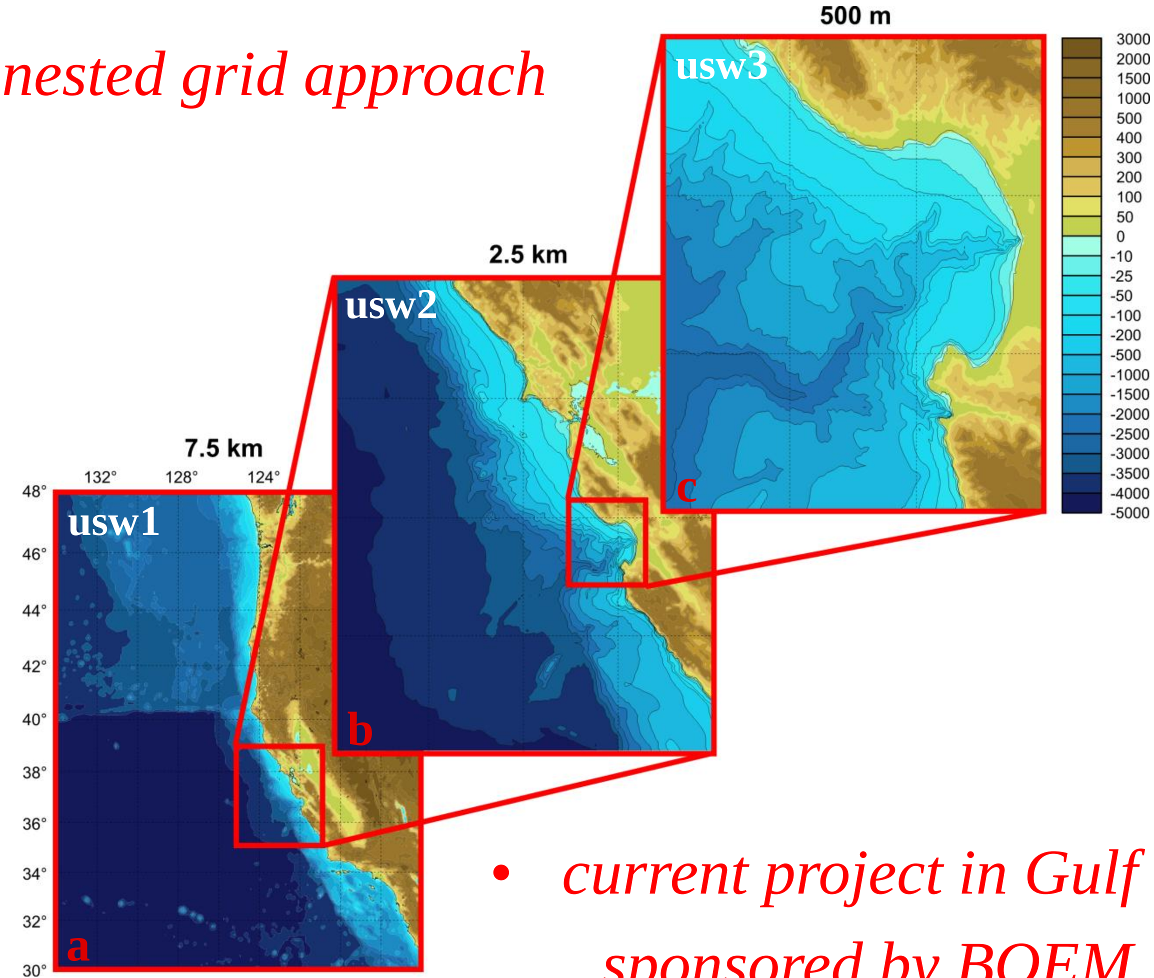
Erosion, resuspension of particle bed by turbidity current

- *multiple, polydisperse flows*
- *feedback of deposit on subsequent flows*
- *formation of ripples, dunes etc.*



Upscaling: Embedding high-resolution simulation within coarser resolution model (w. Arango, Harris, Syvitski)

- *nested grid approach*



- *current project in Gulf of Mexico sponsored by BOEM*

Summary

- *Computational effort for DNS ~ Re^3 → for high-Re flows at field scales we can't perform DNS simulations that resolve all scales*
- *Need turbulence models that capture the effects of the small scales*
- *Two main approaches:*
  - *RANS simulations: based on temporal averaging*
  - *LES simulations: based on spatial filtering*
- *Both of these approaches require closure models involving empirical constants → difficult to determine → uncertainties*
- *Upscaling from microscopic, particle models to continuum models*