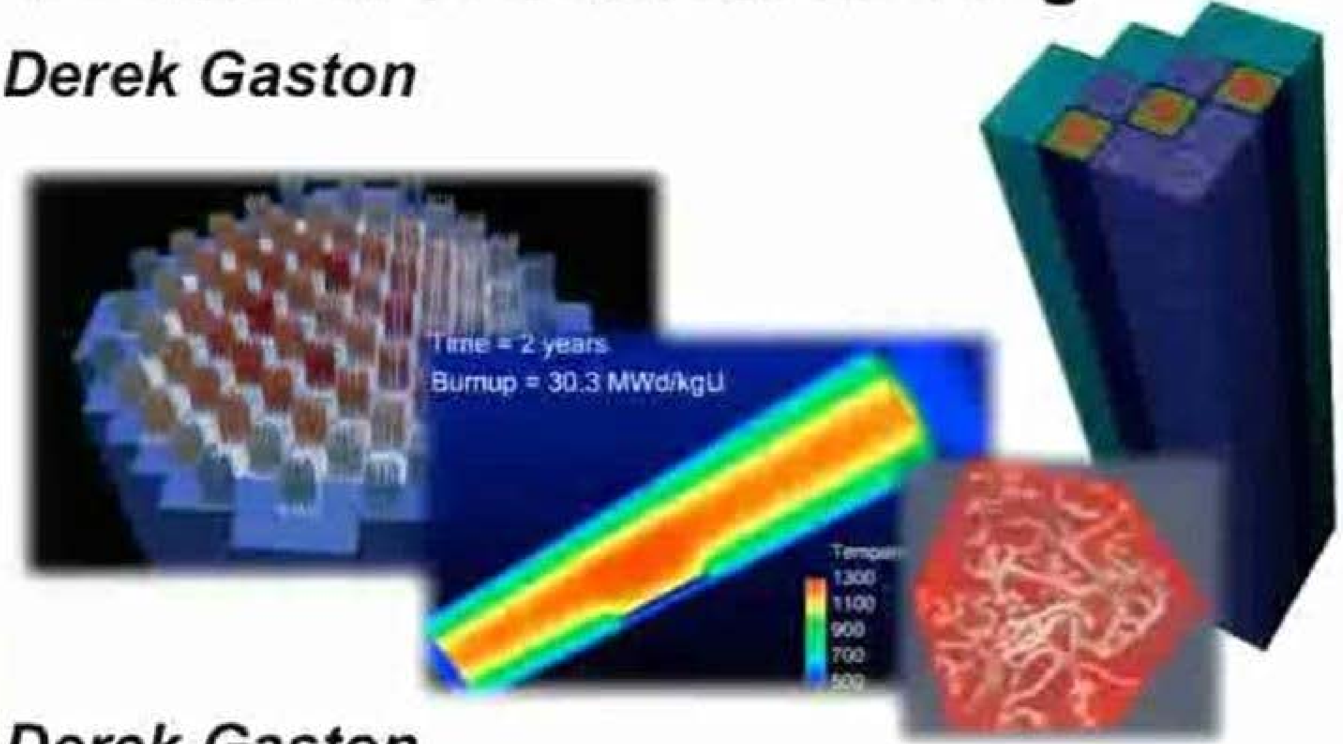
MOOSE: An Open Source Platform For Rapid Development of Multiphysics Simulation Tools

www.mooseframework.org

Derek Gaston



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NSE @ MIT Massachusetts Institute of Technology

www.inl.gov

Idaho National Laboratory

The Core Team

- INL:
  - Cody Permann
  - David Andrs
  - John Peterson
  - Jason Miller
  - Andrew Slaughter

- MIT:
  - Derek Gaston

- Argonne National Laboratory
  - Dmitry Karpeyev

- University of Texas, Austin
  - Roy

MOOSE Minis Tomorrow

MS259/MS284

Parallel, Multiscale, Multiphysics Simulation Using MOOSE

Room 250 C

Outline

- MOOSE Overview
- Ease Of Use
- Parallel Capability
- Community
- Applications

MOOSE Overview

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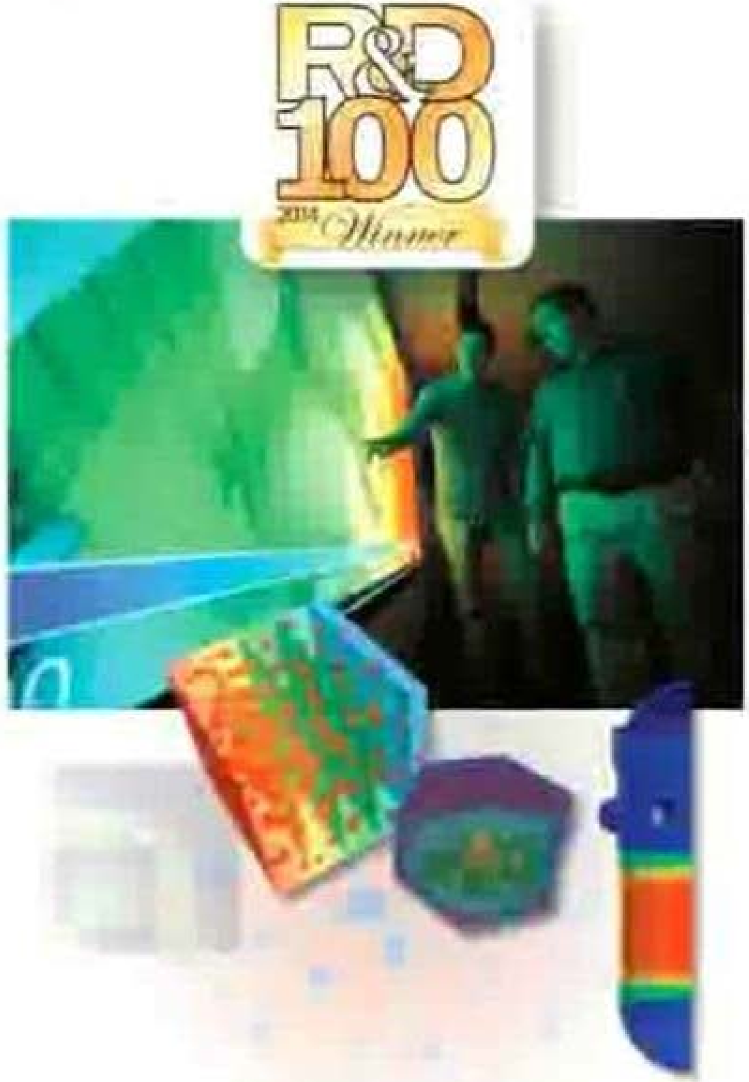
Idaho National Laboratory

MOOSE

INL Idaho National Laboratory

Multiphysics Object Oriented Simulation Environment

- MOOSE is a finite-element, multiphysics framework that **simplifies the development** of numerical applications.
- It provides a high-level interface to **sophisticated nonlinear solvers** and **massively parallel computational capability**.
- Used to model thermomechanics, neutronics, geomechanics, reactive transport, microstructure, computational fluid dynamics, and more every day!
- **Open source** and freely available at **mooseframework.org**
- A complete platform for accelerating computational science.



MOOSE Collaborators

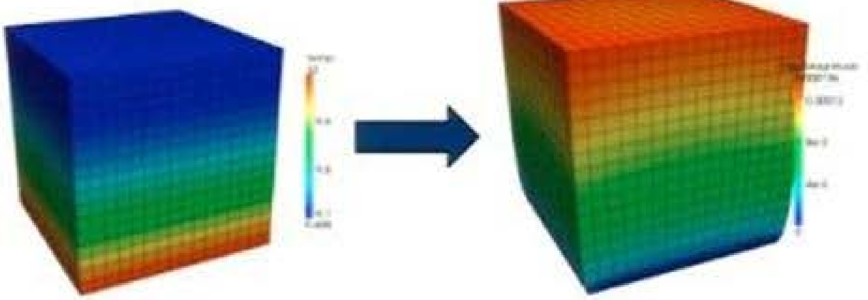
AECL EACL
Argonne NATIONAL LABORATORY
CSIRO
CASL
National Nuclear Laboratory
NEAMS NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM
Los Alamos NATIONAL LABORATORY
Oak Ridge National Laboratory
Pacific Northwest NATIONAL LABORATORY
Sandia National Laboratories

ANATECH
GENERAL ATOMICS
Studsvik

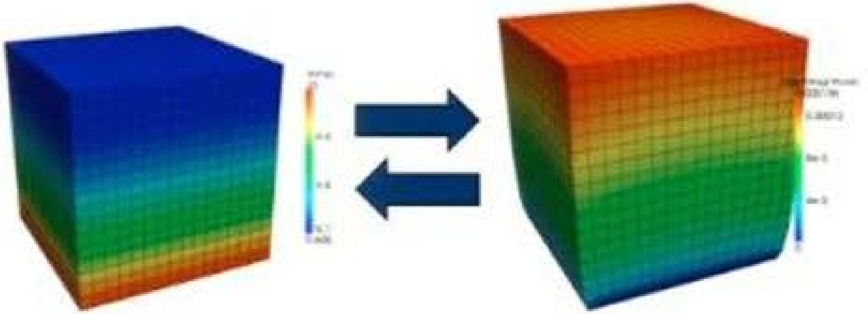
COLORADO SCHOOL OF MINES
Idaho State UNIVERSITY
MIT
T
UNIVERSITY OF OXFORD
NC STATE UNIVERSITY
MICHIGAN
OSU Oregon State UNIVERSITY
PennState
BYU IDAHO
TEXAS A&M UNIVERSITY
University of Idaho
UNM
UNIVERSITY OF SOUTH CAROLINA
THE UNIVERSITY OF UTAH
VCU Virginia Commonwealth University
UNIVERSITY OF WYOMING
WASHINGTON STATE UNIVERSITY
THE UNIVERSITY WISCONSIN MADISON

