Parallel Algorithms and Software for Multiphysics Computational Nuclear Engineering

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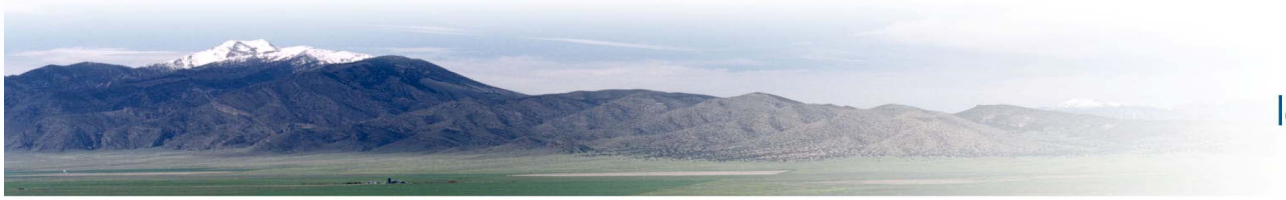
Oregon St. Univ., Oct. 21, 2008



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Outline

- Multiphysics Computational Nuclear Engineering
- Operator Splitting and Analysis *
- Jacobian-Free Newton-Krylov (JFNK) Methods*
- Physics-based Preconditioning of JFNK*
- MOOSE, Multiphysics Object-Oriented Software Environment
- BISON, Fuel Performance Simulation
- PRONGHORN, Pebble-bed Gas Reactor Simulation

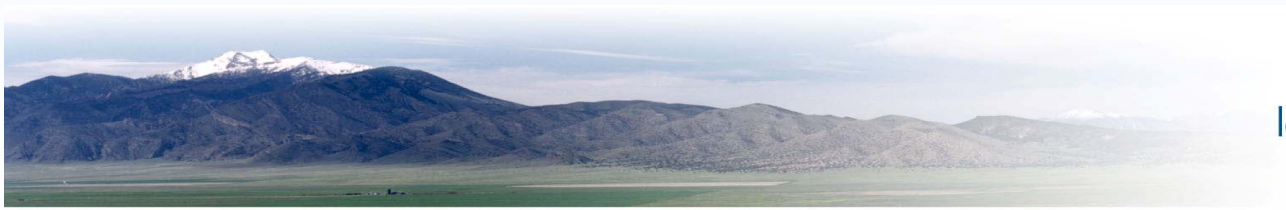
* *Each topic a talk of its own*

Some Requirements for Predictive Simulation

- Proper Physics Model / Equation Set
- Accurate spatial discretization / adequate grid refinement (3-D)
- High end computing platforms and parallel, scalable, algorithms.
- Accurate time integration (or coupling) for multiphysics systems
  - This area has received little attention.
  - Verification of temporal integration (confidence)
  - We must understand this area when we are taking $10^5 - 10^6$ time steps.
  - ”Code coupling” or first-order operator splitting the norm

Multiphysics Computational Nuclear Engineering: Two Examples

- Fuel Performance
  - Nonlinear Mechanics, Contact, Crack models
  - Thermal transport
  - Fission gas transport
  - Species transport
- Reactor design and transient analysis
  - Neutronics
  - Heat conduction
  - Fluid flow
  - Species transport and chemistry
  - Structural response



Linearization and Time Splitting (code coupling): The Standard Approach

- Model Problem: A and B represent two nonlinear processes

$$\frac{dT}{dt} = A(T)T + B(T)T \tag{1}$$

- Linearization

$$\frac{T^{n+1} - T^n}{\Delta t} = A(T^n)T^{n+1} + B(T^n)T^{n+1} \tag{2}$$

- Time Splitting (first-order), Same as ”code coupling”.

$$\frac{T^* - T^n}{\Delta t} = A(T^n)T^*, \quad \frac{T^{n+1} - T^*}{\Delta t} = B(T^n)T^{n+1} \tag{3}$$

- Both are sources of time integration error

Modified Equation Analysis (1 of 2)

- Modified Equation Analysis (MEA) example ($T_t \equiv \frac{dT}{dt}$)

$$T_t = T\,, \quad \frac{T^{n+1} - T^n}{\Delta t} = T^{n+1}\,. \tag{4}$$

- Taylor series used to eliminate T^n

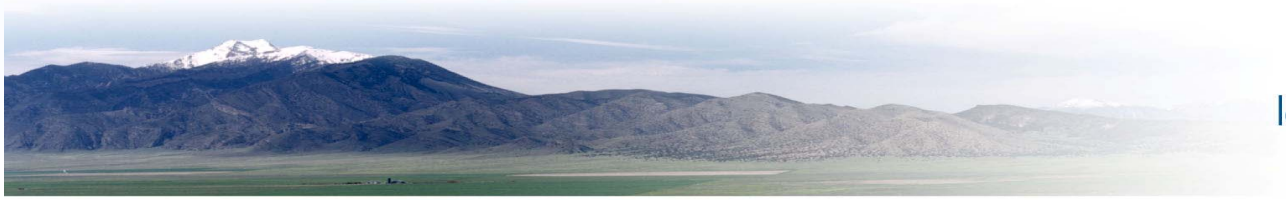
$$T^n = T^{n+1} - \Delta t T_t^{n+1} + \frac{\Delta t^2}{2} T_{tt}^{n+1} - \frac{\Delta t^3}{6} T_{ttt}^{n+1} + O(\Delta t^4)$$

- Original ODE on left side "modified" by nonzero RHS.

$$[T_t - T] = \frac{\Delta t}{2} T_{tt} + \mathcal{O}(\Delta t^2), \tag{5}$$

Modified Equation Analysis (2 of 2)

- History:
  - Nonlinear stability, Hirt, JCP, vol. 2, pp. 339-355 (1968)
  - Accuracy, Warming and Hyett, JCP, vol. 14, pp. 159-179 (1974)
- We will use semi-discrete (time) MEA to begin to analyze numerical errors which arise due to linearization and time splitting.
- D.A. Knoll, et. al., ”On balanced approximations for the time integration of multiple time scale systems”, *J. Comput. Phys.*, vol 185, pp. 583-611 (2003)



Splitting Linear Reaction - Diffusion (1 of 5)

- Model Linear Equation:

$$\frac{\partial T}{\partial t} - D\frac{\partial^2 T}{\partial x^2} = \alpha T, \quad T_{x=0} = T_L, \quad T_{x=1} = T_R$$

- Dynamical Time Scale

$$\frac{1}{\tau_{dyn}} \equiv -(\frac{1}{T}\frac{dT}{dt}) = -\frac{D}{T}\frac{\partial^2 T}{\partial x^2} - \alpha \approx \frac{1}{\tau_{dif}} + \frac{1}{\tau_{reac}},$$

- Normal Mode Time Scales

$$\tau_{dif} \equiv \frac{L^2}{D} \; ; \; \tau_{reac} \equiv -\frac{1}{\alpha},$$

and L is taken as the length of the domain (or solution structure).

