Renewal Proposal for a XSEDE Allocation on the Supercomputer *Stampede2* at TACC

Fully resolved simulations of passive and active particles in fluid flows

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Abstract

This is a renewal proposal for an XSEDE research allocation. The renewal proposal amounts to **xx SUs in node hours** to be used on *Stampede2*, and to **xx[TB]**] of storage on *Ranch*. The allocation will support the group of principal investigator (PI) Prof. Eckart Meiburg, to investigate transport processes involving strongly coupled fluid and particle phases. The interactions between the two phases play a crucial role in a number of research areas, several among them at the center of petroleum science. In order to advance our fundamental understanding of the grain-scale processes underlying the large-scale dynamics of such particulate flows, the PI has established a research direction in recent years aimed at performing three-dimensional, high-resolution and massively parallel grain-resolving simulations of concentrated particulate suspensions. The availability of such a simulation tool will allow the PI's group to initiate a multitude of new research avenues such as the optimization of oil/sand separation processes, the dynamics of "marine snow," which forms the basis of several geo-engineering concepts proposed for deep-ocean CO_2-sequestration [15], or the collective motion of swarms of self-propelled organisms and their impact on large-scale oceanic mixing.

1 Research objectives

Using XSEDE resources, the team aims at numerically exploring the interaction of passive and active particle-laden flows and sediment beds at the microscopic scale of individual grains via grain-resolving simulations. One goal is the development of accurate models for their erosional and depositional behavior, which can then be incorporated into existing macroscopic simulation codes. Another objective of the present project is the investigation of collective motion of large groups of self-propelled organisms in order to help quantifying their impact on global oceanic mixing in conjuncture with field observations and laboratory experiments. XSEDE resources enable the PI's group to analyze multiscale, realistic systems involving large numbers of individual, active or passive, interacting particles. These research directions are currently supported by the following grants to the PI: Army Research Office W911NF-18-1-0379, NSF CBET-1803380, Naval Surface Warfare Center N00174-16-C-0013, NSF CASIS Grant 1638156, and a grant for a research fellowship by the Deutsche Forschungsgemeinschaft (Germany) KO5515/1-1.

Previous work

The present project started three years ago with our first XSEDE proposal. Using XSEDE resources, we have been able to successfully address interesting fundamental questions regarding double-diffusive turbidity currents[12], as well as the impact of particle-laden flows on the mechanism of double-diffusion[1?]. In addition, we have been able to establish new numerical techniques that allow us to study multiphase flows on the grain scale. For the purpose of carrying out phase-resolved direct numerical simulations of particle-laden flows, the in-house code PARTIES (PARTicle-laden flows via immersed boundarIES) was developed by the PI's group for the challenging situation of horizontal flows over heavy and densely packed sediment beds. This was achieved by using the phase-resolving Immersed Boundary Method (IBM)[22] together with a sophisticated approach to model particle collisions[3]. In the latter reference, we have successfully reproduced experimental results from various experimental benchmark data with high accuracy. The study also contains first results of flows over dense sediment beds. The code has been successfully established and employed on *Stampede2*. In this three-year frame, important efforts have been put into making PARTIES a robust, fast and massively parallel code that follows the new paradigms of supercomputer programming. The code is now shared, improved and maintained by the entire team in the PI's lab and collaborators around the world. It uses a version control system, and is now being developed specifically for modern supercomputing heterogeneous architectures. Efforts have been made, established with a 5-day Hackathon at the ORNL, to support GPU acceleration in PARTIES in order to take advantage of XSEDE's GPU resources on the *Comet* cluster in the future. In the meantime, continuous efforts will be put into improving performance and extending PARTIES by tackling new physical phenomenon. For the upcoming allocation period we kindly request your support for the following three distinct projects:

Project 1: Cohesive Sediment Dynamics in Turbulent Flow

Cohesive sediment is ubiquitous in ecologically sensitive environments such as rivers, lakes, estuaries, fisheries and benthic habitats. Reliable predictions of contaminant and nutrient transport in such settings require accurate models of cohesive sediment dynamics, which we currently lack. For cohesive sediment, which commonly refers to particles below approximately 63 micron in size, interparticle cohesive and adhesive forces due to electric charges frequently dominate over the hydrodynamic and gravitational forces known to govern noncohesive sediment. These interparticle forces can trigger a process known as flocculation, which results in the formation of aggregates much larger than the individual grains. At the same time, turbulent stresses can act to break up these flocs generated by the cohesive forces, so that a delicate balance emerges between coalescence and break-up. Consequently, the dynamics of cohesive sediment in turbulent flows is significantly more complex than that of its noncohesive counterpart, with important implications for particle/floc size distributions and their effective settling rates. Cohesive forces furthermore strongly affect the erodibility of sediment deposits on the sea floor, which in turn influences fluvial and oceanic sediment transport processes. The proposed computational research project constitutes the first attempt to quantify the dynamics of cohesive sediment in turbulent flows. It will address a broad range of fundamentally important questions:

a. how do the turbulence properties affect the equilibrium balance between sediment flocculation/coalescence and break-up?

