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

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Predictive nuclear reactor analysis enables...

- Tighter design tolerance for improved thermal performance and efficiency
- Higher fuel burn-up
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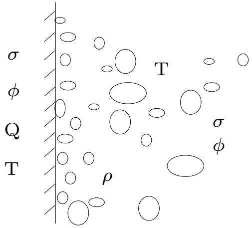
Multiple physics simulations are complicated...

- 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



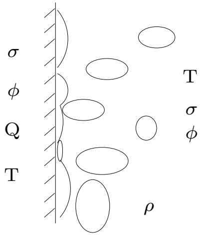


Figure: **Departure from nucleate boiling scenario.**

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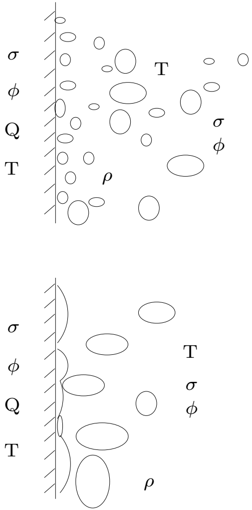

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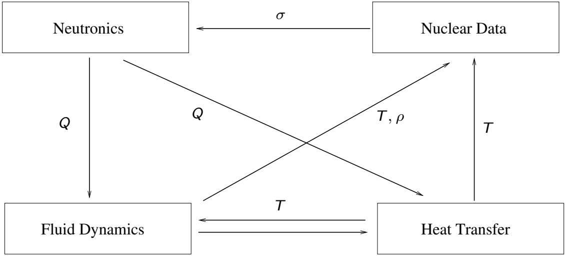

Figure: **Multiphysics dependency analysis of departure from nucleate boiling.**

Hardware-Based Motivation

- 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
  - Memory savings over conventional methods

Research Outline

- Parallelization of 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 nonlinear solver for discrete systems leveraging Monte Carlo
  - Application to nonlinear problems of interest
  - Memory benefits
  - Performance benefits

Linear Operator Equations

- We seek solutions of the general linear operator equation

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

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

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

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

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A Requirement

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

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

Projection Methods

- Powerful class of iterative methods
- Provides theory that encapsulates most other iterative methods
- Leveraged in many modern physics codes at the petascale

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Search Subspace $\mathcal{K}$

Extract the solution from the search subspace:

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

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Search Subspace $\mathcal{K}$

Extract the solution from the search subspace:

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

Constraint Subspace $\mathcal{L}$

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

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

The Orthogonality Constraint

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

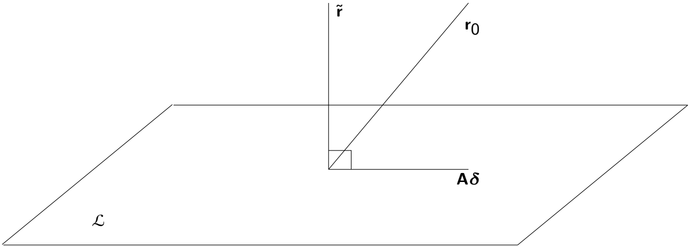

Figure: **Orthogonality constraint of the new residual with respect to $\mathcal{L}$.**

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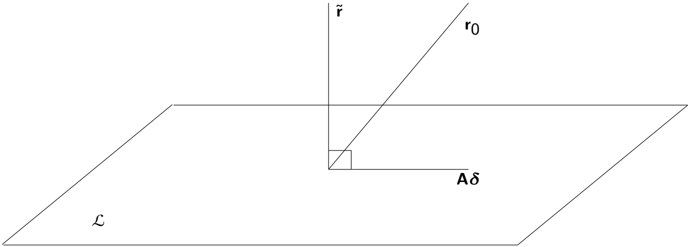

Figure: **Orthogonality constraint of the new residual with respect to $\mathcal{L}$.**

Minimization Property

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

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

Putting It All Together

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

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

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

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Projection Method Iteration

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

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

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

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

Krylov Subspace Methods

$$\mathcal{K}_m(\mathbf{A}, \mathbf{r}_0) = span\{\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \mathbf{A}^2\mathbf{r}_0, \ldots, \mathbf{A}^{m-1}\mathbf{r}_0\}$$

$$\mathcal{L} = \mathbf{A}\mathcal{K}_m(\mathbf{A}, \mathbf{r}_0)$$

- Yields the normal system $\mathbf{A}^T\mathbf{A}\mathbf{x} = \mathbf{A}^T\mathbf{b}$
- Must generate an orthonormal basis $\mathbf{V}_m \in \mathbb{R}^{N\times m}$ for $\mathcal{K}_m(\mathbf{A}, \mathbf{r}_0)$
- $\mathbf{W}_m = \mathbf{A}\mathbf{V}_m$
- Typically choose a Gram-Schmidt-like procedure such as Arnoldi or Lanzcos

GMRES

Algorithm 1 GMRES Iteration

$\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$
$\beta := ||\mathbf{r}_0||_2$
$\mathbf{v}_1 := \mathbf{r}_0/\beta$ {Create the orthonormal basis for the Krylov subspace}
for $j = 1, 2, \cdots, m$ **do**
  $\mathbf{w}_j := \mathbf{A}\mathbf{v}_j$
  for $i = 1, 2, \cdots, j$ **do**
    $h_{ij} \leftarrow \langle \mathbf{w}_j, \mathbf{v}_j \rangle$
    $\mathbf{w}_j \leftarrow \mathbf{w}_j - h_{ij}\mathbf{v}_i$
  end for
  $h_{j+1,j} \leftarrow ||\mathbf{w}_j||_2$
  $\mathbf{v}_{j+1} \leftarrow \mathbf{w}_j / h_{j+1,j}$
end for{Apply the orthogonality constraints}
$\mathbf{y}_m \leftarrow argmin_y ||\beta\mathbf{e}_1 - \mathbf{H}_m\ \mathbf{y}||_2$
$\mathbf{x}_m \leftarrow \mathbf{x}_0 + \mathbf{V_m}\mathbf{y}_m$

Parallel Projection Methods

- Parallel vector update

$$\mathbf{y}[n] \leftarrow \mathbf{y}[n] + a * \mathbf{x}[n],\ \forall n \in [1, N_g]$$

$$\mathbf{y}[n] \leftarrow \mathbf{y}[n] + a * \mathbf{x}[n],\ \forall n \in [1, N_l]$$

- Parallel dot product

$$d_l = \mathbf{y}_l \cdot \mathbf{x}_l,\ d_g = \sum_p d_l$$

- Parallel vector norm

$$||x||_{\infty,l} = \max_n \mathbf{y}[n],\ \forall n \in [1, N_l]$$

$$||x||_{\infty,g} = \max_p ||x||_{\infty,l}$$

Parallel Matrix-Vector Multiplication

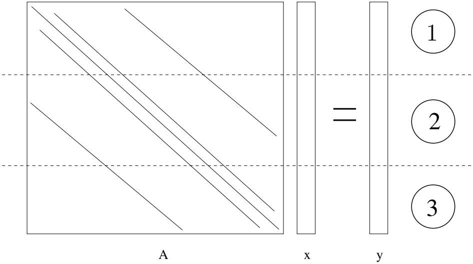

Figure: **Matrix-vector multiply $\mathbf{Ax} = \mathbf{y}$ operation on 3 processors.**

