A Variational Multiscale Large Eddy Computational Framework for Numerical Simulations of Turbidity Currents

Fernando A. Rochinha

Mechanical Engineering Departmen
Universidade Federal do Rio de Janeiro - BRAZIL

GEOFLOWS 2013 - Fluid-Mediated Particle Transport in Geophysical Flows. KITP. UCSB. October 2013.

COPPE - Federal University of Rio de Janeiro

Collaborators :

Federal University of Rio de Janeiro:

Mechanical Engineering : Gabriel Guerra (Post Doc), Zio Souleymane (Dsc. Student)

High Performance Computing Center : Alvaro Coutinho (Prof.) , Renato Elias (Prof.), Jose Camata (Post Doc)

Computer Science : Jonas Dias(Dsc. Student), Marta Mattoso (Prof.) , Eduardo Ogasawara (Post Doc)

Federal University of Para:
Erb Lins (Prof.)

Petrobras :

Paulo Paraizo (Senior Engineer)

Acknowledgments

The authors would like to thank the support of PETROBRAS Technological Program on Basin Modeling in the name of its general coordinator, Dr. Marco Moraes.

We acknowledge the fruitful discussions within the program with E. Meiburg, Ben Kneller, J. Silvestrini and J. Alves. Partial support is also provided by MCT/CNPq and FAPERJ.

We also acknowledge the fruitful discussions about UQ with Prof. Nicholas Zabaras (University of Cornell) .

Computer resources were provided by the High Performance Computer Center, NACAD/UFRJ.

Outline

- Background and Motivation: Turbidity Currents. Sediments and Geological Formations
- Modeling Turbidy Currents : Particle Laden Flows
- Residual Based Variational Multiscale Method LES Formulation for Tubidity Currents
- Computational Simulations
- Final Remarks and Future Steps (integrating physical models and obervational data)

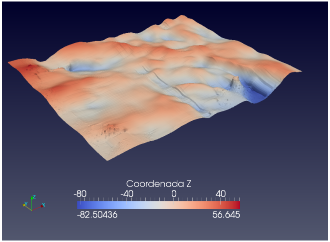
Background

- Large Scale Algorithms + Petascale Computing push the envelope of Simulation - Based Engineering (SBE) Science
- Confidence (reliability) of simulations predictions make SBE an effective tool
- Uncertainty Quantification + Validation: decision making
- Chain of codes involving high performance computation and a huge amount of data. Need of a efficient control strategy and tools for the analysis of output like provenance catalog and queries within heterogeneous data

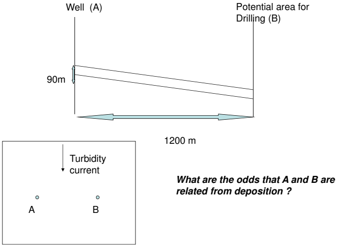
Our context : Oil and Gas (and many other) applications: simulation of complex (multiscale - multiphysics) flows

- A large amount of Brazilian oil reservoirs (indeed worldwide) were formed by the action of Turbidity Currents;
- Understanding reservoir geological formations may help decision making on reservoir development;
- Most of the studies in this area are still based on experiments or nature observation. Computer simulations might be transformed in an effective tool (at least simulations can help geologists to deeper analyse theirs theories);
- Highly coupled and non-linear problem: incompressible flow, polydisperse transport, interaction of sand deposition and bottom morphology;
- Room for improvements in turbulence models (RBVMS) and uncertainty quantification (UQ)

What (oil) Geologists want from simulating turbidity currents?



Deposition map
sea bottom morphology



Decision about where to drill

Strategy

We are putting together three pieces:

- High Performance CFD code based on Large Eddy Simulation approach: Residual Based Variational Mulsticale Method to model Particle Laden Flows. **Guerra et al, Numerical simulation of particle-laden flows by the residual based variational multiscale method. International Journal for Numerical Methods in Fluids, DOI: 10.1002/fld.3820**
- Uncertainty Propagation. Stochastic Collocation **SIAM Conference on Computational Science & Engineering. Boston, 2013**
- Scientific Workflows Managing UQ **.Guerra et al.. Uncertainty Quantification in Computational Predictive Models for Fuid Dynamics Using a workflow Management Engine. International Journal for Uncertainty Quantification, v. 2, p. 53-71, 2012.**

