BERKELEY LAB

LAWRENCE BERKELEY NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

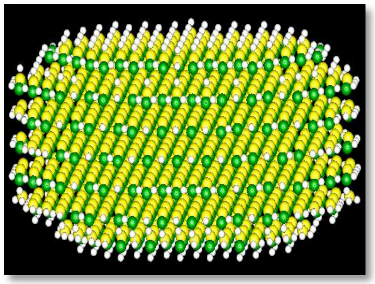
Computation for CCS, Buildings, and Renewables

Juan Meza

Carbon Cycle 2.0
October 11-13, 2009
Chaminade, Santa Cruz, CA

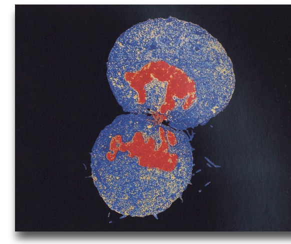
Computational Science Mission

energy technology

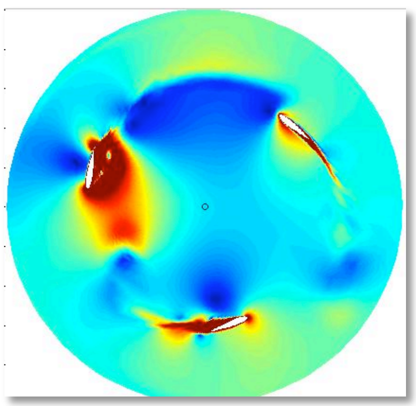


nano systems

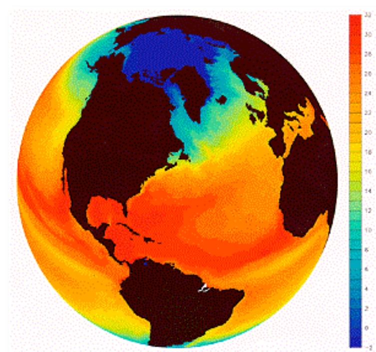
biological systems



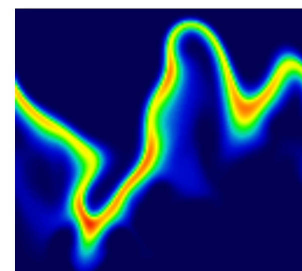
The Computational Research Division engages in computational science partnerships, developing algorithms, tools and techniques that enable advanced computational modeling and simulation, and lead to new understanding in areas such as



Higher-order methods



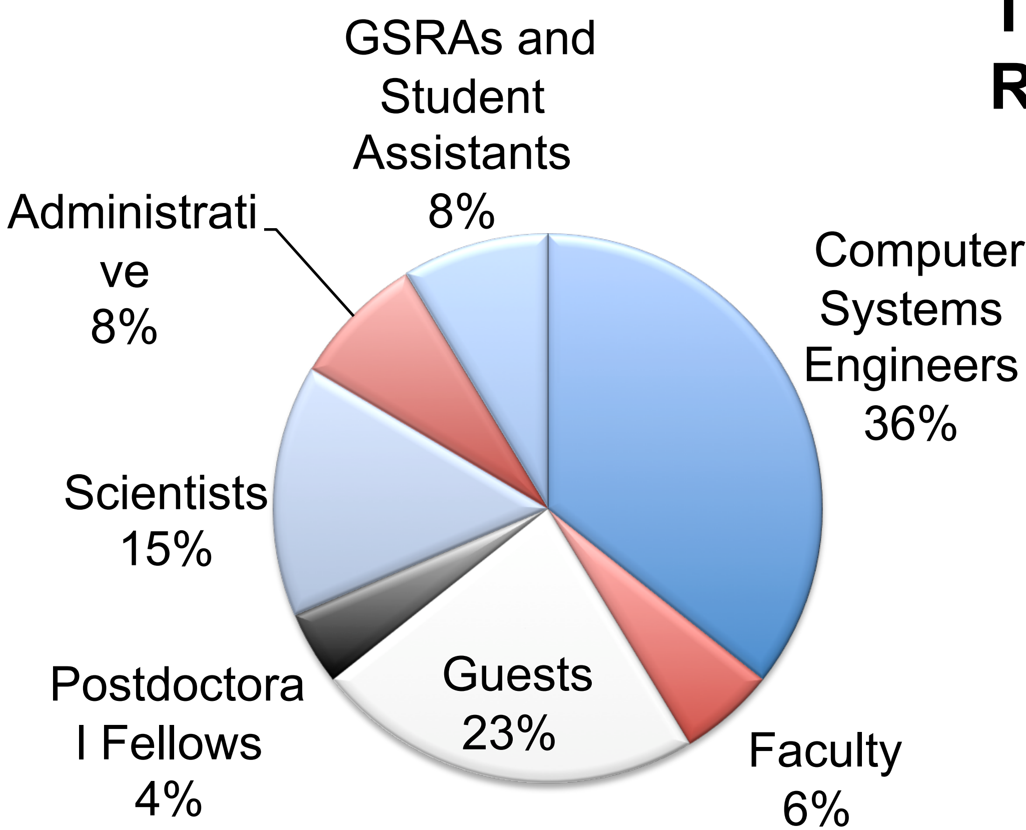
global climate



combustion processes

Computing Sciences Employees – 371 total as of July 1, 2009

Total Budget: ~$100M
Research: ~$24M/year

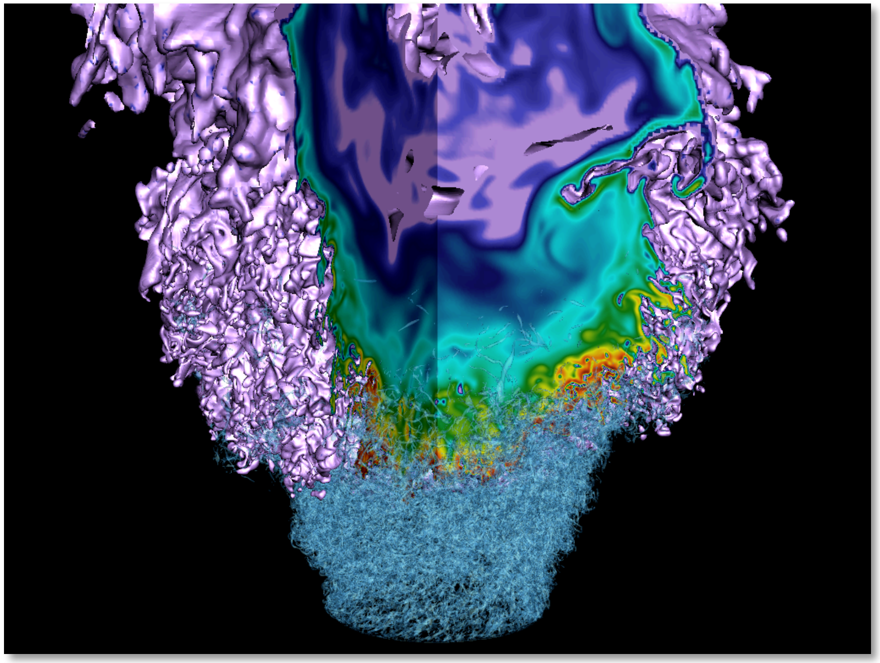


Transformative Mathematics and Computer Science

Leverage expertise in applied mathematics, computational methods and algorithms and apply them to science and engineering problems throughout DOE

