Proceedings of the 3rd International Symposium on Uncertainty Quantification and Stochastic Modeling
D.A. Rade; A. M. G. Lima (Editors), ABCM, Maresias, SP, Brazil, February 15-19, 2016

Modelling particle-laden turbulent flows with parametric uncertainties.

Gabriel M. Guerra[1], Souleymane Zio[1], Henrique F. Da Costa[1], Paulo L. B. Paraizo[2], Jose J. Camata[3], Renato N. Elias[3], Alvaro L. G. A. Coutinho[3], Fernando A. Rochinha[1]

[1] Mechanical Engineering Department, Federal University of Rio de Janeiro, Brazil

[2] Petrobras UO-SEAL Sergipe Operational Unity, Aracaju, Sergipe, Brazil

[3] High Performance Computing Center and Department of Civil Engineering,Federal University of Rio de Janeiro, Brazil

Abstract: Particle-laden flows are a very complex natural phenomenon and considered one of the most responsible for sediment transport and deposition that lead to the formation of basins hosting oil reservoirs. Those turbulent flows are triggered by small differences in the fluid density induced by the presence of sediment particles. A detailed modelling of this phenomenon may offer new insights to help geologists to understand the deposition mechanisms and the final stratigraphic form of the reservoirs. The increasing reliance on numerical simulation for the analysis of these complex physical systems has led in recent years to a strong development of knowledge in this area. In this sense, Uncertainty Quantification (UQ) provides a framework to enable robust computer simulations that take into account the unavoidable uncertainties present in input parameters and in the model structure (model discrepancy). The present work extends the efforts of the authors to build a reliable computational model for the prediction of deposition of sediments transported by particle laden-flows. It presents a UQ analysis, employing a probabilistic perspective, to consider the impact of using phenomenological models on quantities of interest such as bottom shear stresses and deposition maps. Those models combine experimental observations with physical intuition and try to capture the influence of the sediment concentration on the local flow viscosity and settling velocity. Both parameter uncertainties and different forms of model discrepancy (stochastic spatial fields) are considered in the simulations through non-intrusive stochastic collocation methods while a parallel Navier-Stokes solver handles the underlying deterministic model. A scientific workflow management engine tool designed for high-performance computers supports the whole procedure.

Keywords: Particle-laden flows, Model discrepancy, Uncertainties

INTRODUCTION

A significant number of applications rely on the use of computational predictive models. The success of such approach depends on a good understanding of how uncertainties present on the available information beforehand affect the reliability of the output predictions. Despite there are different approaches for handling uncertainties, here only a probabilistic perspective is considered. The traditional computational statistical tool for Uncertainty Quantification (UQ) in science and engineering is the Monte Carlo method. This method starts with the generation of an ensemble of random realizations associated to the uncertain model inputs, and afterwards applies deterministic solvers repetitively to obtain the ensemble of results. This output ensemble allows the computation of the model responses statistics, like, for instance, mean and standard deviation. Monte Carlo implementation is straightforward and independent of the stochastic dimension of the input space, but its convergence rate is very slow (proportional to the inverse of the square root of the number of realizations) which makes the method infeasible due to the large computational costs. It is still more critical when those models are built upon physics principles described through Partial Differential Equations (PDEs). Another technique developed to enhance the computational efficiency of UQ analysis is the Stochastic Galerkin method (SG), which employs spectral representations of inputs and solution through Polynomial Chaos expansions [8]. A Galerkin projection minimizes the error of the truncated expansion, and the resulting set of coupled equations is solved to obtain the expansion coefficients. SG methods are highly suited to dealing with PDEs, even in the case of nonlinear dependence on the random data. The main SG drawback is the need to solve a system of coupled equations requiring efficient and robust solvers and, most importantly, the modification of an existing deterministic code. This last issue entails difficulties on using commercial or legacy codes. A non-intrusive method referred to as Stochastic Collocation (SC), see [54], arises aiming at addressing this point. SC methods combine multivariate polynomial interpolation and deterministic solvers. Similarly to SG methods, SC methods achieve fast convergence when the solution has sufficient smoothness in random space. The presence of steep gradients or finite discontinuities in the input-output mapping may lead these methods to converge very slowly or even fail to converge.

This work examines an interesting UQ situation involving particle-laden flow models used in preliminary analyses of subsea sedimentary systems. Such systems are a particular case of gravity currents [49], often also called density currents. They consist of flows generated from (possibly small) differences in the local fluid density. The density difference promotes a pressure gradient that triggers and drives the flow. This spatial density variability might result from local changes in salinity or temperature. Moreover, it can also be due to the presence of sediment particles in suspension, what motivates the resulting currents to be known as particle-laden or particle-driven flows. Indeed, gravity currents are present in many different contexts and occur naturally as well as caused by human actions [40]. Natural examples are avalanches, deep water turbidity currents and volcanic eruptions. On the other hand, industrial accidents can cause dispersion of heavy gases in the atmosphere that propagate through a forehead. A comprehensive list of examples may be found in [49], [6] and [40]. The particles can be carried out for long distances and, eventually they will settle, being responsible for sediment deposits generating geological formations of considerable interest for the oil and gas industry. Sedimentation and erosion promoted by particle-laden flows can mold the seabed producing different geological structures such as canyons, dunes and ripples. Such geological flows phenomena are the main focus here. They typically develop strong turbulence, which impacts the particles ability to move relatively to the carrying fluid. For instance, data recorded for turbidity currents in the ocean suggests Reynolds numbers of the order of 10^9 [40]. Two mechanisms involving the transport of sediment are particularly important. Near the bottom the particles tend either to settle or to be re-entrained from the seabed, and depending on what prevails, settling or resuspension, the current, and its turbulent structures, might evolve in an entirely different manner, and consequently those flow changes affect the transport of particles. In the present analysis we only address settling effects.

Here, following [41], a monodisperse mixture model is considered, comprising the Navier-Stokes equations to describe the incompressible viscous flow of the carrier fluid and the advective-diffusive transport to represent the mass balance of sediments. Therefore, in contrast with others in the literature, this model is set on a Eulerian-Eulerian framework. The coupling between both equations is through the Boussinesq approximation introduced in the vector of body forces in order to reproduce the gravitational effects associated with small variations in density. Nasr-Azadani et al [41], employ Direct Numerical Simulation to deal with turbulence, which leads to excessive computational time. On the other hand, Large Eddy Simulation (LES) models [50], built upon spatial filters are used in the simulations of [45] and [46], offering better balance between computational effort and accuracy. This is particularly helpful in the context of UQ analysis, that requires running a large number of simulations corresponding to the SC grid points. The present investigation uses the Residual Based Variational Multiscale finite element method (RBVMS), that consistently approximates the effects of the subgrid scales on the resolved scales ([36], [32] and references therein) and can also be viewed as a LES method [50]. Another crucial aspect towards building a tractable computational tool within the present context is to fully explore the capabilities of high performance computers. Here, optimized parallel deterministic solvers, generating a significant amount of data, are supported and steered by Chiron [44], a Scientific Workflow management engine designed for high performance computer applications.

The primary objective here is to present an accurate, reliable, and computationally efficient approach to build a deposition map describing the spatial distribution of sediments left by a special type of particle-laden flow, that is, a turbidity current. This map might help geologists to understand the formation of geological structures (reservoirs) that occurred a long time ago. More specifically, this map, which is probabilistic due to the unavoidable presence of uncertainties, might guide the pinpointing of spots of interest for oil exploitation and the geological connection among already explored wells and potential zones for drilling. The ingredients for achieving our objective is the combination of stochastic collocation, a high performance and accurate flow solver and the use of a Scientific Workflow management engine. Putting all together, a stochastic, high-fidelity coupled multi-physics based computational model is built, enabling the efficient construction of probabilistic deposition maps through computer simulations.

