Large Scale MPI-Parallelization of LBM and DEM Systems
Accelerating Research by Using HPC

Bohumir Jelinek, George Mason, John Peters, Daniel Johnson, Marcus Brumfield, Alex Carrillo, Clay Goodman, Farshid Vahedifard

Introduction

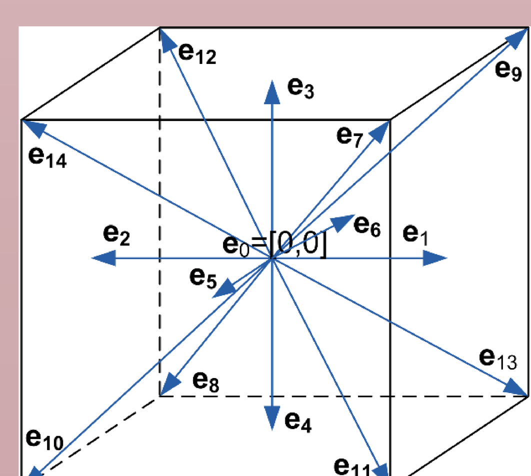
Casting, solidification, and the behavior of dry, saturated, and partially saturated granular media are examples of interesting and important problems in multiple areas of civil, mechanical, and chemical engineering. For interacting particle-fluid systems, the Discrete Element Method (DEM) and Lattice-Boltzmann Method (LBM) provide valuable high-resolution numerical models. Their main issue is high computational demand, which can be addressed by use of HPC resources.

Model description

Lattice-Boltzmann method

D3Q15 lattice: density distribution functions f_0-f_{14} correspond to fifteen velocity vectors $\mathbf{e}_0$ to $\mathbf{e}_{14}$. Macroscopic fluid density ρ is a sum of the distribution functions at that lattice point.

$$\rho = \sum_{i=0}^{14} f_i$$



Fluid velocity at the lattice point is a weighted sum of lattice velocities:

$$\boldsymbol{u} = \frac{\sum_{i=0}^{14} f_i \boldsymbol{e}_i}{\sum_{i=0}^{14} f_i} = \frac{\sum_{i=0}^{14} f_i \boldsymbol{e}_i}{\rho}$$

Time evolution of the distribution functions is given by:

$$f_i(\boldsymbol{r} + \boldsymbol{e}_i \Delta t, t + \Delta t) = f_i(\boldsymbol{r}, t) + \frac{1}{\tau_u}\left(f_i^{eq}(\boldsymbol{r}, t) - f_i(\boldsymbol{r}, t)\right)$$
$$i = 0, 1, \dots, 14$$

Viscosity is related to the relaxation parameter τ:

$$\nu = \frac{\tau_u - 0.5}{3} \frac{\Delta x^2}{\Delta t}$$

Discrete element method

DEM represents granular media at the scale of individual particles. Particles interaction follow contact laws. A simple example is linear spring contact model:

$$F_N = \alpha K_N \delta_n^m$$

Particle linear and angular velocity are determined by integrating Newton's equations of motion:

$$m\frac{\partial v_i}{\partial t} = mg_i + \sum_{c=1}^{N_c} f_i^c, \qquad I_m \frac{\partial \omega_i}{\partial t} = \sum_{c=1}^{N_c} M_i^c$$

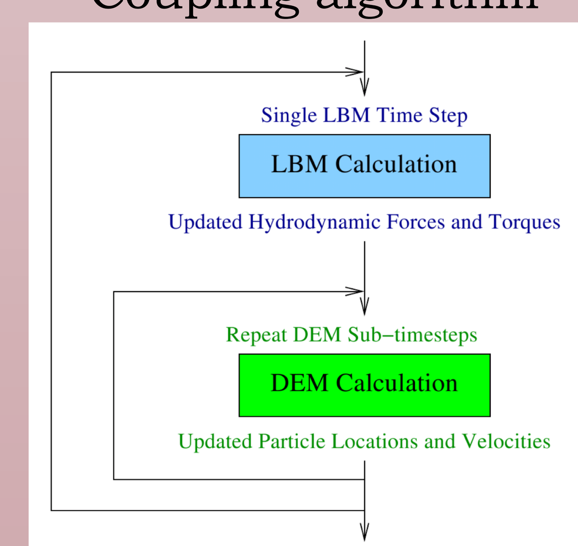
Coupled LBM-DEM system

Coupling is implemented using immersed moving boundary (IMB) method. IMB introduces an additional collision operator Ω_i^S with a weighting factor $\beta(\epsilon,\tau)$ depending on solid coverage ϵ and relaxation parameter τ:

$$f_i(\boldsymbol{r} + \boldsymbol{e}_i \Delta t, t + \Delta t) = f_i(\boldsymbol{r}, t) + [1 - \beta(\epsilon,\tau)]\frac{1}{\tau}\left(f_i^{eq}(\boldsymbol{r}, t) - f_i(\boldsymbol{r}, t)\right) + \beta(\epsilon,\tau)\Omega_i^S$$

$$\Omega_i^S = f_{-i}(\boldsymbol{r}, t) - f_i(\boldsymbol{r}, t) + f_i^{eq}(\rho, \boldsymbol{U}_S) - f_{-i}^{eq}(\rho, \boldsymbol{u})$$

Coupling algorithm



$$\beta(\epsilon,\tau) = \frac{\epsilon}{1 + \frac{1-\epsilon}{\tau - 0.5}}$$

Force and torque by fluid on particles is

$$\boldsymbol{F}_F = \frac{\Delta x^3}{\Delta t}\sum_n \left(\beta_n \sum_{i=0}^{14} \boldsymbol{\Omega}_i^S \boldsymbol{e}_i\right)$$

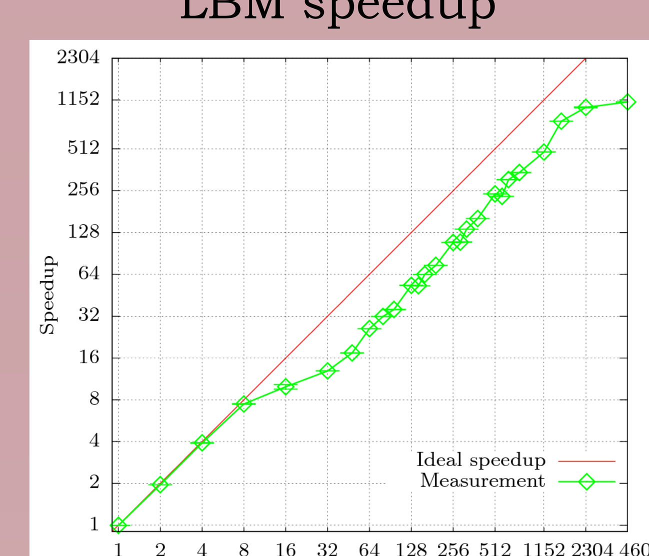
$$\boldsymbol{T}_F = \frac{\Delta x^3}{\Delta t}\sum_n (\boldsymbol{r}_n - \boldsymbol{r}_c) \times \left(\beta_n \sum_{i=0}^{14} \boldsymbol{\Omega}_i^S \boldsymbol{e}_i\right)$$

DEM (serial)+LBM project description with animations:
http://www.cavs.msstate.edu/projects/dem_lbm/