NUMERICAL MODEL OF TURBIDITY CURRENTS

Governing equations

Mathematical setting for the numerical simulation of particle-laden flows within an Eulerian - Eulerian framework:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{\sqrt{Gr}} \Delta \mathbf{u} + c\ \mathbf{e^g} \quad in \quad \Omega \times [0, t_f]$$

$$\nabla \cdot \mathbf{u} = \mathbf{0} \quad in \quad \Omega \times [0, t_f]$$

$$\frac{\partial c}{\partial t} + (\mathbf{u} + u_S\ \mathbf{e^g}) \cdot \nabla c = \nabla \cdot \left(\frac{1}{Sc\sqrt{Gr}} \nabla c \right) \quad in \quad \Omega \times [0, t_f]$$

where Grashof number expresses the ratio between buoyancy and viscous effects.

$Gr = \left(\frac{u_b}{\nu H} \right)^2$ $\quad Sc = \frac{\nu}{\kappa}$ $\quad u_S$: settling velocity $\quad c = \frac{C}{C_0}$: scaled concentration

boundary condition (bottom) : sediments deposition $\frac{\partial c}{\partial t} = u_S \frac{\partial c}{\partial z}$

and initial conditions $c(.,0)$

Residual Based Variational Multiescale formulation

Differently from traditional LES models, that are built upon spatial filters, RBVMS methods rely on scales splitting of the physical variables combined with variational projections.

The splitting involving the large scales and the fine scales for the present problem are:

$$\begin{aligned} \mathbf{u} &= \mathbf{u}_h + \mathbf{u}' \\ \mathbf{p} &= \mathbf{p}_h + \mathbf{p}' \\ \mathbf{c} &= \mathbf{c}_h + \mathbf{c}' \end{aligned}$$

where the subscript h denotes the large scale and the superscript $'$ refers to the subgrid complement.

Residual Based Variational Mulsticale Formulation

Explicit Scales Splitting

$$\mathbf{u} = \mathbf{u}_h + \mathbf{u}' \quad \mathbf{p} = \mathbf{p}_h + \mathbf{p}' \quad \mathbf{c} = \mathbf{c}_h + \mathbf{c}'$$

Weak Form

$$\begin{aligned}
\left(\rho \frac{\partial \mathbf{u}^h}{\partial t}, \mathbf{w}^h\right)_\Omega + \left(\rho(\mathbf{u}^h + \mathbf{u}') \cdot \nabla \mathbf{u}^h, \mathbf{w}^h\right)_\Omega + (2\mu\varepsilon(\mathbf{u}^h), \varepsilon(\mathbf{w}^h))_\Omega - (\tilde{p}_h, \nabla \cdot \mathbf{w}^h)_\Omega \\
\left(\rho \frac{\partial \mathbf{u}'}{\partial t}, \mathbf{w}^h\right)_\Omega - \left(\rho \mathbf{u}', (\mathbf{u}^h + \mathbf{u}').\nabla\ \mathbf{w}^h\right)_\Omega - (2\mu\mathbf{u}', \underbrace{\nabla_h \cdot \varepsilon(\mathbf{w}^h)}_{=0 \ \textit{for linear elements}})_\Omega \\
+ \left(\nabla \cdot \mathbf{u}^h, q^h\right)_\Omega - \left(\mathbf{u}', \nabla q^h\right)_\Omega - (p', \nabla \cdot \mathbf{w}^h)_\Omega \\
\left((c_h + c')(\rho_p - \rho)\mathbf{g}, \mathbf{w}^h\right)_\Omega + \left(\mathbf{t}, \mathbf{w}^h\right)_{\Gamma_h} \\
\forall (w^h, q^h) \in W^h \times P^h
\end{aligned} \qquad (1)$$

Transport Equation

$$
\left(\frac{\partial c_h}{\partial t}, \upsilon_h\right)_\Omega + ((\mathbf{u}_h + \mathbf{u}' + u_s e^g) \cdot \nabla c_h, \upsilon_h)_\Omega + (\tilde{\kappa} \nabla c_h, \nabla \upsilon_h)_\Omega
$$

$$
- \sum_{e=1}^{Nel} (\nabla.(u_h + u' + u_s e^g) c', v_h)_{\Omega_e} + \underbrace{(u_h + u' + u_s e^g).\nabla v_h, c')_{\Omega_e}}_{SUPG\ like}
$$

$$
+ \sum_{e=1}^{Nel} \underbrace{(\tilde{\kappa} c', \Delta \upsilon_h)_{\Omega_e}}_{vanishes\ for\ linear\ elements} = 0
$$

