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13. ABSTRACT (Maximum 200 words)

This project has led to significant progress on several critical questions related to granular flows. First, a high order code based on Discontinuous Galerkin method has been produced to study granular in axisymmetric hoppers. Before that, only ad hoc discretization Methods were used. This led to the discovery of several new phenomena (such as shock formation and propagation). Several weaknesses of established models were also brought to the fore. Second, the effect of the geometry of the hopper on the flow were analyzed. Secondary circulation and resonance phenomena were observed in the models. This too is new. Third, advances were made in the analysis of sound propagation in sand and the importance of wall friction in the process. Fourth, a model of powder consolidation has been proposed, analyzed and discretized, leading to an industrial code. Fifth, a robust method for the volume determination of granular heap in complicated geometries has been proposed and implemented.

The project has also yielded results not directly related to granular materials, such progress in long time integration of Discontinuous Galerkin methods and study of Partial Differential Algebraic equations.

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1. LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS PERIOD, INCLUDING JOURNAL REFERENCES.

1. with N.R. Ide, *Computation of Nonclassical Solutions to Hamilton-Jacobi Problems*, SIAM J. Sci. Comput., 21 (1999), p.502–521.
2. with J.V. Matthews and M. Shearer, *Similarity Solutions for Hopper Flows*, Proceedings of the SIAM/AMS Conference on Nonlinear PDEs, Dynamics and Continuum Physics, J. Bona, K. Saxton, R. Saxton, Eds., AMS Contemporary Mathematics Series, #255 (2000), p.79–95.
3. with J.V. Matthews, *Simulation of gravity flow of granular materials in silos*, in Discontinuous Galerkin Methods, Theory, Computation and Applications, B. Cockburn, C.W. Shu, G. Karniadakis Eds., Lecture Notes in Computational Science and Engineering, #11 (2000), Springer Verlag, p. 125-134.
4. with D.G. Schaeffer and M. Shearer, *Numerical determination of flow corrective inserts for granular materials in conical hoppers*, Int. J. Nonlinear Mech., 35 (2000), p.869-882.
5. with C.T. Kelley, A.T. Royal, K.A. Coffey, *On a powder consolidation problem*, SIAM J. Appl. Math., 62 (2001), 1-20.
6. with J.V. Matthews, *On the Computation of Steady Hopper Flows I: Stress Determination for Coulomb Materials*, J. Comput. Phys., 166 (2001), p.63-83.
7. with K.A. Coffey, *Numerical Simulation of Aerated Powder Consolidation*, (13 pages), *Int. J. Nonlinear Mech.*, 38 (2003), 1185–1194.
8. with J.V. Matthews and D.G. Schaeffer, *Secondary circulation in granular flows through nonsymmetric hoppers*, to appear in SIAM J. Appl. Math.
9. *Numerical issues in plasticity models for granular flows*, submitted to Journal of Volcanology and Geothermal Research.
10. with S.A. Ahmed, R. Buckingham, C.D. Hauck, C.M. Kuster, M. Prodanovic, T.A. Royal, V. Sliantyev, *Volume determination for bulk materials in bunkers*, to be submitted.

2. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT DURING THIS PERIOD.

Pierre A. Gremaud (PI), K.A. Coffey (PhD student).

3. REPORT OF INVENTIONS. NA.

4. SCIENTIFIC PROGRESS AND ACCOMPLISHMENT. This project is about the numerical and theoretical study of granular flows. Significant advances have been achieved in relation to numerical modeling. People who have collaborated to the project during this period of funding include Profs. D.G. Schaeffer (Duke University) and M. Shearer (North Carolina State University), Dr. J.V. Matthews (Duke University) and K.A Coffey (Ph.D. student, Gremaud adviser). We also work in consultation with Engineers at Jenike & Johanson, Inc., Westford, MA., and in particular T.A. Royal, Vice President, to develop efficient and robust solvers for various types of problems related to granular flows.

One of the first and main problems one encounters when dealing with granular materials is to obtain a proper mathematical model. Several models exist, that appear to capture well some, but in general not all, aspects of the phenomena under consideration. Our approach is twofold. First, we aim at obtaining, through careful Analysis and Numerical Analysis of existing models, efficient and reliable computational tools that will allow for meaningful investigations the models themselves, through comparisons with experiments for instance. Second, and at a less fundamental level, having such computational tools represent a breakthrough in this field, and open new opportunities in terms of numerical simulations in industrial settings.