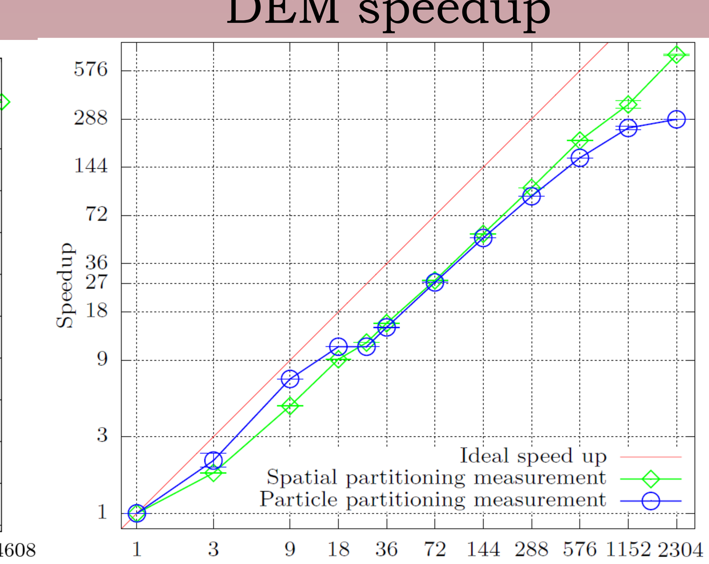
Parallelization

Spatial domain decomposition was used to parallelize LBM [1-5]. Both spatial and particle-based domain decompositions were evaluated for DEM. Spatial domain decomposition divides space, while particle partitioning divides particles between processors.