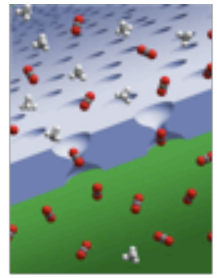
Potential to transform research in:

- Extreme climate prediction
- Energy efficiency
- Carbon sequestration strategies
- Design new photovoltaic materials
- Improving efficiency, reliability of nation's power grid
- Nuclear reactor safety
- Addressing tokamak plasma instabilities

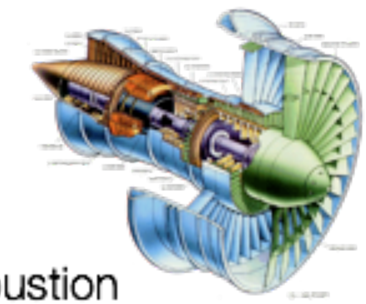


Carbon Cycle 2.0 and Computing

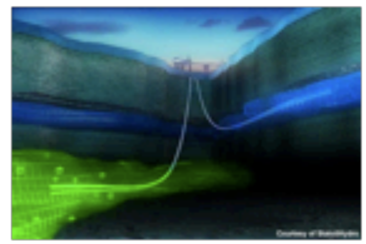
Batteries and storage



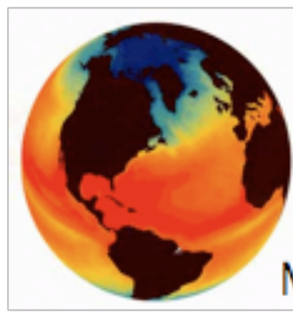
Carbon capture



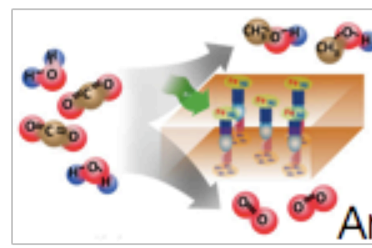
Combustion



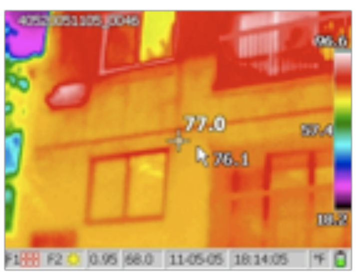
Sequestration



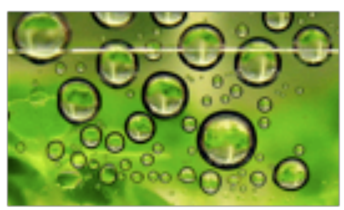
Climate Modeling

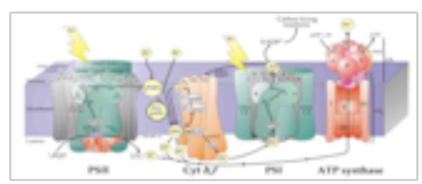


Artificial Photosynthesis



Building efficiency

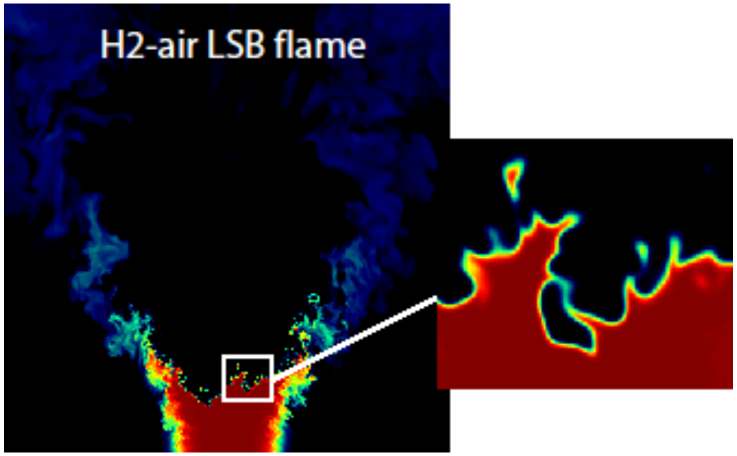




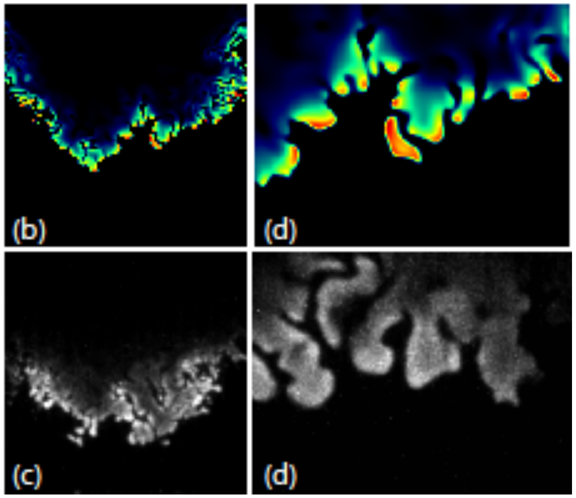
Biofuels

Simulation of lean premixed hydrogen flames stabilized on a low-swirl burner

- **Low Mach number formulation exploits mathematical structure of the problem**
  - Advanced numerical methodology, including projection methodology, adaptive mesh refinement, and parallel implementation using BoxLib
  - Detailed chemistry and transport
  - No explicit models for turbulence or turbulence / chemistry interaction
  - 25 cm x 25 cm x 25 cm
- **Combined methodology enables simulation at effective resolution of 8B cells (2048^3)**
- **Simulation captures cellular structure of thermodiffusively unstable lean hydrogen flames and provides insight into experimental diagnostics**



