Massively Parallel Monte Carlo Methods for Discrete Linear and Nonlinear Systems

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Introduction

- 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

Physics-Based Motivation

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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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.

Physics-Based Motivation: DNB

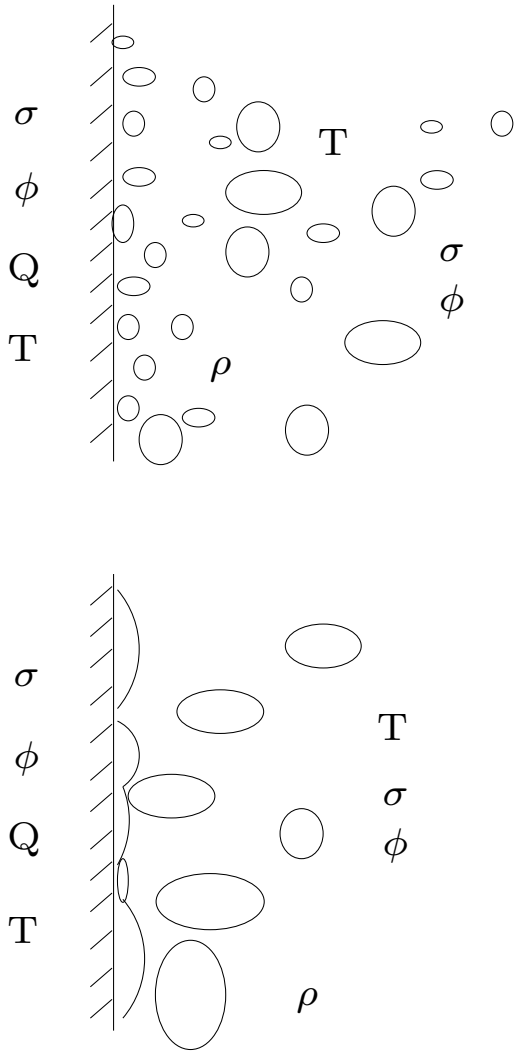

Figure: **Departure from nucleate boiling scenario.**

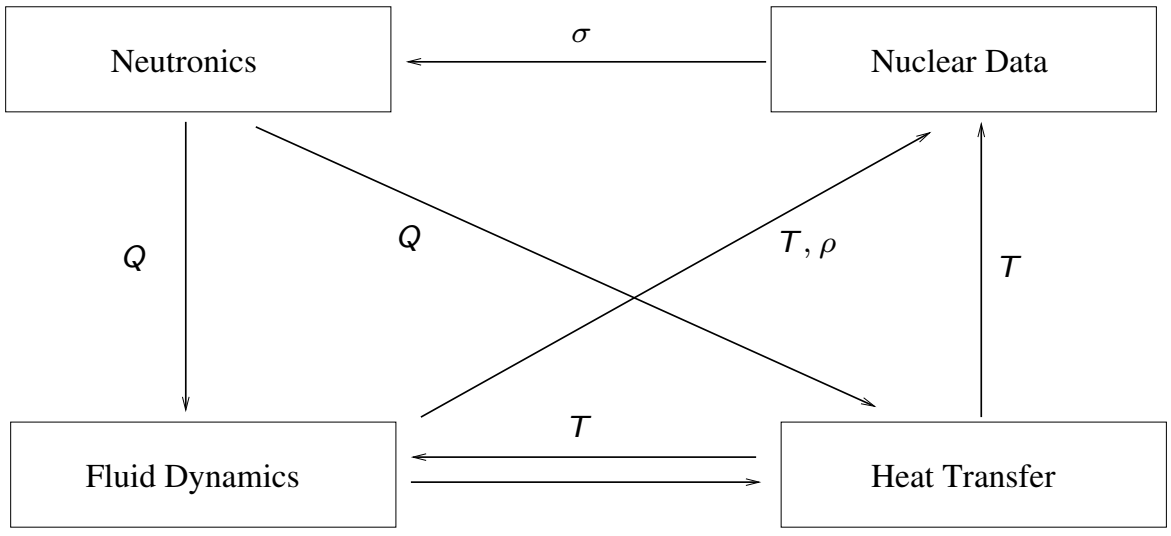

Figure: **Multiphysics dependency analysis of departure from nucleate boiling.**

Hardware-Based Motivation

- Modern hardware is moving in two directions: lightweight machines and heterogeneous machines characterized by low power and high concurrency.
- High concurrency and low cost units means a higher potential for both soft and hard failures.
- Monte Carlo methods bury soft failures within the variance of the tallies while hard failures are high variance events.
- New machines will also be memory restricted with a continued decrease of memory/FLOPS predicted.
- Compared to conventional methods, we aim show that Monte Carlo methods offer a memory savings.