b. how does the floc size distribution vary as a function of the turbulence and sediment properties?

c. how does the effective settling velocity of the cohesive sediment depend on the turbulence and sediment properties?

d. how are the turbulence properties altered by the sediment?

e. how is the effect of cohesive sediment on turbulence different from that of noncohesive sediment?

f. how is the erodibility of a sediment bed affected by cohesive forces?

Project 2: Gravity currents over erodible beds

Gravity currents play a decisive role in transporting mass, momentum, and energy in our environment [21]. Specifically, turbidity currents are believed to be the most critical mechanism for sediment transport to the ocean floor [11]. This project will extend the extensive PI's work on gravity currents [13;18] in the lock exchange configurations to erodible beds with resolved grains. In contrast to recent grain resolved simulations in pressure-driven channel flow with erodible beds [10;23], our simulations will address the peculiarity of gravity currents as an inherent unsteady process to transport sediment in collaboration with experimentalists [25]. Recent numerical attempts [14] described the particle phase with an Eulerian approach that requires substantial modeling of the complex rheology of dense suspension, which we avoid at the expense of increase numerical costs to simulate individual particles. This project is supported by a grant for a research fellowship by the Deutsche Forschungsgemeinschaft (Germany) KO5515/1-1.
Our specific research objectives are

a. What are the key properties that control the entrainment of bed sediment into the gravity current?

b. How do the gravity current dynamics change with particle entrainment?

c. Are the current, simplified models of sediment transport able to recover the results of our numerical experiments?

Project 3: Internal wave induced by downslope gravity current

Gravity currents in environmental settings often propagate down a shallow slope into a density stratified ambient fluid [? ? ? ?]. The ability for internal waves to exist within stratified mediums results in complex interactions between gravity currents and internal waves [? ? ? ? ? ? ?]. The proposed project extends on the recent PI's work on numerical simulations of a single-release gravity current down a slope, encountering a single internal wave propagating at the interface of a two-layer stratified ambient. A manuscript detailing the results of this work has been submitted to *Journal of Fluid Mechanics* and is currently being reviewed. In this project, our simulation will address the corollary problem of internal waves induced by the propagation of a gravity current through a two-layer stratification. Our specific research objectives are

a. What physical mechanism allows gravity currents to transfer energy into internal waves ?

b. In which parameter range do gravity current form internal waves ?

c. What does the efficiency of the energy transfer depend on ?

d. What are the implications for transport in stratified environments ?

2 Computational methodology

Application

All simulations will be carried out with our in-house flow solver PARTIES. It solves the unsteady Navier-Stokes-Boussinesq equations for an incompressible Newtonian fluid

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u}\mathbf{u}) = \frac{1}{\rho_f}\nabla p + \nu_f \nabla^2 \mathbf{u} + \mathbf{f}_f + \mathbf{f}_{IBM}, \tag{1}$$

and the continuity equation

$$\nabla \cdot \mathbf{u} = 0, \tag{2}$$

with $\mathbf{u} = (u, v, w)^T$ designating the velocity vector in Cartesian coordinates, ρ_f the fluid density, p the pressure, ν_f the kinematic viscosity, $\mathbf{f}_f$ a volume force accounting for buoyancy, $\mathbf{f}_{IBM}$ an artificial volume force introduced by the IBM and t the time. Additionally, a concentration field c is advanced over time, which obeys

$$\partial_t c + \hat{\mathbf{u}} \cdot \nabla \mathbf{c} = \nabla \cdot D \nabla \mathbf{c}. \tag{3}$$

Here, $D(\mathbf{x}, t)$ is the diffusivity of both phases, and $\hat{\mathbf{u}}(\mathbf{x}, t)$ is the compound velocity of the particle and fluid phase. Both are defined in the whole domain as follows

$$D = \xi_f D_f + (1 - \xi_f) D_s \tag{4}$$
$$\hat{\mathbf{u}} = \xi_f \mathbf{u} + (1 - \xi_f) \mathbf{v} \tag{5}$$

Here $\mathbf{v}$ denotes the local velocity of the particle phase that we reconstruct from the linear velocity $\mathbf{u}_p$ and the angular velocity $\boldsymbol{\omega}_p$ of particle p. The fluid indicator function ξ_f is zero inside the spherical particles and unity outside. Note that PARTIES can handle an arbitrary number of additional scalar fields.