Splitting Linear Reaction - Diffusion (2 of 5)

- First order, unsplit:

$$\frac{T^{n+1} - T^n}{\Delta t} - D\frac{\partial^2 T^{n+1}}{\partial x^2} = \alpha T^{n+1}$$

$$T^{n+1}_{x=0} = T_L, \quad T^{n+1}_{x=1} = T_R$$

- First order split (R-D):

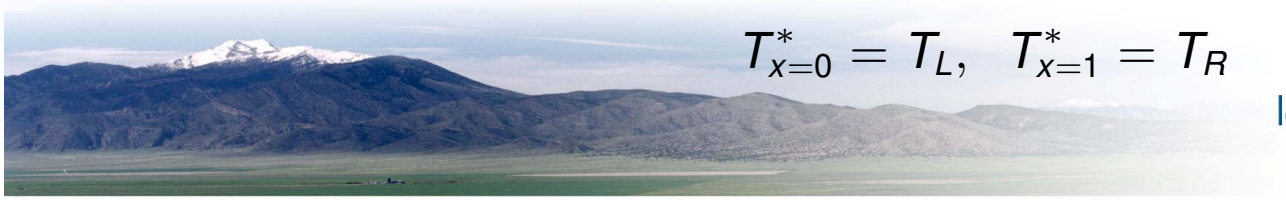
$$\frac{T^* - T^n}{\Delta t} = \alpha T^*, \quad \frac{T^{n+1} - T^*}{\Delta t} - D\frac{\partial^2 T^{n+1}}{\partial^2 x} = 0$$

$$T^{n+1}_{x=0} = T_L, \quad T^{n+1}_{x=1} = T_R$$

- First order split (D-R):

$$\frac{T^* - T^n}{\Delta t} - D\frac{\partial^2 T^*}{\partial^2 x} = 0, \quad \frac{T^{n+1} - T^*}{\Delta t} = \alpha T^{n+1}$$

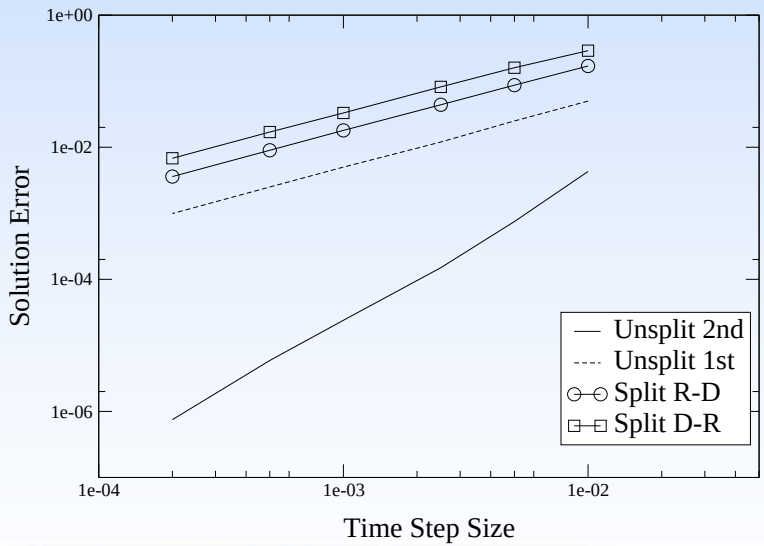
$$T^*_{x=0} = T_L, \quad T^*_{x=1} = T_R$$

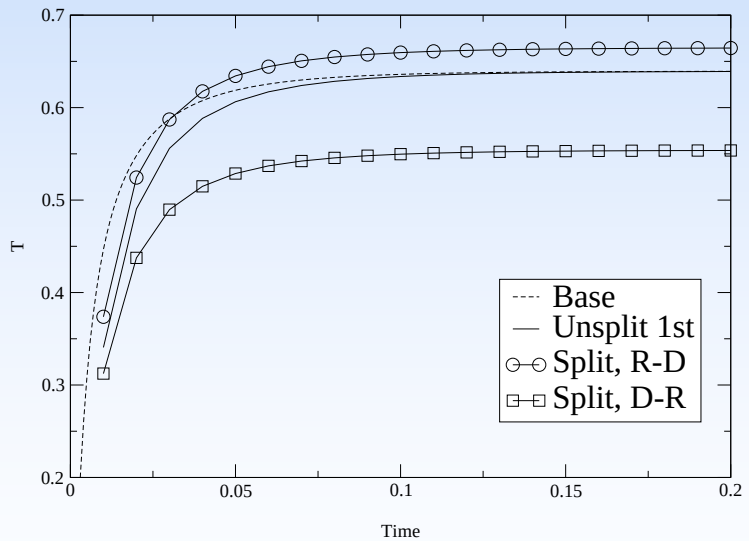


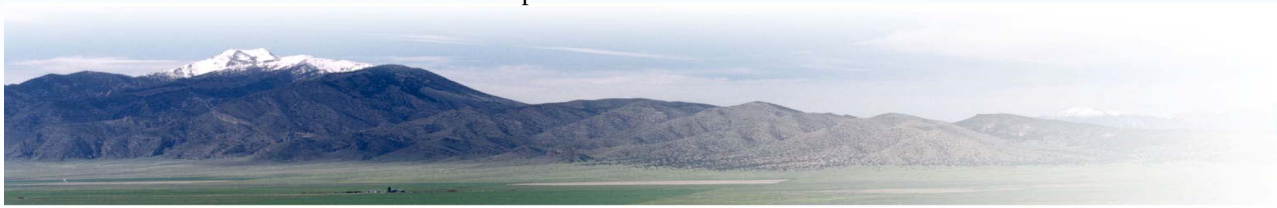
Splitting Linear Reaction - Diffusion (3 of 5)

$$T(t=0)=0, D=1, \alpha=-20, T_L=1, T_R=0,$$

$$\Delta t = 0.01, \alpha\Delta t = -0.2$$







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Splitting Linear Reaction - Diffusion (4 of 5)

- MEA on First order, unsplit, Yields:

$$[T_t - D\frac{\partial^2 T}{\partial x^2} - \alpha T] = \frac{\Delta t}{2} T_{tt} + O(\Delta t^2)$$

- MEA on R-D splitting Yields:

$$[T_t - D\frac{\partial^2 T}{\partial x^2} - \alpha T] = \frac{\Delta t}{2} T_{tt} + \alpha \Delta t D \frac{\partial^2 T}{\partial x^2} + O(\Delta t^2)$$

- MEA on D-R splitting Yields:

$$[T_t - D\frac{\partial^2 T}{\partial x^2} - \alpha T] = \frac{\Delta t}{2} T_{tt} + \alpha \Delta t D \frac{\partial^2 T}{\partial x^2} + O(\Delta t^2)$$

$$T_{x=0} = T_L/(1 - \alpha \Delta t), \quad T_{x=1} = T_R/(1 - \alpha \Delta t)$$

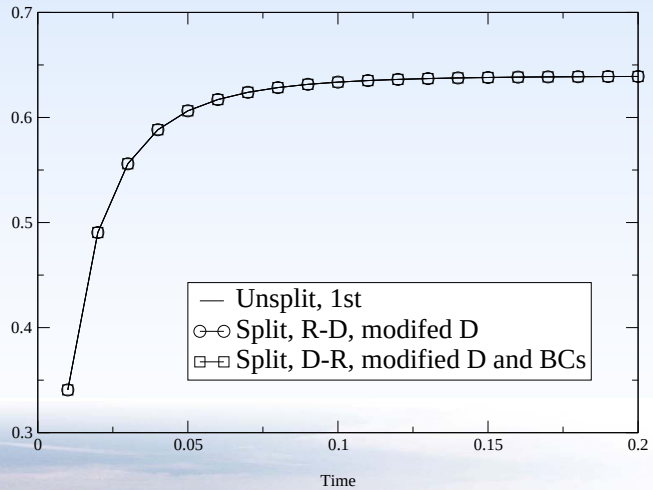
- Splitting errors scale with $\alpha \Delta t$, normal mode.