Coupling

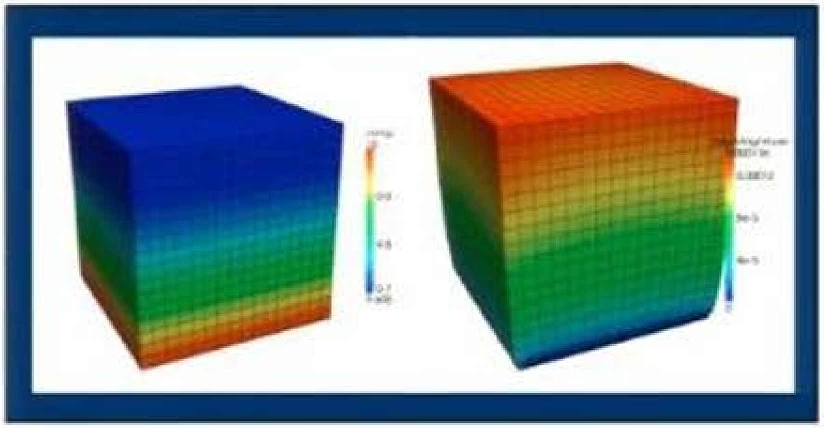
- Loose Coupling / Operator Split
  1. Solve PDE1
  2. Pass Data
  3. Solve PDE2
  4. Move To Next Timestep



- Tight Coupling
  1. Solve PDE1
  2. Pass Data
  3. Solve PDE2
  4. Pass Data
  5. Return to 1 Until Convergence
  6. Move To Next Timestep



- Fully Coupled
  1. Solve PDE1 and PDE2 simultaneously in **one** system
  2. Move To Next Timestep

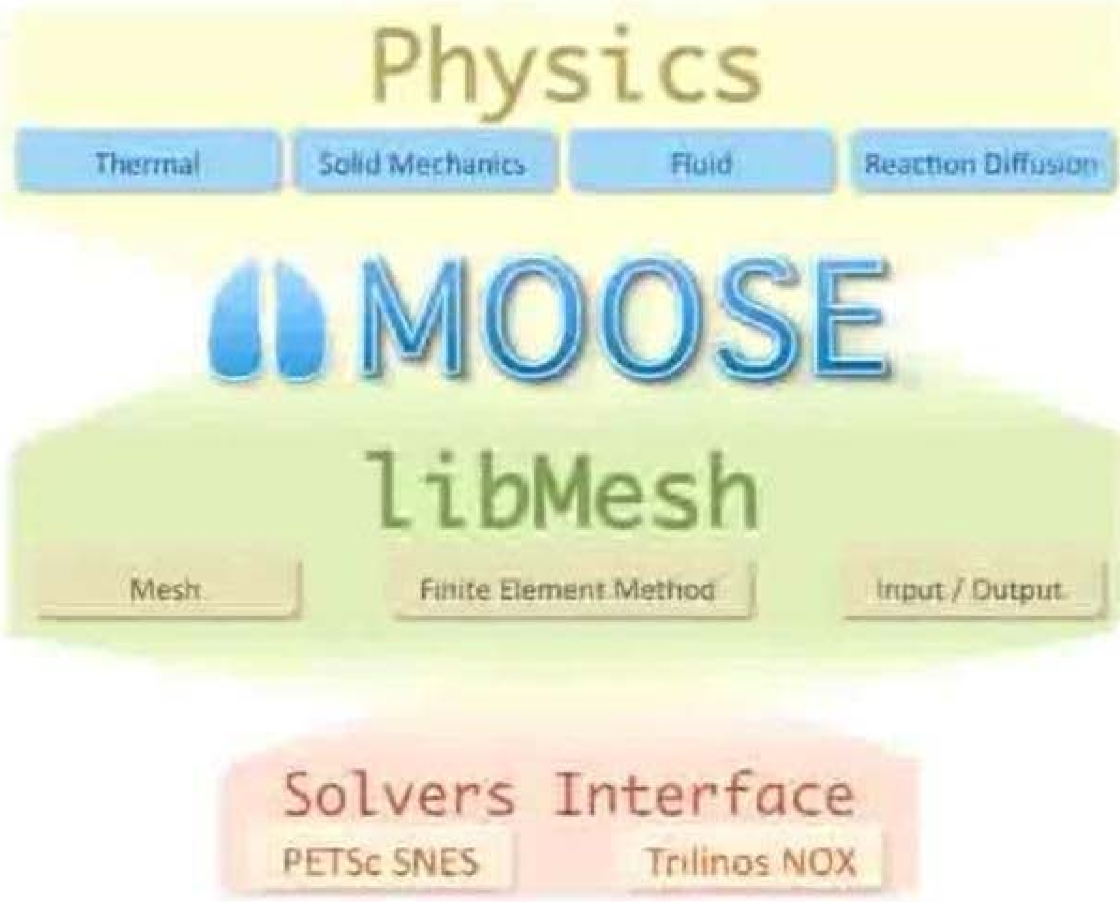


General Finite-Element Capabilities

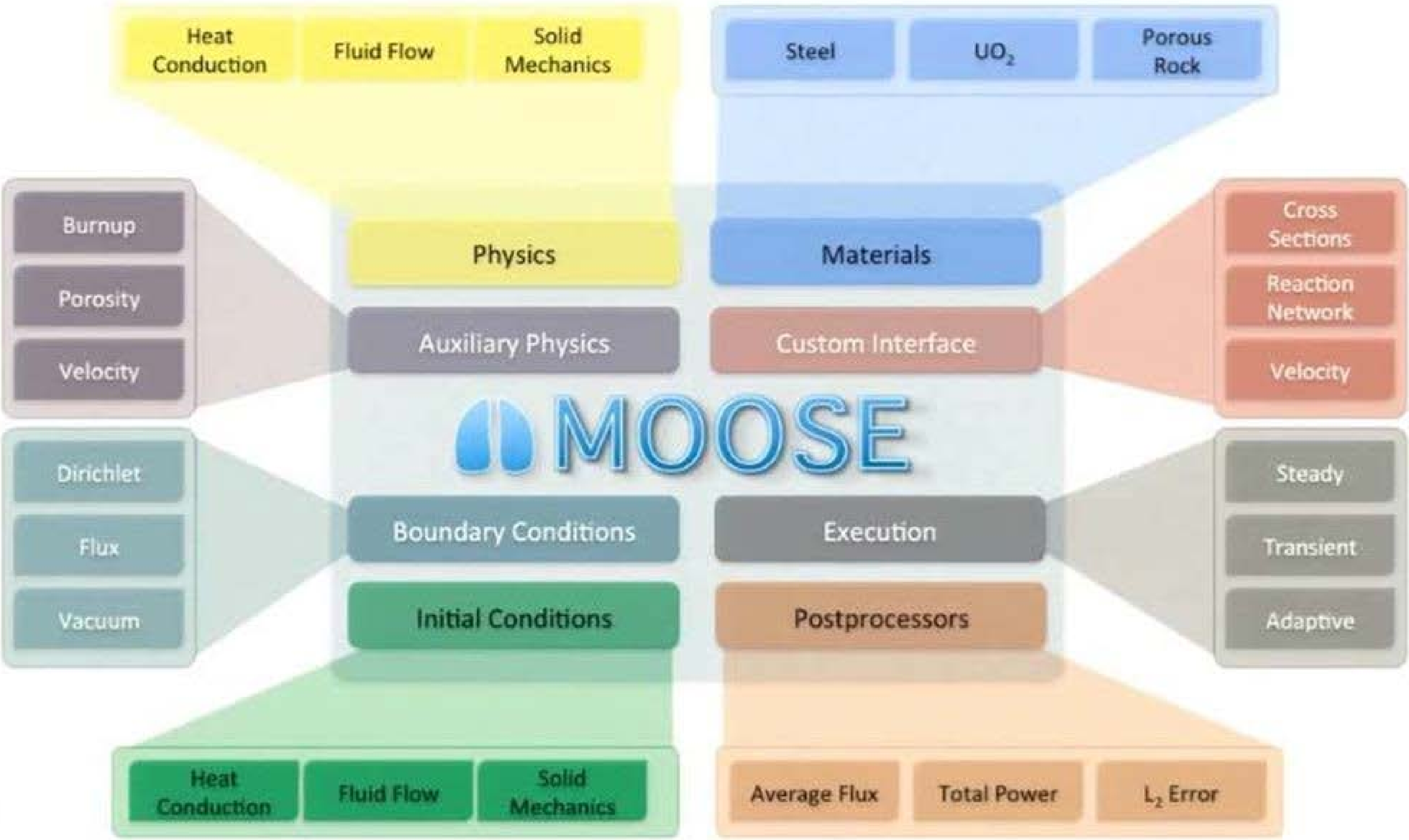
- 1D, 2D and 3D
  - User code agnostic of dimension
- Finite Element Based
  - Continuous and Discontinuous Galerkin (and Petrov Galerkin)
- Fully Coupled, Fully Implicit
- Unstructured Mesh
  - All shapes (Quads, Tris, Hexes, Tets, Pyramids, Wedges…)
  - Higher order geometry (curvilinear, etc.)
  - Reads and writes multiple formats
- Mesh Adaptivity
- Hybrid Parallel
  - MPI + Threading
  - User code agnostic of parallelism
- High Order
  - User code agnostic of shape functions
  - *p*-Adaptivity
- Built-in Postprocessing
  - Also interfaces with 3rd party pre/post processors
- And much more…

