

THE TRIBOELECTRIC CHARGING OF VOLCANIC MATERIALS

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2015-2016 Graduate Fellow

RESEARCH SUMMARY

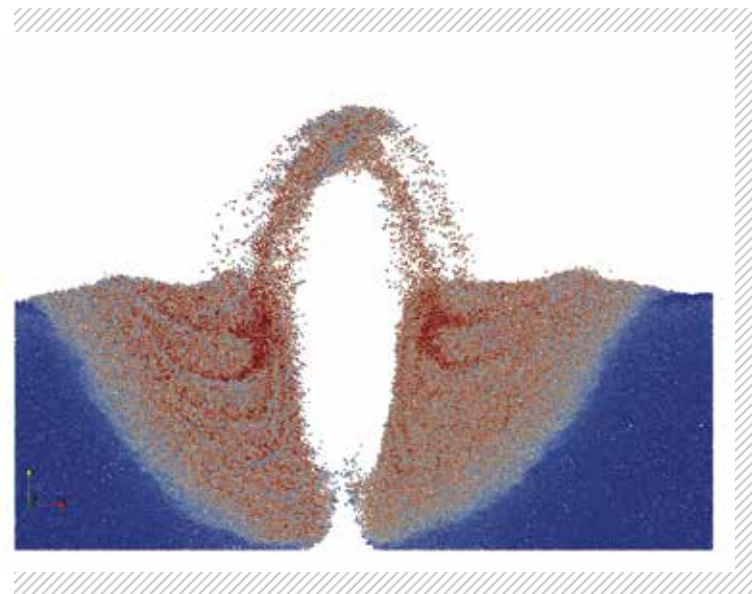
FIGURE 1: Snapshot from the DEM with 100,000 micron particles simulating a laboratory-scale spouted bed. The color code shows the number of electrons transferred during collisions, with warmer colors indicating more electrons. The number of electrons transferred during contacts is proportional to the particles' collisional kinetic energy and the contact time.

When fluidized, insulating granular materials readily become electrified as individual grains undergo collisions. Although contact and frictional electrification processes—collectively termed *triboelectrification*—have been studied for millennia, the mechanisms that drive the exchange of charge between contacting surfaces remain obscure [1]. Perhaps the most dramatic demonstrations of granular charging are the brilliant displays of lightning during violent volcanic eruptions [2]. The industrial sector routinely monitors the hydrodynamics of granular materials non-intrusively using electrostatic probes, electric field mills, and capacitive tomography [3]. In principle, similar methodologies could be widely applied to volcanic systems. Indeed, the observed variability in electrical behavior between eruptions and between volcanoes suggests that the generation and separation of charge is modulated by specific eruption parameters, such as the properties of the ejected materials (both ash and volatiles), environmental conditions, and the energy of the eruption. Thus, understanding the

coupling between eruption dynamics and electrical activity, much of which can be studied remotely, may yield information about the internal dynamics of an eruption that would otherwise be opaque to observation [4].

Most work on the electrification of volcanic plumes has focused on studying macro-scale effects, namely the detection and processing of lightning signals or changes to the ambient electric field. However, because triboelectrification is inherently a microscopic phenomenon involving the interaction of minute ash particles, developing robust tools to probe inside volcanic clouds requires that we build constitutive relationships that link often elusive, nanoscale charge transfer processes to evident meter- and kilometer-scale discharges and electric fields. While we have learned much about the changing behavior of ash from experimental efforts, determining how electrification is effected by the kinetics of the system (which include particle collision frequency, collisional energies, and aggregation rates) can still present a challenge without specialized equipment.

