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Person Months Worked: 1.00
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Article Title: Simulation technique for slurries interacting with moving parts and deformable solids with applications
Authors: Patrick Mutabaruka, Ken Kamrin
Keywords: Discrete elements method, Lattice Boltzmann, Fluid–particle interaction, Smagorinsky turbulence model, Hyperelastic model, Neo-Hookean elastic rubber model
Abstract: A numerical method for particle-laden fluids interacting with a deformable solid domain and mobile rigid parts is proposed and implemented in a full engineering system. The fluid domain is modeled with a lattice Boltzmann representation, the particles and rigid parts are modeled with a discrete element representation, and the deformable solid domain is modeled using a Lagrangian mesh. The main issue of this work, since separately each of these methods is a mature tool, is to develop coupling and model-reduction approaches in order to efficiently simulate coupled problems of this nature, as in various geological and engineering applications. The lattice Boltzmann method incorporates a large eddy simulation technique using the Smagorinsky turbulence model. The discrete element method incorporates spherical and polyhedral particles for stiff contact interactions. A neo-Hookean hyperelastic model is used for the deformable solid. We provide a detailed description of how to couple the three
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Article Title: A general fluid–sediment mixture model and constitutive theory validated in many flow regimes
Authors: Aaron S. Baumgarten, Ken Kamrin
Keywords: granular media, multiphase and particle-laden flows, suspensions
Abstract: We present a thermodynamically consistent constitutive model for fluid-saturated sediments, spanning dense to dilute regimes, developed from the basic balance laws for two-phase mixtures. The model can represent various limiting cases, such as pure fluid and dry grains. It is formulated to capture a number of key behaviours such as: (i) viscous inertial rheology of submerged wet grains under steady shearing flows, (ii) the critical state behaviour of grains, which causes granular Reynolds dilation/contraction due to shear, (iii) the change in the effective viscosity of the fluid due to the presence of suspended grains and (iv) the Darcy-like drag interaction observed in both dense and dilute mixtures, which gives rise to complex fluid–grain interactions under dilation and flow. The full constitutive model is combined with the basic equations of motion for each mixture phase and implemented in the material point method (MPM) to accurately model the coupled dynamics of the mixed system.
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Article Title: A general constitutive model for dense, fine particle suspensions validated in many geometries
Authors: Aaron Baumgarten, Ken Kamrin
Keywords: discontinuous shear thickening, constitutive model, two phase flow
Abstract: Fine particle suspensions (such as cornstarch mixed with water) exhibit dramatic changes in viscosity when sheared, producing fascinating behaviors that captivate children and rheologists alike. Examination of these mixtures in simple flow geometries suggests inter-granular repulsion and its influence on the frictional nature of granular contacts is central to this effect --- for mixtures at rest or shearing slowly, repulsion prevents frictional contacts from forming between particles, whereas, when sheared more forcefully, granular stresses overcome the repulsion allowing particles to interact frictionally and form microscopic structures that resist flow. Previous constitutive studies of these mixtures have focused on particular cases, typically limited to two-dimensional, steady, simple shearing flows. In this work, we introduce a predictive and general, three-dimensional continuum model for this material, using mixture theory to couple the fluid and particle phases. Playing a centra
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Article Title: Modeling stress relaxation in dense, fine-particle suspensions
Authors: Aaron S. Baumgarten, Ken Kamrin
Keywords: (none)
Abstract: In this work, we examine the predictions of the constitutive model proposed in Baumgarten and Kamrin [Baumgarten and Kamrin, Proc. Natl. Acad. Sci. U.S.A. 116, 20828–20836 (2019)], as it relates to the transient relaxation of shear stresses in dense, fine-particle suspensions such as water-cornstarch or water-poly (methyl methacrylate) mixtures. Such mixtures are known to exhibit dramatic increases in viscosity when impacted or sheared, and in rate-controlled experiments, these mixtures are also observed to support shear stresses long after all macroscopic flow has stopped. We show that the experimental observations of substantially longer stress decay in these mixtures compared with standard Newtonian fluids can be captured by the model through its evolution of the internal state variable, f, which reflects the fraction of frictional contacts at the microscale. Analysis of the behavior of f suggests that the presence of system spanning granular contact networks and the associated rate
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Article Title: Reference map technique for incompressible fluid–structure interaction
Authors: Chris H. Rycroft, Chen-Hung Wu, Yue Yu, Ken Kamrin
Keywords: computational methods, Navier–Stokes equations
Abstract: We present a general simulation approach for fluid–solid interactions based on the fully Eulerian reference map technique. The approach permits the modelling of one or more finitely deformable continuum solid bodies interacting with a fluid and with each other. A key advantage of this approach is its ease of use, as the solid and fluid are discretized on the same fixed grid, which greatly simplifies the coupling between the phases. We use the method to study a number of illustrative examples involving an incompressible Navier–Stokes fluid interacting with multiple neo-Hookean solids. Our method has several useful features including the ability to model solids with sharp corners and the ability to model actuated solids. The latter permits the simulation of active media such as swimmers, which we demonstrate. The method is validated favourably in the flag-flapping geometry, for which a number of experimental, numerical and analytical studies have been performed. We extend the flapping a
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Partners