Splitting Linear Reaction - Diffusion (5 of 5)

- Use D^* in R-D splitting and equate the resulting modified equation to the modified equation from first order unsplit to get:

$$D^* = \frac{D}{1.0 - \alpha \Delta t}$$

- What is the result of using D^* in R-D split simulation ? and What is the result of using D^* and modified BCs in D-R split simulation ?



Linearization and Time Splitting: Some Conclusions

- Can appear to be inaccurate physics model under validation process (Dangerous !)
- Boundary conditions can be impacted
- Time step constraints for accuracy related to normal modes
- Second-order splitting is possible, but continues to be prone to numerical stability and accuracy challenges.
  - Numerical Stability Issues
    D.L Ropp and J.N. Shadid, *J. Comput. Phys.*, vol. 203, pp. 449-466 (2005)
  - Asymptotic Range / Time Step Size
    R.M., Rauenzahn, V.A. Mousseau, D.A. Knoll, *Comput. Phys. Comm.* vol. 172, pp. 109-118 (2005)
    V.A. Mousseau, D.A. Knoll, *Nuc. Sci. Eng.*, vol. 154, pp. 174-189 (2006)

Jacobian-Free Newton-Krylov Methods: A Modern Option

- **Pros:**
  - No splitting or linearization error
  - A clean way to include a variety of nonlinear phenomena
  - Can implement a variety of higher-order time discretizations
  - Opens the door for Sensitivity analysis, data assimilation ....
- **Cons:**
  - Solving Nonlinear problem with iteration
  - Solving full dimensional system implicitly
  - MUST produce effective preconditioner

Newton's Method : Equations

Newton's method solves a system of nonlinear equations of the form,

$$\mathbf{F}(\mathbf{x}) = 0,$$

by a sequence of steps defined by (each a linear problem)

$$\mathbf{J^k}(\mathbf{x}^k)\delta\mathbf{x}^k = -\mathbf{F}(\mathbf{x}^k),$$

where,

$$\mathbf{J}_{i,j}(\mathbf{x}^k) = \frac{\partial \mathbf{F}_i}{\partial \mathbf{x}_j^k},$$

and,

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \delta\mathbf{x}^k.$$

This is continued until

$$\|\mathbf{F}(\mathbf{x}^k)\| < tol_n \|\mathbf{F}(\mathbf{x}^0)\|$$

Jacobian-Free Newton-Krylov: Key Point

Krylov linear iterative methods (CG, GMRES ...) only need the action of the Jacobian matrix to construct the m^{th} iteration of $\delta\mathbf{x}^k$

$$\delta\mathbf{x}_m^k = a_0\mathbf{r}_0 + a_1\mathbf{J}\mathbf{r}_0 + a_2\mathbf{J}^2\mathbf{r}_0 + \ldots + a_m\mathbf{J}^m\mathbf{r}_0$$

where

$$\mathbf{r}_0 = \mathbf{J}^k\delta\mathbf{x}_0^k + \mathbf{F}(\mathbf{x}^k)$$

and

$$\delta\mathbf{x}_0^k = -\mathbf{P}^{-1}\mathbf{F}(\mathbf{x}^k)$$

where $\mathbf{P}^{-1}$ is the preconditioner.
The action of the Jacobian Matrix can be approximated with a single function evaluation

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

Jacobian-Free Newton-Krylov: Key Refs

- Standard “PDE motivated” references:
  P. N. Brown and Y. Saad, *SIAM J. Sci. Stat. Comput.*, **11**, pp. 450-481 (1990)
  Tony F. Chan and Kenneth R. Jackson, *SIAM J. Sci. Stat. Comput.*, **5**, pp. 533-542 (1984)
- Also see the monograph,
  C. T. Kelley, *Iterative Methods for Linear and Nonlinear Equations*, SIAM, Philadelphia, 1995
- Recent JFNK review article from the application perspective
  D.A. Knoll and D.E. Keyes, Jacobian-free Newton-Krylov methods: a survey of approaches and applications, *J. Comput. Phys.*, **193**, pp. 357-397 (2004)

Preconditioning JFNK (1 of 2)

- Using right preconditioning one solves

$$(\mathbf{J}\mathbf{P}^{-1})(\mathbf{P}\delta\mathbf{x}) = -\mathbf{F}(\mathbf{x}). \tag{6}$$

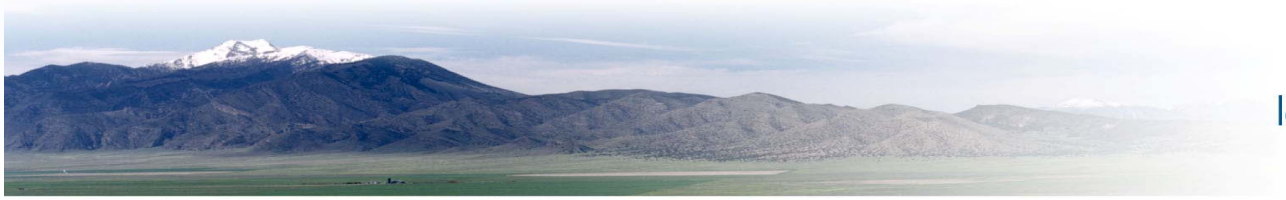
  P symbolically represents the preconditioning matrix (or process) and $\mathbf{P}^{-1}$ the inverse of preconditioning matrix.
- Actually realized through a two-step process. First solve

$$(\mathbf{J}\mathbf{P}^{-1})\mathbf{w} = -\mathbf{F}(\mathbf{x}), \tag{7}$$

  for **w** with the Krylov method. Then solve for $\delta\mathbf{x}$

$$\delta\mathbf{x} = \mathbf{P}^{-1}\mathbf{w}, \tag{8}$$

- Operationally only require the action of $\mathbf{P}^{-1}$ on a vector.

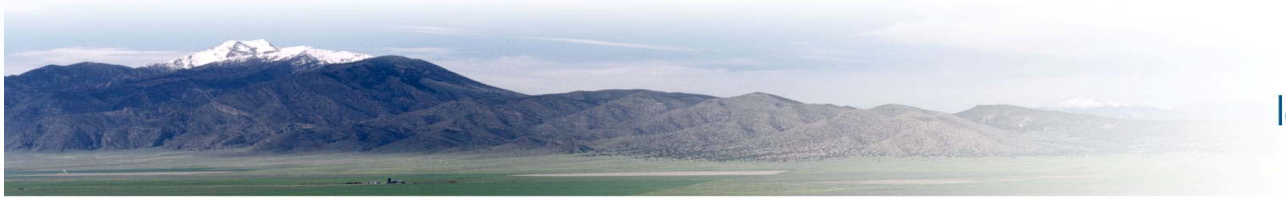


Preconditioning JFNK (2 of 2)

- Right-preconditioned matrix-free version is:

$$\mathbf{J}\mathbf{P}^{-1}\mathbf{v} \approx [\mathbf{F}(\mathbf{x} + \epsilon\mathbf{P}^{-1}\mathbf{v}) - \mathbf{F}(\mathbf{x})] \; / \; \epsilon. \tag{9}$$

