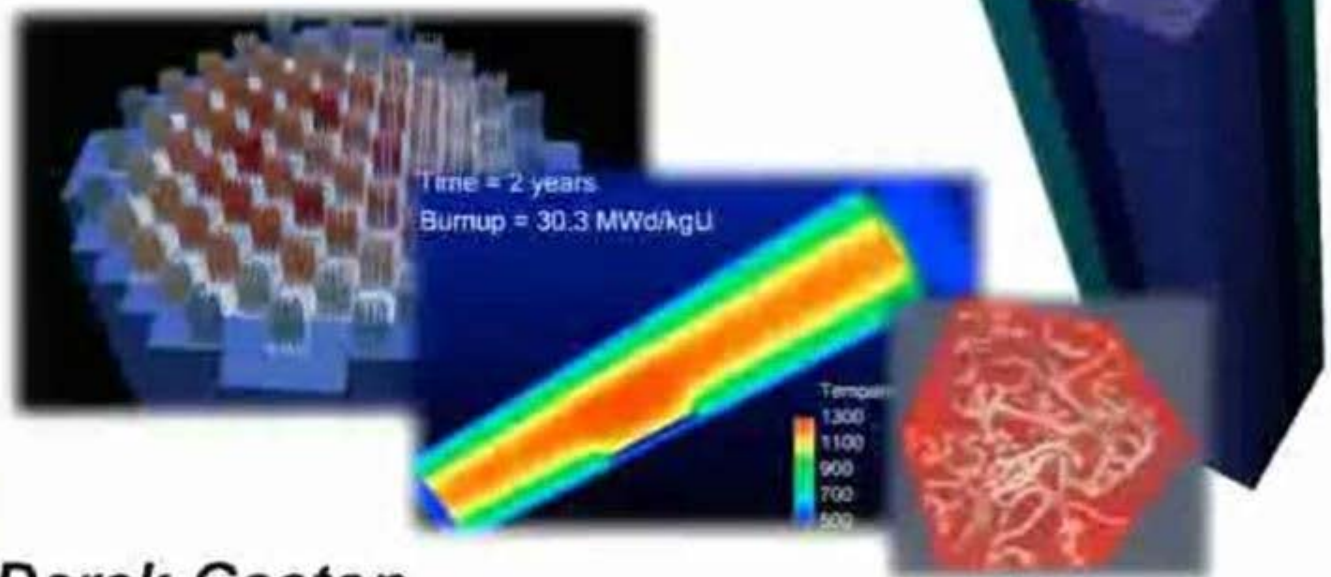


MOOSE: An Open Source Platform For Rapid Development of Multiphysics Simulation Tools

www.mooseframework.org

Derek Gaston



Derek Gaston

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

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

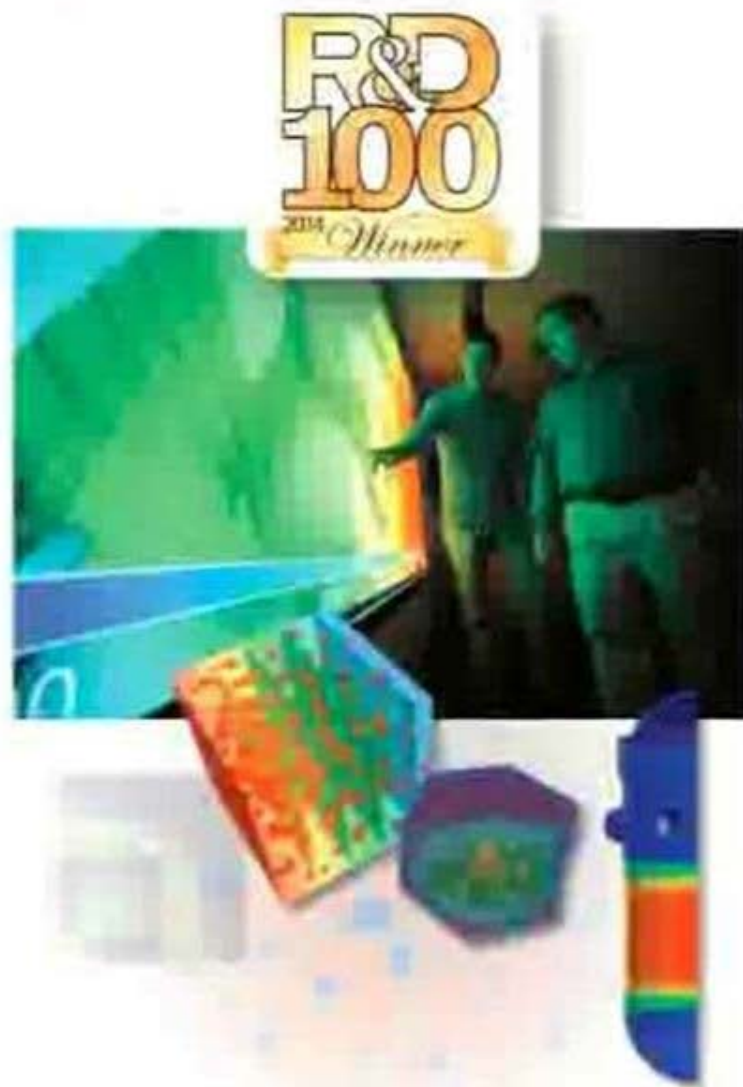
MOOSE Overview

www.inl.gov



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.