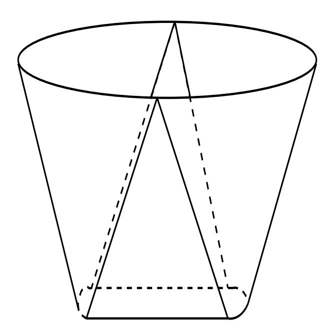

FIG. 4.1. Transitional hopper.

Three main fields of applications have been considered: hopper flows, powder consolidation and sound propagation in granular materials. Our main contributions during the last year have been

- identification of secondary circulation phenomena and resonance in three dimensional hoppers; this observation is astonishing and could potentially revolutionize silo design;

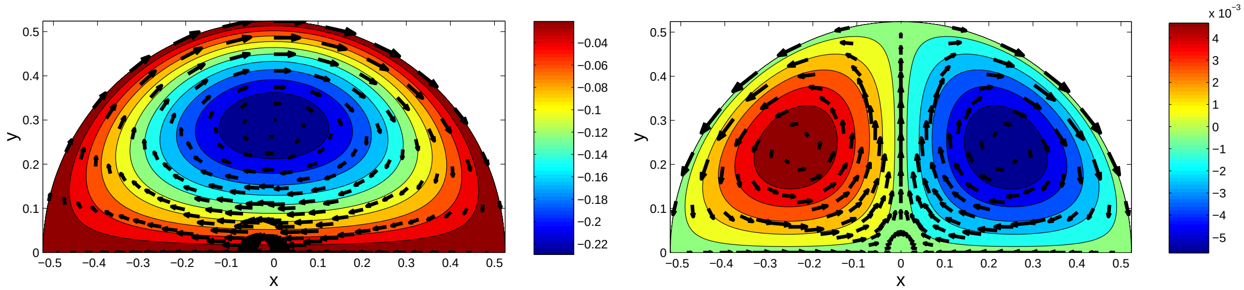

FIG. 4.2. Stream function showing secondary flow; top: tilted hopper ($m = 1$), bottom: "elliptical" hopper ($m = 2$). Angle of wall friction $= 15°$ ($\mu = \tan 15°$), half opening angle $\theta_w = 30°$. By symmetry, only half of the hopper is represented.

- further progress in the implementation (Objective-C) of our model for powder consolidation to axisymmetric domains of varying cross section in an industrial setting,
- numerical analysis of sound propagation phenomena in granular materials; our analysis,the first one done using higher order methods (third order Discontinuous Galerkin method) solves a controversial question which had been incorrectly answered in the literature as a result of substandard numerics.

We now proceed to describe in more details the first and third points.

4.1. Secondary circulation in hopper flows. We have studied 3D steady flow in a pyramidal hopper

$$\Omega = \{(r, \theta, \phi) : 0 \leq \theta < \mathcal{C}(\phi)\}.$$

This work prepares the way to study flow in fully three-dimensional geometries, such as the transition hopper illustrated in Figure 4.1 or a silo with multiple outlets. We have begun the study of flows using a perturbation-theory analysis. For conical hoppers (i.e., $\mathcal{C}(\phi) \equiv \theta_w$, a constant), classical similarity solutions can be constructed. Those so-called Jenike solutions are such that only the radial component of the velocity is nonzero, all variables are independent of ϕ, and the r-dependence of the solution has the similarity form

$$v_r = -r^{-2}\,\hat{v}(\theta), \qquad T = r\,\hat{T}(\theta).$$

Suppose the function $\mathcal{C}$ specifying the boundary of Ω has the expansion

$$C(\phi) = \theta_w + \epsilon\,\cos(m\phi) + \mathcal{O}(\epsilon^2);$$

for example, a slightly tilted (circular) cone admits such an expansion with $m = 1$, where ϵ measures the angle of tilt; likewise for a (vertical) pyramidal hopper having a slightly elliptical cross section, with $m = 2$. An expansion of the solution

$$v = v^{(0)} + \epsilon v^{(1)} + \mathcal{O}(\epsilon^2), \qquad T = T^{(0)} + \epsilon T^{(1)} + \mathcal{O}(\epsilon^2),$$

