

# Massively Parallel Monte Carlo Methods for Discrete Linear and Nonlinear Systems

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- Predictive modeling and simulation enhances engineering capability
- Modern work focused on this task leverages multiple physics simulation (CASL, NEAMS)
- New hardware drives algorithm development (petascale and exascale)
- Monte Carlo methods have the potential to provide great improvements that permit finer simulations and better mapping to future hardware
- A set of massively parallel Monte Carlo methods is proposed to advance multiple physics simulation on contemporary and future leadership class machines



## Predictive nuclear reactor analysis enables...

- Tighter design tolerance for improved thermal performance and efficiency
- Higher fuel burn-up
- High confidence in accident scenario models

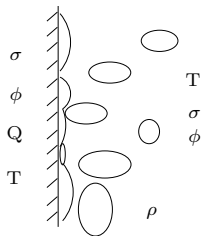
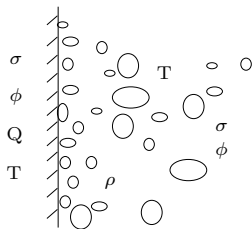


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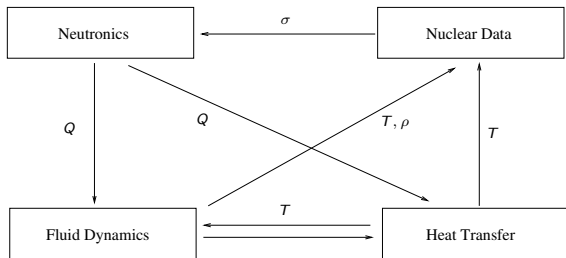
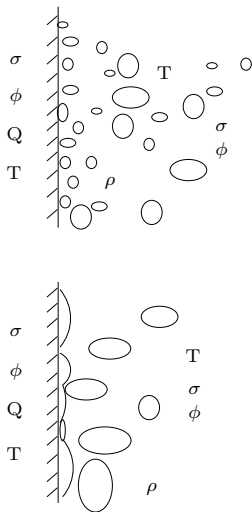
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## Multiple physics simulations are complicated...

- Neutronics, thermal hydraulics, computational fluid dynamics, structural mechanics, and many other physics
- Consistent models yield nonlinearities in the variables through feedback effects
- Tremendous computational resources are required with  $O(1 \times 10^9)$  element meshes and  $O(100,000)+$  cores used in today's simulations.



**Figure: Departure from nucleate boiling scenario.**



**Figure: Multiphysics dependency analysis of departure from nucleate boiling.**

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- Modern hardware is moving in two directions:
  - Lightweight machines
  - Heterogeneous machines
  - Both characterized by low power and high concurrency
- Some issues:
  - Higher potential for both soft and hard failures
  - Memory restrictions are expected with a continued decrease in memory/FLOPS
- Potential resolution from Monte Carlo:
  - Soft failures buried within the tally variance
  - Hard failures are high variance events
  - Possible memory savings over conventional methods



- Parallelization of classic Monte Carlo methods for discrete systems
  - Parallel strategies taken from modern reactor physics methods
  - Research is required to explore varying parallel strategies
  - Scalability is of concern
- Development of a novel nonlinear solver leveraging Monte Carlo
  - Application to nonlinear problems of interest
  - Memory benefits
  - Performance benefits



- We seek solutions of the general linear operator equation

$$\mathbf{Ax} = \mathbf{b}$$

$$\mathbf{A} \in \mathbb{R}^{N \times N}, \mathbf{A} : \mathbb{R}^N \rightarrow \mathbb{R}^N, \mathbf{x} \in \mathbb{R}^N, \mathbf{b} \in \mathbb{R}^N$$

$$\mathbf{r} = \mathbf{b} - \mathbf{Ax}$$

- $\mathbf{r} = \mathbf{0}$  when an exact solution is found.