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I certify that the information in the report is complete and accurate:
Signature: Ken Kamrin
Signature Date: 10/20/21 4:52PM

Major Goals:

Fluid-driven sediment transport, in which a flow passing over a granular bed entrains and moves the grains, plays a pivotal role in many natural and engineered landscapes. Common examples include conveyance of sediment through engineered channels, infilling of artificial reservoirs, and dispersal of stored sediment following dam removal or landslides. Applications like these require field-scale models for calculating sediment transport rates over a wide range of flow conditions and sediment characteristics. This is a very challenging task, because sediment transport at the scale of a river depends on the fine-scale interaction of a turbulent flow with many individual grains. Moreover, variations in these fluid-grain interactions through time, or with height above or below the sediment bed, can create different regimes of grain motion, including creep of closely packed grains, a rapidly shearing slurry, or a dilute suspension. Empirical sediment transport models do not explicitly account for this grain-scale physics and can therefore be inaccurate.

The objectives of this project are to (1) better understand the fundamental processes that underlie empirical sediment transport equations, particularly those related to grain shape; and (2) derive alternative, continuum models of sediment transport that apply to a range of flow conditions and sediment characteristics. We approach both objectives with the same set of tools: flume experiments and numerical simulations. Our goals can be organized into three themes:

* = accomplished in the previous reporting period

Theme 1: Laboratory Flume Experiments

- Goal 1a*: Conduct flume experiments with spheres, including development of techniques for particle and fluid tracking to quantify sediment transport at the grain scale.
- Goal 1b*: Conduct flume experiments with natural grains, including development of techniques for particle and fluid tracking.
- Goal 1c*: Develop a method for high-resolution characterization of natural grain shapes for use in simulations.
- Goal 1d*: Quantify effects of grain shape on bedload transport by comparing flume experiments with spheres and natural/irregular grains.

Theme 2: Simulations

- Goal 2a*: Custom-code an LBM-DEM scheme capable of precise representation of the regimes present in the fluid-sediment transport range of problems.
- Goal 2b*: Conduct an array of LBM-DEM simulations with spheres, including benchmarking against experimental data.
- Goal 2c: Examine the relevant parameters for the spread of transport relation data from field and lab observations, with an array of LBM-DEM simulations of spheres under wide wall-free boundary conditions.
- Goal 2d: Conduct an array of LBM-DEM simulations with natural grains, including benchmarking against experimental data.

Theme 3: Mechanistic Insights and Continuum Model Development

- Goal 3a*: Determine a mixture homogenization scheme to extract the phase-wise continuum fields from LBM-DEM simulations.
- Goal 3b*: Regarding the dense slurry and the dilute suspension, formulate a continuum model informed by relating sets of relevant continuum fields extracted from simulations. Validate it by comparing mixture continuum fields from LBM-DEM to fully continuum simulations of the model.
- Goal 3c: Regarding the creep flow beneath the bed surface, adapt the nonlocal granular fluidity model for submerged particles and validate it with the DEM-LBM results.