Fuel

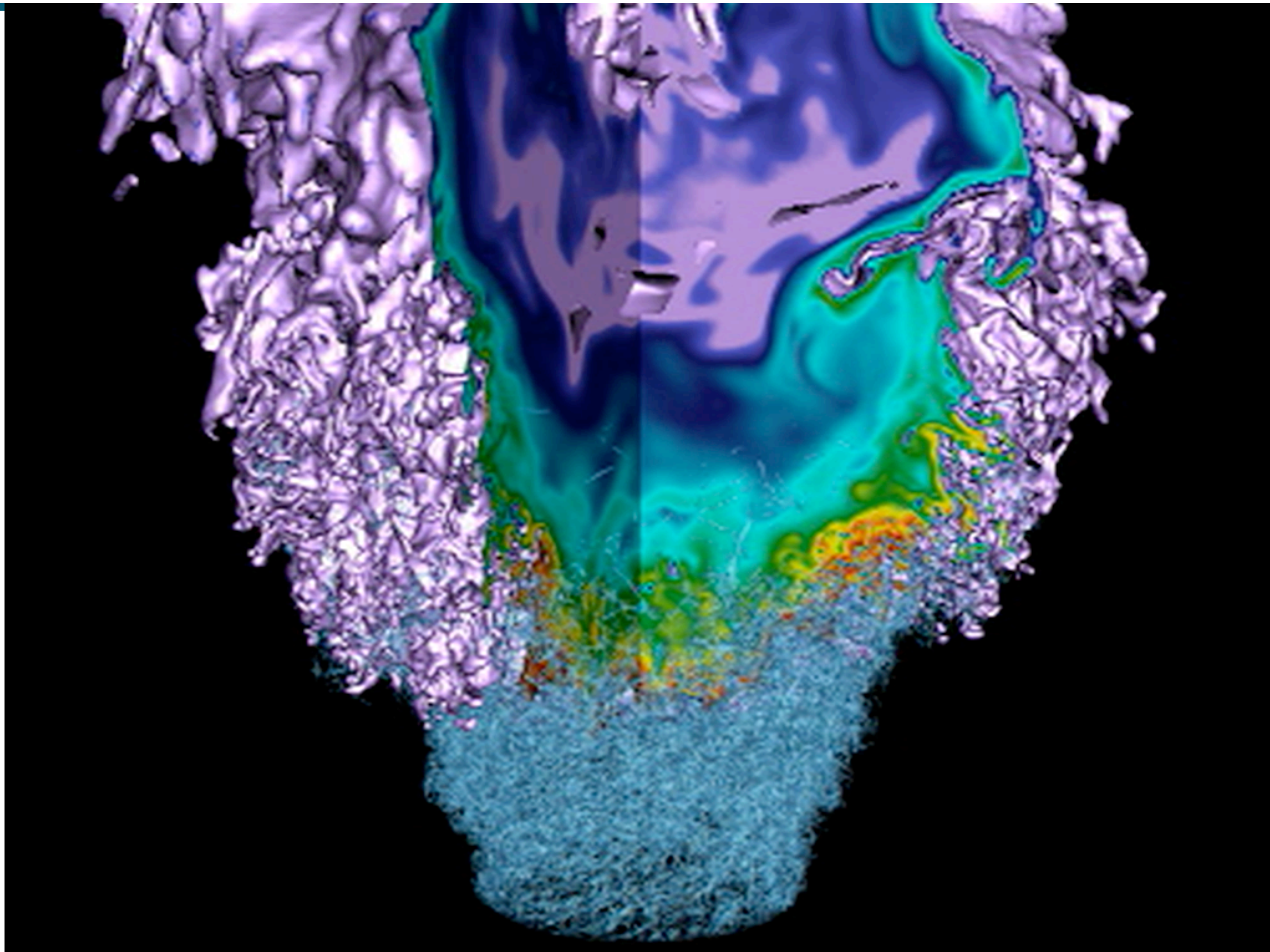


Experimental comparison of OH Radical

PI: J. Bell, LBNL

Simulations performed at NERSC under an INCITE grant

Simultaneous rendering of OH and Vorticity



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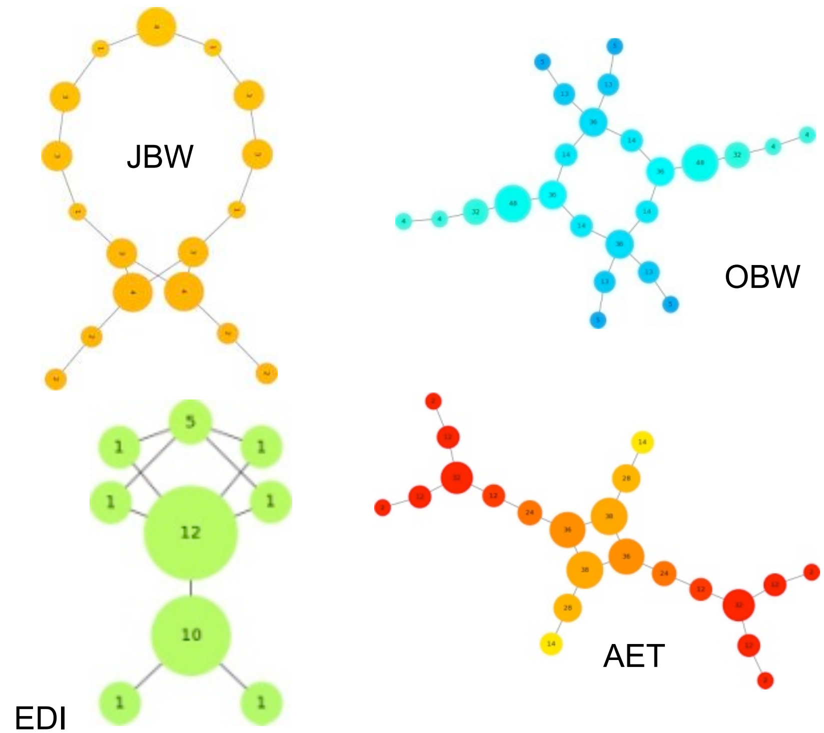
Knowledge-guided screening tools for identification of porous materials for CO_2 separation

M. Haranczyk, J.A. Sethian, J.C. Meza
Collaborators: B. Liu, K. Theisen, B. Smit (UCB), J. Kloke, G. Carlsson (Stanford)

Goal: Screening of large databases of porous materials (e.g. zeolites) to identify structures with optimal performance for CO_2 separation.

Computational Challenges: Develop mathematical techniques to characterize and represent the geometrical and physical features of porous structures and to use statistical and data mining methods to identify similarity between structures



These graphs represent the topology of four zeolite structures obtained with Mapper method. Nodes of each graph are obtained by clustering of atoms of similar density and are colored according to values of density.
Similarity is based on Hausdorff-Gromov distance

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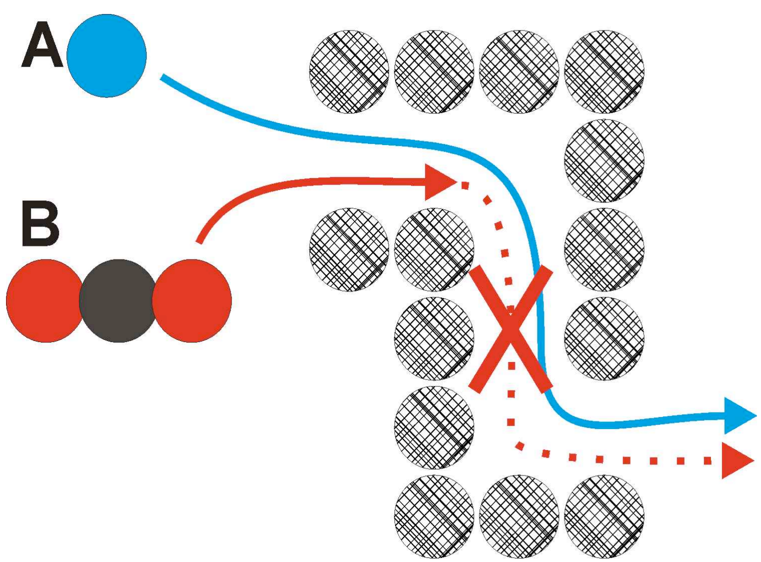
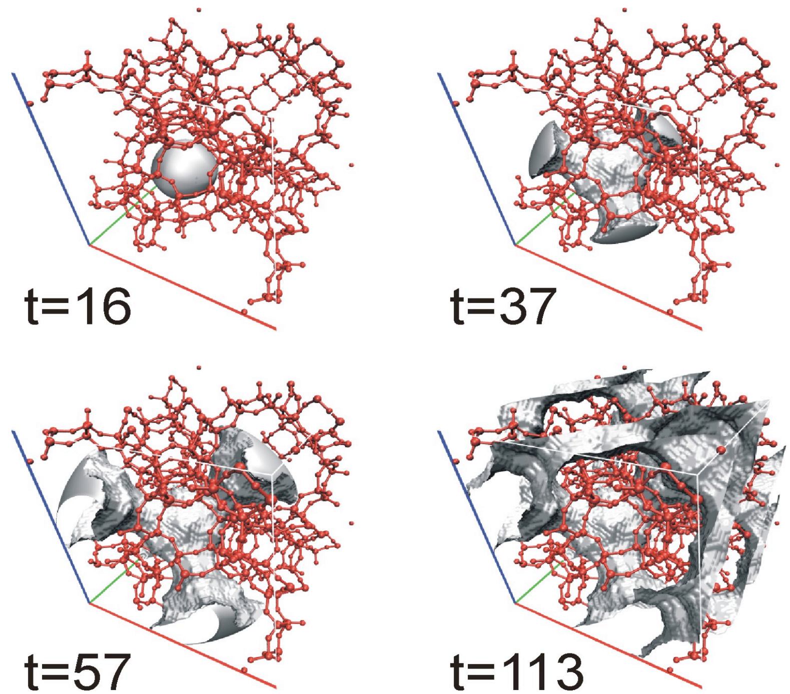
Structure Descriptors, Representations and Similarity Measures

