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
- 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

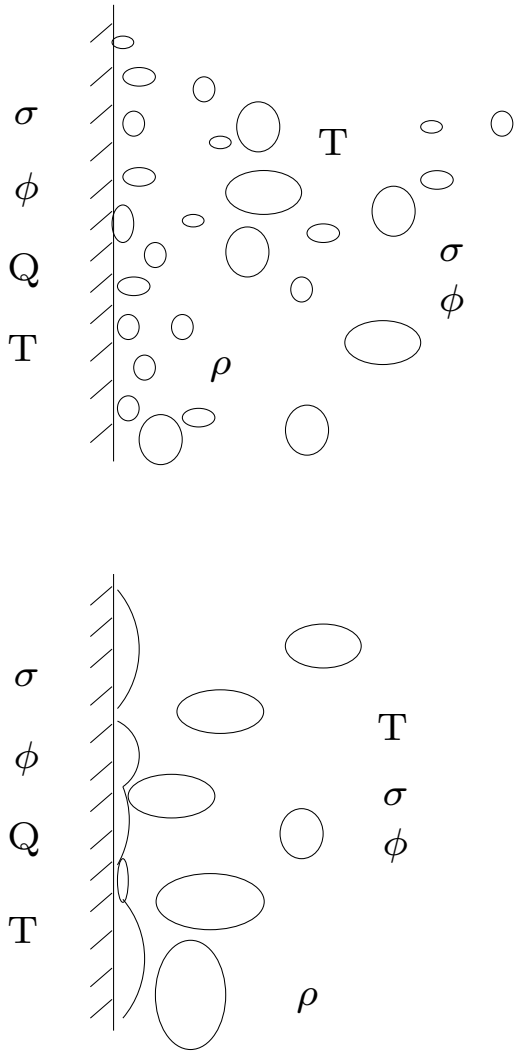

Figure: **Departure from nucleate boiling scenario.**

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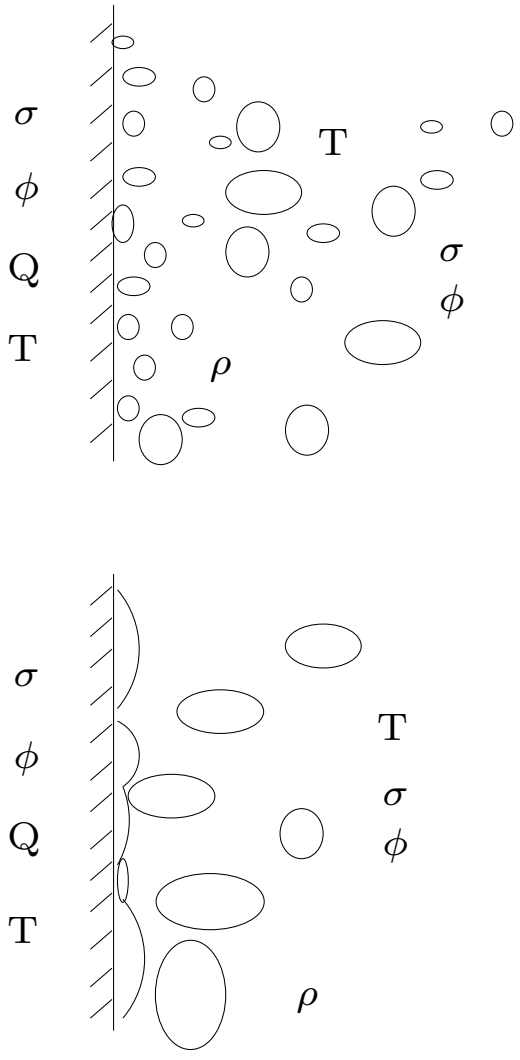