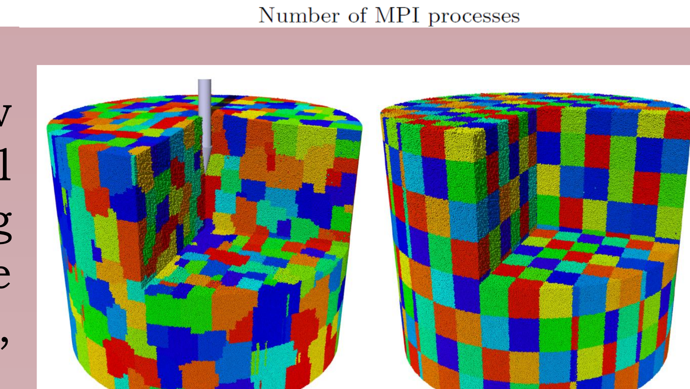
LBM speedup



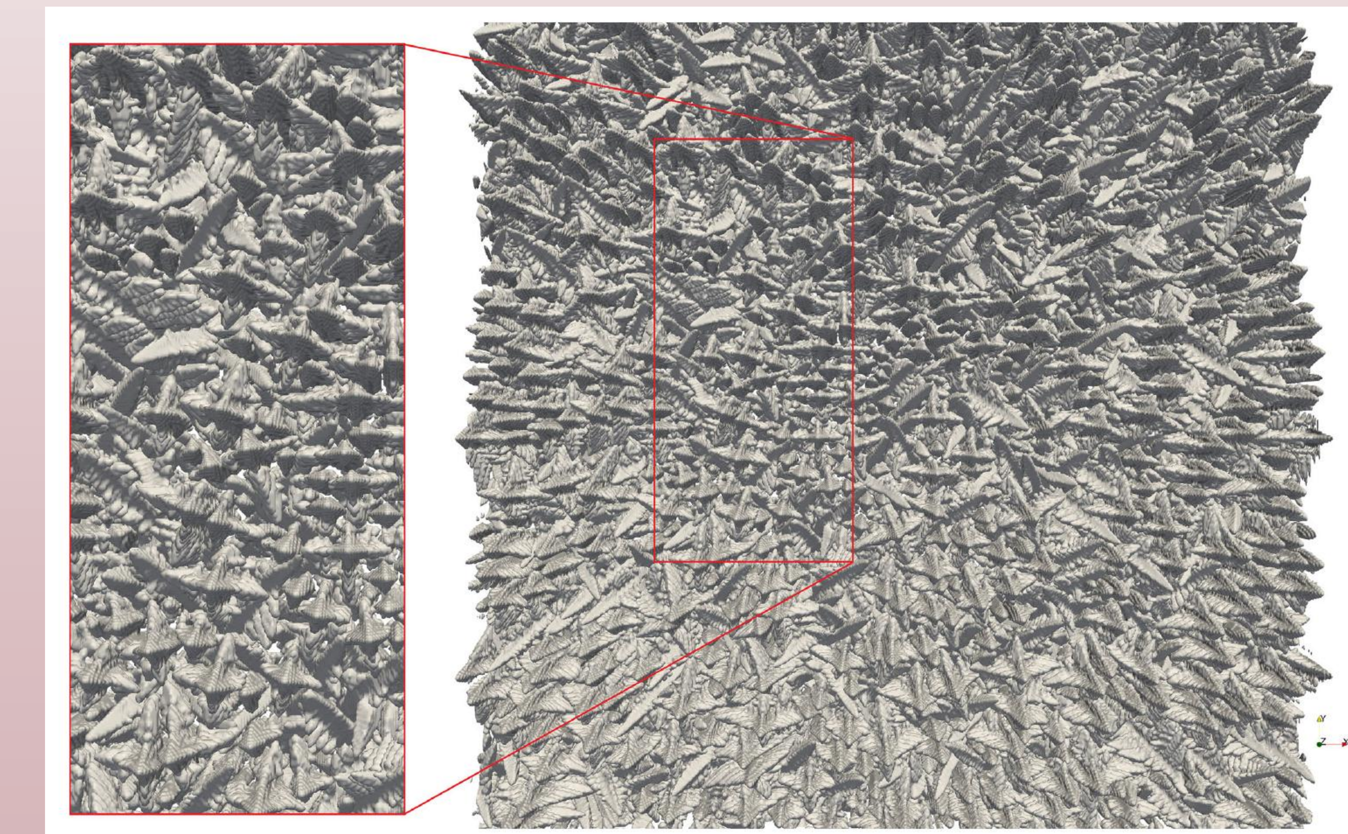
DEM speedup



Images on the right show particle (left) and spatial (right) parallel partitioning for DEM simulations of the cone penetration test, which is shown afterwards.

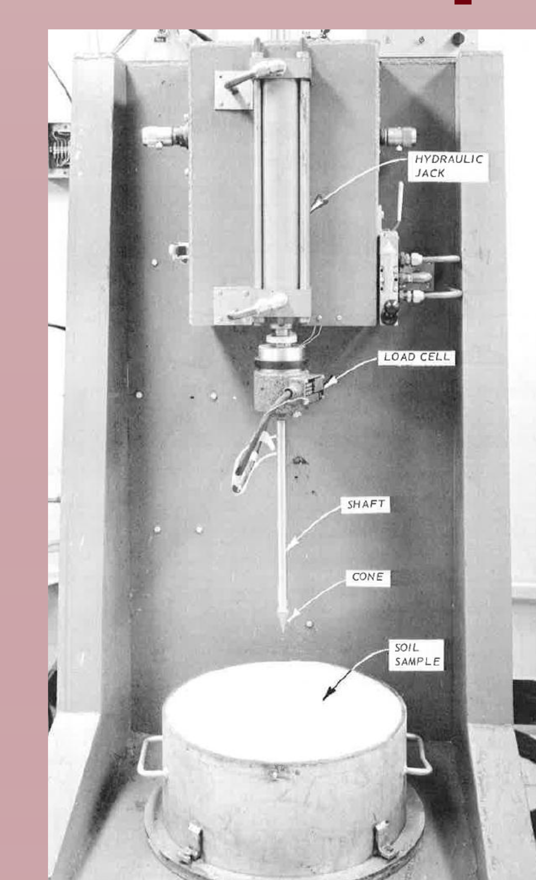


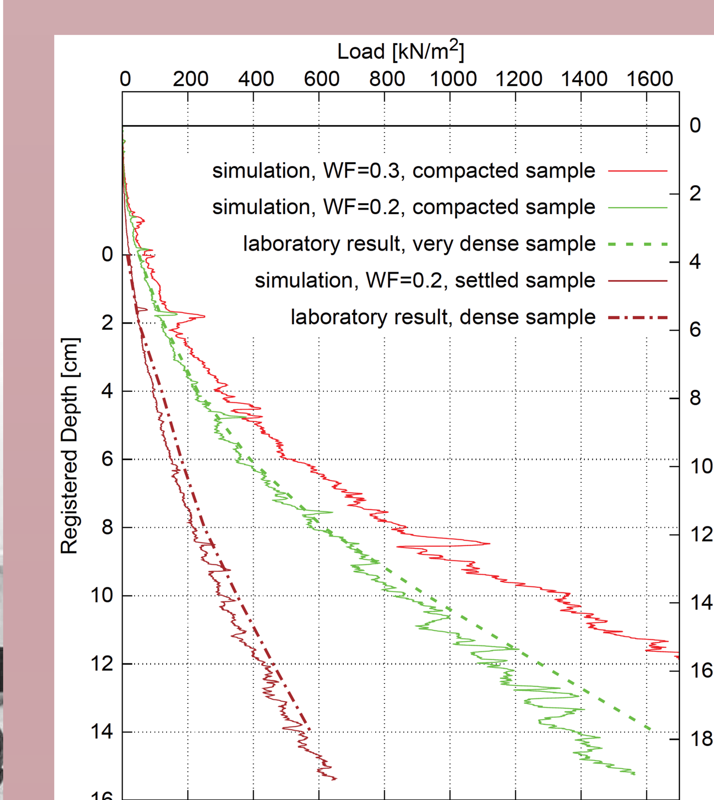
Large scale 3D simulation of dendrite growth



