Percolation Through Voids Around Randomly Disordered Sand Grains

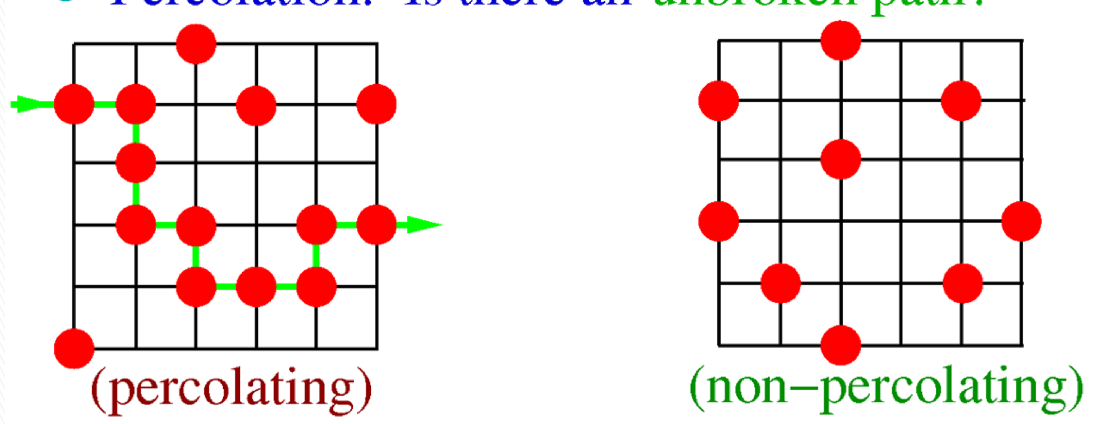
Nicholas McGuigan, Dr. Donald Priour

Abstract:

Fluid flow or charge transport through porous materials takes place within voids around impermeable grains. With increasing density of grains, fluid flow diminishes, ultimately ceasing at the percolation transition separating configurations macroscopically navigable; and those which block fluid flow in the bulk limit. Theoretical studies of void networks have generally been confined to monodispersed systems of identical particles, with no calculations of percolation thresholds for geometrically diverse grains. In addition to positional and orientational disorder, we incorporate structural disorder by imposing random variations in the geometries and sizes of grains, akin to realistic porous materials. We consider cubes distorted into rectangular solids with random proportions. More comprehensibly, we also examine configurations of structurally disordered tetrahedra and parallelepipeds with both random perturbations in edge lengths and dihedral angles. Reflecting the fact that grains in practice are irregular polyhedral with various numbers of faces, we also implement structural disorder by using Voronoi tessellation to carve out irregularly shaped grains. Intuitively, this approach mimics the formation of grains in nature from fractured larger objects.

Void Percolation: A Brief Tour

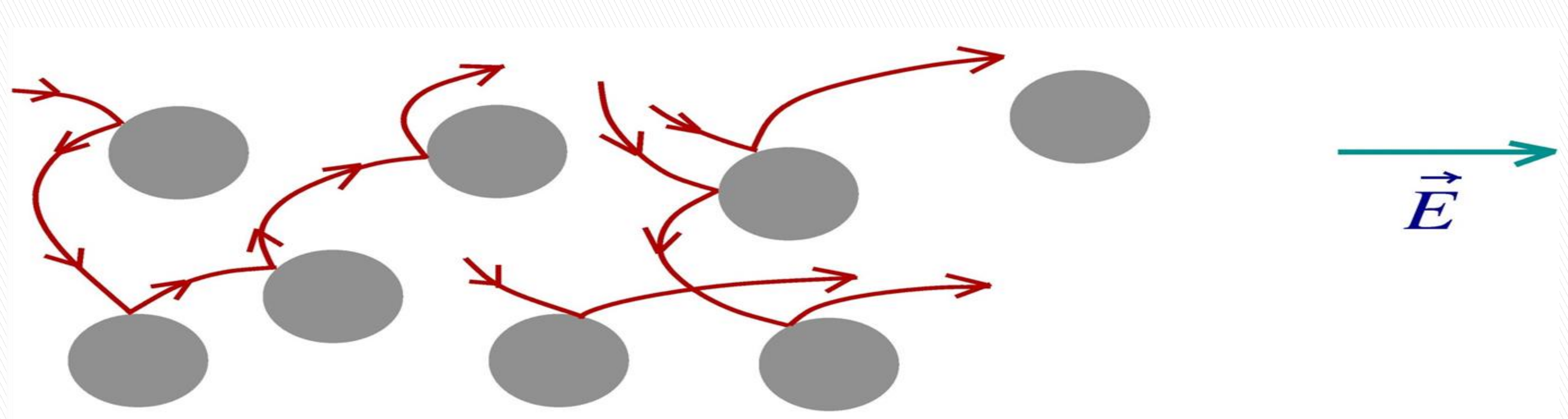
- Percolation: Is there an unbroken path?