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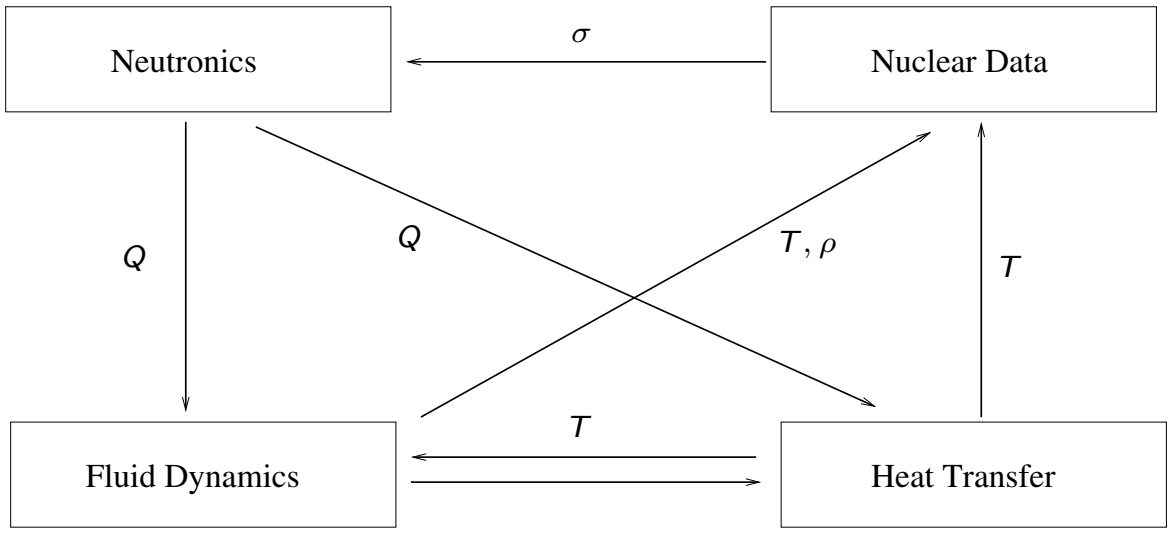

Figure: **Multiphysics dependency analysis of departure from nucleate boiling.**

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 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:

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

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

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

- 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

- 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

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

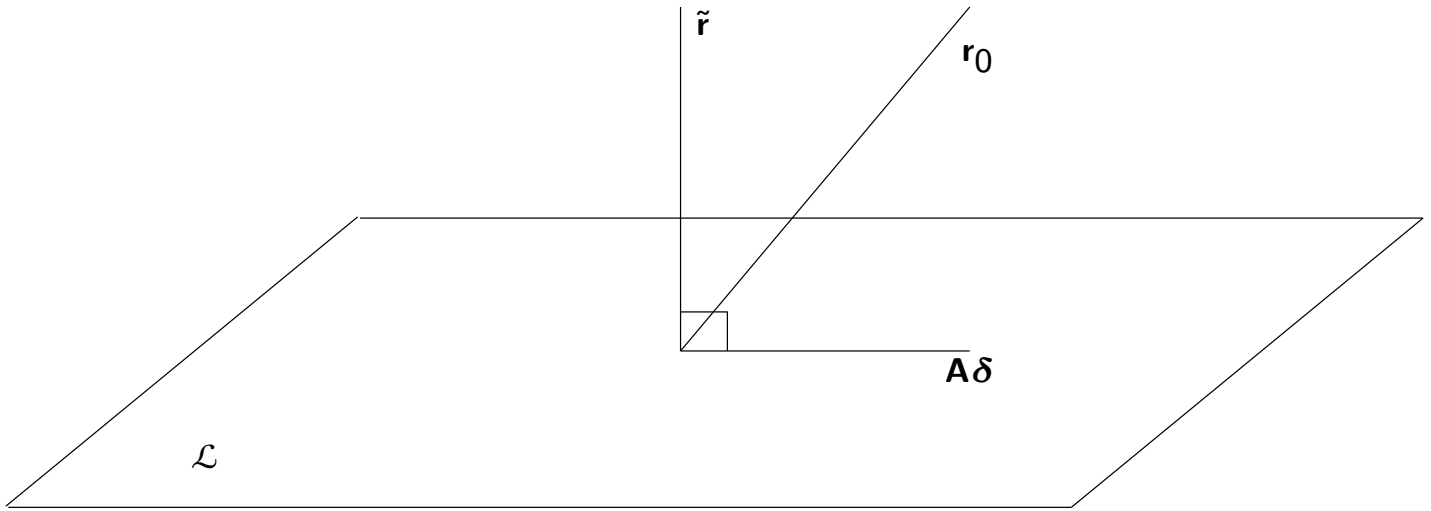

Figure: **Orthogonality constraint of the new residual with respect to $\mathcal{L}$.**