Code Platform

- Provides an object-oriented, pluggable system for defining all aspects of a simulation tool.
- Leverages multiple DOE and university developed scientific computational tools
  - ~2 Million LOC!
- Allows scientists and engineers to efficiently develop state of the art simulation capabilities.
  - **Maximize Science/$**



Application

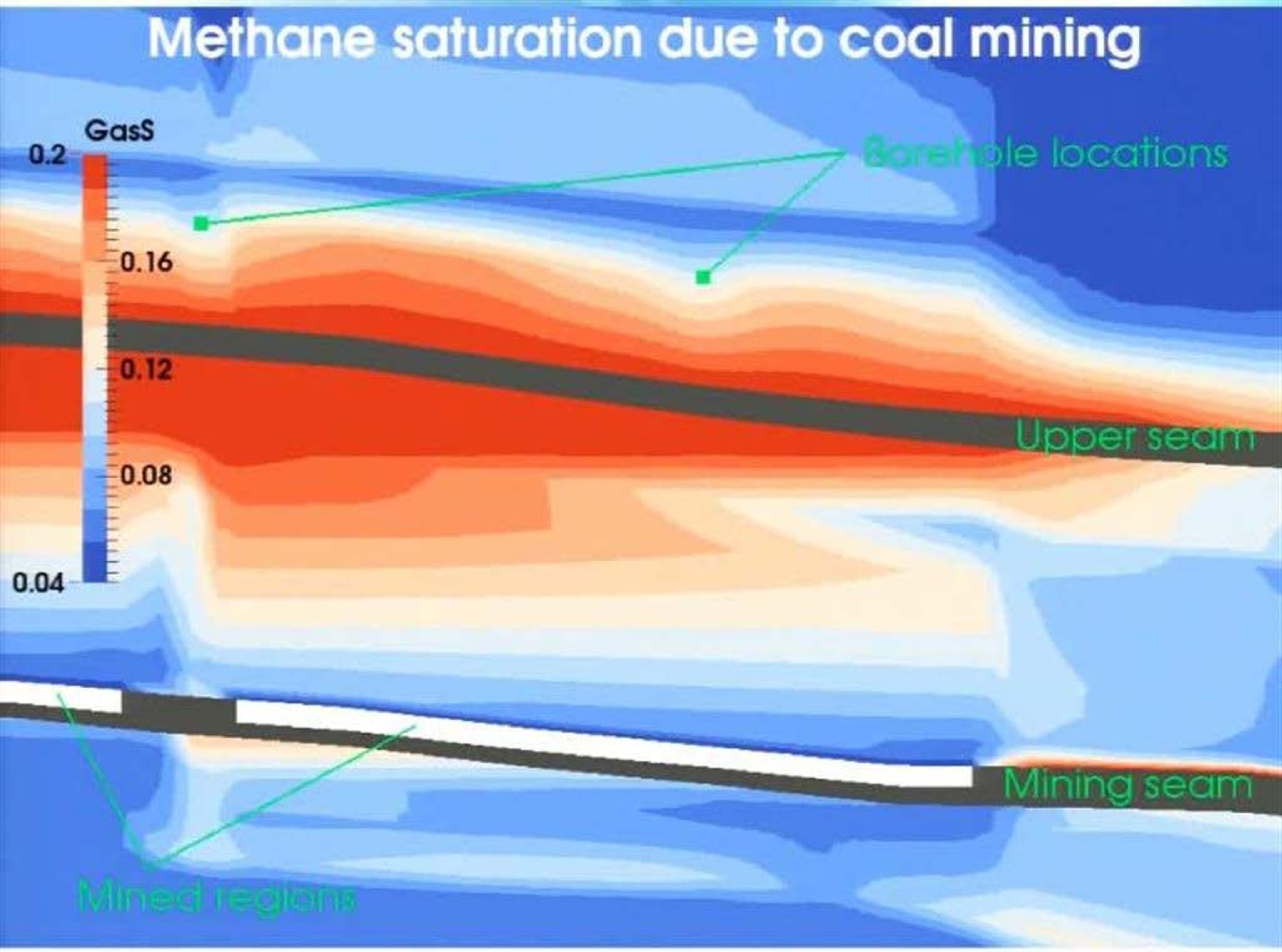


Flexible Interfaces For Customization

- Actions
- Auxiliary Kernels
- Auxiliary Variables
- BCs
- Constraints
- Dampers
- DGKernels
- DiracKernels
- Executioners
- Functions
- GeomSearch
- ICs
- Indicators
- Kernels
- Markers
- Materials
- Mesh
- MeshModfiers
- MultiApps
- Outputs
- Oversampling
- Postprocessors
- Preconditioners
- Predictors
- Splits
- TimeIntegrators
- TimeSteppers
- Transfers
- UserObjects
- Variables

Physics Modules

- MOOSE Ships with community developed physics modules to accelerate development.
- Simple to extend and modify to fit your application.
- Some Examples:
  - Phase Field
    - Has become a whole framework by itself with its own training classes!
  - Tensor Mechanics
  - Heat Conduction
  - Multiphase flow through porous media (Richards Eq.)
  - Chemical Reactions
  - Navier Stokes
  - Contact


Methane saturation due to coal mining
GasS
0.2
0.16
0.12
0.08
0.04
Borehole locations
Upper seam
Mining seam
Mined regions

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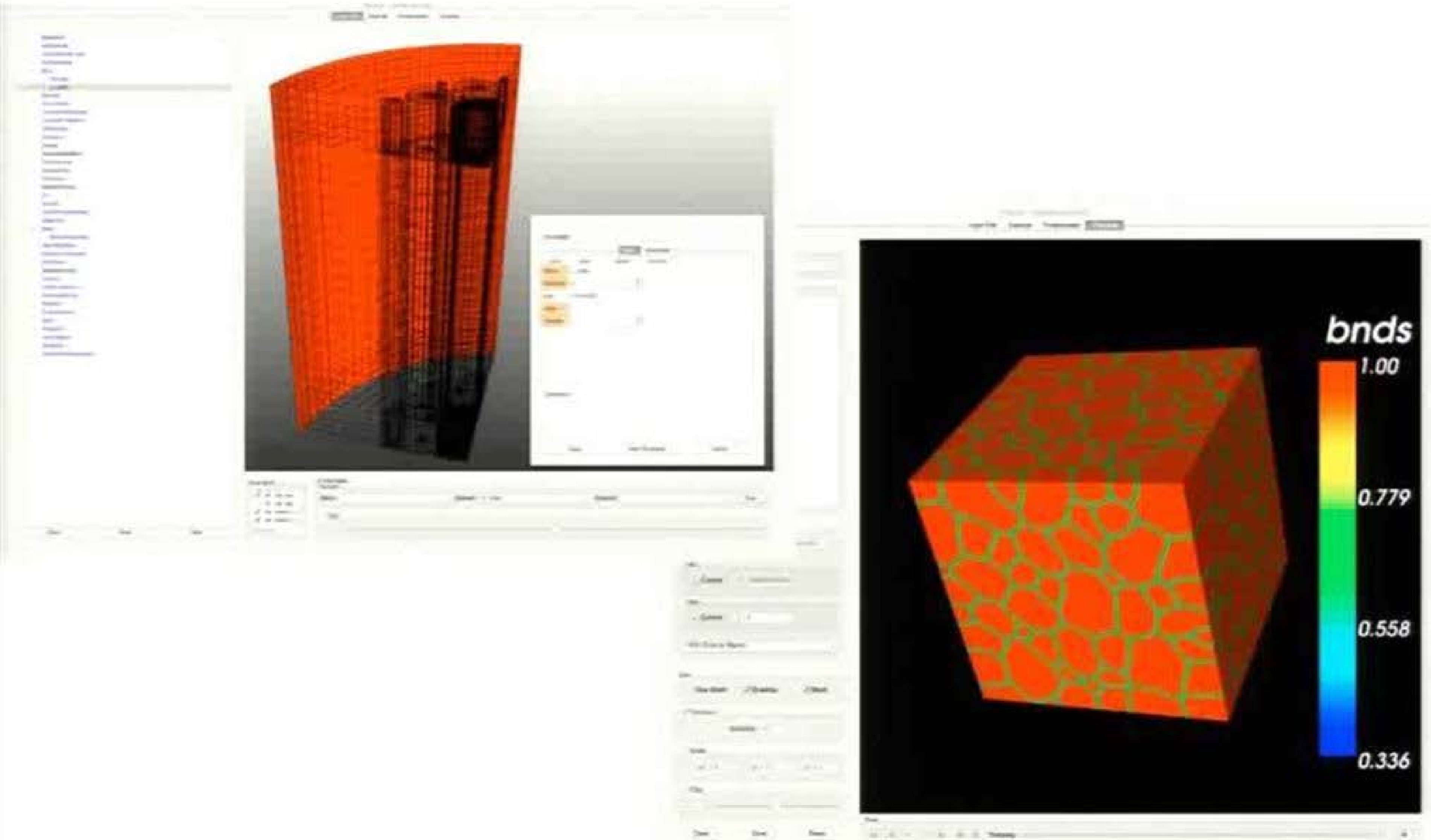
Ease Of Use

