MOOSE

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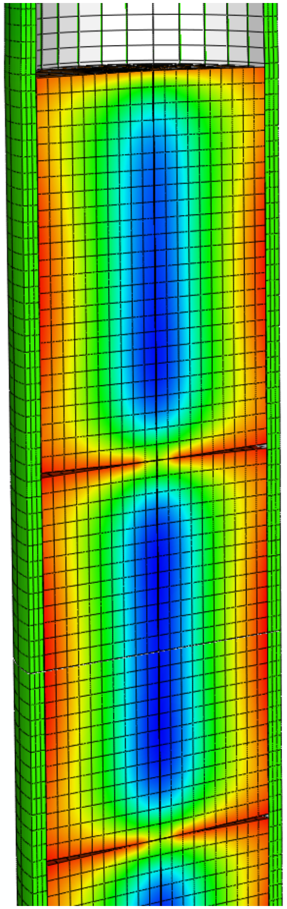
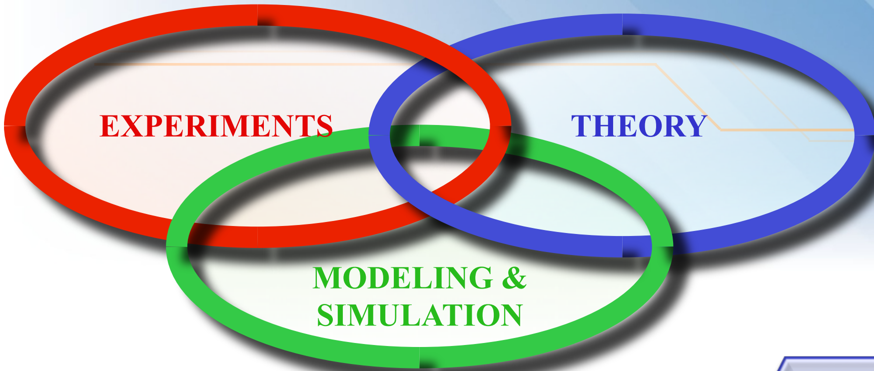
MOOSE – Multiphysics Object Oriented Simulation Environment



- A framework for solving computational nuclear engineering problems in a well planned, managed, and coordinated way
  - *Leveraged across multiple programs*
- Designed to significantly reduce the expense and time required to develop new applications
- Designed to develop analysis tools
  - *Uses very robust solution methods*
  - *Designed to be easily extended and maintained*
  - *Efficient on both a few and many processors*
- Currently supports ~7 applications which are developed and used by ~20 scientists.



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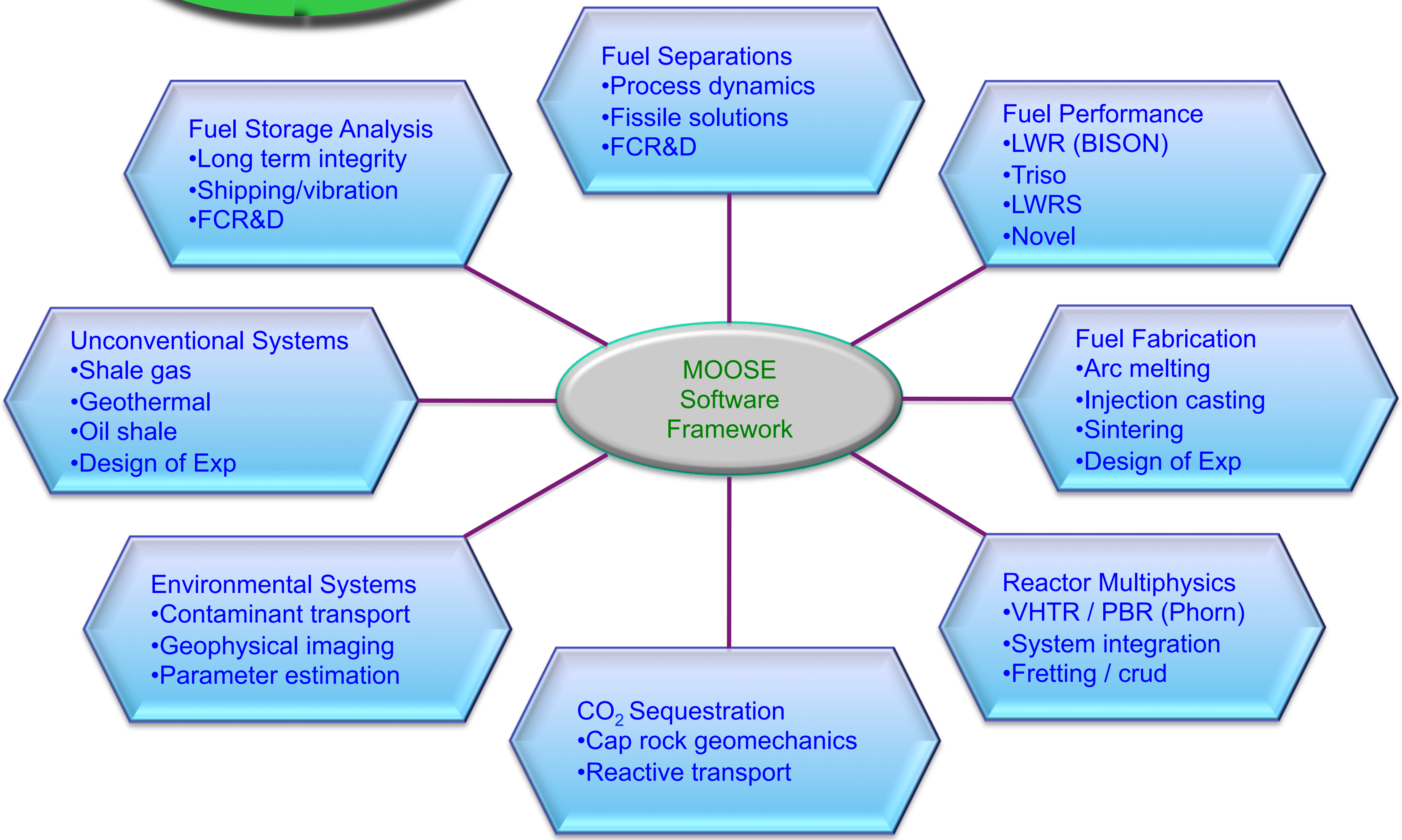


MOOSE Ecosystem

Application	Physics	Start	Time To Results	Lines of Code
BISON	Thermo-mechanics, Chemical Diffusion, coupled mesoscale	June 2008	4 Months	931
PRONGHORN	Neutronics, Porous Flow, Eigenvalue	September 2008	3 Months	2,883
SALMON	Multiphase Porous Flow	June 2009	3 Months	800
MARMOT	4th Order Phasefield Mesoscale	August 2009	1 Month	838
RAT	Porous ReActive Transport	August 2009	1 Month	439
FALCON	Geo-mechanics, coupled mesoscale	September 2009	3 Months	810

The Jacobian-free Newton Krylov method

- Extremely robust solution method for stiff, highly nonlinear, and tightly coupled problems
  - Provides the convergence of Newton's method without the need to form a Jacobian (saves time and memory)
  - Directly supports advanced preconditioning strategies (physics-based and multilevel)
  - Implicit method is unconditionally stable
- Residual function abstraction provides a very clean software design pattern

$$\sum_{j=1}^{n} (u_j)_t \,(\phi_j, \phi_i) + u_j (k \nabla \phi_j, \nabla \phi_i) - (q, \phi_i) - \langle g, \phi_i \rangle = 0$$

$$\mathbf{u} = [u_1, \ldots, u_n]^T$$

$$\mathbf{F}(\mathbf{u}) = 0$$

Jacobian-free Newton Krylov solution method

- Newton's method is used to solve the nonlinear system

$$\mathbf{F}(\mathbf{u}) = 0, \; or \; \mathbf{F}(\mathbf{u}^{n+1}) < tol$$

- The resulting linear system and nonlinear iteration are

$$\mathbf{J}\delta\mathbf{u}^{n+1} = -\mathbf{F}(\mathbf{u}^{n}) = 0, \; \mathbf{u}^{n+1} = \mathbf{u}^{n} + \delta\mathbf{u}^{n+1}$$

- Using a Krylov method (GMRES) to solve the linear system only requires a matrix-vector product (the Jacobian never appears alone)

$$\delta\mathbf{u}^{n+1,k} = a_0\mathbf{r}_0 + a_1\mathbf{J}\mathbf{r}_0 + a_2\mathbf{J}^2\mathbf{r}_0 + \ldots + a_k\mathbf{J}^k\ \mathbf{r}_0$$

- This matrix-vector product (for generic **v**) may be approximated by

$$\mathbf{J}\mathbf{v} \approx \frac{\mathbf{F}(\mathbf{u} + \epsilon\mathbf{v}) - \mathbf{F}(\mathbf{u})}{\epsilon}$$

Preconditioned JFNK

- Preconditioning is key for efficient application to engineering multiphysics problems.

$$(\mathbf{J}\mathbf{M}^{-1})(\mathbf{M}\delta\mathbf{u}) = -\mathbf{F}(\mathbf{u})$$

- Right-preconditioned matrix-free version is:

$$\mathbf{J}\mathbf{M}^{-1}\mathbf{v} \approx \left[\mathbf{F}(\mathbf{u} + \epsilon\mathbf{M}^{-1}\mathbf{v}) - \mathbf{F}(\mathbf{u})\right] / \epsilon$$

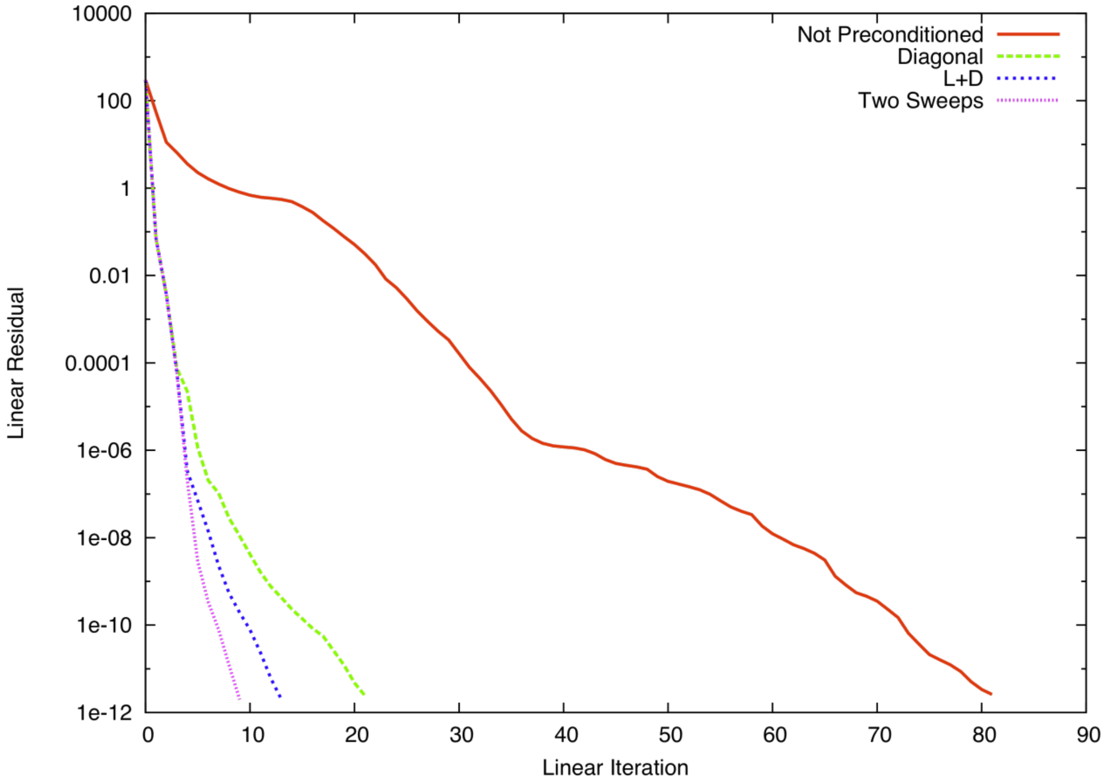
- Traditional preconditioning
  - Step 1: Choosing the matrix, $\mathbf{M} = \mathbf{J}$
  - Step 2: Approximating $\mathbf{M}^{-1}$, typically using ILU or Schwarz-ILU based methods, or perhaps system multigrid

Physics-based preconditioning

- Step 1: Choosing the matrix, $\mathbf{M} \neq \mathbf{J}$!
  - **M** is instead some approximate combination of linear operators (they look like scalar elliptic problems).
- Step 2: Approximating $\mathbf{M}^{-1}$ is a two step process:
  1. Ordering represents some standard operator split approximation to a time step with the approximate inversion of each sub-system.
  2. Use of modern parallel multilevel solvers to approximately invert each elliptic operator (sub-system).
- Using multilevel methods with standard smoothers can now be very effective.