Calculation of accessible volume and transport pathways based on analysis of configuration space of a molecule inside zeolite structure using Fast Marching Method – Robotic Navigation (Sethian)



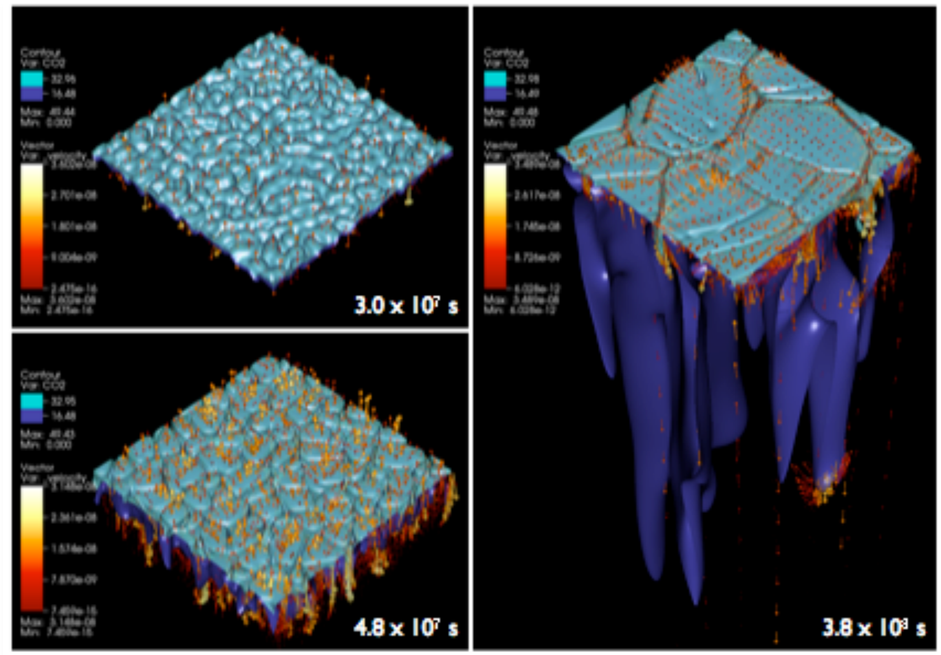


POC: M. Haranczyk (LBNL)

Front propagation to obtain accessible volume

AMR provides accurate onset times

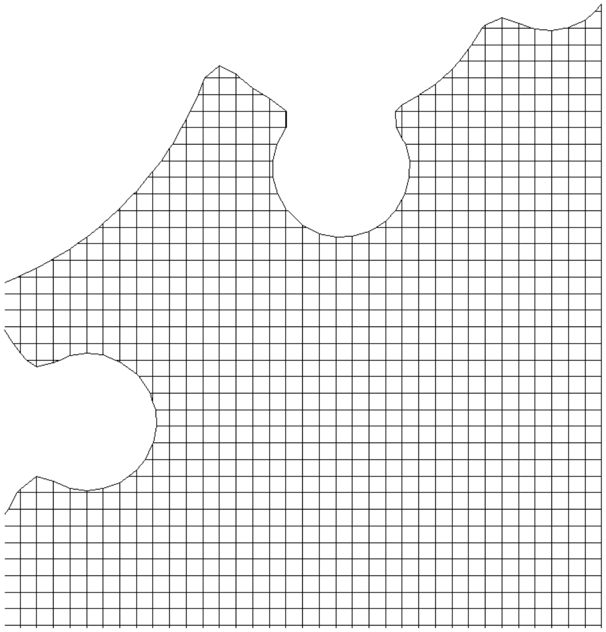
- **Accurate and rigorous determinations of the onset time of convection, and the long-term stabilized CO_2 mass flux.**
- **Showed that the density-driven convective process significantly increases the rate at which CO_2 is transformed into a negatively buoyant state.**
- **Determined dependence of the mass flux on the formation properties.**
- **Proposed a simplified model for integration into a full carbon sequestration simulation.**
- **3D simulations use 2048 CPUs for more than 48 hours on Franklin at NERSC.**

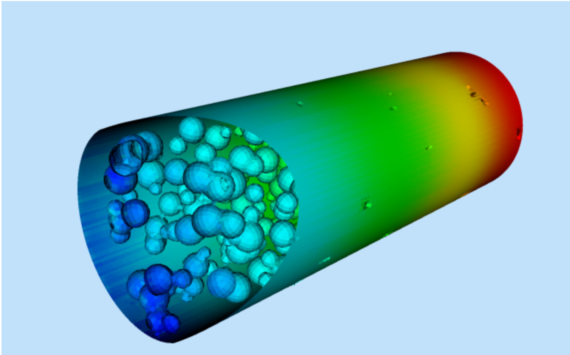


Evolution of convective fingers with time. The arrows show how the velocity field drives the formation and evolution of the fingers. Joint work with Karsten Pruess at ESD.

Embedded boundaries are a cut cell approach to geometry on Cartesian grids

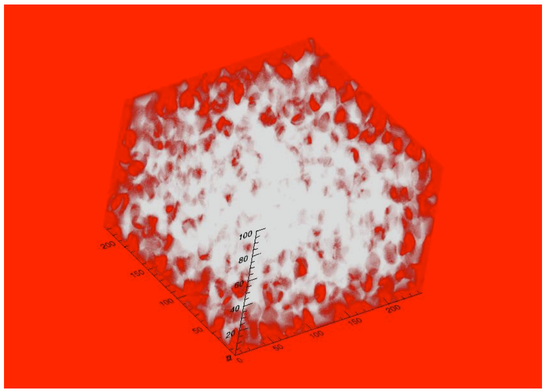
- **Irregular boundaries are represented by the intersection of the domain with Cartesian cells**
- **Finite Volume Method is used to discretize PDEs**
- **Special discretization methods are used in the small subset of irregular cells**
- **Majority of computational cells have regular structure, FVM reduces to finite differences**
- **In most cases, EB / FV approach not practical without adaptive mesh refinement**



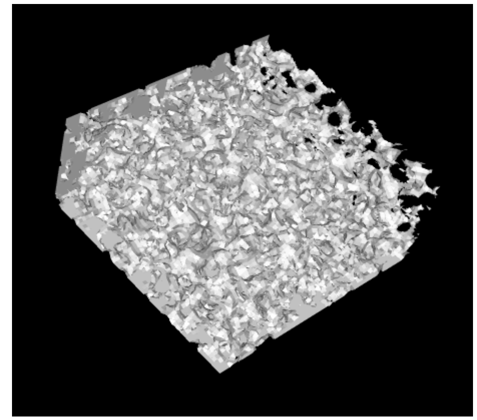


3D packed bed flow model (above) with cutaways (below); 20-50 μm spheres, .5mm cylinder diam.