Research Outline

- Parallelization of classic Monte Carlo methods.
- Parallel strategies taken from modern reactor physics methods in Monte Carlo.
- Research is required to explore how domain decomposition patterns and the discrete system properties are related.
- Research is required to explore how these methods perform in modern multiple physics simulations where strong nonlinearities are present.

The Linear Problem

We will seek solutions of the general linear problem:

$$\mathbf{A}\mathbf{x} = \mathbf{b}\,,$$

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

We will assert that $\mathbf{A}$ is *nonsingular*. The solution is then:

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

We can also define the residual of the system as:

$$\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}\,,$$

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

Stationary Methods

- 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*

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

Stationary Methods Convergence

- 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
- The iteration error is generated by a recurrence relation

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

- 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

Projection Methods

We choose a *search subspace* $\mathcal{K}$ and a *constraint subspace* $\mathcal{L}$ and determine the solution to the linear problem by extracting the solution from the search subspace:

$$\tilde{\mathbf{x}} = \mathbf{x}_0 + \boldsymbol{\delta},\ \boldsymbol{\delta} \in \mathcal{K}\ ,$$

and by constraining it with the constraint subspace:

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

We can generate a more physical and geometric-based understanding of these constraints by writing the new residual as:

$$\tilde{\mathbf{r}} = \mathbf{r}_0 - \mathbf{A}\boldsymbol{\delta}$$

If $\tilde{\mathbf{r}}$ is to be orthogonal to $\mathcal{L}$, then $\mathbf{A}\boldsymbol{\delta}$ must be the projection of $\mathbf{r}_0$ onto the subspace $\mathcal{L}$ that eliminates the components of the residual that exist in $\mathcal{L}$.

The Orthogonality Constraint

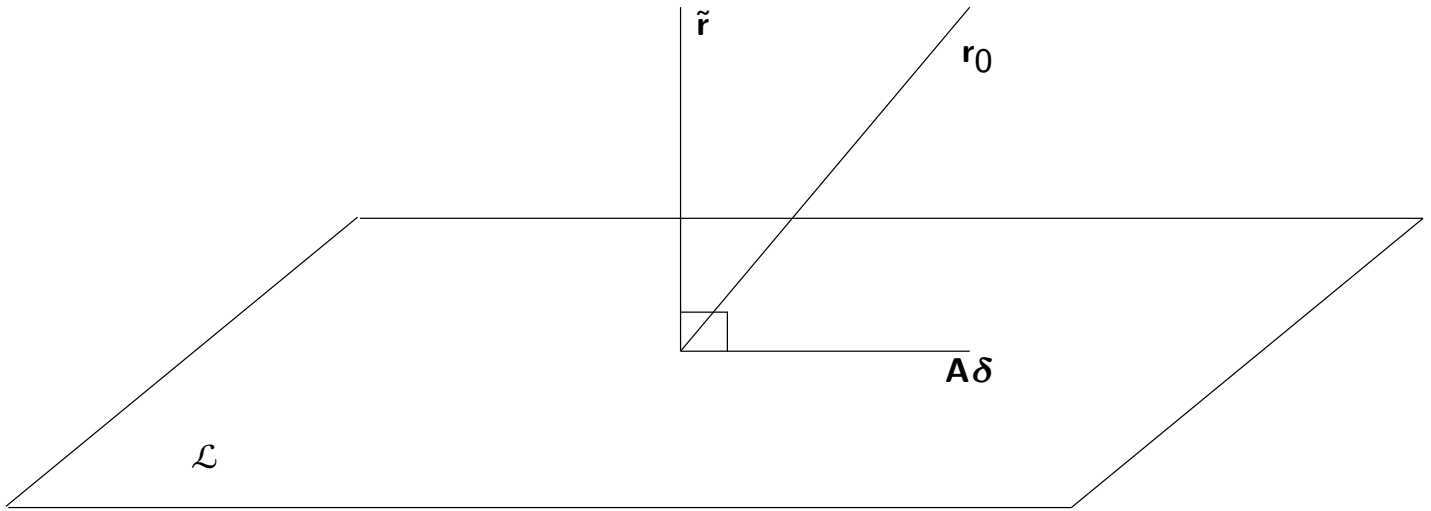

Figure: **Orthogonality constraint of the new residual with respect to $\mathcal{L}$.**