The remainder of this paper is organized as follows. Section 2 presents the mathematical model for the particle-laden flows of interest, that is, polydisperse turbidity currents. The following Section discusses the stochastic modeling and the uncertainty quantification. Section 4 is dedicated to the presentation and discussion of the results and the last Section summarizes the main findings.

MATHEMATICAL MODEL: MONODISPERSE MIXTURE

This section presents the mathematical setting for the numerical simulation of particle-laden flows within a Eulerian - Eulerian framework introduced in [41] for monodisperse currents. The term polydisperse refers to the possibility of the mixture of sediment particles to contain N different grain sizes. The flows of interest here are mainly driven by small differences in the density promoted by the heterogeneous presence of sediment particles within the fluid, that explains why they are deemed particle-laden flows. The double mention above to Eulerian is to emphasize that the mass of sediment particles is modeled as a continuum in dilute proportion embedded in a mixture with clear fluid. That motivates to assume that the sediment motion can be accurately described by an advection-diffusion transport equation. This pure Eulerian formulation is in contrast with other formulations that employ Lagrangian tracking of particles [39]. Moreover, the interaction between the two phases, carrier fluid and sediments, considers a two-way coupling that also takes into consideration the particle effects on the flow. In the remaining of this section, governing equations for the monodisperse mixture along with the proposed computational formulation are discussed.

Governing Equations for Incompressible Flows Coupled with Sediment Transport

The spatial domain in which the flow takes place along the time interval $[0, t_f]$ is denoted by $\Omega \subset \mathbb{R}^{n_{dim}}$, where n_{dim} is the number of spatial dimensions, and Γ the boundary of Ω. A velocity-pressure non-conservative form of the Navier-Stokes (NS) equations describes the incompressible turbulent fluid flows carrying dilute suspensions of sediments. Confining the present modeling to small particle volume fractions allows for assuming that particles inertia and particle-particle interactions can be neglected. Moreover, we also apply the Boussinesq hypothesis which accounts for the fluid - particle interaction by means of a forcing term proportional to the local difference in the fluid density due to the presence of sediments. Fluid motion drives the particles, but they are also endowed with extra mobility modeled by their settling velocity $u_{S_i} (i = 1, ..., N)$, assumed constant in the gravity direction $\mathbf{e}^g$ and proportional to their sizes, such that coarser grains drop faster. The constant settling velocities are either estimated by experiments or analytically, in the last case admitting slow relative motion (Stokes flow) [38]. Thus, N uncoupled advection-diffusion equations model the sediment transport. The motion of each grain size embedded in the mixture is mapped by the fields $c_i = C_i/C_0$, the scaled concentrations, expressing the volume fraction occupied by each particle size. C_i and C_0 are, respectively, the actual concentration and a normalization value, the latter typically taken as the total initial volume fraction of the particles. Diffusion is supposed to be quite small, and its inclusion in the modeling is often motivated by numerical reasons [18]. Therefore, the dimensionless equations that govern the particle-laden flow are:

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

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in} \quad \Omega \times [0, t_f] \tag{2}$$

$$\frac{\partial c_i}{\partial t} + (\mathbf{u} + u_{S_i}\, \mathbf{e}^g) \cdot \nabla c_i = \nabla \cdot \left(\frac{1}{Sc_i \sqrt{Gr}} \nabla c_i \right) (i = 1, .., N) \text{ in } \Omega \times [0, t_f] \tag{3}$$

where $\mathbf{u}$, p and t are, respectively, non-dimensional velocity, pressure and time. Above, p, many times referred in the literature as the dynamic pressure, results after removing the hydrostatic component of the pressure. Moreover, $c_T = \sum_{i=1}^{N} c_i$ is the total concentration of sediment and *Gr* is the Grashof number that expresses the ratio between buoyancy and viscous effects given by:

$$Gr = \left(\frac{u_b}{\nu H} \right)^2 \tag{4}$$

with ν is the fluid kinematic viscosity, H is a characteristic length of the flow and $u_b = \sqrt{gHC_0(\tilde{\rho}_p - \tilde{\rho}_f)/\tilde{\rho}_f}$ is the buoyancy velocity; g stands for the gravity acceleration and $\tilde{\rho}_p$ and $\tilde{\rho}_f$ for, respectively, particles and fluid densities. It is assumed that the different grains have the same density. A second dimensionless number resulting from turning the governing equations into a non-dimensional form is Sc_i, the Schmidt number, that expresses the ratio between diffusion and viscous effects given by:

$$Sc_i = \frac{\nu_i}{\kappa_i} \tag{5}$$

where κ_i are the diffusion coefficients, supposed to be very small.

Essential and natural boundary conditions for Equation (1) are $\mathbf{u} = \mathbf{g}$ on $\Gamma_\mathbf{g}$ and $\mathbf{n} \cdot \left(-p\, \mathbf{I_d} + \frac{1}{\sqrt{Gr}} \nabla \mathbf{u} \right) = \mathbf{h}$ on $\Gamma_\mathbf{h}$, where $\Gamma_\mathbf{g}$ and $\Gamma_\mathbf{h}$ are complementary subsets of the domain boundary Γ. Functions $\mathbf{g}$ and $\mathbf{h}$ are given, and $\mathbf{n}$ is the unit outward normal vector of Γ. A divergence-free velocity field $\mathbf{u}_0(\mathbf{x})$ is the initial condition for the velocity and $c_i(\mathbf{x}, 0)$ describing grain size composition and concentration of the suspended sediment in the begining of the current have to be prescribed for the transport equation. For equation (3), boundary conditions modeling the transport of particles into and out the flow domain are: $c = c_{i_n}$ on $\Gamma_{i_n}^{c_i}$, $(u_{S_i} \mathbf{e}^g\, c_i - \left(\frac{1}{Sc_i \sqrt{Gr}} \right) \nabla c_i) \cdot \mathbf{n} = 0$ on $\Gamma_h^{c_i}$ and $\frac{\partial c_i}{\partial t} - u_{S_i} \nabla c_i \cdot \mathbf{n} = 0$ on Γ_{bottom}, with $\Gamma = \Gamma_{i_n}^{c_i} \cup \Gamma_h^{c_i} \cup \Gamma_{bottom}$ and $\Gamma_{i_n}^{c_i} \cap \Gamma_h^{c_i} \cap \Gamma_{bottom} = \emptyset$. The former, a Dirichlet condition, describes the quantity of sediment entering in the flow domain. The second and third boundary conditions are enforced to reproduce physical mechanisms of particle motion through the remaining boundary, either by diffusion or advection. Sedimentation is allowed at the bottom on Γ_{bottom}. This last condition implies in loss of sediment, but does not take into account any modification of the bottom geometry by deposition. Moreover, no explicit particle resuspension mechanism, allowing particles going back to the flow after hitting the bottom, like erosion, is included. No significant amount of resuspension is expected for the flow conditions analyzed here [38]. Therefore, at the bottom, the boundary condition is nothing but the net flux of sediment mass deposited by the current. Moreover, for each spatial point $\mathbf{x}$ on Γ_{bottom}, the contribution of the i-th grain size to the layer thickness resulting from the deposition is given by integrating the particles fluxes till the time t resulting in surfaces defined over the bottom as:

$$D_i(\mathbf{x}, t) = \int_0^t u_{S_i}\, c_i(\mathbf{x}, t)\, d\tau \tag{6}$$

The resulting deposit thickness is obtained by summing up all the i-th grain size contributions. Therefore, at each time t, the total height corresponding to the deposition on a specific point at the bottom is $D_T = \sum_{i=1}^{N} D_i$. The final spatial maps computed at the end of the current ($t = t_\infty$), $D_i(\mathbf{x}, \infty)$, are considered in the present study of high interested and will be dubbed as Quantities of Interest (QoI), inasmuch they characterize the deposition patterns which can be used to infer a geological model of the basin [13]. Those maps contain both thickness and composition of the deposits. At this point, it is important to recognize that the genesis of the final geologic formation occurs along a long period of time resulting from different events. The above model is supposed to reproduce a single event. However, to obtain the final form we have to consider a sequence of simulations in which each event deposits, and might erode, stacking sediment mass over the previous ones.