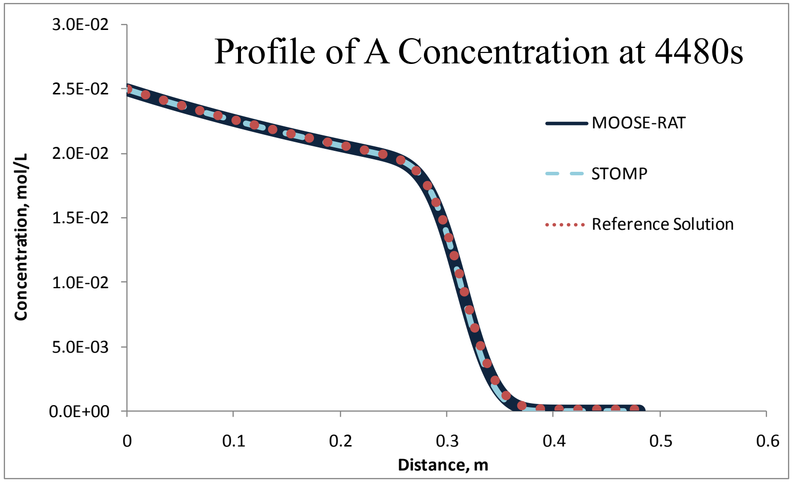
Applying multiphysics preconditioning

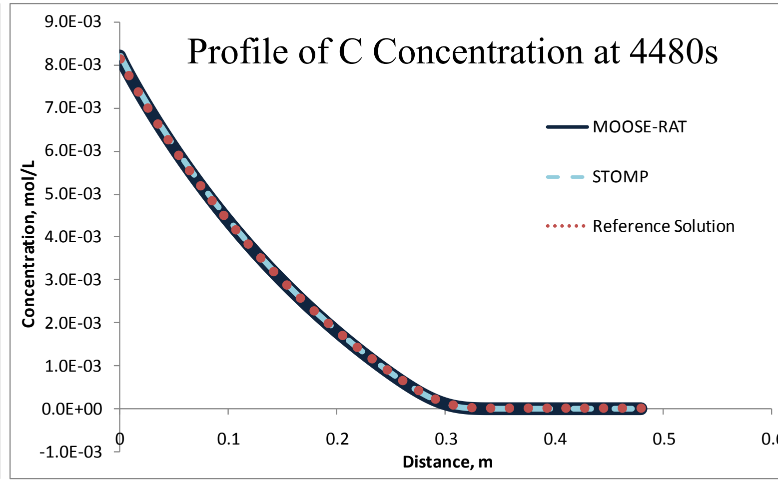
- Applying these ideas to a coupled fuel performance problem:



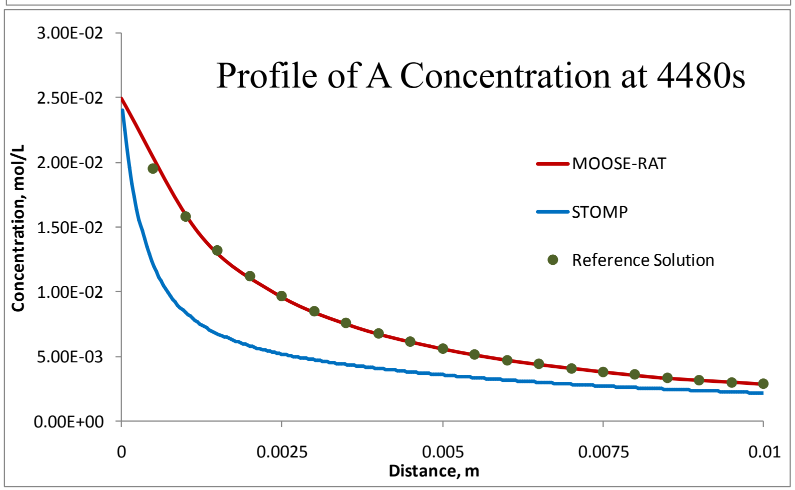
MOOSE solves problems that challenge others

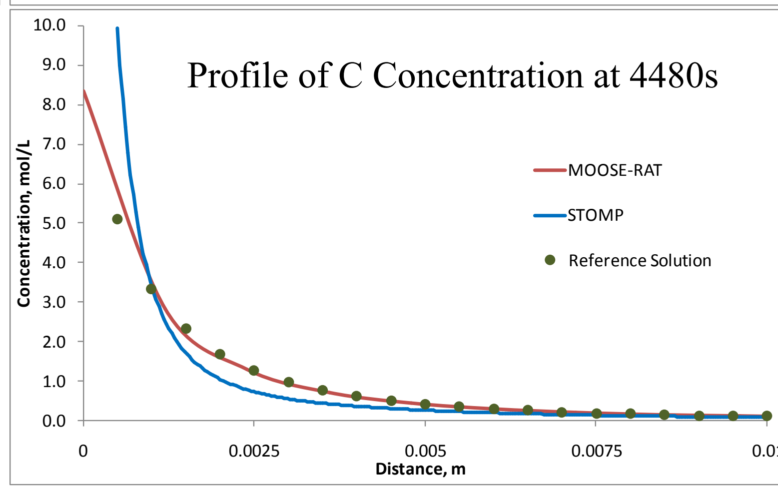
Slow Kinetics – Weak Coupling





Fast Kinetics – Strong Coupling





Weak coupling - excellent agreement between fully-coupled and operator-split approaches

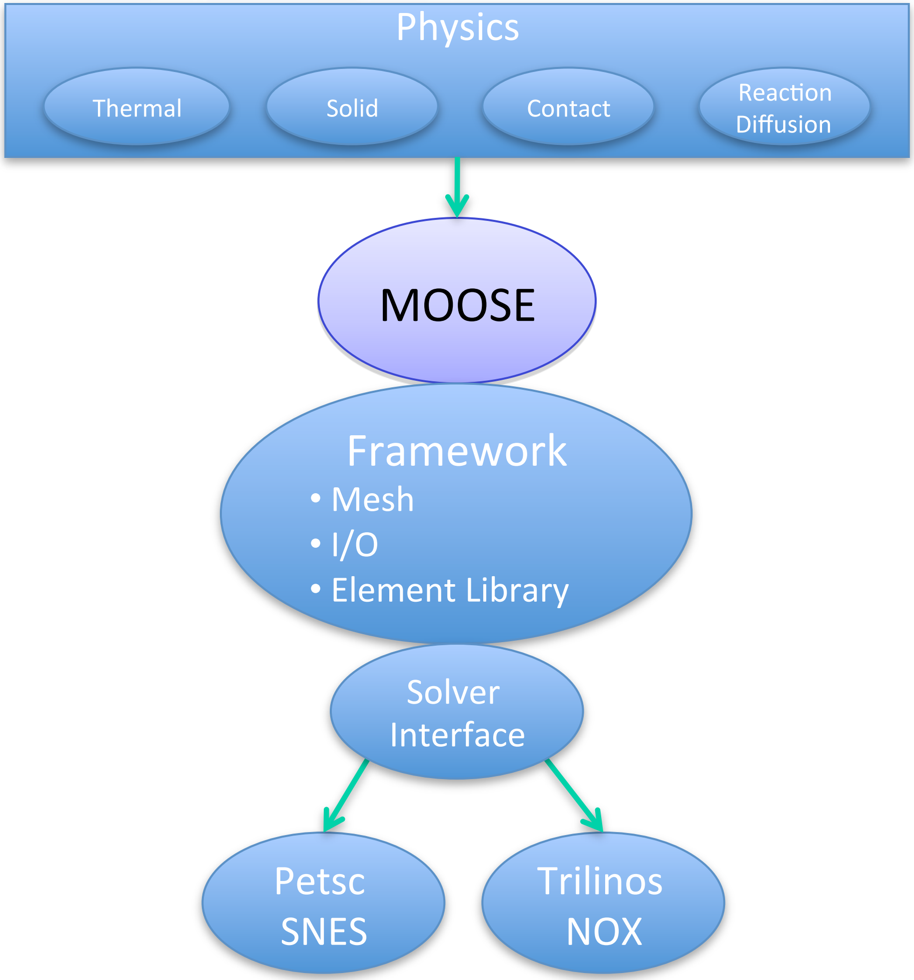
Strong coupling – better agreement between fully-coupled and the reference solution

Software Infrastructure Background

- Requirements:
  - 3D (and 2D (and 1D))
  - Massively Parallel, Including Hybrid Parallelism
  - Fully Coupled and Implicit
  - Advanced solution strategies (Adaptivity, etc.)
  - Portable
  - Flexible Physics Interface
  - Flexible Materials Database
- MOOSE: Multiphysics Object Oriented Simulation Environment

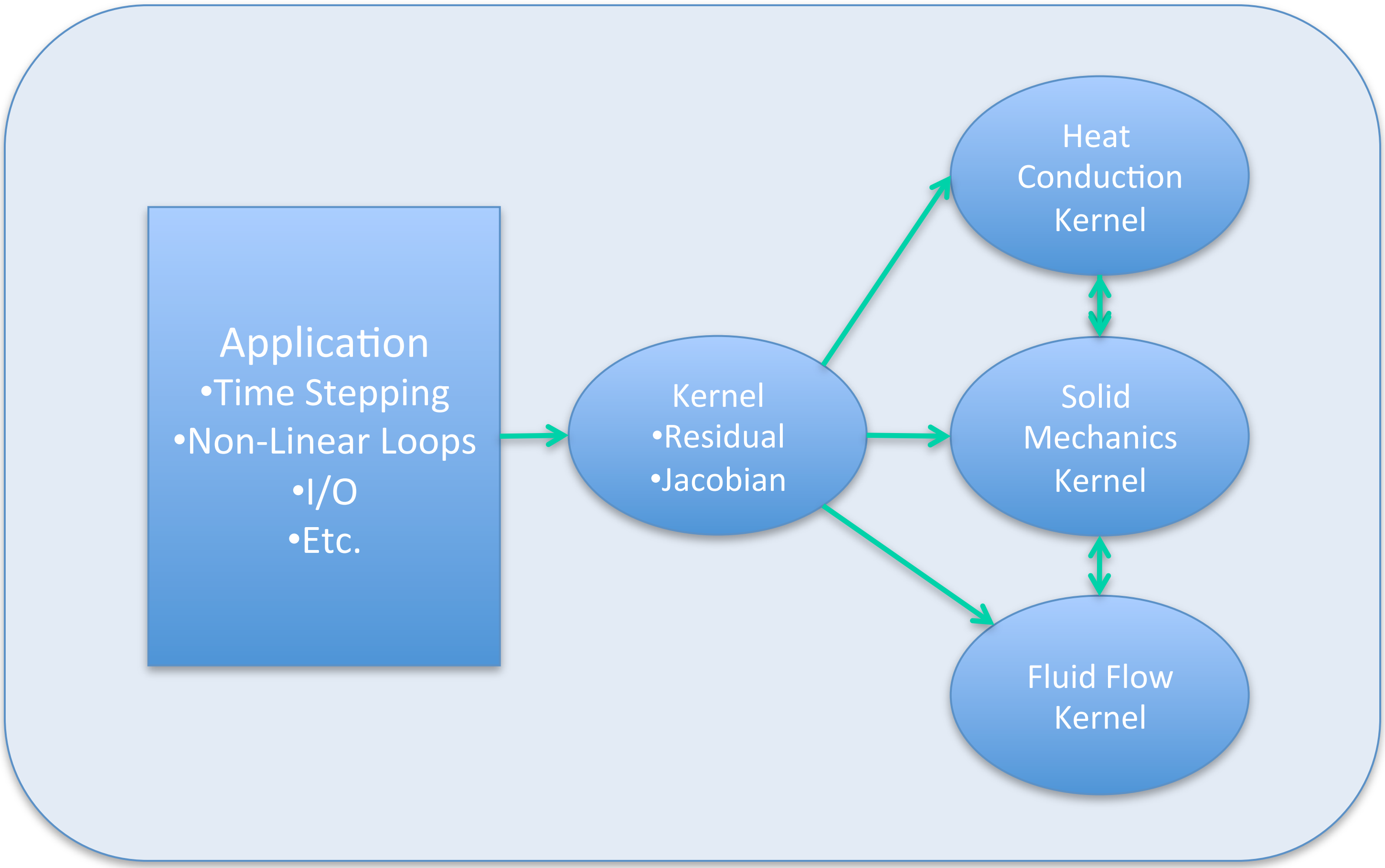
Code Platform

- Plug-and-play modules
  - Simplified coupling
- MOOSE provides a set of interfaces
- Framework provides core set of common services
  - libMesh: http://libmesh.sf.net
- Solver Interface abstracts specific solver implementations.
  - Common interface to linear and non-linear solvers
  - More flexible
- Utilize state-of-the-art linear and non-linear solvers
  - Robust solvers are key for “ease of use”