Parallel Matrix-Vector Multiplication

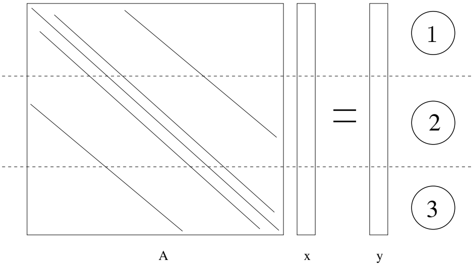

Figure: **Matrix-vector multiply $\mathbf{Ax} = \mathbf{y}$ operation on 3 processors.**

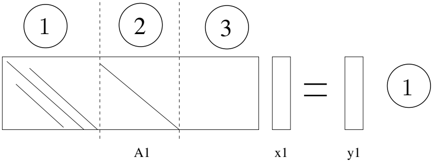

Figure: **Components of multiply operation owned by process 1.**

Projection Methods Summary

- Widely used in practice
- Krylov methods require only the action of the operator
- Parallelism achieved through a handful of operations
- Global reduction operations observed not to impede scalability
  - Dot product
  - Vector norms
- Nearest neighbor computations have poor algorithmic strong scaling
  - Matrix-vector multiply
  - Weak scaling is better
- Short and long recurrence relations available for orthogonalization

Monte Carlo Methods for Discrete Linear Systems

- First proposed by J. Von Neumann and S.M. Ulam in the 1940's
- Earliest published reference in 1950
- General lack of published work
- Modern work by Evans and others has yielded new applications

Monte Carlo Linear Solver Preliminaries

- Split the operator

$$\mathbf{H} = \mathbf{I} - \mathbf{A}$$

$$\mathbf{x} = \mathbf{H}\mathbf{x} + \mathbf{b}$$

- Generate the *Neumann series*

$$\mathbf{A}^{-1} = (\mathbf{I} - \mathbf{H})^{-1} = \sum_{k=0}^{\infty} \mathbf{H}^k$$

- Require $\rho(\mathbf{H}) < 1$ for convergence

$$\mathbf{A}^{-1}\mathbf{b} = \sum_{k=0}^{\infty} \mathbf{H}^k \mathbf{b} = \mathbf{x}$$

Monte Carlo Linear Solver Preliminaries

- Expand the Neumann series

$$x_i = \sum_{k=0}^{\infty} \sum_{i_1}^{N} \sum_{i_2}^{N} \dots \sum_{i_k}^{N} h_{i,i_1} h_{i_1,i_2} \dots h_{i_{k-1},i_k} b_{i_k}$$

- Define a sequence of state transitions

$$\nu = i \rightarrow i_1 \rightarrow \cdots \rightarrow i_{k-1} \rightarrow i_k$$

- Define the *Neumann-Ulam decomposition*[1]

$$\mathbf{H} = \mathbf{P} \circ \mathbf{W}$$

[1] The Hadamard product $\mathbf{A} = \mathbf{B} \circ \mathbf{C}$ is defined element-wise as $a_{ij} = b_{ij} c_{ij}$.

Direct Method

- Compute row-normalized transition probabilities and weights

$$p_{ij} = \frac{|h_{ij}|}{\sum_j |h_{ij}|}, \;\; w_{ij} = \frac{h_{ij}}{p_{ij}}$$

- Generate an expectation value for the solution

$$W_m = w_{i,i_1} w_{i_1,i_2} \cdots w_{i_{m-1},i_m}$$

$$X_\nu(i_0 = i) = \sum_{m=0}^{k} W_m b_{i_m}$$

Direct Method

- Compute the probability of a particular random walk permutation

$$P_\nu = p_{i,i_1} p_{i_1,i_2} \cdots p_{i_{k-1},i_k}$$

- Generate the estimator

$$E\{X(i_0 = i)\} = \sum_\nu P_\nu X_\nu$$

- Check that we recover the exact solution

$$\begin{aligned} E\{X(i_0 = i)\} &= \sum_{k=0}^{\infty} \sum_{i_1}^{N} \sum_{i_2}^{N} \ldots \sum_{i_k}^{N} p_{i,i_1} p_{i_1,i_2} \ldots p_{i_{k-1},i_k} w_{i,i_1} w_{i_1,i_2} \ldots w_{i_{k-1},i_k} b_{i_k} \\ &= x_i \end{aligned}$$

Direct Method: Evolution of a Solution

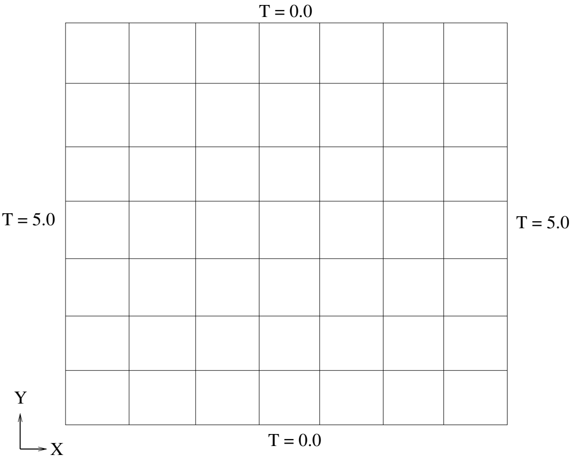

Figure: **Problem setup for 2D heat equation.** *Dirichlet conditions are set for the temperature on all 4 boundaries of the Cartesian grid. No thermal source was present.* 50×50 *grid.*

Direct Method: Evolution of a Solution

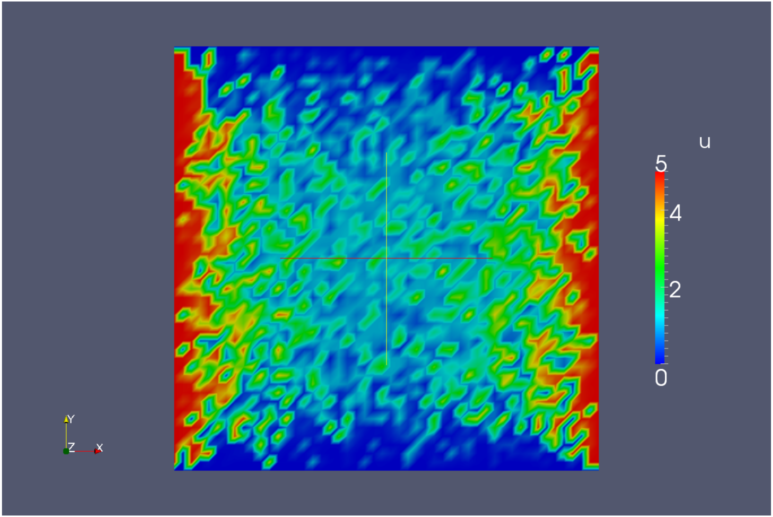

Figure: **Direct solution to Poisson Equation.** *1 history per state,* 2.5×10^3 *total histories. 0.785 seconds CPU time.*