<u>Accomplishments</u>

With the flume experiments accomplished in the previous reporting period, the high-resolution tracking of both spherical grains and natural grains (Goals 1a and 1b) have provided insights into the intermittent nature of sediment transport near the threshold of motion, which is characterized by rare but large transport events (Fig 1). The rich data provided by the high-resolution grain tracking has allowed us to observe and uncover things that others didn't have access to in past studies. By separating the flux out into two components, grain activity and grain velocity, we were able to identify the physical source of the intermittency in the sediment flux time signal. We found that rolling grains on top of the bed experience intermittent velocities and are the ones that provide the on-off intermittent signal (Figure 2). To complement the experimental work looking at sediment transport statistics, we have also developed a cellular automata model of bed load sediment transport near the threshold of motion. This model is much simpler than the models described below, but is instead an attempt to capture the minimal information required to describe the statistics of bed load sediment transport. Given its simplicity, we are able to run the model for very long times and for many values of the parameters, allowing us to efficiently explore the parameter space and uncover what the minimal components are required to reproduce the statistics of sediment transport and how the statistics might depend on physical parameters.

In the previous reporting period, we refined and improved a custom Lattice Boltzmann Method/Discrete Element Method (LBM-DEM) code and developed a procedure for simulating the laboratory flume experiments with spheres (Goal 2a) with a good match in terms of the $q^* - \tau^*$transport relations and the flow profiles (Goal 2b). In this reporting period, using the LBM-DEM algorithm benchmarked by the experiments, we have explored the parameter space (macroscopic river settings such as slope, and microscopic particle parameters such as the mean size, surface roughness and damping coefficient) to see what is responsible for the spread of the transport relation observed in field and lab observations (Goal 2c). Table 1 lists the relevant parameters, the nondimensionalization and the corresponding dimensionless groups. For the sediment (sand in hard limit) transport on Earth surface, the dimensional groups are:

$$q^* = \tilde{\Psi}_0\big(\underbrace{\tau^*, S}_{\text{macroscopic}}, \underbrace{Ga, \mu_p, \Pi_6}_{\text{microscopic}}\big) = \tilde{\Psi}\big(\tau^*; S, Ga, \mu_p, \Pi_6\big).$$

Guided by the dimensional analysis, LBM-DEM simulations are performed in wide wall-free geometries (24d*8d*~20d, where d is grain diameter, with periodic sidewall boundary conditions, mimicking wide rivers) as shown in Fig. 3a. When the Shields number is fixed, neither the (gentle) macroscopic bed slope (Fig. 3b) nor the tested microscopic particle parameters such as diameter, surface sliding friction coefficient and the damping coefficient (Fig. 3c) is influencing the dimensionless transport rate q^*. By exclusion, this suggests that the particle shape and the size distribution may be chiefly responsible for the spread of the experimental transport relation even on gentle slopes, in agreement with the conclusion of the experimental study (Goal 1d): the $q^* - \tau^*$ relation is parameterized primarily by the repose angle of the sediment particles, which is strongly dependent on the particle shape and size distribution but independent of Ga (mean size) or Π_6 (stiffness). Though the particle surface friction coefficient μ_p influences the repose angle, the influence for round particles is very limited when $\mu_p > 0.05$. As a result, μ_p has negligible influence on the transport of spherical sediment particles, but may potentially have an influence on the transport of non-spherical particles. We have also begun developing the LBM-DEM for the transport of natural shaped particles. Fig. 4 shows the settling of an elongated particle (approximated by overlapping spheres) in fluid.