Incremental Application Development

Solid Mechanics Application



Oxygen Diffusion

- Strong form

$$s_t - \nabla \cdot \left(D\left(\nabla s + \frac{sQ^*}{FRT^2}\nabla T\right)\right) = 0$$

- Weak form

$$(s_t, \phi) + \left(D\nabla s + \frac{sQ^*}{FRT^2}\nabla T, \nabla\phi\right) - \langle g, \phi\rangle = 0$$

Oxygen Kernel

Residual()

$$(D(s,T)(\nabla s + f(s,T)\nabla T), \nabla \phi)$$

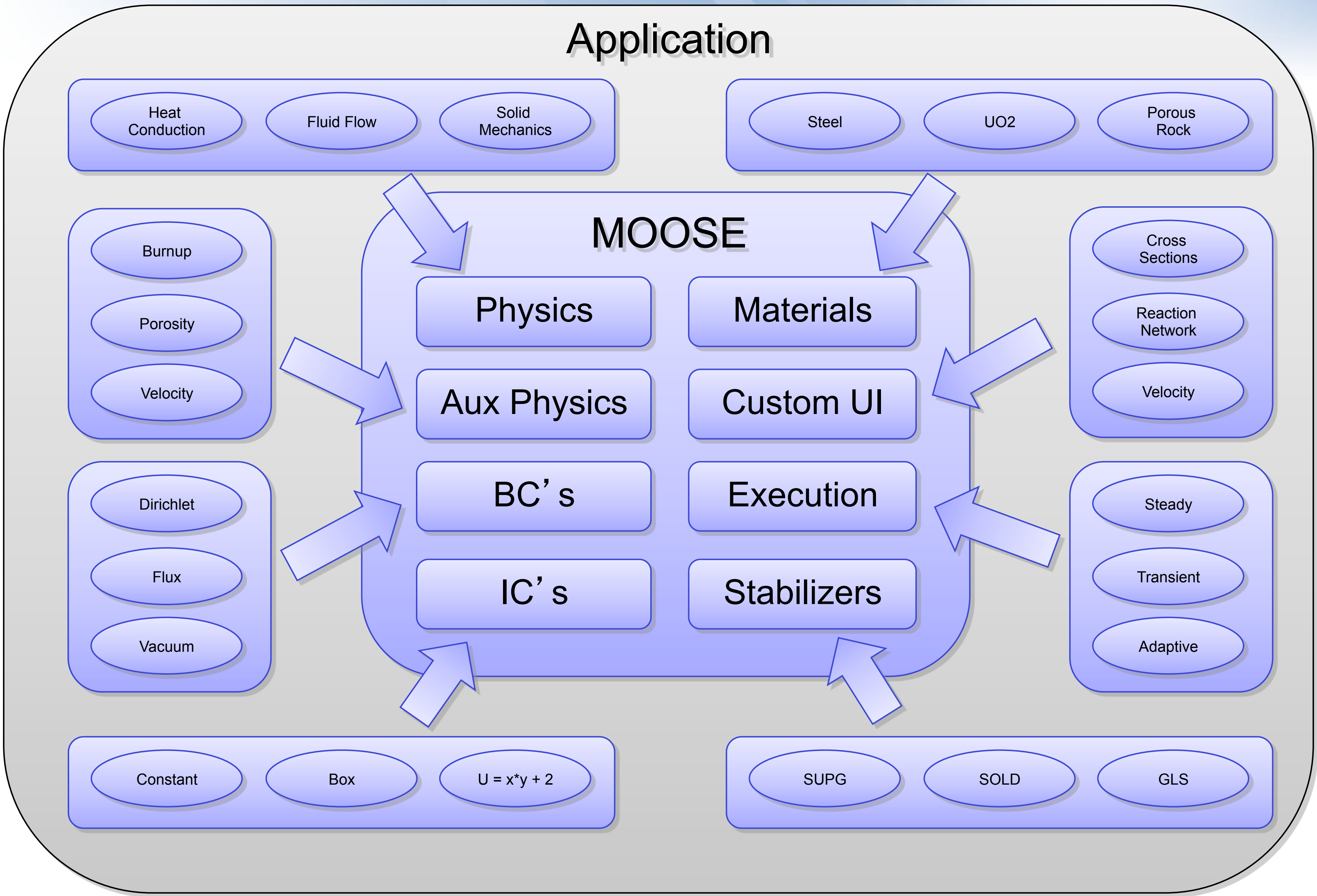
```
D*(grad_s[qp] + f(s[qp],T[qp])*grad_T[qp])*dphi[i][qp]
```

Jacobian()

$$D(s,T)(\nabla \phi, \nabla \phi)$$

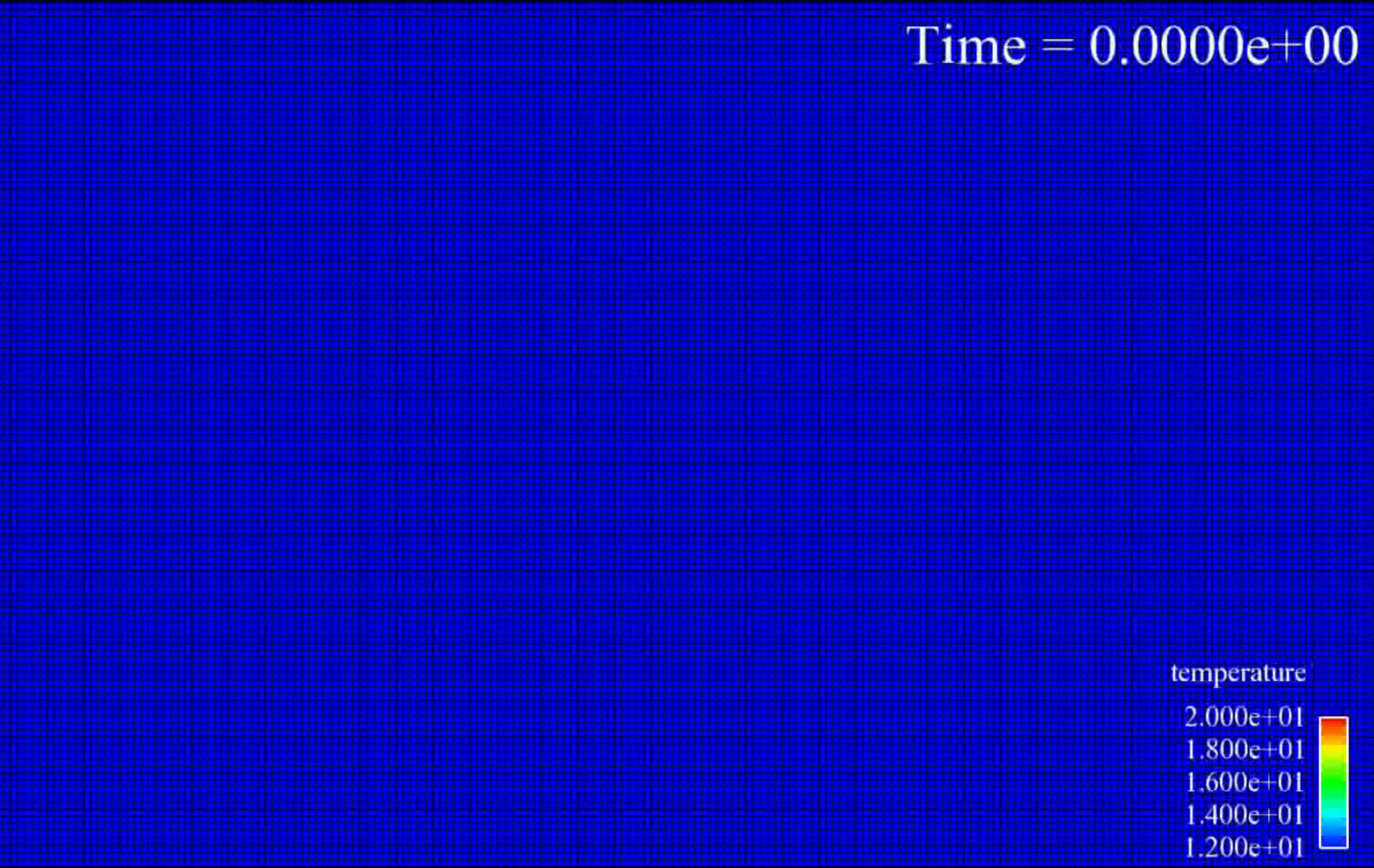
```
D * dphi[j][qp] * dphi[i][qp]
```

Current MOOSE Architecture



Falcon

- Developed to model field-scale geomechanics with porous, density driven flow.
- Used to study contaminate transport in large geological reservoirs.
- Implemented Physics Modules:
  - Heat Conduction
  - Solid Mechanics
  - Poroelasticity
  - Porous flow (Darcy)
  - Density driven flow
- Planned Modules:
  - Multiphase flow
  - Link to mesoscale fracture simulation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1.600e+01
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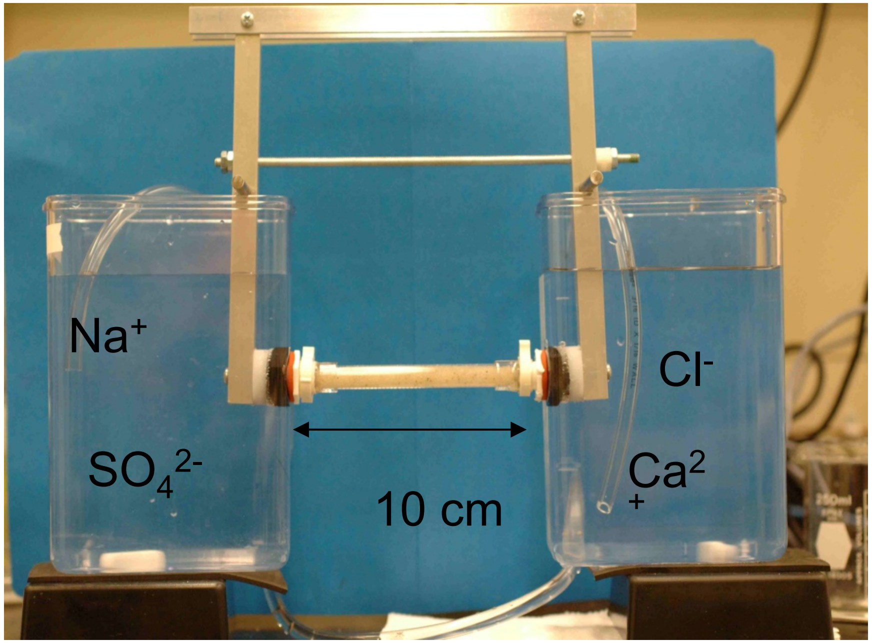
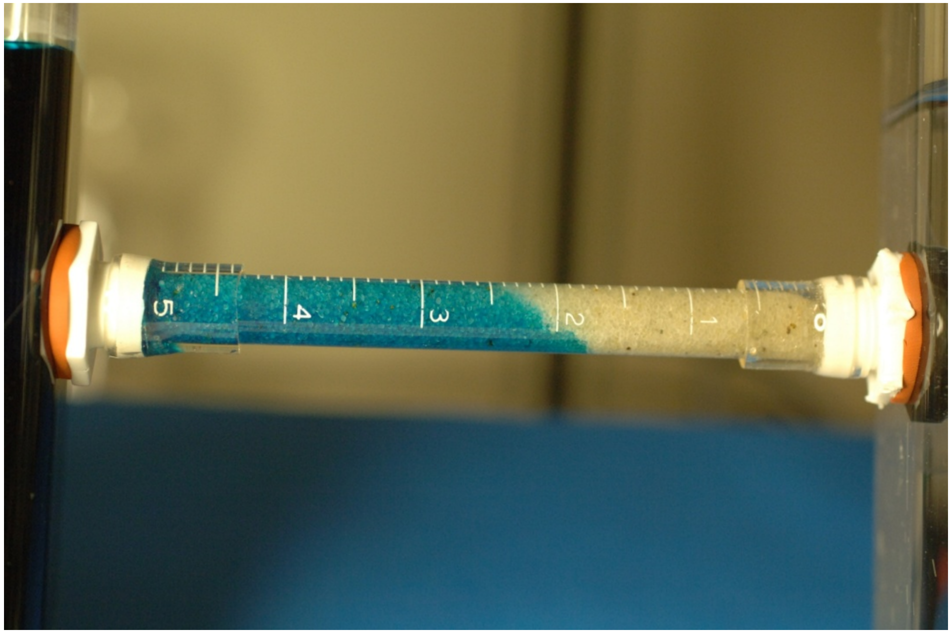
1.200e+01

