ERC: Engineering Research Center for Structured Organic Particulates

IREE Supplemental Award

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ABSTRACT: We visited the Eidgenösische Technische Hochshule (Swiss Federal Technical University) in Zürich, Switzerland under the sponsorship of the NSF IREE program. We describe our accomplishments and the connections we made for future international collaborations. We were hosted during our stay by Prof. Dr. Hans Herrmann, Director of the Computational Physics group at the Institut für Baustoffe.

INTRODUCTION

This award was provided to Rutgers University under the IREE program. The purpose of the award was to build an international collaboration between the NSF Engineering Research Center (ERC) for Organic Particulate Systems at Rutgers University and the Granular Research Group at the Swiss Technical University (ETH). The Center's mission focuses on advancing the scientific foundation for the optimal design of Structured Organic Particulate Systems with advanced functionality while developing methodologies for their active control and manufacturing. At the heart of this mission is the need to control the formation of engineered particulate systems – for example to provide uniform and reliable mixing of pharmaceutical powders. For this reason, we pursued a collaboration between Associate Professor Troy Shinbrot, who has expertise in granular flow and segregation as well as in industrial triboelectrification, with one of the world's pre-eminent computational scientists, Prof. Dr. Hans Herrmann, who develops computational methods for powders and grains. Professor Herrmann is former Director of the Institute for Computational Physics at Stuttgart, and is now Director of a companion institute at the Swiss Institute of Technology (ETH, Zürich). Dr. Herrmann is very interested in extending his work on powders and grains to applications in pharmaceutical engineering.

To facilitate this collaboration, we brought two graduate students from the Rutgers BME department who are interested in these topics. First, we selected an international graduate student, Carlos Caicedo-Carvajal, a US citizen born in Colombia, to participate: Mr. Caicedo has already published in granular flow, and has already obtained experience in computational methods for these flows. Second, we brought another international graduate student, Mehdi Doumi, a US citizen born in Algeria, who has developed computational methods for the study of charged and polarized granular materials of importance to the study of pharmaceutical mixing. The students and the PI visited the ETH between Jan 1, 2008 and June 22, 2008, and performed both simulations and experiments to study particulate flow and mixing.

RESEARCH ACTIVITIES AND ACCOMPLISHMENTS OF THE INTERNATIONAL COOPERATION

We performed several separate studies while at the ETH. Several of these were entirely new (e.g. Sand Swimming, and River Delta studies) and others were planned continuations of existing lines of research (e.g. Granular Electrostatics work). Because the work was so broad and extensive, we provide short synopses of each topic, along with researchers involved, here.

1. Granular Electrostatics Experiments. Researchers: T. Shinbrot, Rutgers; H. Hermann (Professor) & Dr. F. Wittel (Postdoc), ETH.

In these studies, we investigated a new phenomenon that occurs when flowing grains become highly charged. This occurs both industrially, e.g. in agricultural or pharmaceutical processing plants, and naturally, e.g. in desert sandstorms. One example of this work is illustrated in Fig. 1 below, where we show that grains of sand can become so highly charged that they cannot be contained within a jar, and instead the grains form a fountain, erupting violently from the jar. This work was published in [Shinbrot & HJ Herrmann, "Static in Motion" Nature 451 (2008) 773-4].