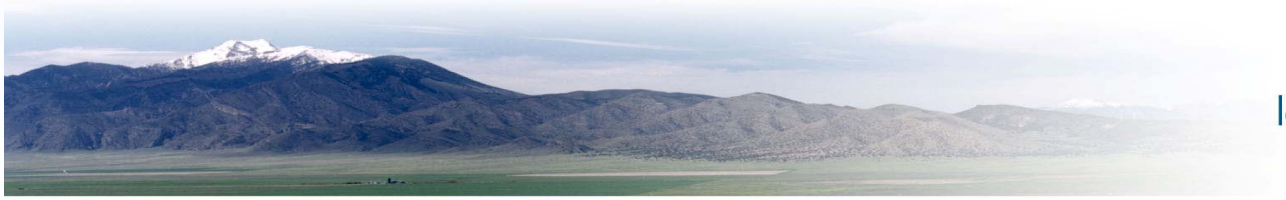
- Required in step 1 of previous slide
- Actually done in two steps ($\mathbf{v}$ is given):
  1. Preconditioning: Solve (approximately) for $\mathbf{y}$ in $\mathbf{y} = \mathbf{P}^{-1}\mathbf{v}$.
  2. Perform matrix-free product $\mathbf{J}\mathbf{y} \approx [\mathbf{F}(\mathbf{x} + \epsilon\mathbf{y}) - \mathbf{F}(\mathbf{x})] \; / \; \epsilon$.
- Only the matrix elements required for the action of $\mathbf{P}^{-1}$ are formed.



Physics-based Preconditioning: Motivation

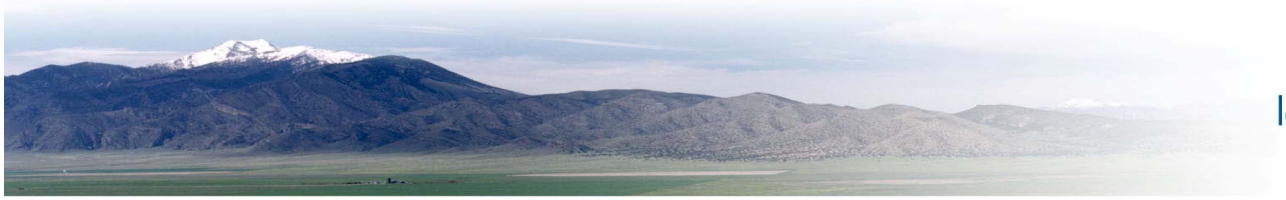
What is an effective choice for P^{-1} ?

- There exist numerous, legacy algorithms to solve multiphysics systems.
- Most are based on linearization and time splitting
- Typically developed with some insight into the time scales or physical behavior of the problem.
- As a benefit of this insight, a reduced implicit system, or a sequence of segregated implicit systems may be solved in place of the fully coupled system.
- We have shown that these legacy algorithms may make excellent preconditioners for JFNK.



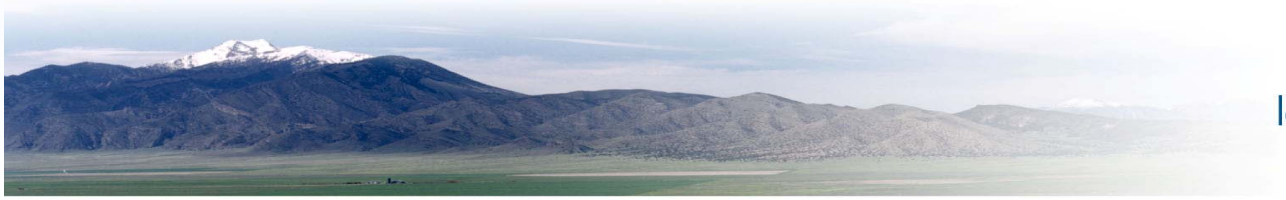
Physics-based Preconditioning: Examples

- Nonequilibrium Radiation Diffusion (Applied Astrophysics)
  V.A. Mousseau, D. A. Knoll and W.J. Rider, *J. Comput. Phys.*, **160**, pp. 743-765 (2000)
- Magnetohydrodynamics (Fusion and Space Weather)
  L. Chacon, D.A. Knoll, and J.M. Finn, *J. Comput. Phys.*, **178**, pp. 15-36 (2002)
- Low speed flow (Hurricane Simulation)
  J.M. Reisner, V.A. Mousseau, A. Wyszogrodzki and D.A. Knoll, *Mon. Wea. Rev.*, **133**, pp. 1003-1022 (2005)
- Solidifying flow (Metal Casting)
  K.J. Evans, D. A. Knoll and M.A. Pernice, *J. Comput. Phys.*, **219**, pp. 404-417 (2006)



Dual use of the method

- Not JFNK vs Linearization / Time Splitting
- Linearization / time splitting can be used as solver or preconditioner within a single code.
- Our view: Combination of JFNK and linearization plus time splitting is the most dependable route to time accurate (2^{nd} order), stable, and efficient methods.

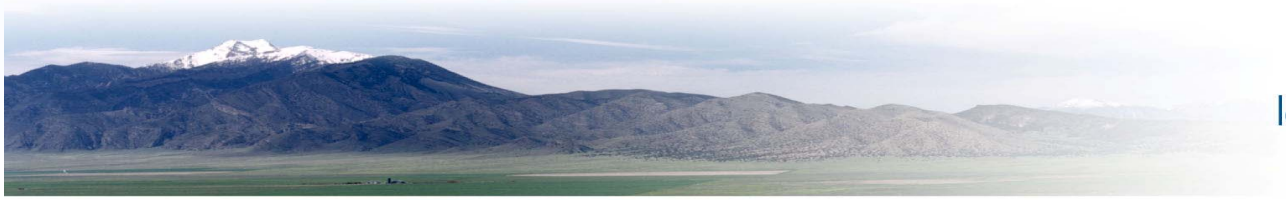


Multiphysics Framework Requirements

- 1D, 2D and 3D with same code
- Massively Parallel
- Fully Coupled
- Fully Implicit
- JFNK Finite Element Based
- Flexible Physics Interface
  - Ability to rapidly develop new capabilities
- Flexible Materials Database
- Error Estimation and Adaptivity
- Portable

MOOSE: *Multiphysics Object Oriented Simulation Environment*

- Meets all of the above requirements and more.