Finite Element Formulation and Turbulence Subgrid Modeling

The solver for the sediment transport coupled problem employed here relies on a weak formulation based on the Residual Based Variational Multiscale Method (RBVMS) introduced within the context of stabilized finite element methods. RBVMS have been used with success in the simulation of turbulent flows [10] , [21] and [32], free-surface flows [37] and multi-transport [25] and [9], two key aspects of the present problem. Indeed, the finite element formulation employed here is a direct extension of the one proposed in [32] for polydisperse currents. The interested reader will find all details about the formulation, with special emphasis on the role of the subgrid modeling in the turbulent transport of the sediments in [32]. Therefore, here, only specific aspects will be detailed. RBVMS relies on a scales splitting of the physical variables combined with variational projections [32]. This splitting involving the large scales (those explicitly captured by the numerical grid) and the fine scales (subgrid scales), that is,

$$\begin{aligned} \mathbf{u} &= \mathbf{u}_h + \mathbf{u}' \\ p &= p_h + p' \\ c_i &= c_{h\,i} + c_i' \end{aligned} \tag{7}$$

where the subscript h denotes the large scale component of the solution, while the superscript $'$ refers to the subgrid complement. The above splitting of scales is to be inserted in a standard weak formulation built upon Equations (1) to (3), assuming as in [32], a simple algebraic model for the fine scales, that is,

$$\begin{aligned} p' &= \tau_c R_c \\ \mathbf{u}' &= \tau_m \mathbf{R}_m \\ c'_i &= \tau_{t_i} R_{t_i} \end{aligned} \tag{8}$$

where R_c, $\mathbf{R}_m$ and $R_{t_i}, i = 1, ..., N$ are the discrete residuals of the coarse scale equations. The $\tau's$ are mesh dependent parameters, computed as in [32]. The final finite formulation is obtained substituting the above expressions in the weak formulation for the coarse scales. It can be shown that RBVMS stabilizes the numerical solution for convection-dominated flows and also allows equal-order interpolation for velocity and pressure, as is the case of the present work. Furthermore, the final formulation is now understood ([48], [16]) to lead to Large Eddy Simulation (LES) framework, in which the fine scales model above provides a subgrid model for turbulence. The use of a LES approach, although computationally intensive, is considered crucial to improve the turbulence prediction. The turbulence structures within the turbidity currents, as the computational simulations to be presented later in this paper, involving recirculation and separation of the flow have great impact on the final depositional pattern.

The solution of all test problems presented in this work employs the EdgeCFD software. EdgeCFD is a parallel Fortran90 finite element code where the computational solution kernel consists of a staggered implicit predictor–multicorrector time integration scheme as described in [27] for both incompressible fluid flow and particle transport equations. The generalized trapezoidal rule is employed in the time discretization, with an adaptive time stepping procedure based on a proportional-integral-derivative (PID) controller (see [53] for further details). The nonlinearities due to the convective term on the Navier–Stokes equation is treated by an Inexact Newton–GMRES algorithm as described in Elias et al [26]. In this solution algorithm, at the beginning of the nonlinear iterations in each time step, the algorithm computes large linear tolerances, producing fast nonlinear steps. As the iterations progress towards the solution, the inexact nonlinear method adapts the GMRES tolerances to reach the desired accuracy. A nodal-block diagonal preconditioner is employed for the flow equation and a diagonal preconditioner for each transport equation. Linear tetrahedra together with an edge-based data structure are used in all computations [26]. EdgeCFD is also able to solve fluid-structure interaction (FSI) problems where the mesh movement is treated by the Arbitrary Lagrangian Eulerian (ALE) formulation, which is useful to describe bed morphodynamics [17].

INPUTS STOCHASTIC MODELING AND UNCERTAINTY PROPAGATION

Uncertainty Quantification for high fidelity computations built upon physical-based models combines three main components. The first consists in putting together robust numerical tools, typically fast solvers, for handling large discrete versions of the underlying deterministic problem, which are often implemented in a parallel environment due to the associated large computational costs. The other two components address the involved stochastic aspects: modeling and characterizing the input uncertainties and a method to efficiently propagate those uncertainties. At this point, it is worth mentioning that only the impact of input uncertainties on the simulations outputs are considered here particualry be investigate model discrepancies [35]. Below, a brief description about how these three aspects are treated in this study is presented.

Nonintrusive UQ methods, roughly describing, use a (expected small) number of runs of a deterministic computational model, each one having as inputs judiciously chosen points of the stochastic input space. Statistics of the outputs are then estimated from the deterministic computations, generating a significant amount of data and thus requiring careful management [31].

Phenomenological modeling: closure equations and uncertainties

The interdependence of the motion of the two components of the mixture, fluid and sediments, is expressed in the above balance equations through a buouyancy force proportional to the total sediments concentration at each spatial point acting on the fluid, the depostion mechanism embedded in the botton boundary condition, the convective velocity in the transport equation, and, the particular focus here, phenomenological relations to describe the effect of higher concentrations on the viscosity and settling velocity of the particles. The modeling of this modified rheological behavior introduces two closure equations to the mathematical problem. Here we adopt, despite the variety of possibilites found in the literature [5], for the viscosity the model of Krieger and Dougherty [1]

$$\mu_m = \mu_0 \left(1 - \frac{c}{c_m}\right)^{-2.5*c_m} \tag{9}$$

where c_m is the maximum volumetric concentration. This particular model has been used in [2] to help in the understanding of turbulence modulation in nondilute sediment transport.

The above nonlinear phenomenological models are supposed to reproduce the rheological response of the mixture with a limited degree of accuracy. They are employed to pursue a compromise between computational costs and fidelity to reality. More sophisticated models, like those based on the two-fluid approach [2], are supposed to deliver more accuracy but the simulations would, tipically, lead to more intense computations as well. In order to fullfill the compromise and provide reliable results with computational simulations, it is crucial to estimate the impact of potential pitfalls of those models in the final predictions. [4] presents an analysis of how the dynamics of turbidity currents are sensitive with respect to empirical relations describing mass exchange with the surroundings and carries out a validation of turbulent closure models for particle-laden flows.

Uncertainty Quantification (UQ) is considered a central component for the analysis of complex computer models. In general terms, it deals with connecting inputs uncertainties with their respective impact observed in the outputs of the computational simulations. We can identify two main sources of uncertainties associated to those phenomenological models. The first is related to the estimation of parameters, which often employs standard experimental techniques that entails some level of uncertainty due to noise in measurements or extrapolation arising from differences between the experimental scenarios and those of the applications. More relevant in the present context as a source for uncertainties is the model discrepancy. [3], that is intended to express the lack of information about the physics due to the assumed functional form used in the models.