The Orthogonality Constraint

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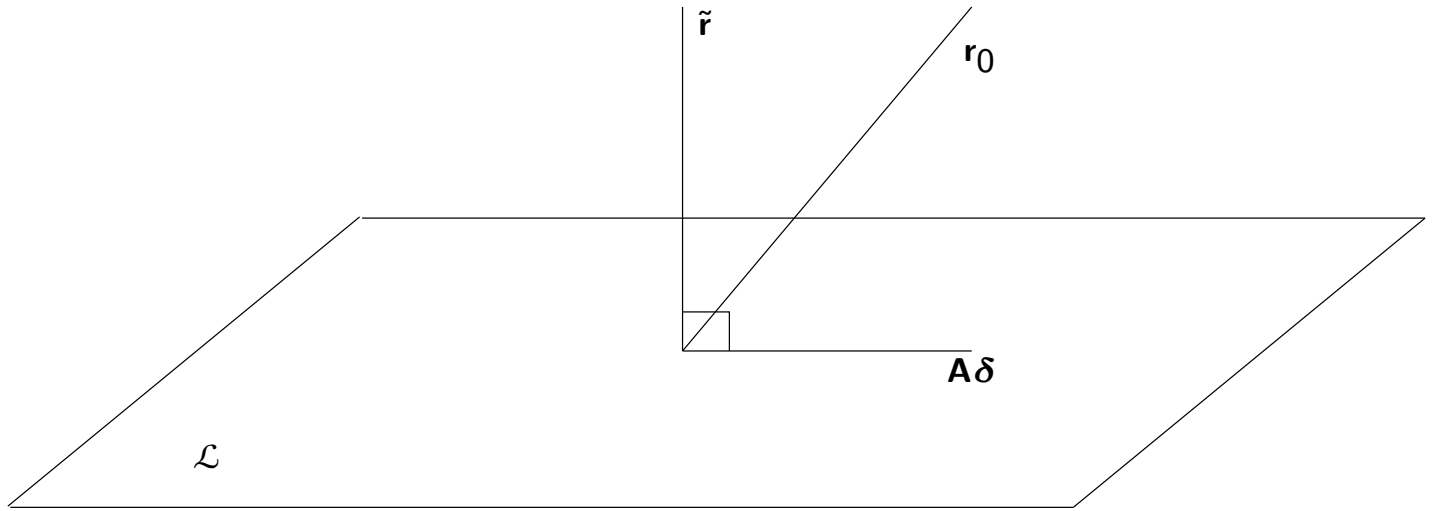

Figure: **Orthogonality constraint of the new residual with respect to $\mathcal{L}$.**