To complement our experimental work and answer outstanding questions, I developed a novel discrete element model (DEM) that includes a charging module and interparticle electrostatic force module. The model implements the trapped electron model first described by [5], to account for charging between chemically similar particles (Fig. 1). Specifically, this mechanism proposes that charging is driven by electrons trapped in unfavorable energy states on one surface that transfer into empty low-energy states on another surface when they come into contact. A particularity of this process is that if asymmetric contact is involved, such as small particles colliding with larger grains, the smaller particles become negative and the larger ones acquire a positive charge. As particles charge, their dynamics may become influenced by electrostatic forces. My model integrates a formulation for polarizable, dielectric spheres [6]. At large distances, the electrostatic force can be approximated by that



between two point charges. However, at close ranges, the effects of mutual polarization can radically change the magnitude and sign of the forces between grains. Indeed, there are given combinations of particle size and charge that generate attractive forces even if the particles carry charge of the same sign (Fig. 2)! The model reproduces the bimodal charging behavior observed in a number of experiments [7]. Using the charging rates obtained from the DEM allows us to start exploring charging behavior in a large-scale Eulerian-Eulerian simulations of volcanic plumes, to reproduce the lightning storms present in large volcanic eruptions. As a case study, we will use the 2009 Redoubt eruption. Applicable to study other systems, my model is also being used to explore morphological peculiarities of the “plastic” sand dunes of Saturn’s moon Titan [8], structures perhaps molded by electrostatic forces.

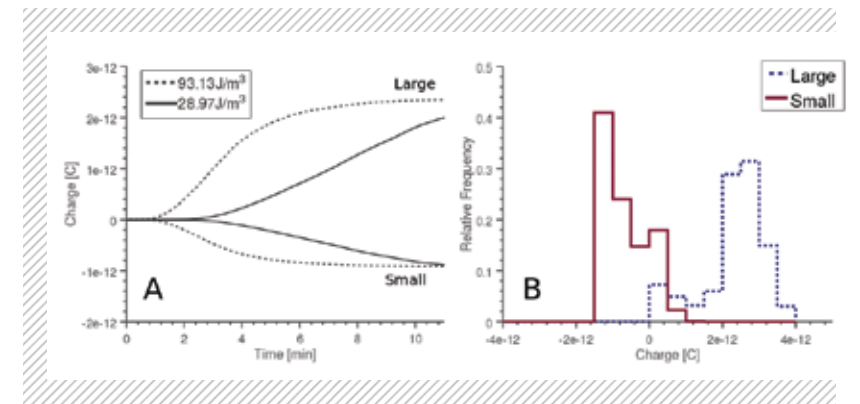
WHY BLUE WATERS

Discrete element models have the advantage that the interactions between particles can be resolved directly. However, even simulating a physically small, laboratory setup often involves tracking several hundred-thousands to millions of particles, exceeding the abilities of conventional desktop machines or small clusters. These simulations and would not have been viable without a machine like Blue Waters.

While I have done computing work during much of my academic career, most of the work prior to receiving the Blue Waters Fellowship involved the programming of embedded systems. One of the processors with which I am most familiar runs on a 1

Joshua Méndez Harper is a fifth-year Ph.D. student at the Georgia Institute of Technology, working with advisor Josef Dufek. He enjoys “projects that straddle disciplines,” and hopes to continue pursuing multidisciplinary work as either a faculty member at a public research university or at a national laboratory.

“This fellowship has not only brought key aspects of my research into different, clearer light, it has also guided me toward avenues that I considered inaccessible a year ago,” he says. “Furthermore, the code I have developed during my fellowship has garnered interest among researchers beyond the confines of my primary field of study, opening new and exciting possibilities for future interdisciplinary work.”



Mhz clock, has little more than 1 kB of Flash memory and 32 bytes of ram, costs around \$1, and is about 3 mm on a side. Starting to run code on one of the **world’s most powerful** machines was intimidating at times. The Blue Waters staff, particularly my point-of-contact, rapidly helped to dissipate any uncertainty—resolving compilation issues or jumping in to improve the code’s performance. As someone who is relatively new to HPC, I think they are one of the most valuable parts of this fellowship and have convinced me to use HPC resources for the rest of my career.

PUBLICATIONS AND DATA SETS

Méndez Harper, J.S. and Josef Dufek (2016), The effects of granular dynamics on the triboelectric charging of volcanic ash: Experiments and numerical simulations. *Proceedings of the 2016 Meeting of the Electrostatics Society of America*, Purdue University, USA.

FIGURE 2: Output from the spouted bed simulation. Implementing the trapped electron model, the simulation reproduces the bipolar charging behavior observed in many natural and man-made systems. Specifically, smaller particles are observed to charge negatively while larger ones charge positively.