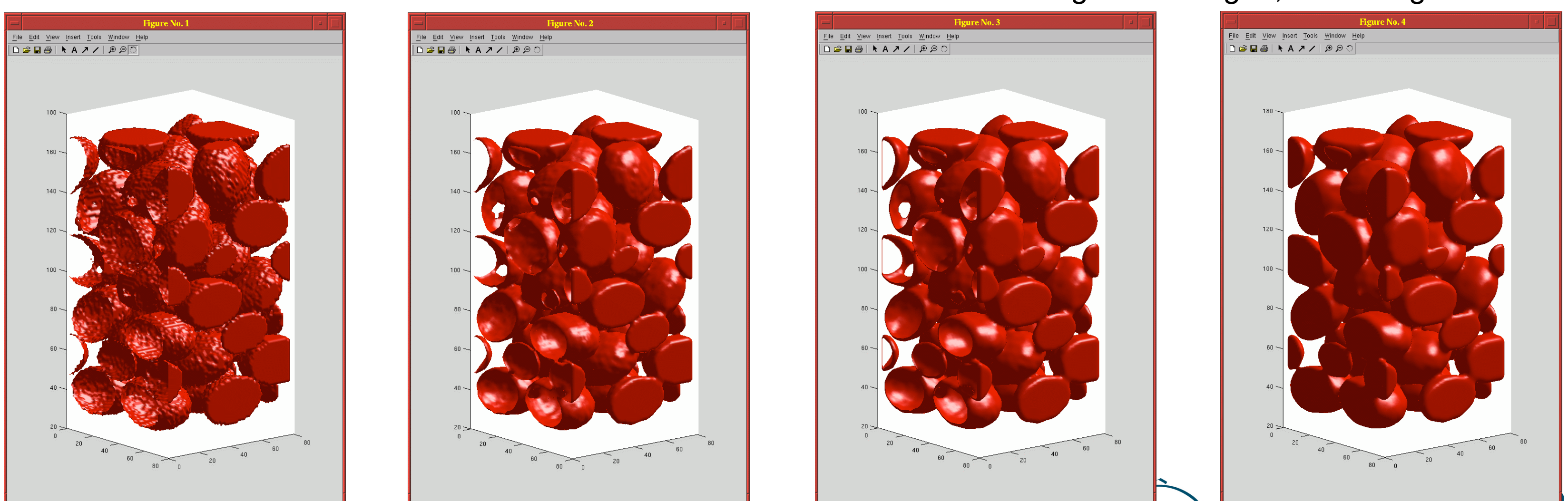
Extension to realistic geometries will require high resolution images from ALS



Experimental image of packed sintered glass beads
Courtesy of R. Detwiler, J. Nelson (LLNL)



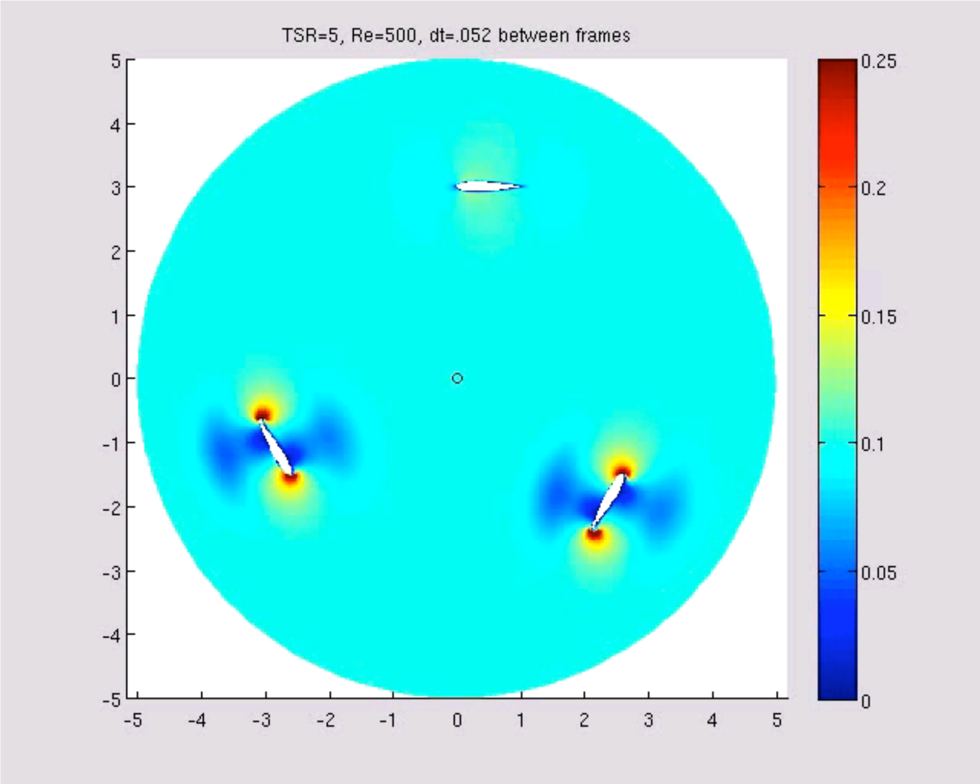
Embedded boundaries on Cartesian grid obtained from level set and implicit function representation of low resolution image data on grid; with T. Ligocki



Raw porous media image data with various levels of smoothing; Courtesy of PNNL, A. Tartakovsky; with T. Ligocki

