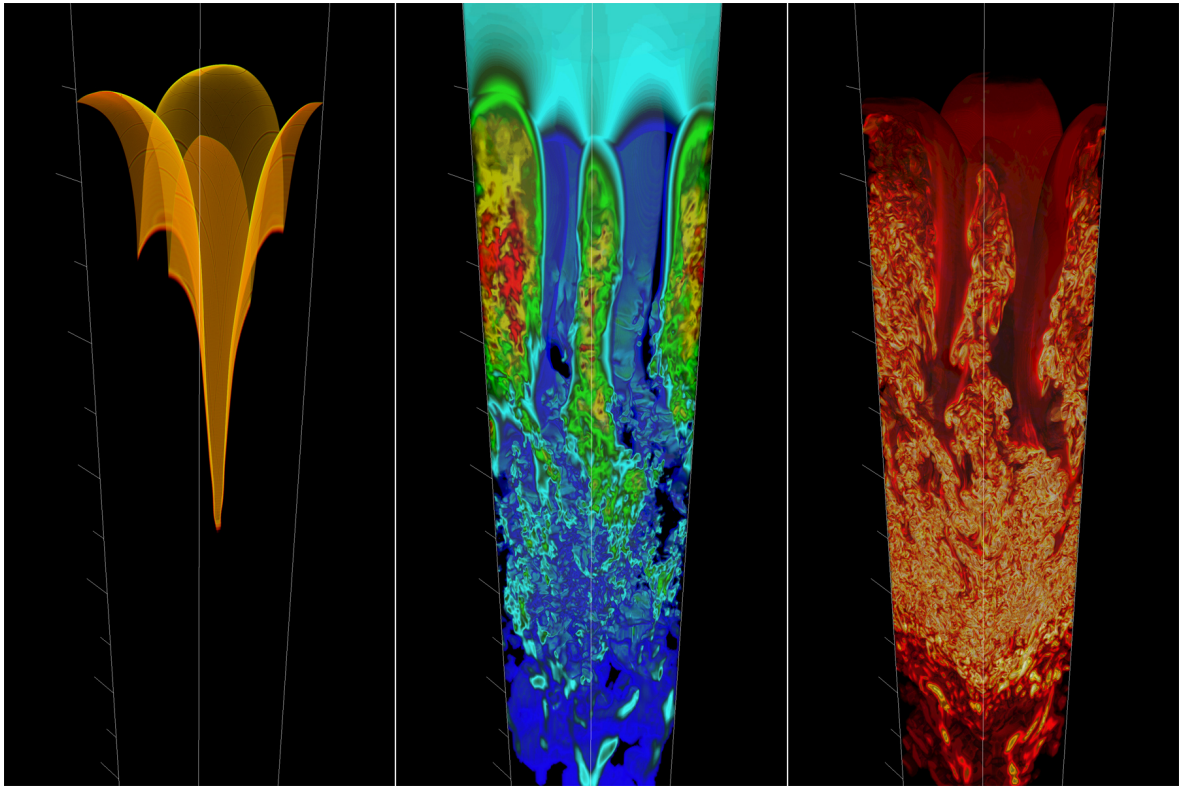
# Science



**Timothy J. Williams**

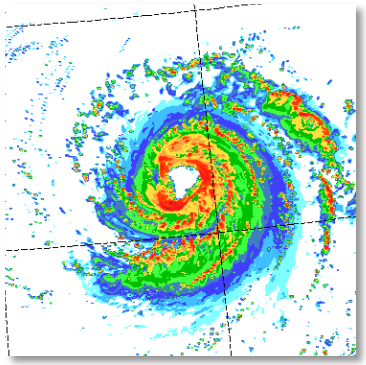
*Argonne Leadership Computing Facility*

Argonne National Laboratory

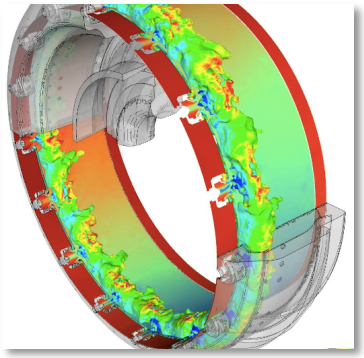
**Getting Started Workshop**

*Closing Remarks, 10/4/2011*

# ALCF Projects Span Many Domains

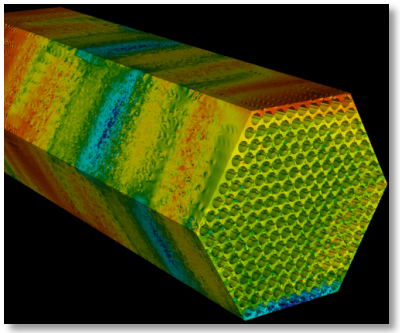


## Climate
Predicting hurricane tracks to mitigate risks, hindcasting with climate model data to gauge impact of global change.

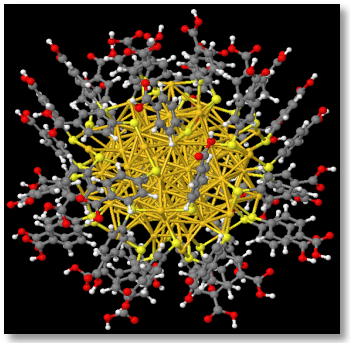


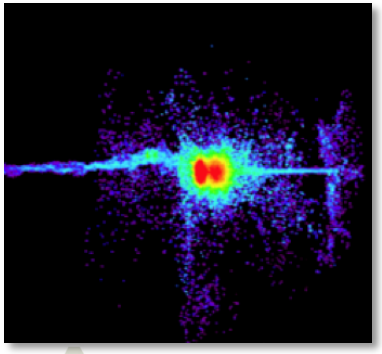
## Gas Turbines
Modeling two-phase flow and combustion for the design of more efficient aircraft engines.

## Nuclear Energy
High-fidelity fluid flow and heat transfer simulation of next-generation reactor designs, aiming to reduce the need for costly experimental facilities.