When dealing with disordered systems, however:
- Transport channels are not well defined
- Percolation occurs through pores, or voids, between barrier particles
- Long-range connections begin at a critical threshold denoted ρ_c

Inspiration:

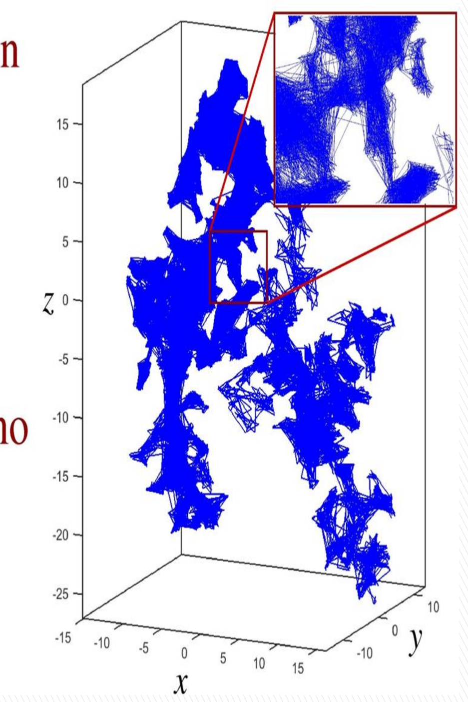
- Improve results obtained using specular reflection approach.
- Follow parabolic bounces of tracer particles driven by an electric field.
  - Electric field proved to be irrelevant to calculation
- Switched from altering system sizes to a time-scaled run approach.



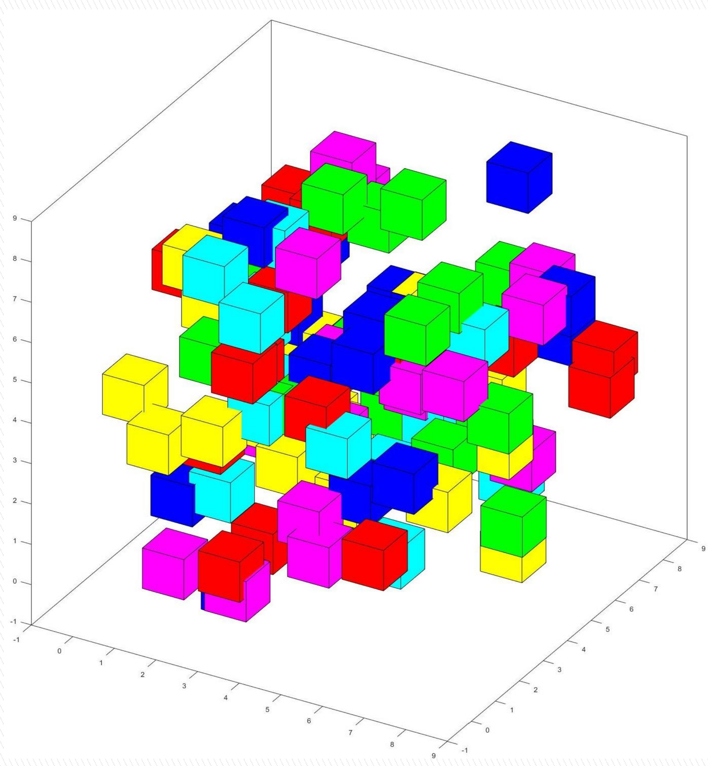
Dynamic Infiltration Simulations: Advantage of Finite Time Scenario