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

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

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

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

Update $\mathbf{V}$ *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

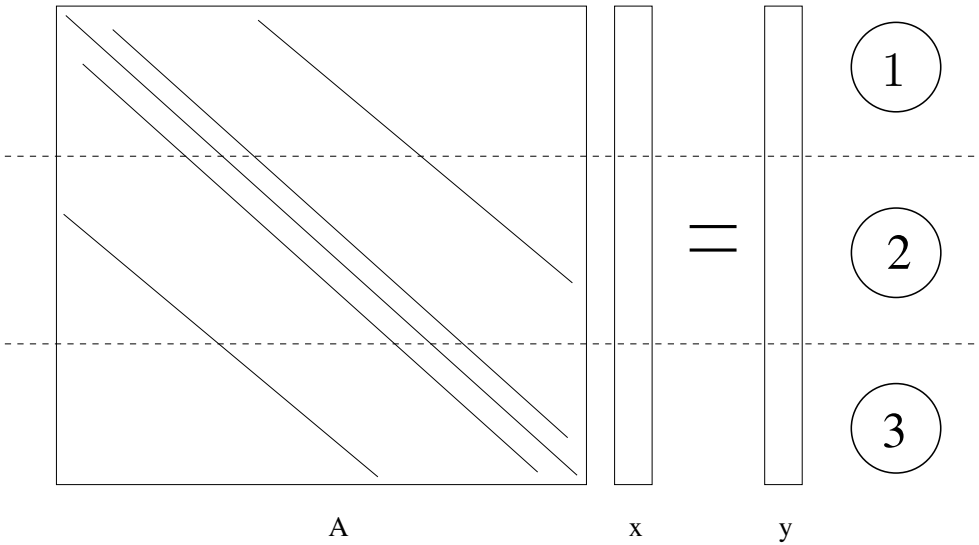
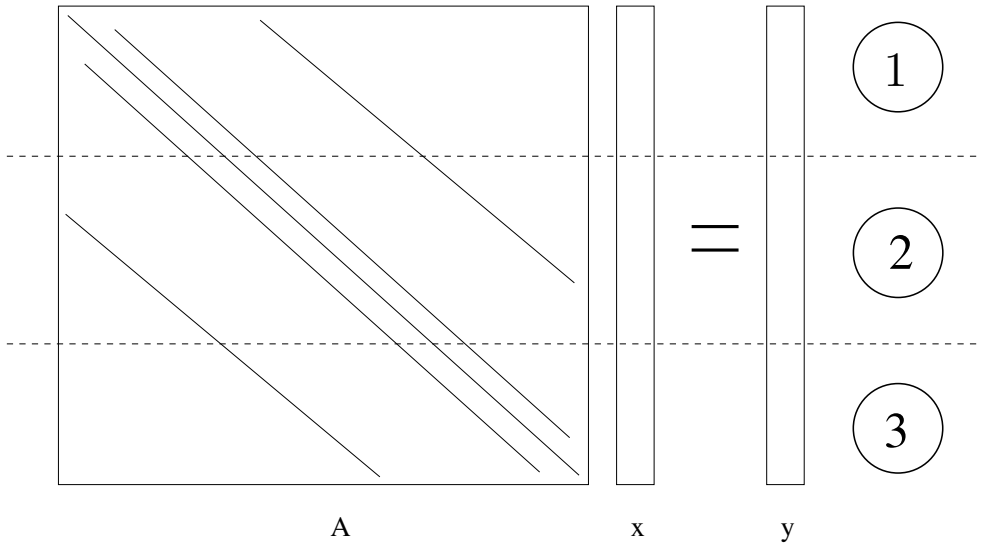


Figure: **Matrix-vector multiply Ax = y operation on 3 processors.**

Parallel Matrix-Vector Multiplication



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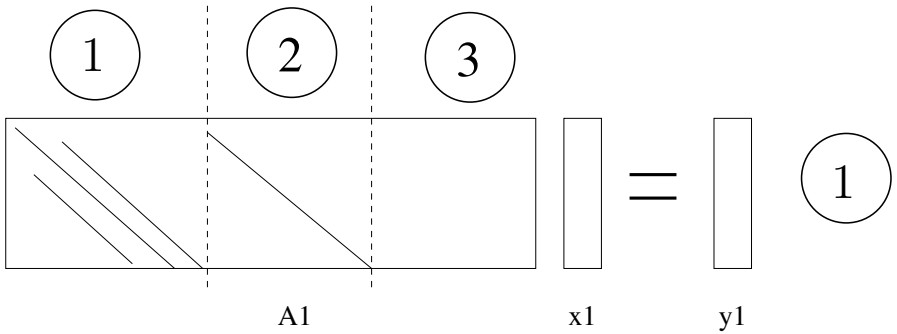

Figure: **Components of multiply operation owned by process 1.**

Projection Method Notes

- 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

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 Nuemann series

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

- 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

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

- Generate an expectation value for the solution

$$W_m = \sum_{m=0}^{k} w_{i,i_1} w_{i_1,i_2} \cdots w_{i_{m-1},i_m}$$

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

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

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

Direct Method: Evolution of a Solution

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

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

- 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

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

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

- Build the estimator and expectation value

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

$$\begin{aligned} E\{X_j\} &= \sum_{k=0}^{\infty} \sum_{i_1}^{N} \sum_{i_2}^{N} \cdots \sum_{i_k}^{N} b_{i_0} h_{i,i_1} h_{i_1,i_2} \ldots h_{i_{k-1},i_k} \delta_{i_k,j} \\ &= x_j \ , \end{aligned}$$

Adjoint Method: Evolution of a Solution

Sequential Monte Carlo

- Neumann-Ulam methods bound by the Central Limit Theorem
- Halton proposed an iterative residual method
- 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