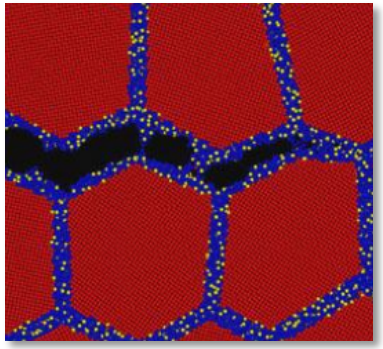


## Nano Catalysts
Mapping out properties of gold nanoparticles to design catalysts for fuel cells and methane conversion.





## Fusion Energy
Understanding the detailed physics of Fast Ignition inertial confinement fusion.

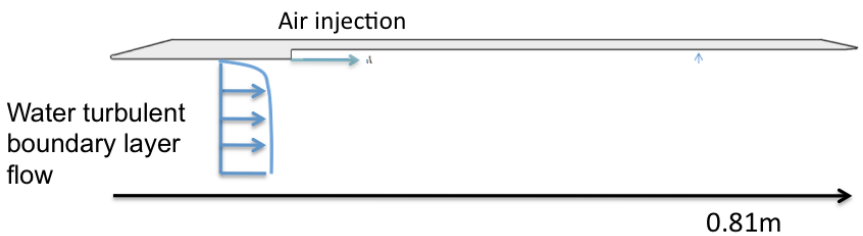


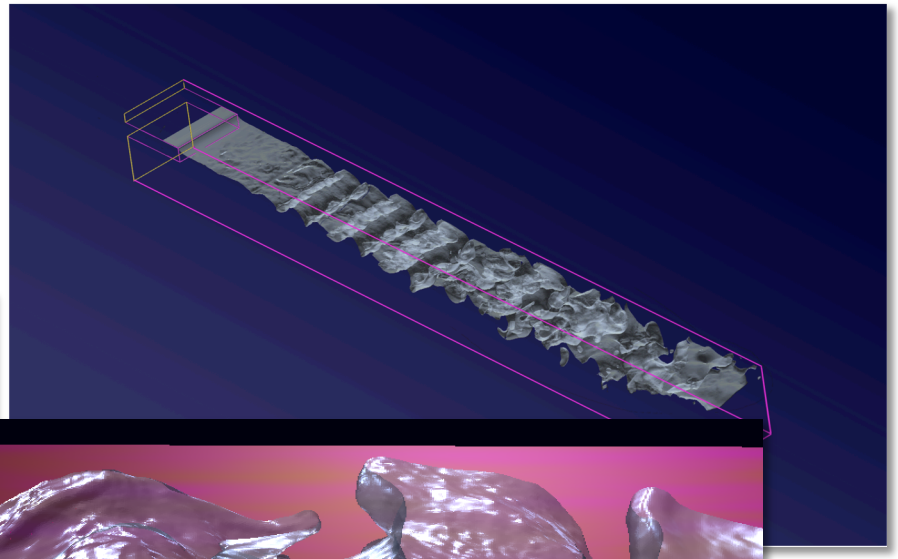
## Materials Science
Molecular simulation of fracture dynamics in structural materials in next-generation nuclear reactors.