Probabilistic approaches have become a common option within the realm of UQ. Parameters are represented by random variables (or fields), what requires for a complete characterization the estimation of joint probabilities density functions (PDF). Due to the different phenomenoligies involved in 5, we adopt two different strategies to model the inherent uncertainties. Building descriptions for model discrepancies requires a deep knowledge of the problem in hand, which, typically, makes it more difficult to handle than parameter uncertainties. Moreover, model discrepancy was shown in [**?**] to play a key role in computer models calibration and validation, integrand parts on the mitigation of negative impacts of uncertainties on the predictions. The authors employ a Bayesian perspective and they sugest to add in the observation equation a statistical representation of the model discrepancy. Some limitations of such approach in the context of a physics based model like the one proposed here are discussed in [3]. Amongst them, the difficults of naturally imposing physical constraints represents a significant drawback.

Here, we propose a discrepancy model to be embedded in the viscosity model reffered before. That garantees that the resulting closure model reproduces the physics observed for sediment-water mixtures in standard rheological experiments. Figure 1 unveils that the phenomenological models built upon those tests display same trends of growth but also bear important differences in terms of the viscosity values predicted for a specific concentration, especially for medium and high concentrations. Indeed, the grey area indicates such dispersion that can be captured in the following stochastical model

$$\mu_m = \mu_0 \left(1 - \frac{c}{c_m}\right)^{-\lambda*c_m} \tag{10}$$

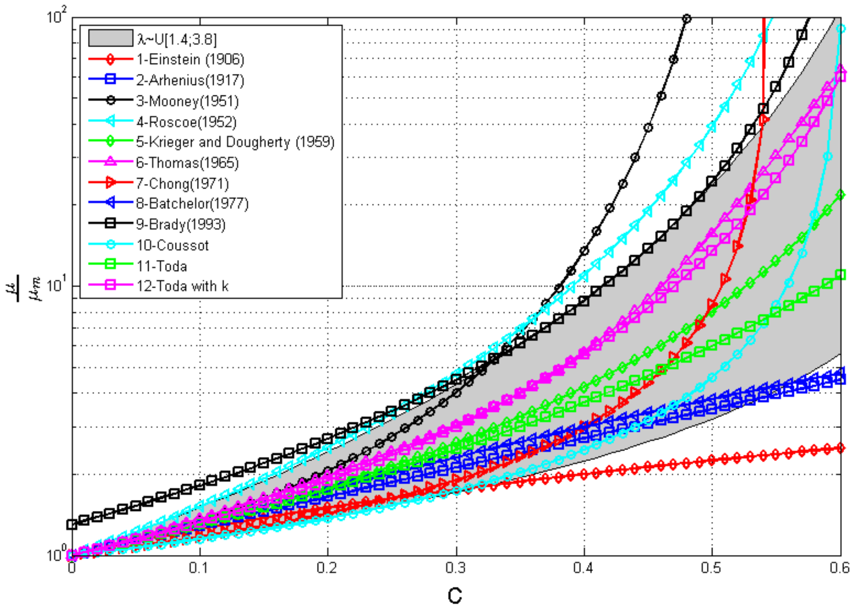


Figure 1 – Sample of statistics for reduced velocity $U_r = 6.9$

with $c_m = 0.74$and having $\lambda = 2.6$ a typical value for monodisperse dispersions of particles.

$$\lambda \quad = \quad \overline{\lambda}\,(1 + \delta\xi)$$

where λ is a random variable that encapsulates the model discrepancy with ξ is an independent uniform random variables with support [-1,1]. Moreover $\overline{\lambda} = 2.6$, $\delta = 0.46$. i.e. λ varying in the interval [1.4, 3.8].

It is important to emphasize that we propose, as discussed in [3], that the model error is embedded in this one parameter. That choice reflects the diversity found in the literature, or in other words our uncertainty about models, and the need for having a tractable computational model. We are performing a UQ analysis, in which we intend to estimate the impact of such model uncertainty in the predictions.

Towards modeling nondilute currents

- Complex underlying physics : non-Boussinesq and non-Newtonian behavior, particle-particle interaction, bed-load behaves like flow through porous media.

- In the present context, two-phase flows models are computer intensive.

- One phase-flow employing enhanced models for the rheology of the mixture can provide a good balance between computational costs and predictive capabilities.

- As example, Krieger and Dougherty equation for viscosity of suspensions, Pseudo-Newtonian fluid with viscosity dependence on the sediment concentration,

In this sense the physical reasoning: What would be the effect in the model response if we consider one phenomenological law covering the behavior of all other. Thus, model discrepancy (error) is embedded in a parameter uncertainty:

COMPUTATIONAL RESULTS AND ANALYSIS

All the computations involved in the UQ analysis were performed taking into consideration the same physical scenario corresponding to the lock-exchange configuration schematically depicted in Figure 2. The lock area contains the fluid mixed with sediments of two different grain sizes, which are assumed to form a homogeneous suspension, and is connected to the basin deposition region through a narrow channel. Upon the lock barrier release, the current starts to flow along the channel, with no deposition as the channel bottom is assumed to be impervious. After reaching the channel end the current spreads laterally, still moving forward, as depicted in the right part of Figure 2. As the current evolves, leaving sediments on the bottom, it tends to lose strength and eventually dissipates ($t = t_\infty$).

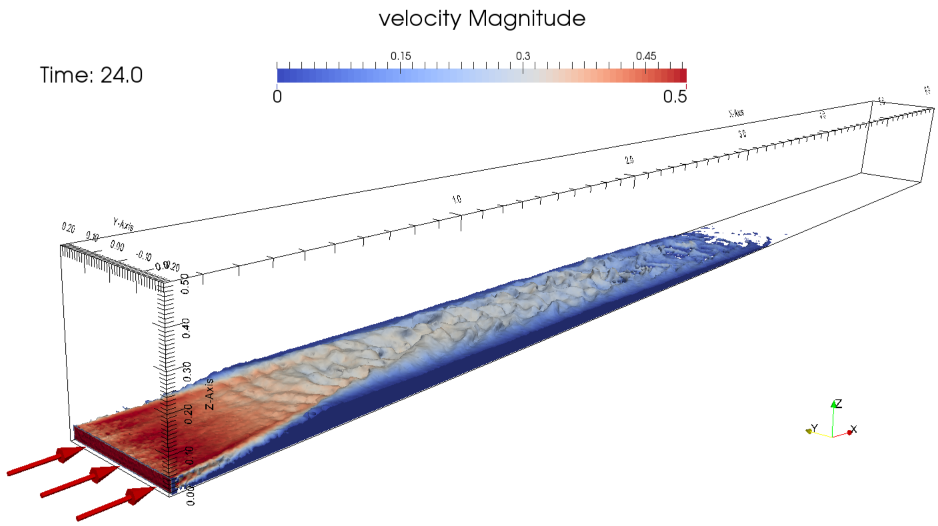


Figure 2 – Computational setup

This computational configuration, that mimics typical experimental setups with a channel with $L_x^c = 6.0$ (streamwise direction), $L_y^c = 0.4$ (spamwise direction), $L_z^c = 0.5$ (height of the channel) and a inlet window with heigth $L_z^w = 0.04$. The area have flat topography. One sediment grain size are uniformly mixed with water and injected by the windows with $Q = 1l/m$. Those values, combined with the settling velocities and initial concentrations defined previously, lead to Grashoff number $Gr = 10^{10}$, which meets laboratory standards, but it does not correspond to typically values of turbidity currents in nature. Despite that, this Grashoff number allows the formation of turbulent structures that interact with the sediments and are responsible for the deposition patterns.