Sub-grid Modeling (designed based on numerics reasoning)

Fine Scale Approximation (static hypothesis - residuals of the balance equations)

$$p' = \tau_c \rho R_c = \nabla \cdot \mathbf{u}^h$$

$$u' = \frac{\tau_m}{\rho} R_m = -\rho \frac{\partial \mathbf{u}^h}{\partial t} - \rho(\mathbf{u}^h + \mathbf{u}') \cdot \nabla \mathbf{u}^h + \nabla \cdot (2\mu\varepsilon(\mathbf{u}^h)) - \nabla \tilde{p}_h + c(\rho_p - \rho)\mathbf{g}$$

$$c' = \tau_t R_t = -\frac{\partial c_h}{\partial t} - (u_h \; + \; u' + u_s \mathbf{e}^{\mathbf{g}}) \cdot \nabla(c_h) + \tilde{\kappa} \nabla^2 (c_h)$$

$$\tau_m = \left(\left(\frac{2}{\Delta t}\right)^2 + \left(c_1 \frac{\left\|u^h\right\|}{h_e}\right)^2 + \left(c_2 \frac{\nu}{h_e^2}\right)^2 \right)^{-\frac{1}{2}} \qquad \tau_c = \frac{h_e}{3} \left\|u^h\right\|$$

$$\tau_t = \left(\left(\frac{2}{\Delta t}\right)^2 + \left(c_1 \frac{\left\|u^h\right\|}{h_e}\right)^2 + \left(c_2 \frac{k}{h_e^2}\right)^2 \right)^{-\frac{1}{2}}$$

Our Software Playground

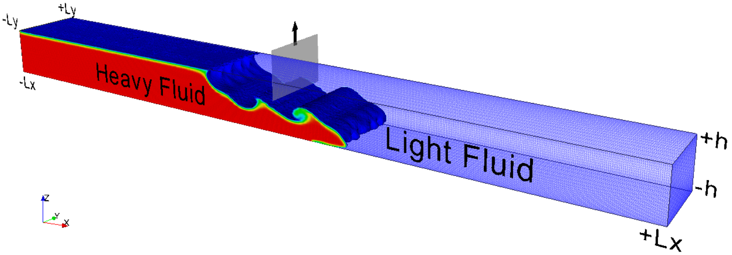
EdgeCFD is a parallel and general purpose CFD solver developed at UFRJ with the following main characteristics:

- Edge-based data structure;
- Hybrid parallel (MPI, OpenMP or both);
- Low Order Finite Elements; Unstructured Meshes
- Staggered Multiphysics solver strategies;
- SUPG/PSPG/LSIC FEM formulation for incompressible flow;
- RBVMS or Smagorinsky turbulence treatment;
- u-p fully coupled solver;
- RB-VMS + schock capturing for multiple advetion-diffucion eq.;
- Free-surface flows (VOF and Level Sets);
- Adaptive time step control;
- Inexact-Newton solvers;

R.N.Elias, P.L.B. Paraizo and A.L.G.A. Coutinho. *Stabilized edge-based Finite element computation of gravity currents in lock-exchange configurations*. International Journal for Numerical Methods in Fluids, 2008.

COMPUTATIONAL SIMULATIONS

Lock-Exchange Scenario



Lock-Exchange

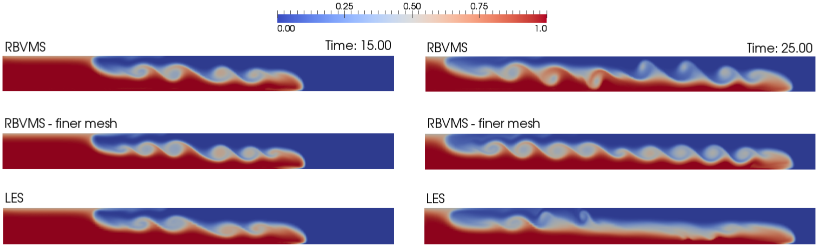
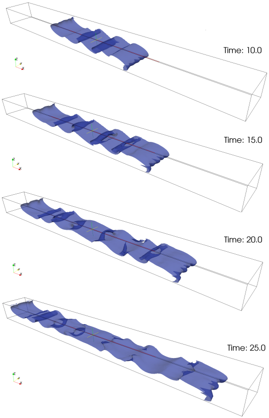


Figure: Side view: Concentration field at $t = 15$ and $t = 25$ for different spatial discretizations for $Gr = 1.5 \times 10^6$.