- 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

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

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

- Implicit Euler time differencing

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

Direct vs. Adjoint Analysis

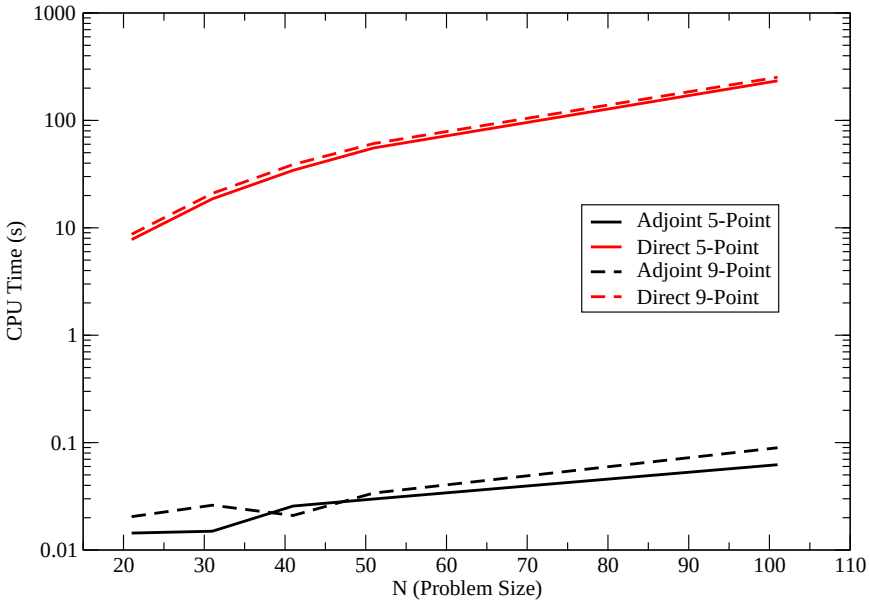

Figure: **CPU Time (s) to converge vs. Problem Size (N for an $N \times N$ square mesh).**

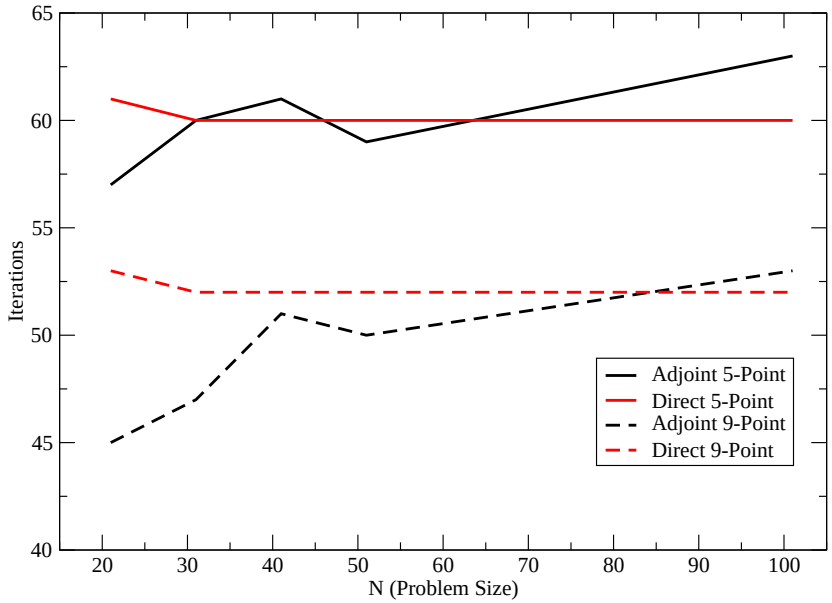

Figure: **Iterations to converge vs. Problem Size (N for an $N \times N$ square mesh).**