Simplified Installation

- We provide installable binaries for:
  - Mac OSX
  - Ubuntu (14.x) / Mint 17
  - Ubuntu (12.x)
  - openSUSE 13.1
  - Fedora Core 20
  - Fedora Core 21
  - Virtual Machine
  - Manual Installation Instructions (Basic)
  - Linux Cluster

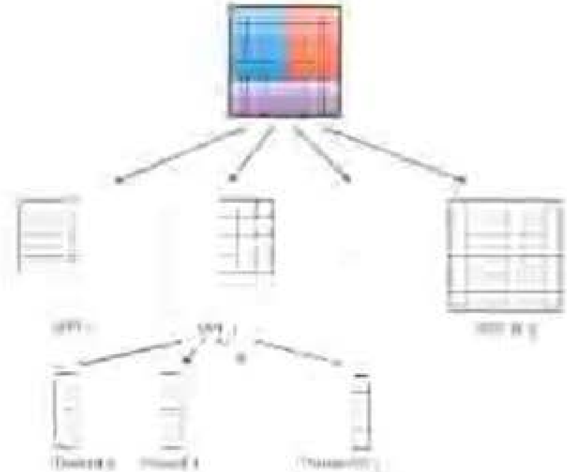
Graphical User Interface (Peacock)

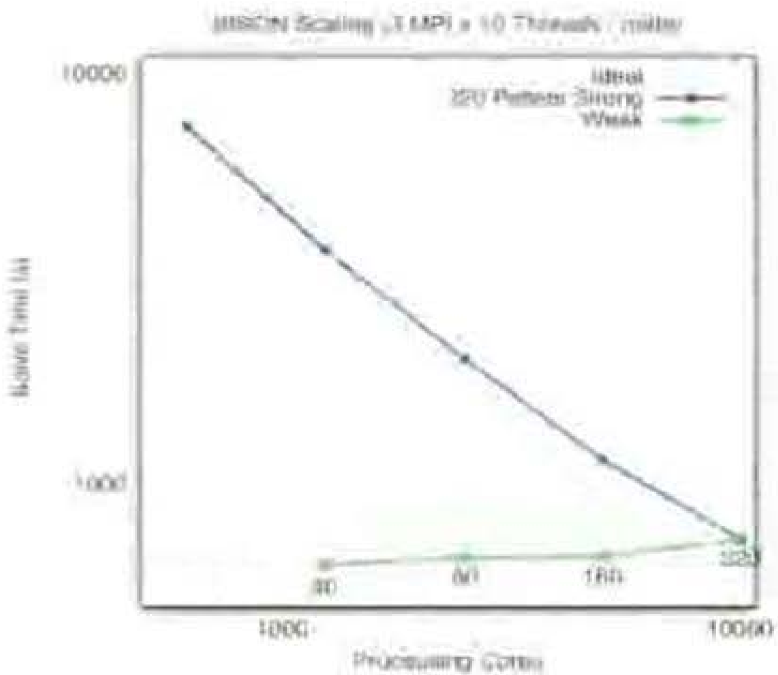


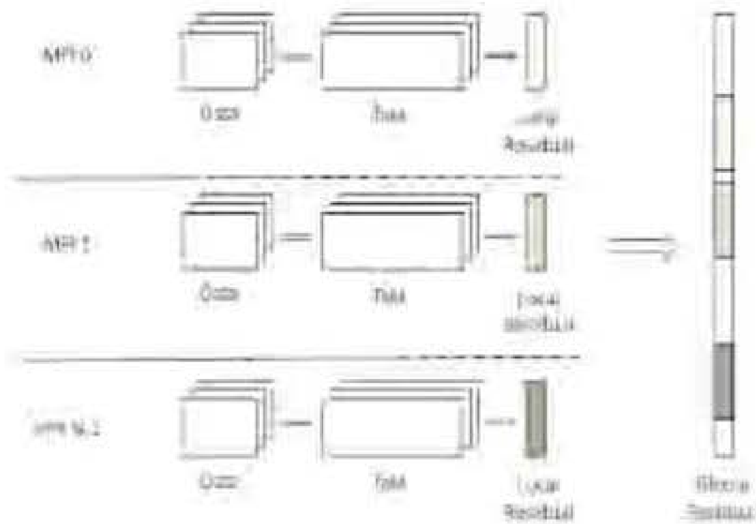
Parallel Capability

Parallel Work Distribution

- User code agnostic of parallelism.
- MPI used for coarse grained splitting.
- Threading used for on-node parallelism.
  - Can utilize: TBB, OpenMP or straight Pthreads
- Largest runs on over 100,000 processors

