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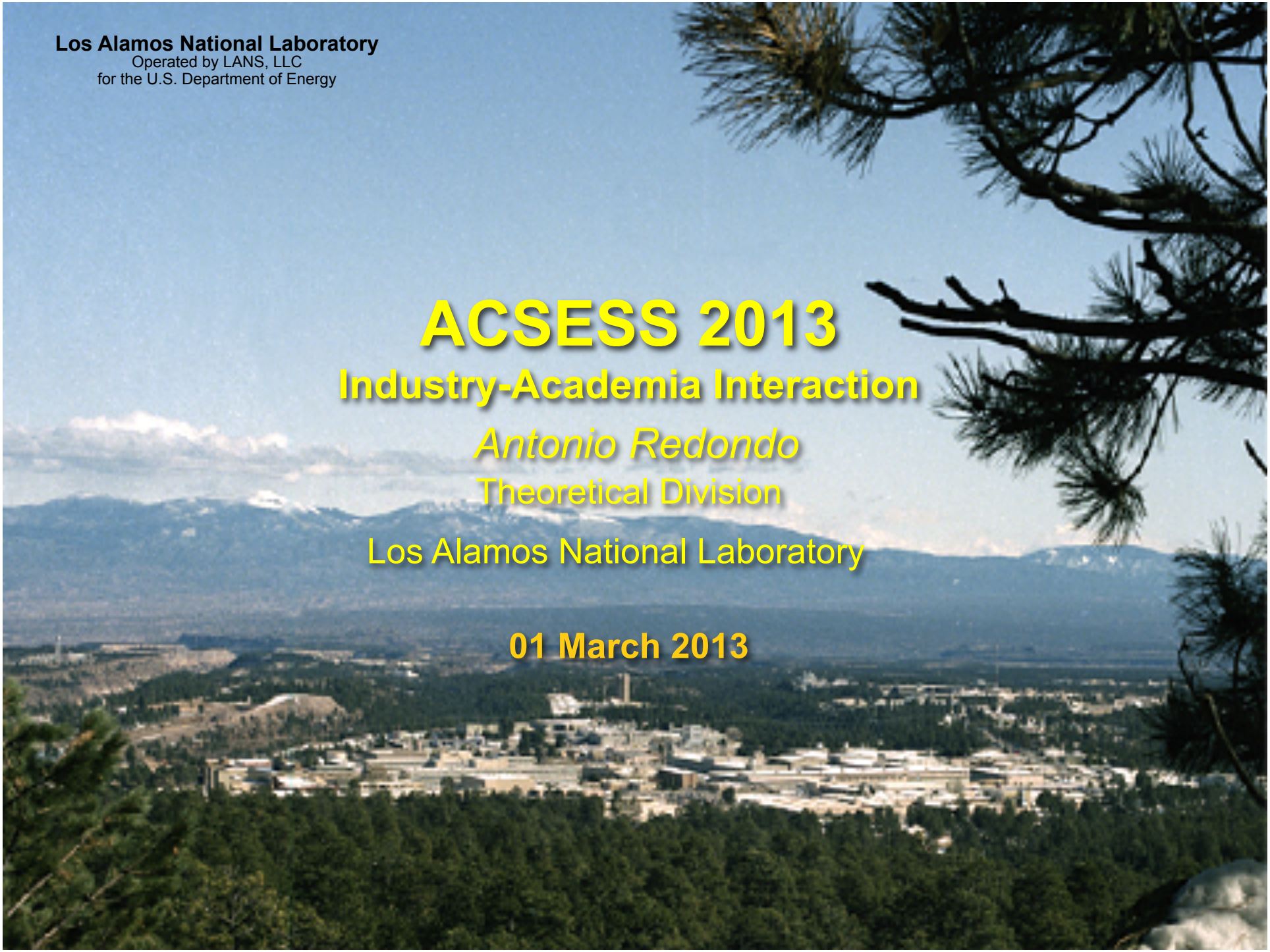

ACSESS 2013

Industry-Academia Interaction

Antonio Redondo
Theoretical Division
Los Alamos National Laboratory

01 March 2013

Los Alamos National Laboratory

The **laboratory of choice** when our nation faces the most **complex security challenges**

Supporting Nuclear Deterrence

Supercomputers simulate nuclear weapons performance—scientists then experiment to refine and verify data—to assure effectiveness of our deterrent without nuclear testing.