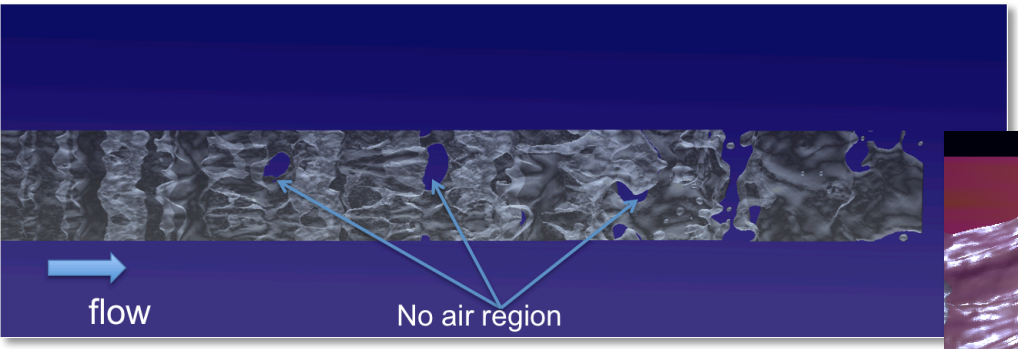
# Air-Layer Drag Reduction

*Parviz Moin, Stanford University*

- **3D LES simulation of turbulent multiphase flows on a flat plate**





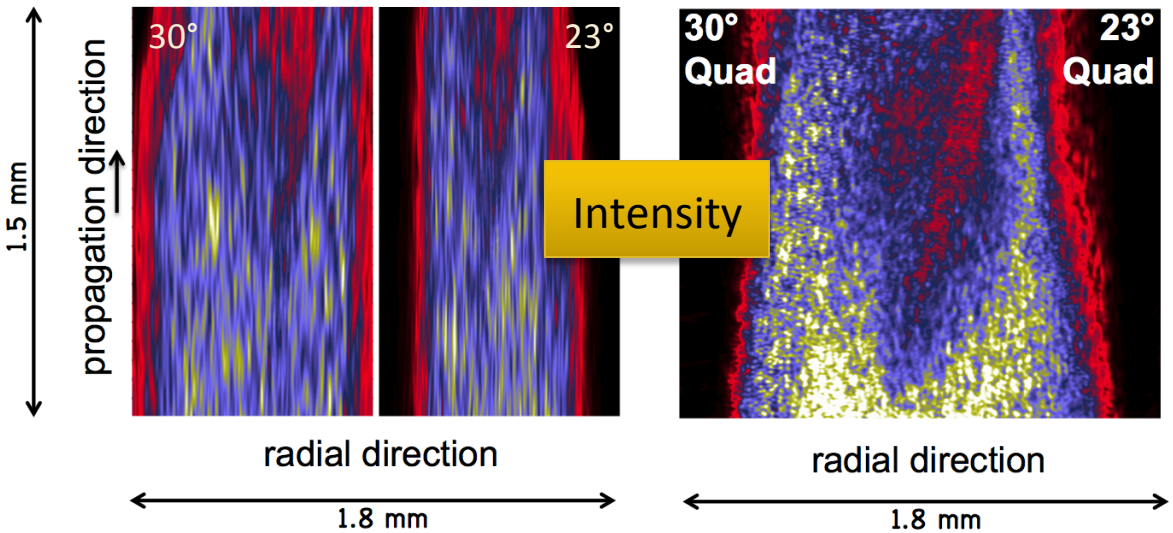

Breakup of air layer →
Water spots→
Much larger skin friction

Kelvin-Helmholtz instability

# Laser-Plasma Interaction in ICF

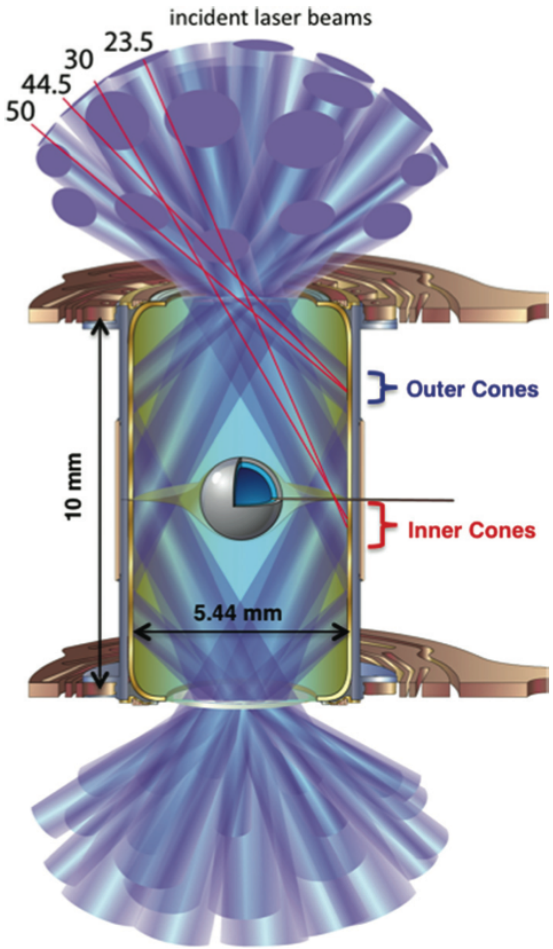
*Denise Hinkel, Lawrence Livermore National Laboratory*

- **Code: pF3D (radiation & hydrodynamics)**
- **Laser backscatter**
  - Problem for indirect-drive inertial confinement fusion
  - Overlap of beams important!




Single-quad propagation

Double-quad propagation




Physics of Plasmas 18, 056312 (2011)

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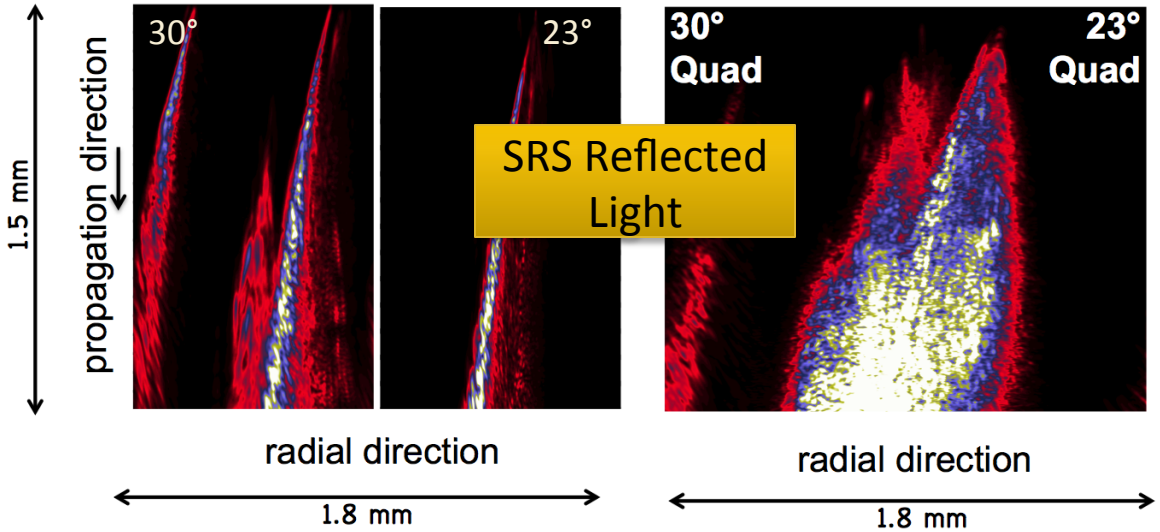


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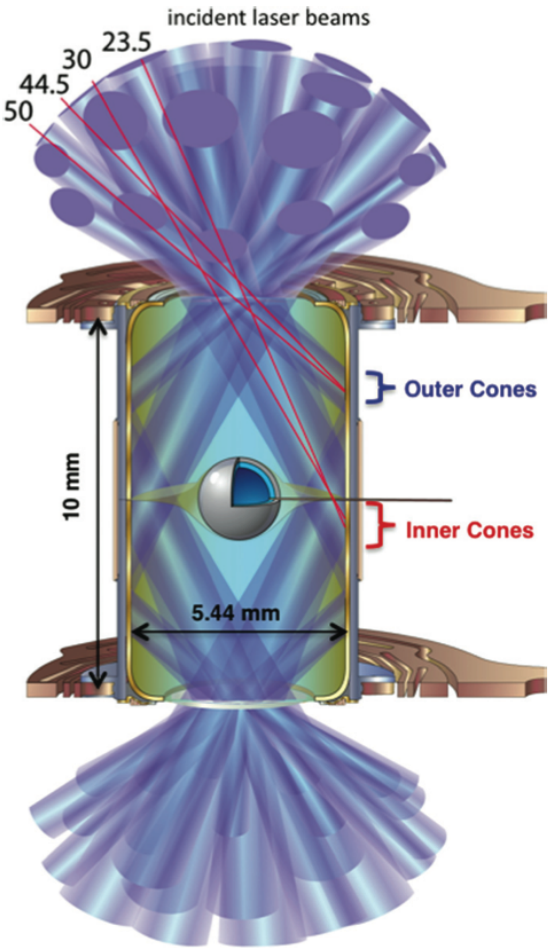