Governing equations (1)-(3) hold on the computational domain Ω, which is a cuboid with edge length L_x, L_y, L_z. This domain is divided in N_x, N_y, N_z cells for each direction making up a Cartesian grid with variables arranged with the Marker and cell method[6]. Each field $(\mathbf{u}, p, c)$ is thus discretized at $N_{tot} = N_x \times N_y \times N_z$ grid points by a double precision floating point number. At the boundary of Ω, we are able to specify a variety of conditions (e.g. periodic, no-slip, impermeable, etc.) depending on the particular problem.

Furthermore, we consider N_p spherical particles $\mathbb{S}_p$ with center of mass $\mathbf{X}_p$ immersed into the computational domain. The motion of each individual spherical particle is calculated by solving an ordinary differential equation for its translational velocity $\mathbf{u}_p = (u_p, v_p, w_p)^T$

$$m_p \frac{\mathrm{d}\mathbf{u}_p}{\mathrm{d}t} = \oint_{\Gamma_p} \boldsymbol{\tau} \cdot \mathbf{n} \, \mathrm{d}s + V_p (\rho_s - \rho_f) \, \mathbf{g} + \mathbf{F}_{c,n} + \mathbf{F}_{c,t} \qquad . \tag{6}$$

and for its angular velocity $\boldsymbol{\omega}_p = (\omega_{p,x}, \omega_{p,y}, \omega_{p,z})^T$,

$$I_p \frac{\mathrm{d}\boldsymbol{\omega}_p}{\mathrm{d}t} = \oint_{\Gamma_p} \mathbf{r} \times (\boldsymbol{\tau} \cdot \mathbf{n}) \, \mathrm{d}s + \mathbf{T}_c \qquad . \tag{7}$$

Here, V_p is the particle volume, $\mathbf{g}$ the gravitational acceleration, $\boldsymbol{\tau}$ is the stress tensor, ρ_s the particle density, $I_p = 8\pi\rho_s R_p^5/15$ the moment of inertia, and R_p the particle radius. The vector $\mathbf{n}$ is the outward-pointing normal on the interface $\partial\mathbb{S}_p$, the term $\mathbf{F}_c$ denotes the forces resulting from particle-particle interaction. The torque generated by collision, hence, is $\mathbf{T}_c = R_p \, (\mathbf{n}_p \times \mathbf{F}_{c,t})$. The fluid phase [Eqs. (1)-(3)] and the immersed particles [Eqs. (6)-(7)] are coupled through the source term $\mathbf{f}_{IBM}$ enforcing the no-slip condition at the particle surfaces

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_p + \omega_p \times (\mathbf{x} - \mathbf{X}_p) \quad \text{for } \mathbf{x} \in \partial\mathbb{S}_p. \tag{8}$$

The surface of the particles is represented by discrete Lagrangian markers that communicate with the Eulerian fields $(\mathbf{u}, p, c)$ by interpolation and spreading operations. For the present proposal only spherical particles, each with an arbitrary radius, are used. We published[3] this method that involves a novel collision scheme, together with successful validations against several test cases for binary particle-wall collisions and the collective motion of particles in a horizontal channel flow.

The solution of the scalar field governing equation requires the treatment of a spatially varying diffusivity and the construction of a continuous velocity across the particle and the fluid phase. We do this by Volume of Fluid approach similar to[2] but with an additional features to handle the squirmer model[5], which we validated and currently working on its description in a publication[?]

Numerical methods and efficiencies

The computational performance of PARTIES is detailed in the separate document *Code Performance* to which the reader is referred for further details. The discretization of spatial derivatives is performed with a central finite-difference method. The time advancement is done by a fractional-step method for the pressure using an explicit low-storage three-step Runge-Kutta scheme for the convective terms and a semi-implicit Crank-Nicholson scheme for the viscous terms[9]. To advance the discretized fields from time t^n to $t^{n+1} = t^n + \Delta t^n$ three Runge-Kutta substeps are performed that essentially perform the same key procedures.