Reducing Global Threats

From epidemics to terrorist attacks, cyber security sabotage to energy security, LANL has unique capabilities that focus on identifying, anticipating, and responding to emerging threats.

Fostering Energy Security

Protecting our energy infrastructure while developing clean, sustainable energy sources are key areas of research and technology to ensure a secure future.

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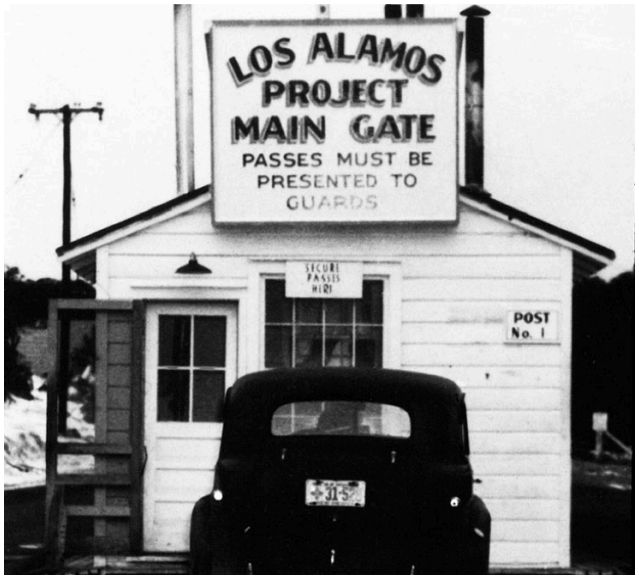

The nation turns to us for solutions to the most complex national security technical challenges of our times, whether a threat may be nuclear, biological, or chemical.

Accelerators, Electrodynamics »

Bioscience, Biosecurity, Health »

Chemical Science »

Earth, Space Sciences »

Energy »

Engineering »

High-Energy-Density Plasmas, Fluids »

Information Science, Computing, Applied Math »

Materials Science »

National Security, Weapons Science »

Nuclear & Particle Physics, Astrophysics, Cosmology »

Sensors, Instrumentation Systems »

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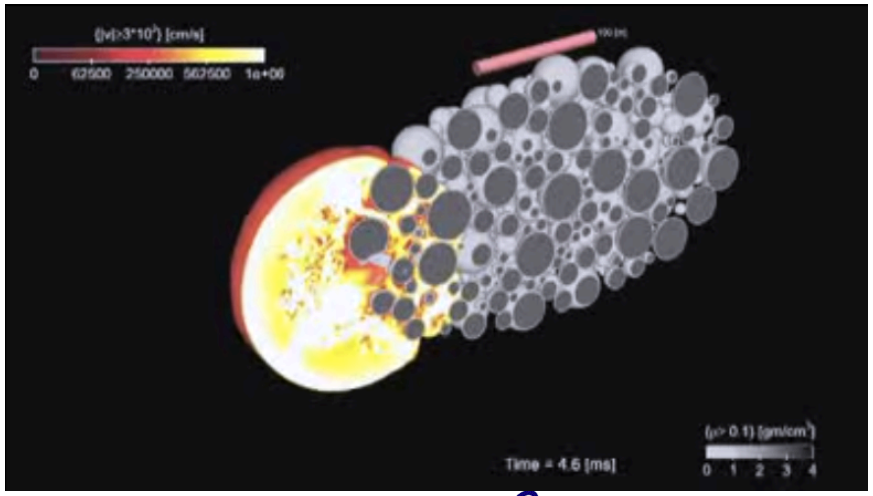
- LANL has one of the largest supercomputing centers on the planet, with massive resources for both classified and unclassified scientific simulation, along with world-class computational physicists, computer scientists, and mathematicians. The result is a unique and tight integration of theory, modeling, and computational science.