Direct Method: Evolution of a Solution

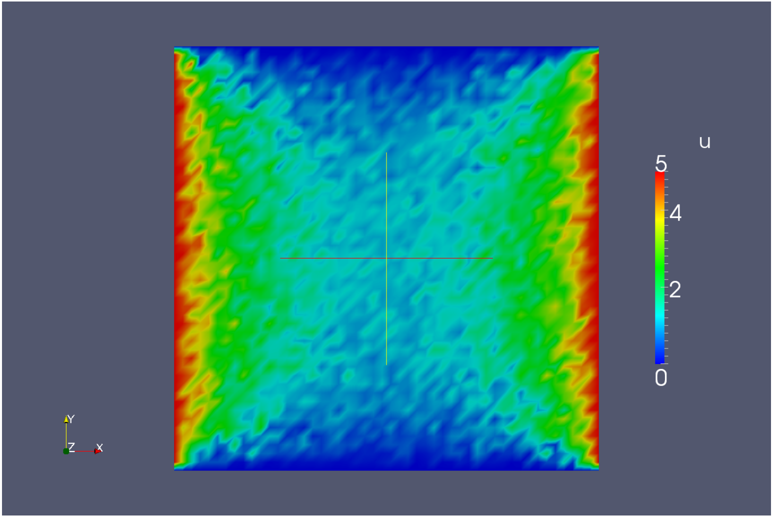

Figure: **Direct solution to Poisson Equation.** *10 histories per state,* 2.5×10^4 *total histories. 5.9 seconds CPU time.*

Direct Method: Evolution of a Solution

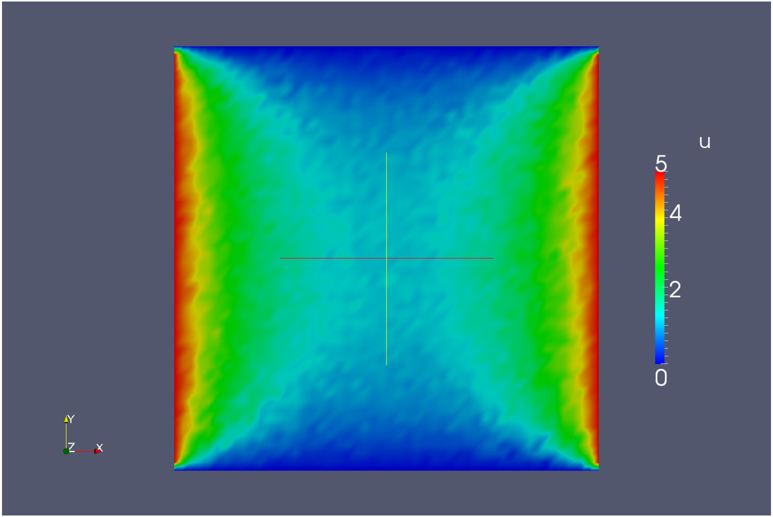

Figure: **Direct solution to Poisson Equation.** *1000 histories per state,* 2.5×10^5 *total histories. 54.7 seconds CPU time.*

Direct Method: Evolution of a Solution

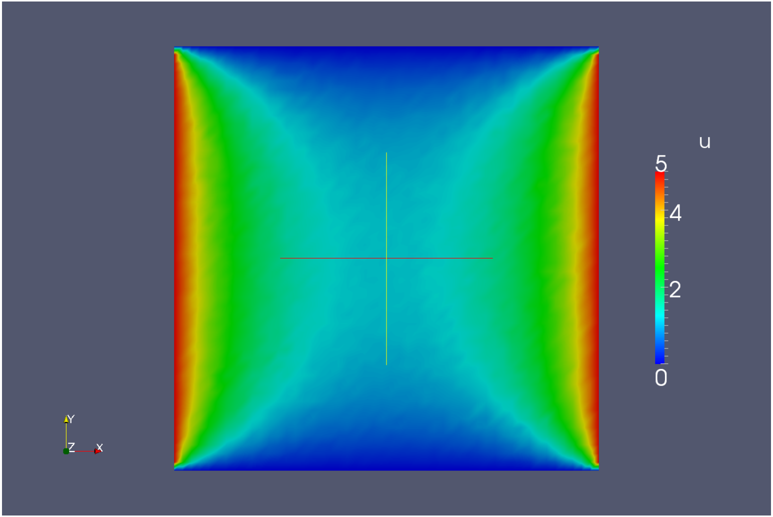

Figure: **Direct solution to Poisson Equation.** *100 histories per state,* 2.5×10^6 *total histories. 644 seconds CPU time.*

Adjoint Method

- Solve the adjoint linear system

$$\mathbf{A}^T\mathbf{y} = \mathbf{d}$$

$$\mathbf{y} = \mathbf{H}^T\mathbf{y} + \mathbf{d}$$

- Set the adjoint constraint

$$\langle \mathbf{A}^T\mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{A}\mathbf{y} \rangle$$

$$\langle \mathbf{x}, \mathbf{d} \rangle = \langle \mathbf{y}, \mathbf{b} \rangle$$

Adjoint Method

- Generate the Neumann series for the adjoint operator

$$\mathbf{y} = (\mathbf{I} - \mathbf{H}^T)^{-1}\mathbf{d}$$

$$\mathbf{y} = \sum_{k=0}^{\infty} (\mathbf{H}^T)^k \mathbf{d}$$

- Expand the series

$$y_i = \sum_{k=0}^{\infty} \sum_{i_1}^{N} \sum_{i_2}^{N} \dots \sum_{i_k}^{N} h_{i_k,i_{k-1}} \dots h_{i_2,i_1} h_{i_1,i} d_{i_k}$$

- Pick another constraint to yield the original solution

$$\mathbf{d} = \boldsymbol{\delta}_i, \ \langle \mathbf{y}, \mathbf{b} \rangle = \langle \mathbf{x}, \boldsymbol{\delta}_i \rangle = x_i$$

Adjoint Method

- Use the adjoint Neumann-Ulam decomposition

$$\mathbf{H}^T = \mathbf{P} \circ \mathbf{W}$$

$$p_{ij} = \frac{|h_{ji}|}{\sum_j |h_{ji}|}, \;\; w_{ij} = \frac{h_{ji}}{p_{ij}}$$

- Build the estimator and expectation value

$$X_\nu = \sum_{m=0}^{k} W_m \delta_{i,i_m}$$

$$E\{X_j\} = \sum_{k=0}^{\infty} \sum_{i_1}^{N} \sum_{i_2}^{N} \dots \sum_{i_k}^{N} b_{i_0} h_{i_0,i_1} h_{i_1,i_2} \dots h_{i_{k-1},i_k} \delta_{i_k,j}$$
$$= x_j$$

Adjoint Method: Evolution of a Solution

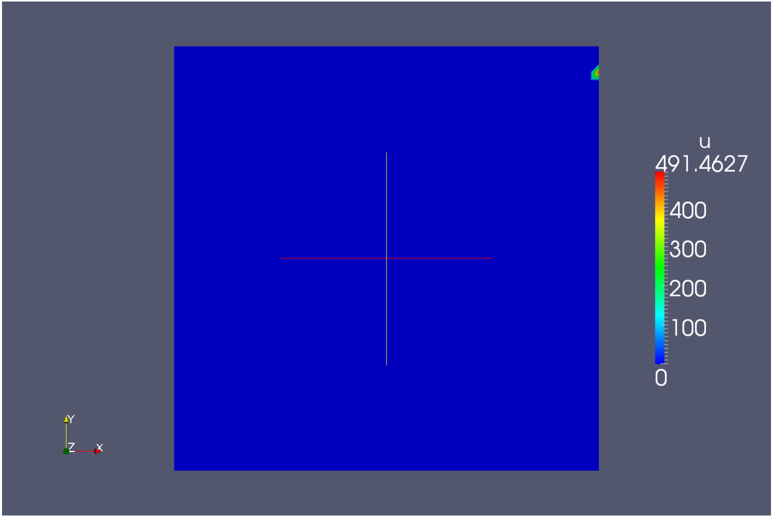

Figure: **Adjoint solution to Poisson Equation.** 1×10^0 *total histories, 0.286 seconds CPU time.*