Those procedures are the solution of a Poisson equation for the quasi pressure, the solution of a Helmholtz equation for each velocity component and the scalar field via a Conjugate Gradient (CG) method, several interpolation steps between Lagrangian and Eulerian points, and evaluating explicit terms of the time-stepping scheme. Besides the MPI library, PARTIES employs two third party libraries. The FFTW library is used as a part of the Fast-Poisson solver to calculate the quasi pressure and the parallel Hierarchical Data Format (HDF) library is used for data input/output. The HDF5 data model and software libraries are used to write data collectively and from distributed memory. The code is fully parallelized by the Message Passing Interface (MPI) routines utilizing the spatial decomposition of Ω, i.e., assigning to each MPI process a subdomain of Ω and the particles within.

Outputted data is in double-precision floating-point format and is written at certain output steps for flow fields, i.e. the pressure p and the fluid velocity (u, v, w) as well as particle data. Data storage requirements are dominated by the fluid flow variables (we thus neglect the particle data for the storage requirement) and each output of the fluid flow data requires $N_{var} \times N_{tot} \times 8$ bytes. A minimum of $N_{var} = 4$ is needed but it might increase when additional scalar fields are solved for or particle volume fractions are saved. Thus for each simulation, we require a storage of

$$D = N_{save} \times N_{var} \times N_{tot} \times 8 \tag{9}$$

in bytes, where N_{save} is the number of outputs that are necessary to accurately describe the processes of interest in time, which is determined by the user depending on the scientific goal of the simulation. The service units on Stampede2 are calculated with the help of the scaling test, where we determine the wall-clock time $\hat{K}$ needed to advance the simulation by one time step per gridpoint on one 'virtual' node. Thus the node hours S (i.e. the service units SUs) can be calculated by multiplying number of gridpoints and time steps with $\hat{K}$

$$S = N_{tot} N_{step} \hat{K}. \tag{10}$$

In principle $\hat{K}$, which we call *timing coefficient*, depends on the problem size N_{tot} as well as the number of nodes $\hat{P}$. As described in the Code Performance, we will work with $\hat{K} = 2.5 \times 10^{-7}$ (in node seconds) when no preliminary simulation of the specific problem is available. This parameter was obtained for approximately 16 million grid points per node, which showed an optimal parallel efficiency on the SKX nodes.

The number of time steps N_{step} can be calculated from the fact that time-stepping scheme is conditionally stable with respect to the Courant-Friedrich-Levy (CFL) conditions that forces the maximum time step Δt being such that any information is advected less than the width Δx of a cell, i.e. schematically , $\Delta t < \mathrm{CFL}\,\Delta \mathrm{x}/\mathrm{U_{max}}$. To determine the time step we set $\mathrm{CFL} = 0.5$, so that the time step can be explicitly calculated when the maximum velocity U_{max} is known

$$\Delta t = \Delta x\, \mathrm{CFL}/\mathrm{U_{max}}, \tag{11}$$

which yields the number of time steps given the simulation time τ_s

$$N_{step} = \frac{\tau_s U_{max}}{\Delta x \mathrm{CFL}} \tag{12}$$

3 Computational research plan

Project 1: Cohesive Sediment Dynamics in Turbulent Flow

Firstly, one-way coupled, lagrangian point particle simulations of cohesive sediment in a cellular flowfield comprising Taylor-Green vortices of size L and velocity U_o are performed. The goal is to study the competing influences of particle inertia, which on one hand will promote the preferential accumulation of particles in regions of downward fluid motion, thus accelerating their effective settling motion, but which on the other hand will transport particles into regions of high strain, thereby promoting their break-up and reducing their settling rate.The fluid is characterized by its viscosity μ and density ρ_f, the particles by their diameter $\Gamma_D = D/L$ and density $\rho = \rho_p/\rho_f$ and finally the gravity force by the gravitational acceleration g.The non-dimensional parameters of this problem are the Cohesive Number(Co), Stokes Number(St) and the Velocity

Ratio(W) (which is the ratio of Stokes settling velocity and the characteristic velocity U_o).

$$Co = \frac{max(||\mathbf{F}_{cohesive}||)}{\rho_f U_o^2 L^2}, St = \frac{1}{18}\frac{\rho_p D^2 U_o}{\rho_f \nu_f L}, W = \frac{V_s}{U_o} = \frac{1}{18}(\rho - 1)\frac{D^2 g}{\nu_f U_o} \tag{13}$$