Modeling of Coupled Diffusion and Mineral Precipitation in Porous Media with RAT

"SIMPLE" Diffusion-Reaction experiment



Focused precipitation front – visible only by using dye



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

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

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

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

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

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

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

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

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

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

$$(10)\quad C_{CaSO_4(aq)}-10^{3.1}C_{Ca^{2+}}\cdot C_{SO_4^{2-}}=0$$

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

$$(12)\quad C_{HCl(aq)}-10^{0.7}C_{H^{+}}\cdot C_{Cl^{-}}=0$$

$$(13)\quad C_{HSO_4^{-}}-10^{1.976}C_{H^{+}}\cdot C_{SO_4^{-}}=0$$

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

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

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

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

Challenges:

- **Both fast and slow kinetics**
- **Strongly coupled processes**

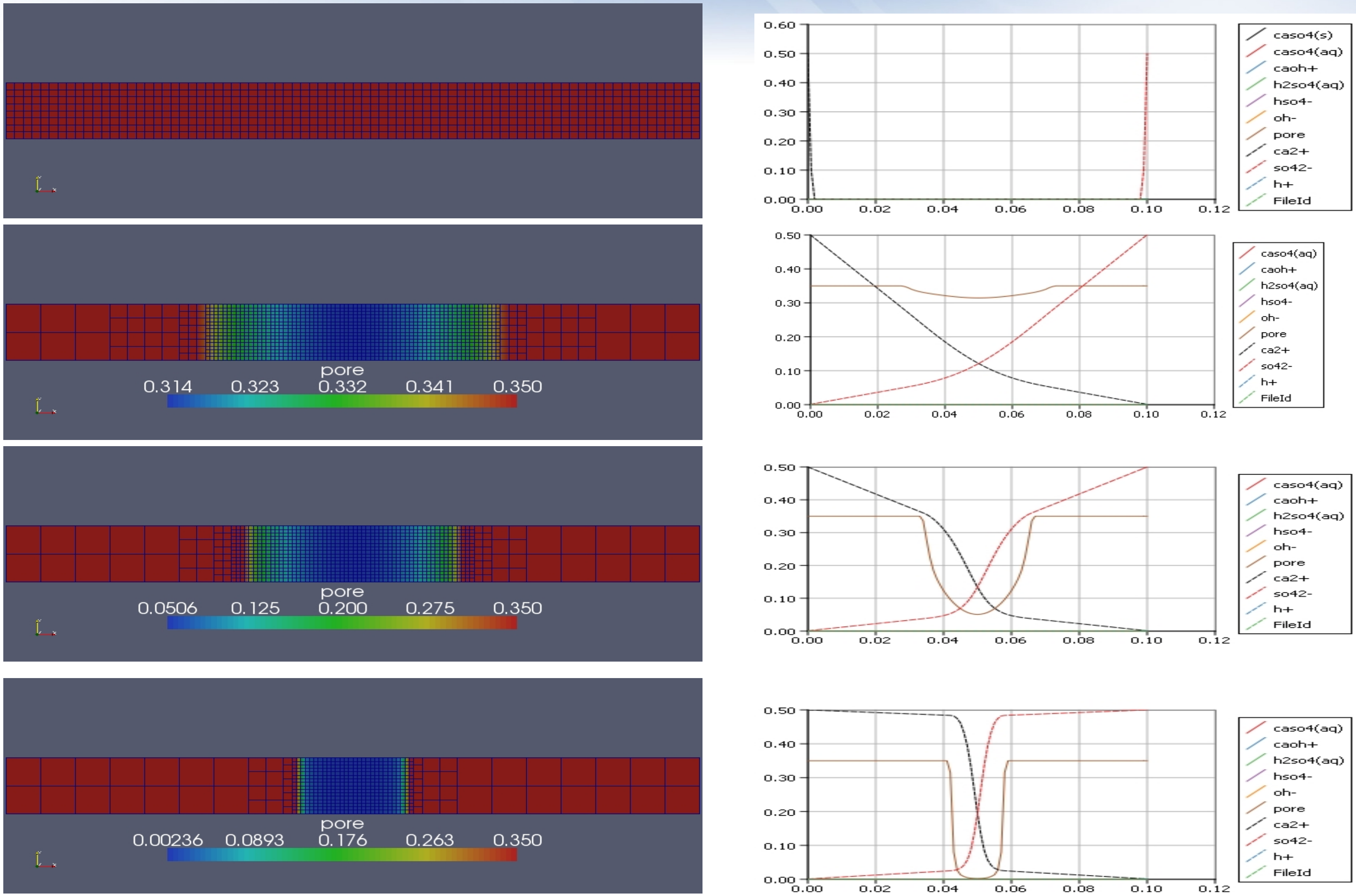
Conventional Approach:

- **Operator splitting**

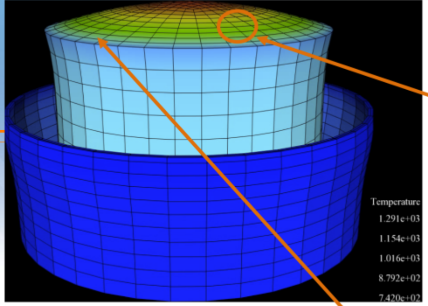
Our approach:

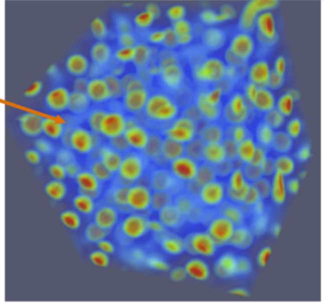
- **Fully coupled, fully implicit**
- **Adaptive mesh refinement**
- **JFNK nonlinear solver**