Adjoint Method: Evolution of a Solution

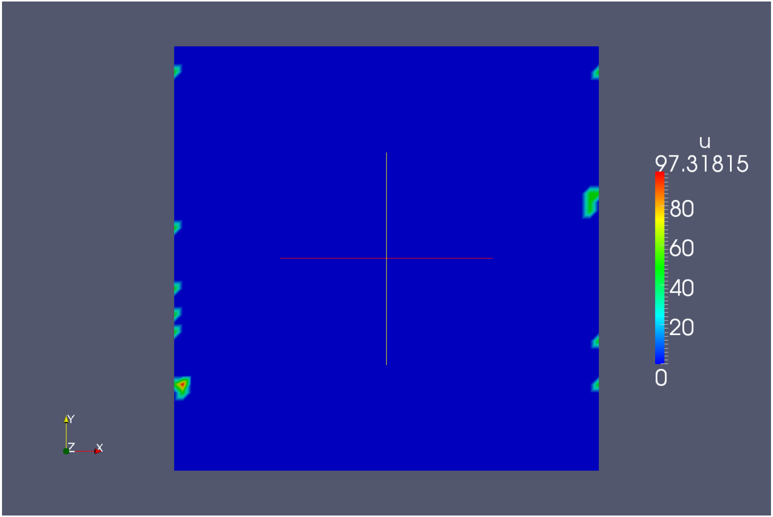

Figure: **Adjoint solution to Poisson Equation.** 1×10^1 *total histories, 0.278 seconds CPU time.*

Adjoint Method: Evolution of a Solution

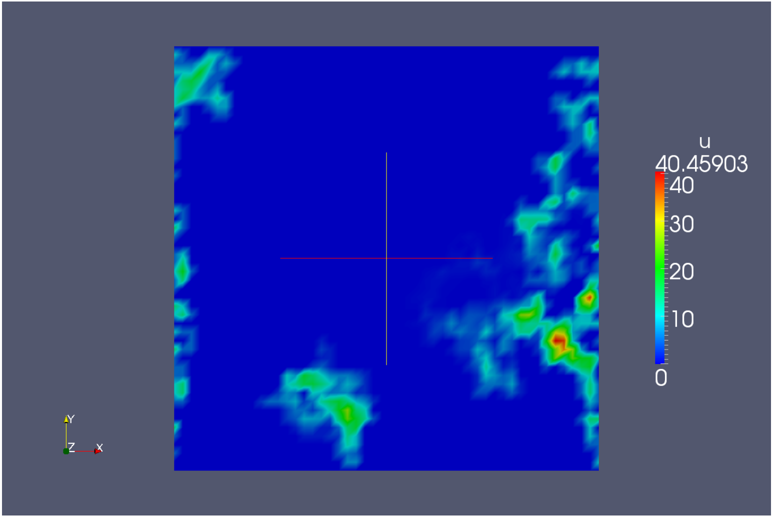

Figure: **Adjoint solution to Poisson Equation.** 1×10^2 *total histories, 0.275 seconds CPU time.*

Adjoint Method: Evolution of a Solution

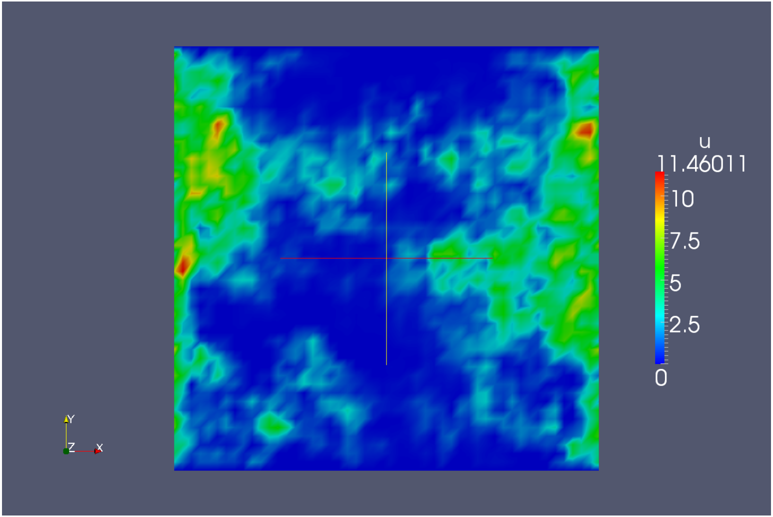

Figure: **Adjoint solution to Poisson Equation.** 1×10^3 *total histories, 0.291 seconds CPU time.*

Adjoint Method: Evolution of a Solution

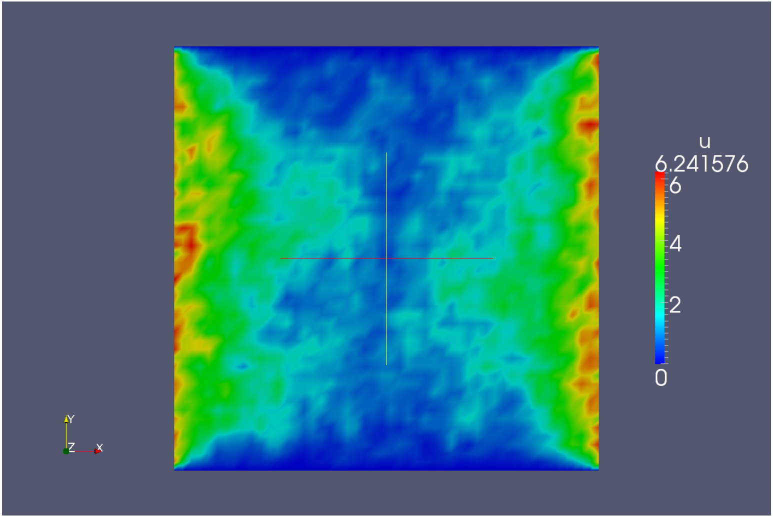

Figure: **Adjoint solution to Poisson Equation.** 1×10^4 *total histories, 0.428 seconds CPU time.*

Adjoint Method: Evolution of a Solution

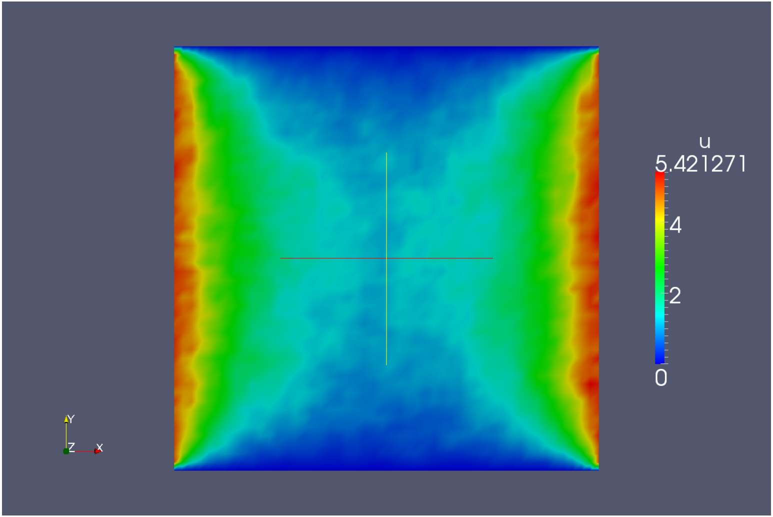

Figure: **Adjoint solution to Poisson Equation.** 1×10^5 *total histories, 1.76 seconds CPU time.*