Lock-Exchange



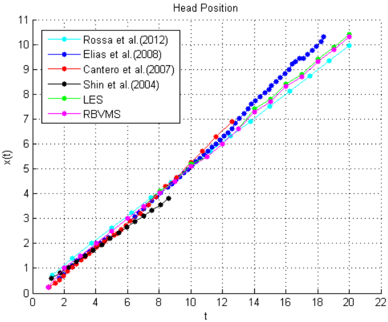


Figure: Evolution of the fluids interface

Lock-Exchange

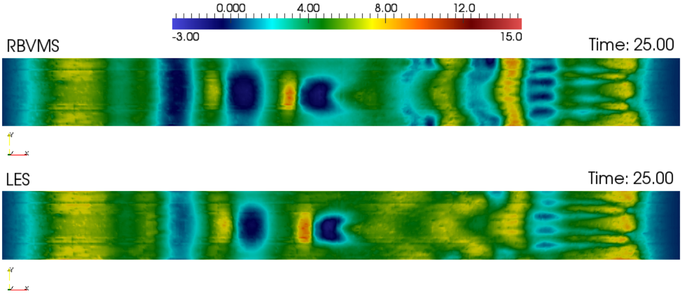


Figure: Non-dimensional shear stress at the bottom

Lock-Exchange

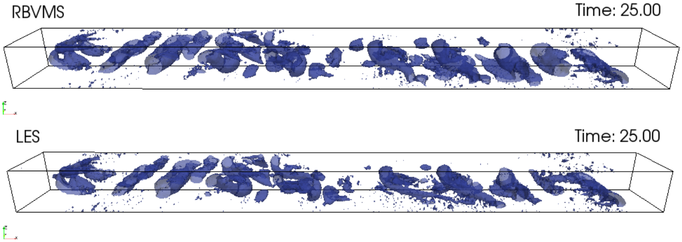


Figure: View of vortical structures, Q-criterium iso-surfaces (Q=0.3).

Lock-Exchange $Gr = 9.0 \times 10^7$

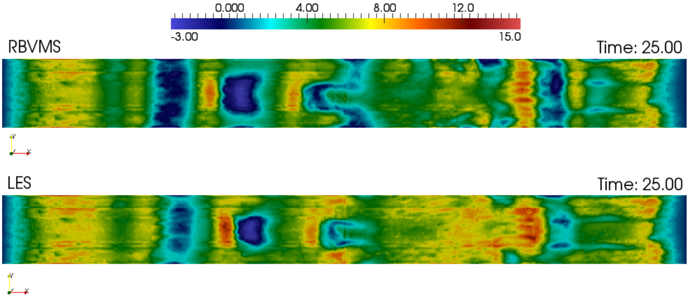


Figure: Top view: shear stress distribution at the bottom

Lock-Exchange (deposition) $Gr = 1.0 \times 10^8$

Time evolution of the concentration field

Lock-Exchange – $Gr = 1.0 \times 10^8$

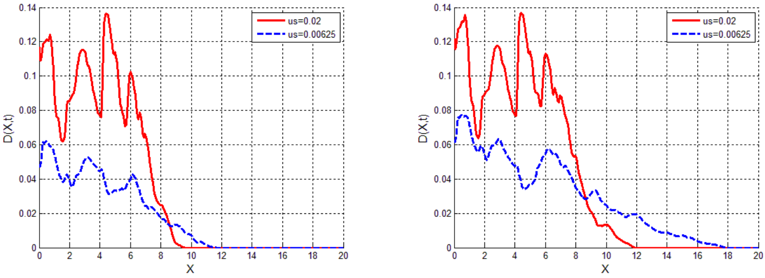


Figure: Deposit profile at the middle plane: t=25 (left) and t=50 (right)