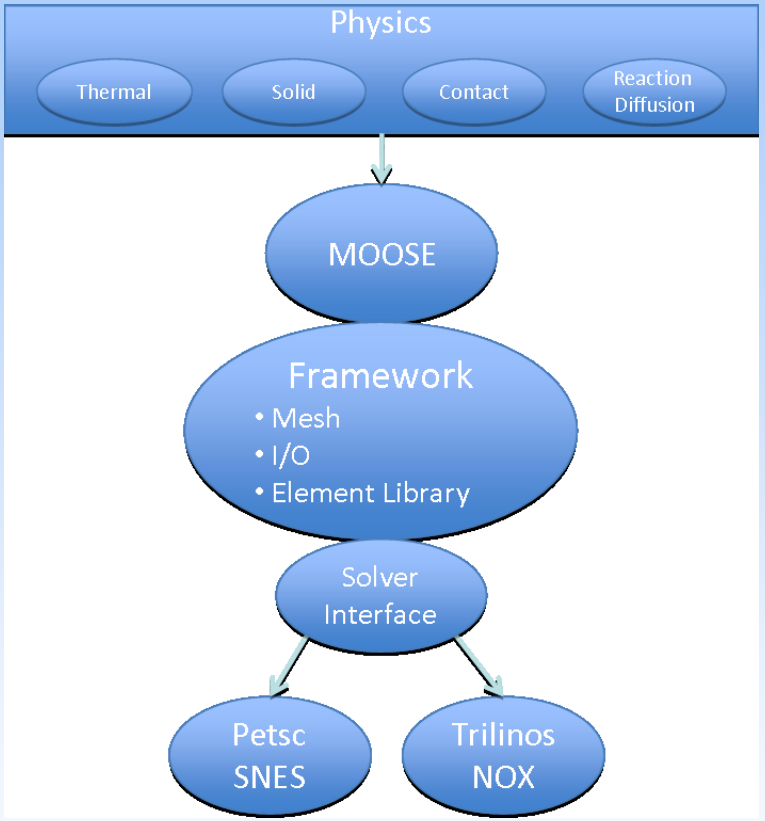


Parallel Algorithms

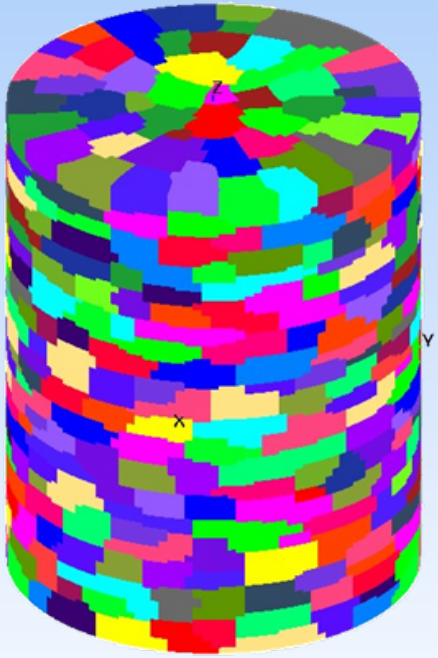
- First and second order Lagrange finite element discretization.
- Residual is calculated in parallel.
  - Off processor contributions assembled in parallel.
  - Element based domain decomposition.
- Parallel solver packages used for JFNK and elliptic system preconditioning.
  - PETSc, ANL
  - Trilinos, SNL

MOOSE – Multiphysics Object Oriented Simulation Environment

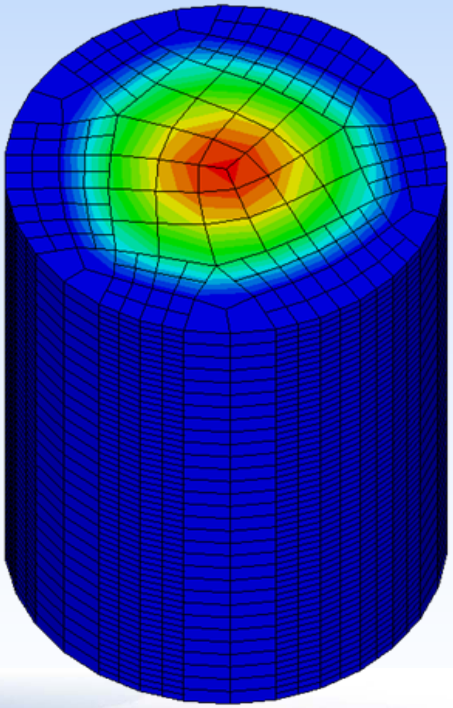
- Multiphysics framework for complex applications development
- Engineering application environment, not "research code"
  - Mesh generation, adaptation, and sensitivity analysis are tightly integrated to form a robust engineering application
- Plug-and-play modules
  - Simplified coupling
- MOOSE Physics Interface conceals framework complexity
- Utilizes state-of-the-art linear and non-linear solvers
  - Robust solvers are key for "ease of use"



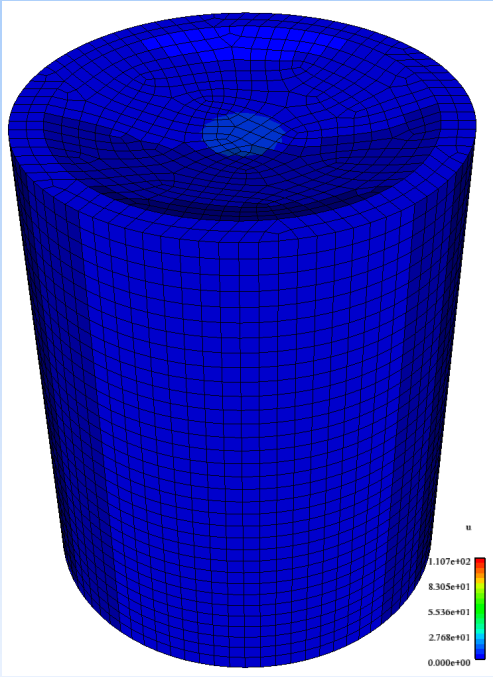
Advanced Capabilities



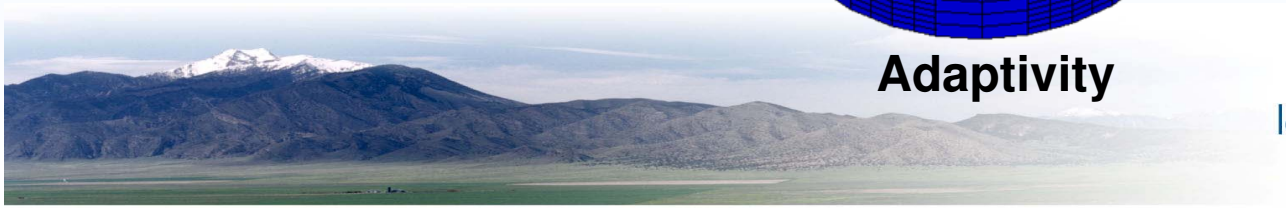
Parallel Decomposition



Adaptivity



Transient Analysis



Future Work

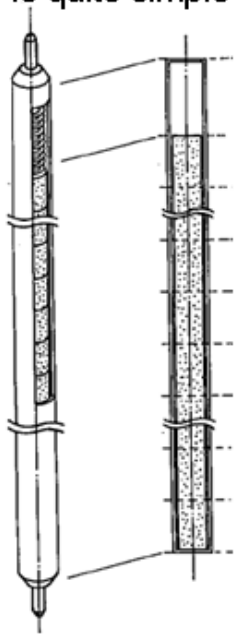
- Advanced physics based preconditioning.
  - De-coupled elliptic solves using multi-grid.
- Adjoint capability.
  - Enhances sensitivity analysis.
  - Enables goal oriented error estimation and adaptivity.
- Finite volume based discrete operator options
- Linking with other libraries.
  - Explore other solver and preconditioning packages.
  - Utilize material databases such as MATPRO.
- Code optimization.

BISON: Motivation and Target Application

- Motivation
  - Develop a predictive capability analysis for reactor fuel performance
  - Efficiently and accurately predict extended burn-up scenarios
- Target Application
  - 3-D, Full pin, extended burn-up cladding integrity
  - Comprehensive pellet–cladding interaction capability
- Capabilities
  - 3-D transient thermomechanics
- Development began in June 2008 !

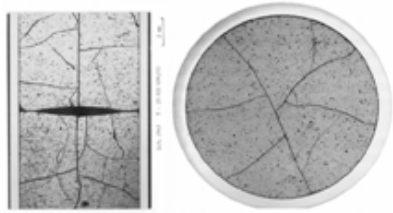
BISON: Nuclear Fuel Issues

At beginning of life, a fuel element is quite simple . . .