Adjoint Method: Evolution of a Solution

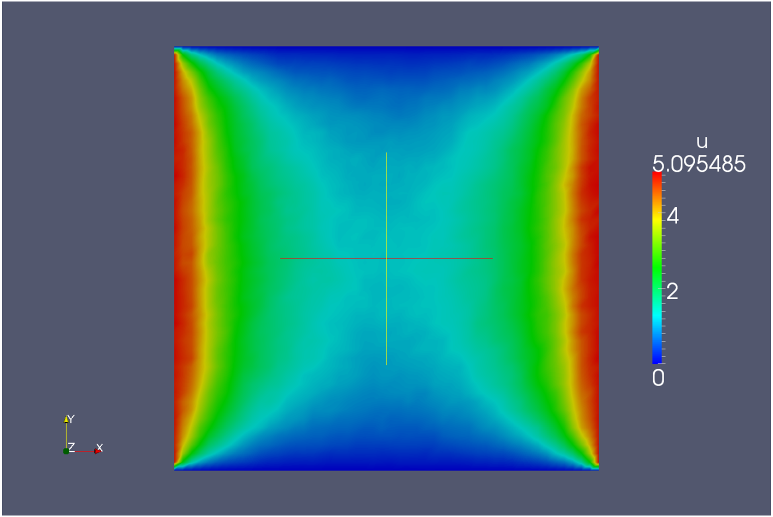

Figure: **Adjoint solution to Poisson Equation.** 1×10^6 *total histories, 15.1 seconds CPU time.*

Adjoint Method: Evolution of a Solution

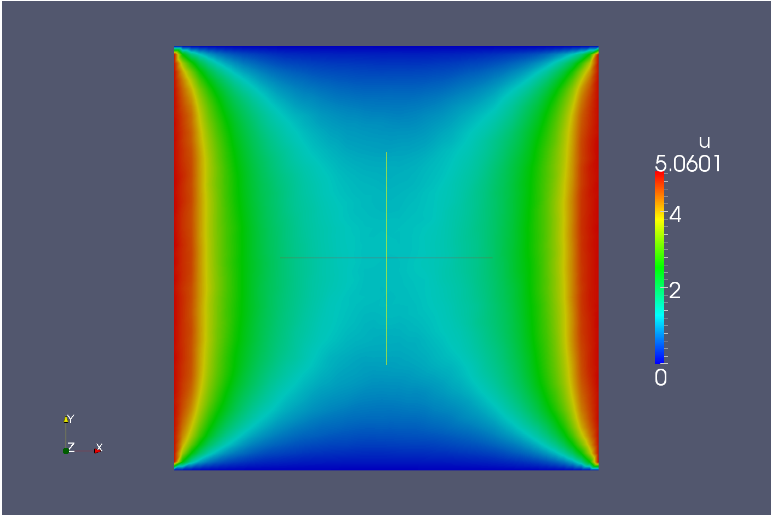

Figure: **Adjoint solution to Poisson Equation.** 1×10^7 *total histories, 149 seconds CPU time.*

Sequential Monte Carlo

- Neumann-Ulam methods bound by the Central Limit Theorem
- Halton proposed an iterative residual method in 1962
- Iteration error decoupled from Monte Carlo error
- Exponential convergence

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

$$\mathbf{A}\boldsymbol{\delta}^k = \mathbf{r}^k$$

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

Monte Carlo Synthetic-Acceleration

- Evans and Mosher 2009 work
- Split the operator to yield Richardson's iteration

$$\mathbf{x} = (\mathbf{I} - \mathbf{A})\mathbf{x} + \mathbf{b}$$
$$\mathbf{x}^{k+1} = (\mathbf{I} - \mathbf{A})\mathbf{x}^{k} + \mathbf{b}$$

- Define the iteration error

$$\delta\mathbf{x}^{k} = \mathbf{x} - \mathbf{x}^{k}$$
$$\delta\mathbf{x}^{k+1} = (\mathbf{I} - \mathbf{A})\delta\mathbf{x}^{k}$$

Monte Carlo Synthetic-Acceleration

- Subtract $(\mathbf{I} - \mathbf{A})\delta\mathbf{x}^{k+1}$

$$\begin{aligned}\mathbf{A}\delta\mathbf{x}^{k+1} &= (\mathbf{I} - \mathbf{A})(\mathbf{x}^{k+1} - \mathbf{x}^{k}) \\ &= \mathbf{r}^{k+1}\end{aligned}$$

- The following converges in one iteration with exact inversion of $\mathbf{A}$:

$$\mathbf{x}^{k+1} = (\mathbf{I} - \mathbf{A})\mathbf{x}^{k} + \mathbf{b}$$

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

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

Monte Carlo Synthetic-Acceleration

MCSA Iteration

$$\mathbf{x}^{k+1/2} = (\mathbf{I} - \mathbf{A})\mathbf{x}^{k} + \mathbf{b}$$

$$\mathbf{r}^{k+1/2} = \mathbf{b} - \mathbf{A}\mathbf{x}^{k+1/2}$$

$$\hat{\mathbf{A}}\delta\mathbf{x}^{k+1/2} = \mathbf{r}^{k+1/2}$$

$$\mathbf{x}^{k+1} = \mathbf{x}^{k+1/2} + \delta\mathbf{x}^{k+1/2}$$

- Adjoint Neumann-Ulam solver computes the correction
- Decouples Monte Carlo error from solution error
- Exponential convergence
- Demonstrated by Evans and colleagues to be competitive with Krylov methods

Preconditioning Monte Carlo Methods

- No symmetry requirements
- Require $\rho(\mathbf{H}) < 1$
- Choose Jacobi preconditioning at a minimum

$$\mathbf{M} = diag(\mathbf{A})$$

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

- Yields a preconditioned MCSA iteration with no in-state transitions

$$\mathbf{x}^{k+1/2} = (\mathbf{I} - \mathbf{M}^{-1}\mathbf{A})\mathbf{x}^{k} + \mathbf{b}$$

$$\mathbf{r}^{k+1/2} = \mathbf{b} - \mathbf{M}^{-1}\mathbf{A}\mathbf{x}^{k+1/2}$$

$$\mathbf{M}^{-1}\mathbf{A}\delta\mathbf{x}^{k+1/2} = \mathbf{r}^{k+1/2}$$

$$\mathbf{x}^{k+1} = \mathbf{x}^{k+1/2} + \delta\mathbf{x}^{k+1/2}$$

Direct vs. Adjoint Analysis

- Analysis needed to select Monte Carlo method
- Time-dependent 2-dimensional Poisson equation
- Spectral radius fixed
- Sparsity varied with 2 Laplacian stencils

$$\nabla_5^2 = \frac{1}{\Delta^2}[u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}]$$

$$\begin{aligned}\nabla_9^2 = \frac{1}{6\Delta^2}[&4u_{i-1,j} + 4u_{i+1,j} + 4u_{i,j-1} + 4u_{i,j+1} + u_{i-1,j-1} \\ &+u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1} - 20u_{i,j}]\end{aligned}$$