LANL asteroid killer



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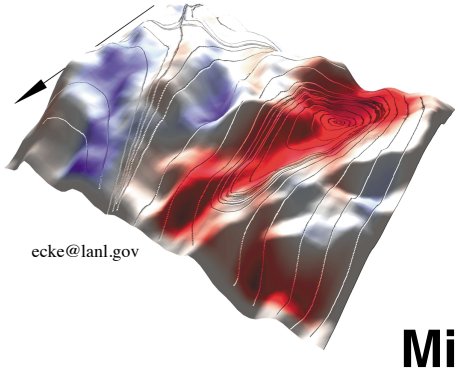
Theory, modeling and simulation



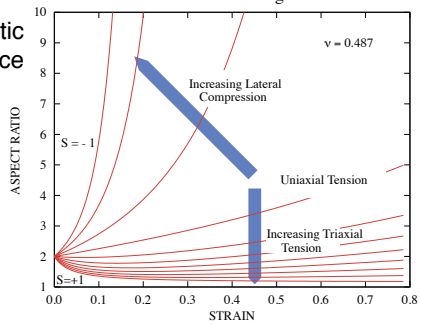
ecke@lanl.gov

We Can Help You

Turbulence in Flowing Soap Films: Soap films, such as ones that form soap bubbles, present a convenient model for many laboratory studies of two-dimensional hydrodynamics. We have developed a diagnostic to simultaneously measure the velocity and thickness fields in the soap film. The image represents a computer-processed snapshot of the flow field in soap film perturbed by a comb.

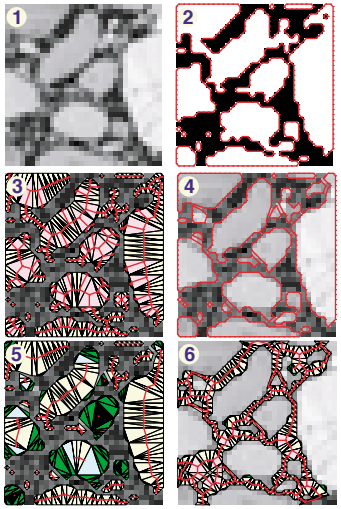
bclements@lanl.gov

Damage Evolution in Viscoelelastic Polymers by Void Coalescence



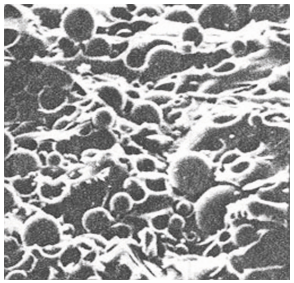
Might Interest You

Granular Materials Image Analysis



http://www.nis.lanl.gov/~bschlei
schlei@lanl.gov, prasad@lanl.gov, alexei@lanl.gov

Mechanical Properties of Filled Polymers



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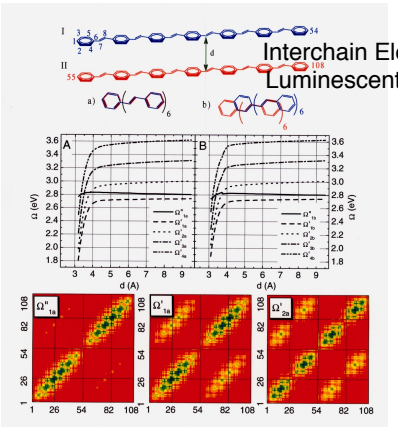
Check out the wide range of research at Theoretical Division. 505-667-4401