We will run simulations with O(10^3) particles each, for different initial value combinations of the Stokes number St_o, the settling parameter W_o and the cohesion parameter Co_o. We will then record the long-time statistical equilibrium values of St, W and the effective settling rate, and analyze these as functions of the equilibrium value of the cohesion parameter Co. These computationally cheap simulations will help us to narrow down the parameter space where the dynamics are very interesting.
Followingly we will explore this parameter space with four way coupled fully resolved simulations as the only accurate way to simulate the motion of particles, whose diameter is greater than the Kolmogorov length scale in a turbulent flow is to numerically resolve the fluid motion around each individual moving particle. We will set up a homogeneous, isotropic turbulent flow, for example via the forcing procedure described in eswaranPope1988, cf. also Bosse et al., 2006. After the flow has reached statistical equilibrium, we will seed it with cohesive sediment grains and then track the dynamics of these grains as they flocculate and break up in the turbulent flow. Both neutrally and negatively buoyant particles will be considered. These simulations will provide information on such quantities as equilibrium floc size distributions, effective settling rates and turbulence modulation as functions of the governing dimensionless parameters, including particle volume fraction, cohesive force strength and the ratio of particle size to Kolmogorov length scale.

Project 2: Gravity currents over erodible beds

Figure **??** sketches the model flume with a typical full-lock exchange configuration for the bed-erosion simulations. The third z-dimension is not drawn since the setup is periodic in this direction. In what follows, we describe lengths relative to the flume height L_y. On the left, heavy fluid of density ρ_1 is located in a lock of length $x_0 = L_y$. This local density change is mediated by the concentration field $c(\mathbf{x}, t)$ that will start to move for $t > 0$. This concentration represent an excess salinity, which is typically used in laboratory experiments[25], such that the diffusivity inside particle is zero $D_s = 0$, i.e. no salt diffuses across the solid bodies. With the beginning of the simulation the dense fluid will spread with a front velocity of $v_F \approx 0.5\mathcal{U}$. Here, $\mathcal{U}$ is the buoyancy velocity $\mathcal{U} = \sqrt{L_y(\rho_1 - \rho_f)/\rho_f}$. The bed of particles is built of polydisperse particles with a small variance around the median diameter D_p, which are randomly placed and then settle without interaction with the fluid phase (i.e. in a vacuum). However, similarly to the experimental work[25], particles (dark gray circles in Fig.**??**) close to the lock will be fixed to avoid the special conditions of the of gravity current acceleration, also after the mobile particles (white filled circles), we fix particles to determine how they sediment out Rephrase this sentence, not super clear ?. The actual size of the flume is constrained by the numerical costs, which we fixed in Sec. 4 and explain next. Our simulations from the current allocation period suggest that a bed height of around 7 particle layers is adequate.
Beside the dimensions of the flume and the particle collision model that we tuned for typical sediments, the problem is described by five non-dimensional parameters ($Re_L = \mathcal{U}L_y/\nu, Sc = \nu/D_f, G = gL_y/\mathcal{U}^2, \rho_s' = \rho_s/\rho_f, \delta = D_p/L_y$) that arise when the governing equation are non-dimensionalized by the introduced scales. Since we are not able to simulate the large length scale ratios and Reynolds numbers that appear in the environment, but want to observe as much as features from a realistic gravity current, we aim for three objectives that are in conflict with each other: (i) In the environment gravity currents are turbulent flows so that we need a sufficiently high Reynolds number, at least $Re_L > 5000$. (2) We need to match the ratio of settling velocity V_s relative to the buoyant velocity $\mathcal{U}$?). Using the Stokes formula this ratio gets

$$V_s/\mathcal{U} = -\frac{\delta^2 G Re(\rho_s' - 1)}{18} \tag{14}$$

$$V_{sd}/\mathcal{U} = -\frac{\delta^2 G Re[-1/G + (1 - \rho_s')]}{18} \tag{15}$$

and inside the undiluted current body $c = 1$.
However the range of settling velocities may vary a lot in the environment, e.g. for a large turbidity current a front velocity of 1m/s is a characteristic number while settling might differ a lot with the sediment size (from

coarse to very fine sand we might find $V_s = 2$mm/s ... 20cm/s, which results in ratios of $V_s/\mathcal{U} = 0.2...2\times10^{-3}$). (3) Resolution requirements grow considerably by reducing the particle size. Indeed, considering that each particle is resolved by σ number of gridpoints the total number of gridpoints is

$$N_{tot} = L_x L_y L_z \times \left(\frac{\sigma}{d_p}\right)^3 \tag{16}$$

The main conflict between objectives is the salinity induced buoyancy that leads to difference in normalized settling velocity of

$$\frac{\Delta^2 Re_L}{18}, \tag{17}$$

Which needs to be small enough to reach into the targeted settling velocity, especially to avoid a rising particles due to positive buoyancy. We found that $\delta = 0.01$ to be feasible value.