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

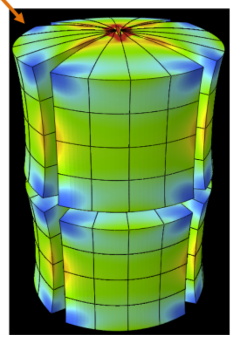


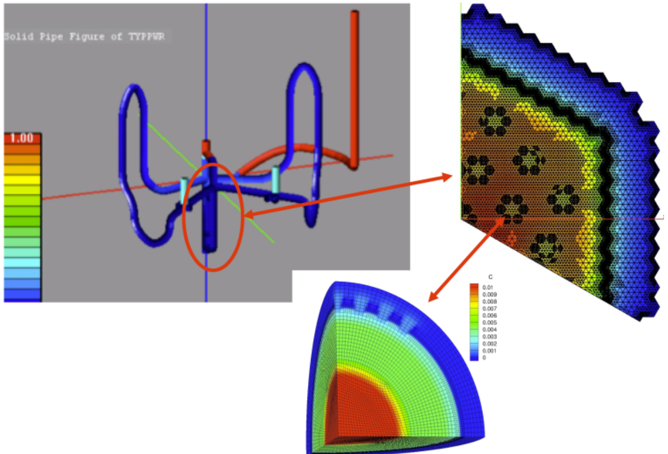
BISON fuel performance

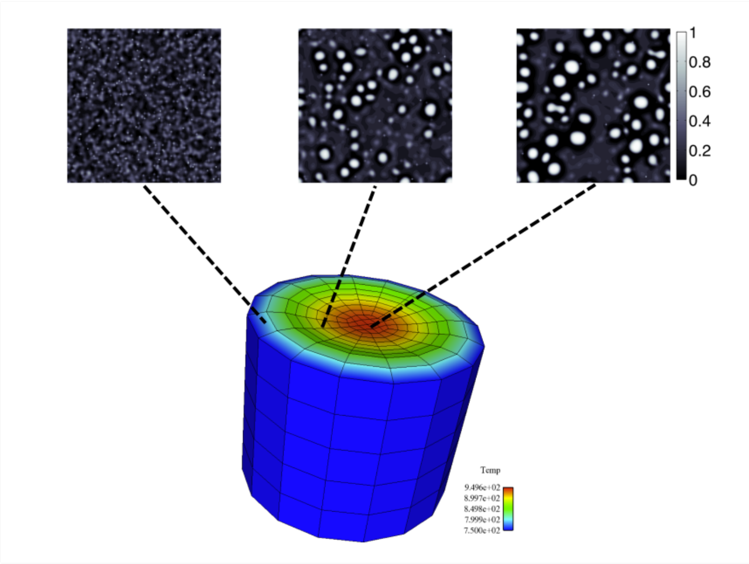


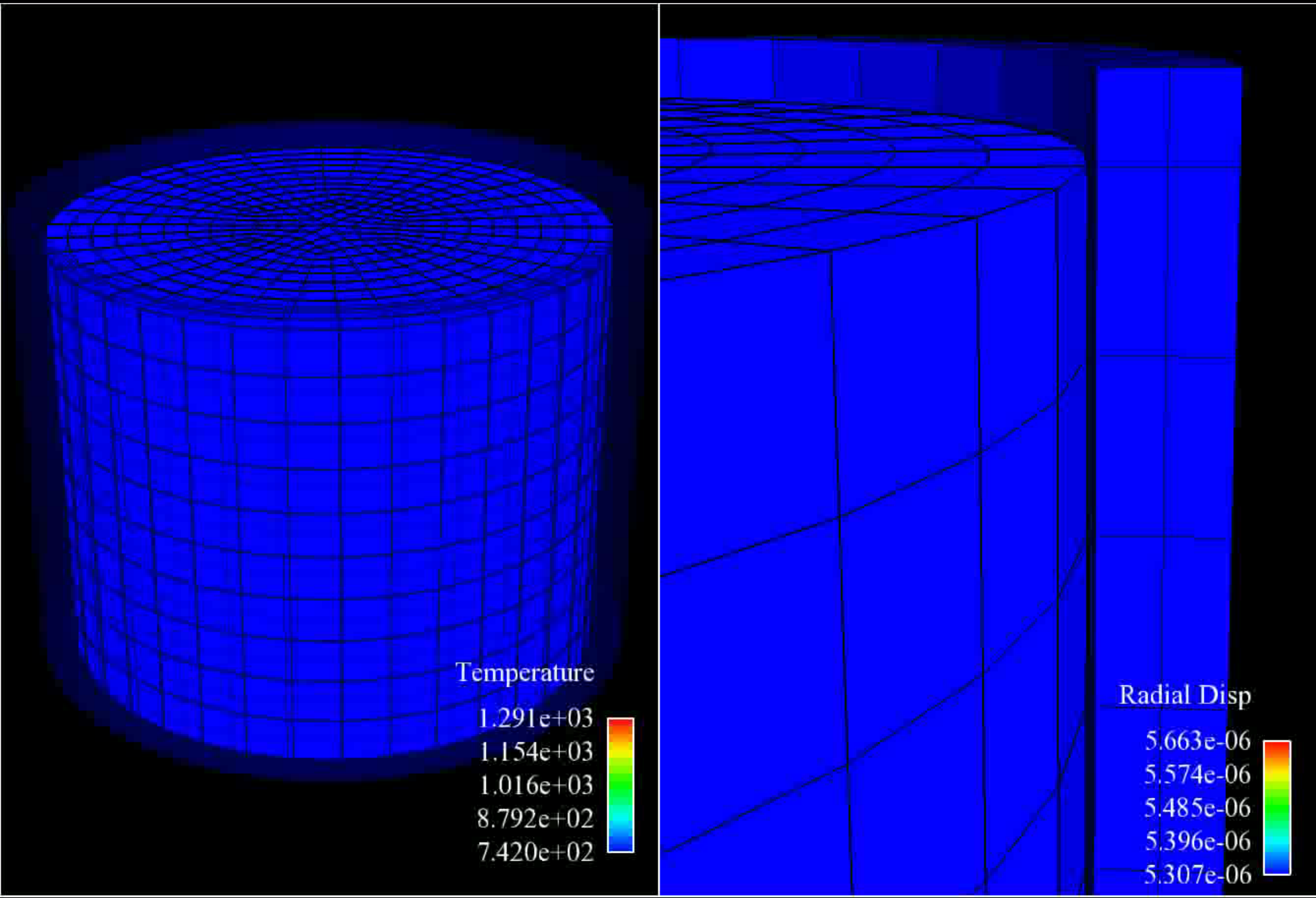


- LWR, Triso, and TRU fuel performance code
- Parallel 1D-3D thermomechanics code
- Thermal, mechanical, and chemical models for FCI
- Constituent redistribution
- Material, fission product swelling, fission gas release models
- Mesoscale-informed material models








Temperature
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1.154e+03
1.016e+03
8.792e+02
7.420e+02
Radial Disp
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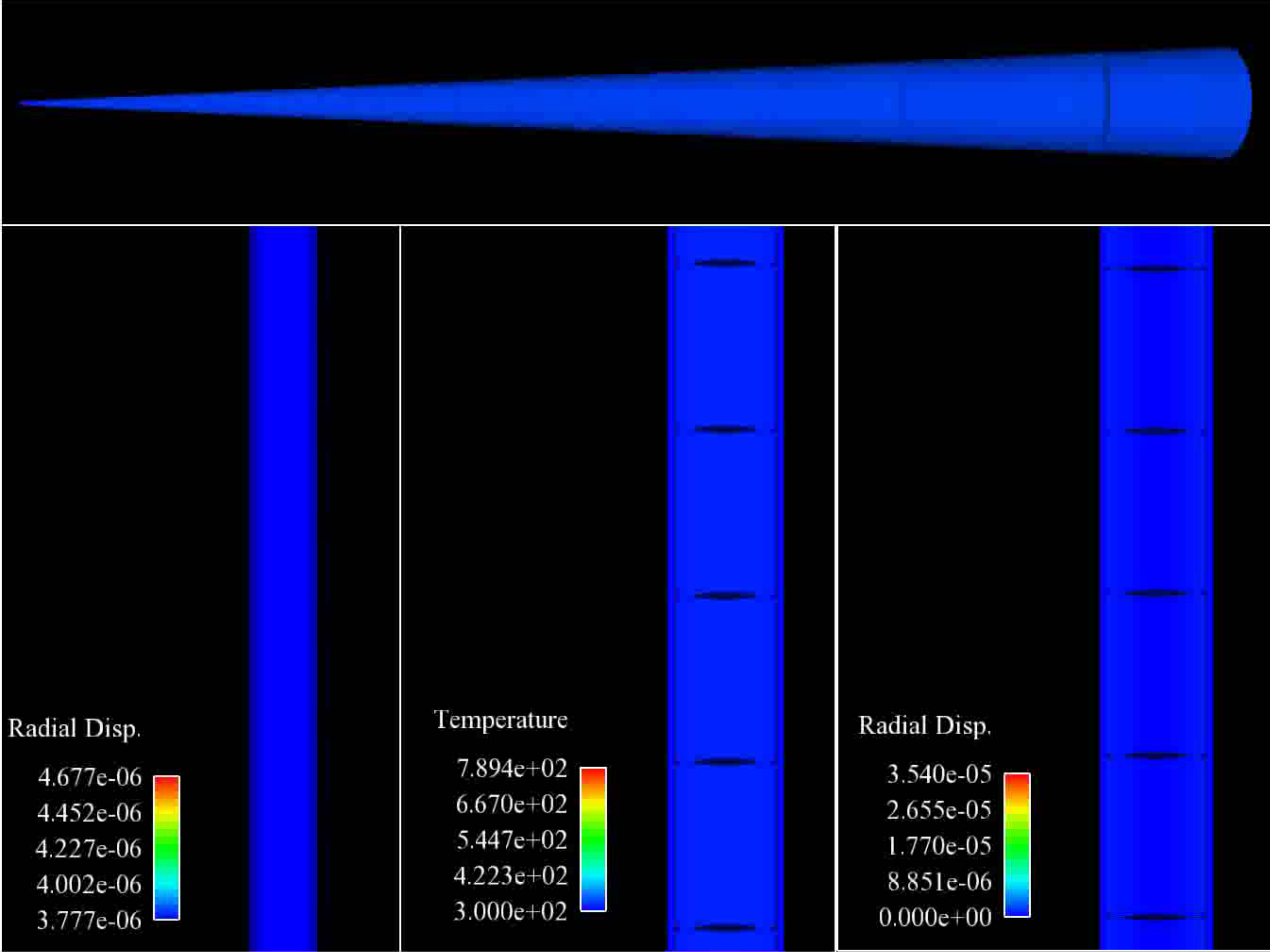
5.574e-06
5.485e-06
5.396e-06
5.307e-06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Temperature
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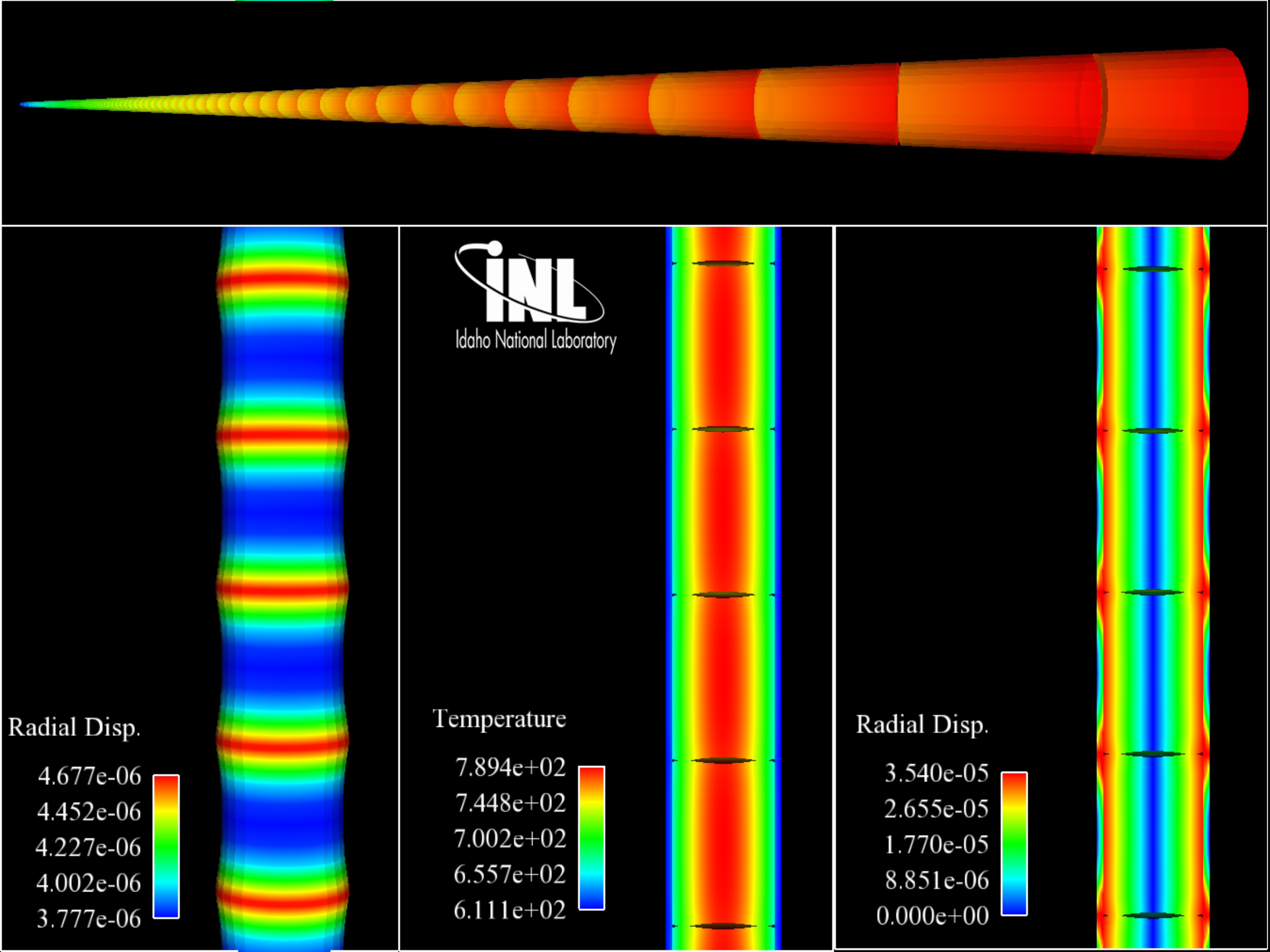
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Radial Disp.
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4.452e-06
4.227e-06
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Temperature
7.894e+02
7.448e+02
7.002e+02
6.557e+02
6.111e+02
Radial Disp.
3.540e-05
2.655e-05
1.770e-05
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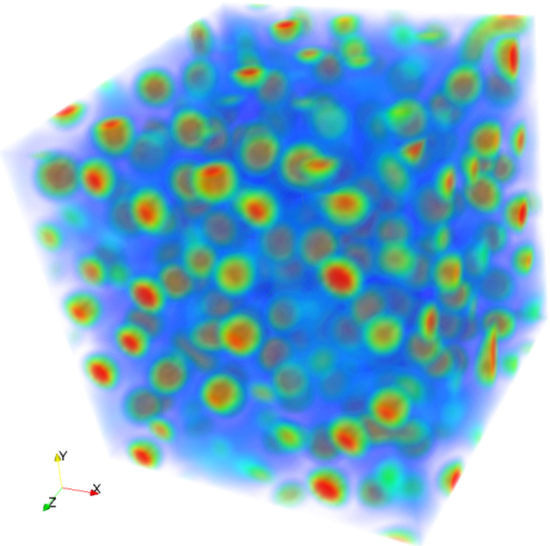
MARMOT: Integrated Mesoscale Phase Field Code



Finite Element Solution of Phase Field Equations

- Strong Form

$$\mathbf{R}_{c_i} = \frac{\partial c_i}{\partial t} - \nabla\cdot\left(M_{ij}\nabla\left(\frac{\partial g_0}{\partial c_i} - \kappa\nabla^2 c_i + \frac{\partial E_{el}}{\partial c_i}\right)\right) = \mathbf{0} \qquad \mathbf{R}_{\eta_i} = \frac{\partial \eta_i}{\partial t} + L_i\left(\frac{\partial f_0}{\partial \eta_i} - \kappa\nabla^2\eta_i + \frac{\partial E_{el}}{\eta_i}\right) = \mathbf{0}$$

$$\mathbf{R}_u = \nabla\cdot\left(\mathbf{C}\nabla\mathbf{u}\right) - \nabla\cdot\left(\mathbf{C}\varepsilon^*\right) = \mathbf{0}$$