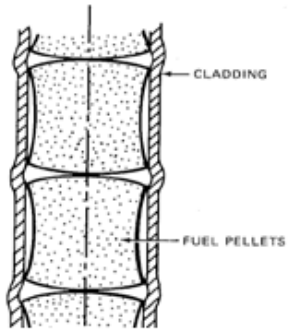
Nakajima et al, Nuc Eng Des, **148**, 41 (1994)

but irradiation brings about substantial complexity



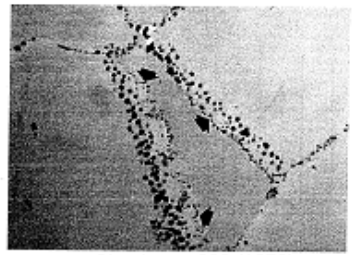
Michel et al, Eng Frac Mech, **75**, 3581 (2008)

Fuel Fracture



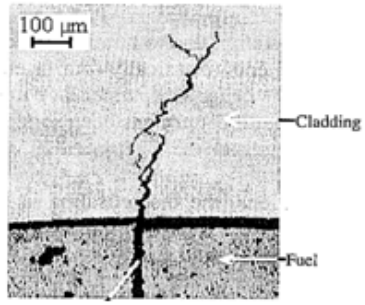
Olander, p. 584 (1978)

Multidimensional contact and deformation



Olander, p. 323 (1978)

Fission gas



Stress Corrosion Cracking Cladding Failure

BISON: Initial Equation Set (1 of 2)

- Nonlinear thermal conduction

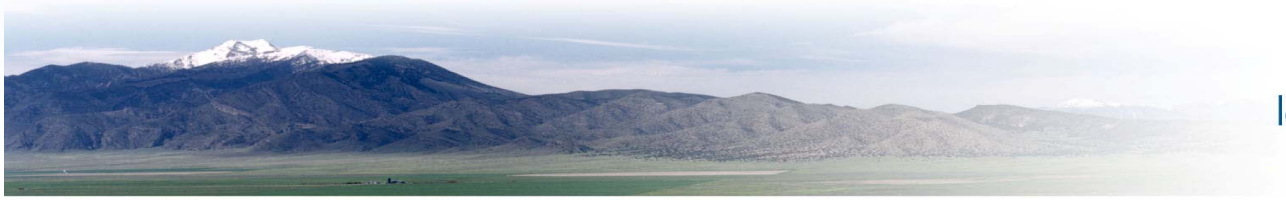
$$\rho C_p T_t + \nabla \cdot k \nabla T - Q = 0$$

  with appropriate boundary conditions

- Nonlinear oxygen non-stoichiometry

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

  with appropriate boundary conditions



BISON: Initial Equation Set (2 of 2)

- Linear elasticity

$$\mathrm{A}^{\mathrm{T}}\mathrm{D}\mathrm{A}u + f = 0,$$

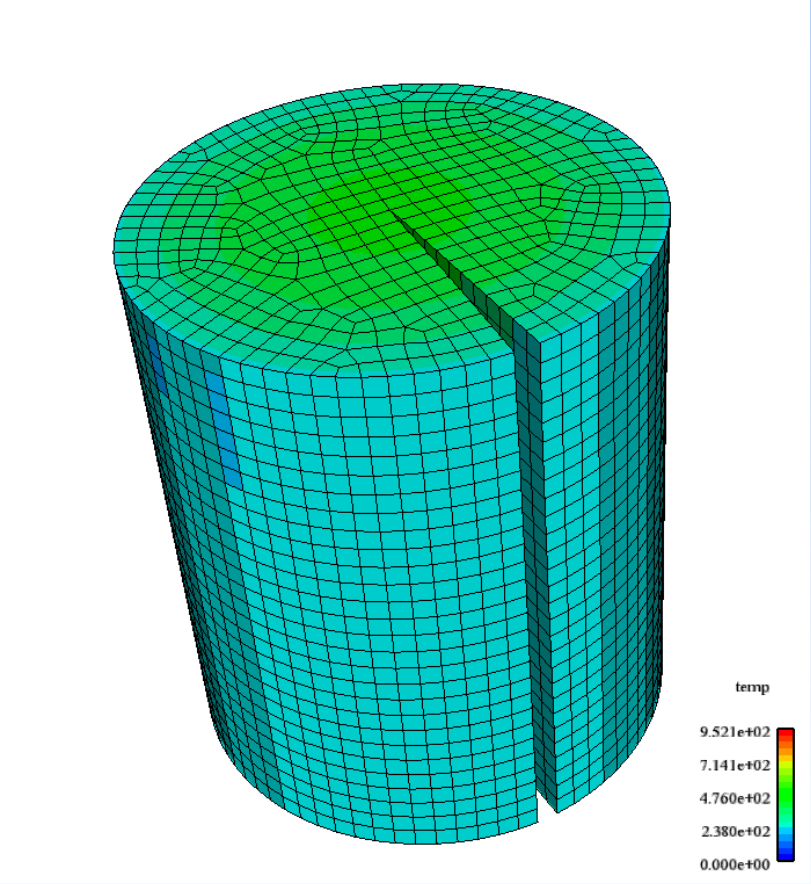
with

$$\mathrm{A} = \begin{bmatrix} \partial_x & 0 & 0 \\ 0 & \partial_y & 0 \\ 0 & 0 & \partial_z \\ \partial_y & \partial_x & 0 \\ 0 & \partial_z & \partial_y \\ \partial_z & 0 & \partial_x \end{bmatrix}, \quad \mathrm{D} = c_1 \begin{bmatrix} 1 & c_2 & c_2 & 0 & 0 & 0 \\ c_2 & 1 & c_2 & 0 & 0 & 0 \\ c_2 & c_2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & c_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & c_3 \end{bmatrix}$$

and $c_1 = \frac{E(1-\nu)}{(1+\nu)(1-\nu)}, c_2 = \frac{\nu}{(1-\nu)}, c_3 = \frac{(1-2\nu)}{2(1-\nu)}$
with appropriate boundary conditions