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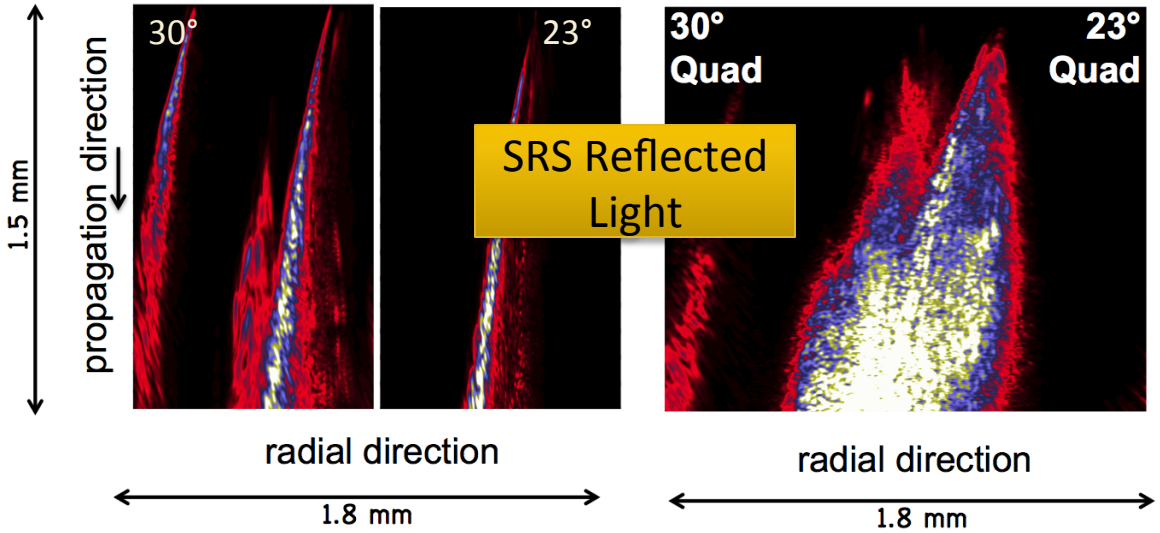


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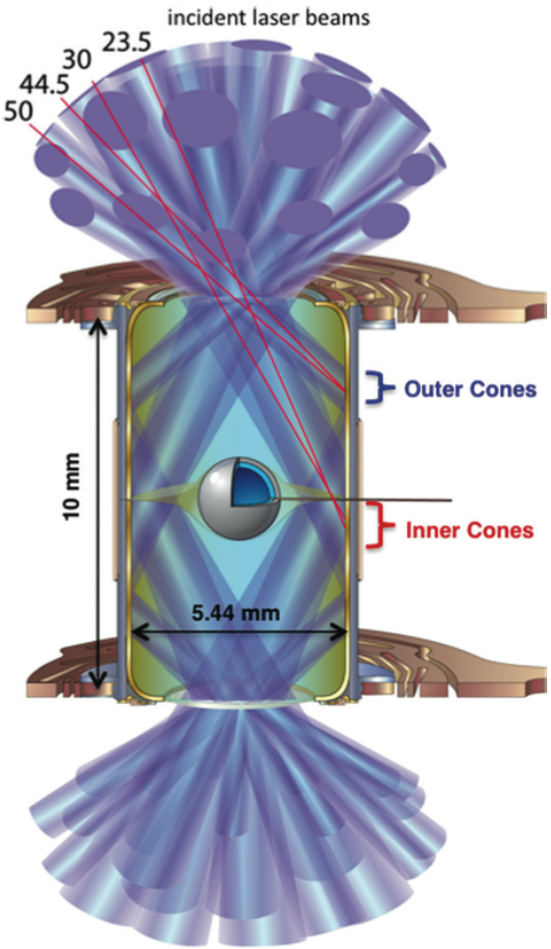