- Weak Form

$$\mathbf{R}_{c_n} = \left(\frac{\partial c_n}{\partial t}, \varphi_i\right) + \left(M_{ij}\nabla\frac{\partial g_0}{\partial c_i}, \nabla\varphi_i\right) + \kappa\left(\nabla^2 c_n, \nabla\cdot\left(M_{ij}\nabla\varphi_i\right)\right) + \left(M_{ij}\nabla\frac{\partial E_{el}}{\partial c_i}, \nabla\varphi_i\right) = \mathbf{0}$$

$$\mathbf{R}_{\eta_n} = \left(\frac{\partial \eta_n}{\partial t}, \varphi_i\right) + L_i\left(\frac{\partial f_0}{\partial \eta_i}, \varphi_i\right) + L_i\kappa\left(\nabla\eta_i, \nabla\varphi_i\right) + L_i\left(\frac{\partial E_{el}}{\eta_i}, \varphi_i\right) = \mathbf{0}$$

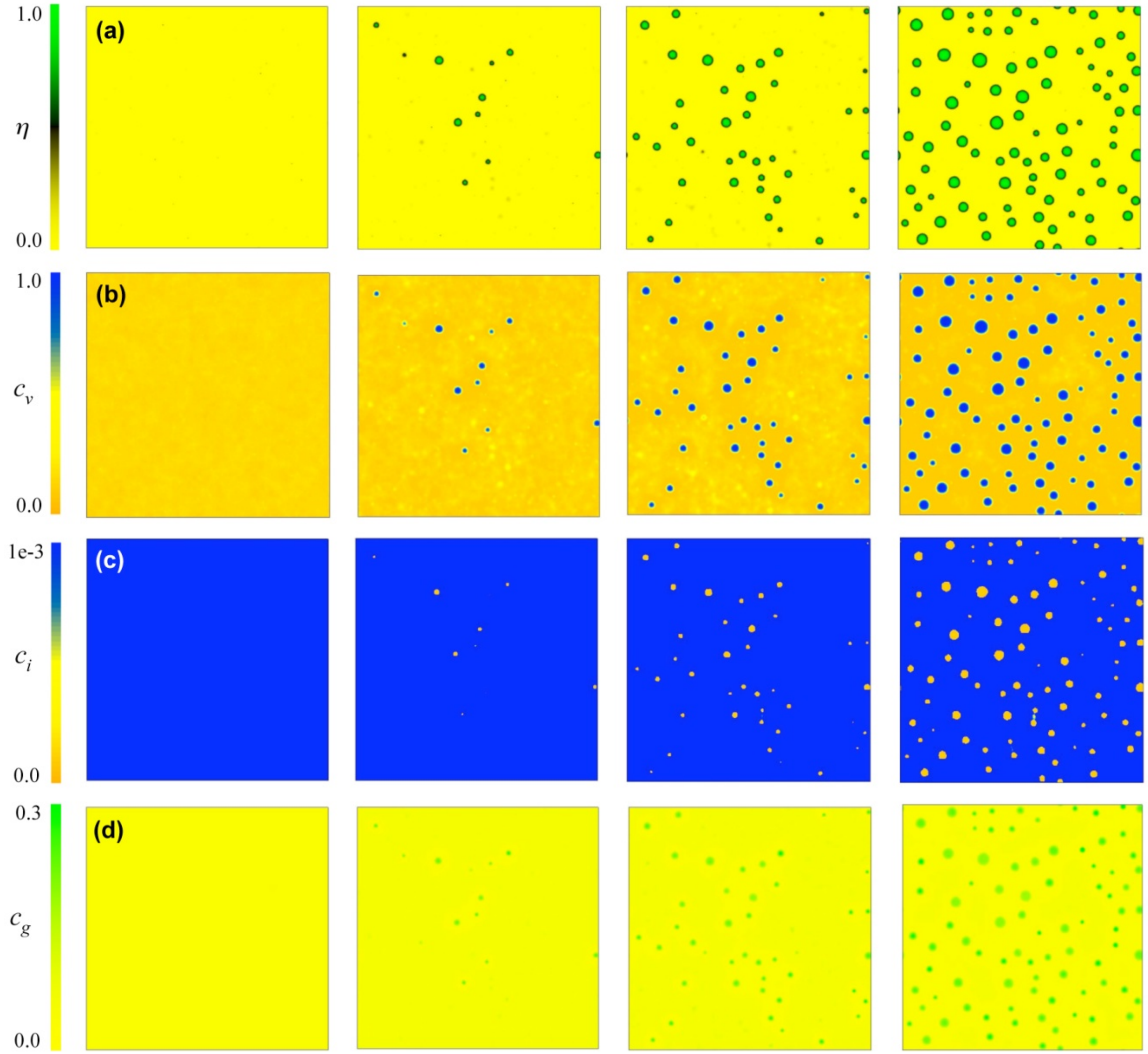
$$\mathbf{R}_u = \left(\mathbf{C}\nabla\mathbf{u}, \nabla\varphi_i\right) + \left(\nabla\cdot\mathbf{C}\varepsilon^*, \varphi_i\right) = \mathbf{0}$$

- FEM discretization

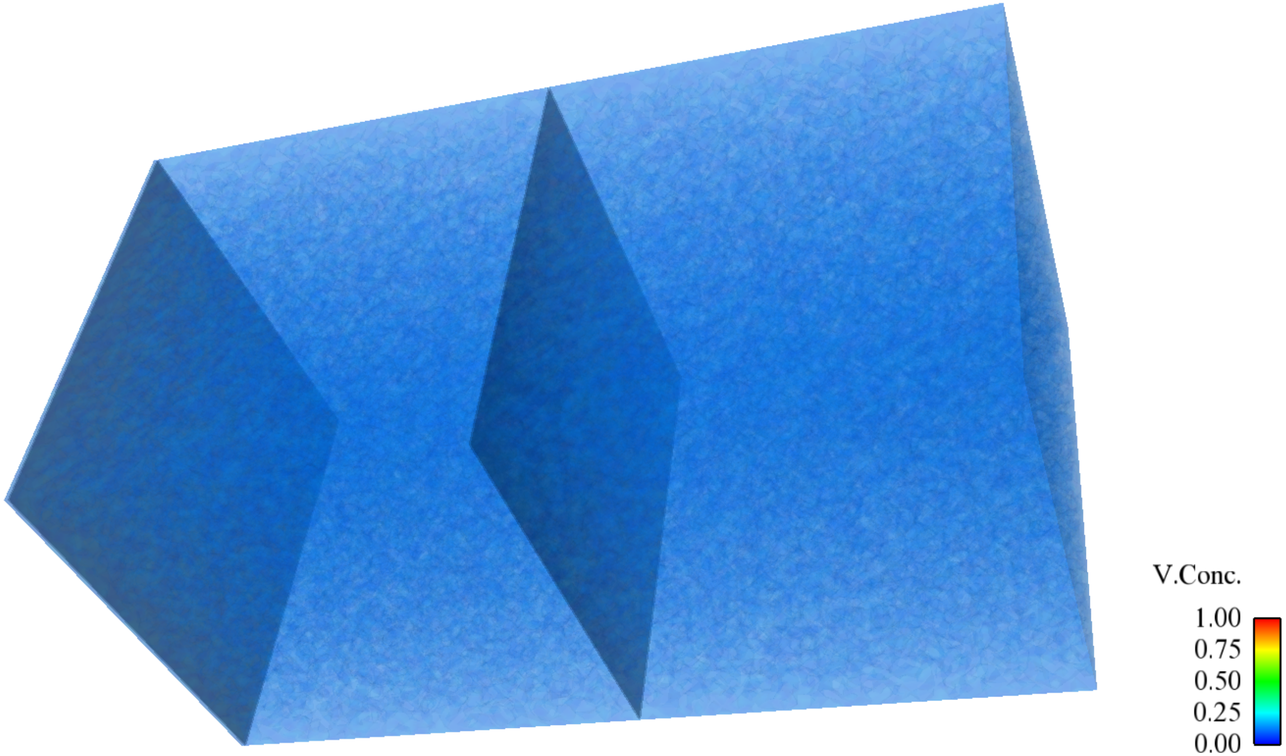
$$c_i(\mathbf{r}) = \sum_{j=1}^{N} c_i^j\varphi_j(\mathbf{r}) \qquad \eta_i(\mathbf{r}) = \sum_{j=1}^{N}\eta_i^j\varphi_j(\mathbf{r}) \qquad \mathbf{u}(\mathbf{r}) = \sum_{j=1}^{N}\mathbf{u}^j\varphi_j(\mathbf{r})$$

Discretized using 3rd order Hermite element	*Discretized using 1st order Lagrange elements*	*Discretized using 1st order Lagrange elements*
2D: 20 DOF	*2D: 8 DOF*	*2D: 8 DOF*
3D:36 DOF	*3D: 12 DOF*	*3D: 12 DOF*