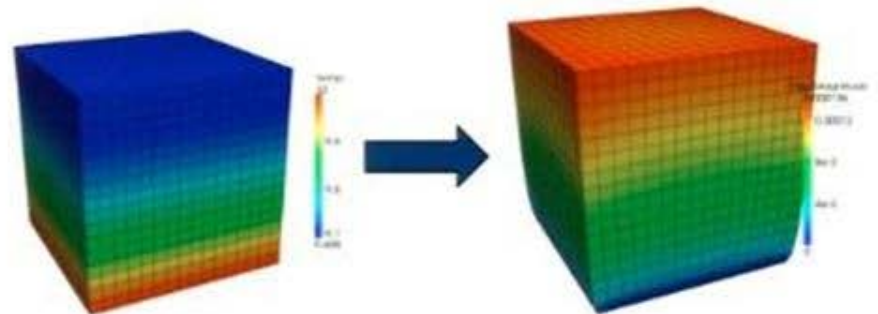
MOOSE Collaborators



Coupling

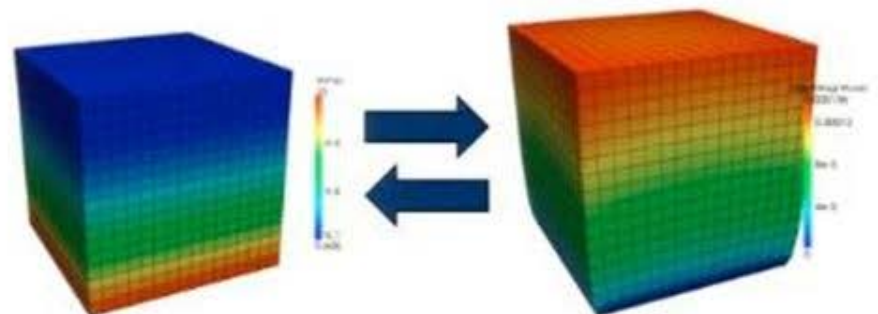
- Loose Coupling / Operator Split

1. Solve PDE1
2. Pass Data
3. Solve PDE2
4. Move To Next Timestep



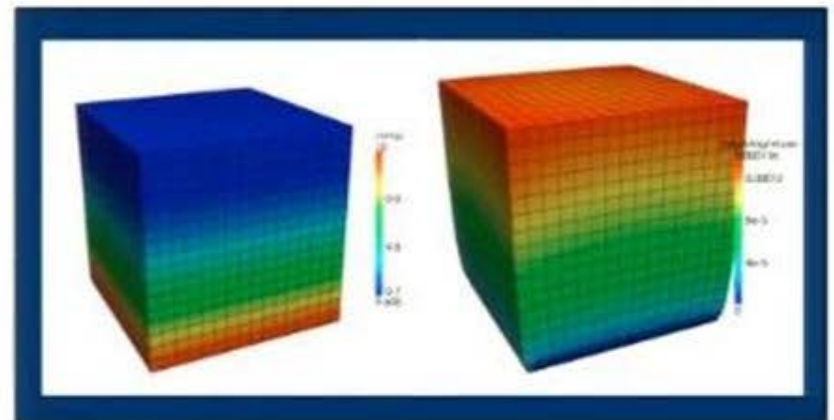
- Tight Coupling

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



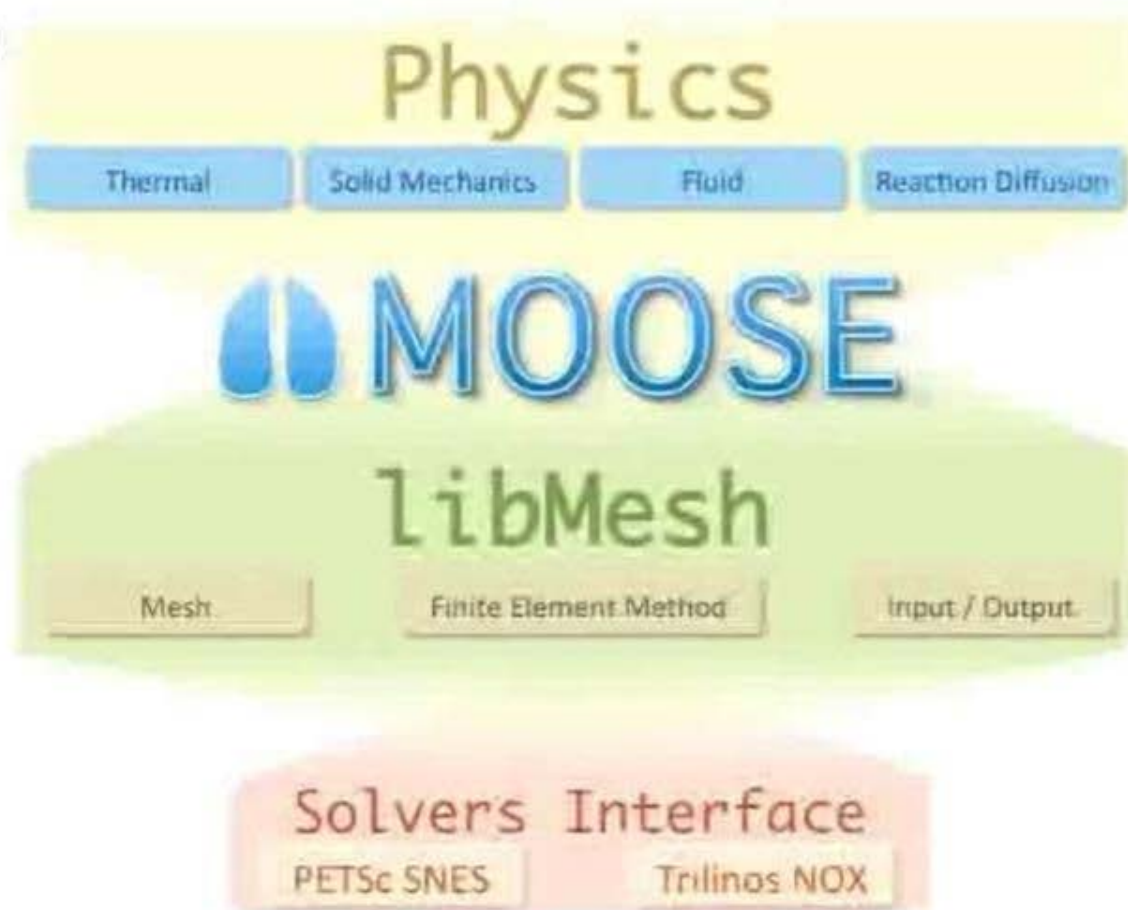
General Finite-Element Capabilities

- 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...