In the previous period, for the modeling of the dense slurry and the dilute suspension flow, we have formulated a continuum model informed by relating sets of relevant continuum fields extracted from simulations (Goal 3a), validated by the LBM-DEM WWF simulation flow fields (Goal 3b). In this reporting period, for the creep flow under the bed surface, we extend the nonlocal granular fluidity (NGF) model for dry granular materials to account for fluid forcing (Goal 3c). Fig. 5 shows the capability of predicting the exponentially decaying velocity profile that appears deeper in the bed. The success of applying the NGF model to the river bed indicates that the physics of the nonlocal effects in submerged particles may be similar to that of dry particles.

Table 1. Non-dimensionalization of the dependent and independent variables in sediment transport problems (Var: variables, Dim: dimensions, DN: dimensionless numbers, FDN: related famous dimensionless numbers)

Var	q_s	H	S	ρ_f	η	g	ρ_s	d_p	μ_p	g_p	k_p
Meaning	flux per unit width	water depth	slope	fluid density	viscosity	gravity	solid density	particle size	surface friction coef.	damping coef	stiffness
Dim	$\frac{\mathrm{L}^2}{\mathrm{T}}$	L	-	$\frac{\mathrm{M}}{\mathrm{L}^3}$	$\frac{\mathrm{M}}{\mathrm{LT}}$	$\frac{\mathrm{L}}{\mathrm{T}^2}$	$\frac{\mathrm{M}}{\mathrm{L}^3}$	L	-	$\frac{\mathrm{M}}{\mathrm{T}}$	$\frac{\mathrm{M}}{\mathrm{T}^2}$
DN	$q_s \frac{\rho_f}{\eta}$	$H\left(\frac{\rho_f^2 g}{\eta^2}\right)^{\frac{1}{3}}$	S	1	1	1	$\frac{\rho_s}{\rho_f}$	$d_p\left(\frac{\rho_f^2 g}{\eta^2}\right)^{\frac{1}{3}}$	μ_p	$\frac{g_p}{\eta}\left(\frac{g\rho_f^2}{\eta^2}\right)^{\frac{1}{3}}$	$\frac{k_p}{\eta}\left(\frac{\rho_f}{\eta g}\right)^{\frac{1}{3}}$
Symbol		Π_1	Π_2	-	-	-	Π_3	Π_4	Π_5	Π_6	Π_7
FDN	q^*	τ^*	S	-	-	-		Ga			
Varied or not	dependent variable	varied	varied	fixed, water	fixed, water	fixed, on Earth	fixed, sand	varied	varied	varied	fixed, hard limit