Direct vs. Adjoint Analysis

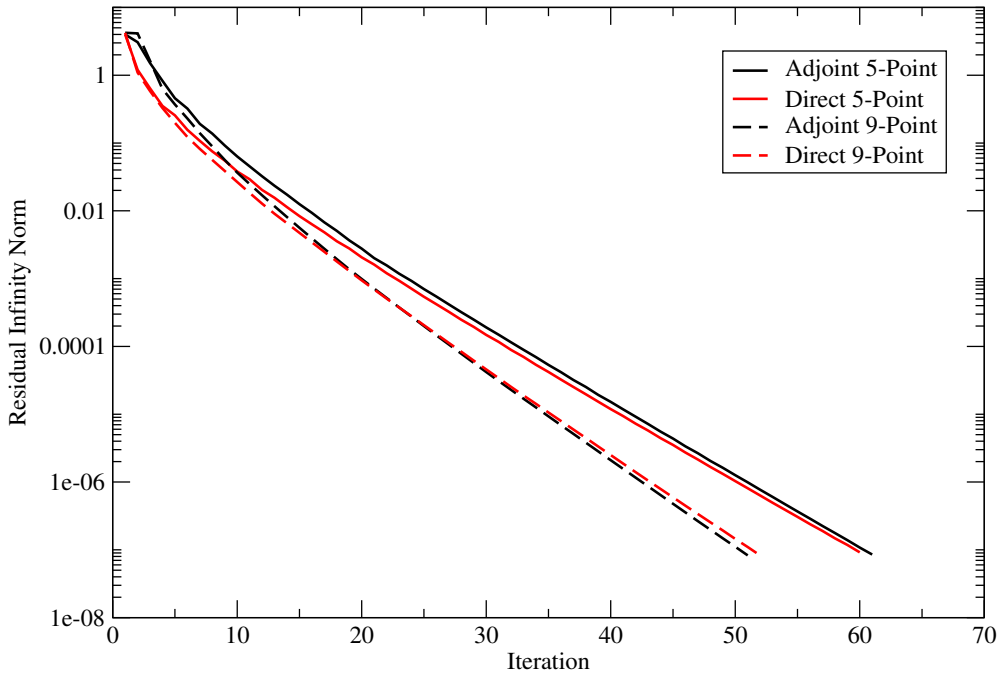

Figure: **Infinity norm of the solution residual vs. iteration number for a problem of fixed size.**

- 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

Parallelization of Monte Carlo Methods

- No literature observed for parallel Neumann-Ulam solvers
- Numerous references for modern parallel Monte Carlo methods in reactor physics
- MCSA parallelism comes from parallel matrix/vector operations