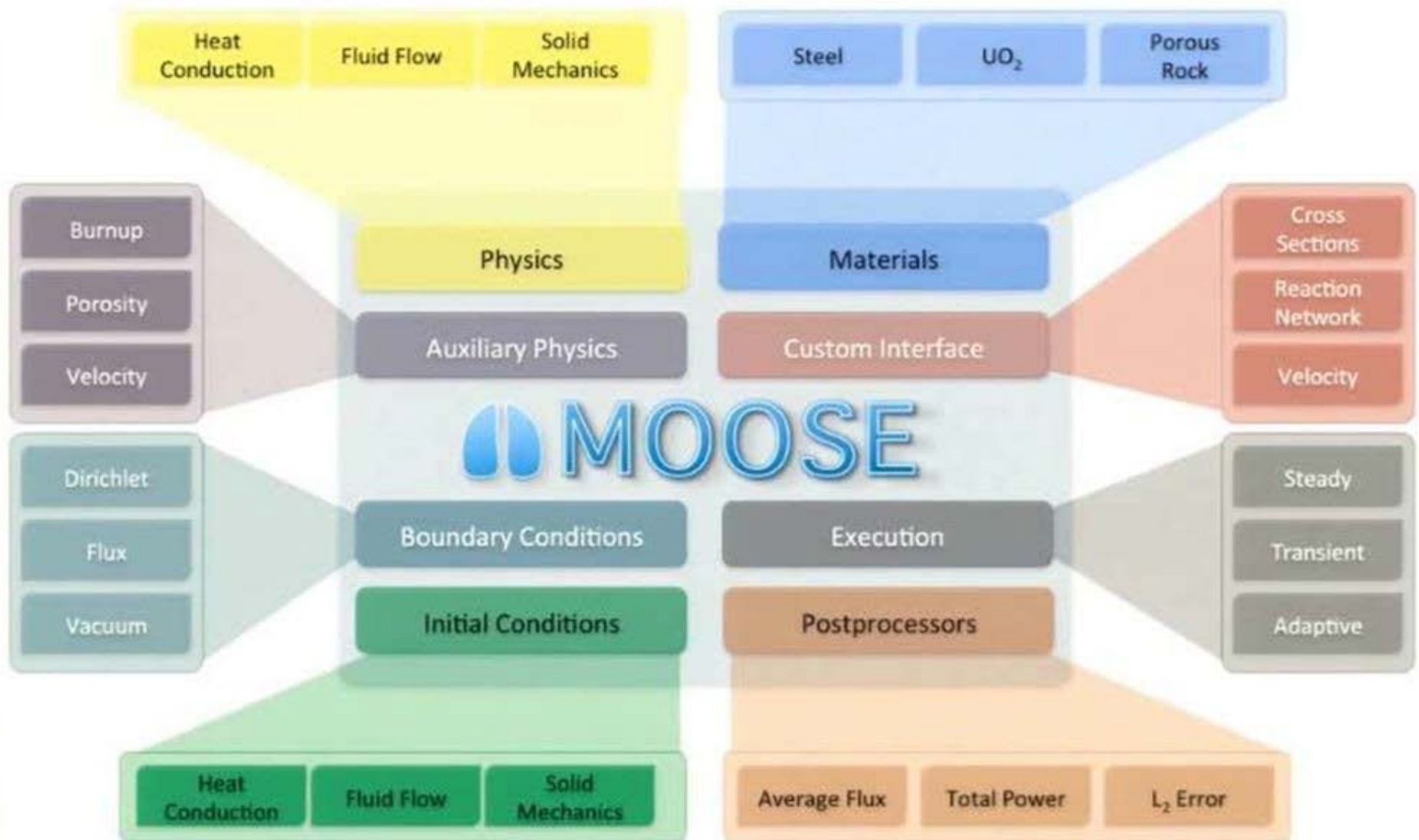
Code Platform

- 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



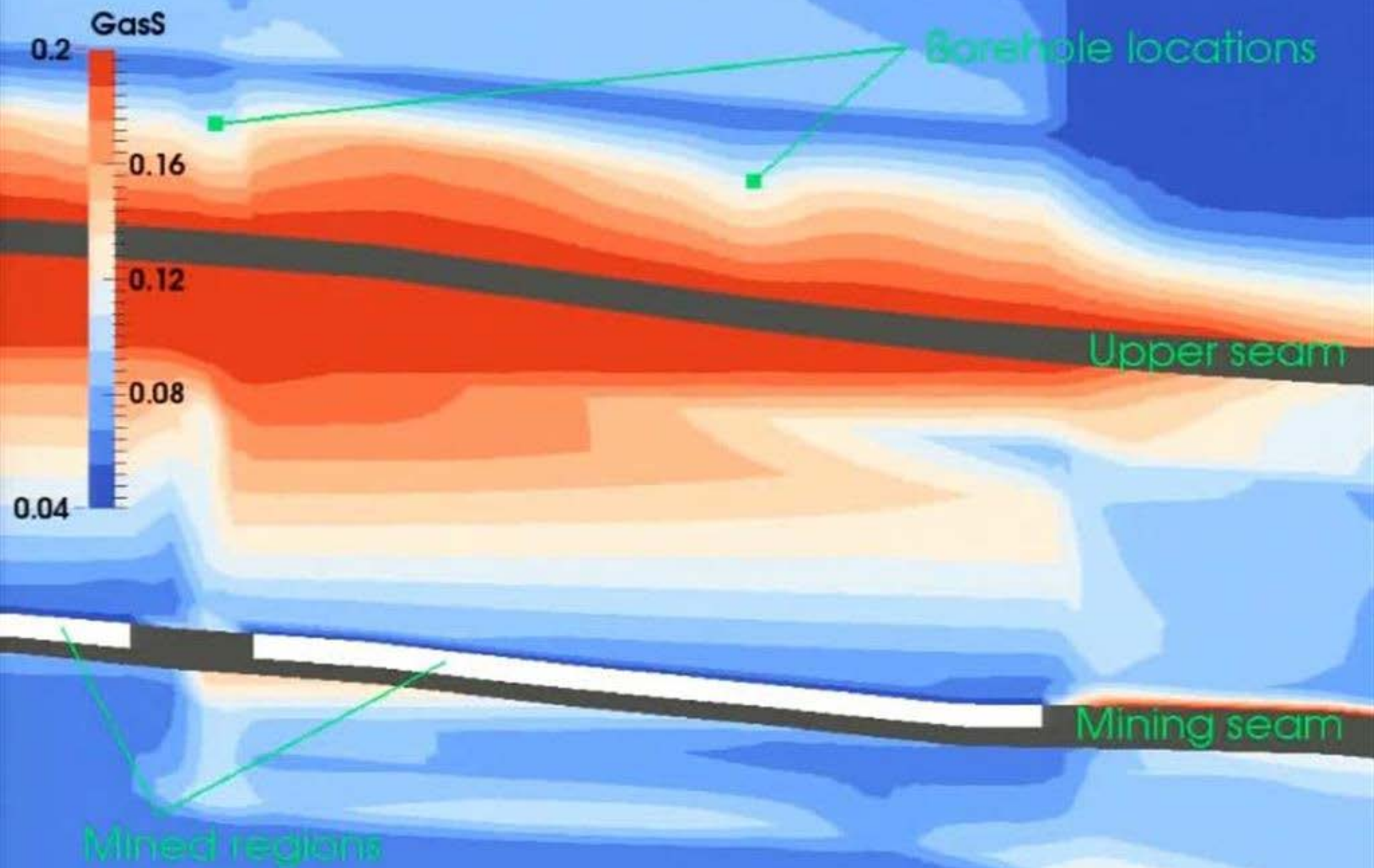
Flexible Interfaces For Customization

- Actions
- Auxiliary Kernels
- Auxiliary Variables
- BCs
- Constraints
- Dampers
- DGKernels
- Dirackernels
- Executioners
- Functions
- GeomSearch
- ICs
- Indicators
- Kernels
- Markers
- Materials
- Mesh
- MeshModifiers
- 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



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Ease Of Use

www.inl.gov

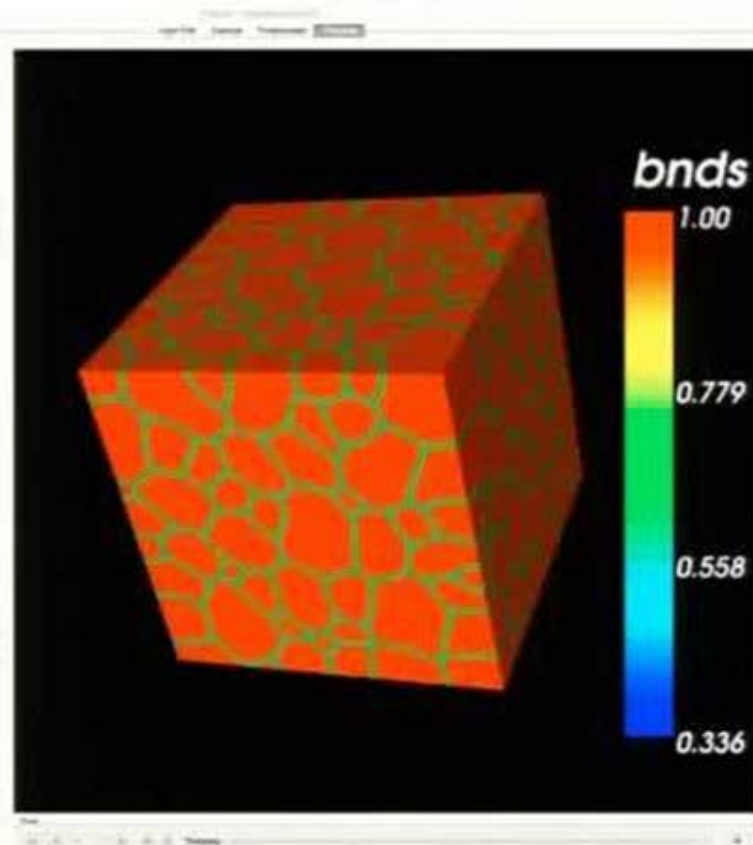
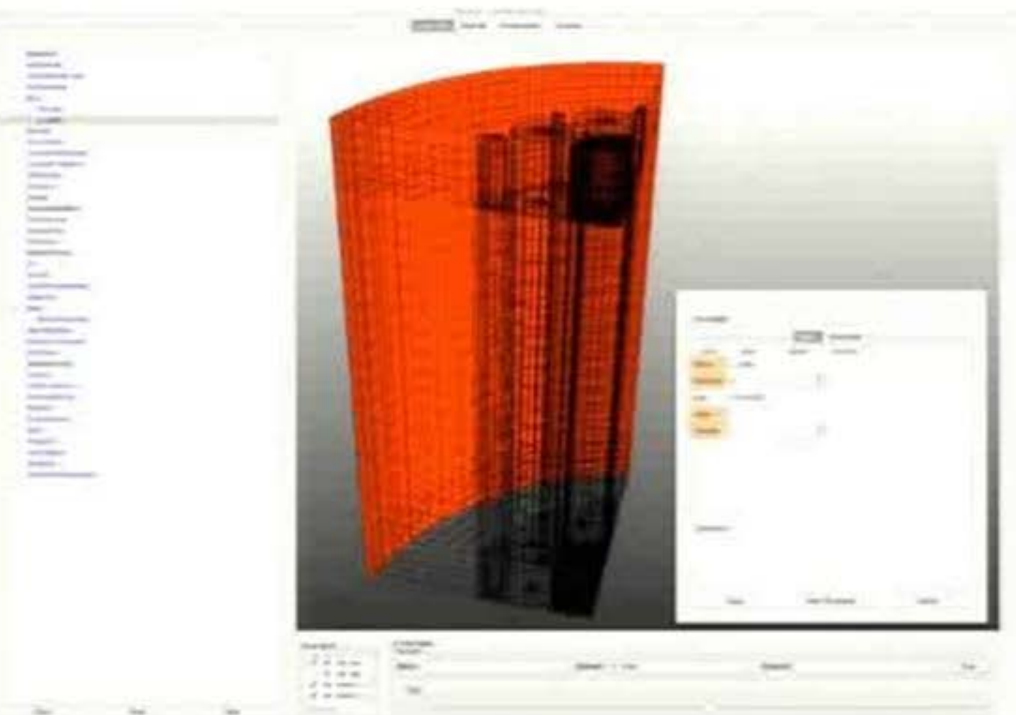