Lock-Exchange – $Gr = 1.0 \times 10^8$

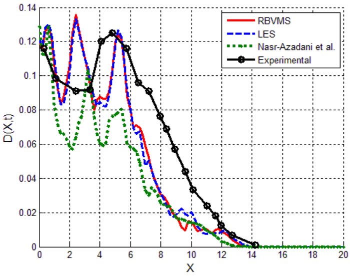
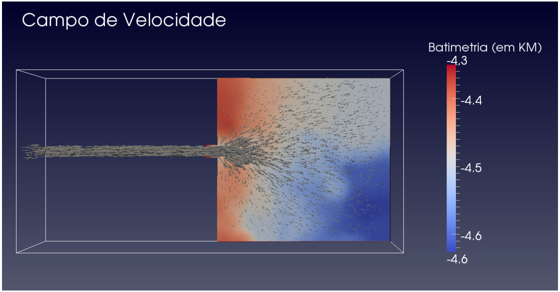
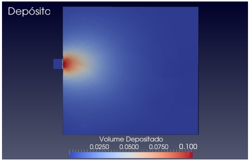


Figure: Depositon map profile (left) and mass along time (right), comparison among experiments and numerical simulations

Subgrid Modeling

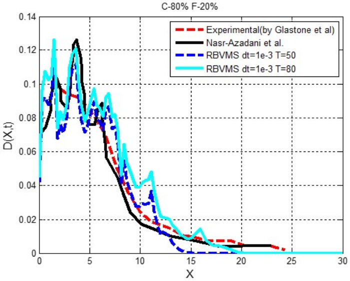
Sustained Flow and Complex Bottom Topography (prelimarly results)





POLYDISPERSE FLOWS

Polydisperse flow: Coarse 80% and Fine 20%



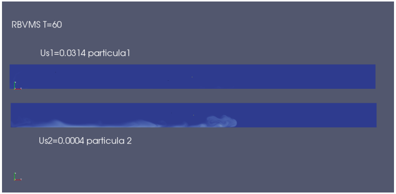


Figure: Depositon map profile (left) and mass along time (right), comparison among experiments and numerical simulations

Ref.: M.M. Nasr-Azadani, B.Hall, E.Meiburg. Polydisperse turbidity currents propagating over complext opography: Comparison of experimental and depth-resolvedsimulation results. Computer & Geosciences (53), 141 – 153, 2013.

Tank Configuration – $Gr = 1.0 \times 10^8$ (prelimarly results)

ALE (FSI) FORMULATION FOR MORPHODYNAMICS

UNCERTAINTY QUANTIFICATION

General Aspects

- Model uncertainty (epistemic), numerical errors, uncertainty in parameters (initial conditions,physical constants...), all of them interacting and compromising the simulations reliability
- Verification and Validation (V&V) and Uncertainty Quantification (UQ)
- Probabilistic Perspective : parameters modeled as random variables or fields. Looking for a PDF instead of a point solution
- Governing Equations represented by Stochastic Partial Differential Equations

Mathematical Preliminaries

To quantify the uncertainty in a system of differential equations we adopt a probabilistic approach.

Definition: Complete probability space $(\Omega, \mathcal{F}, \mathcal{P})$

- Ω is a event space,
- $\mathcal{F} \subset 2^{\Omega}$ is the σ-algebra of subsets in Ω
- $\mathcal{P} : \mathcal{F} \to [0, 1]$ is the probability measure

In this framework, the uncertainty in a model is introduced by representing the input data (parameters,geometry,boundary and initial condition) as random fields.

Mathematical Preliminaries

For a general differential equation defined on $\mathcal{D} \subset \mathbb{R}^d$, $d = 1, 2, 3$ with boundary $\partial\mathcal{D}$. The problem consists on find a stochastic function, $\mathbf{u} \equiv \mathbf{u}(\omega, \mathbf{x}) : \Omega \times \mathcal{D} \longrightarrow \mathbb{R}$, such that, for everywhere $\omega \in \Omega$, (Main idea: uncertainty as an extra stochastic dimension)

Governing Stochastic Equations

$$
\begin{aligned}
\mathcal{L}(\omega, \mathbf{x}; \mathbf{u}) &= f(\omega, \mathbf{x}) \qquad \mathbf{x} \in \mathcal{D} \\
\mathcal{B}(\omega, \mathbf{x}; \mathbf{u}) &= g(\omega, \mathbf{x}) \qquad \mathbf{x} \in \partial\mathcal{D}
\end{aligned}
$$

with $\mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d$, $d \geq 1$, the space coordinates.