Figure 3 portrays a top view of concentration for standard simulation with constant concentration and considering the Krieger law for nominal value and the diferences at the bottom, all of result at final time of simulation. It is important to note, however, that both snapshots (flow and sediment transport) present complex spatial characteristics, demonstrating the importance of employing a three-dimensional model. Figure 4 shows the lateral view of concentration for standard

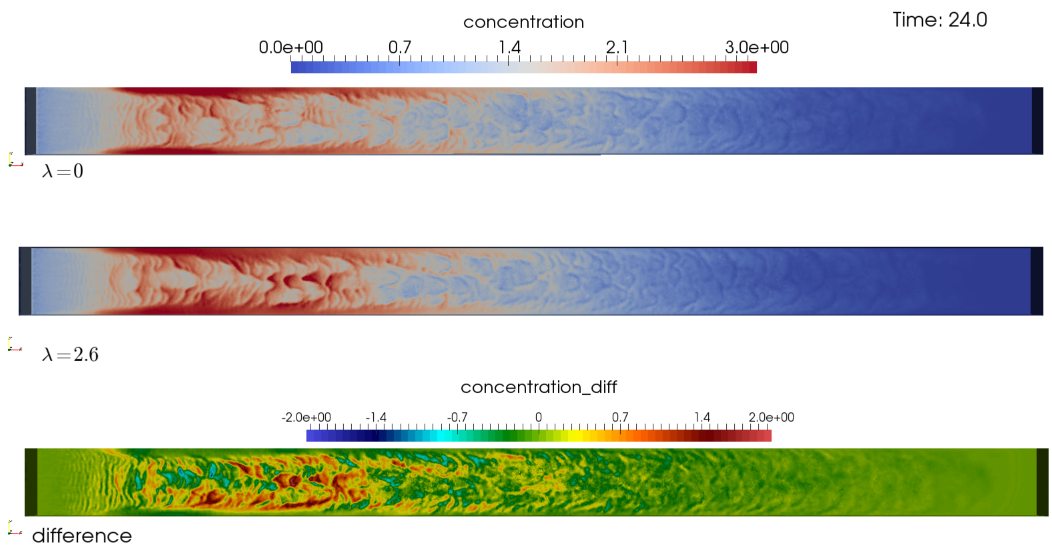


Figure 3 – Diferences bettwen constant and variable viscocity using Krieger law, top view of concentration

simulation with constant concentration and considering the Krieger law for nominal value and the diferences at the bottom, all of result at final time of simulation. It is important to note, however, that both snapshots (flow and sediment transport) present complex spatial characteristics, demonstrating the importance of employing a three-dimensional model. Figures 5 and 6 depicts the mean values of the stochastic fields and their respective standard deviations. At the end of simulation a large amount of sediments had already been deposited. Figure 7 shows the spatial distribution of the sediments deposition mean and standard deviation at the bottom at $t = 24$. An important aspect to be noticed in this figure is the segregation of

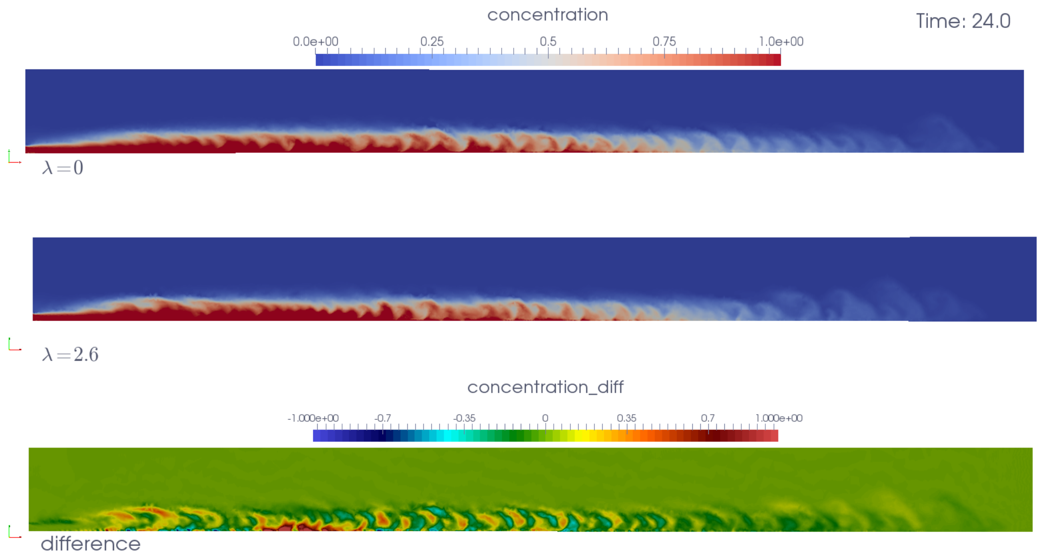


Figure 4 – Diferences bettwen constant and variable viscocity using Krieger law, top view of concentration

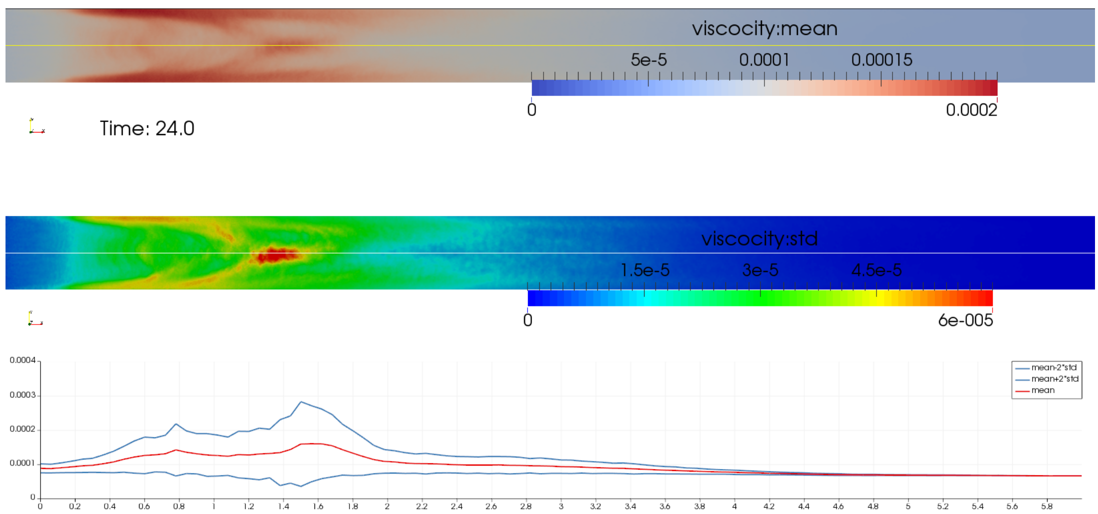


Figure 5 – Top view of viscocity at bottom mean and standard deviation

grain sizes resulting from the combination of the two transport mechanisms (flow and deposition), which will determine the heterogeneous deposition pattern. The sediment deposits, as expected, earlier and closer to the entrance of the basin.