Bubble Nucleation and Growth

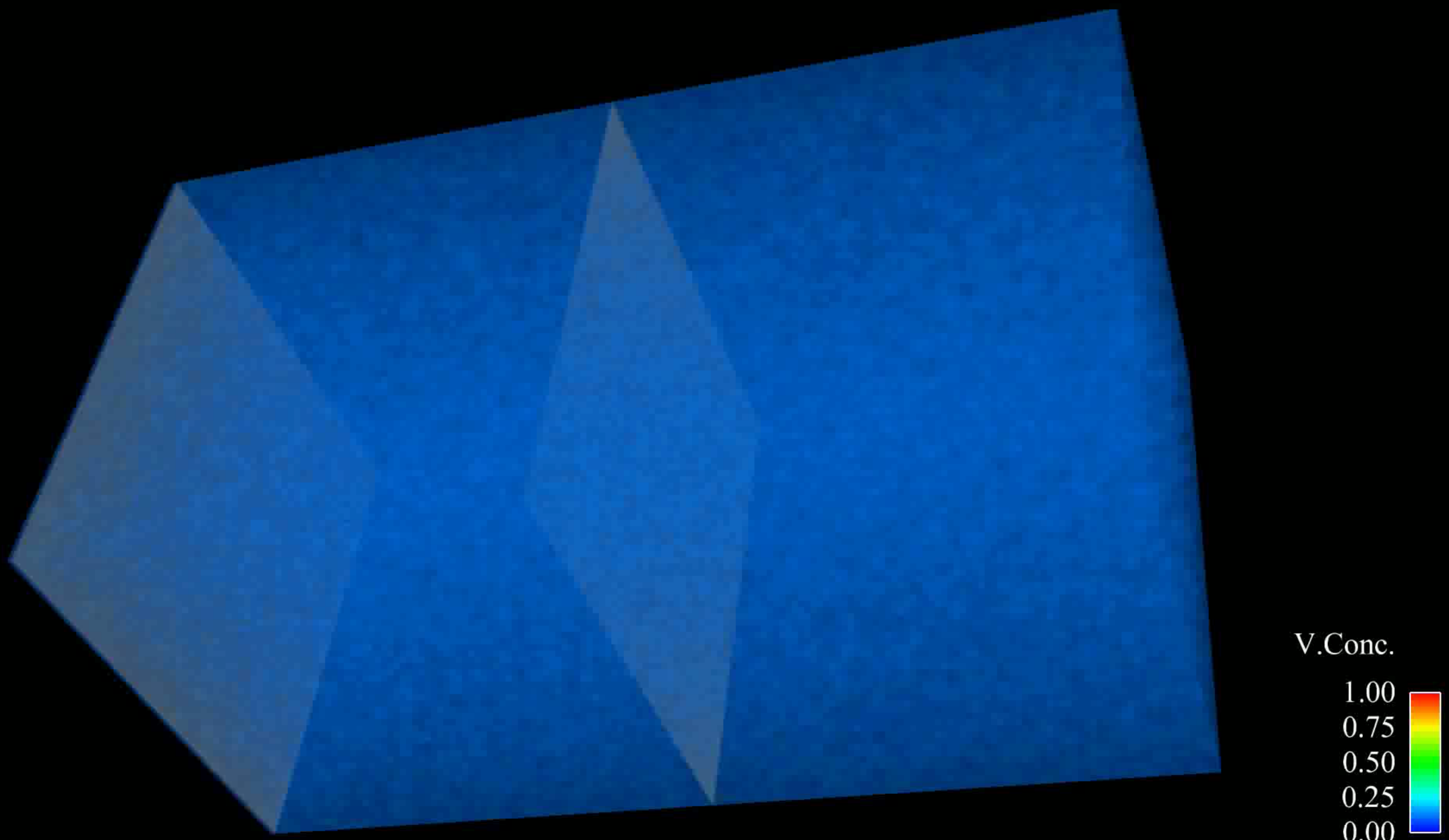


3-D Void Nucleation In a Bicrystal



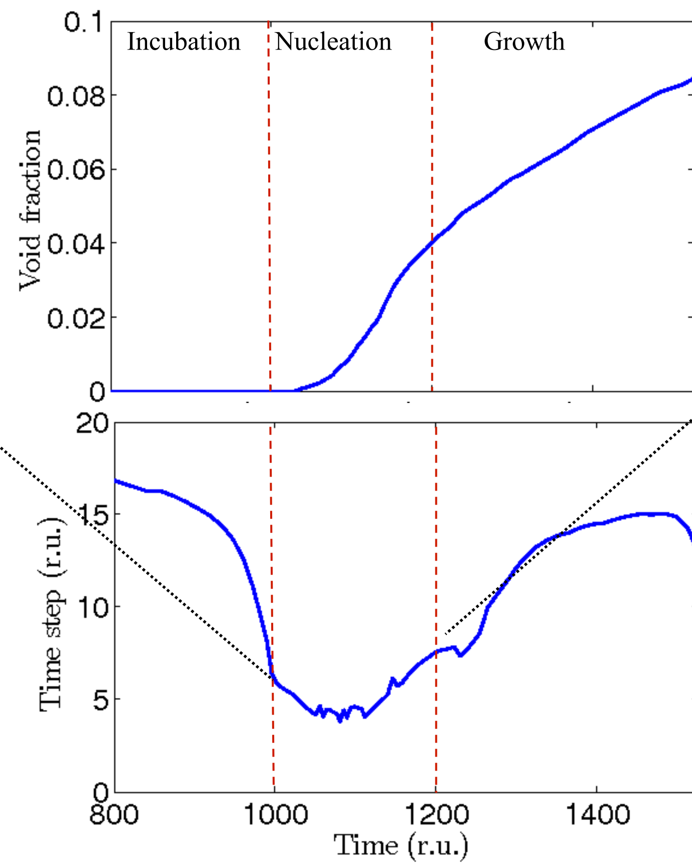
- Grain boundaries act as a vacancy sink
  - In this simulation, the rate at which vacancies are absorbed by the boundary is slower than the rate at which the vacancies diffuse
- Vacancies will diffuse and cluster, resulting in void nucleation

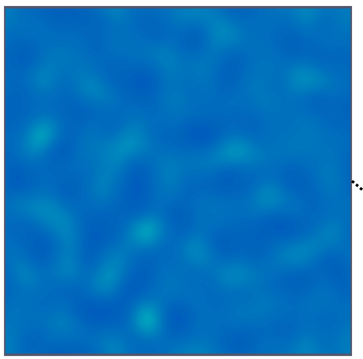
Void Nucleation and Growth in a Bicrystal



Adaptive Time Step

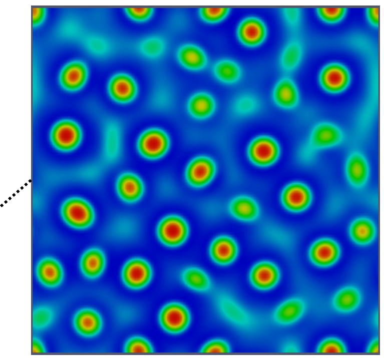
- Solution time step adapts to the current phenomena



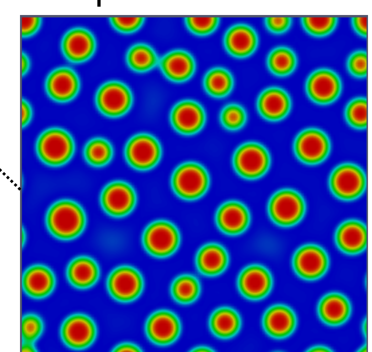


Void nucleation requires small spatial resolution

Void growth can be resolved with a larger time step



Void coalescence needs smaller spatial resolution



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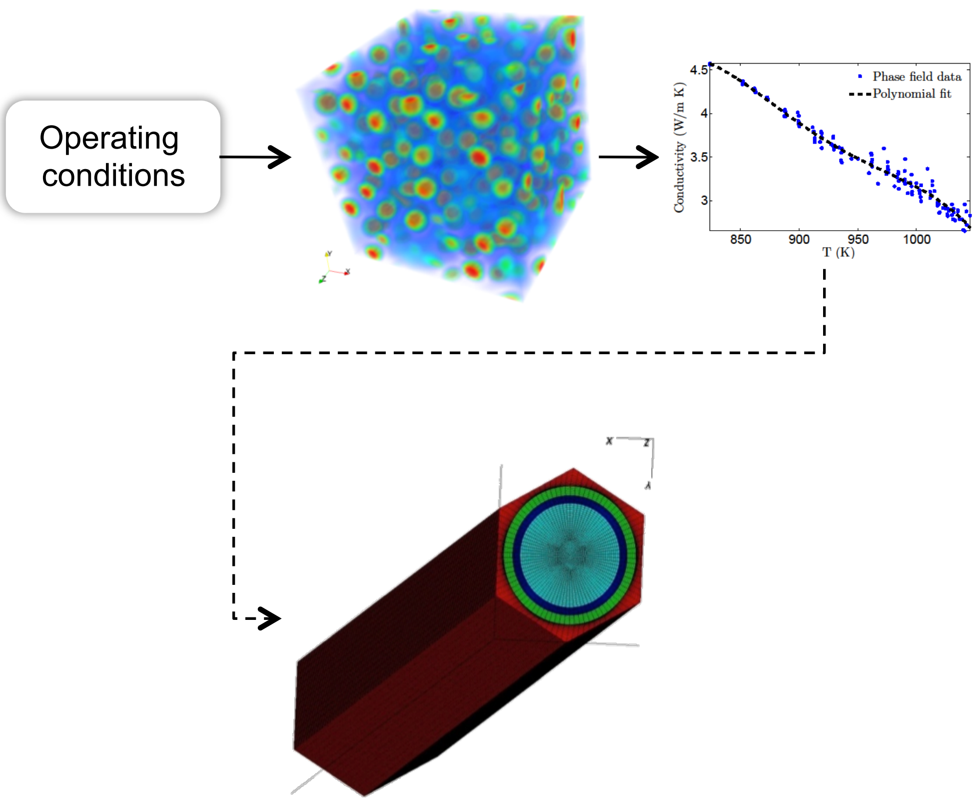
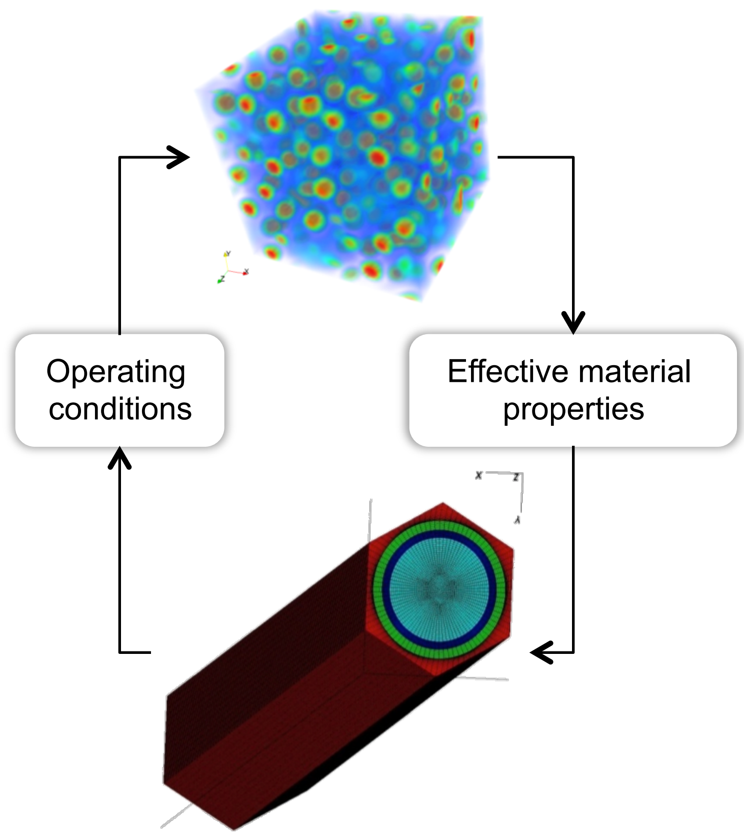
Multiscale Modeling: Meso- to Macroscale

- Mesoscale simulation results take the place of empirical constitutive models in macroscale simulation