Wind Turbine Simulations

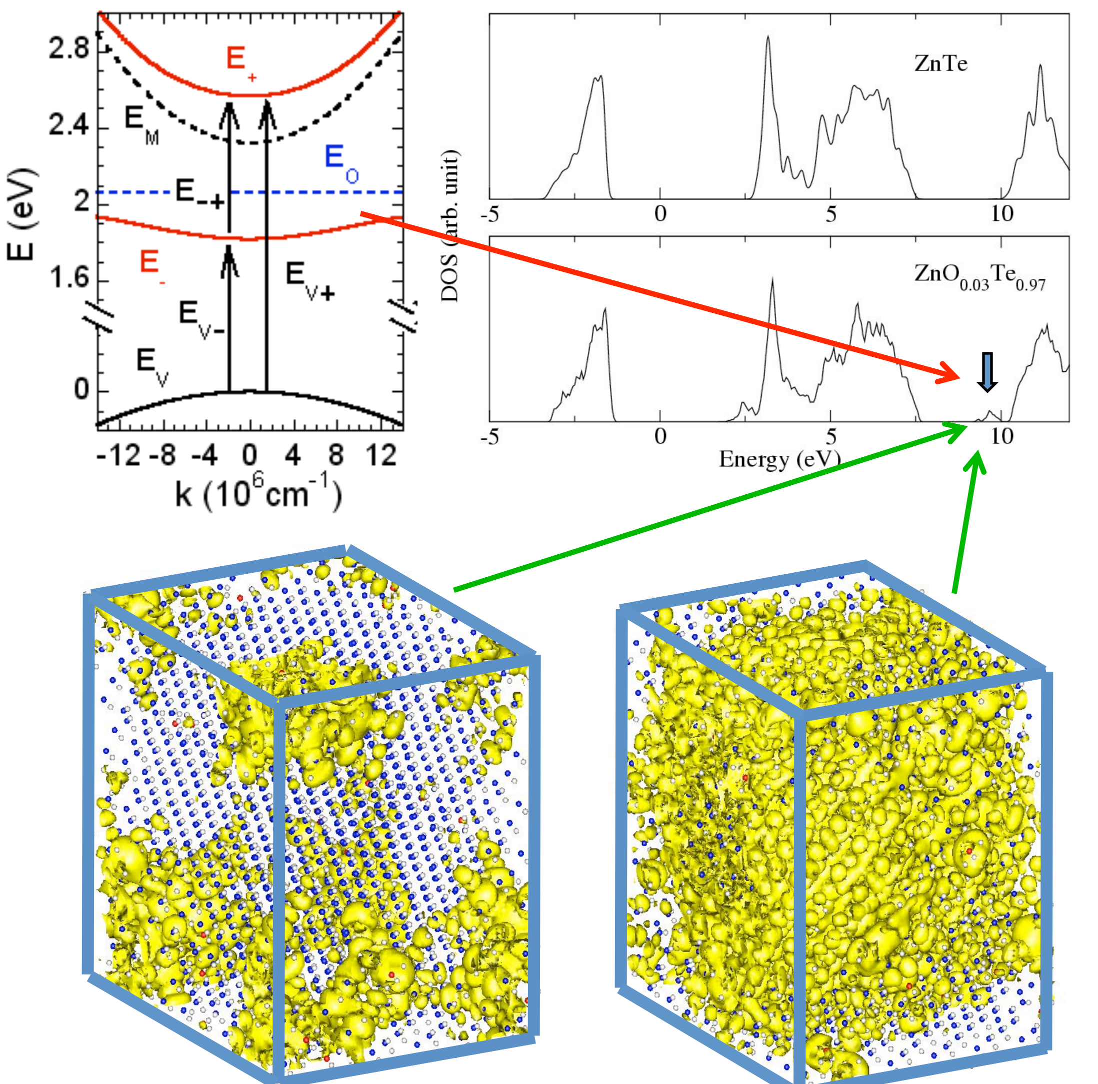
- Need for ***higher fidelity predictions*** in computational mechanics
- Develop new high-order accurate methods for problems with
  - complex real-world geometries
  - turbulent flows, waves, multiple scales
  - non-linear and fluid-structure interactions
- Our new schemes, algorithms, and solvers make high-order discontinuous Galerkin methods practical for realistic problems



Vertical wind turbine (velocity plot)

PI: Per-Olof Persson, UCB, LBNL

Can one use an intermediate state to improve solar cell efficiency?



Highest O induced state

ZnTe bottom of cond. band state

- Single band material theoretical PV efficiency is 30%
- With an intermediate state, the PV efficiency could be 60%
- One proposed material ZnTe:O
  - Is there really a gap?
  - Is it optically forbidden?
- LS3DF calculation for 3500 atom 3% O alloy [one hour on 17,000 cores of Franklin]
- Yes, there is a gap, and O induced states are very localized.

L-W. Wang, B. Lee, Z. Zhao, H. Shan, J. Meza, D. Bailey, E. Strohmaier.
INCITE project, NERSC, NCCS.

Finding vulnerabilities in a complex system

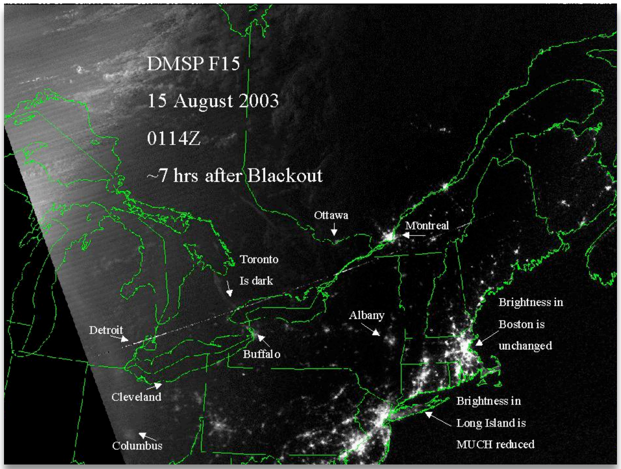
2003 NE US Blackout demonstrated vulnerability of power grid.

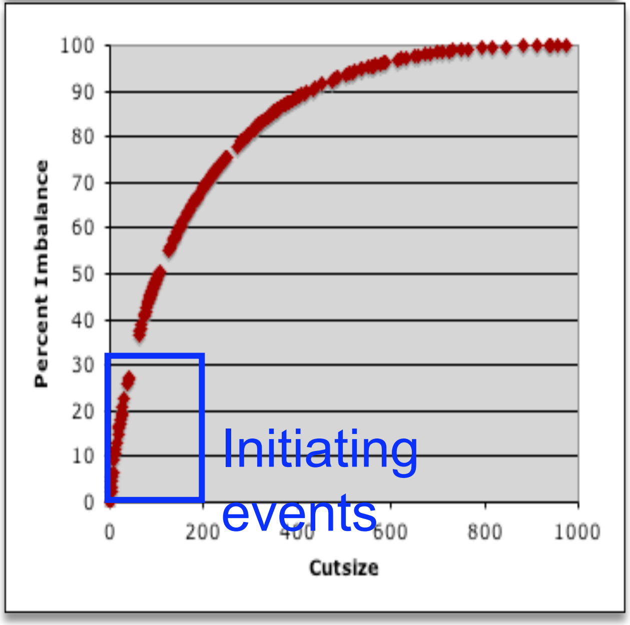
Applied for an LDRD in 2004 and obtained funding from 2005 – 2007 to investigate the application of combinatorial optimization and no-linear optimization for large scale problem.

Can now analyze vulnerabilities of large systems in minutes.

Solutions with small cut size can be used to detect initiating events and groups of vulnerabilities.

Received $875K DOE funding in 2009 (PI Meza).





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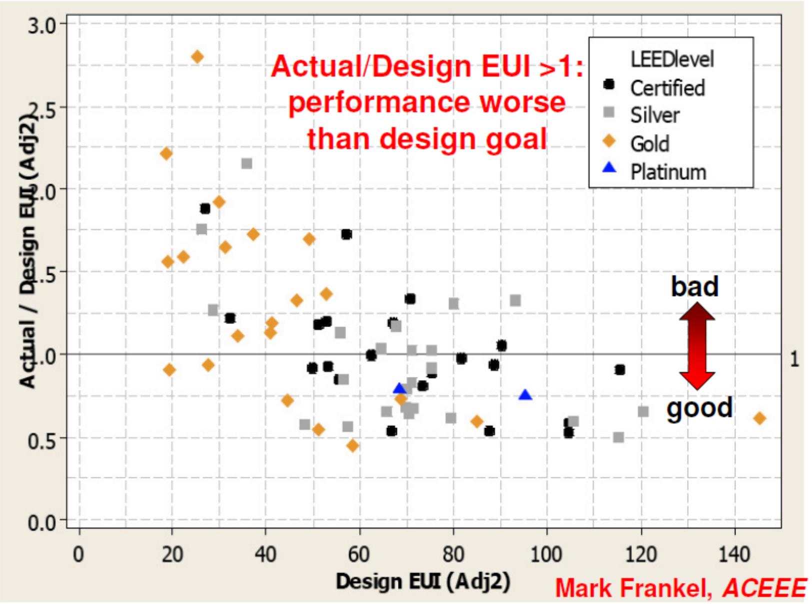
Uncertainty Analysis and Quantification