Simplified Installation

- 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)



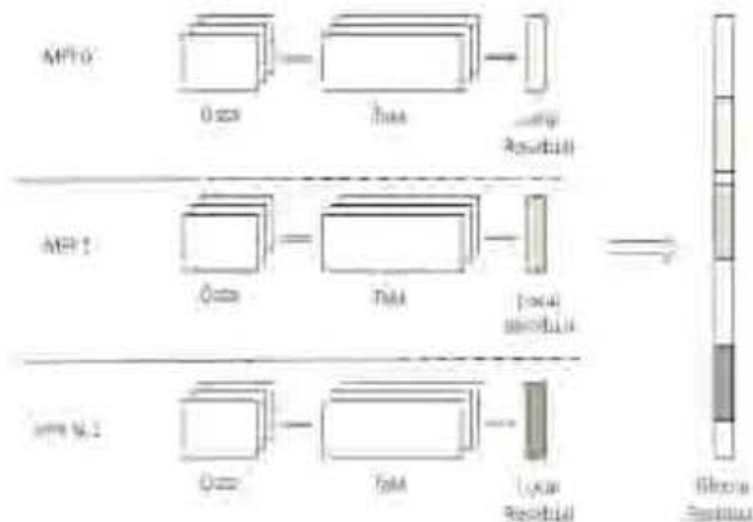
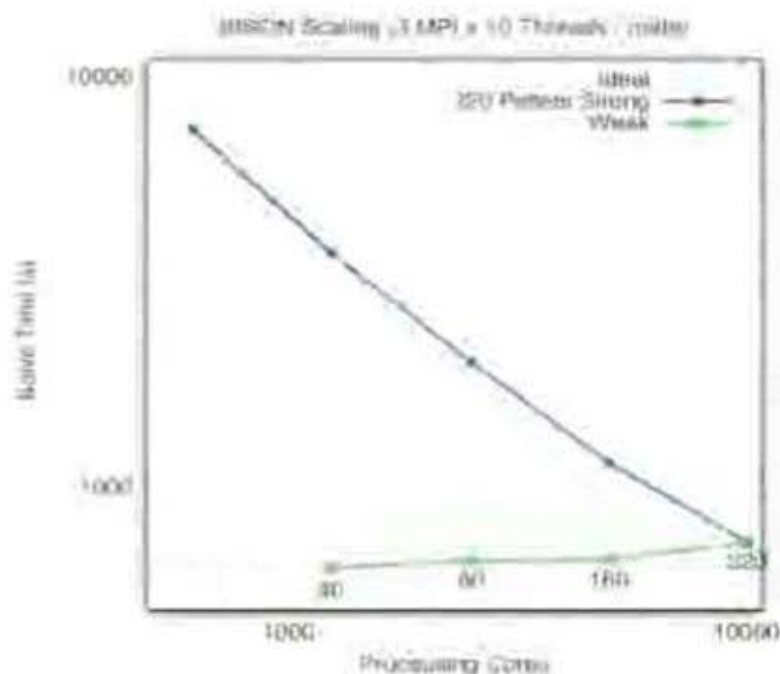
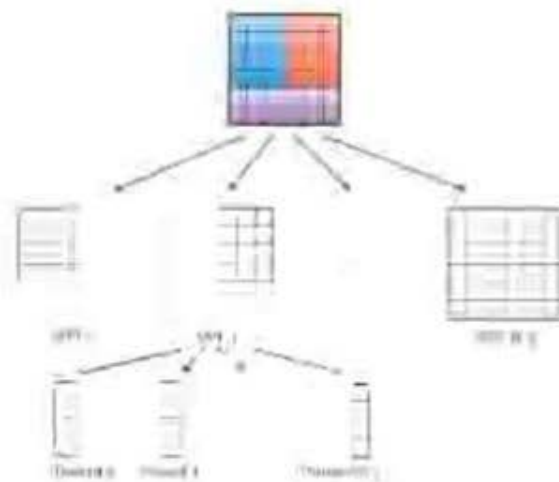
Parallel Capability