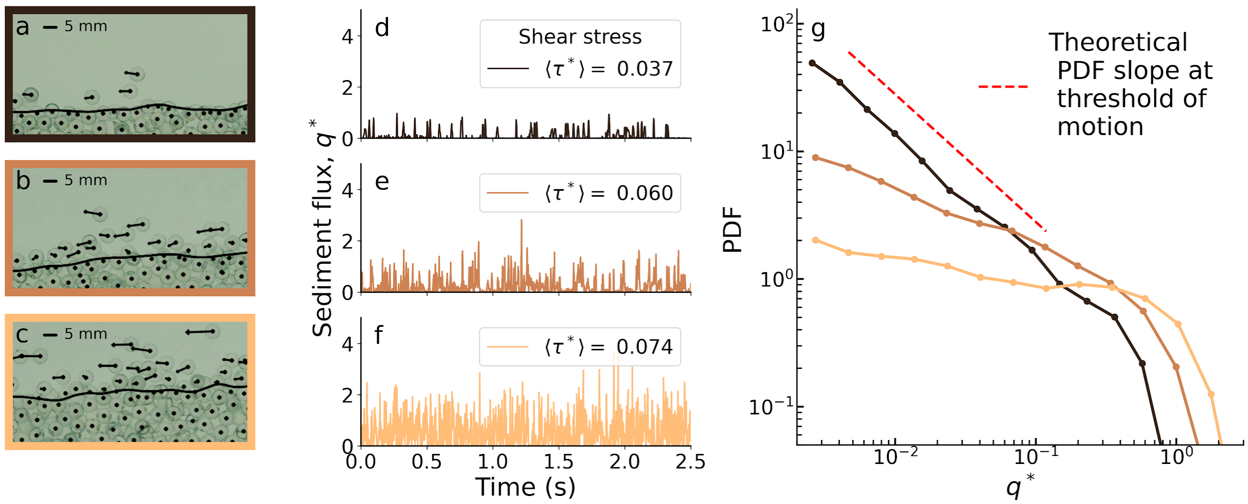

Figure 1. Intermittent bed load sediment flux. Sample data from three flume experiments using glass spheres, representing typical runs with low sediment flux (a and d), intermediate sediment flux (b and e), and high sediment flux (c and f). a-c, High-speed video frames showing grain centers and velocities and the location of the bed. d-f, Samples of the corresponding sediment flux time series. g, Probability density function (PDF) calculated from the sediment flux time-series. The red dashed line shows the theoretical slope of the PDF tail at the threshold of motion.

