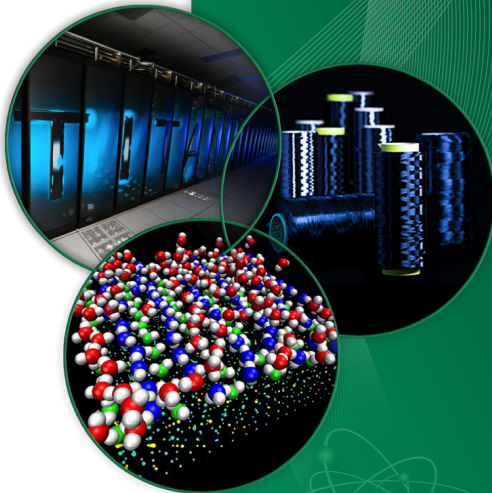# Parallel Algorithms for Monte Carlo Linear Solvers

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Acknowledgements

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Motivation

- As we move towards exascale computing, the rate of errors is expected to increase dramatically

  - The probability that a compute node will fail during the course of a large scale calculation may be near 1

- Algorithms need to not only have increased concurrency/scalability but have the ability to recover from hardware faults
  - Lightweight machines
  - Heterogeneous machines
  - Both characterized by low power and high concurrency

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Towards Exascale Concurrency and Resiliency

- Two basic strategies:

  1. State with current "state of the art" methods and make incremental modifications to improve scalability and fault tolerance
     - Many efforts are heading in this direction, attempting to find additional concurrency to exploit

  2. Start with methods having natural scalability and resiliency aspects and work at improving performance (e.g. Monte Carlo)
     - Soft failures a component of the tally variance
     - Hard failures potentially mitigated by replication
     - Concurrency enabled by several levels of parallelism

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Outline

- Monte Carlo Linear Solvers

- Domain Decomposition and Replication

- Scaling Studies

- Algorithm Variations

- Conclusions and Future Work

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Monte Carlo Methods

Monte Carlo for Linear Systems

- Suppose we want to solve $\mathbf{A}\mathbf{x} = \mathbf{b}$

- If $\rho(\mathbf{I} - \mathbf{A}) < 1$, we can write the solution using the Neumann series

$$\mathbf{x} = \sum_{n=0}^{\infty} (\mathbf{I} - \mathbf{A})^n \mathbf{b} = \sum_{n=0}^{\infty} \mathbf{H}^n \mathbf{b}$$

where $\mathbf{H} \equiv (\mathbf{I} - \mathbf{A})$ is the Richardson iteration matrix

- Build the Neumann series stochastically

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

- Define a sequence of state transitions
$$\nu = i \rightarrow i_1 \rightarrow \cdots \rightarrow i_{k-1} \rightarrow i_k$$

Forward Monte Carlo

- Choose a row-stochastic matrix $\mathbf{P}$ and weight matrix $\mathbf{W}$ such that $\mathbf{H} = \mathbf{P} \circ \mathbf{W}$
- Typical choice (Monte Carlo Almost-Optimal):

$$\mathbf{P}_{ij} = \frac{|\mathbf{H}_{ij}|}{\sum_{j=1}^{N} |\mathbf{H}_{ij}|}$$

- To compute solution component $\mathbf{x}_i$:
  - Start a history in state i (with initial weight of 1)
  - Transition to new state j based probabilities determined by $\mathbf{P}_i$
  - Modify history weight based on corresponding entry in $\mathbf{W}_{ij}$
  - Add contribution to $\mathbf{x}_i$ based on current history weight and value of $\mathbf{b}_j$
- A given random walk can only contribute to a single component of the solution vector with $\mathbf{x} \approx \mathbf{M_{MC}b}$

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Sampling Example (Forward Monte Carlo)

- Suppose

$$\mathbf{A} = \begin{bmatrix} 1.0 & -0.2 & -0.6 \\ -0.4 & 1.0 & -0.4 \\ -0.1 & -0.4 & 1.0 \end{bmatrix} \rightarrow \mathbf{H} \equiv (\mathbf{I} - \mathbf{A}) = \begin{bmatrix} 0.0 & 0.2 & 0.6 \\ 0.4 & 0.0 & 0.4 \\ 0.1 & 0.4 & 0.0 \end{bmatrix}$$

then

$$\mathbf{P} = \begin{bmatrix} 0.0 & 0.25 & 0.75 \\ 0.5 & 0.0 & 0.5 \\ 0.2 & 0.8 & 0.0 \end{bmatrix}, \quad \mathbf{W} = \begin{bmatrix} 0.0 & 0.8 & 0.8 \\ 0.8 & 0.0 & 0.8 \\ 0.5 & 0.5 & 0.0 \end{bmatrix}$$