Interchain Electronic Excitations in Luminescent Polymer Aggregates

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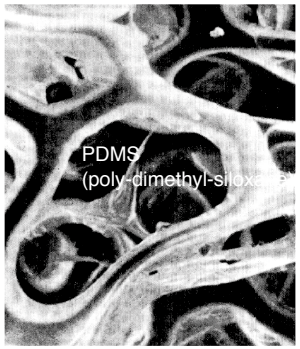
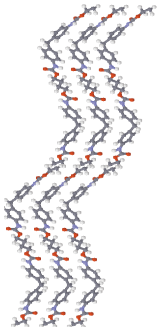
Theory, modeling and simulation

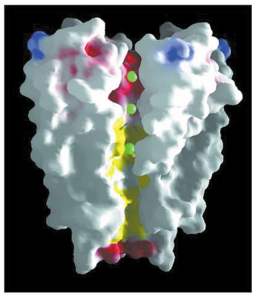
Aging in Polymer Materials

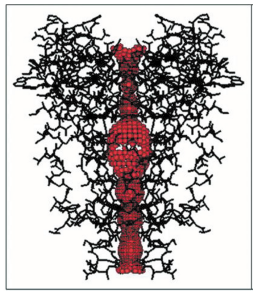


Estane
(polyester-polyurethane)



We can calculate chemical aging and mechanical properties of polymers in different environments.





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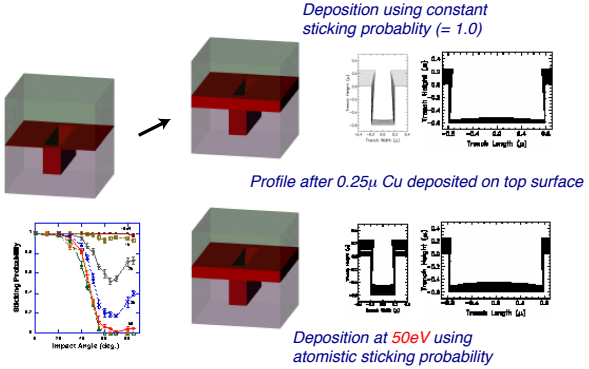
and

Why Study Inner Hydration Shells of Ions in Water?

- They are incompletely understood, yet fundamentally important to physical chemistry
- Knowledge of their structures and dynamics is a prerequisite to understanding inner shell exchange reactions
- Inner shell exchange reactions appear decisive to selectivity of biological ion channels

Materials Modeling



Bridging the Length Scale Atomistic to Mesoscopic

Example shows effect of using atomistic simulation data on the deposition profile of Cu in a trench-fill simulation for semiconductor applications.

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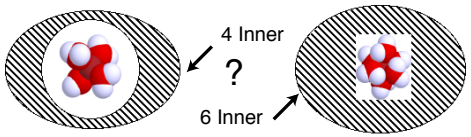
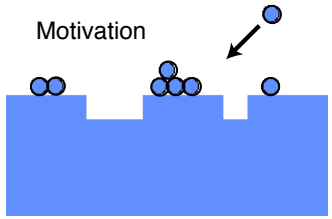
Li^+ (aq) Hydration



A balanced theoretical treatment of both nearest neighbors and solution to resolve hydration issue.

Many materials problems are amenable to atomistic simulation, but are not viable with current hardware and software when there is a coupling between different temporal scales.



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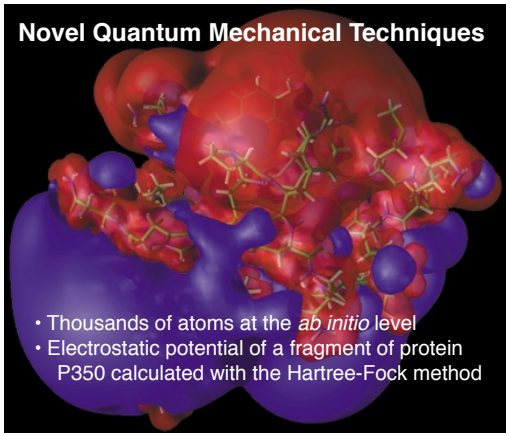