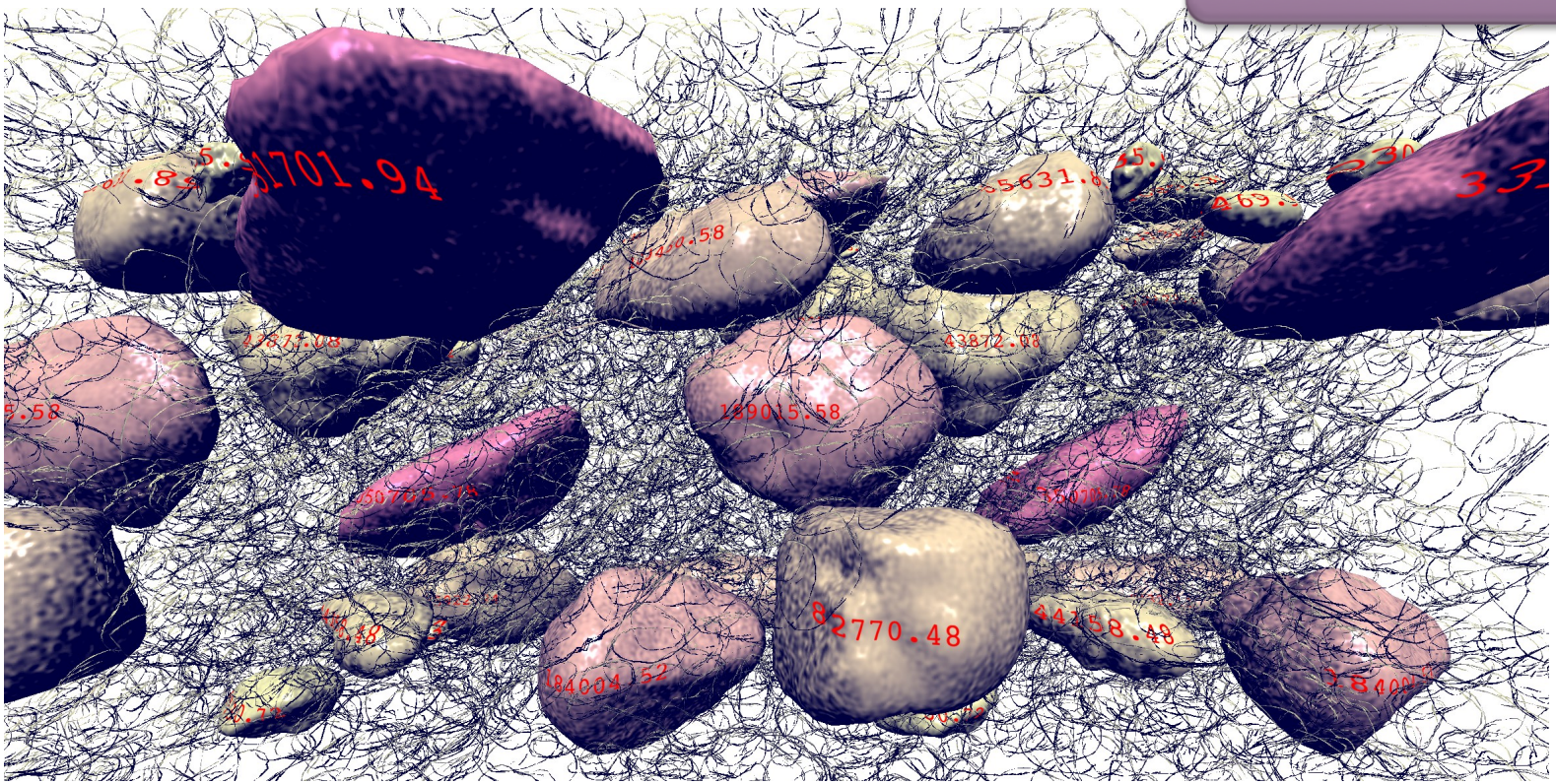

32K *Intrepid* nodes (132k cores)

# Rheology of Concrete

*William George, National Institute of Standards and Technology*

- **How do shape and size of aggregate impact behavior?**
- **Simulate how stress propagates through the fluid.**
  - Non-Newtonian matrix fluid
  - Code: smoothed particle hydrodynamics (SPH)

Stress level "painted" on surfaces

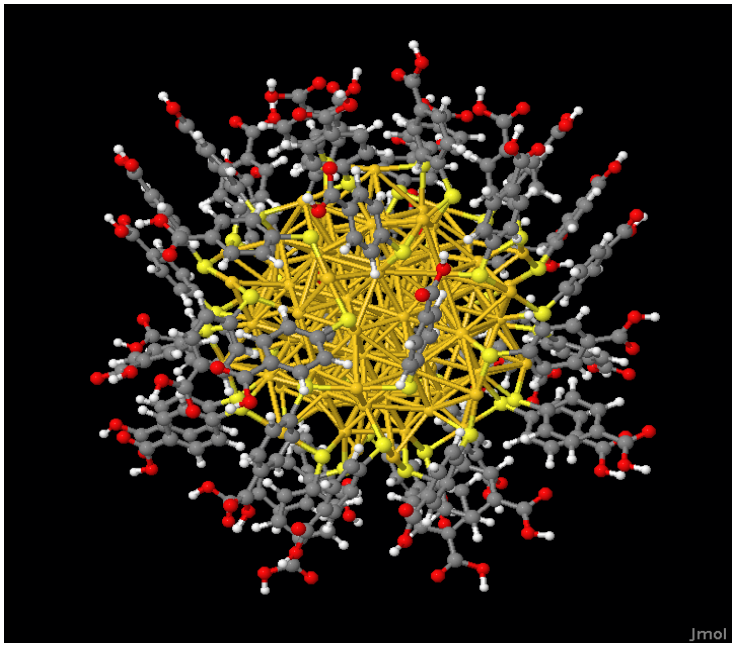


# Catalytic Nanoparticles

*Jeff Greeley, Argonne National Laboratory*

- **Code: GPAW (DFT)**
- **Gold has exciting catalytic abilities, still poorly understood**
  - e.g. CO into $CO_2$
- **Simulated nanoclusters up to 1415 atoms**
  - 16 racks on *Intrepid* (40% of system)

ALCF Catalyst:
- Reduced memory footprint
- New layer of parallelization
- Expanded production from 128 cores to 16,384