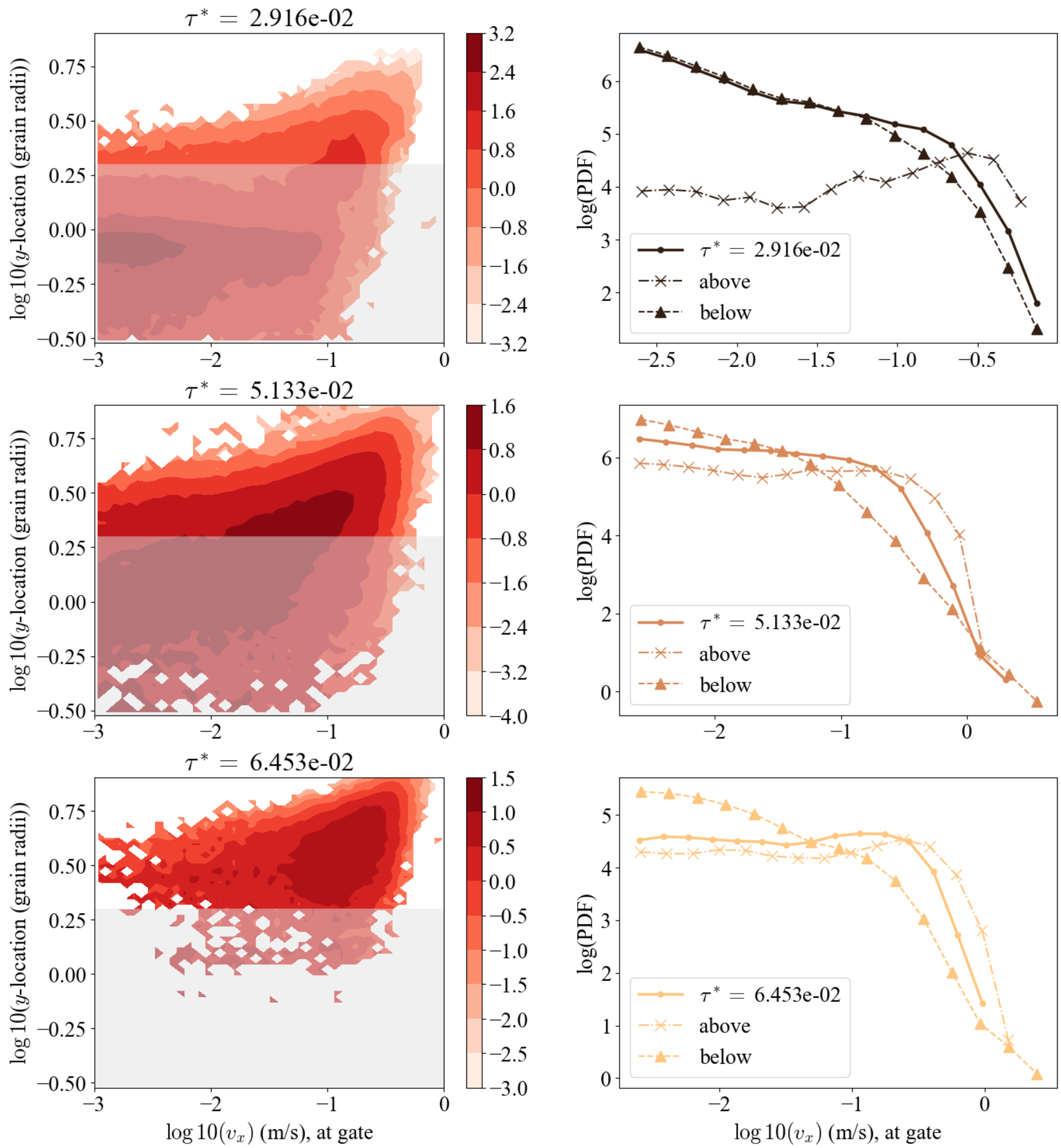

Figure 2: Left column: joint probability density function (for average vertical location of the grains (y axis) and average velocity of the grains (x axis) in a frame. The "bed" region is denoted by the transparent gray box. Right column: the PDF of the grain velocities, showing contributions from below (triangles) and above ('x') the bed. Each row represents a successively higher transport stage, going from most intermittent to less intermittent as one goes down the rows.

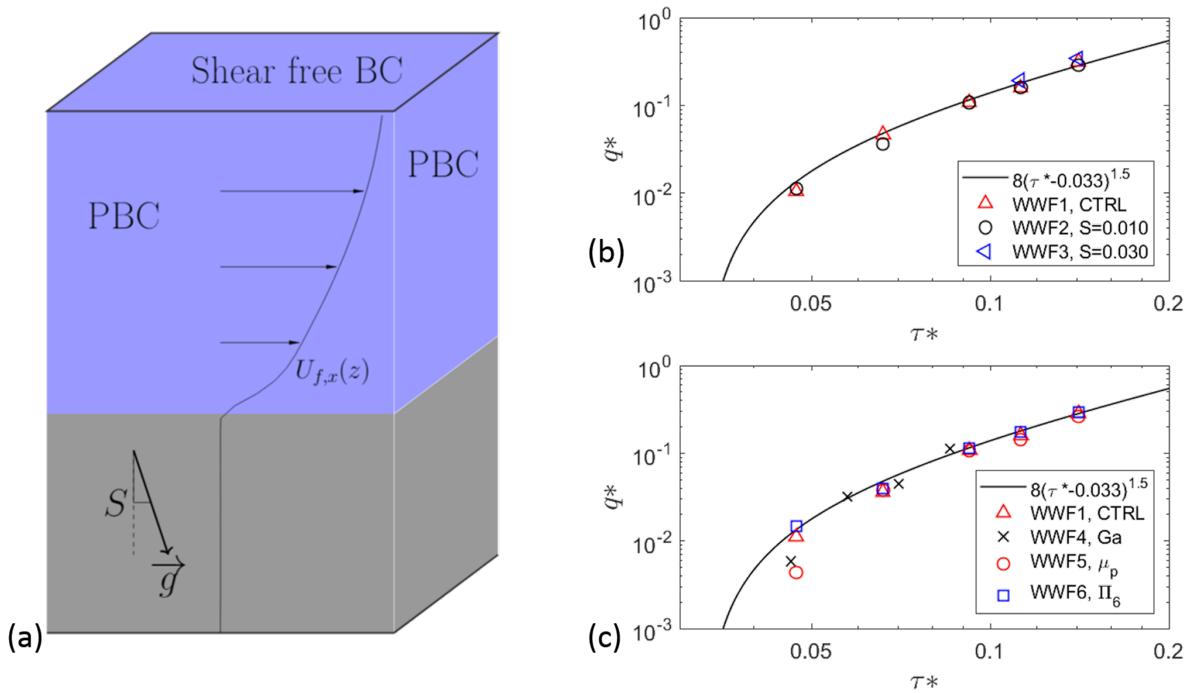

Figure 3. (a) Geometry and boundary conditions of the wide wall-free (WWF) simulations (PBC: periodic boundary condition). (b) Sediment transport relation from the WWF simulations with the macroscopic geometrical parameter S varied. (c) Sediment transport relation from the WWF simulations with the microscopic particle parameters Ga, μ_p and Π_6 varied. WWF1 is the control group while the other groups vary the dimensionless groups in Table 1 one by one, as denoted in the legends.