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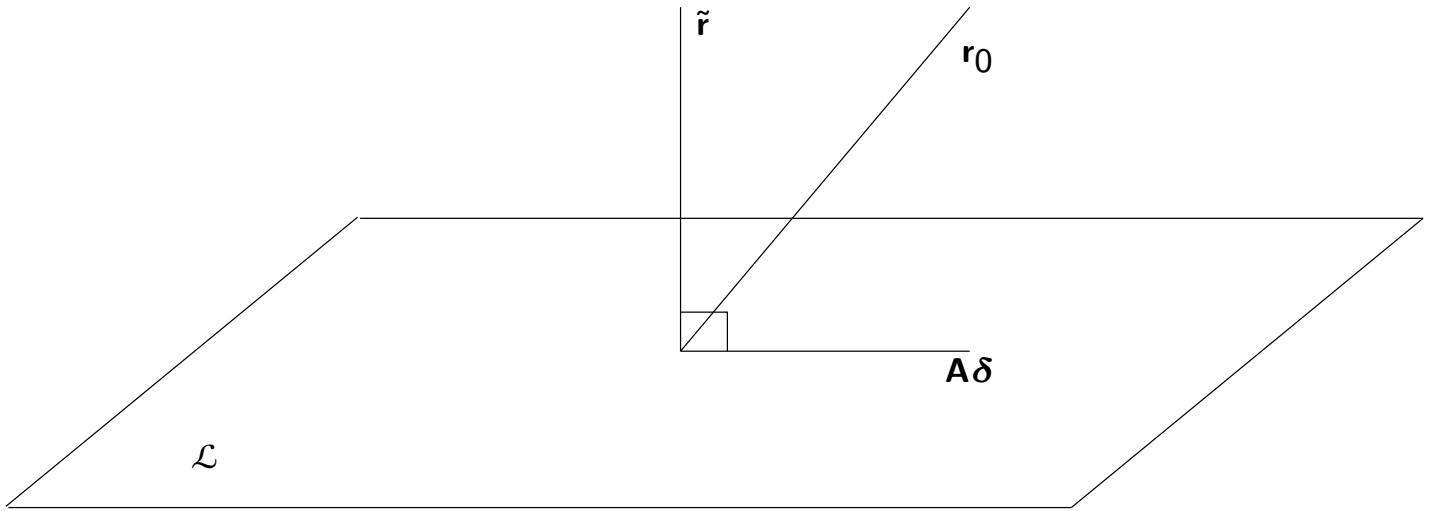

Figure: **Orthogonality constraint of the new residual with respect to $\mathcal{L}$.**

Minimization Property

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

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

Projection Iteration

Consider a matrix $\mathbf{V}$ to form a basis of $\mathcal{K}$ and a matrix $\mathbf{W}$ to form a basis of $\mathcal{L}$.

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

From the orthogonality constraint it then follows that:

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

We can then form an iteration sequence:

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

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

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

with $\mathbf{V}$ and $\mathbf{W}$ updated prior to each iteration.

Krylov Subspace Methods

GMRES

Parallel Projection Methods

Monte Carlo Linear Solver Preliminaries

Direct Method

Adjoint Method

Sequential Monte Carlo

Monte Carlo Synthetic-Acceleration

Parallelization of Stochastic Methods

Monte Carlo Solution Methods for Nonlinear Problems

Monte Carlo Nonlinear Solver Preliminaries

Inexact Newton Methods

The FANM Method

Research Proposal

Experimental Framework

Progress to Date

Monte Carlo Methods Verification

Proposed Numerical Experiments

Proposed Challenge Problem

Conclusion