www.inl.gov



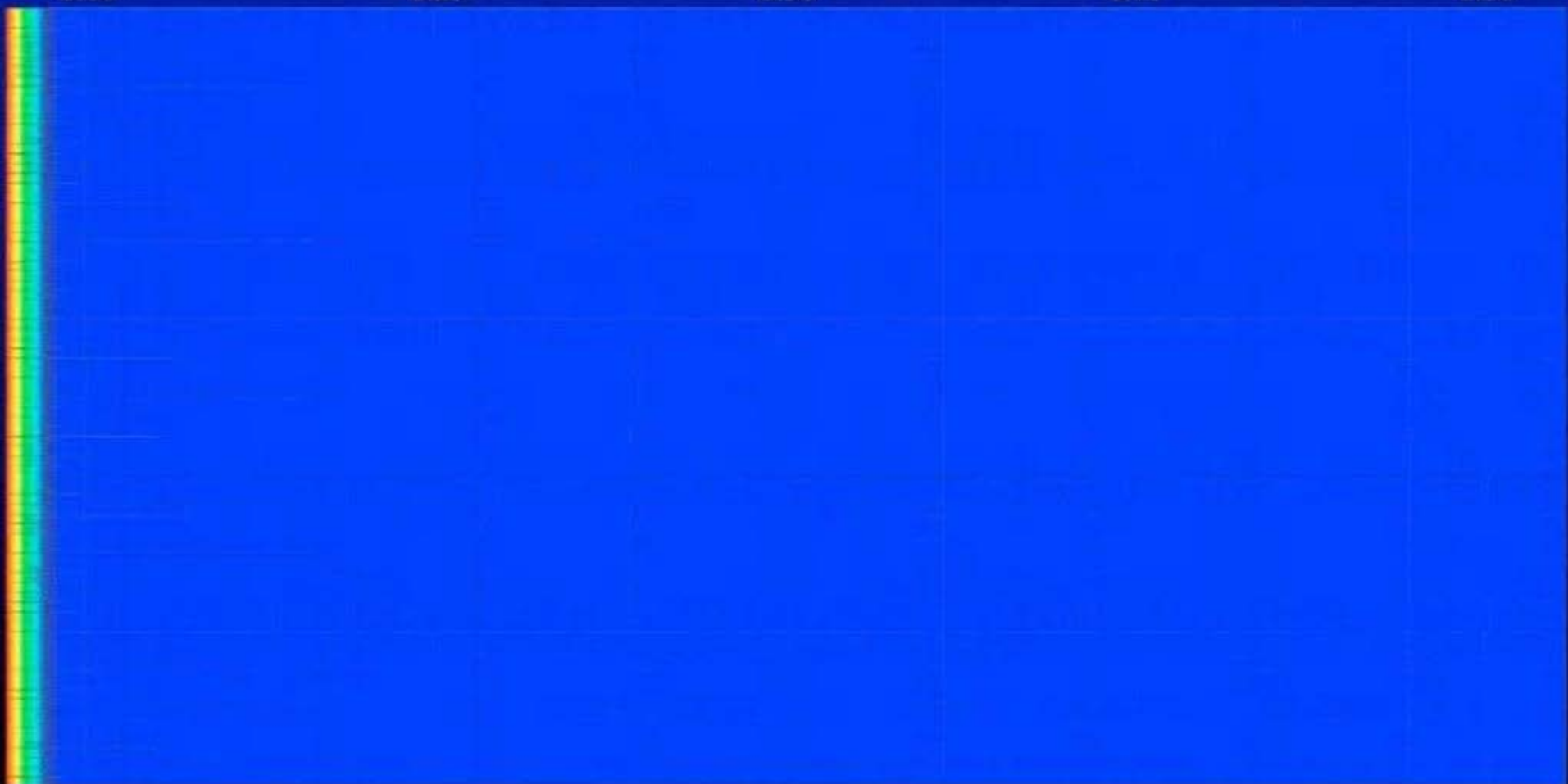
Parallel Work Distribution

- 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



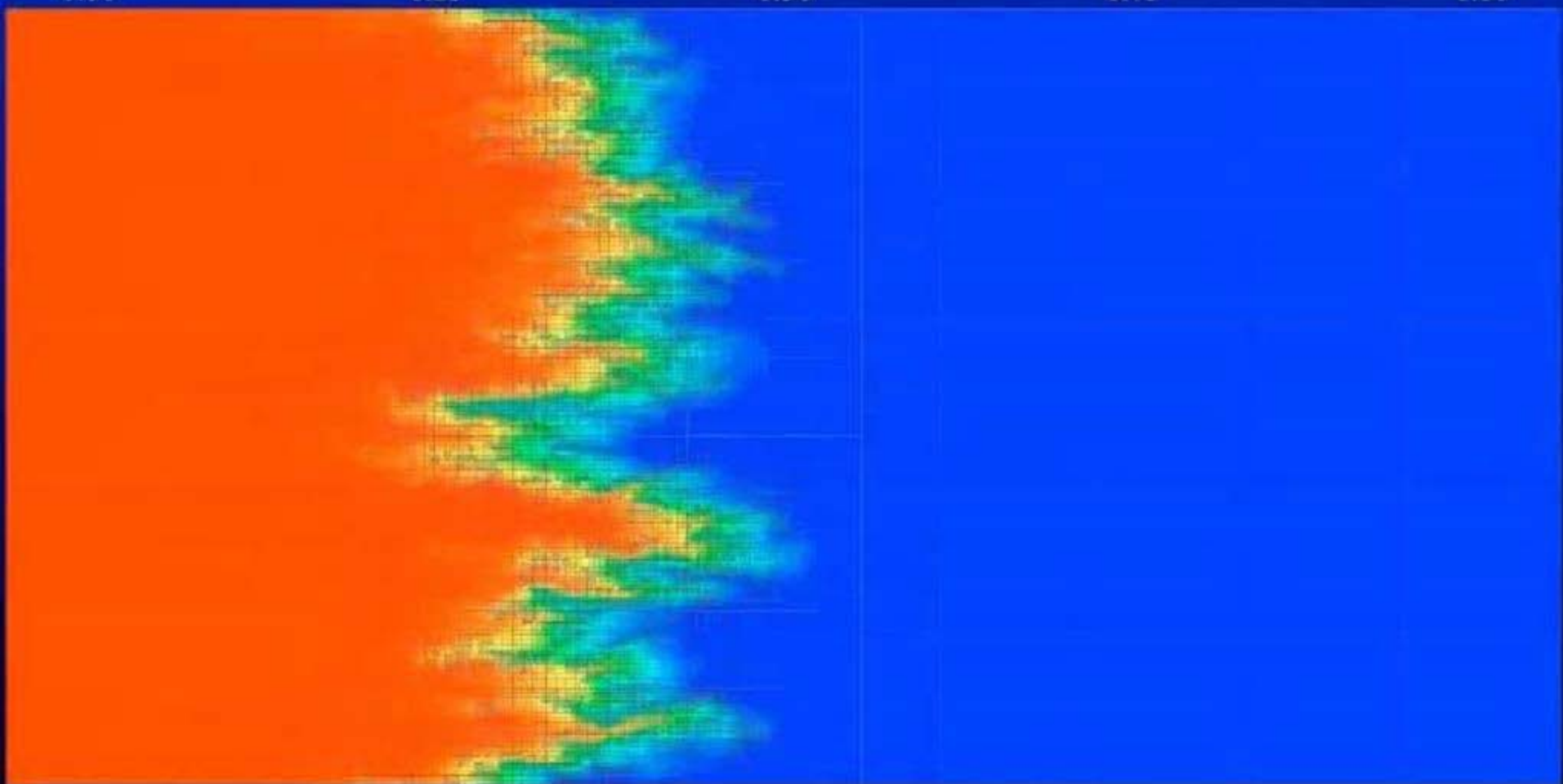
All Features Implicitly Parallel

Time = 0.00 s



All Features Implicitly Parallel

Time = 6.44 s

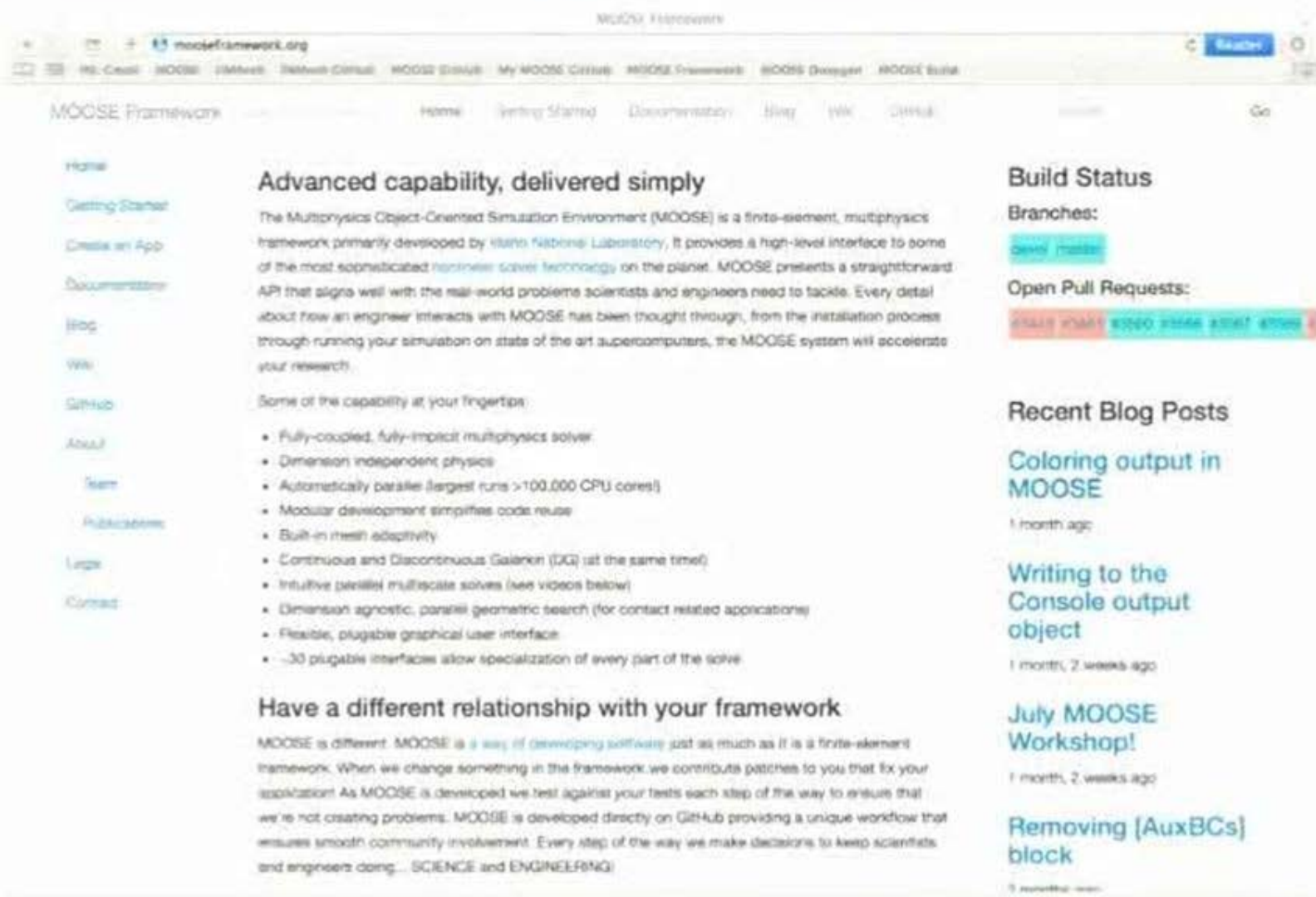


Community

www.inl.gov



MooseFramework.org



The screenshot shows the homepage of the MooseFramework.org website. The browser address bar shows 'mooseframework.org'. The navigation menu includes 'Home', 'Getting Started', 'Documentation', 'Blog', 'Wiki', and 'Contact'. A sidebar on the left lists various sections like 'Home', 'Getting Started', 'Create an App', 'Documentation', 'Blog', 'Wiki', 'Github', 'About', 'Team', 'Publications', 'Legal', and 'Contact'. The main content area features a heading 'Advanced capability, delivered simply' followed by a paragraph describing MOOSE as a finite-element, multiphysics framework. Below this is a list of capabilities such as 'Fully-coupled, fully-implicit multiphysics solver' and 'Dimension independent physics'. A section titled 'Have a different relationship with your framework' explains the development workflow. On the right, there are three sections: 'Build Status' showing 'Build Status' and 'Open Pull Requests', 'Recent Blog Posts' with titles like 'Coloring output in MOOSE' and 'Writing to the Console output object', and 'July MOOSE Workshop!'.

Advanced capability, delivered simply

The Multiphysics Object-Oriented Simulation Environment (MOOSE) is a finite-element, multiphysics framework primarily developed by Idaho National Laboratory. It provides a high-level interface to some of the most sophisticated *business solver technology* on the planet. MOOSE presents a straightforward API that signs well with the real-world problems scientists and engineers need to tackle. Every detail about how an engineer interacts with MOOSE has been thought through, from the installation process through running your simulation on state of the art supercomputers, the MOOSE system will accelerate your research.

Some of the capability at your fingertips:

- Fully-coupled, fully-implicit multiphysics solver
- Dimension independent physics
- Automatically parallel (largest runs >100,000 CPU cores)
- Modular development simplifies code reuse
- Built-in mesh adaptivity
- Continuous and Discontinuous Galerkin (DG) (at the same time!)
- Intuitive (parallel) multiscale solves (see videos below)
- Dimension agnostic, parallel geometric search (for contact related applications)
- Flexible, plugable graphical user interface
- ~30 plugable interfaces allow specialization of every part of the solve

Have a different relationship with your framework

MOOSE is different. MOOSE is a way of developing software just as much as it is a finite-element framework. When we change something in the framework we contribute patches to you that fix your application. As MOOSE is developed we test against your tests each step of the way to ensure that we're not creating problems. MOOSE is developed directly on Github providing a unique workflow that ensures smooth community involvement. Every step of the way we make decisions to keep scientists and engineers doing... SCIENCE and ENGINEERING!