- Implicit Euler time differencing

$$\mathbf{A}\mathbf{u}^{n+1} = \mathbf{u}^n$$

Direct vs. Adjoint Analysis

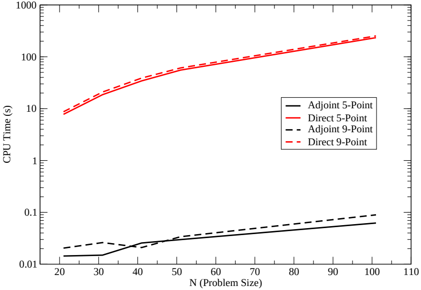

Figure: **CPU Time (s) to converge vs. Problem Size (N for an $N \times N$ square mesh).**

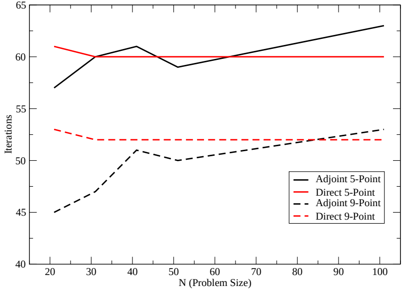

Figure: **Iterations to converge vs. Problem Size (N for an $N \times N$ square mesh).**

Direct vs. Adjoint Analysis

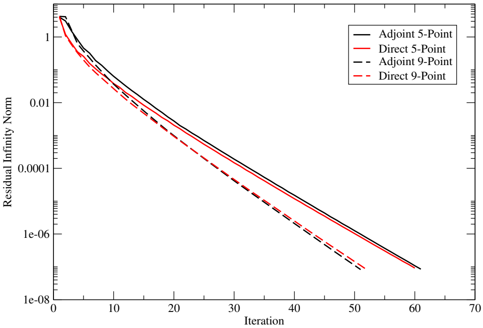

Figure: **Infinity norm of the solution residual vs. iteration number for a problem of fixed size.**

- CPU time dominating factor in method selection
- Significant speedup with adjoint method
- Does not affect convergence behavior
- Use adjoint with MCSA and Sequential Monte Carlo

Generalization of MCSA for Linear Problems

- Published work to date has used a physics-based formulation
  - Radiation transport equations used as model system
  - Transition probabilities built from problem-specific parameters
  - Probabilities and weights must be re-derived for each new equation set
- Desire a generalization for all linear operator equations
  - Requires a general parallel framework
  - Requires implementation with a general linear algebra framework
  - Operator, vector, and graph abstractions
- Neumann-Ulam solvers and MCSA implemented using the Trilinos Petra frameworks
- Can be leveraged in modern physics implementations

Parallelization of Monte Carlo Methods

- No literature observed for parallel Neumann-Ulam solvers
- Numerous references for modern parallel Monte Carlo methods in reactor physics
- Build a strategy for applying modern methods to the Neumann-Ulam method
- MCSA iteration-level parallelism comes from parallel matrix/vector operations

Domain Decomposition

- Each parallel process owns a piece of the domain
- Random walks must be transported across domains through communication

Brunner's Work (2006 and 2009)

- Looked at 4 communication patterns:
  - Fully-locking synchronous
  - asynchronous-send/synchronous-receive
  - master/slave
  - binary tree master/slave
- Binary tree master/slave performed best but race conditions observed
- A later improvement to their work showed a fully asynchronous pattern to work best
- Poor scaling for unbalanced problems

Multiple-Set Overlapping-Domain Decomposition

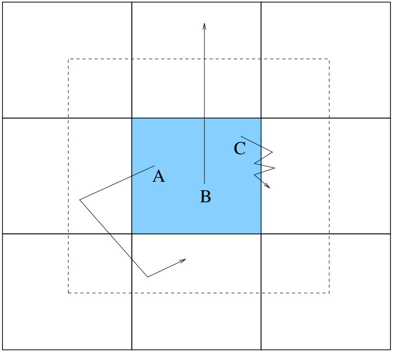

Figure: **Overlapping domain example illustrating how domain overlap can reduce communication costs.**

- Developed by Wagner and colleagues in 2010
- Each set contains the full domain
- Multiple sets replicate the domain
- Domains overlap within a set
- Reduces communication by a significant fraction
- Increases scalability through smaller processor sets
- Redundancy for resiliency (and useful work)

Domain-to-Domain Communication

- The amount of domain leakage dictates communication
- Per Siegel's 2012 work, define a leakage fraction

$$\lambda = \frac{average\ \#\ of\ particles\ leaving\ local\ domain}{total\ of\ \#\ of\ particles\ starting\ in\ local\ domain}$$

- Siegel observed λ to be bound empirically to the mean free path of the system
- Optimum ratio of local to global domain size exists
- Experiments show feasibility for large-scale calculations
  - Not bandwidth or latency limited in load-balanced case

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- Optimum ratio of local to global domain size exists
- Experiments show feasibility for large-scale calculations
  - Not bandwidth or latency limited in load-balanced case
- How do we define λ empirically for linear operator equations?

Load Balancing

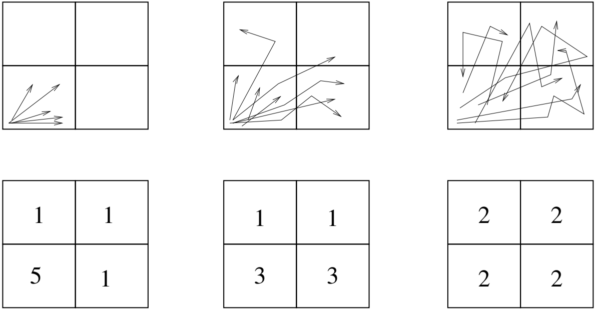

Figure: **Example illustrating how domain decomposition can create load balance issues in Monte Carlo.**

- Procassini's 2005 work addressed some concerns
- Dynamic balancing replicates domains independently
- Linear operator equations may benefit - fixed source problems

Reproducibility

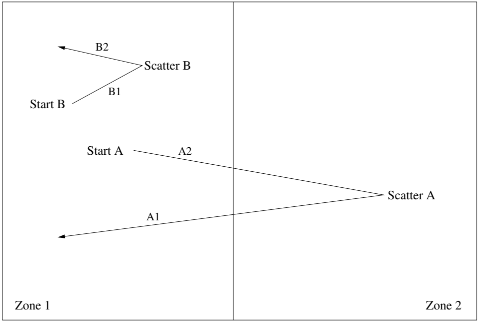

Figure: **Gentile's example illustrating how domain decomposition can create reproducibility issues in Monte Carlo.**

- 2005 work by Gentile outlines reproducibility in parallel Monte Carlo
- Maintaining random number sequences
- Floating point addition does not commute
- Useful for benchmarking and unit testing

Parallel Adjoint Method

Strategy

- Direct analogs between particle transport and Neumann-Ulam solvers
- Aim for MSOD implementation and fully asynchronous communication patterns

Questions

- How much domain overlap is suitable for linear operator equations?
- Is memory a limitation for overlap and replication?
- Do the linear operator properties help select overlap?
- Will full-clip roulette perturb the MCSA solution?
- How much does MSOD facilitate scaling?