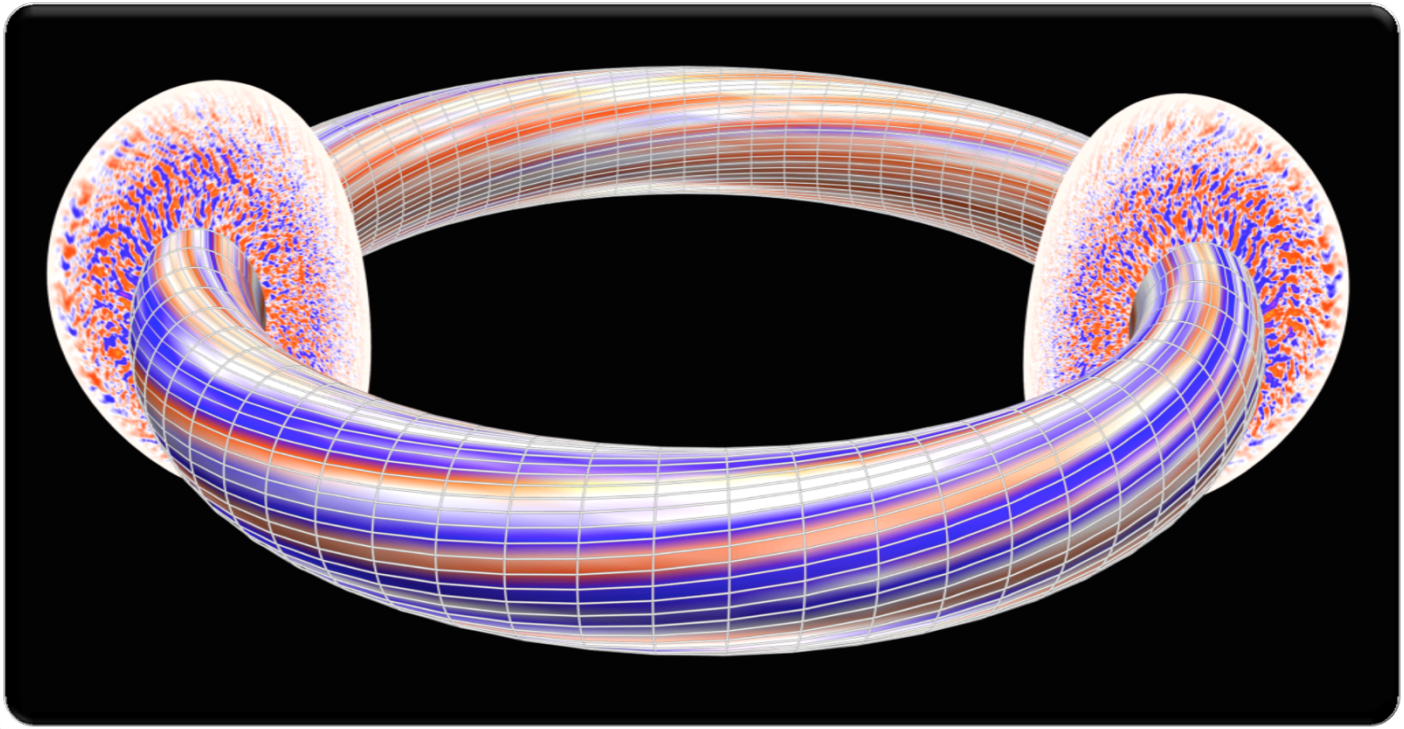


# Microturbulent Transport in Tokamaks

*William Tang, Princeton Plasma Physics Laboratory*

- **Code: GTC**
- **Particle-in-cell simulation of plasma**
  - Study energy loss through turbulence
  - Trying to validate key assumption about scaling in ITER

$O(10^9)$ particles
$O(10^8)$ grid cells



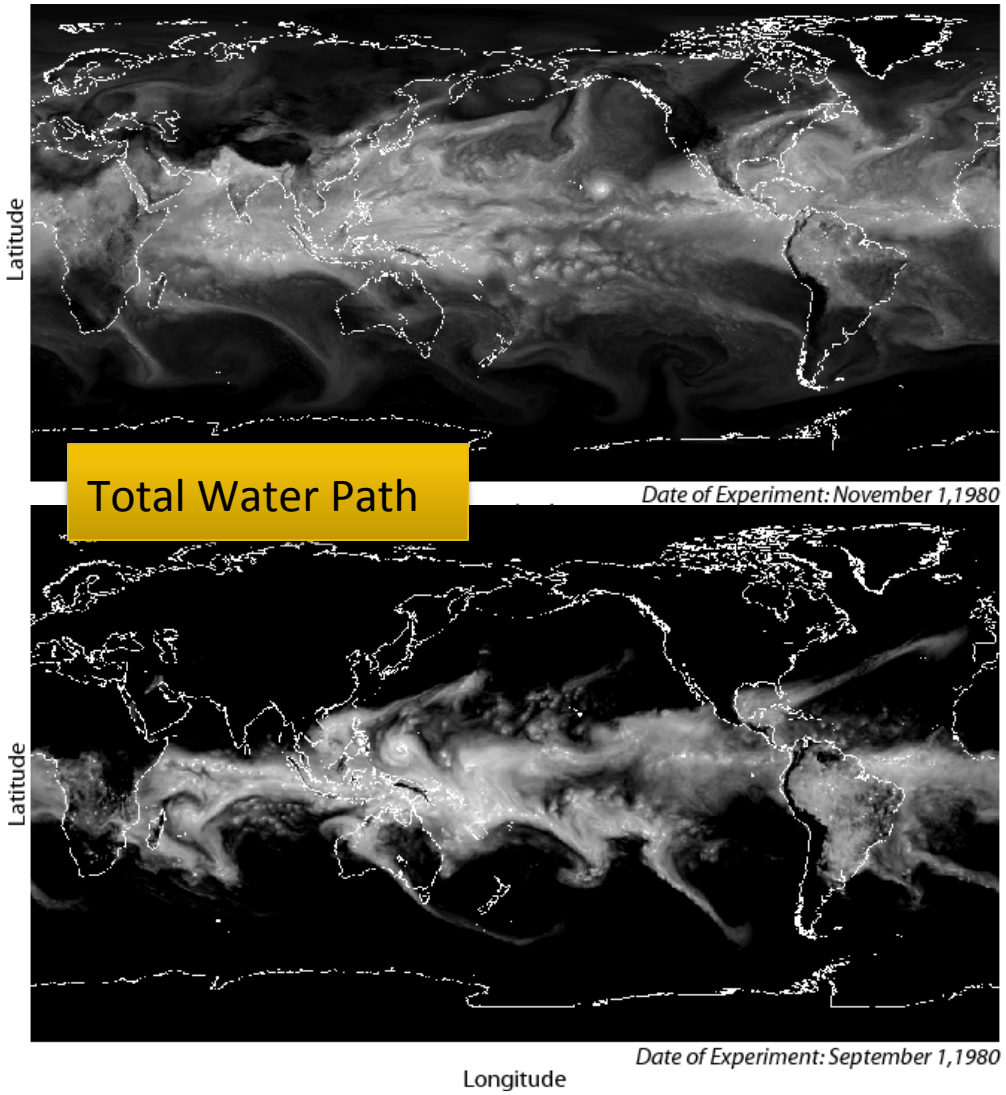
# Ultra-High Resolution Climate-Weather Modeling