Project 3: Internal wave induced by downslope gravity current

Figure 1 sketches the model flume with a lock-exchange configuration, where the gate separating the gravity current fluid and the ambient fluid has height h_0 and is located on a slope. The ambient fluid is stably stratified with two distinct layers of top and bottom density ρ_0 and ρ_2 respectively. The initial density of the gravity current fluid ρ_1 and is such that $\rho_1 \geq \rho_2 \geq \rho_0$. The changes in density are due to salinity and assumed to evolve linearly with the local salt concentration. The third z-dimension is not drawn since the setup is homogeneous and periodic in this direction. The local salinity c determines the density through the equation of state $\rho = \rho_0(1+\alpha c)$ where α is a constant expansion coefficient. Due to our interest in the energy budget of the system, including individual contributions of the gravity current salinity and ambient salinity to the potential energy, we split the salinity field into the distinct contributions of the salt initially present in the gravity-current fluid c_c and in the lower ambient c_a, such that $c(\mathbf{x}, t) = c_c(\mathbf{x}, t) + c_a(\mathbf{x}, t)$. At $t = 0$, $c_c = C_1$ in the lock fluid and zero elsewhere, while $c_a = C_2$ in the lower ambient layer and zero elsewhere. We thus have that $\rho_1 = \rho_0(1 + \alpha C_1)$ and $\rho_2 = \rho_0(1 + \alpha C_2)$. The equations are made non-dimensional by introducing the reference length h_0, the buoyancy velocity $u_b = \sqrt{\frac{\rho_1-\rho_0}{\rho_0} g h_0}$ and the reference salinity C_1. The key non-dimensional parameters that control the dynamics of the current, besides the flume geometry, are the Reynolds number Re, the Schmidt number Sc, the density ratio Γ and the slope m, defined as

$$Re = \frac{u_b h_0}{\nu},\ Sc = \frac{\nu}{\kappa_s},\ \Gamma = \frac{\rho_2 - \rho_0}{\rho_1 - \rho_0} = \frac{C_2}{C_1},\ m = \frac{h_s}{L_s} \tag{18}$$

The geometry of the flume stems from the experimental setup[?] and our numerical simulations (*Interaction of a downslope gravity current with an internal wave*, submitted), but is adapted to allow for a longer distance from the slope to the right wall. This will allow for a longer propagation of the generated internal wave and thus a more accurate description of its properties. The applicability of our results to environmentally relevant scales depends on the ability of the simulations to replicate the strongly three-dimensional and turbulent nature of the gravity current. The lobe-and-cleft instability that is responsible for the destabilization of the head of the gravity current, and thus for the breakdown of large two-dimensional Kelvin-Helmholtz rollers can only exist in a sufficiently wide and high Reynolds number flow. The Reynolds number and width (z-direction) of the numerical domain thus constrain the computational cost. The Reynolds number is set to $Re = 10000$ such that the flow is fully turbulent. The wavenumber associated to the fastest growing mode of the lobe-and-cleft instability can be estimated a priori[?] and is found to be $k \approx 95$ for $Re = 10000$. The associated wavelength is thus $\lambda = 2\pi/60 \approx 0.662$, i.e. one fifteenth of the lock height h_0. Given that periodic conditions are imposed in the spanwise direction, it is essential to allow for the instability to develop naturally, i.e. to set the width of the domain to multiple times the wavelength of the fastest growing mode. The width W of the domain in the spanwise direction is set to $W = 1$ such that ≈ 15 lobe-and-cleft structures are able to form during the propagation of the current. The Schmidt number is considered to be an invariable parameter of the fluid and given the highly-turbulent nature of the flow, the simplifying assumption $Sc = 1$ is made as it is not expected to impact the dynamic of the flow and energy budget. In particular, the flux of potential energy induced by molecular diffusion in such systems is often neglected. We

Figures/setup_iw.pdf

Figure 1: *Initial conditions for the simulation scenario addressing the formation and energy budget of internal waves induced by a downslope gravity current passing through a two-layer stratification interface.*

thus focus our numerical investigation on the effect of the density ratio Γ and slope m on the internal wave induced by the gravity current. The flume size is set to $L_x \times L_y \times L_z = 25h_0 \times 2.5h_0 \times h_0$. As in section 3 the gravity current is expected to initially propagate at $v_F \approx 0.5u_b$ such that the non-dimensional time τ required for the current to reach the right wall of the flume is $\tau \approx 2\frac{L_x}{h_0} = 50$.