Parallel MCSA

MCSA Iteration

$$\mathbf{x}^{k+1/2} = (\mathbf{I} - \mathbf{A})\mathbf{x}^k + \mathbf{b}$$

$$\mathbf{r}^{k+1/2} = \mathbf{b} - \mathbf{A}\mathbf{x}^{k+1/2}$$

$$\hat{\mathbf{A}}\delta\mathbf{x}^{k+1/2} = \mathbf{r}^{k+1/2}$$

$$\mathbf{x}^{k+1} = \mathbf{x}^{k+1/2} + \delta\mathbf{x}^{k+1/2}$$

- Richardson iteration and residual computation require parallel matrix-vector multiply and parallel vector update
- This work will generate a parallel adjoint Neumann-Ulam solver
- Application of correction requires parallel vector update
- Convergence checks through parallel norm computation

Monte Carlo Solution Methods for Nonlinear Problems

- Many multiphysics problems of interest are nonlinear
- Segregated methods lack the consistency of fully implicit methods
- Newton methods often leverage Krylov solvers
  - Robust implementations
  - No operator required
  - Memory intensive
- Monte Carlo methods need the full operator
- Automatic construction of the linear operator available
  - Ideal for Monte Carlo
  - Relaxes memory requirements
  - Potential scaling improvements
  - Resiliency benefits

Nonlinear Preliminaries

- We seek solutions of the general nonlinear problem

$$\mathbf{F}(\mathbf{u}) = \mathbf{0}$$
$$\mathbf{u} \in \mathbb{R}^n,\ \mathbf{F} : \mathbb{R}^N \to \mathbb{R}^N$$

- We interpret the exact solution $\mathbf{u}$ to be the roots of $\mathbf{F}(\mathbf{u})$
- Taylor expand the residuals at the $k+1$ iterate about the k iterate

$$\mathbf{F}(\mathbf{u}^{k+1}) = \mathbf{F}(\mathbf{u}^k) + \mathbf{F}'(\mathbf{u}^k)(\mathbf{u}^{k+1} - \mathbf{u}^k) + \frac{\mathbf{F}''(\mathbf{u}^k)}{2}(\mathbf{u}^{k+1} - \mathbf{u}^k)^2 + \cdots$$

- Assert $\mathbf{u}^{k+1}$ is the exact solution

$$-\mathbf{F}(\mathbf{u}^k) = \mathbf{F}'(\mathbf{u}^k)(\mathbf{u}^{k+1} - \mathbf{u}^k)$$

Nonlinear Preliminaries

- $\mathbf{F}'(\mathbf{u}^k)$ is the *Jacobian* $\mathbf{J}(\mathbf{u})$

$$J_{ij} = \frac{\partial F_i(\mathbf{u})}{\partial u_j}$$

- $(\mathbf{u}^{k+1} - \mathbf{u}^k)$ is the solution update from the k iterate to the $k+1$ iterate

$$\delta \mathbf{u}^k = \mathbf{u}^{k+1} - \mathbf{u}^k$$

- Form Newton's method

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

Newton-Krylov Methods

- A form of inexact Newton methods

$$||\mathbf{J}(\mathbf{u}^k)\delta\mathbf{u}^k + \mathbf{F}(\mathbf{u}^k)|| \leq \eta^k||\mathbf{F}(\mathbf{u}^k)||,\ \eta^k \in [0, 1)$$

- Choose a Krylov method to solve for the Newton correction
- GMRES with a long recurrence relation observed as more robust
- Generates a monotonically decreasing residual from maintaining the optimization and orthogonality conditions

Newton-Krylov Methods

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Where does the Jacobian come from?

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- Choose a Krylov method to solve for the Newton correction
- GMRES with a long recurrence relation observed as more robust
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Where does the Jacobian come from?

- The Jacobian can come from hand-coded derivatives
  - Tedious and error prone
  - Repeated for each equation set and hard to do for multiphysics

Matrix-Free Approximation

- Krylov methods only need the action of the linear operator
- The action of the Jacobian can be approximated using a forward difference

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

- Forms the basis of Jacobian-Free Newton-Krylov (JFNK) methods
  - Sensitive to scaling and discretization error
  - Still have to form part of Jacobian periodically for preconditioning
  - Eventually break even with generating and storing the full Jacobian

Automatic Differentiation

- Automatically generate Jacobians from nonlinear function evaluations
  - Overload math operators and apply the chain rule (FAD)
  - Yields evaluations as accurate as function discretization
- Modern packages take an element-level assembly approach
  - Function evaluations are local, communication builds global data

$$\mathbf{J}(\mathbf{u}) = \sum_{i=1}^{N} \mathbf{Q}_i^T \mathbf{J}_k \mathbf{P}_i$$

$$e_k : \mathbb{R}^{n_k} \to \mathbb{R}^{m_k},\ \mathbf{J}_{k_i} = \partial e_{k_i} / \partial P_i u,\ \mathbf{P} \in \mathbb{R}^{m_{k_i} \times N}$$

- Performance studies give acceptable results for use in large-scale, production physics codes

Forward-Automated Newton-MCSA

The FANM Method

Forward-Automated Newton-MCSA

Algorithm 3 FANM

$k := 0$
while $||\mathbf{F}(\mathbf{u}^k)|| > \epsilon||\mathbf{F}(\mathbf{u}^0)||$ **do**
  $\mathbf{J}(\mathbf{u}^k) \leftarrow AD(\mathbf{F}(\mathbf{u}^k))$ {Automatic differentiation}
  $\mathbf{J}(\mathbf{u}^k)\delta\mathbf{u}^k = -\mathbf{F}(\mathbf{u}^k)$ {Solve for the Newton correction with MCSA}
  $\mathbf{u}^{k+1} \leftarrow \mathbf{u}^k + \delta\mathbf{u}^k$
  $k \leftarrow k + 1$
end while

The FANM Method

Forward-Automated Newton-MCSA

Algorithm 4 FANM

1. $k := 0$
2. **while** $||\mathbf{F}(\mathbf{u}^k)|| > \epsilon||\mathbf{F}(\mathbf{u}^0)||$ **do**
3. $\quad \mathbf{J}(\mathbf{u}^k) \leftarrow AD(\mathbf{F}(\mathbf{u}^k))$ {Automatic differentiation}
4. $\quad \mathbf{J}(\mathbf{u}^k)\delta\mathbf{u}^k = -\mathbf{F}(\mathbf{u}^k)$ {Solve for the Newton correction with MCSA}
5. $\quad \mathbf{u}^{k+1} \leftarrow \mathbf{u}^k + \delta\mathbf{u}^k$
6. $\quad k \leftarrow k + 1$
7. **end while**

- Robustness of Newton's method (inexact)
- Accuracy and convenience of FAD
- Parallelism, memory, and resiliency benefits of MCSA
- Requires only nonlinear function evaluations

Jacobian Storage vs. Subspace Storage

- Jacobian will be in a compressed row storage format

$$\mathbf{A} = \begin{bmatrix} 2 & 0 & 8 & 0 & 0 & 0 \\ 4 & 5 & 0 & 1 & 0 & 0 \\ 0 & 2 & 1 & 0 & 1 & 0 \\ 0 & 0 & 3 & 7 & 0 & 2 \\ 0 & 0 & 0 & 4 & 9 & 0 \\ 0 & 0 & 0 & 0 & 9 & 1 \end{bmatrix}$$

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$$\begin{array}{lccccccccccccccc} \mathbf{A}\ \textit{values}: & 2 & 8 & 4 & 5 & 1 & 2 & 1 & 1 & 3 & 7 & 2 & 4 & 9 & 9 & 1 \\ \textit{column}: & 1 & 3 & 1 & 2 & 4 & 2 & 3 & 5 & 3 & 4 & 6 & 4 & 5 & 5 & 6 \\ \textit{row start}: & 1 & 3 & 6 & 9 & 12 & 14 & 16 & & & & & & & & \end{array}$$

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- m Krylov iterations require $(m+1)$ subspace vectors
- Storage requirement is $\left[(m+1)N\right]$ for $\mathbf{x} \in \mathbb{R}^{N \times N}$

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- m Krylov iterations require $(m+1)$ subspace vectors
- Storage requirement is $\left[(m+1)N\right]$ for $\mathbf{x} \in \mathbb{R}^{N\times N}$

If we need 10 Krylov iterations to converge...