*S-J Lin, Geophysical Fluid Dynamics Laboratory*

- **HIRAM global atmospheric code**
  - Cubed sphere grid

*Hydrostatic:*
12 km resolution

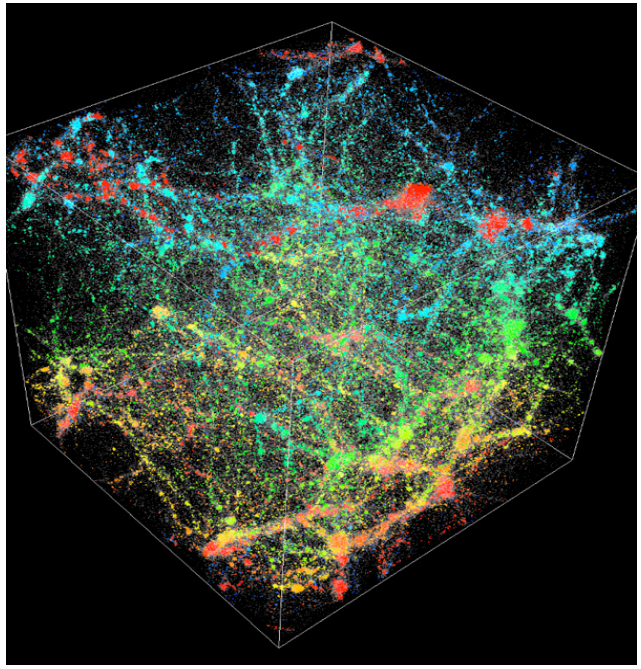
*Non-Hydrostatic:*
3.5 km resolution
Global cloud resolving



# Cosmic Structure Probes of the Dark Universe

*Salman Habib, Argonne National Laboratory*

- **Code: Hardware/Hybrid Accelerated Cosmology Code (HACC)**
- **Gravitational evolution of large-scale structure of the universe**
  - Characterize dark energy & dark matter by predicting observational signatures for a variety of new/existing experimental cosmological probes
    - 1st simulations resolving galaxy-scale mass concentration at scale of state-of-the-art sky surveys
  - Study primordial fluctuations by predicting the effects on cosmic structures today



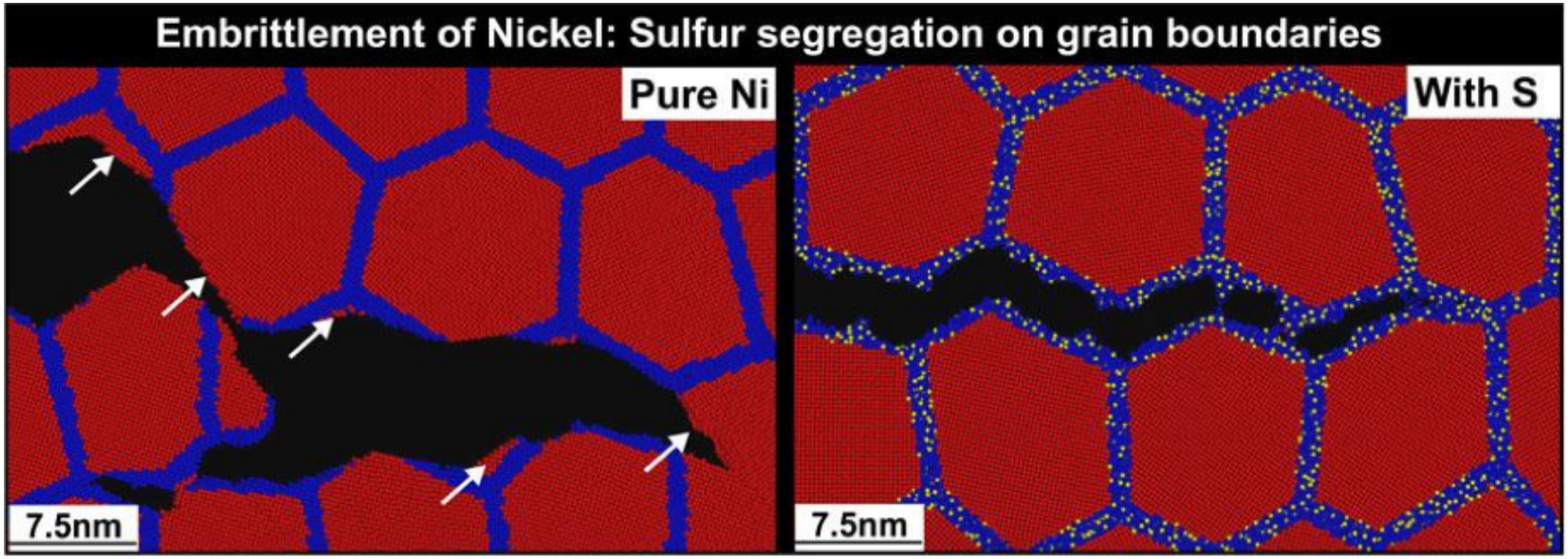
$O(10^{11}-10^{12})$ grid cells
$O(10^{11}-10^{12})$ particles

# Reactive MD Simulation of Nickel Fracture

*Priya Vashista, University of Southern California*

- **Sulfur atoms in nickel grain boundaries embrittle the nickel**
  - Phys. Rev. Letters 16 Apr 2010
- **65K cores on Intrepid BlueGene/P**
  - 48 million atoms
  - Chemically reactive molecular dynamics
  - Fracture mechanics modeled