- If a history is started in state 3, there is a 20% chance of it transitioning to state 1 and an 80% chance of moving to state 2

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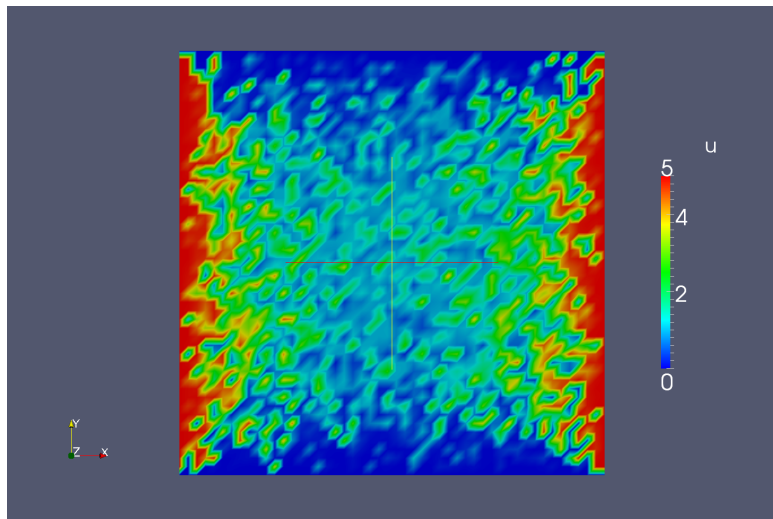# Solving the Heat Equation: Forward Method

Figure : **Forward solution.** 2.5×10^3 *total histories.*
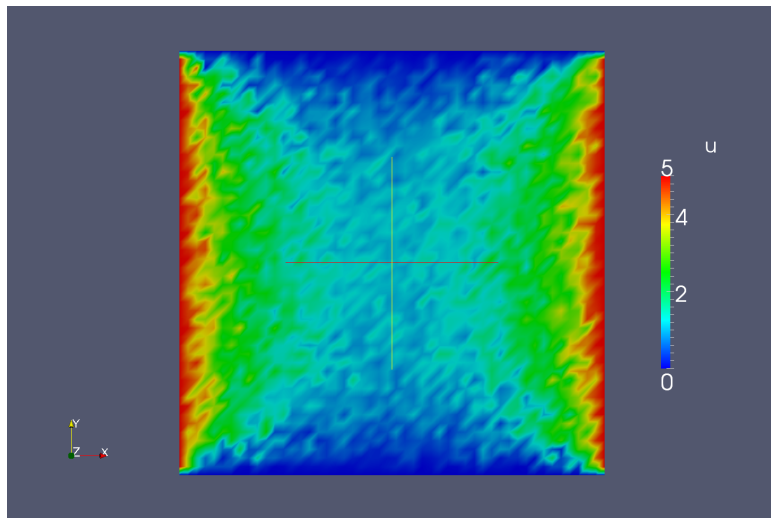
Solving the Heat Equation: Forward Method

Figure : **Forward solution.** 2.5×10^4 *total histories.*
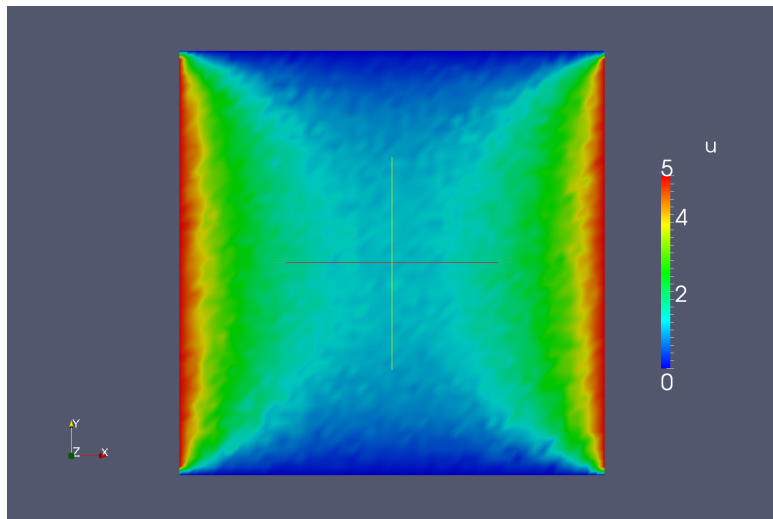
Solving the Heat Equation: Forward Method