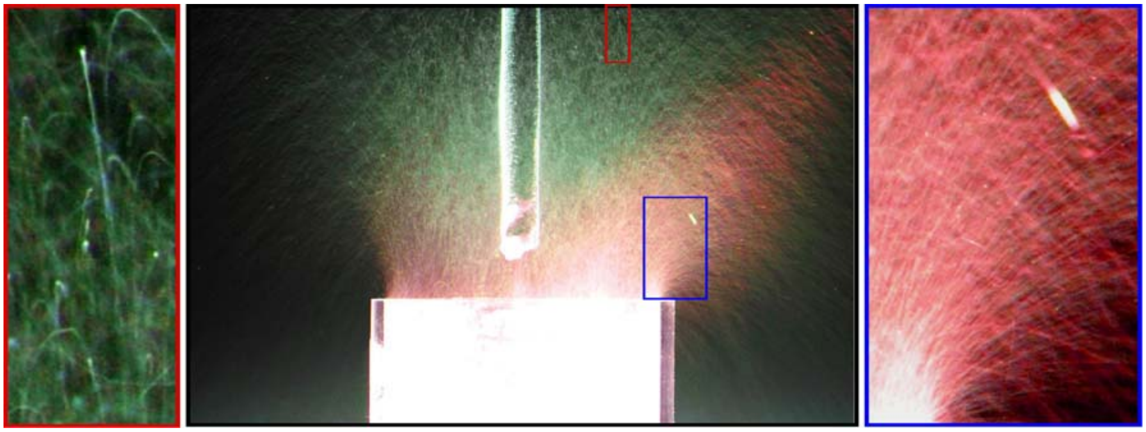


Figure 1 – Granular fountain. In this laboratory demonstration of the explosive potential of charged grains, glass beads 500 micrometres in diameter are charged by repeated pouring them through a vertical acrylic tube into an acrylic container. The grain charges become so large that the beads cannot remain at rest, and they spontaneously form a fountain that erupts from the container, even after the inflow has ceased. If the tube is electrically grounded, these ejections do not occur. The left inset shows trajectories of individual grains; the right inset shows an apparent example of a granular aggregate coexisting alongside individual grains. (Colours are digitally enhanced.) Figure credit: Falk K. Wittel.

2. Granular Electrostatics Simulations. Researchers: T. Shinbrot & M. Doumi, Rutgers; H. Hermann (Professor) & T. Pähtz (Graduate Student), ETH.

In these studies, we simulated the charging that occurs during interactions between grains made of identical materials, as has been demonstrated in [T. Shinbrot, TS Komatsu & Q. Zhao, "Spontaneous tribocharging of similar materials," Europhysics Letters *(in press)*]. This occurs again both industrially and naturally, and we developed a hypothesis for a mechanism that could account for this peculiar process. We performed discrete element simulations that confirmed that the hypothesis seems to be accurate, and we are currently completing experiments in the laboratory to confirm simulation results. A typical outcome of simulations is shown in Fig. 2 below. A complete manuscript describing our findings is under preparation, with a target submission date of Aug. 31, 2008.

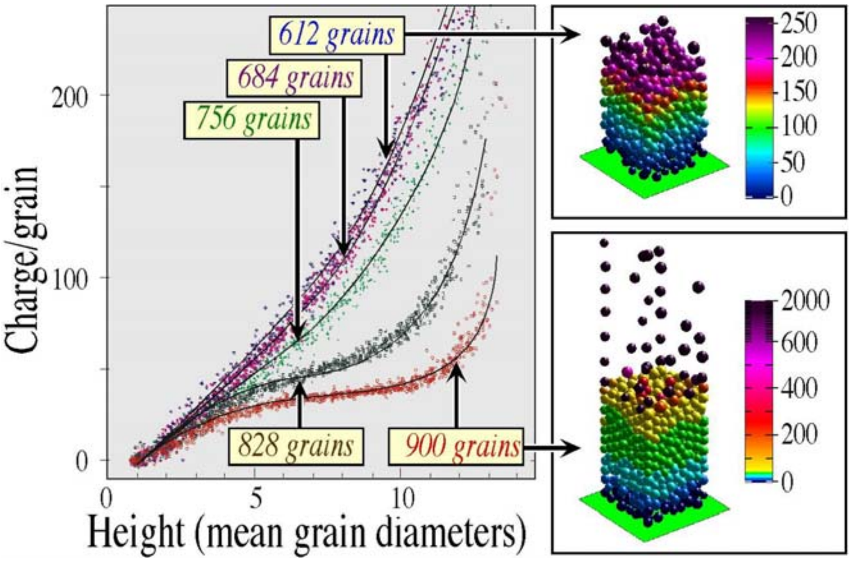
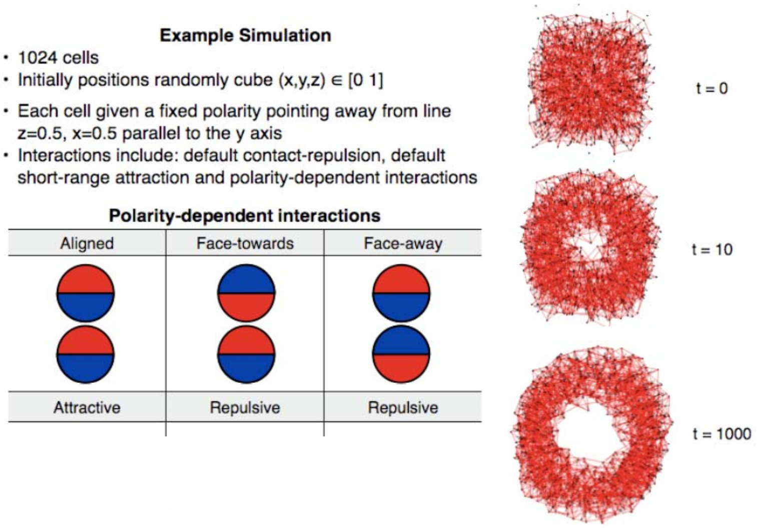