Build Status

Branches:

Build Status

Open Pull Requests:

Build Status

Recent Blog Posts

Coloring output in MOOSE

1 month ago

Writing to the Console output object

1 month, 2 weeks ago

July MOOSE Workshop!

1 month, 2 weeks ago

Removing [AuxBCs] block

1 month, 2 weeks ago

Active Mailing List

Google

www.google.com



+Data



Groups

NEW TOPIC



Mark all as read

Actions

Filters

20

Settings

moose-users Shared publicly

30 of 554 topics (99+ unread)

Manage Members About

This group is for users of the MOOSE framework (Multiphysics Object Oriented Simulator Environment) to ask questions, discuss the project, and to participate in collaborative efforts. See <http://www.mooseframework.com> for more information.

Edit welcome message Clear welcome message

- Error in MultiPhase Example (4)**
 By SudiptaBiswas · 4 posts · 4 views
 0:24 AM
- elastic wave equation (0)**
 By sikal · 0 posts · 0 views
 1:48 PM
- Random Number generation for Kernel (4)**
 By SudiptaBiswas · 4 posts · 2 views
 1:48 PM
- UserObject variables get erased at each step? (4)**
 By xelchao87 · 4 posts · 2 views
 1:48 PM
- Boundary AuxKernel (11)**
 By karpenev · 11 posts · 7 views
 1:48 PM
- Error in Coupleable.C (old and older values) (6)**
 By john.m..@uconn.edu · 6 posts · 2 views
 1:48 PM
- specifying start_time (or time) in Steady calculations (2)**
 By andrew.wilkins · 2 posts · 2 views
 1:48 PM
- Output in csv format (19)**
 By Muelo Perera de Almeida · 19 posts · 20 views
 1:48 PM
- Problem with ni_ref_tol (11)**
 By petar.chakraborty · 11 posts · 4 views
 1:48 PM
- Postdoc position available (1)**
 By karpenev · 1 post · 0 views
 1:48 PM
- AuxVariables and Materials and DiracKernels (6)**
 By andrew.wilkins · 6 posts · 0 views
 1:48 PM

Active Mailing List

Google

Groups



+ Derek



Groups

NEW TOPIC



Mark all as read

Actions

Filters



moose-users Shared publicly

30 of 554 topics (99+ unread)

Manage · Members · About

This group is for users of the MOOSE framework (Multiphysics Object Oriented Simulation Environment) to ask questions, discuss the project, and to participate in collaborative efforts. See h

Edit w

319 Members In The First Year

elastic wave equation (0)

By xikai · 0 posts · 12 views

Random Number generation for Kernel (4)

By SudiptaBiswas · 4 posts · 3 views

UserObject variables get erased at each step? (4)

By leichao087 · 4 posts · 2 views

Boundary AuxKernel (11)

By karpov · 11 posts · 7 views

Error in Coupleable C (old and older values) (0)

By john.m. @ucornc.edu · 0 posts · 2 views

specifying start_time (or time) in Steady calculations (2)

By andrew.wilkins · 2 posts · 10 views

Output in csv format (10)

By Muelo Pereira de Almeida · 10 posts · 21 views

Problem with nl_nu_tol (11)

By pritam.chakraborty · 11 posts · 8 views

Postdoc position available (1)

By karpov · 1 post · 0 views

AuxVariables and Materials and DiracKernels (5)