Growth of columnar dendrites in 1mm³ domain was discretized with 3300 x 3300 x 3300 grid cells, or 36 billion grid points total and 4000 initial seeds [2]. Simulation was performed on 6400 cores Stampede, UTACC.

Large scale DEM simulations of cone penetration test (CPT)

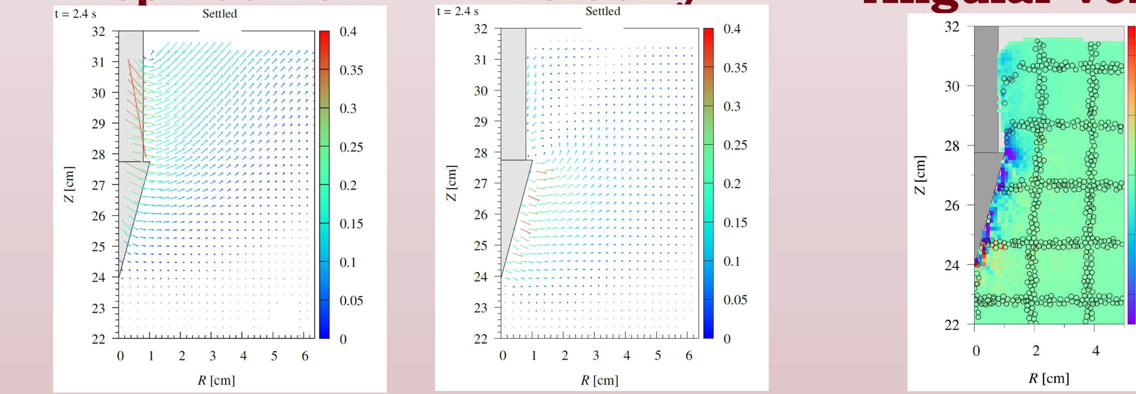




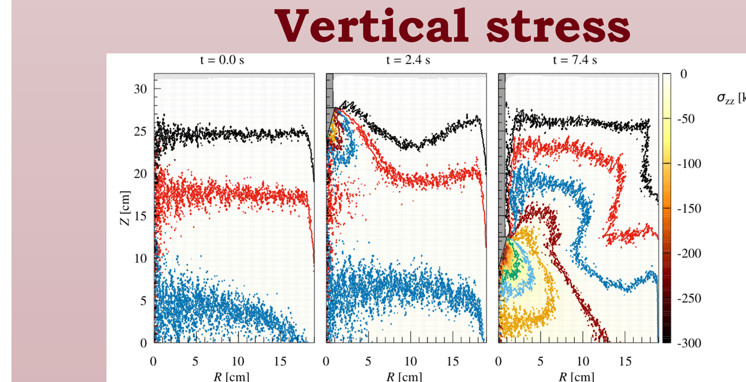
The soil sample was represented by 9.5 million spherical particles placed in a cylindrical mold. Rigid probe with cone-shaped tip was inserted with velocity 3cm/s. Simulations of probe insertion took ~10 days on 1152 cores. Parallel executions were performed on an SGI ICE X system having 3,456 nodes with 116 GB of DDR4-2133 RAM and two eighteen-core Intel Xeon E5-2699v3 processors, connected by 4x FDR InfiniBand network with Hypercube topology.