- 66 elements required for subspace vectors
- 72 total elements required for Jacobian and probability matrix

Parallel FANM Method

Algorithm 5 FANM

1: $k := 0$
2: **while** $||\mathbf{F}(\mathbf{u}^k)|| > \epsilon||\mathbf{F}(\mathbf{u}^0)||$ **do**
3: $\quad \mathbf{J}(\mathbf{u}^k) \leftarrow AD(\mathbf{F}(\mathbf{u}^k))$ {Automatic differentiation}
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5: $\quad \mathbf{u}^{k+1} \leftarrow \mathbf{u}^k + \delta\mathbf{u}^k$
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7: **end while**

- Modern FAD packages are parallelized using element-level assembly
- This work will generate a parallel MCSA solver
- Application of the Newton correction requires a parallel vector update
- Convergence checks through parallel norm computation

Research Proposal

- Experimental framework
- Methods verification
- Numerical experiments
- Challenge problem

Experimental Framework

- Need a framework to generate linear and nonlinear systems in parallel
  - Linear algebra data structures
  - Parallel communication framework
  - Mesh generation and partitioning
  - Automatic differentiation and more...
- Choose the finite element method to leverage a finite element assembly engine

$$\mathbf{A}(\mathbf{u}) = \mathbf{0}, \ \forall \mathbf{u} \in \Omega$$

$$\mathbf{B}(\mathbf{u}) = \mathbf{0}, \ \forall \mathbf{u} \in \Gamma$$

$$\int_\Omega \mathbf{v}^T \mathbf{A}(\mathbf{u}) d\Omega + \int_\Gamma \bar{\mathbf{v}}^T \mathbf{B}(\mathbf{u}) d\Gamma = \mathbf{0}$$

$$\int_\Omega \mathbf{C}(\mathbf{v}^T) \mathbf{D}(\mathbf{u}) d\Omega + \int_\Gamma \mathbf{E}(\bar{\mathbf{v}}^T) \mathbf{F}(\mathbf{u}) d\Gamma = \mathbf{0}$$

Monte Carlo Methods Verification

- Analytic solution to the heat equation for the linear methods
- Sequence of Navier-Stokes benchmarks for the nonlinear methods
  - Thermal convection cavity problem (De Vahl Davis, 1983)
  - Lid driven cavity problem (Ghia et al., 1982)
  - Backward-Facing step problem (Gartling, 1990)
- Tuning benchmark parameters varies the strength of nonlinearities

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \mathbf{T} - \rho \mathbf{g} = \mathbf{0}$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho C_p \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = 0$$

$$\mathbf{T} = -P\mathbf{I} + \mu[\nabla \mathbf{u} + \nabla \mathbf{u}^T]$$

$$\mathbf{q} = -k \nabla T$$

Proposed Numerical Experiments

Proposed Numerical Experiments

Domain Overlap Studies for the Parallel Neumann-Ulam Method

- Correlate domain overlap behavior to linear system properties
- Analyze random walk transport with respect to the operator:
  - Eigenvalues
  - Sparsity
  - Asymmetry
- Evaluate communication cost
- Evaluate memory cost

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- Analyze random walk transport with respect to the operator:
  - Eigenvalues
  - Sparsity
  - Asymmetry
- Evaluate communication cost
- Evaluate memory cost

Domain Replication Studies for the Parallel Neumann-Ulam Method

- Feasibility from a memory perspective
- Impact on scalability
- Impact on load balancing

Proposed Numerical Experiments

Parallel Performance and Numerical Accuracy Studies for the MCSA Method

- Characterize Neumann-Ulam parameters required for good correction
- Feasibility of MCSA with full-clip Neumann-Ulam
- Performance for asymmetric systems
- Memory usage compared to Krylov methods

Parallel Performance and Numerical Accuracy Studies for the MCSA Method

- Characterize Neumann-Ulam parameters required for good correction
- Feasibility of MCSA with full-clip Neumann-Ulam
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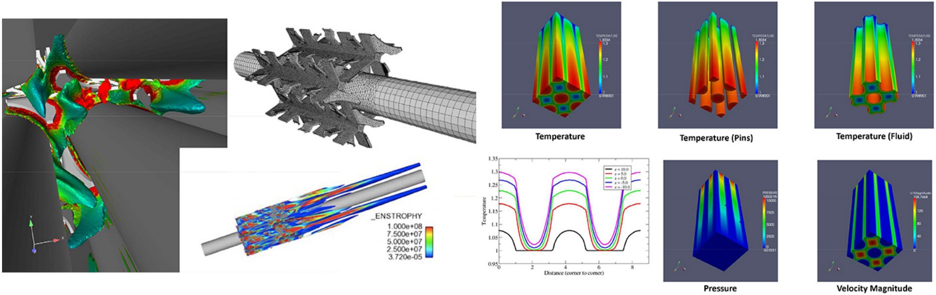
- Memory usage compared to Krylov methods

Parallel Performance and Numerical Accuracy Studies for the FANM Method

- Feasibility for problems of interest
- Memory usage vs. Newton-Krylov methods
- Scalability vs. Newton-Krylov methods

Proposed Challenge Problem

- Problems of interest are coupled large scale problems in reactor physics
- The Consortium for Advanced Simulation of LWRs (CASL) is a modeling and simulation program aimed at:
  - Higher power uprates and efficiency
  - Higher burn-up
  - Predictive accident scenario analysis
- CASL and industry partners identified challenge problems:
  - Departure from nucleate boiling
  - Grid-to-rod-fretting
- Our challenge problem should reflect how this work aids the solution of these problems



- CASL has utilized the Drekar multiphysics code (SNL)
- Coupled fluid flow and heat transfer helps characterize many phenomena
- Drekar is massively parallel and leverages Newton-Krylov methods
- Propose using the largest Drekar problem to date as a challenge problem for the new Monte Carlo methods

Images source: www.casl.gov

Conclusion

- Proposed research and development of new Monte Carlo methods
  - Parallelization of Monte Carlo methods for linear systems
  - FANM for nonlinear systems
- Verification through benchmarks
- Numerical experiments for understanding
- Challenge problem for application
- Directed towards hard problems in nuclear reactor analysis:
  - Application to multiphysics
  - Potential improvements for scalability
  - Potential improvements for memory consumption
  - Looking forward to exascale