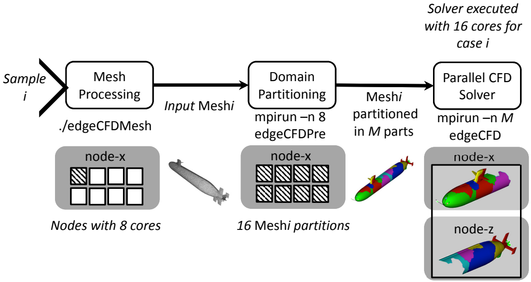
Numerical methods

- **Intrusive Methods**
  - Polynomial Chaos + Galerkin Formulation
- **Non-Intrusive Methods**
  - Sampling: Monte Carlo, Quasi MC, LHS
  - Stochastic Collocation : Polynomial Chaos, Quadratures or Polynomial interpolation
  - Bayesian Surrogates and Gaussian Process Modeling

Scientific Workflows supporting High Performance Computing

- Scientific/Engineering Computational Experiments Modeled as Scientific Workflows
- Simulations generate a lot of data: understanding how to manage and query simulation data in runtime
- Track who performed the computational experiment and who is responsible for its results Provenance data is automatically registered by SWfMS

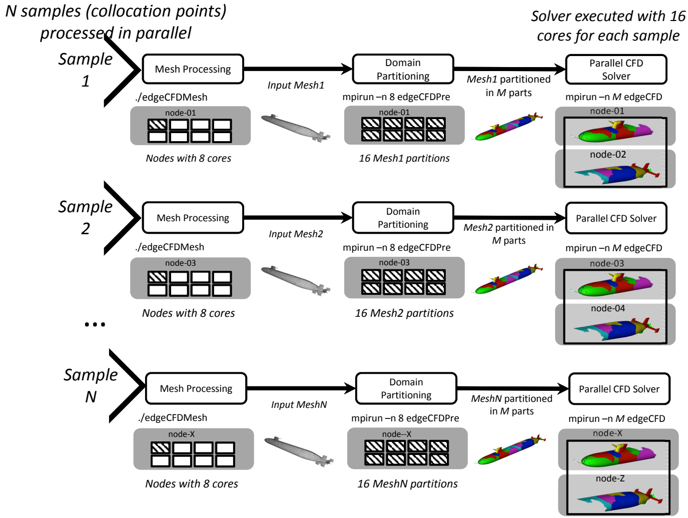
Provenance



Chiron is running in each core of each node:managing scheduling, fault-tolerance, provenance data gathering

Typical queries : check for convergence of the deterministic solver ; computation on the fly of high order statistics (two point correlation represents important QoI)for checking convergence regarding stochastic components

Edge-CFD + CHIRON : Two level paralelism

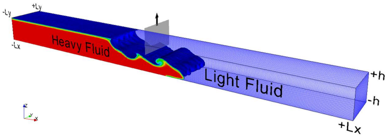


Proof of Concept Prototype (ongoing research and implementation)

- Non-intrusive UQ strategies : Edge-CFD not to be recoded
- Stochastic Collocation : low stochastic dimension
- Double level parallelization: exploring the stochastic space ; exploring built-in parallel Edge-CFD features
- Still more: space-time-stochastic adaptivity (provenance data and online queries); computing solution statistics (post-processing)
- Uncertainty on the initial conditions (initial scenario of the currents – Lesshaff et al. . Towards inverse modeling of turbidity currents: The inverse lock-exchange problem. Computer & Geosciences, 37(4): 521-529,2011) and on settling velocity

Lock Exchange Configuration

$Gr = 2.5x10^6$ and 320,000 tetrahedra



Example 1: Homogeneous uncertain initial condition – $c = \overline{c} + \sigma_c \phi$ with mean and variance given by $(\overline{c}, \sigma_c) = (1, 0.2)$. No sediments deposition ($u_S = 0$)

Example 2 :Non uniform initial condition $c(x, y, 0; \phi)$:$c(x, y, \phi) = c_0 + \sum_1^2 \phi_n \sqrt{\lambda_n} f_n(x, y)$, where $\lambda_n = \frac{4\eta_1 \eta_2 \sigma_Y^2}{[\eta_1^2 (w_i^{(1)})^2 + 1][\eta_2^2 (w_j^{(2)})^2 + 1]}$ with $(\eta^2 w^2 - 1)s(wL) = 2\eta wc(wL)$ and $f_n(x) = \frac{1}{\sqrt{(\eta^2 w_n^2 + 1)L/2 + \eta}} [\eta w_n cos(w_n x) + sin(w_n x)]$. The random variables ϕ with support [-1,1] are assumed independent and uniformly distributed.