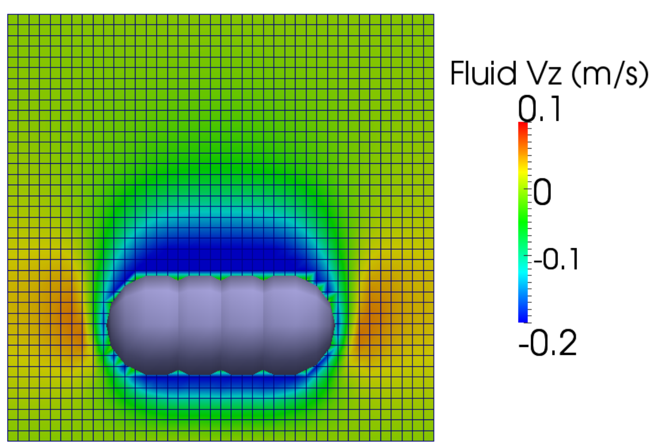

Figure 4. A multi-sphere elongated particle settling in fluid, colored by fluid velocity in vertical direction.

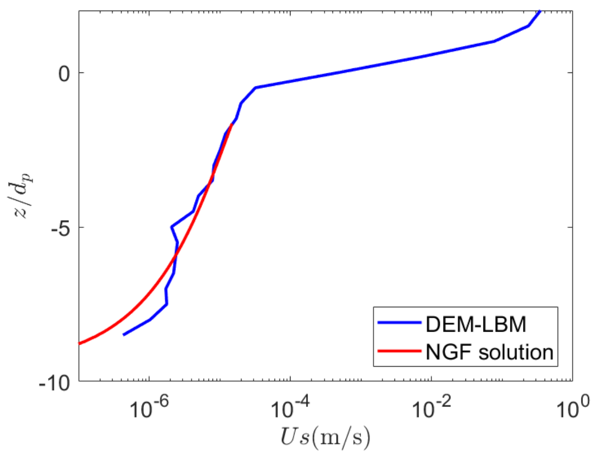

Figure 5. The solid phase velocity profile comparison between a DEM-LBM wide wall-free simulation (d_p=5mm, S=0.016) and the corresponding steady state NGF solution.

Training opportunities:

Postdoc Eric Deal had the chance to develop his advising skill set while advising several undergraduate and graduate students in the course of the project. He also gained experience designing and conducting laboratory experiments and developing particle tracking algorithms. PhD student Santiago Benavides, who has a background in physics and math, has gained experience applying techniques from statistical physics to problems in geoscience and granular materials.

The project has also provided training opportunities to several undergraduate students through the MIT undergraduate research opportunities program (UROP). This includes Matt Rushlow, who worked with us on this project from fall 2017 until spring 2020, and whose work culminated in a poster presented at the fall 2019 American Geophysical Union (AGU) Meeting, and his undergraduate thesis. Shannon Duffy is another undergraduate who worked with us for several months through the same program. These students have had the chance to develop programming and data science skills, critical thinking and paper reading, some light project management, and in the case of Rushlow, writing and presentation skills as well.

PI Kamrin's PhD student Qiong Zhang has benefitted from direct interaction with the Earth Science community at MIT through his collaboration with PI Perron on this project and in coursework stemming from this project. Aaron Baumgarten has gotten his PhD degree in the summer of 2021.

Publications

* = MIT student or postdoctoral researcher supported by this project

*Benavides, S.J., *Deal, E., *Rushlow, M., Venditti, J., *Zhang, Q., Kamrin, K., and Perron, J.T., The impact of intermittency on bed load sediment transport. In review at *Geophys. Res. Lett.*

*Zhang, Q., Deal, E., Perron, J.T., Venditti, J., *Benavides, S.J., *Rushlow, M., and Kamrin K., Fluid-driven transport of round sediment particles: from discrete simulations to continuum modeling. In preparation for submission to *J. Geophys. Res*.