can be sought, where $v^{(0)}, T^{(0)}$ have the form of the Jenike solution. A numerical code based on a differential-algebraic formulation has been written to solve the boundary value problem one obtains for $\hat{v}^{(1)}, \hat{T}^{(1)}$. This analysis has brought to the fore some extremely interesting phenomena. In particular all three components of $v^{(1)}$ need to be nonzero: in other words, *secondary circulation appears when axial symmetry is broken!* This circulatory flow is illustrated in Figure 4.2 (left) for a tilted hopper $m = 1$ and Figure 4.2 (right) for an elliptical hopper $m = 2$. In other words, the grains do not move along radial lines, as is the case for Jenike's solutions but follow more complicated and fully three dimensional trajectories. Very singular behavior occurs when the parameters in the problem are varied. For example, consider Figure 4.3 (left), which shows, for $m = 1$ and other parameters fixed, the circulation velocity $v_\phi^{(1)}$ as a function of the opening angle of the hopper: $v_\phi^{(1)}$ suffers a "$1/x$-blow-up" as θ_w passes through a critical value.

While this blow up could not have been anticipated, *a posteriori*, its cause is easily understood: the two-point boundary problem for $\hat{v}^{(1)}, \hat{T}^{(1)}$ has inhomogeneous boundary conditions, but at the singular point in

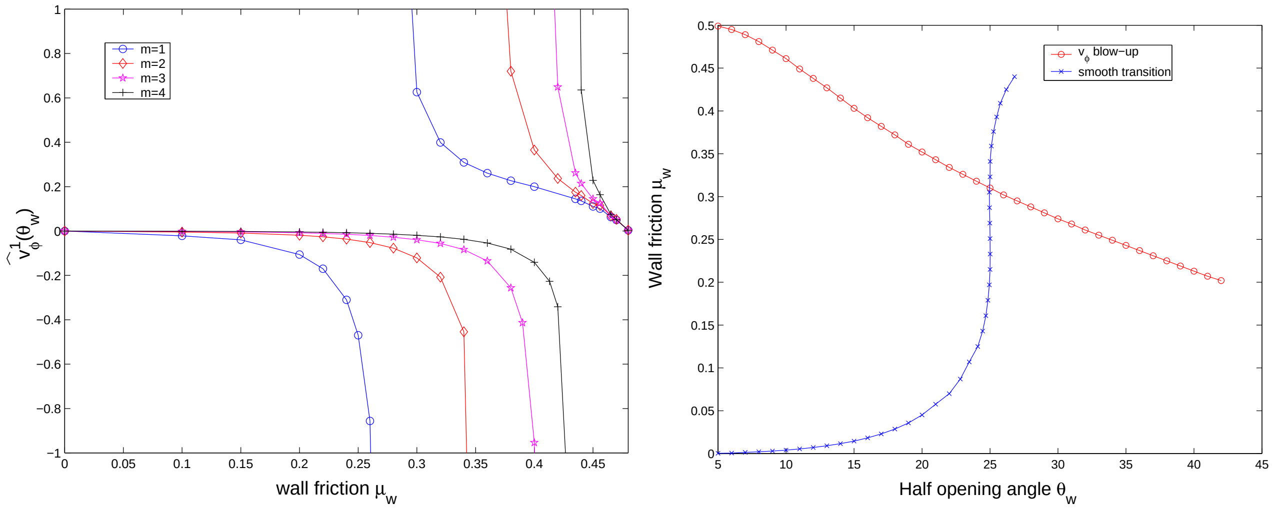

FIG. 4.3. Left: dependence of the resonance on the geometry of the domain through the coefficient m: blowup of $\hat{v}_\phi^{(1)}(\theta_w)$ as a function of the wall friction μ_w (internal friction $\delta = 30°$, half opening angle $\theta_w = 30°$). Right: critical values leading to sign changes of the circulation (internal friction $\delta = 30°$, $m = 1$).

Figure 4.3 (left), the problem with homogeneous boundary conditions has a nonzero solution. This behavior is analogous to that of a forced linear harmonic oscillator

$$\ddot{x} + \omega_0^2 x = A \sin \omega t :$$

the steady-state oscillations have amplitude $A/(\omega_0^2 - \omega^2)$, which diverges as ω passes through the natural frequency ω_0 of the oscillator. Unlike the above problem, in our model the inhomogeneity is in the equation rather than a boundary condition. Based on this analogy, we describe this divergence as a kind of resonance.