Uncertainty Propagation - Homogeneous Initial Conditions

Propagation of uncertainties in the QoIs: deposition map

Multipoint Statistics – Spatial Correlation

Final Remarks and Next Steps

- RB-VMS as LES model for Tubridity Currents. Room for improvement in the subrgrid modeling
- FSI - ALE formulation for handling bed form evolution
- We have made progress on exploring Chiron (Scientific Workflow Management Systems) capabilities for UQ analysis - two level paralelism and first steps towards adaptivity. More to come.
- Characterization of $c(x, 0)$ through inverse stochastic algorithms (again Chiron has a role to play)

Future Trends

Bayesian Analysis of Turbidity Currents Deposition

A question raised by a geologist

Imaginemos que no eixo do escoamento, ao longo da linha central, exista um poço (posição XX). À cerca de 1139 metros afastado dele, existe um outro poço (posição YY), conforme o esquema abaixo. O poço na posição YY estä mais alto cerca de 90m em relação ao poço XX.
A pergunta é a seguinte. Uma corrente, entrando pelo eixo, vai depositar na posição XX. Essa mesma corrente tem condições de depositar também na posição YY, apesar do mesmo estar mais alto ??

Penso que poderíamos variar o número de Reynolds dessa corrente, e ver se em alguma condição, ela consegue deixar sedimento no poço mais alto.

Isso teria um grande interesse, pois nos ajudaria a entender se as areias que observamos nos dois poços tem alguma chance de estarem conectadas, uma informação muito relevante para o desenvolvimento dessa área.

A response (in elaboration)...

- Integrating (well log from XX) data with the numerical model
- Robust predictions relying upon taking into consideration uncertainties (measurements + numerical inputs)
- Probabilistic framework: odds to reach YY translated into joint probabilities ($p(\mathbf{D}_{XX}, \mathbf{D}_{YY})$)
    - Flow driven by spatial distribution in the begining of the flow (initial conditions (scenario). It is not known!! Inversion (quite expensive).
    - Initial conditions modeled as random (uncertain) fields (sensitivity analysis) - Uncertainty Quantification
    - Different scenarios must be analyzed. Physical experiments would help a lot.
    - Results might be (easly) integrated in a decision making framework (risk analysis)

Bayesian Analysis Framework

Stochastic framework - parameters or (and) physical quantities are modeled as random variables (fields).

Physics - based models phrased as stochastic partial differential equations (SPDE).

Bayesian techniques emerging as leading tools for analysis

Analysis Bayesian workflow (inspired in Bayesian modeling of air-sea interaction. Berliner et. al., Journal of Geophysical Research, 2003.)

$$\pi_{post} := \pi(\mathbf{D}, \mathbf{m}|\mathbf{d}) \propto [\mathbf{d}|\mathbf{D}]\ L(\mathbf{D}|\mathbf{m})\ \pi_{prior}(\mathbf{m}) \qquad (2)$$

d ... well log data : deposits heights and sediments distribution.
m . . . initial conditions (initial scneario) and settling velocity
[**d**|**D**] . . . data model (measurments errors)

Analysis

- Equation (2) is often not amenable to be treated by analytcal means
- Indeed, one might want only to compute quantiles... $P(D_j \leq \bar{D})$ or analyse plausible scnearios. Sampling will do.
- Sampling from π_{post} is not a trivial task... Markov Chain Monte Carlo algorithms represent a good option. But they will be quite expensive (a forward problem is to be solved for each sample (accpeted or not)
- Computational Surrogates :I.Bilionis, N. Zabaras, B. A. Konomi, G. Lin. Multi-output separable Gaussian process: Towards an efficient fully Bayesian paradigm for uncertainty quantitication. Journal of Computational Physics 241 (2013) 212–239.