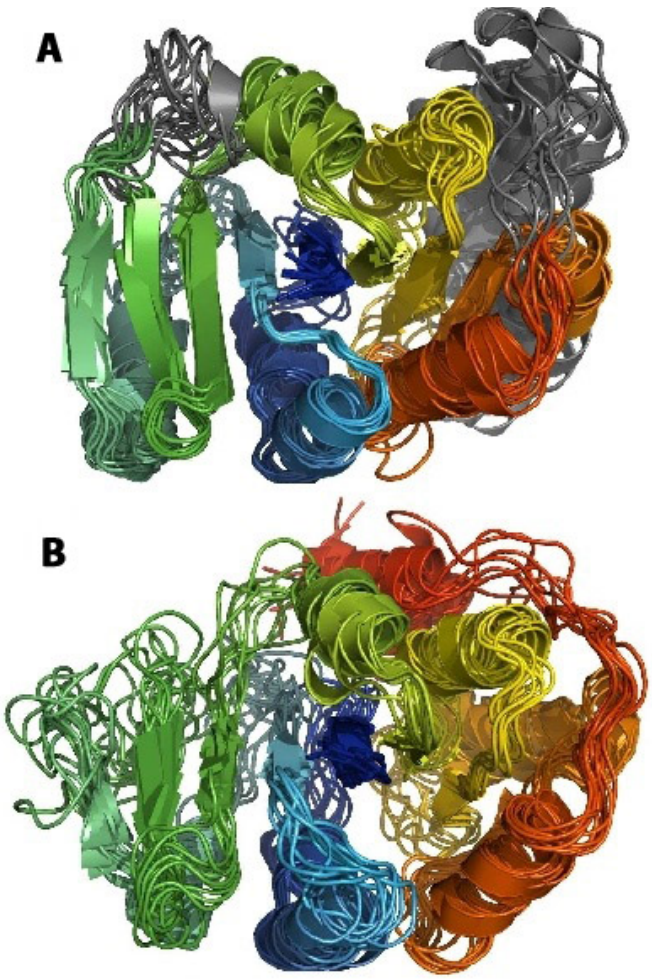
Relevant to next-gen nuclear reactors.



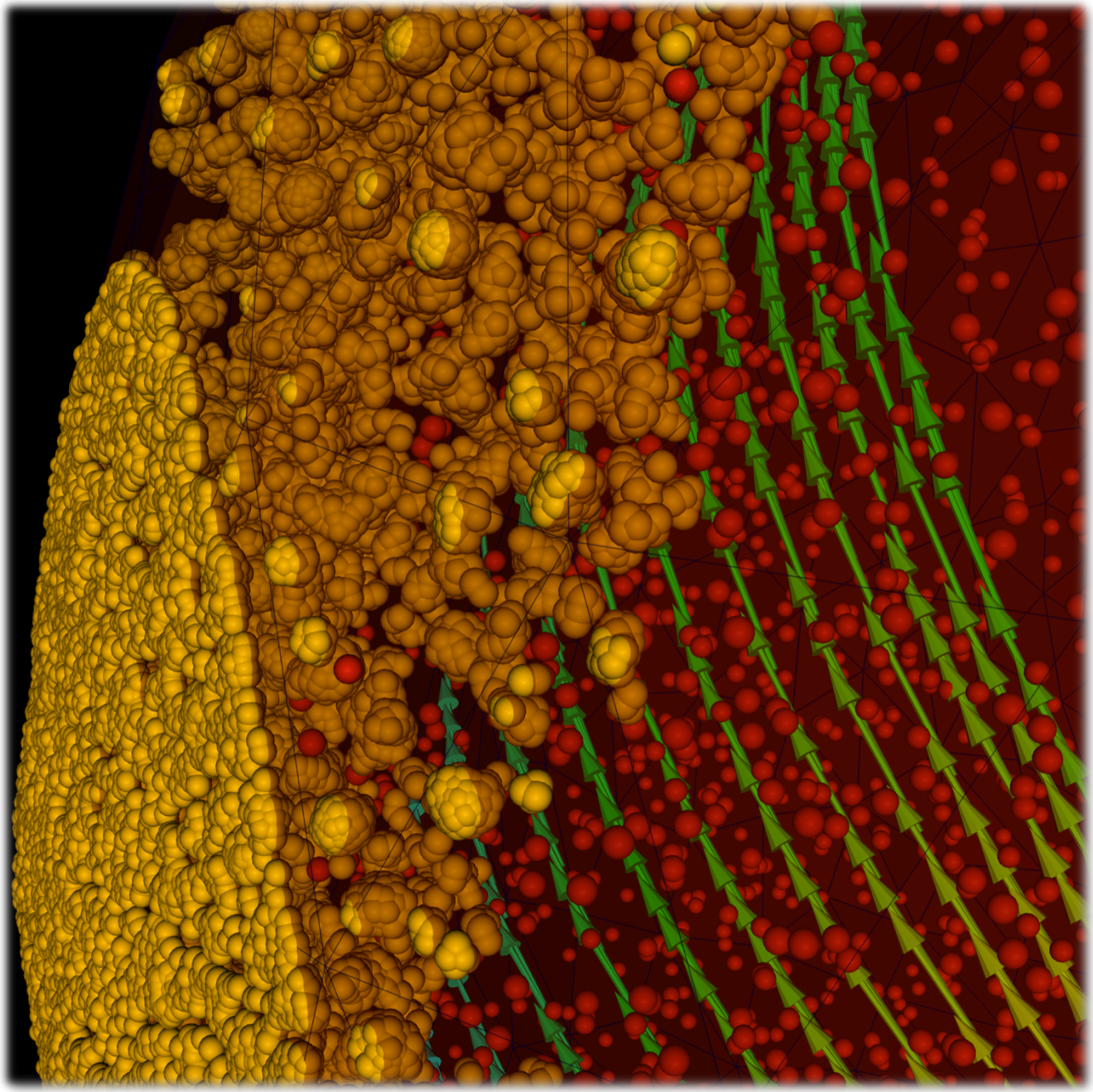
# Computational Protein Structure Prediction and Protein Design

*David Baker, University of Washington*

- **INCITE, PI David Baker (U. Washington)**
  - Rosetta protein folding application
    - *Science* **327**, 1014 (2010)
      *NMR Structure Determination for Larger Proteins Using Backbone-Only Data*
  - Structure of ALG13
    (A) computationally
    (B) experimentally by NMR




Systems with > 150 amino acids
- Full experimental NMR difficult
- Backbone data easier:
  *Input to Rosetta*



G. Karniadakis