Finite Volume:
- Calculate, e.g., fraction of escaping tracers
- Latency in waiting; residual undertainty

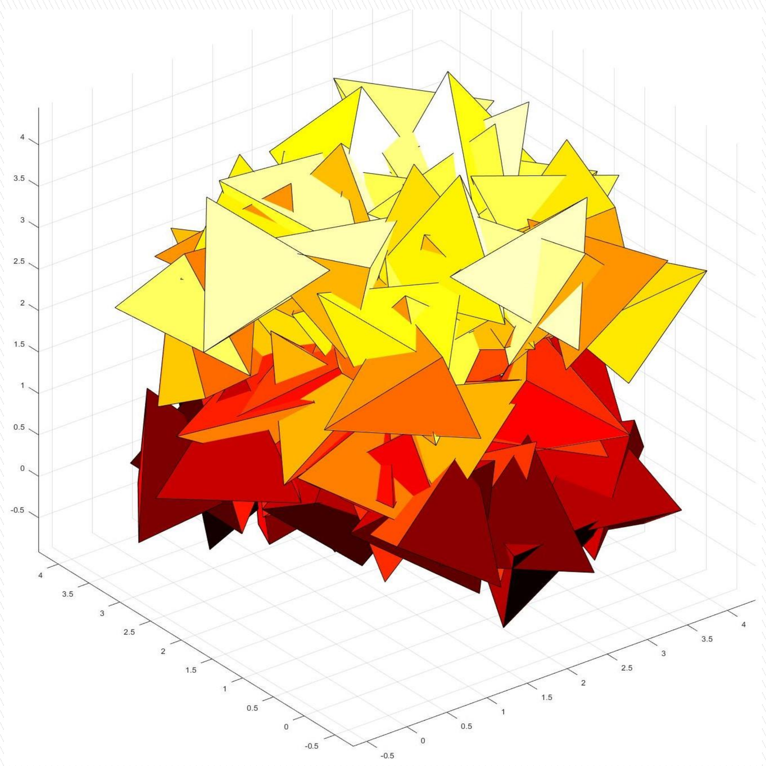
Finite Time:
- Reduced dwell time (no need to await escape)
- Feasible to examine up to 10^7 polyhedra



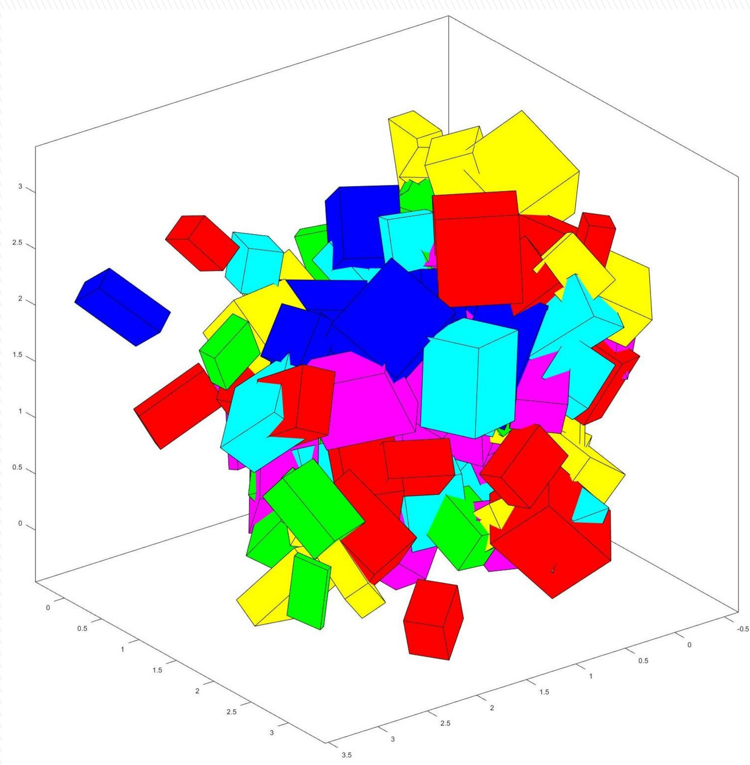
Positional, Orientational, and Structural Disorder