Domain Decomposition

Multiple-Set Overlapping-Domain Decomposition

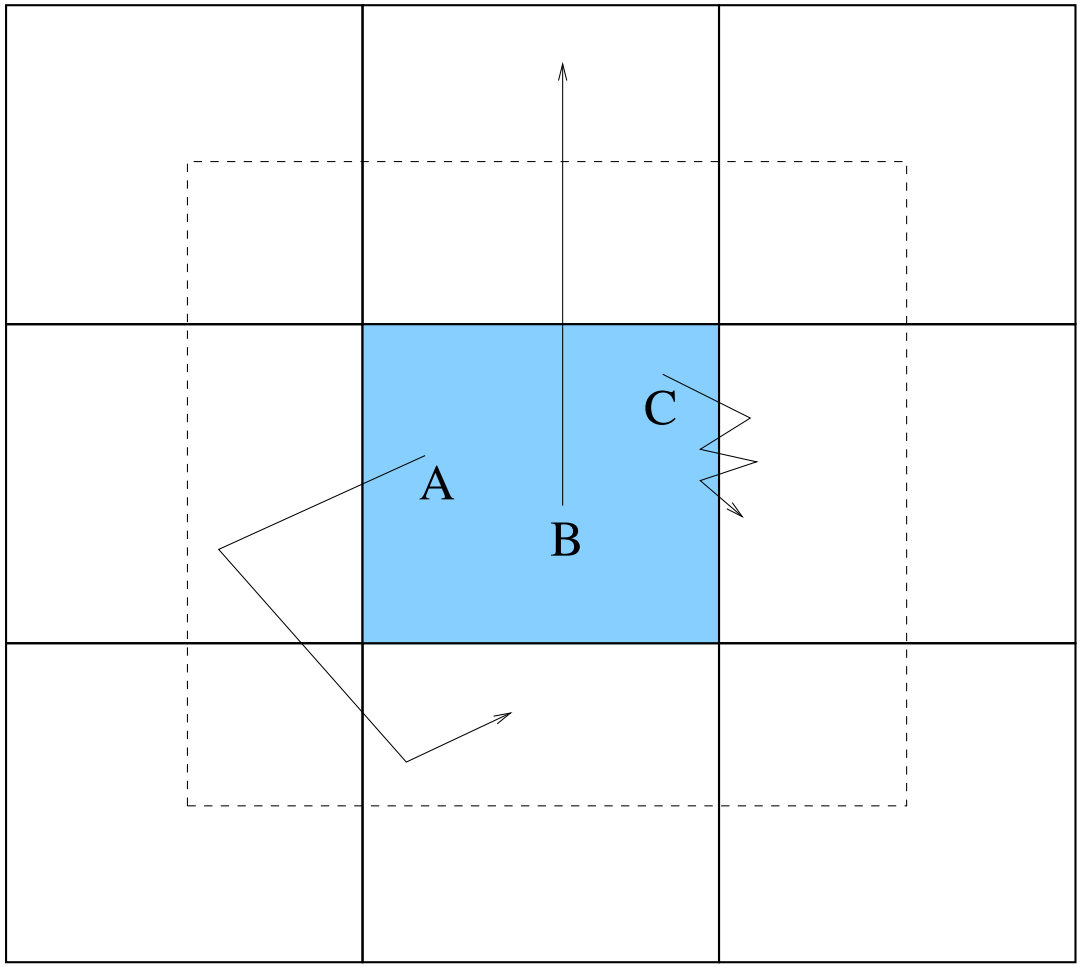

Figure: **Overlapping domain example illustrating how domain overlap can reduce communication costs.**

Domain-to-Domain Communication

Load Balancing

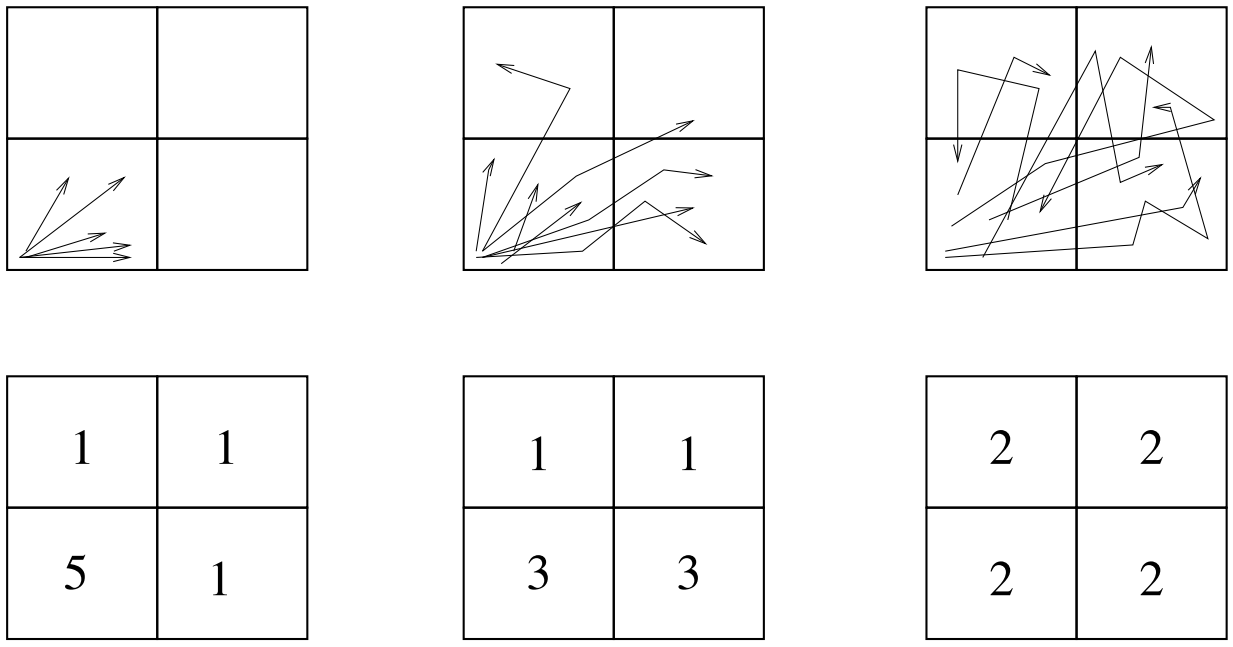

Figure: **Example illustrating how domain decomposition can create load balance issues in Monte Carlo.**