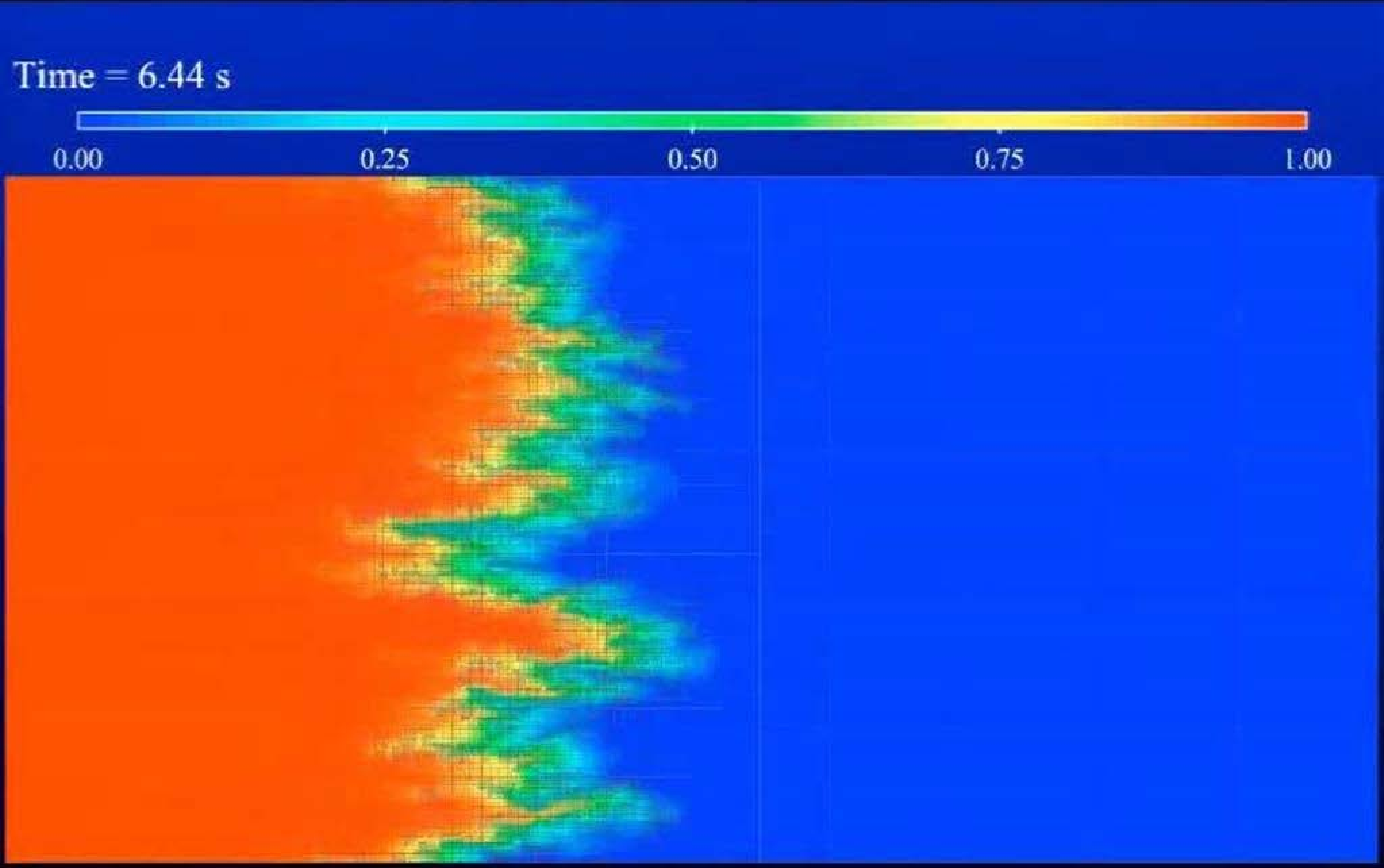






All Features Implicitly Parallel

All Features Implicitly Parallel

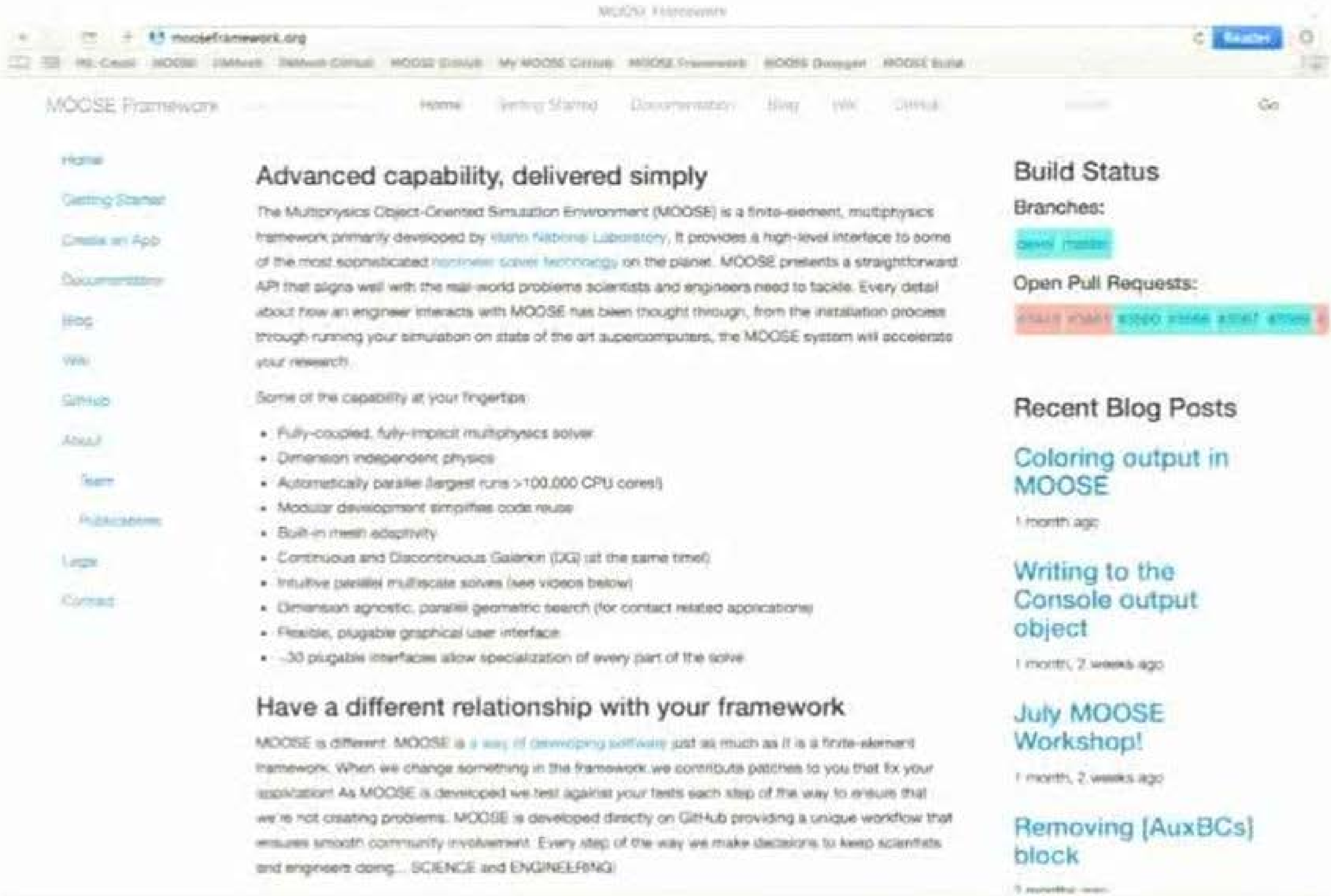


Community

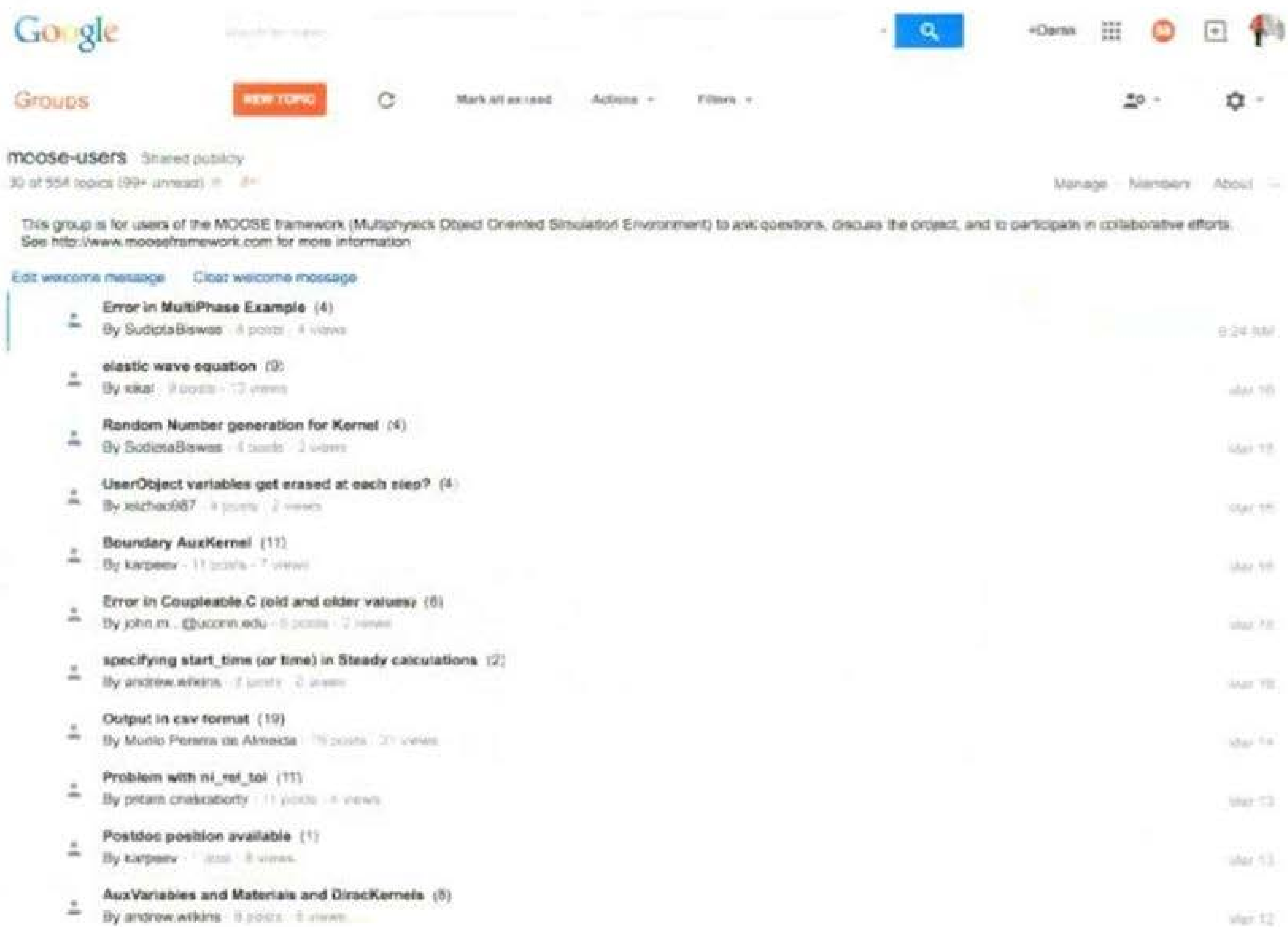
www.inl.gov

Idaho National Laboratory

MooseFramework.org



Active Mailing List



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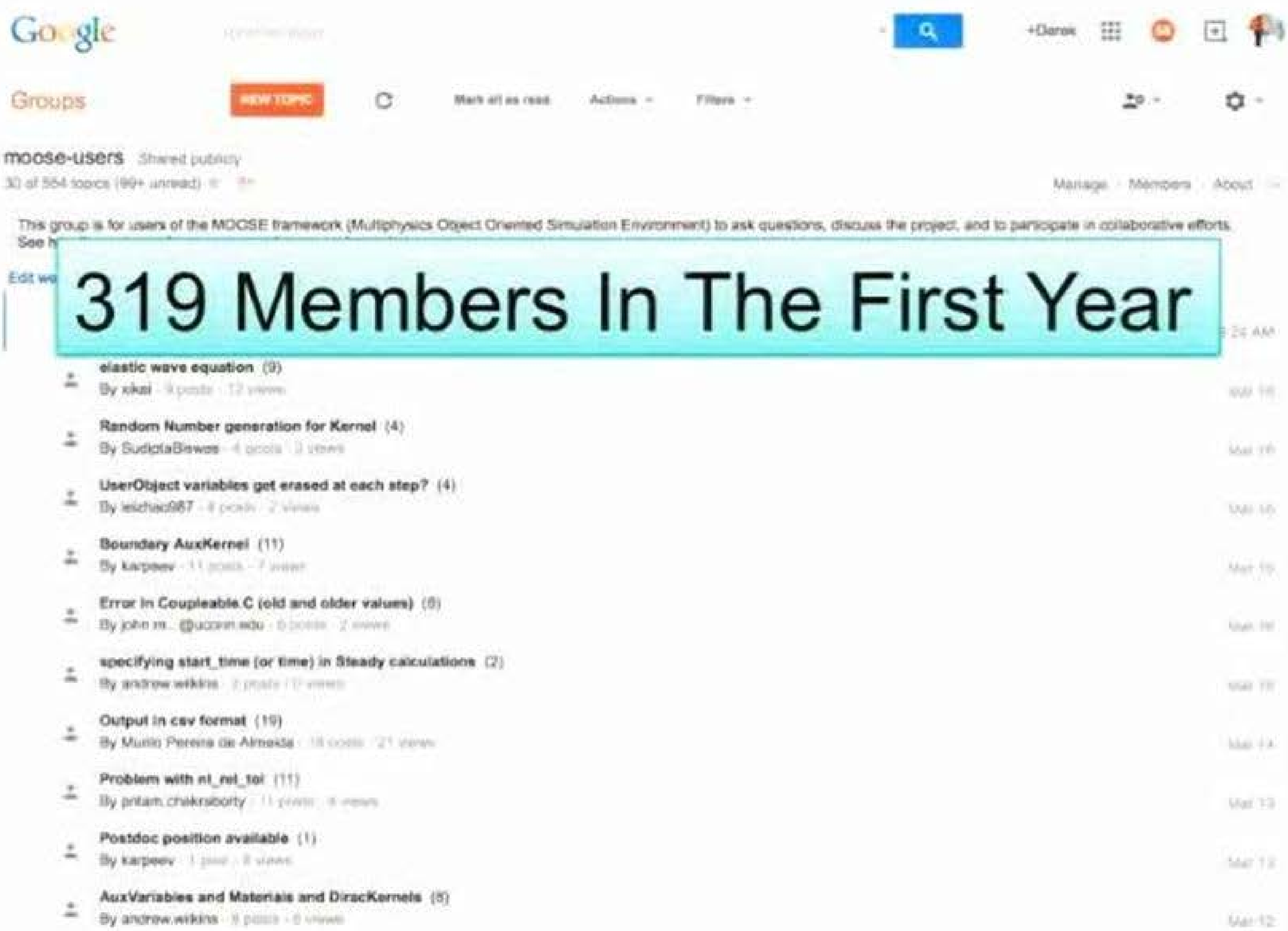