The likelihood of occurrence of a determined event lies in the core of UQ analyses and can be explored in order to help decision making, like in [24] where a hazard map related to geoflows was built with the help of computational simulations. Here, the estimation of probabilities related to the deposits can be computed by sampling over the input stochastic space. Interrogating the inputs-outputs map provided by SGSC using those samples allow us to estimate high-order statistics, like, for instance, probability density functions (PDFs) of the composition. Figure 8 depicts such PDFs that not only are measures of the uncertainties impacts on the simulations predictions, but also can provide analysts important information like the plausibility of finding a certain amount of one of the grain-sizes deposit at specific regions.

CONCLUSIONS AND FUTURE WORK

A high-fidelity coupled multi-physics based computational model was employed to enhance the understanding, qualitatively and quantitatively, of sedimentary depositional systems resulting from turbidity currents. This model takes into consideration the physics of the flow, sediment transport and deposition mechanisms. The computations lead to high resolution spatial and temporal three-dimensional predictions about general features of the flow and its deposits, and great emphasis is placed in quantifying uncertainty on those predictions. These unavoidable uncertainties are induced by the lack of knowledge related to typical inputs of forward solvers associated to the modeling, like, for instance, initial

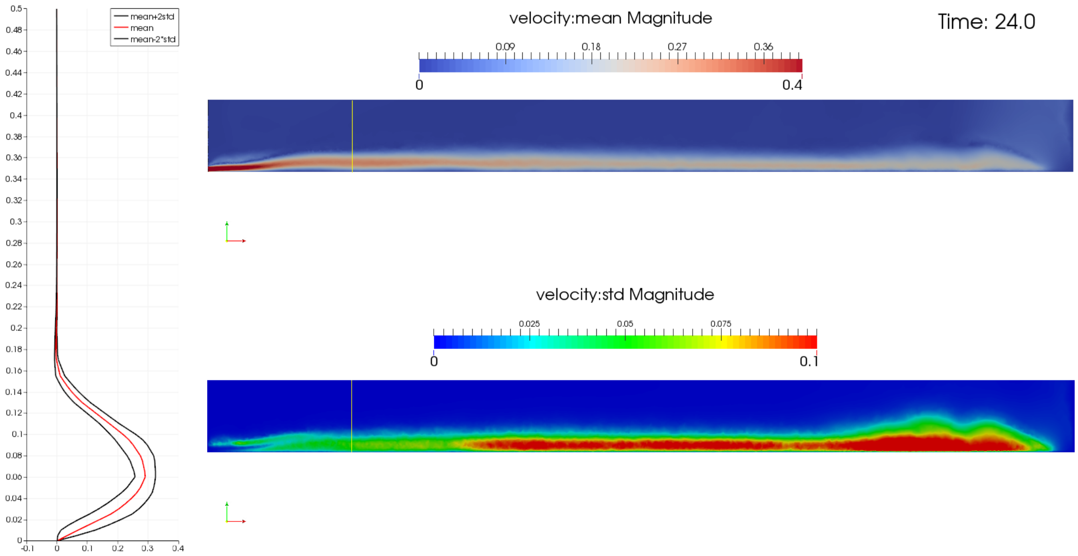


Figure 6 – Side view of mean and standard deviation of velocity field

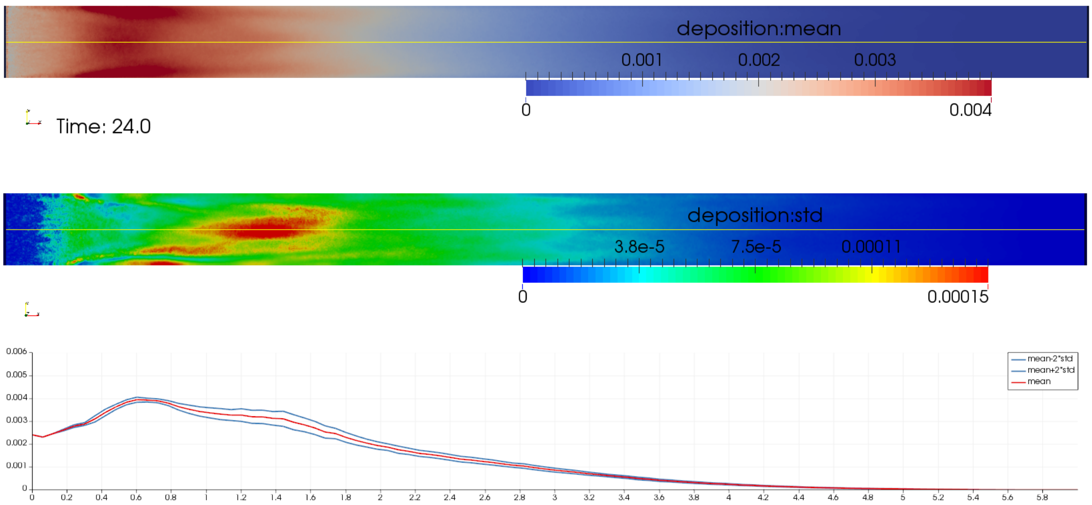
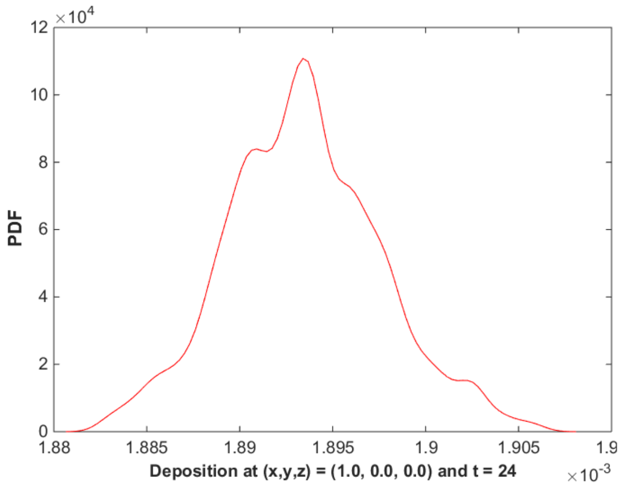


Figure 7 – Top view of deposition mean and standard deviation

conditions and parameters introduced through phenomenological assumptions used to build the model. Uncertainty is addressed here within a probabilistic perspective in which inputs are modeled as random variables or fields. Therefore, outputs of the simulations are consequently also random, and the underlying mathematical problem is transformed into a system of stochastic partial differential equations. The discrete equations are solved in parallel on a high performance computing environment.

The numerical experiments involve a single turbidity event for a relative high Gr number, in an environment that replicates laboratory setups. They illustrate the ability of the proposed stochastic model to assess the effect of parameter uncertainties in the study of geologic depositions systems. The deposition patterns are studied through the computed deposition maps, represented here by spatial stochastic fields. The analysis is supported by scrutinizing spatial correlation functions, mean and standard deviation of the output fields, and high order statistics (PDFs) at given observation points. The study of depositional systems deriving from turbidity currents gains particular relevance in the context of improving reservoir models that can be explored towards optimizing the production. Besides geostatistical techniques, different approaches (see [43] and [42]), ranging from the use of complex physics-based models like the one proposed here, to less computationally intensive simulations, that employ geological rules learnt from observations and accumulated knowledge by experts, can be used to tackle these problems.