Reproducability

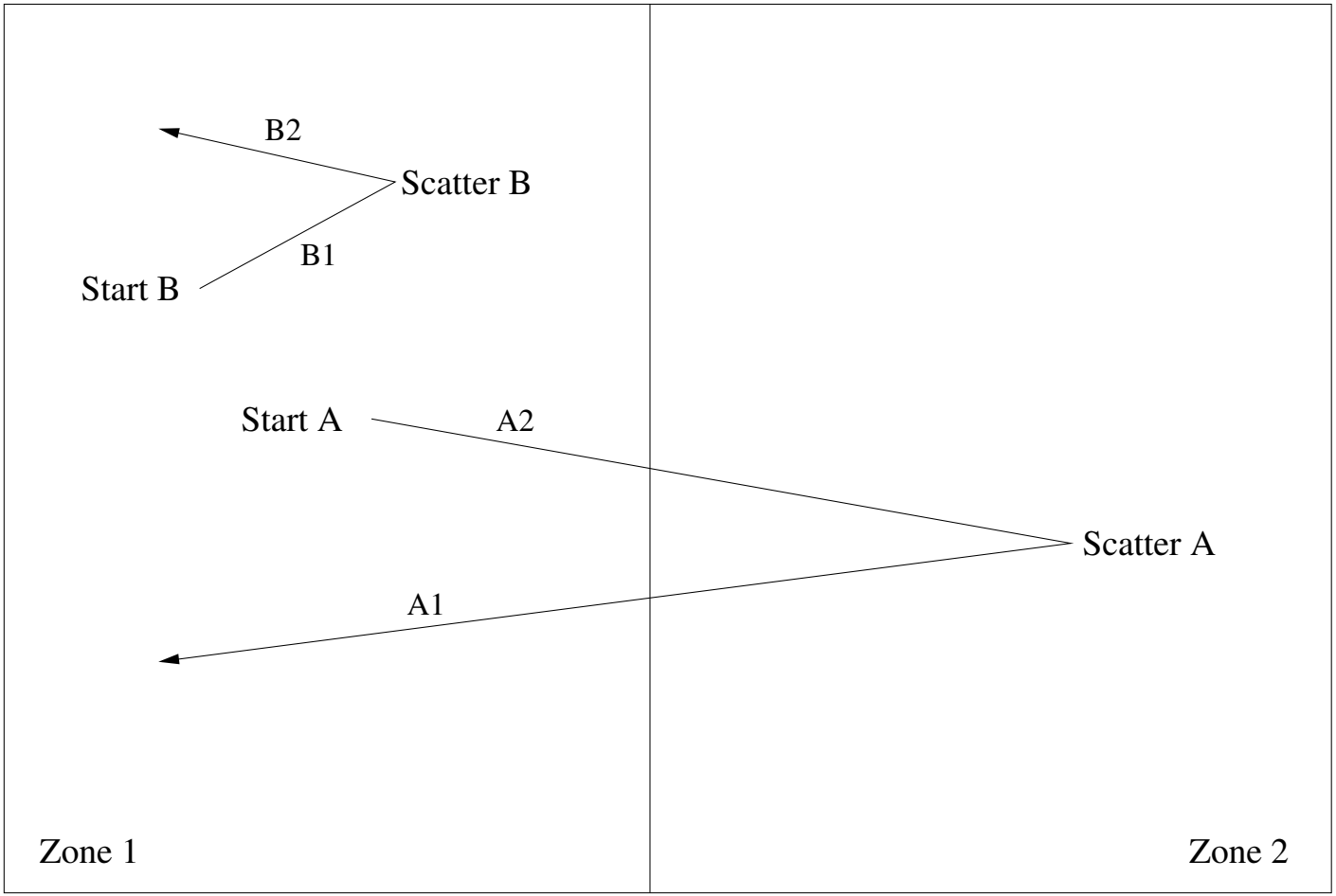

Figure: **Gentile's example illustrating how domain decomposition can create reproducibility issues in Monte Carlo.**

Parallel Adjoint Method

Parallel MCSA

Monte Carlo Solution Methods for Nonlinear Problems

Nonlinear Preliminaries

Nonlinear Preliminaries

Newton-Krylov Methods

Newton-Krylov Methods

Matrix-Free Approximation

Automatic Differentiation

The FANM Method

Jacobian Storage vs. Subspace Storage

Parallel FANM Method

Research Proposal

Experimental Framework

Progress to Date

Progress to Date

Progress to Date

Monte Carlo Methods Verification

Proposed Numerical Experiments

Proposed Challenge Problem

Conclusion