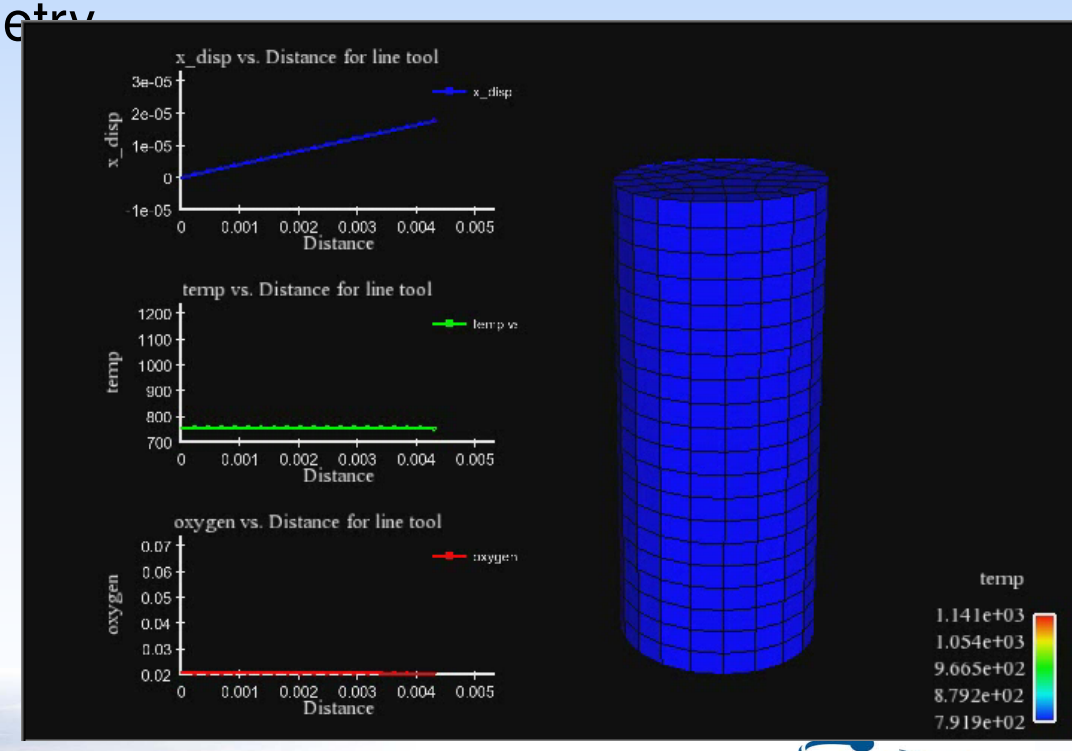
BISON: Example Results

- Coupled transient thermal–solid mechanics



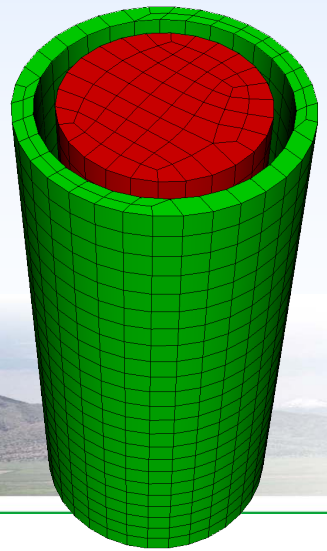
3D Transient Oxygen Diffusion Results

- Transient, fully-coupled thermomechanics and oxygen diffusion
- Inset shows 3D transient displacement X 100, colored by temperature. X-Y plots show radial displacement, temperature, and oxygen hyperstoichiometry



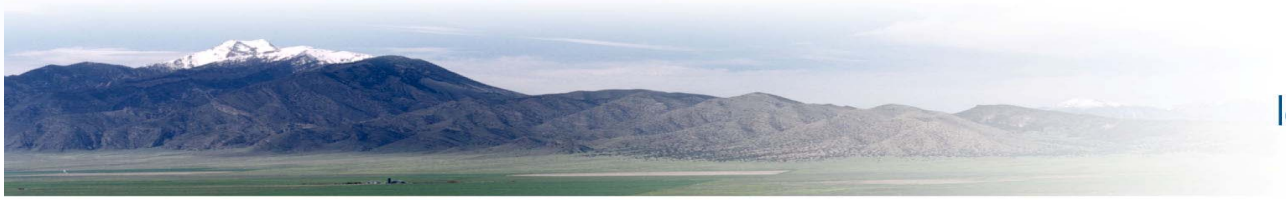
BISON: Near term plan

- Fission gas model, gap heat transfer, nonlinear mechanics, Dec 2008
- FRAPCON / FRAPTRAN test suite, March 2009
- 3-D Pellet-Cladding Mechanical Interaction, June 2009
- Benchmark with ABAQUS pellet-gap-clad model, July 2009
- 3-D multiphysics transient simulation in parallel, initial study of crack impacts on cladding deformation, Dec 2009 (1.5 years into project)



PRONGHORN: Motivation and Target Application

- Motivation
  - Base thermal solver for 3-D steady-state and transient pebble bed gas-cooled reactor. Many researches rely on standard codes (e.g. THERMIX) and use as a black box. (THERMIX is only 2D)
  - Coupled thermal-neutronics solver
- Target Applications
  - Use to study 3-D transient phenomena
  - study multiphysics boundary layer with extended physical model
- Development began in mid-September 2008 !



PRONGHORN: Initial Equation Set (1 of 2)

- Steady-state Thermal-Fluid Model (Darcy-like flow model) (solving for $P, \rho\vec{u}, T_f, T_s, \quad P = \rho R T_f$)
- Momentum (W is porous media friction model)

$$\nabla P - \epsilon\rho\vec{g} + W\rho\vec{u} = 0$$

- Continuity ($\nabla \cdot \rho\vec{u} = 0$)

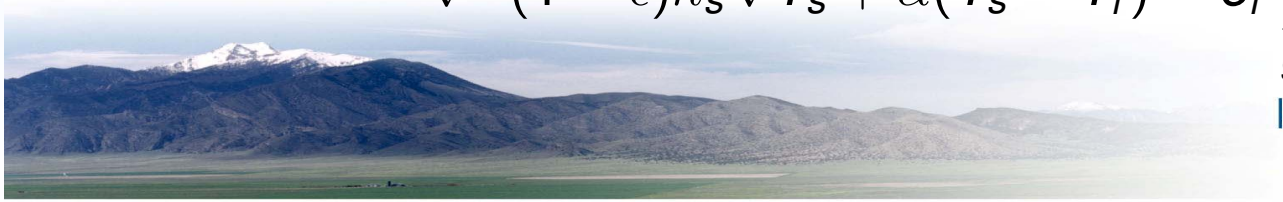
$$-\nabla \cdot \frac{1}{W}\nabla P + \nabla \cdot \frac{\epsilon\rho\vec{g}}{W} = 0$$

- Fluid Energy

$$\nabla \cdot (\rho c_{pf} u T_f) - \nabla \cdot \epsilon\kappa_f \nabla T_f + \alpha(T_f - T_s) = 0$$

- Solid Energy

$$-\nabla \cdot (1-\epsilon)\kappa_s \nabla T_s + \alpha(T_s - T_f) - e_f \sum_{g=1}^{g=G} \Sigma_{fg}\phi_g = 0$$

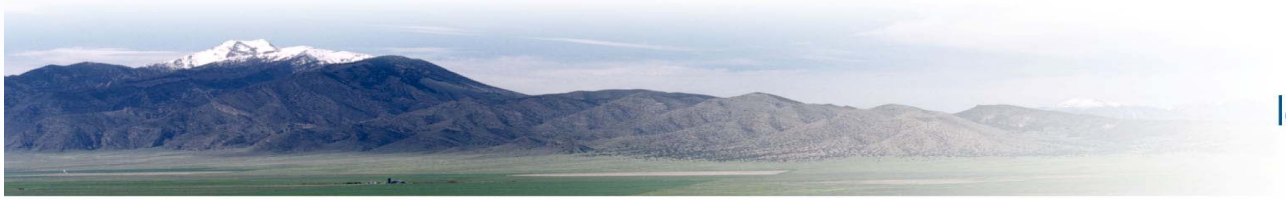


PRONGHORN: Initial Equation Set (2 of 2)

- Neutronics Model (Multigroup diffusion)