319 Members In The First Year

Active Developer Community

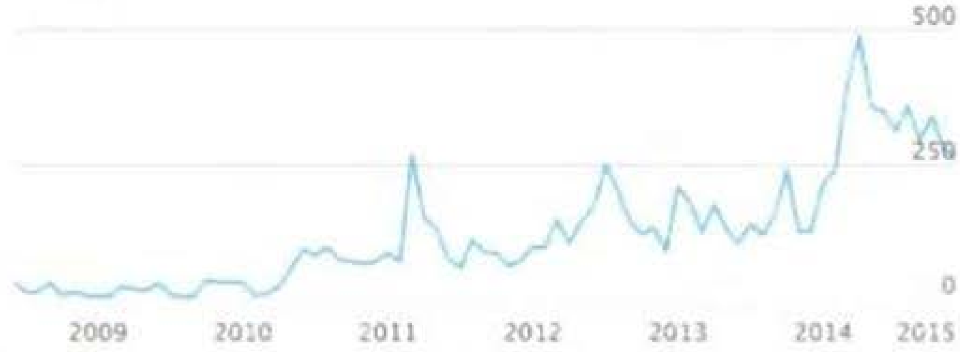
idaholab / **moose**

Unwatch 33 | Unstar 73 | Fork 119

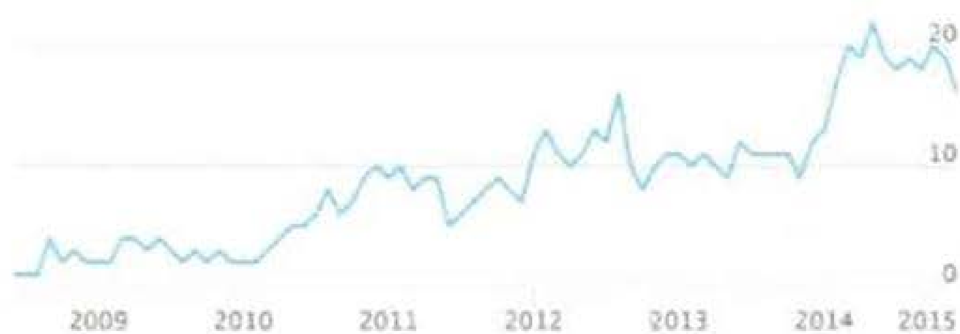
idaholab / **stork**

Unwatch 13 | Star 4 | Fork 103

Commits per Month



Contributors per Month



Automated Contributor Feedback

Augmented EquationSystems reinit #4727

Open roystgnr wants to merge 1 commit into idaholab:devel from roystgnr:augmented_es_reinit

Conversation 12 Commits 1 Files changed 1

roystgnr commented 19 days ago Owner

As of libMesh/libmesh#478 (and as requested in libMesh/libmesh#437), libMesh now supports the use of EquationSystems::add_system() after EquationSystems::init(). However, to make that code simple and O(N) instead of O(N^2), we do still require a call to EquationSystems::reinit() afterwards before the newly-added systems can be used.

moosebuild commented 19 days ago Owner

Results of testing [illegible] using moose_PR_pre_check recipe:

Failed on: linux-gnu

View the results here: https://www.moosebuild.com/view_job/12321

Reinit EquationSystems after adding new Systems ...

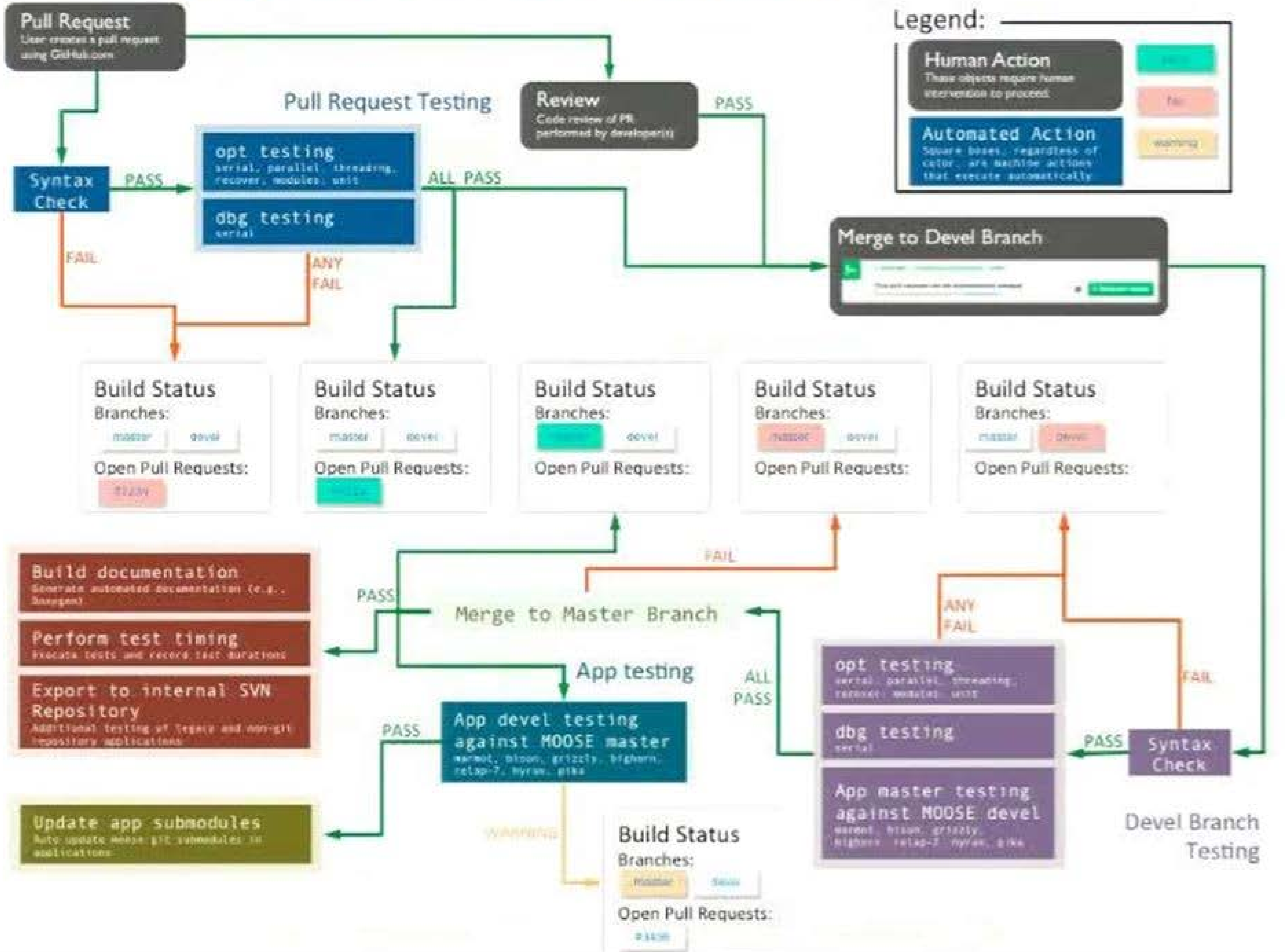
moosebuild commented 19 days ago Owner

Results of testing [illegible] using moose_PR_pre_check recipe:

Passed on: linux-gnu

View the results here: https://www.moosebuild.com/view_job/12325

Pull Request Centric Workflow



More Information on Build System

- A. Slaughter, D. Gaston, J. Peterson, C. Permann, D. Andrs, and J. Miller. Continuous Integration for Concurrent MOOSE Framework and Application Development on GitHub. In Workshop On Sustainable Software for Science: Practice and Experiences 2 (WSSSPE2), Supercomputing 2014
- http://figshare.com/articles/Continuous_Integration_for_Concurrent_MOOSE_Framework_and_Application_Development_on_GitHub/1112585