As θ_w crosses the critical value in Figure 4.3 (left), the direction of circulation changes. It turns out that there are also additional parameter values for which *the sign of the circulation changes smoothly*, passing continuously through zero. Curves of θ_w, μ_w along which the circulation changes sign by either mechanism are shown in Figure 4.3 (right). Those are fundamentally new observations. They lead to fascinating questions discussed in Section 4.3.1.

4.2. Wave propagation in granular materials. The time dependent versions of most plasticity models for granular flows are hopelessly ill-posed. We have investigated in some simple cases how equilibrium is reached. More precisely, considering the granular equivalent of the waterhammer problem, see Figure 4.4, it has been argued by some authors[1] that the classical "Janssen stress profile" for a granular material at rest is *not* the asymptotic solution that is reached at equilibrium. Considering the experiment depicted in Figure 4.4, the two main unknowns are u and v, the strain and the velocity. If σ stands for the average horizontal stress, the equations in Lagrangian coordinates take the form

$$\partial_t u - \partial_x v = 0, \tag{4.1}$$

$$\partial_t v + \partial_x \sigma \in -\kappa \,\mathrm{sgn}(v)\, \sigma, \tag{4.2}$$

where κ is a material parameter depending on both the internal friction of the material and the frictional effects between the wall and the grains. The stress σ is taken as a function of the strain u.

The propagation of acoustic waves in dry granular materials and the corresponding influence of wall friction can then be studied in the above framework. The way an asymptotic profile is reached can be numerically determined and is illustrated in Figure 4.5 which shows the evolution of a pressure step toward a

[1] See for instance T. Boutreux, E. Raphael and P.G. de Gennes, *Propagation of a pressure step in a granular material: the role of wall friction*, Phys. Rev. E, 55 (1997), pp.5759–5773.

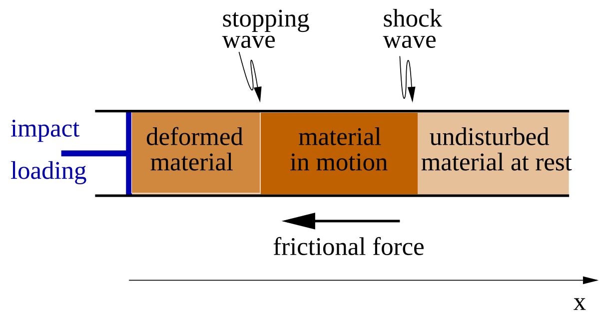

FIG. 4.4. "Waterhammer" experiment: a semi infinite cylinder contains a compressible granular material; a pressure step is applied at the end.