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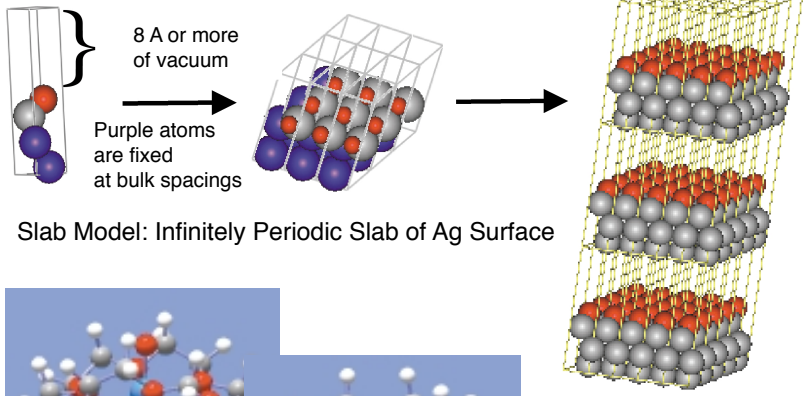
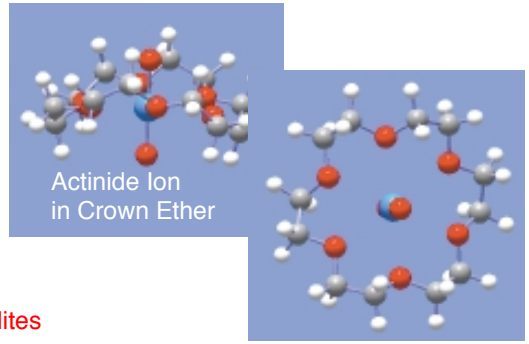


Slab Model: Infinitely Periodic Slab of Ag Surface



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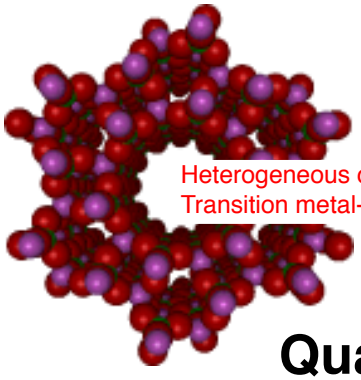
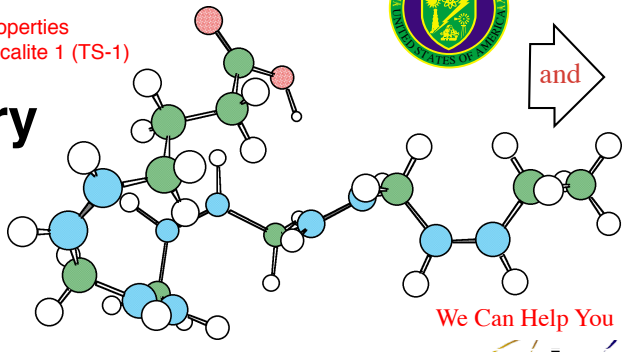


Heterogeneous catalysis:
Transition metal-substituted zeolites

- Shape-selective catalysts
- Have reduction and oxidation (redox) properties
- Up-to-date, the most used is titanium silicalite 1 (TS-1)

Quantum Chemistry

- Diets rich in ω-3 fatty acids are known to have beneficial health effects.
- They can help control ventricular fibrillation and other cardiac arrythmias associated with calcium overload in the cytosol.
- They are also associated with the control of abnormal behavior in the physiology of the nervous system.