Aligned Cubes (Positional)



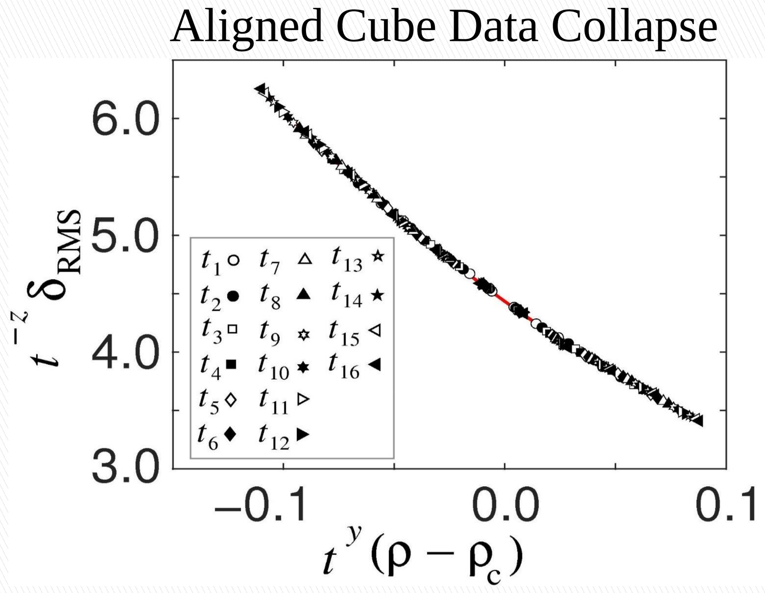
Randomly Oriented Tetrahedra



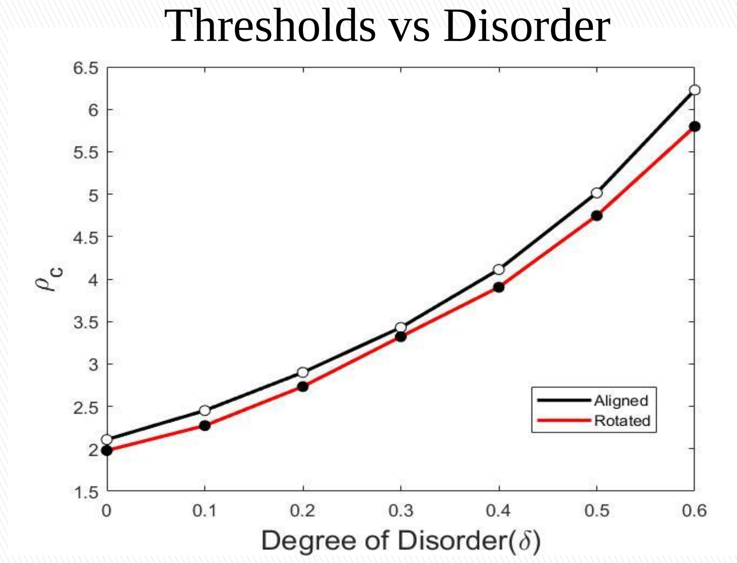
Structurally Disordered Rectangular Solids