Design Intent: 66% (ASHRAE 90.1); Measured 44%

LEED ratings are based on ***design*** performance, not ***actual*** performance (EUI = End Use Intensity)



Mark Frankel, *ACEEE* (2008)

Figures from WBCSD, DOE (Chu), Tsinghua (Yi), NREL

Failure Modes Arising from Detrimental Sub-system Interactions

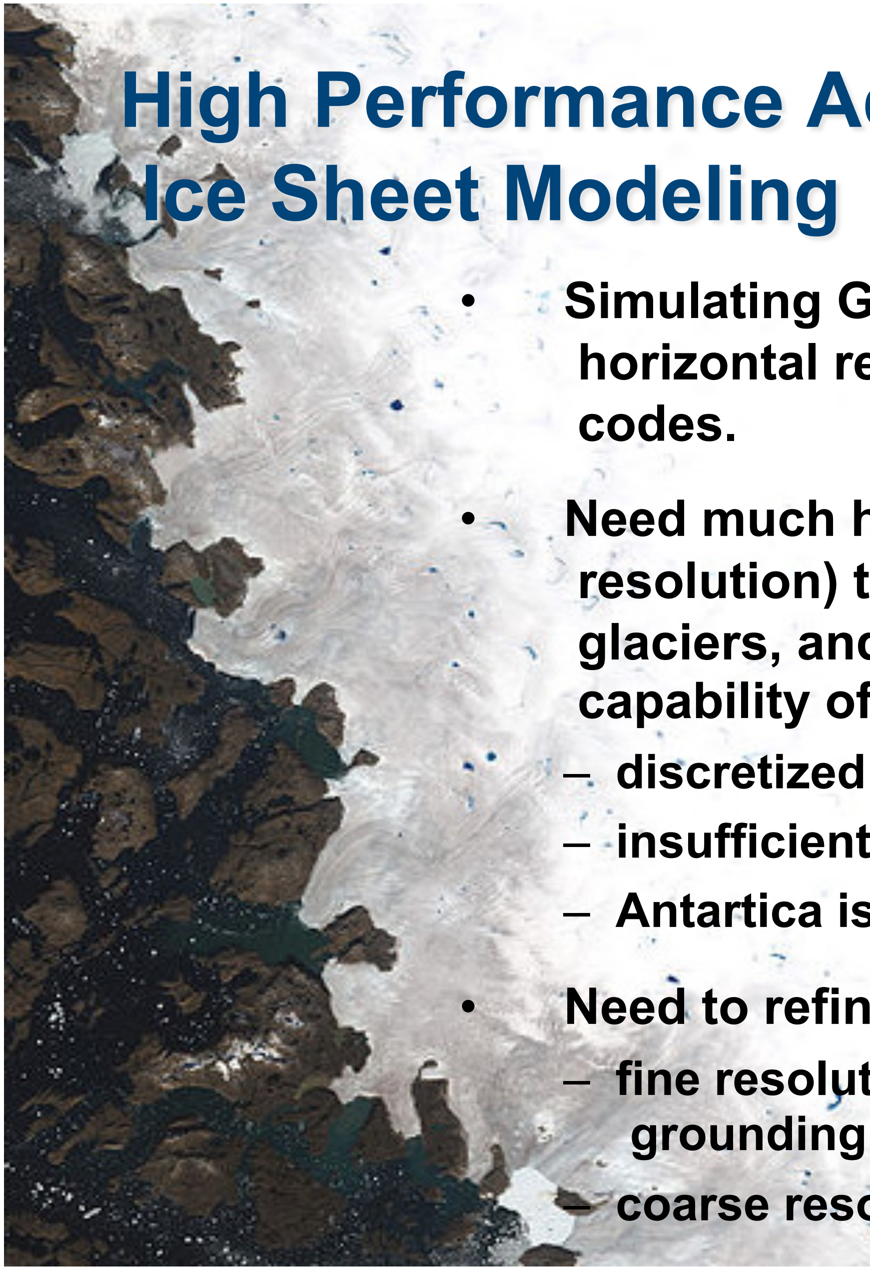
Changes made to envelope to improve structural integrity diminished integrity of thermal envelope ("retainer wall as a fin")

Lack of visibility of equipment status/operation and uncertainty in loads (plug, occupancy, leaks), leading to excess energy use

The barrier is identifying critical (controlling) parameters for large scale dynamical systems (including physics and networks) and then using information to create and deploy and operate robust solutions

Advanced Building Energy Simulation

Discovery Research	Use-inspired Basic Research	Applied Research	Technology Maturation & Deployment
Uncertainty			
• Fast propagation of uncertainty in large scale heterogeneous dynamical systems • Sensitivity analysis of coupled fluid-thermal, dynamic systems	• Fast propagation of uncertainty for system level building models • Modeling of failure modes for building components and system level performance	• Creation of tools for failure modes and uncertainty for building classes • Uncertainty descriptions of system level models for building design	▪ Design tools for GSA/ DOE buildings and systems
Multi-scale dynamics			
• Multi-scale dynamic analysis of large scale heterogeneous dynamic systems • Extraction of accurate low order models suitable for design, optimization and control	• Dynamic analysis of system level building models • Use of low order models for system design, optimization and supervisory control	• Dynamic analysis of standard low energy consumption systems • Validation of supervisory control performance, predicted stability boundaries and robustness margins	• Controls and Diagnostics implementations for GSA/DoD buildings
Optimization			
• Methods for stochastic optimization including occupant load, weather, and climate	• Methods for mixed discrete/ continuous optimization problems	• Application of multi-criteria optimization including energy efficiency, cost, HVAC systems	• Off-point design and commissioning tools
SC		**EERE**	