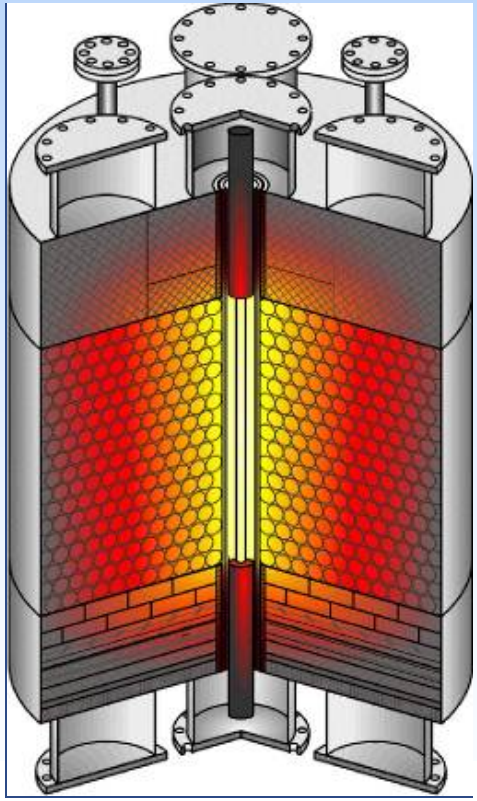
$$-\nabla \cdot D_g \nabla \phi_g + \Sigma_{ag}\phi_g - \chi_g \sum_{g'=1}^{g=G} \nu\Sigma_{fg'}\phi'_g - \sum_{g'=1,g'\neq g}^{g'=G} \Sigma_s^{g'\rightarrow g}\phi_{g'} = 0$$

- D Σ_a $\Sigma_f\Sigma_s$ are generally function of density and temperature (leads to nonlinear equations)



SANA Test

A series of thermal experiments were conducted at SANA test facility.

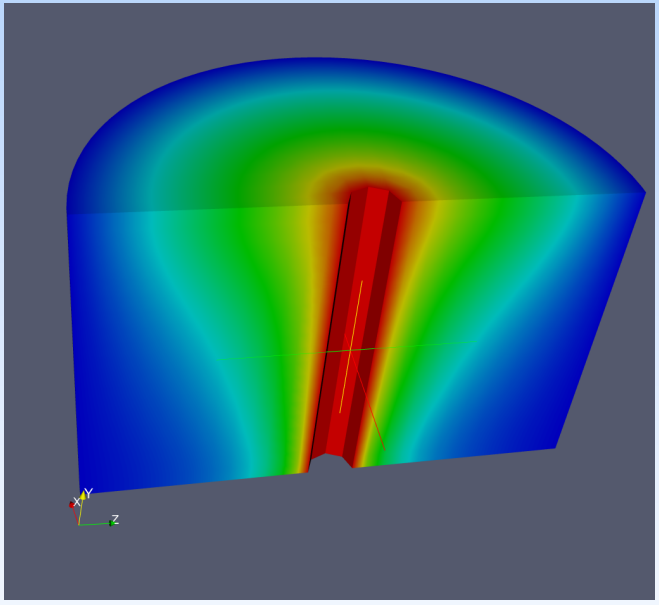


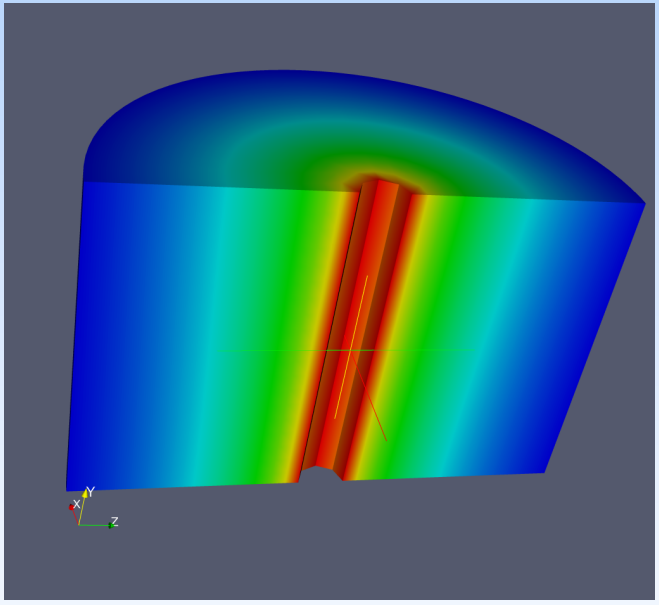
- Installed electrical power 50kW
- Diameter of the pebble bed 1.5m
- Height of the pebble bed 1.0m
- Complete height 3.2m
- Pebble diameter 60mm

Initial result SANA Test

- Fluid Temperature

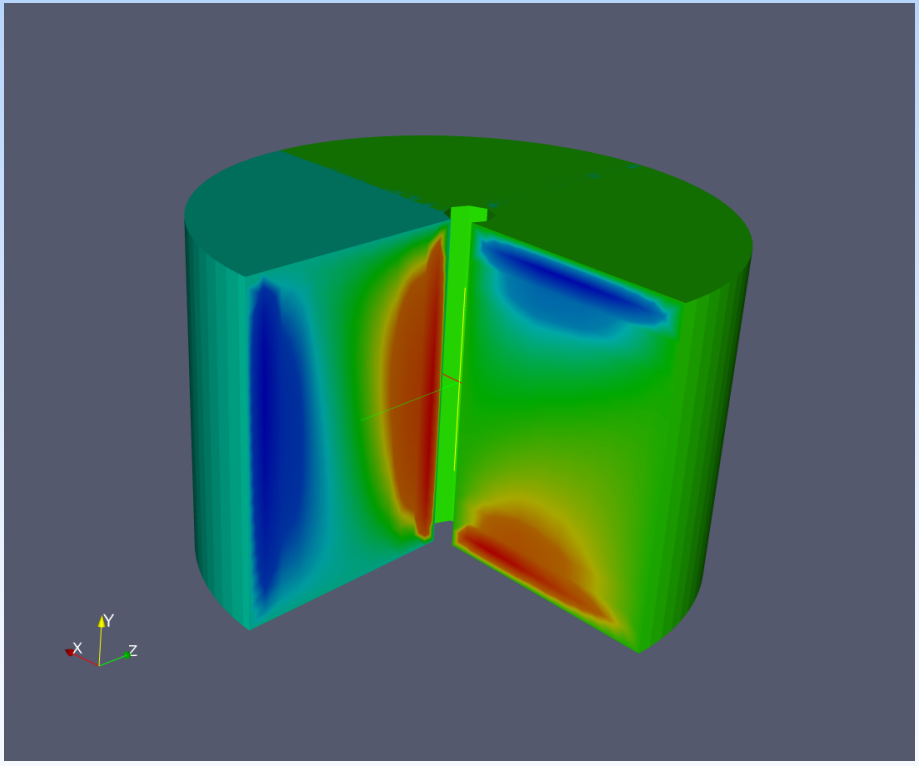
Solid Temperature





Initial result SANA Test, cont.

- Fluid Momentum



PRONGHORN: CPU effort and near term plan

- Rough computational cost
  - total DOF $\approx$ 90000 (6 DOFs/node)
  - CPU time $\approx$ 5min (on workstation with 4 procs)
- Initial validation of steady-state thermal solver with SANA experiment, Jan 2009
- Coupled thermal-neutronics simulation PBMR 400 benchmark, March 2009
- Couple to INL nodal neutronics model, March 2009
- 3-D multiphysics transient simulation in parallel, May 2009 (9 months into project)

Conclusions

- Multiphysics simulation is the next frontier in computational nuclear engineering
- Current algorithms leave open the question of accuracy and stability.
- Jacobian-Free Newton-Krylov (JFNK) methods and physics-based preconditioning provide a modern option.
- Multiphysics Object-Oriented Software Environment, MOOSE, is allowing for rapid, 3-D, parallel, multiphysics application tool development