Figure : **Forward solution.** 2.5×10^5 *total histories.*
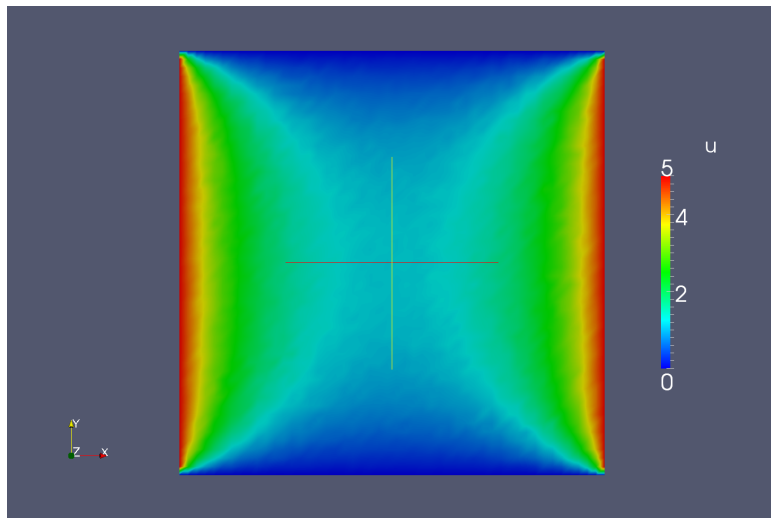
Solving the Heat Equation: Forward Method

Figure :   **Forward solution.** 2.5×10^6 *total histories.*

Domain Decomposition and Replication

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Domain Decomposed Monte Carlo

- Each parallel process owns a piece of the domain (linear system)

- Random walks must be transported between adjacent domains through parallel communication

- Domain decomposition determined by the input system
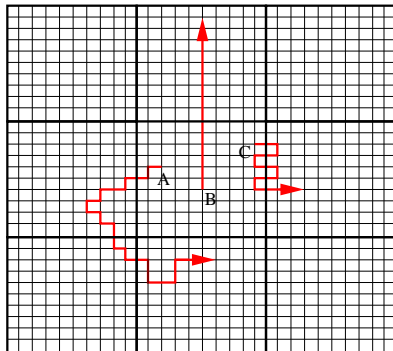
- Load balancing not yet addressed

Figure : Domain decomposition example illustrating how domain-to-domain transport creates communication costs.

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Asynchronous Monte Carlo Transport Kernel

- General extension of the Milagro algorithm (LANL)

- Asynchronous nearest neighbor communication of histories

- System-tunable communciation parameters of buffer size and check frequency (performance impact)

- Need an asynchronous strategy for exiting the transport loop without a collective (running sum)
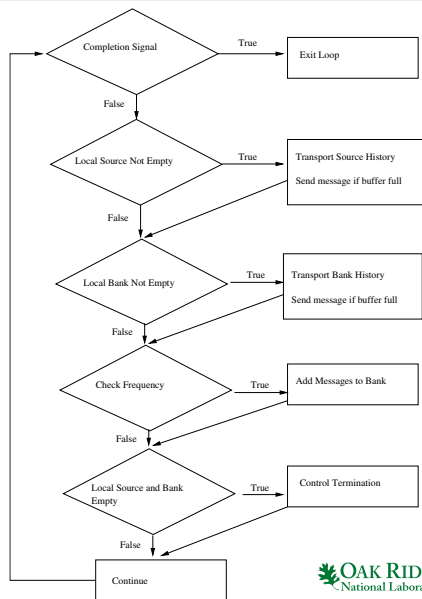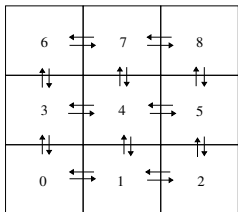
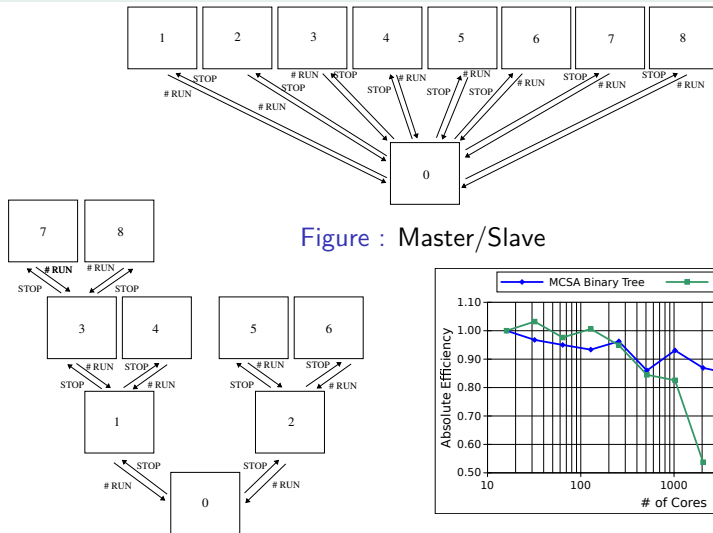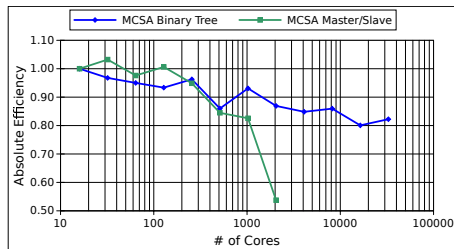# Exiting the Transport Loop without Collectives