*Deal, E., Perron, J.T., Venditti, J., *Benavides, S.J., Bradley, R, Kamrin K., and *Zhang, Q., Grain shape effects in bed load sediment transport. In preparation.

*Zhang, Q., Townsend, S., Kamrin, K., Expanded scaling laws for locomotion in sloped or cohesive beds, *Phys Rev Fluids*, 5, 114301 (2020).

*Baumgarten, A., Couchman, B., Kamrin, K., A coupled finite volume and material point method for two-phase simulation of liquid–sediment and gas–sediment flows, *Comp Meth App Mech Eng,* 384, 113940 (2021).

*Wang, X., Kamrin, K., Rycroft, C., An incompressible Eulerian method for fluid-structure interaction with mixed soft and rigid solids, In review at *Phys Fluids*.

<u>Dissemination of results</u>

Student and Postdoc presentations:

* = MIT student or postdoctoral researcher supported by this project

*Deal, E., *Zhang, Q., Perron, J.T., *Benavides S., Kamrin K., and Venditti J. (2020), A close look at the effect of grain shape on bedload transport, American Geophysical Union, Fall Meeting 2020, abstract #EP008-05.

*Deal, E., Perron, J.T., Venditti J., *Zhang, Q., *Benavides S., and Kamrin K. (2020), Observing and modeling bedload sediment transport at the grain-scale, European Geosciences Union, General Assembly, id.21982.

PI presentations:

PI Kamrin presented invited talks on this work at Columbia University and U Penn.

<u>Plans next reporting period</u>

The LBM-DEM procedure using overlapping spheres to approximate aspherical grains (Goal 2c) needs further development and validation. A similar continuum homogenization procedure can be carried out for the natural sediments (Goals 3b). The final goal is to use these continuum approaches in the case of the sediment transport problems of particles of any shape with actual river bed boundary conditions. Incorporating NGF directly in the mixture theory for a submerged granular flow rule that even covers the creep flow regime is also a direction for future research.

Our efforts during the final reporting period will also be directed at publishing journal articles reporting the results described in the Accomplishments section as well as the results of the final research efforts described in this section.

<u>Honors:</u>

Graduate student Santiago Benavides was awarded NASA's Future Investigators in NASA Earth and Space Science and Technology (FINESST) fellowship.

Technology Transfer

PI Kamrin has continued his collaboration with Dr George Gazonas of ARL on the topic of discrete and continuum impact modeling, and has a MIPR agreement formalizing the interaction. The collaboration uses tools being developed in this project (both discrete and continuum modeling) to help understand ceramic damage processes during impact. Kamrin is currently advising Gazonas' team on DEM customization to model grain breakage. PI Perron has had previous contacts with Dr Joe Dunbar (USACE Geotechnical and Structures Laboratory, Vicksburg) and Drs Sally Shoop and Charles Ryerson (CRREL). The codes used to perform grain identification, particle tracking, and 3D grain shape analysis are open source, and PI Perron is seeking opportunities to share these techniques with Army personnel involved in research on sediment transport and other granular phenomena.

Participants and months worked

In addition to the two PIs Prof. Perron and Prof. Kamrin, and the two main workers, PhD student Qiong Zhang (who worked on the project since its start) and Postdoc Eric Deal (who worked on the project full-time until he was hired as a staff scientist by a research group in Switzerland in December 2019), there were several students who worked on the project at various times, some supported by the grant and some supported by outside funds. This includes undergraduate students Shannon Duffy (MIT 3 mo) and Matt Rushlow (MIT 20 mo), and graduate students Santiago Benavides (MIT 18 mo), Aaron Baumgarten (MIT 18 mo), Xiaolin Wang (MIT 2mo), Max Hurson (SFU 2 mo) and Ryan Bradley (SFU 3 mo). Months worked from just the last fiscal year have been entered directly into the report portal.