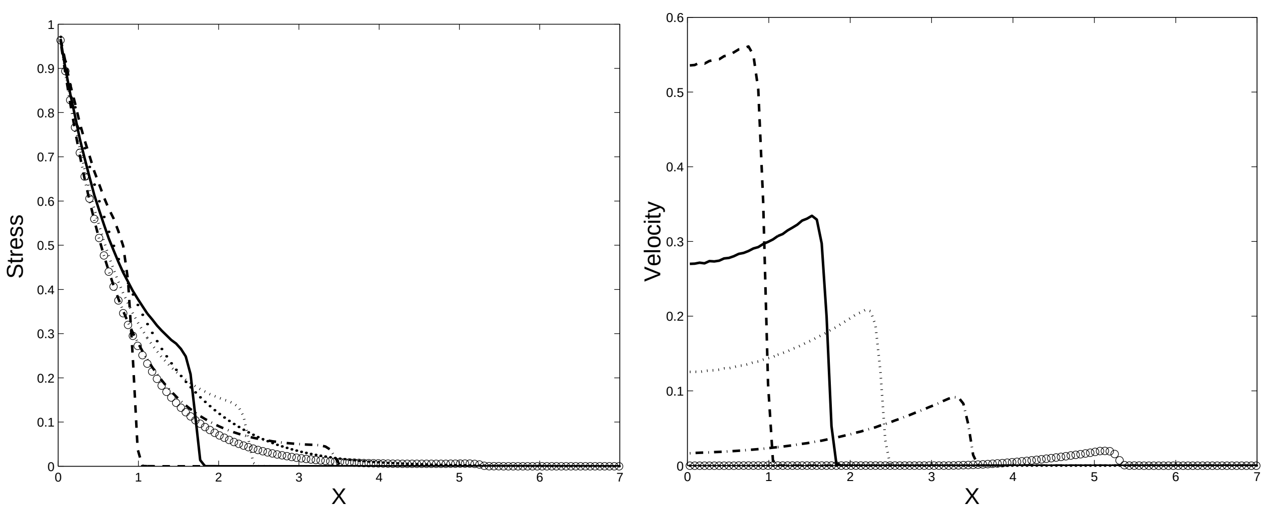

FIG. 4.5. Propagation of a pressure wave in a granular material with a quadratic stress-srain relationship ($m = 2$) and convergence toward a Janssen's like asymptotic state; solutions are plotted at time $t = 1$, 2, 3, 5, 10 and 200. Left: stress, right: velocity

Janssen-like state. A pressure front, followed by a stopping wave, propagate through the material. When the latter catches up with the former, all motion stops.

The above system is a hyperbolic system of nonlinear conservation laws. Using a high order (3) Discontinuous Galerkin method together with a careful implementation of the right-hand term corresponding to a graph, we have been to show that the solutions to the above system do indeed convergence to Janssen's solution. We explain the discrepancy between our results and some previously published results by other authors by the excess of numerical diffusion introduced by their methods.

4.3. Ongoing and future work.

4.3.1. Hopper flows. The main progress on hopper flows during this period of funding has been the discovery of secondary circulations in most pyramidal hoppers. We do not argue that secondary circulation actually takes in lab experiments. We claim, however, that the current models predict them, a fact that had escaped everybody so far, mainly because a full numerical study would require the numerical resolution of a nonlinear elliptic DEA (Differential Algebraic Equations) system of 9 unknowns. We are in close contact with Prof. R.H. Behringer in the Physics Department at Duke who is interested setting up experiments that will bring to the fore secondary circulation. In case circulation phenomena are indeed observed, that will add a fundamental aspect to the present field. Alternatively, the absence of such phenomena would call for a complete and thorough revision of the whole field.

Should the experiments support the theory, we plan to discretize the full three dimensional problem in the next period of funding.

4.3.2. Powder consolidation. Our previous efforts toward the implementation of a reliable and efficient powder consolidation code have been expanded. Having obtained a satisfactory model, we have started its implementation in Objective-C to ease the inclusion of the corresponding code into existing dedicated engineering packages. We expect to have a first version ready by July 2002, when our industrial contact Tony Royal will visit us for 10 days this summer.

4.3.3. Wave propagation in granular material. The problem of wave propagation as set in Section 4.2 is interesting in several respects.

For instance, most existing models assume a stress-strain relationship of the type $\sigma(u) = -\sigma_0 \operatorname{sgn}(u) |u|^m$, $\sigma_0 > 0$. However, theoretical and experimental studies differ as to what the value of m is, namely 3/2 and 2, respectively. The present problem is an ideal testbed to settle this question. Again, our colleague Bob Behringer has expressed strong interest in directing a series of experiments which,by comparision with our numerical results will allow the determination of m.

Mathematically, the problem is also very interesting and open. Closely related systems with damping have recently received a quite a lot of attention. In all those contributions the damping terms are proportional to the velocity instead being proportional to the stress σ as is the case for dry friction. The present case is much tougher to analyze, as no energy estimate can be easily derived. We plan on investigating As part of this project conditions of existence of weak solutions to problems of the present type will be sought.

As a generalization on the numerical side, we will also develop efficient and reliable numerical methods for the resolution of hyperbolic systems with either stiff, discontinuous or set-valued right hand side will be constructed, studied and implemented.

4.3.4. PDAEs. PDAs are ubiquitous in plasticity theory. One of our main long term goals is the development of numerical methods to efficiently handle this type of mathematical structure. Several methods will be tested including the use "streamfunctions" leading to *systems* of Hamilton-Jacobi equations, adaptation of DAE techniques such as constraint stabilization methods to PDAEs, use of variational formulations such as constraint least gradients.

4.3.5. Frictional chutes. The design of optimal chutes is important in countless applications. We have started the study of finding optimal three dimensional chutes when the particles are subject to Coulomb's dry friction. In first approximation, the chute is considered as a wire and the particles as beads allowed to slide along that wire. For given location and direction of the starting point and outlet of the chute, the problem consists in finding the optimal geometry linking the two. Optimal is does not refer to minimizing time, as in the classical brachistochrone problem, but rather to minimizing the work done by friction. A typical industrial application is the handling of brittle material such as pasta for instance.

