CHRIS RYCROFT, UC Berkeley and Lawrence Berkeley Laboratory, Berkeley, CA 94720, USA *A multiscale simulation technique for granular flow*

Due to an incomplete picture of the underlying physics, the simulation of dense granular flow remains a difficult computational challenge. Currently, modeling in practical and industrial situations would typically be carried out by using the Discrete-Element Method (DEM), individually simulating particles according to Newton's Laws. The contact models in these simulations are stiff and require very small timesteps to integrate accurately, meaning that even relatively small problems require days or weeks to run on a parallel computer. These brute-force approaches often provide little insight into the relevant collective physics, and they are infeasible for applications in real-time process control, or in optimization, where there is a need to run many different configurations much more rapidly.

Based upon a number of recent theoretical advances, a general multiscale simulation technique for dense granular flow will be presented, that couples a macroscopic continuum theory to a discrete microscopic mechanism for particle motion. The technique can be applied to arbitrary slow, dense granular flows, and can reproduce similar flow fields and microscopic packing structure estimates as in DEM. Since forces and stress are coarse-grained, the simulation technique runs two to three orders of magnitude faster than conventional DEM. A particular strength is the ability to capture particle diffusion, allowing for the optimization of granular mixing, by running an ensemble of different possible configurations