Applications

www.inl.gov

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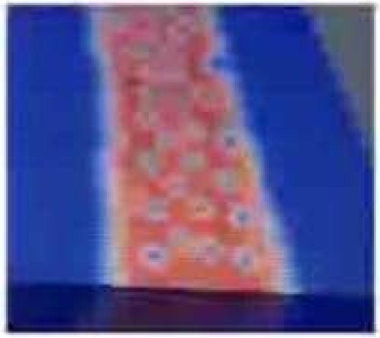
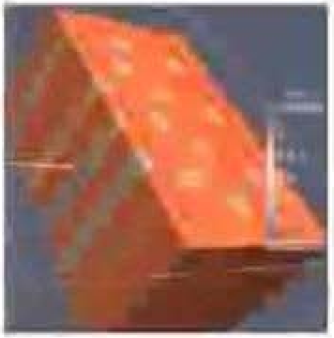
Condor
(Argonne National Laboratory)

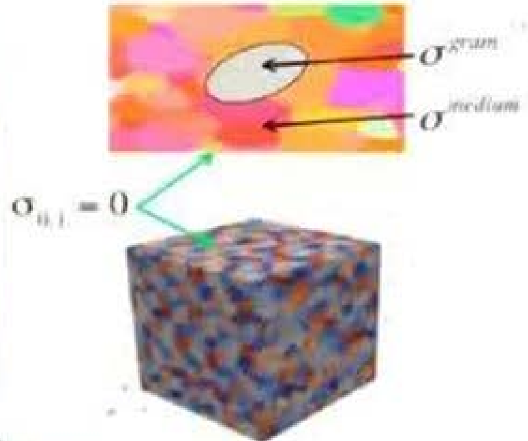
- *Condor* (SciDAC): Simulates the behavior of super-conducting materials with inclusions (e.g., particles, columnar defects) with the goal of finding the optimal inclusion geometries that result in the highest efficiency of the superconductor.
  - The model is a coupled system of PDEs – complex variable Ginzburg-Landau equation, over-damped Maxwell's equation, Poisson's equation, and temperature diffusion equation.
  - Chaotic vortices should relax to a vertical arrangement that has a hexagonal lattice *xy*-cross-section (Abrikosov lattice).
  - Particular challenges result from the need to resolve complex inclusion geometries and the imposition of quasi-periodic boundary conditions in the direction of the current.





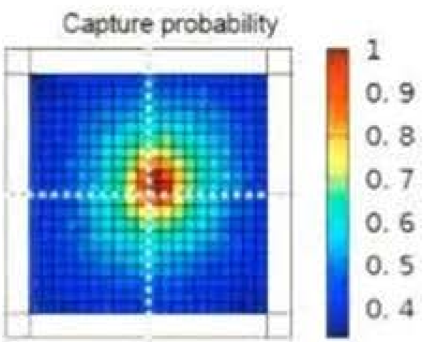
The so-called "Abrikosov lattice", which earned ANL's Dr. Abrikosov his Nobel Prize

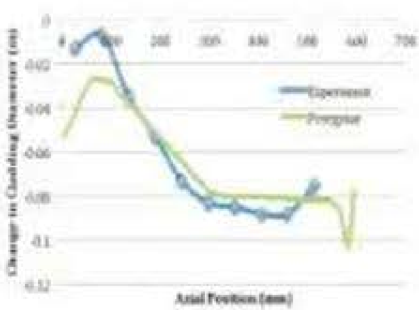
Vulture (CASL)



Vulture: Multi-scale simulation of nuclear fuel cladding deformation and failure

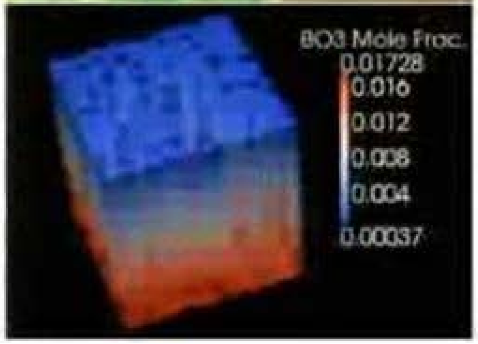
- Visco Plastic Self Consistent (VPSC) model, which accounts for crystallographic mechanisms, interactions between grains and coupling between growth and creep (radiation and thermal).
- Improved models for clad deformation required for PCI and safety assessments.
- Atomistic simulation for defect behavior, including mobility and interaction with dislocations.
- Vulture successfully integrated into Peregrine (BISON) and constitutive models include creep, growth and plastic deformation of Zr-4.





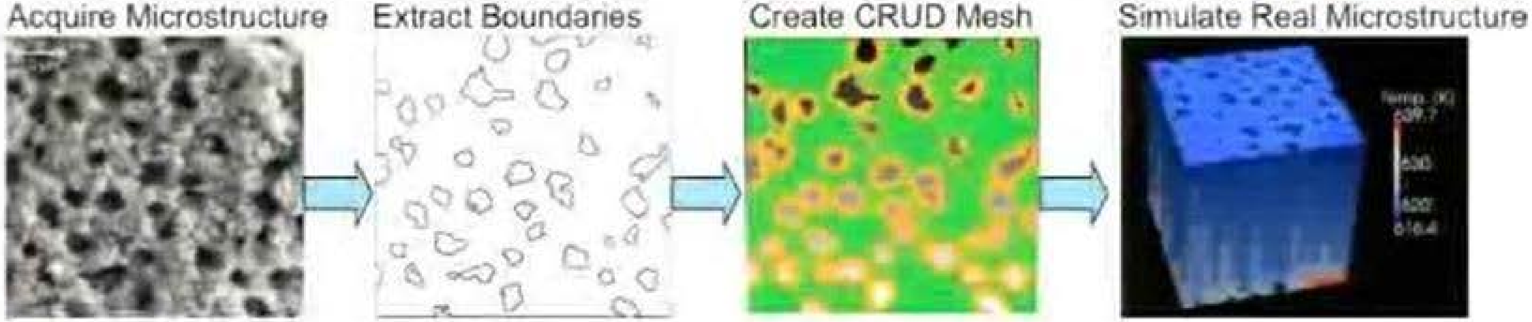
- Collaborators:

MAMBA-BDM (Michael Short (MIT) for CASL)

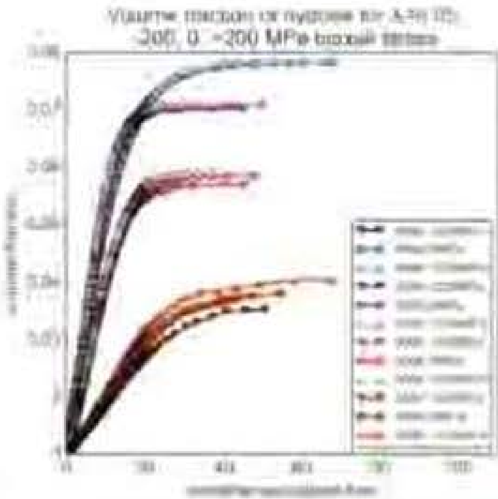


- *MAMBA-BDM*: 2D – 3D application describing CRUD growth in PWRs.
  - The CRUD model is treated as a chemical deposition process in an environment of coupled variable concentration, surface heat flux adjacent to clad, and a complex fractal-based flow geometry.
  - MAMBA-BDM operates on the micro-scale, and directly incorporates DFT-based atomistic-scale thermodynamic information on phase stability into its models, which are subsequently fed up to a related macro-scale framework (MAMBA).
  - Determines oxide deposition and boron concentrations to predict and help avoid CIPS and CILC.
  - Collaborators:

Los Alamos National Laboratory | MIT Massachusetts Institute of Technology | CASL



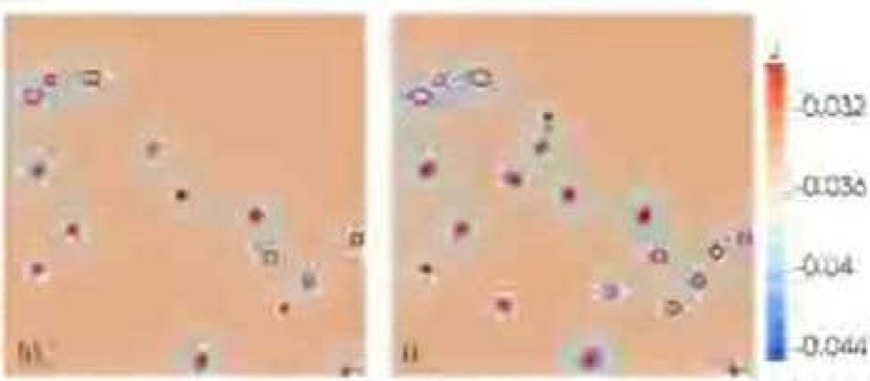
HYRAX
(Andrea Jokisari (Michigan) for CASL)



- *Hyrax:* **Multi-physics simulation of zirconium hydride precipitation and growth**
  - CALPHAD-based Phase Field model which captures realistic energetics and thermodynamics of the α-Zr / δ-hydrirde system
  - Linear Elastic Solid Mechanics model with partial crystal misfit relaxation to account for elastic and plastic effects
  - Classical Nucleation Theory-based explicit nucleation algorithm to capture hydride nucleation behavior
  - Collaborators:

CALPHAD-based energy description

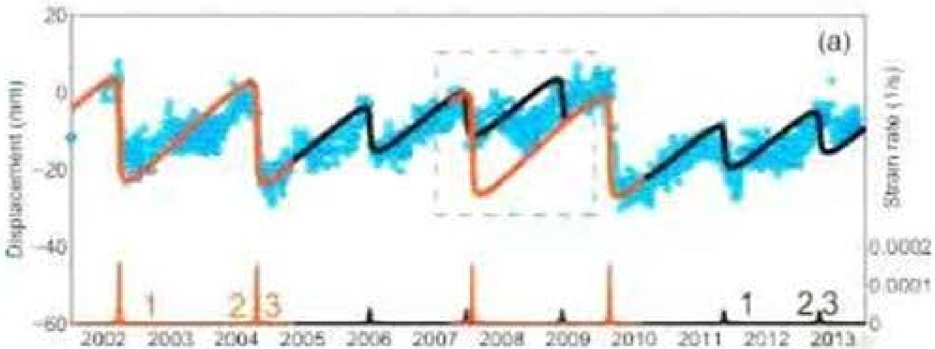
Predictive modeling of hydride microstructure evolution



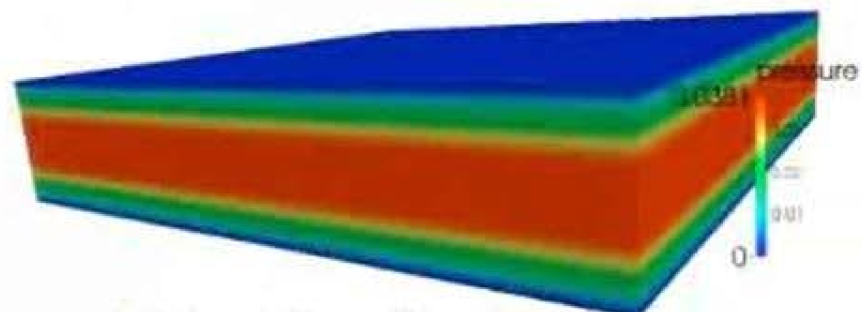
Nucleation of new hydrides

Redback (CSIRO Australia)

- ***Redback:* Capability that solves coupled thermo-mechanical-chemical system describing plate tectonics and earthquake onset with the eventual goal of predicting earthquakes.**
  - CSIRO is the Australian national science agency.
  - They're considering basing most of their scientific simulation capabilities on MOOSE.
  - To date they have developed two applications
    - Mining impact on ground water
    - Redback: Earthquake simulator



GPS Data (blue dots) superimposed by simulation predictions for Gisborne. New Zealand (from previous 1D code)



3D Simulation of localization zone between two plates from Redback

Poulet, T., M. Veveakis, K. Regenauer-Lieb, and D. A. Yuen (2014), Thermo-poro-mechanics of chemically active creeping faults: 3. The role of serpentinite in episodic tremor and slip sequences, and transition to chaos, J. Geophys. Res. Solid Earth, 119, 1–20, doi:10.1002/2014JB011004.

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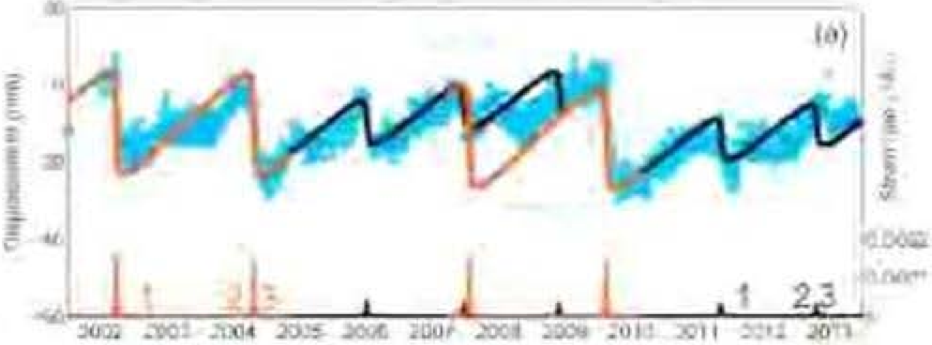

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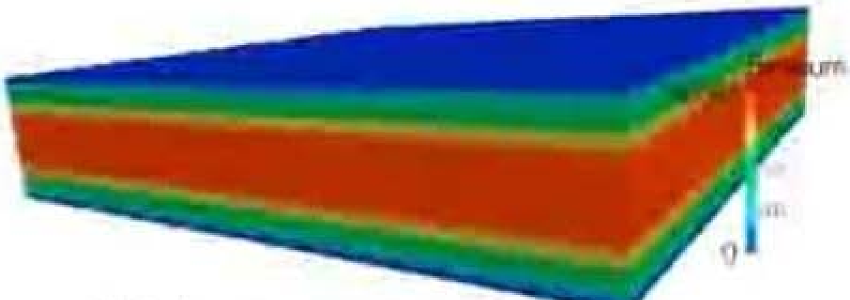

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Modeling of Coupled Diffusion and Mineral Precipitation in Porous Media with MOOSE-based Simulator RAT

$$(1)\quad \frac{\partial\left[\theta\left(C_{Ca^{2+}}+C_{CaCl^{+}}+C_{CaCl_2(aq)}+C_{CaOH^{+}}+C_{CaSO_4(aq)}+C_{CaSO_4(s)}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{Ca^{2+}}+C_{CaCl^{+}}+C_{CaCl_2(aq)}+C_{CaOH^{+}}+C_{CaSO_4(aq)}\right)\right]=0$$

$$(2)\quad \frac{\partial\left[\theta\left(C_{Cl^{-}}+C_{CaCl^{+}}+2C_{CaCl_2(aq)}+C_{HCl(aq)}+C_{NaCl(aq)}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{Cl^{-}}+C_{CaCl^{+}}+2C_{CaCl_2(aq)}+C_{HCl(aq)}+C_{NaCl(aq)}\right)\right]=0$$

$$(3)\quad \frac{\partial\left[\theta\left(C_{H^{+}}+2C_{H_2SO_4(aq)}+C_{HCl(aq)}+C_{HSO_4^{-}}-C_{CaOH^{+}}-C_{NaOH(aq)}-C_{OH^{-}}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{H^{+}}+2C_{H_2SO_4(aq)}+C_{HCl(aq)}+C_{HSO_4^{-}}-C_{CaOH^{+}}-C_{NaOH(aq)}-C_{OH^{-}}\right)\right]=0$$

$$(4)\quad \frac{\partial\left[\theta\left(C_{Na^{+}}+C_{NaCl(aq)}+C_{NaOH(aq)}+C_{NaSO_4^{-}}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{Na^{+}}+C_{NaCl(aq)}+C_{NaOH(aq)}+C_{NaSO_4^{-}}\right)\right]=0$$

$$(5)\quad \frac{\partial\left[\theta\left(C_{SO_4^{2-}}+C_{CaSO_4(aq)}+C_{H_2SO_4(aq)}+C_{HSO_4^{-}}+C_{NaSO_4^{-}}+C_{CaSO_4(s)}\right)\right]}{\partial t}-\nabla\left[\theta D\cdot\nabla\left(C_{SO_4^{2-}}+C_{CaSO_4(aq)}+C_{H_2SO_4(aq)}+C_{HSO_4^{-}}+C_{NaSO_4^{-}}\right)\right]=0$$

$$(6)\quad \frac{d\left(C_{CaSO_4(s)}\right)}{dt}-0.1\times 6.456542\times 10^{-8}\times\left(1-\frac{C_{Ca^{2+}}\cdot C_{SO_4^{2-}}}{10^{-1.8487}}\right)=0$$

$$(7)\quad C_{CaCl^{+}}-10^{-0.7}C_{Ca^{2+}}\cdot C_{Cl^{-}}=0$$

$$(8)\quad C_{CaCl_2(aq)}-10^{-0.653}C_{Ca^{2+}}\cdot\left(C_{Cl^{-}}\right)^{2}=0$$

$$(9)\quad C_{CaOH^{+}}-10^{-12.85}C_{Ca^{2+}}\cdot\left(C_{H^{+}}\right)^{-1}=0$$

$$(10)\quad C_{CaSO_4(aq)}-10^{2.3}C_{Ca^{2+}}\cdot C_{SO_4^{2-}}=0$$

$$(11)\quad C_{H_2SO_4(aq)}-10^{-1.021}\left(C_{H^{+}}\right)^{2}\cdot C_{SO_4^{2-}}=0$$

$$(12)\quad C_{HCl(aq)}-10^{6.1}C_{H^{+}}\cdot C_{Cl^{-}}=0$$

$$(13)\quad C_{HSO_4^{-}}-10^{1.979}C_{H^{+}}\cdot C_{SO_4^{2-}}=0$$

$$(14)\quad C_{NaCl(aq)}-10^{-0.782}C_{Na^{+}}\cdot C_{Cl^{-}}=0$$

$$(15)\quad C_{NaOH(aq)}-10^{-14.799}C_{Na^{+}}\cdot\left(C_{H^{+}}\right)^{-1}=0$$

$$(16)\quad C_{NaSO_4^{-}}-10^{0.82}C_{Na^{+}}\cdot C_{SO_4^{2-}}=0$$

$$(17)\quad C_{OH^{-}}-10^{-13.991}\left(C_{H^{+}}\right)^{-1}=0$$

Challenges:

- Both fast and slow kinetics
- Strongly coupled processes

Conventional Approach:

- Operator splitting

Our approach:

- Fully coupled, fully implicit
- Adaptive mesh refinement
- JFNK nonlinear solver

Free Workshops

- Three to four FREE workshops per year
- Next week: Berkeley!
  - mooseframework.org for more information
- Next one in late spring in Idaho

MOOSE Minis Tomorrow

MS259/MS284

Parallel, Multiscale, Multiphysics Simulation Using MOOSE

Room 250 C