4 Resources and storage allocation amounts

This section details the justification of allocation amounts for each project. The summary of the allocation amounts is:

- The total requirement for the completion of all three research projects is **xx SUs in node hours** to be used on *Stampede2*, Phase 1.
- The total storage requirement is **xx[TB]** on *Ranch*.

Simulations are spread across work packages (WP). Each work package corresponds to a certain number of runs N_{run}.

Project 1: Cohesive Sediment Dynamics in Turbulent Flow

This problem has three non dimensional parameters as mentioned in the previous section namely St,Co and V. For each parameter we will run a simulation for 4 values which makes the total number of simulations to be 12. This parameter space is going to be explored in a domain $L_x \times L_y \times L_z = 0.32 \times 0.32 \times 0.32$ with 626 particles with volume fraction of 0.01. Each particle is resolved by 16 grid points ($\Delta x = 0.625 \times 10^{(-3)}$ with a CFL criterion of 0.5 makes $\Delta t = 0.0001559$)making the total number of grid points to be $512 \times 512 \times 512$. Once we figure out the parameters which is of greater interest to us, we run 4 larger simulations. This parameter space is going to be explored in a domain $L_x \times L_y \times L_z = 0.64 \times 0.64 \times 0.64$ with 5007 particles with volume fraction of 0.01. Each particle is resolved by 16 grid points ($\Delta x = 0.625 \times 10^{(-3)}$ with a CFL criterion of 0.5 makes $\Delta t = 0.0001559$)making the total number of grid points to be $1024 \times 1024 \times 1024$. From the computationally cheap one-way coupled, lagrangian point particle simulations, we obtain that the total simulation time that we need to obtain a saturation of the flocs is $\tau = 80$.

$$S = L_x L_y L_z \times \left(\frac{\sigma}{d_p}\right)^3 \frac{\hat{K}\tau}{\Delta t} \tag{19}$$

WP	N_{run}	$L_x \times L_y \times L_z$	N_{tot}	S_{run} (SUs)	D_{run} (TB)
1	12	$0.32 \times 0.32 \times 0.32$	256^3	4 783	0.3125
2	4	$0.64 \times 0.64 \times 0.64$	1024^3	38 264	2.5
Sum		$S = 210\,452$ node hours		D = 13.75 TB	

Table 1: *Estimated resources on* Stampede2 *for the sub-project on Cohesive Sediment Dynamics in Turbulent Flow.*

Project 2: Bed erosion by gravity currents:

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By carefully assessing the different parameters, we determined a flume geometry that is listed in Tab. 2, which distinguishes two work packages that are distinguished in the z dimension: WP1 represents a slab geometry for which the periodic z-direction is only three times the particle median D_p altering the flow practically two-dimensional. WP2 represents a fully three-dimensional flume for which the z the dimension will extend over half the flume height $L_z = 0.5L_y$ to allow for the lobe and cleft instability to develop, but which is computationally much more expensive. With our consideration the computational time is estimated by introducing (16), (12), together with the estimation of the front velocity for the maximum velocity and that the current propagates though the whole flume with this velocity in (10), which yields

$$S = L_x^2 L_y L_z \times \left(\frac{\sigma}{d_p}\right)^4 \frac{\hat{K}}{\mathrm{CFL}} \tag{20}$$

Thomas, should d_p be replace with δ ? Also, it is not immediately clear why L_x appears with a ^{2} and the reviewers might ask for more intermediate steps. I specified that $\hat{K}$ was in seconds in the text, but we might want to specify here that we understand that SUs = Nh and not Ns

WP	N_{run}	$L_x \times L_y \times L_z$	N_{tot}	S_{run} (SUs)	D_{run} (TB)
1	20	$8L_y \times L_y \times 10^{-3}L_y$	810^6	1 350	0.8
2	4	$8L_y \times L_y \times 0.5L_y$	13.5^9	22 500	13
Sum		$S = 117\,000$ node hours		D = 68 TB	

Table 2: *Estimated resources on* Stampede2 *for the sub-project on bed erosion by gravity currents. The remaining parameters are* $Re_L = 5425, Sc = 7, G = 333.33, \rho_s' = 1.007, \delta = 0.01, \sigma = 15, N_{var} = 6, N_{save} = 20$