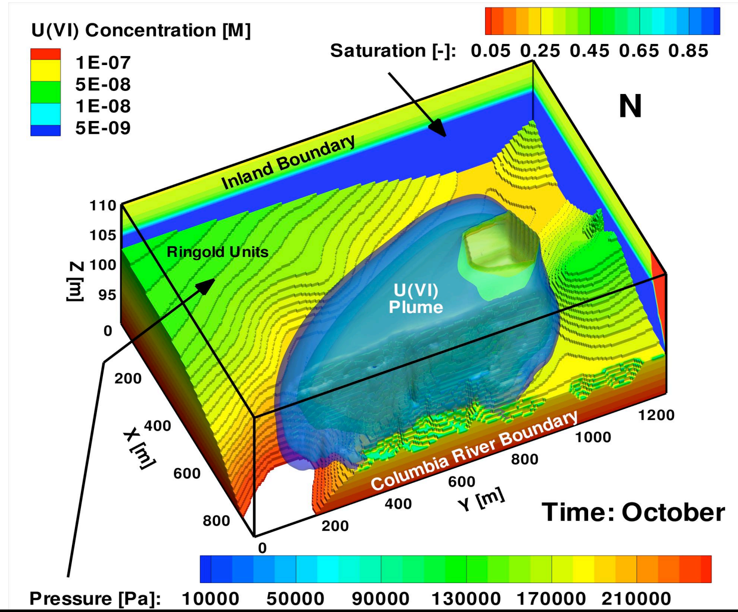


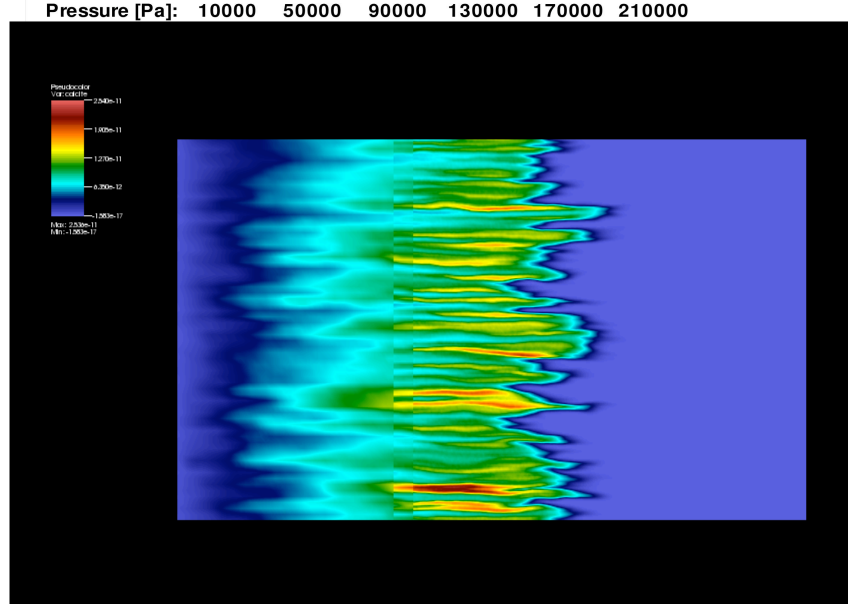
High Performance Adaptive Algorithms for Ice Sheet Modeling

- **Simulating Greenland ice sheet at about 5-km horizontal resolution is doable with current modeling codes.**
- **Need much higher resolution (~1-km horizontal resolution) to accurately model ice streams, outlet glaciers, and grounding lines -- but this is beyond the capability of current codes**
  - **discretized problems too large**
  - **insufficient computing resources**
  - **Antartica is much larger than Greenland**
- **Need to refine regions selectively …**
  - **fine resolutions around ice streams, outlet glaciers, and grounding lines.**
  - **coarse resolutions elsewhere**

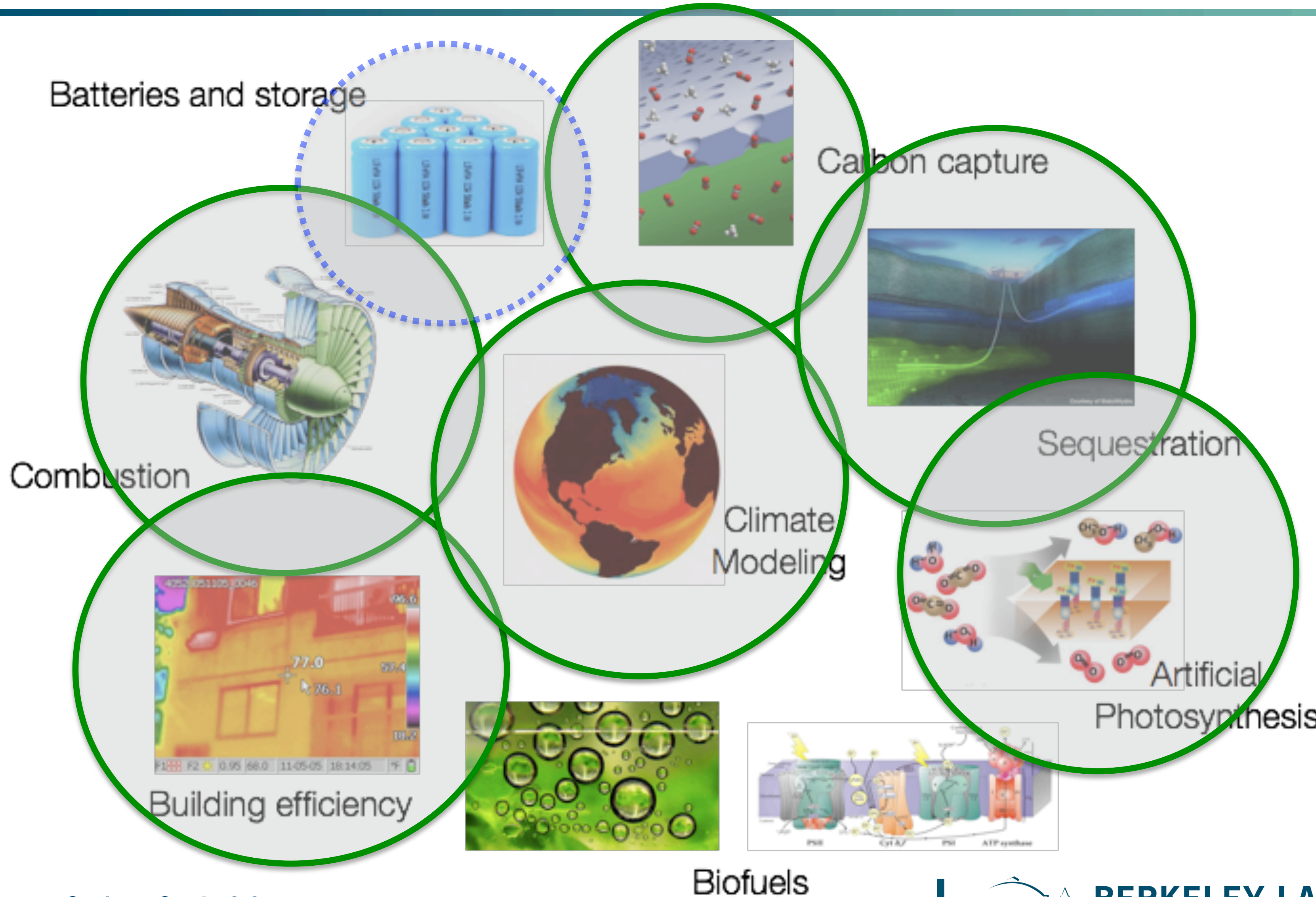
ASCEM Has 3 Thrust Areas

- **High Performance Computing Simulator**
  - Encompasses process models and the core framework for the HPC simulator
- **Integrated Toolset Platform**
  - Includes a complete user environment from HPC down to the desktop
- **Site Applications**
  - Provides ties to the user community





Carbon Cycle 2.0 and Computing



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Main themes and challenges

1. Multiscale
2. Adaptive algorithms
3. Higher order methods
4. O(N) algorithms
5. Optimization
6. Combinatorial methods
7. Uncertainty quantification
8. Multi-physics coupling

Barriers

- Scientific Hurdles
  - New computing architecture paradigms
  - Development of scalable algorithms
  - Programming models
  - Green computing
- Programmatic
  - Finding more staff with right skills set
  - Continuous, long-term source of funding for collaborations
  - Access to large-scale computing resources

Other Centers of Excellence

- Two other major DOE centers for computing: ORNL and ANL
- Several NSF centers in computational science
- Many other labs around the world
  - Julich Supercomputing Centre
  - Centro Nacional de Supercomputacion, Barcelona
  - Swiss National Supecomputing Centre (CSCS), Switzerland
  - Earth Simulator, Japan

Collaboration Opportunities

- **Software developed at LBNL could be used to initiate new collaborations**
- **Technology transfer in algorithms, software, performance tools, etc.**
- **Industry could provide data for validation of computer models and prototyping of general algorithms for specific applications**

Acknowledgements

John Bell
Maciej Haranczyk
Esmond Ng
George Pau
Per-Olof Persson
James Sethian
David Trebotich
Lin-Wang Wang
Michael Wehner
Zhengji Zhao

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