Figure 2 – Charge distributions in beds of grains that are agitated from below using a 'splash function', as occurs during desert saltation, when high velocity windoblown grains strike the desert floor. Main plot: Charge per grain vs. height for various numbers of grains. All simulations are shown after 25 million timesteps in horizontally periodic box 8 mean grain diameters across. To mimic the splash that saltating sand grains receive when they hit the desert floor, grains receive a vertical velocity of random amplitude up to a maximum of 0.2 grain diameters per timestep when they strike the bottom of the box. Notice that as the number of grains – and hence the height of the granular bed – increases, the density of grains in the center of the bed grows and charge/grain becomes increasingly nonlinear: this appears to occur because the center of the bed becomes compressed, between gravity pushing down from above and splashing grains pushing up from below. Grains near the top are observed to bounce frequently on the nearly solid central region, gaining charge with every collision. The charge throughout the bed is shown in the insets to the right. Top inset: charge distribution using 612 grains; bottom inset: charge distribution using 900 grains. Colorbars indicate charge per particle, in dimensionless units. Note that for 900 grains, fewer grains acquire a higher charge than for the 612 grain case.

3. Self-Assembly of Polarized Particles. Researchers: T. Shinbrot & M. Doumi, Rutgers; H. Hermann (Professor) & N. Stoop (Graduate Student), ETH, S. Shvartsman (Professor), Princeton.

One of the established effects of granular charging is that grains become highly polarized, causing them to self-assemble into a variety of unanticipated patterns. This process is very poorly understood, and has implications both to granular flow and mixing (which our group has documented in several publications) and to biological development, where tubulogenesis and other essential processes depend on the interaction between polarized cells, which develop into complex structures throughout the body. We have developed a simulation that reproduces some of these processes, for example in Fig. 3 below, we show that polarized cells that attract neighbors only if co-aligned spontaneously assemble into tubes. We are currently performing both laboratory and computational studies to confirm these findings, both in collaboration with our ETH colleagues, and in concert with Prof. Shvartsman's laboratory, which studies biological pattern formation and morphogenesis of polarized cells.

As an outcome of this work, Mr. Stoop has agreed to visit Rutgers in 2008-9, and Professor Shvartsman has agreed to collaborate on research with him and with Prof. Shinbrot involving self-assembly in biological systems.



Example Simulation

- 1024 cells
- Initially positions randomly cube (x,y,z) ∈ [0 1]
- Each cell given a fixed polarity pointing away from line z=0.5, x=0.5 parallel to the y axis
- Interactions include: default contact-repulsion, default short-range attraction and polarity-dependent interactions

Figure 3 – Spontaneous self-assembly of tubes in 3D discrete element simulations of polarized elements. On the right, a progression of polarized cells is shown, starting from a random agglomerate at the top, and concluding with a tabulated structure at the bottom. Cell centers are shown in black; connections between nearby cells are shown in red. The algorithm used in the simulations is summarized at the left.

4. Viscous Mixing Driven by Interfacial Tension. Researchers: T. Shinbrot & C. Caicedo, Rutgers; H. Hermann (Professor) & N. Stoop (Graduate Student).