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## A Requirement

Assert that  $\mathbf{A}$  is *nonsingular*. The solution is then:

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

- General stationary methods are formed by splitting the linear operator

$$\mathbf{A} = \mathbf{M} - \mathbf{N} .$$

$$\mathbf{x} = \mathbf{M}^{-1}\mathbf{N}\mathbf{x} + \mathbf{M}^{-1}\mathbf{b} .$$

- We identify  $\mathbf{H} = \mathbf{M}^{-1}\mathbf{N}$  as the *iteration matrix*

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

- The qualities of the iteration matrix dictate convergence
- Define  $\mathbf{e}^k = \mathbf{x}^k - \mathbf{x}$  as the error at the  $k^{th}$  iterate

$$\mathbf{e}^{k+1} = \mathbf{H}\mathbf{e}^k$$

- We diagonalize  $\mathbf{H}$  to extract its Eigenvalues

$$\|\mathbf{e}^k\|_2 = \rho(\mathbf{H})^k \|\mathbf{e}^0\|_2,$$

- We bound  $\mathbf{H}$  by  $\rho(\mathbf{H}) < 1$  for convergence



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## Search Subspace $\mathcal{K}$

Extract the solution from the search subspace:

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## Constraint Subspace $\mathcal{L}$

Constrain the extraction with the constraint subspace by asserting orthogonality with the residual:

$$\langle \tilde{\mathbf{r}}, \mathbf{w} \rangle = 0, \quad \forall \mathbf{w} \in \mathcal{L}$$

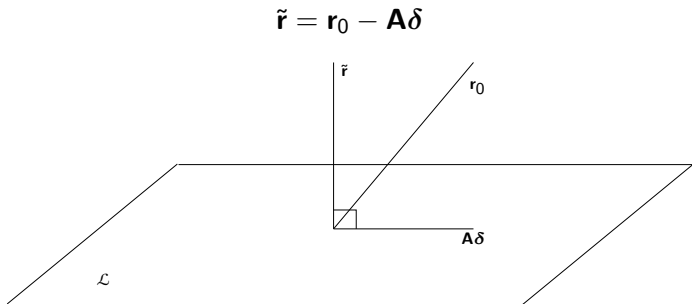


Figure: Orthogonality constraint of the new residual with respect to  $\mathcal{L}$ .



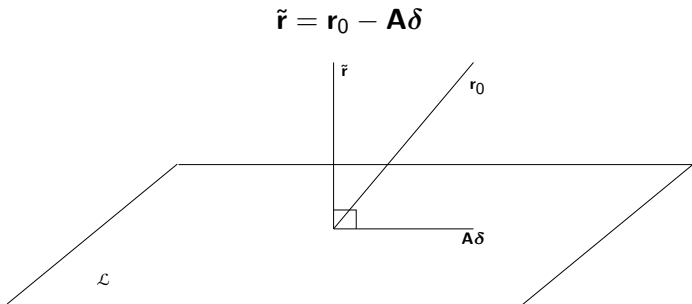


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## Minimization Property

The residual of the system will always be *minimized* with respect to the constraints

$$\|\tilde{\mathbf{r}}\|_2 \leq \|\mathbf{r}_0\|_2, \quad \forall \mathbf{r}_0 \in \mathbb{R}^N,$$

- Choose  $\mathbf{V}$  as a basis of  $\mathcal{K}$  and  $\mathbf{W}$  as a basis of  $\mathcal{L}$

$$\delta = \mathbf{V}\mathbf{y}, \quad \forall \mathbf{y} \in \mathbb{R}^N$$

$$\mathbf{y} = (\mathbf{W}^T \mathbf{A} \mathbf{V})^{-1} \mathbf{W}^T \mathbf{r}_0$$

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## Projection Method Iteration

$$\mathbf{r}^k = \mathbf{b} - \mathbf{A}\mathbf{x}^k$$

$$\mathbf{y}^k = (\mathbf{W}^T \mathbf{A} \mathbf{V})^{-1} \mathbf{W}^T \mathbf{r}^k$$

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \mathbf{V}\mathbf{y}^k$$

*Update  $\mathbf{V}$  and  $\mathbf{W}$*























# Monte Carlo Solution Methods for Nonlinear Problems



















# Proposed Challenge Problem