Project 3: Internal wave induced by downslope gravity current

In section 3 we restricted the parametric space to the density ratio Γ and the slope m in order to investigate the dynamic and energy budget of the generated internal wave. $\Gamma = 0$ and $\Gamma = 1$ are natural limit conditions to the parametric study as the former defines the absence of stratification in the ambient fluid and the latter defines the situation of neutral buoyancy between the current and the lower ambient fluid. However, the current accumulates kinetic energy by release of potential energy and can thus strongly perturb the

lower layer even in the case where $\Gamma > 1$. We thus consider the parametric range $\Gamma = 0.0, 0.4, 0.8, 1.0, 1.2$. The slope $m = h_s/L_s$ is set alternatively to $0.1, 0.125, 0.2, 0.3, 0.5$. Anticipating a non-linear effect of both parameters and their combinations, we define a single work package WP in which simulation $WP_{i,j}$ denotes the simulation at Γ_i and m_j. This results in a total of $N_{sim} = 5 \times 5 = 25$.
A two-dimensional test simulation was run on *Stampede2* and revealed that satisfactory mesh-size convergence was obtained for $\Delta x = 0.0035$. Thus combining equations 10, 12 and noting that $\tau U_{max} \approx L_x$ we find the required SUs (in Nh) per simulation to be

$$S = \frac{L_x^2 L_y L_z}{\Delta x^4} \frac{\hat{K}}{\mathrm{CFL}} \approx 1.45 \times 10^3 SUs. \tag{21}$$

The number of variables required by this simulation to be stored is $N_{var} = 6$ ($\mathbf{u} = (u, v, w)$, p, c_c, c_a). Data analysis is done in runtime within PARTIES in the form of 2D averages and 0D metrics, such that writing of three-dimensional data is only necessary for visualization purposes and resuming of simulations. High frame rate videos of the three-dimensional flow will be rendered using *Blender* and its *Cycles* rendering engine, coupled with an automated rendering procedure developed by the PI's group. Due to the computational cost of such rendering procedures on our local workstations, we limit the number of simulations with high frequency output to four reference simulations ($\Gamma = 1.0$ with $m = 0.2, 0.5$ and $\Gamma = 0.4, 1.2$ with $m = 0.2$). We require low output (lo) simulations to have $N_{save} = 25$, and high output (ho) simulations to have $N_{save} = 250$ i.e. one save every 0.2 time units (we recall that the gravity current propagates at a non-dimensional speed of ≈ 0.5 such that it advances by 0.1 of its height at every save). This yields $D_{lo} = N_{save,lo} \times N_{var} \times N_{tot} \times 8 = 1.591TB$ and $D_{ho} = N_{save,ho} \times N_{var} \times N_{tot} \times 8 = 15.91TB$. The total requirements for this project are given in table 3.

WP	N_{run}	$L_x \times L_y \times L_z$	N_{tot}	S_{run} (SUs)	D_{run} (TB)
1.lo	21	$25h_0 \times 2.5h_0 \times h_0$	1.46×10^9	1 450	1.591
1.ho	4	$25h_0 \times 2.5h_0 \times h_0$	1.46×10^9	1 450	15.91
Sum	$S = 36\,000$ node hours			D = 97.1 TB	

Table 3: *Estimated resources on* Stampede2 *for the sub-project on internal wave generation by downslope gravity current. Parameters are* $Re = 10000$, $Sc = 1$, $\Gamma_i = 0.0, 0.4, 0.8, 1.0, 1.2$, $m_j = 0.1, 0.125, 0.2, 0.3, 0.5$, $N_{var} = 6$, $N_{save} = 25, 250$

5 Local resources and personnel

Computing resources

Within the PI's research group, we use a network of high-end Linux based computers and have access to the Knot Cluster at UCSB, which comprises

- 84 SL390 nodes of dual Intel X5650 six core processors (48GB and Infiniband Interconnect).
- Three DL580 nodes with 4 Intel X7550 eight core processors and 1TB of RAM.
- One DL580 nodes with 4 Intel X7550 eight core processors and 512GB of RAM.
- 12 NVIDIA M2050 GPUs in SL390 nodes with X5650 six core processors.
- 9 Intel Xeon Phi coprocessors

These facilities will be adequate for program development, single processor performance tests, small-scale parallel simulations and post-processing, such as the generation of animations and visualizations. It is however extremely limited for the large-scale simulations that are necessary for the advancement of our research objectives.

Key Personnel

Principal investigator:

- Prof. Eckart Meiburg

Postdoctoral reasearchers:

- Dr. Thomas Köllner

PhD students and researchers:

- Raphael Ouillon
- Rochishnu Chowdhury