The complementary process to granular flow and mixing is, of course, fluid flow and mixing. Our laboratory has a long history in this topic, and we have continued this work in the study of periodic mxing that spontaneously occurs when two miscible liquids interact. Shown below is a simple experiment in which common food coloring is dropped into a beaker of water and allowed to equilibrate. We emphasize that no stirring or agitation has occurred: this manifestly chaotic mixing process appears to occur as a result of interfacial energy differences between the alcohol-based color and the water. Visually, we see that the drop of dye, carefully placed in the center of the beaker, periodically pulsates to produce the pattern shown (false colored to enhance contrast). We have investigated effects of detergent, aspect ratio and other obvious parameters, and continue to be perplexed by the complexity of the spontaneously-induced flow.

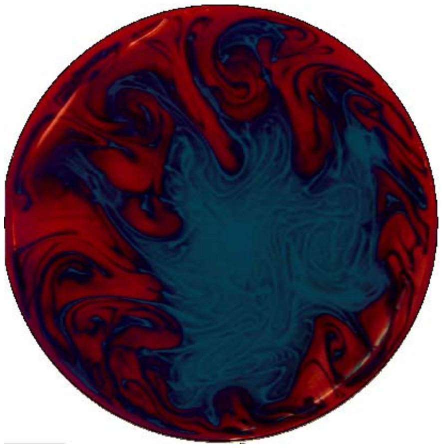


Figure 4 – Effects of pulsation of a drop of food coloring added to a beaker of water. The drop is observed to pulsate spontaneously, producing striated structures that are characteristic of chaotic mixing. This recently observed effect remains unexplained.

5. Dry and Wet River Delta Morphogenesis. Researchers: T. Shinbrot & M. Doumi, Rutgers; H. Hermann, W. Kinzelbach (Professor), P. Molner (Professor) & H. Seybold (graduate student), ETH.

The deposition and erosion of grains is an important process, both in industrial slurries and in natural river deltas. It turns out that there are two distinct processes that can occur in the latter system. Either the river can terminate in a water body – as in the Mississippi river delta – or the river can terminate in the desert – as occurs in the Okavango delta in Botswana. An authority in this field is Prof. Dr. W. Kinzelbach, who works at the ETH in Prof. Herrmann's department. In consultation with Prof. Kinzelbach, and Prof. Molner, who is an expert in fluvial geomorphology, we devised a laboratory experiment to differentiate between these two processes. In Fig. 5, we show typical snapshots from these experiments (also being simulated by an ETH graduate student, H. Seybold).

Figure 5 – Comparison between laboratory deltas formed during flow of grains suspended in water terminating in a dry surface (left) and in a liquid 'sea' (right). Note that the sedimented layer peters out continuously in the dry delta case, but drops off abruptly in the wet delta. Other morphological differences are also evident, for example channels tend to be straighter in the dry deltas than in the wet deltas, and more viable channels are present in the wet deltas than in the dry deltas. In the experiment to the left, the flat supporting surface is heated from below to facilitate evaporation (as would occur in the desert), and the inflow of suspended grains occurs in a pulsatile manner (to simulate seasonal storms). The inflow is colored red in the snapshot to the left. In the experiment to the right, grains suspended in water flow continually; experiments using pulsatile inflow here are underway, as are comparisons with cellular automata simulations.

6. Locomotion of Sand Swimmers. Researchers: T. Shinbrot & M. Doumi, Rutgers; H. Hermann (Professor), Dr. D. Kadau (Postdoc) & R. Mottl (Undergraduate Student), ETH; S. Koehler (Professor), WPI; and J. Soares de Andrade (Professor), Universidade Federal do Ceará, Brazil.

It has long been known that certain lizards and snakes, which are cold-blooded, must submerge beneath the sands of the desert during daytime to prevent fatal increases in their body temperatures. It has been determined, furthermore, that these creatures submerge to depths of at least 10 cm, and can travel beneath the surface at these depths. How they accomplish this remains unexplained, however recent studies have indicated that two separate mechanisms may achieve this feat. First, the traditional Purcell's swimmer, used to explain flow in the Stokes regime in viscous fluids, may permit sand swimming, and second, a mechanism termed "Pushme-Pullyou" (after the Dr. Doolittle creature) has been studied [JE Avron, O. Kenneth & DH Oaknin, "Pushmepullyou: an efficient micro-swimmer," New J. Phys. 7 (2005) 234-42]. The Pushme-Pullyou mechanism involves the creation of linked spheres that alternately expand and contract, as is seen to operate during some modes of propulsion of simple protists.