By andrew.wilkins · 5 posts · 0 views

Active Developer Community

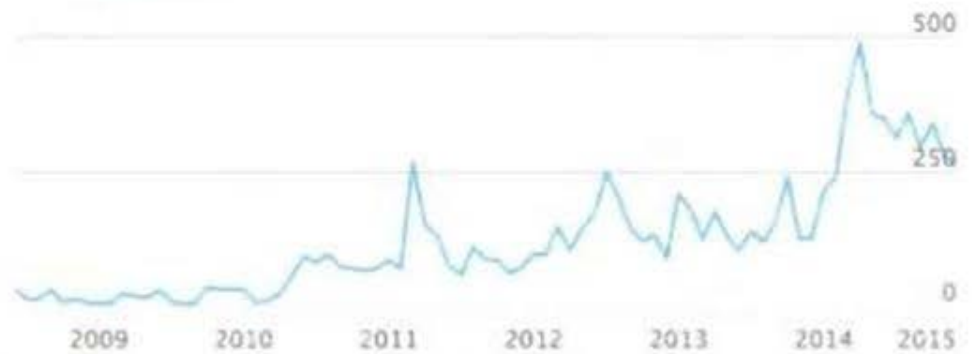
 idaholab / **moose**

 Unwatch ▾ 33  Unstar 73  Fork 119

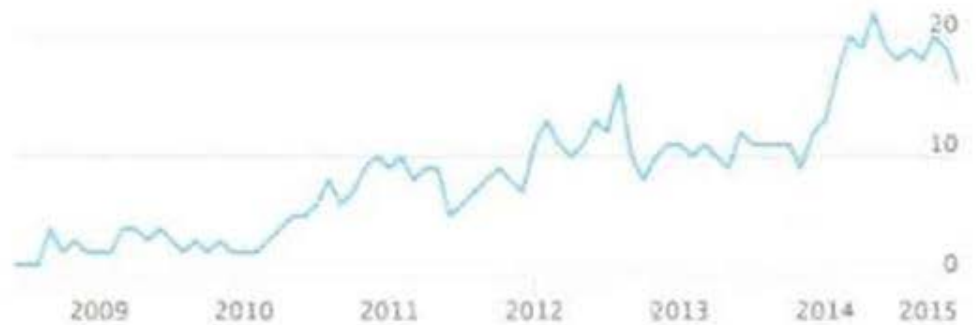
 idaholab / **stork**

 Unwatch ▾ 13  Star 4  Fork 103

Commits per Month



Contributors per Month



Automated Contributor Feedback

Augmented EquationSystems reinit #4727

 **roystgr** wants to merge 1 commit into `idaho:dev` from `roystgr:augmented_es_reinit`

 Conversation 12  Commits 1  Files changed 1



roystgr 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 [7866a44](#) 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 [6868f9f](#) using `moose_PR_pre_check` recipe:

Passed on: linux-gnu

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

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

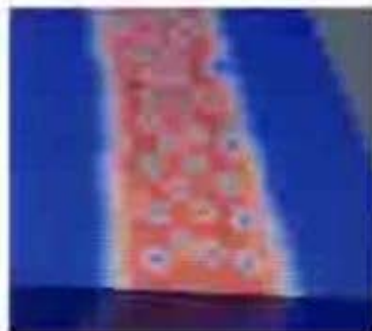
www.inl.gov



Condor (Argonne National Laboratory)

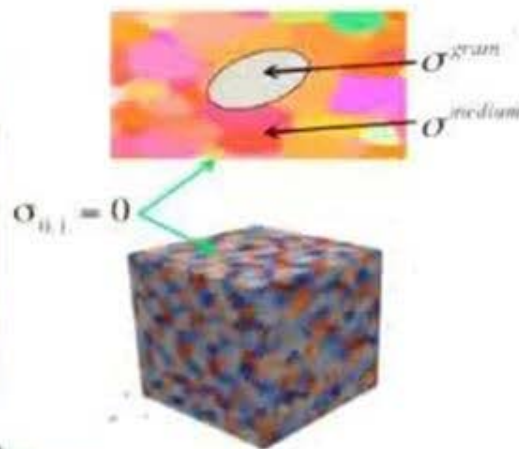


- *Condor* (SciDAC): Simulates the behavior of super-conducting materials with inclusions (e.g., particles, columnar defects) with the goal of finding the optimal inclusion geometries that result in the highest efficiency of the superconductor.
 - The model is a coupled system of PDEs – complex variable 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)

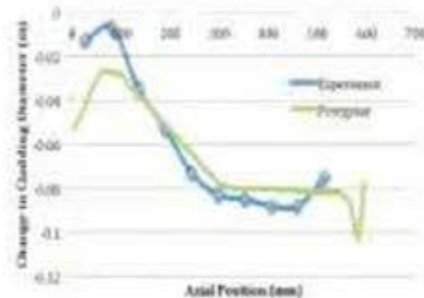
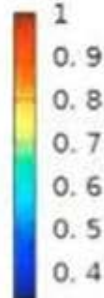
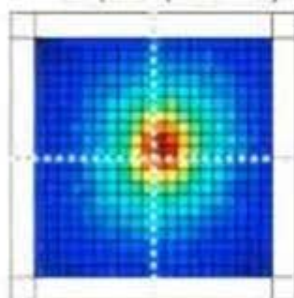


Vulture: Multi-scale simulation of nuclear fuel cladding deformation and failure

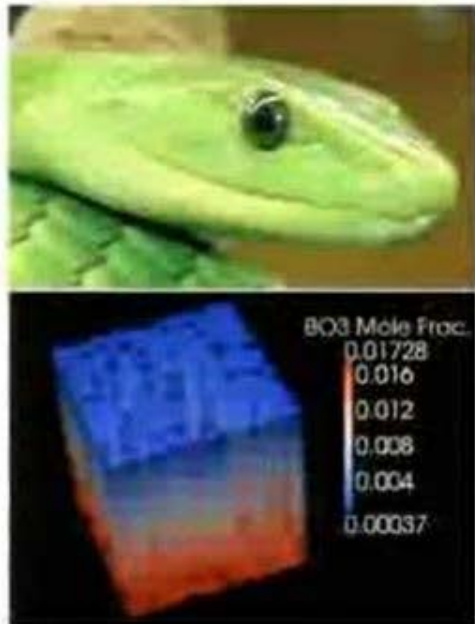
- Visco Plastic Self Consistent (VPSC) model, which accounts for crystallographic mechanisms, interactions between grains and coupling between growth and creep (radiation and thermal).
- Improved models for clad deformation required for PCI and safety assessments.
- Atomistic simulation for defect behavior, 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:

Capture probability



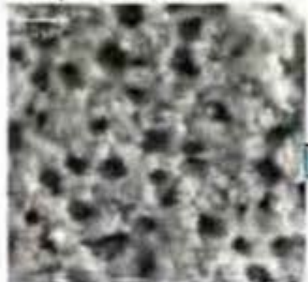
MAMBA-BDM (Michael Short (MIT) for CASL)



- **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:



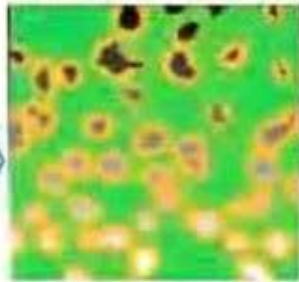
Acquire Microstructure



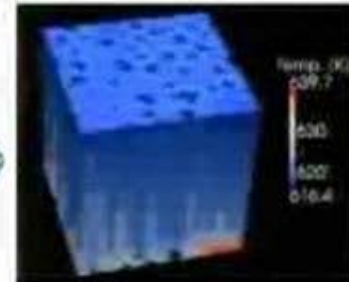
Extract Boundaries



Create CRUD Mesh

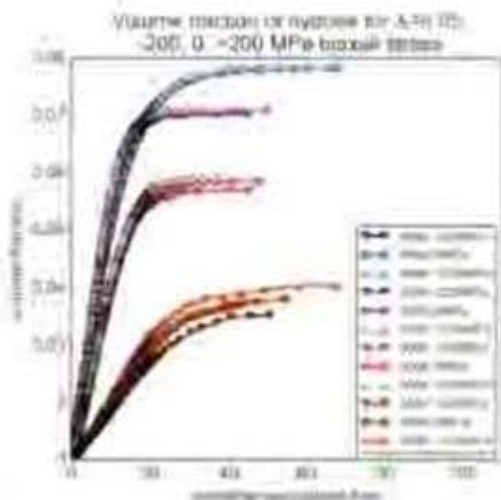


Simulate Real Microstructure



HYRAX

(Andrea Jokisari (Michigan) for CASL)