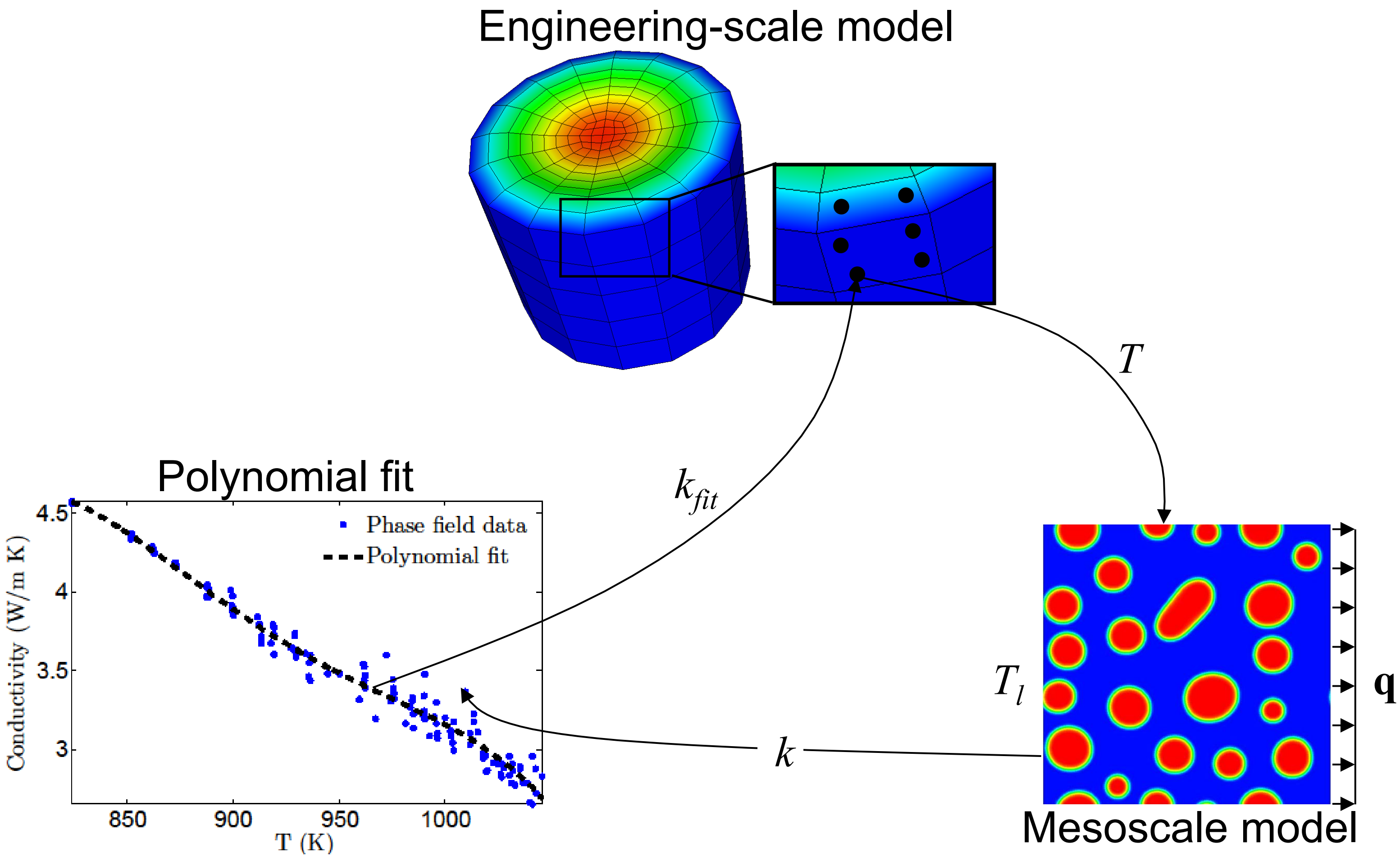
Hierarchical coupling



Concurrent coupling



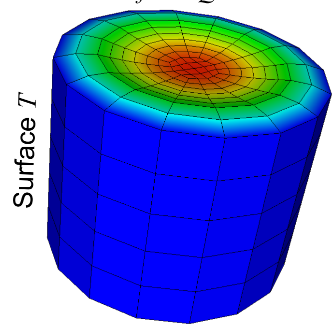
Initial Concurrent Linking Methodology

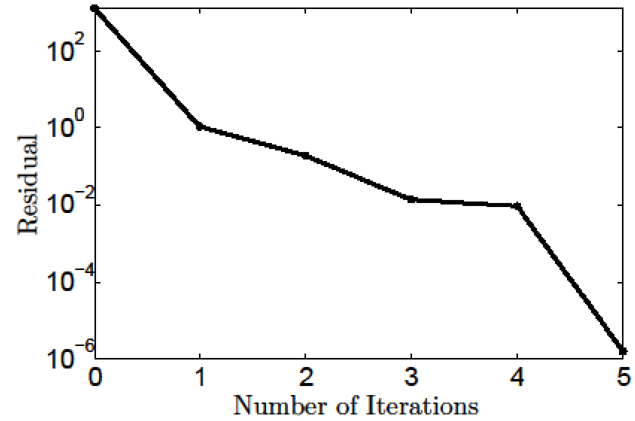


Numerical Performance

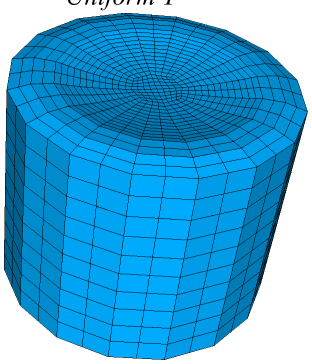
- Non-linear convergence test
  - 720 elements
  - Boundary Conditions
    - Constant surface temp
    - Uniform heat source
- Parallel scalability test
  - 5760 elements
  - Boundary Conditions
    - Constant temperature

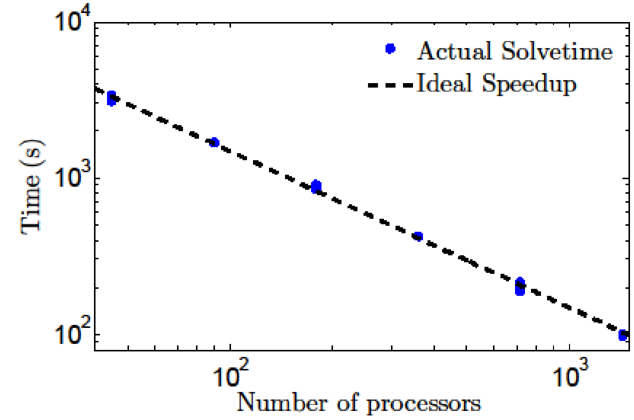
Uniform Q



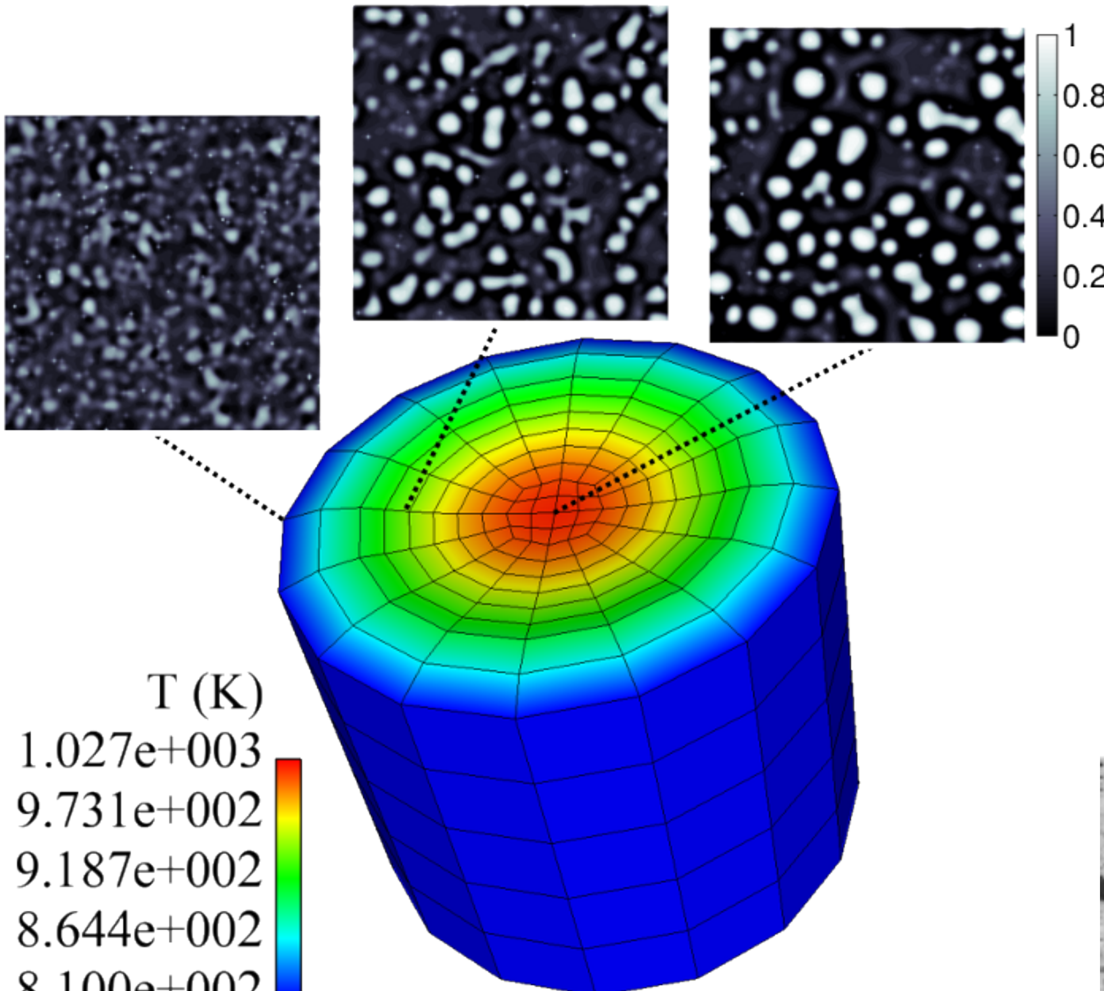


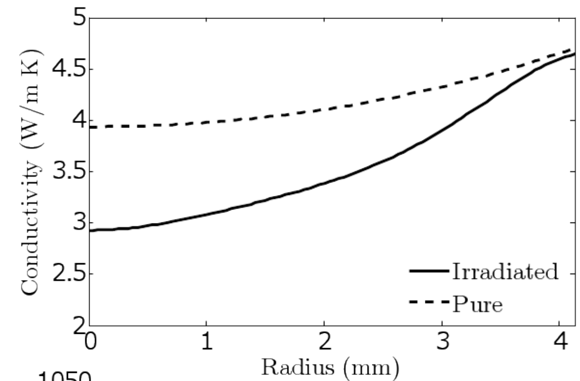
Uniform T

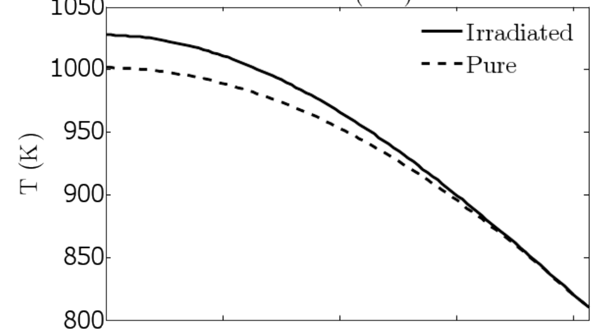




Results







Radially dependent void size from P.F. Sens, 1972

Papers

1. Michael Tonks, Derek Gaston, Cody Permann, Paul Millett, Glen Hansen, Chris Newman, and Dieter Wolf. A coupling methodology for mesoscale-informed nuclear fuel performance codes. *Nucl. Engrg. Design, 2010. Accepted.*
2. G. Hansen and C. Newman. ALE mesh adaptation method for complex geometry. *Engrg. Comput., 2010. Submitted.*
3. D. Gaston, G. Hansen, S. Kadioglu, D. Knoll, C. Newman, H. Park, C. Permann, and W. Taitano. Parallel multiphysics algorithms and software for computational nuclear engineering. *Journal of Physics: Conference Series, 180(1):012012, 2009.*
4. M. R. Tonks, G. Hansen, D. Gaston, C. Permann, P. Millett, and D. Wolf. Fully-coupled engineering and mesoscale simulations of thermal conductivity in UO2 fuel using an implicit multiscale approach. *Journal of Physics: Conference Series, 180(1):012078, 2009.*
5. C. Newman, G. Hansen, and D. Gaston. Three dimensional coupled simulation of thermomechanics, heat, and oxygen diffusion in UO2 nuclear fuel rods. *Journal of Nuclear Materials, 392:6–15, 2009.*
6. D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandie. MOOSE: A parallel computational framework for coupled systems of nonlinear equations. *Nucl. Engrg. Design, 239:1768–1778, 2009.*
7. G. Hansen, C. Newman, D. Gaston, and C. Permann. An implicit solution framework for reactor fuel performance simulation. In *20th International Conference on Structural Mechanics in Reactor Technology (SMiRT 20), paper 2045, Espoo (Helsinki), Finland, August 9–14 2009.*
8. G. Hansen, R. Martineau, C. Newman, and D. Gaston. Framework for simulation of pellet cladding thermal interaction (PCTI) for fuel performance calculations. In *American Nuclear Society 2009 International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics, Saratoga Springs, NY, May 3–7 2009.*
9. C. Newman, D. Gaston, and G. Hansen. Computational foundations for reactor fuel performance modeling. In *American Nuclear Society 2009 International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics, Saratoga Springs, NY, May 3–7 2009.*
10. D. Gaston, C. Newman, and G. Hansen. MOOSE: a parallel computational framework for coupled systems of nonlinear equations. In *American Nuclear Society 2009 International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics, Saratoga Springs, NY, May 3–7 2009.*
11. L. Guo, H. Huang, D. Gaston, and G. Redden. Modeling of calcite precipitation driven by bacteria-facilitated urea hydrolysis in a flow column using a fully coupled, fully implicit parallel reactive transport simulator. In *Eos Transactions American Geophysical Union, 90(52), Fall Meeting Supplement, AGU 90(52), San Francisco, CA, Dec 14-18 2009.*
12. Podgorney, H. Huang, and D. Gaston. Massively parallel fully coupled implicit modeling of coupled thermal-hydrological-mechanical processes for enhanced geothermal system reservoirs. In *Proceedings, 35th Stanford Geothermal Workshop, Stanford University, Palo Alto, CA, Feb 1-3 2010.*
13. H. Park, D.A. Knoll, D.R. Gaston, and R.C. Martineau, Tightly Coupled Multiphysics Algorithms for Pebble Bed Reactors. *Nuclear Science and Engineering*, *2010. Accepted*.

Peer-reviewed pubs 2009-10