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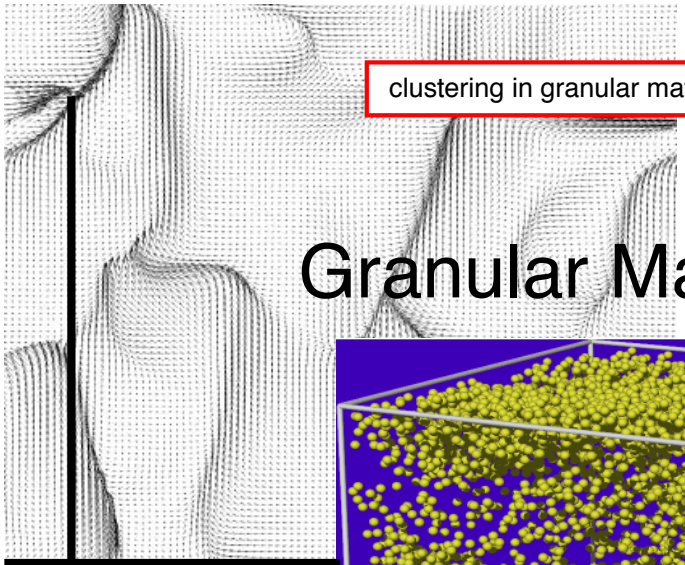

clustering in granular matter

Shock Dynamics of Granular Gases: We have shown that the asymptotic dynamics of freely evolving granular gases is dominated by shock coalescence processes, and used the corresponding hydrodynamic description (the inviscid Burgers equation) to obtain density and velocity statistics. Using scaling techniques, we can predict the critical mass for the formation of finite time singularities in the velocity and density profiles.

Granular Materials

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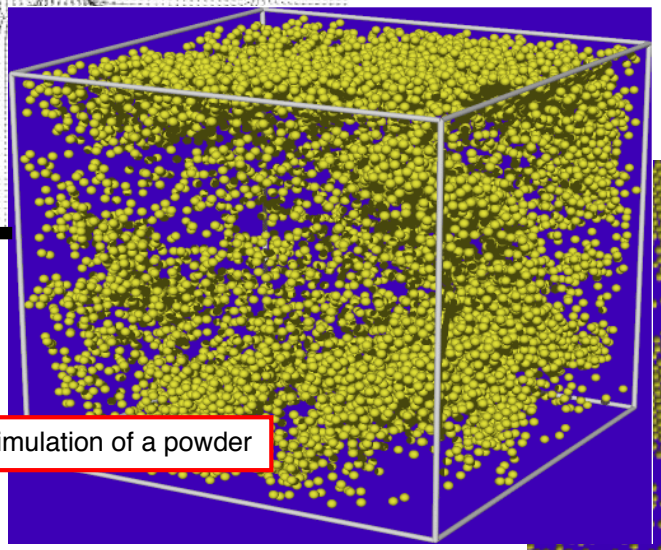
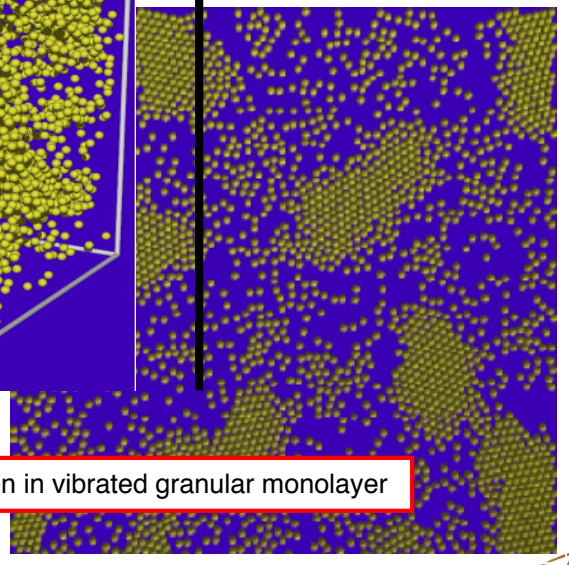


molecular dynamics simulation of a powder



crystallization in vibrated granular monolayer

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