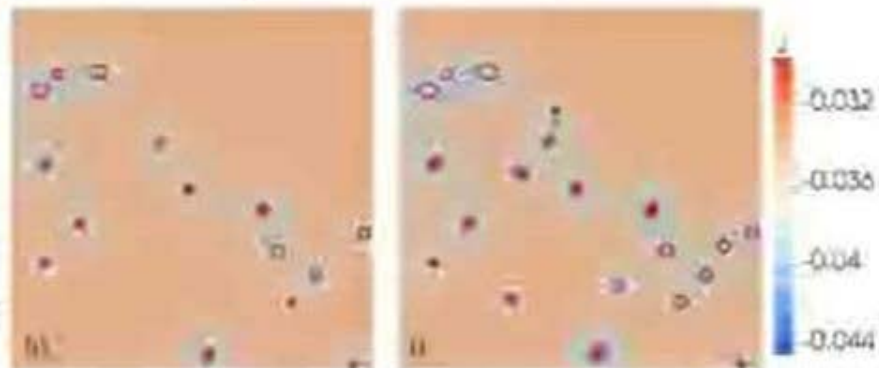
■ Hyrax: Multi-physics simulation of zirconium hydride precipitation and growth

- CALPHAD-based Phase Field model which captures realistic energetics and thermodynamics of the α -Zr / δ -hydride 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:

Predictive modeling of hydride microstructure evolution

CALPHAD-based energy description

Nucleation of new hydrides

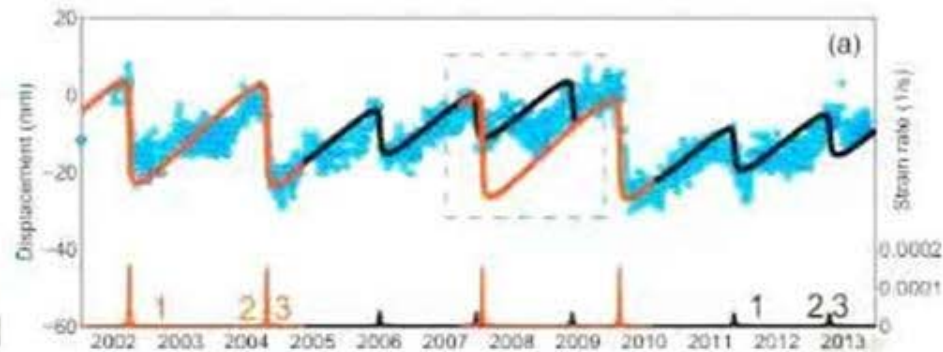


Redback (CSIRO Australia)

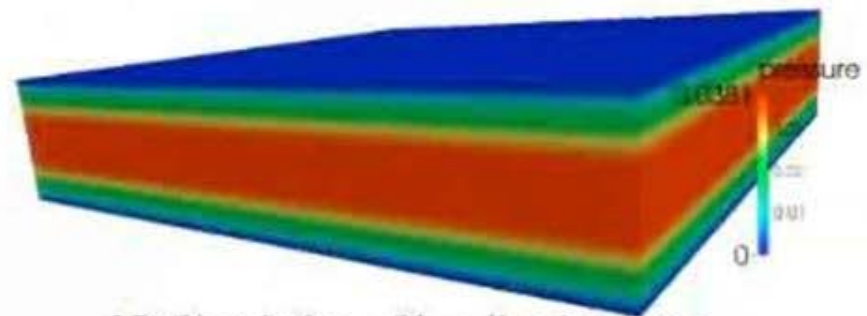


■ **Redback:** Capability that solves coupled thermo-mechanical-chemical system describing plate tectonics and earthquake onset with the eventual goal of predicting earthquakes.

- 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 ID code)



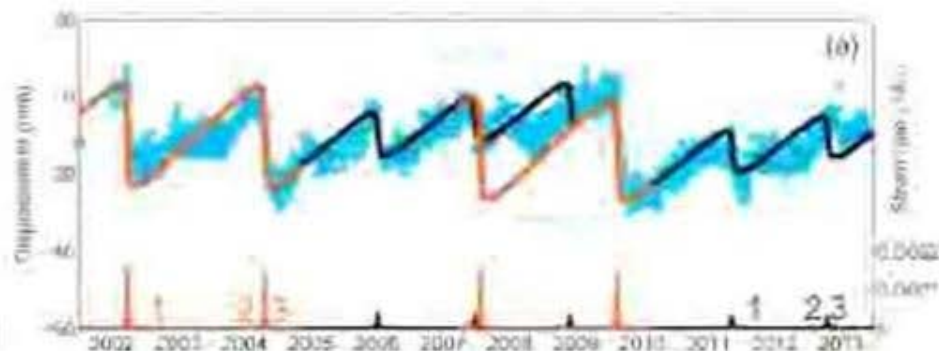
3D Simulation of localization zone between two plates from Redback

Redback (CSIRO Australia)

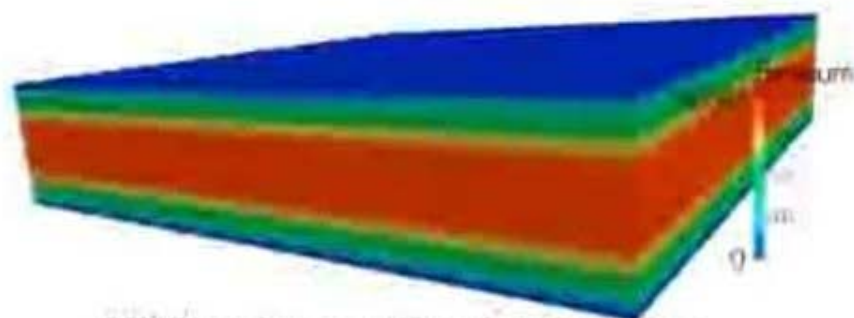


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GPS Data (blue dots) superimposed by simulation predictions for Gisborne, New Zealand (from previous ID code)



3D Simulation of localization zone between two plates from Redback.

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

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

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

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

$$(4) \frac{\partial [\theta (C_{Na^+} + C_{NaCl(aq)} + C_{NaOH(aq)} + C_{Na_2SO_4})]}{\partial t} - \nabla [\theta D \cdot \nabla (C_{Na^+} + C_{NaCl(aq)} + C_{NaOH(aq)} + C_{Na_2SO_4})] = 0$$

$$(5) \frac{\partial [\theta (C_{SO_4^{2-}} + C_{CaSO_4(aq)} + C_{H_2SO_4(aq)} + C_{H_2SO_4} + C_{Na_2SO_4} + C_{CaSO_4(s)})]}{\partial t} - \nabla [\theta D \cdot \nabla (C_{SO_4^{2-}} + C_{CaSO_4(aq)} + C_{H_2SO_4(aq)} + C_{H_2SO_4} + C_{Na_2SO_4})] = 0$$

$$(6) \frac{d(C_{CaSO_4(s)})}{dt} - 0.1 \times 6.456542 \times 10^{-8} \times \left(1 - \frac{C_{Ca^{2+}} \cdot C_{SO_4^{2-}}}{10^{-13.487}} \right) = 0$$

$$(7) C_{CaCl_2} - 10^{-6.7} C_{Ca^{2+}} \cdot C_{Cl^-} = 0$$

$$(8) C_{CaCl_2(aq)} - 10^{-6.655} C_{Ca^{2+}} \cdot (C_{Cl^-})^2 = 0$$

$$(9) C_{CaOH} - 10^{-12.55} C_{Ca^{2+}} \cdot (C_{H^+})^2 = 0$$

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

$$(11) C_{H_2SO_4(aq)} - 10^{-1.121} (C_{H^+})^2 \cdot C_{SO_4^{2-}} = 0$$

$$(12) C_{HCl(aq)} - 10^{0.3} C_{H^+} \cdot C_{Cl^-} = 0$$

$$(13) C_{H_2SO_4} - 10^{1.976} C_{H^+} \cdot C_{SO_4^{2-}} = 0$$

$$(14) C_{NaCl(aq)} - 10^{-6.782} C_{Na^+} \cdot C_{Cl^-} = 0$$

$$(15) C_{NaOH(aq)} - 10^{-14.799} C_{Na^+} \cdot (C_{OH^-})^2 = 0$$

$$(16) C_{Na_2SO_4} - 10^{0.92} C_{Na^+} \cdot C_{SO_4^{2-}} = 0$$

$$(17) C_{OH^-} - 10^{-13.994} (C_{H^+})^2 = 0$$

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