The emphasis here is on the impact on the predictions of uncertainties related to the parameters associated to the main mechanisms that drive deposition. The interplay of turbulent flow transport and settling motion responsible for



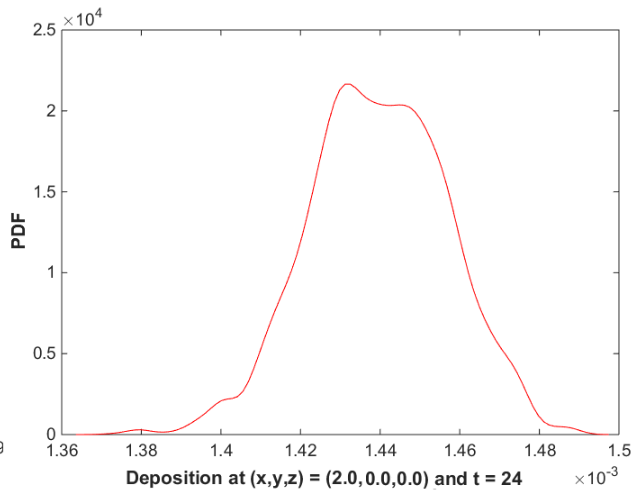


Figure 8 – Probability distribition function for deposition in two points of central line of channel

the final form of the geologic formation, amplifies and spreads uncertainties along the current endurance. The understanding and quantification of such uncertainties is a key point for enabling the use of computational simulations as an effective tool for modeling complex geological formations like those of reservoirs [43], and, eventually, support decision making [47]. Moreover, extending the present UQ analysis for more realistic scenarios, comprising successive turbidity depositions events within a long geological period under hydrodynamical conditions observed in the field (high Gr numbers, considering the modifications in the bottom topography resulting from deposition and erosion), poses a tremendous computational challenge.

That can be tackled by pursuing different approaches. On one side, the computational burden of running the computational codes many times might be alleviated by the use of surrogates, like Gaussian Process Models which are, frequently, built within a Bayesian approach [12]. A probabilistic Bayesian framework also enables to incorporate actual field data available (well logs for instance) to the computational simulations, improving the credibility of the numerical predictions [11] and [15]. The authors expect to report on those challenges in the near future.

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. Special thanks to Prof. N. Zabaras for his invaluable help with Uncertainty Quantification methods. Partial support is also provided by MCT/CNPq and FAPERJ. Computer resources were provided by the High Performance Computer Center, COPPE/UFRJ.

REFERENCES

[1] Krieger I. M., Dougherty T. J. (1959) A mechanism for non-Newtonian flow in suspensions of rigid spheres. T. Soc. Rheol. 3:137152, (doi:10.1122/1.548848).

[2] S. Balachandar and John K. Eaton, Turbulent Dispersed Multiphase Flow Annual Review of Fluid Mechanics Vol. 42: 111-133 (Volume publication date 2010)

[3] K. Sargsyan,Habib N. Najm,R. Ghanem, On the Statistical Calibration of Physical Models International Journal of Chemical Kinetics 02/2015; 47(4).

[4] Traer, M. M. and Fildani, A. and McHargue, T. and Hilley, G. E., Simulating depth-averaged, one-dimensional turbidity current dynamics using natural topographies Journal of Geophysical Research: Earth Surface, vol120, nro 8, 2015

[5] Patryk Widera, Study of sediment transport processes using Reynolds Averaged Navier-Stokes and Large Eddy Simulation. PhD Thesis, Universitet Brussels, August 2011

[6] Allen, J.R., Principles of Physical Sedimentology. *The Blackburn Press* (1985)

[7] Alpak, F.O., Barton, M.D., Caers, J., A flow-based pattern recognition algorithm for rapid quantification of geologic uncertainty, *Computational Geosciences*, **14**: 603 – 621 (2010)

[8] Babuska, I.,Nobile, F., Tempone, A Stochastic Collocation Method for Elliptic Partial Differential Equations with Random Input Data, *SIAM Journal on Numerical Analysis*, **52**(2): 317 – 355 (2010)

[9] Bauer G., Gravemeier V. and Wall, W.A., A Stabilized Finite Element Method for the Numerical Simulation of Multi-Ion Transport in Electrochemical systems, *Computer Methods in Applied Mechanics and Engineering*, **223-224**: 199 – 210 (2012)

[10] Bazilevs, Y., Calo, V.M., Cottrell, J.A., Hughes, T.J.R., Reali, A., Scovazzi, G., Variational multiscale residual-based turbulence modeling for large eddy simulation of incompressible flows, *Computer Methods in Applied Mechanics and Engineering*, **197**: 173 – 201 (2007)

[11] Berliner, L.M., Physical-statistical modeling in geophysics, *Journal of Geophysical Research D: Atmospheres*, **74** : 2321 – 2338 (2003)

[12] Bilionis, I., Zabaras, N., Konomi , B.A., Lin, G., Multi-output separable Gaussian process: Towards an efficient, fully Bayesian paradigm for uncertainty quantification, *Journal of Computational Physics*, **241**: 212 – 239 (2013)

[13] Bonnecaze, R.T., Huppert, H.E., Lister, J.R., Patterns of Sedimentation from Polydispersed Turbidity Currents, *Proceedings of the Royal Society: Mathematical, Physical and Engineering Sciences*, **452**(1953): 2247 – 2261 (1996)

[14] Bungartz, H. J., Griebel, M., Sparse grids, *Acta Numerica*, **13**: 147 – 270 (2004)

[15] Bursik, M., Jones,M., Carn,S., Dean K., Patra, A., Pavolonis, M., Pitman, E.B. and Singh, T. and Singla, P. Webley, P., Bjornsson, H., Ripepe. M., Estimation and propagation of volcanic source parameter uncertainty in an ash transport and dispersal model: application to the Eyjafjallajokull plume of 1416 April 2010, *Bulletin of Volcanology*, **74**(10): 2321 – 2338, 2012.

[16] Calderer, R. , Masud A., Residual-based variational multiscale turbulence models for unstructured tetrahedral meshes, *Computer Methods in Applied Mechanics and Engineering*, **254**: 238 – 253, 2013.

[17] Camata, J. J., Elias, R.N., Coutinho, A. L. G. A., FEM Simulation of Coupled Flow and Bed Morphodynamic Interactions due to Sediment Transport Phenomena, *Journal of Computational Science and Technology*, **7**(2): 306 – 321, 2013.

[18] Cantero, M. I., Balachandar, S., Garcia, M. H., Bock, D., Turbulent structures in planar gravity currents and their influence on the flow dynamics, *Journal of Geophysical Research: Oceans*, **113**(C8): 2156 – 2202 (2008)

[19] Chils, Jean-Paul, Delfiner, Pierre, Geostatistics Modeling Spatial Uncertainty, Wiley (2012)

[20] Codina, R., Stabilized finite element approximation of transient incompressible flows using orthogonal subscales, *Computer Methods in Applied Mechanics and Engineering* **191**(39–40): 4295 – 4321 (2002)

[21] Codina, R., Principe, J., Avila, M., Finite element approximation of turbulent thermally coupled incompressible flows with numerical sub-grid scale modelling, *International Journal of Numerical Methods for Heat and Fluid Flow*, **20**, 492 – 516, 2010.

[22] Codina R., Principe J., Guasch O., Badia S., Time dependent subscales in the stabilized finite element approximation of incompressible flow problems, *Computer Methods in Applied Mechanics and Engineering*, **196** (21–24): 2413 – 2430, 2007.

[23] Coutinho, A. L. G. A., Martins, M. A. D., Sydenstricker, R. M., Elias, R. N., Performance comparison of data-reordering algorithms for sparse matrix–vector multiplication in edge-based unstructured grid computations, *International Journal for Numerical Methods in Engineering*, **66**(3): 431 – 460, 2006.