Macroscopic averages from DEM simulations

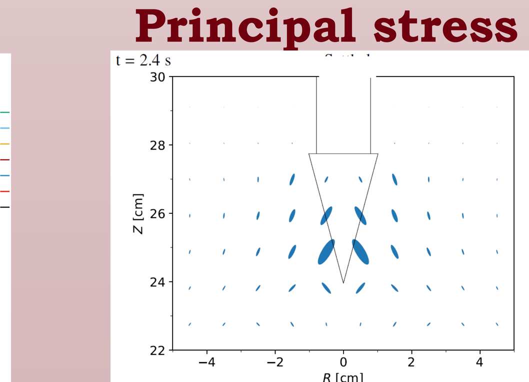
Displacement Velocity Angular velocity



Vertical stress

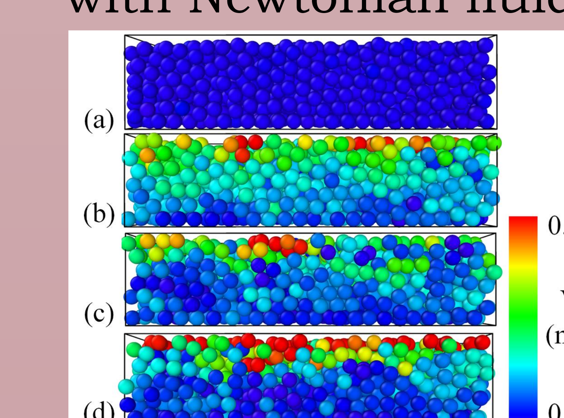


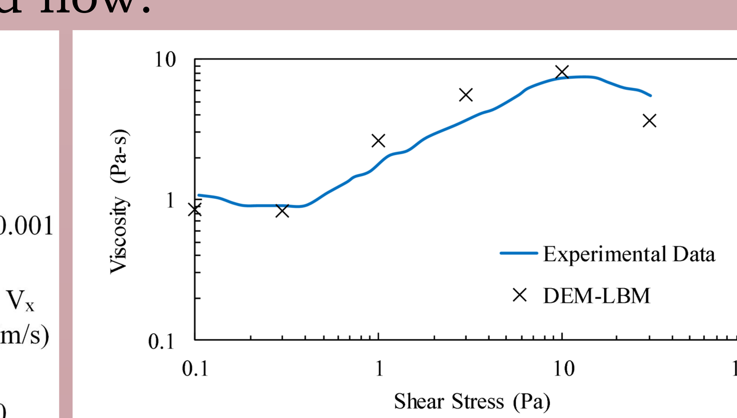
Principal stress



DEM+LBM modeling of discontinuous shear thickening in granular suspension

Velocity was applied to the top boundary of the flat channel flow, which caused the shearing motion, and the shear resistance of the system was measured as $\eta = \tau/\dot{\gamma}$. Resulting viscosity values are predictions from 3D micromechanics combined with Newtonian fluid flow.





Summary

This work demonstrates the use of MPI-parallelized LBM and DEM models to accelerate research in solidification and macroscopic behavior of dry and saturated granular media. Large scale parallel simulations of dendritic growth, the calibration-chamber cone penetration test, and a parametric study of shear thickening in granular suspension were performed. Use of HPC significantly reduced the computational time for these studies and provided high-resolution representation of physical experiments.

References

[1] Jelinek et al., Comp. Phys. Comm. 2013, 185(3), pp. 939-947
[2] Eshraghi et al., JOM 2016, 67(8), pp. 1786-1792
[3] Johnson et al., Journal of Rheology 2017, 61(2), pp. 265-277
[4] Johnson et al., Computers and Geotechnics 2017, 89, pp. 103-112
[5] Eshraghi et al., Metals 2017, 7(11), pp. 474

Center for Advanced Vehicular Systems, Civil and Environmental Engineering, Computer Science and Engineering, Mississippi State University
U.S. Army Corps ERDC, Vicksburg, Mississippi