Results

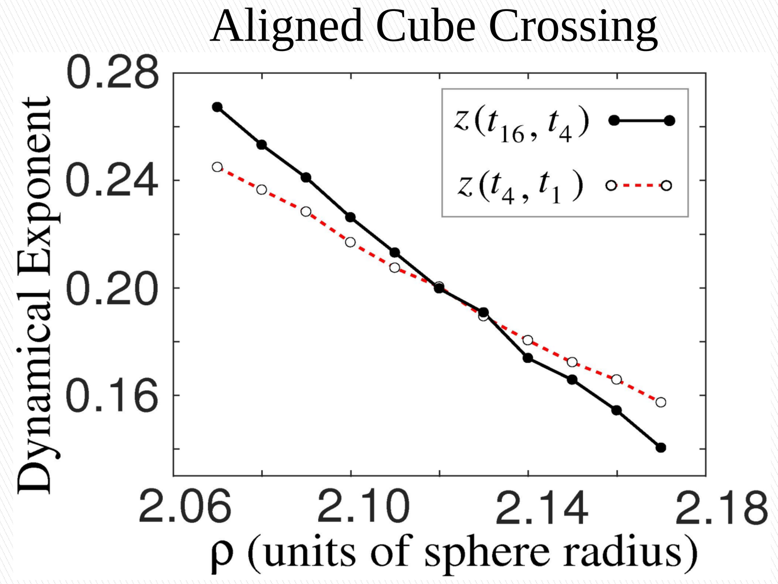
Aligned Cube Data Collapse



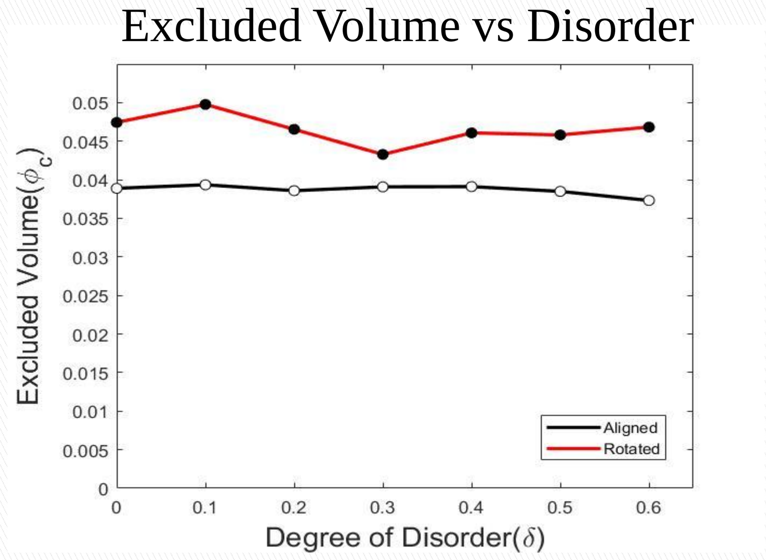
Thresholds vs Disorder



Aligned Cube Crossing



Excluded Volume vs Disorder



Percolation in Porous Materials

Grain Type	ρ_c	ϕ_c	Dynamical Exponent
Aligned Tetrahedra	5.47(2)	0.0605(6)	0.20(1)
Rotated Tetrahedra	5.47(2)	0.0605(6)	0.19(1)
Aligned Cubes	2.122(5)	0.0381(3)	0.20(1)
Rotated Cubes	2.012(8)	0.0452(6)	0.18(1)
Aligned Octahedra	2.402(6)	0.0407(3)	0.19(1)
Rotated Octahedra	2.419(9)	0.0398(5)	0.19(1)
Aligned Dodecahedra	1.198(3)	0.0356(3)	0.18(1)
Rotated Dodecahedra	1.194(4)	0.0360(3)	0.18(1)
Aligned Icosahedra	1.326(3)	0.0346(3)	0.19(1)
Rotated Icosahedra	1.338(8)	0.0336(7)	0.18(1)
Spherical Grains	0.837(1)	0.0301(1)	0.17(1)

- ρ_c in units of radius of circumscribed sphere
- Critical excluded volume $\phi_c = e^{-(\nu_B \rho_c)}$
- Critical dynamical exponent $\delta_{RMS} = A t^{z}$

Conclusions/Future Work:

- Sensitivity to orientational disorder only arises in the case of rectangular solids.
- Implementing structural disorder raises the critical density as expected, yet appears to have little to no effect on the excluded volume in case of rectangular solids.
- We shall examine the remaining platonic solids to verify if this trend holds.