[24] Dalbey, K., Patra, A.K., Pitman, B., Bursik,M.I., Sheridan, M.F., Input uncertainty propagation methods and hazard mapping of geophysical mass flows, *Journal of Geophysical Research*, **113**: B05203 1 – 16, 2008.

[25] Ehrl A., Bauer G., Gravemeier V., Wall, W.A., A Computational Approach for the Simulation of Natural Convection in Electrochemical Cells, *Journal of Computational Physics*, **235**: 764 – 785, 2013.

[26] Elias, R. N., Martins, M. A. D., Coutinho, A. L. G. A., Parallel Edge-Based Inexact Newton Solution of Steady Incompressible 3D Navier-Stokes Equations, *Lecture Notes in Computer Science*, **3648**: 1237 – 245, 2005.

[27] Elias, R. N., Coutinho, A. L. G. A., Stabilized edge-based finite element simulation of free-surface flows, *International Journal for Numerical Methods in Fluids*, **54**(6 – 8): 965 – 993, 2007.

[28] Elias, R.N., Paraizo, P.L.B., Coutinho A.L.G.A., Stabilized edge-based finite element computation of gravity currents in lock-exchange configurations, *International Journal for Numerical Methods in Fluids*, **57**: 1137 – 1152 (2008)

[29] Elishakoff, I., Notes on Philosophy of the Monte Carlo Method, *International Applied Mechanics*, **39**: 753 – 762 (2003)

[30] Freire J., Koop, D., Santos, E., Silva, C.T., Provenance for Computational Tasks: A Survey, *Computing in Science and Engineering*, **10** (3): 11 – 21 (2008)

[31] Gabriel Guerra, Fernando A. Rochinha, Renato Elias, Daniel de Oliveira, Eduardo Ogasawara, Jonas Furtado Dias, Marta Mattoso, Alvaro L. G. A. Coutinho, Uncertainty Quantification in Computational Predictive Models for Fluid Dynamics using a Workflow Management Engine, *International Journal for Uncertainty Quantification*, **2** (1): 53 – 71 (2012)

[32] Guerra, G. M., Zio, S., Camata, J. J., Rochinha, F. A., Elias, R. N., Paraizo, P. L.B., Coutinho, A.L.G. A., Numerical simulation of particle-laden flows by the residual-based variational multiscale method, *International Journal for Numerical Methods in Fluids*, **73**(8) 729 – 774 (2013)

[33] Lesshafft, L., Meiburg, E., Kneller, B., Marsden, A., Towards inverse modeling of turbidity currents: The inverse lock-exchange problem, *Computers and Geosciences*, **37**(4): 521 – 529 (2011)

[34] Karypis, G., Kumar,V., A Fast and High Quality Multilevel Scheme for Partitioning Irregular Graphs, *SIAM J. Sci. Comput.*, **20**(1): 359 - -392 (1998)

[35] Kennedy, M.C., O'Hagan, A., Bayesian calibration of computer models, *Journal of the Royal Statistical Society B*, **63**: 425 – 464 (2001)

[36] , Lins, Erb F., Elias, Renato N., Guerra, Gabriel M., Rochinha, Fernando A., Coutinho, Alvaro L. G. A., Edge-based finite element implementation of the residual-based variational multiscale method, *International Journal for Numerical Methods in Fluids*, **61** (1): 1 – 22 (2009)

[37] Lins, Erb F. , Elias, Renato N., Rochinha, Fernando A., Coutinho, Alvaro L.G.A. Residual-based variational multiscale simulation of free surface flows, *Computational Mechanics*, **54**(4): 545 – 557 (2010)

[38] Meiburg, E., Kneller, B., Mixing and dissipation in particle-laden gravity currents, *Journal of Fluid Mechanics*, **545**: 339 – 372 (2005)

[39] Bosse, T., Kleiser, L., Meiburg, E., Small particles in homogeneous turbulence: Settling velocity enhancement by two-way coupling, *Physics of Fluids*, **18**:027102 (2006)

[40] Meiburg E., Kneller, B., Turbidity currents and their deposits, *Annual Review of Fluid Mechanics*, **42**: 135 – 156 (2010)

[41] Nasr-Azadani M.M, Hall B., Meiburg E, Polydisperse turbidity currents propagating over complex topography: Comparison of experimental and depth-resolved simulation results, *Computers and Geosciences* , **53**: 141 – 153 (2013)

[42] Michael, H. A., Li, H., Boucher, A., Sun, T. , Caers, J., Gorelick, S. M., *Combining geologic-process models and geostatistics for conditional simulation of 3-D subsurface heterogeneity*, *Water Resources Research*, **46** (5): 1944 – 7973 (2010)

[43] Miller, J., Sun, T., Li, H., Stewart J., Genty, C., Li D., Lyttle, C., Direct Modeling of Reservoirs Through Forward Process-Based Models: Can We Get There?, *International Petroleum Technology Conference*, IPTC – 12729 (2008)

[44] Ogasawara, E.S., Dias, J., Silva, V., Chirigati, F.S., Mattoso, M., Chiron: a parallel engine for algebraic scientific workflows. *Concurrency and Computation: Practice and Experience*, **25**(16): 2327 – 2341 (2013)

[45] Ooi, S.K., Constantinescu, G. Weber, L., Analysis of the evolution of a high grashof number finite-channel lock-release current from initial stages to the inviscid phase, *Proceedings of the 7th International Conference on Hydro-Science and Engineering , Philadelphia, USA*, 1 –10 (2006)

[46] R. Henniger, T. Bosse, L. Kleiser, LES of Particle Settling in Homogeneous Turbulence, *Proceedings in applied mathematics and mechanics*, **6**: 523 – 524 (2006)

[47] Osypov, K., Ivanova, N., Yang, Yi, Fournier, A., Nichols, D., Bachrach, R., Yarman, C.E., Nikolenko, D. Uncertainty as a Rosetta Stone Uniting Geoscience Knowledge and E & P Business Value, *International Petroleum Technology Conference*. IPTC – 16817 (2008)

[48] Principe J., Codina, R., Henke, F., The dissipative structure of variational multiscale methods for incompressible flows, *Computer Methods in Applied Mechanics and Engineering*, **199** (13–16): 791 – 801 (2010)

[49] Simpson, J., Gravity Currents, Cambridge University Press, Cambridge, UK (1997)

[50] Sagaut, P., Deck, S., Terracol M., Multiscale and Multiresolution Approaches in Turbulence, *Imperial College Press* (2006)

[51] Sochala, P., Le Maitre, O.P., Polynomial Chaos expansion for subsurface flows with uncertain soil parameters, *Advances in Water Resources*, **62**: 139 – 154 (2013)

[52] Tezduyar, Tayfun E., *Computation of moving boundaries and interfaces and stabilization parameters*, *International Journal for Numerical Methods in Fluids*, **43**(5): 555 – 575 (2003)

[53] Valli, A. M. P., Carey, G. F., Coutinho, A. L. G. A., Control strategies for timestep selection in finite element simulation of incompressible flows and coupled reaction–convection–diffusion processes, *International Journal for Numerical Methods in Fluids*, **47**(3): 201 – 231 (2005)

[54] Xiu, D., Hesthaven, J.S., High-Order Collocation Methods for Differential Equations with Random Inputs, *SIAM Journal on Scientific Computing*, **27**(3): 1118 – 1139 (2005)

RESPONSIBILITY NOTICE