To evaluate whether these distinct mechanisms, developed to understand propulsion in viscous fluids, could operate in sand, we produced a discrete element simulation in which we link spheres together, which we alternately inflate and deflate (see Fig. 6). We find that this mechanism does seem to efficiently propel the system of spheres, and we are engaged in two studies. First, we are evaluating the optimal size and inflation protocol that minimizes energy consumption and maximizes propulsion distance, and second, we are comparing the efficiency of this scheme as compared with the more traditional Purcell's swimmer.

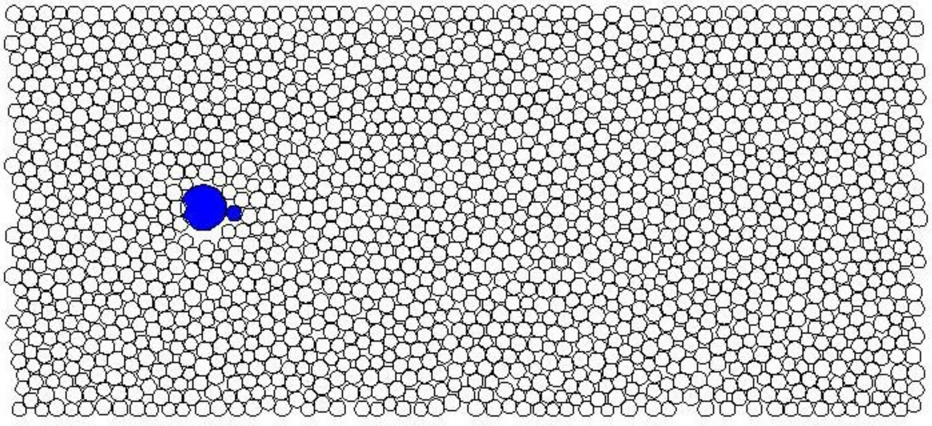


Figure 6 – Discrete element simulation of "Pushme-Pullyou" sand-swimming. The mechanism of motion consists of four sequential actions by the two-sphere assembly (solid blue). First, the smaller sphere (to the right in the figure above) is pushed to the right; second, the large sphere deflates and the small one inflates; third, the smaller sphere (now to the left) is retracted to the right; and fourth, the large sphere (now to right) deflates and the small one (now to left) inflates . The consequence of this sequence of actions, confirmed in our simulations, is that the two-sphere assembly moves to the right. A similar mechanism is observed in the motion of the bacterium, Euglena [Avron, 2005], and our simulations seek to evaluate the relative efficiency of this behavior in locomotion within a sand bed as compared with the traditional Purcell's swimmer.

BROADER IMPACTS OF THE INTERNATIONAL COOPERATION

The two students from Rutgers who were involved in the visit to the ETH were US citizens born in Colombia and in Algeria, and provided our Swiss hosts with a strong multicultural face from their American colleagues. ETH itself is a nexus of international collaborations, and exposed us in turn to visitors from around the world, including in the short time that we were present, from France, Germany, Italy, Norway, Russia, South Africa, Iran, Israel, Cuba, Argentina, Mexico and Brazil. We built active collaborations with scientists from Japan and China as well.

A culmination of our experience is that we have begun to build an exchange program, and are bringing the first, of what we hope will be many, graduate student from Switzerland to Rutgers in the Fall. We have built a multi-institutional collaboration for that student to take part in, including a prominent scientist from Princeton, producing in the process a new direction to our lab's research dealing with simulations for the self-assembly of cells during development. As part of this effort, we had one-on-one meetings with numerous scientists, including Prof. Drs. Martin Schwab of the Institute for Brain Research, Esther Stoeckli of the Institute of Zoology, Ruedi Stoop of the Institute for Neuroinformatics, Petros Koumoutsakos of the Computational Science and Engineering Laboratory, and Konrad Basler of the Institute for Molecular Biology, among others.