4.3.6. Granular heap. When a dry granular material is poured on a surface, the slope of the resulting pile cannot exceed some critical value: *the angle of repose.* The pile takes a conical shape, such as for instance that of sand in the lower part of an hour glass. In this project, we study how to determine the shape of such piles when obstacles are present, see Figure 4.6, right.

A deceptively simple problem is the determination of the volume of material inside a bin of possibly complicated geometry including inserts, internal walls, etc... In practice, this is done by having one or several gauges measuring the height of the material at given points. Without some knowledge of the geometry of the top free boundary, such methods are inaccurate. This problem has a long history, largely due to its connection to soil mechanics in civil and military engineering. Coulomb was the first to relate the angle of slip to the friction properties of the material. Unlike previous work, he did not assume a priori values of that angle.

We are proposed a new Eikonal formulation of those problems. Problems with cylindrical obstacles (of arbitrary cross section) correspond to traveltime problems with obstacles. When the obstacle is not cylindrical, the formulation is more involved, but still Eikonal. We have supposed, studied and implemented numerical methods based on modification of the fast marching method, that preserve both the sweeping (one sweep instead of many iterations!) character of the method and preserve the order of accuracy (up to and included second order), even in the presence of obstacles (domains of infinite slowness).

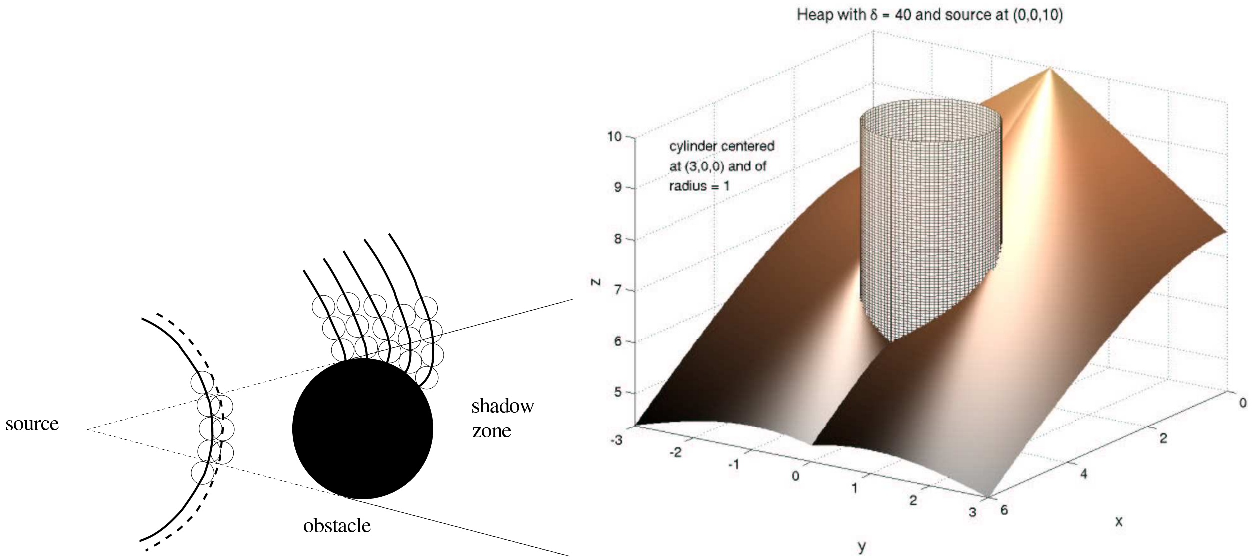

FIG. 4.6. Left: the Huygens principle at play in the two dimensional case. Right: Heap around a circular cylindrical obstacle for a material with an angle of repose of $\delta = 40^\circ$

5. TECHNOLOGY TRANSFER. We will pursue our collaboration with Jenike & Johanson, Inc. We have had meetings about twice a year and expect this to continue in the near future. The focus will be on the efficient resolution of the full problem for granular flows (as described above), and the fine tuning and generalization of the powder consolidation code. We also intent to explore further the possibility of collaborating with the researchers at the U.S. Army Engineer Waterways Experiment Station in Vicksburg, MS, especially in terms of the possible use the present continuum approach to “plowing type problems”.