Our visit expanded the perspectives of all of the Rutgers participants, exposing us to new cultural and linguistic experiences, permitting us to use Switzerland's extremely advanced transportation system and to build connections with European, South American, African and Asian granular researchers, and giving us the opportunity to build a long-lasting set of collaborations and exchanges for the future. Our host at the ETH has invited us to return in the near future, as have colleagues at the nearby University of Zürich, and as we have mentioned, we have begun a student exchange program with the ETH. We have more than accomplished what we had planned (developing a simulation of granular electrostatics: item 2 above), producing complete results in the original field, and establishing a clear foundation for results in several new fields as well (items 1, 3-6 above). We look forward to seeing the fruits of this short visit develop in the years ahead.

DISCUSSION AND SUMMARY

The IREE program provided an unparalleled opportunity for our laboratory to pursue existing studies, to build new collaborations, and to develop entirely novel lines of research for future exploration. We completed a first paper on granular electrostatics (already published) and got a second one (on tribocharging of similar materials) approved for publication. We are writing a third paper (on simulations of granular charging), and plan at least two more for the near future (on delta formation, and on applying polar simulations to biological development). We met both with scientists from abroad, and brought scientists from the US to visit the ETH and join our collaborative circle (Prof. R. Dave of NJIT and Prof. S. Shvartsman of Princeton).

For the future, two recommendations are first that it seems suitable to bring students and scientists from abroad to the US, thus building a two-way exchange mechanism. In Switzerland, we were able to do this by capitalizing on funding for student travel through the Swiss Research Foundation (the equivalent of the US NSF), however this would not be so for all host countries. It would be helpful if visits by colleagues from abroad were supported in some way as a follow-up to the IREE initiative. A second recommendation is that it would be useful if scientists who are not affiliated with an ERC could gain support for foreign travel. I was privileged to have been able to take part in this program, but this was only possible because of my close interactions with Rutgers ERC. Broader accessibility to this fine program could only be a good thing.

ACKNOWLEDGEMENTS

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BRIEF BIOGRAPHIES OF RESEARCHERS

Troy Shinbrot received his Bachelor's in Physics from Reed College in 1978, and worked for several years at Xerox Corporation and then at Arthur D. Little, Inc. He took his PhD from the University of Maryland, College Park in 1992, with a dissertation on the Control of Chaos. He completed a postdoc at Northwestern University in the Department of Chemical Engineering, and was promoted to Research Assistant Professor in 1994. He left Northwestern for Rutgers University in 1998, where he held the position of Research Associate Professor, again in Chemical Engineering, until 2002, when he became Associate Professor in Biomedical Engineering. He was granted tenure in 2005 and served as Graduate Director between 2002 and 2007. His research deals with two areas: first, he studies granular flow and mixing, most recently of charged grains, and second he studies pattern formation, particularly during biological development.

Carlos Caicedo-Carvajal was born in Colombia and became a US citizen in 2007. He received the B.S. degree in Biochemistry from Rutgers University in 2001. Following a year working on measuring adhesive properties of fibroblast on polymer surfaces at the NJ Center for Biomaterials, he enrolled in the Biomedical Engineering graduate program at Rutgers University. Since 2002, he has worked on several academic aspects from the physics of granular flow to his current research on the physical properties of tissue self-assembly and cellular rearrangement and simulation of cellular systems with prescribed attraction/repulsion relations. He is committed to community education, and has volunteered for several outreach projects to teach Science and Engineering to local underprivileged youth. Research interests include pattern formation in granular and biological systems, and his dissertation focuses on the understanding of basic aspects of substrate deposition during tissue self-assembly and the dynamics of wound healing in the adult organism.

Mehdi Doumi was born in Algeria, and became a US citizen in 2006. He graduated from Rutgers in the Biomedical Engineering Department (BME) in 2006, with an honors thesis on neurite pathfinding, and enrolled in the BME graduate program the same year. He has performed finite element simulations of nonlinear interactions between fluid and heat transport during pharmaceutical capsule drying. He has received several awards, including a Bloustein Award for Outstanding Scholarship and a National Award of Distinction for direction and production of a video for the Rutgers Television system. He helped rebuild homes after the Katrina hurricane through Habitat for Humanity, and serves as a Biomedical Engineering Student Society graduate representative. His research interests include computational biology as applied to morphogenesis during development and emergent processes in granular and fluid physics.