Figure : Master/Slave

Figure : Binary Tree

Figure : Weak scaling absolute efficiency

Replication

Different batches of Monte Carlo samples can be combined in summation via superposition if they have different random number streams. For two different batches:

$$\mathbf{M_{MC}x} = \frac{1}{2}(\mathbf{M_1} + \mathbf{M_2})\mathbf{x}$$

Consider each of these batches independent *subsets* of a Monte Carlo operator where now the operator can be formed as a general additive decomposition of N_S subsets:

$$\mathbf{M_{MC}} = \frac{1}{N_S}\sum_{n=1}^{N_s}\mathbf{M_n}$$

We replicate the linear problem and form each subset on a different group of parallel processes. Applying the subsets to a vector requires an AllReduce to form the sum. Each subset is domain decomposed. OAK RIDGE
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Scaling Studies

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Parallel Test Application – Nuclear Reactor Analysis

The simplified P_N (SP_N) equations are an approximation to the Boltzmann neutron transport equation used to simulate nuclear reactors

$$\hat{\Omega} \cdot \vec{\nabla}\psi(\vec{r}, \hat{\Omega}, E) + \sigma(\vec{r}, E)\psi(\vec{r}, \hat{\Omega}, E) = \\ \iint \sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \cdot \hat{\Omega})\psi(\vec{r}, \hat{\Omega}', E')d\Omega'dE' + q(\vec{r}, \hat{\Omega}, E) \quad (1)$$

$$-\nabla \cdot \left[\frac{n}{2n+1}\frac{1}{\Sigma_{n-1}}\nabla\left(\frac{n-1}{2n-1}\phi_{n-2} + \frac{n}{2n-1}\phi_n\right) \right. \\ \left. + \frac{n+1}{2n+1}\frac{1}{\Sigma_{n+1}}\nabla\left(\frac{n+1}{2n+3}\phi_n + \frac{n+2}{2n+3}\phi_{n+2}\right) \right] \\ + \Sigma_n\phi_n = q\delta_{n0} \qquad n = 0, 2, 4, \cdots, N \quad (2)$$

$$-\nabla \cdot \mathbb{D}_n\nabla\mathbb{U}_n + \sum_{m=1}^{4} \mathbb{A}_{nm}\mathbb{U}_m = \frac{1}{k}\sum_{m=1}^{4} \mathbb{F}_{nm}\mathbb{U}_m \qquad n = 1, 2, 3, 4 \quad (3)$$

SP_N Assembly Problem

Scaling problem – 1×1 to 17×17 array of fuel assemblies with pins resolved by a 2×2 spatial mesh

- 23 energy groups, 1 angular moment, 1.6M to 273.5M degrees of freedom

- 64 to 10,800 computational cores via domain decomposition

- We are usually interested in solving generalized eigenvalue problem - we use the operator from these problems to test the kernel scaling
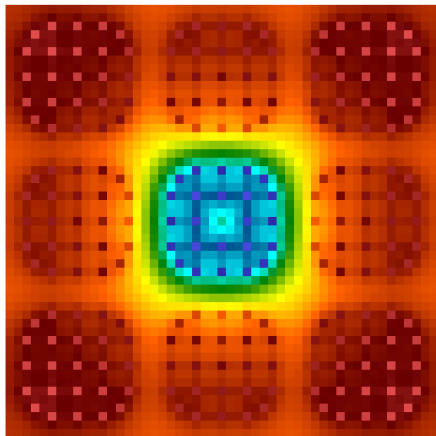

Figure : SP_N solution example

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Monte Carlo Communication Parameters

		Message Check Frequency			
		128	**256**	**512**	**1024**
	256	1.054	1.061	1.076	1.076
	512	1.103	1.146	1.211	1.270
	1024	1.062	1.088	1.133	1.176
Mesage Buffer Size	**2048**	1.030	1.042	1.072	1.107
	4096	1.010	1.012	1.025	1.050
	8192	1.001	1.000	1.008	1.018
	16384	1.017	1.003	1.010	1.009

- 64 cores, 1.6M DOFs, history length of 15, 3 histories per DOF
- Buffer size dominates the trend
- 27% decrease in runtime observed for bad parameter choices
- Worth the time to do this parameter study when running on new hardware

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Monte Carlo Strong Scaling

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Monte Carlo Weak Scaling

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Algorithm Variations

Matrix-Free Algorithm

Stochastic Approximate Inverse Algorithm

Monte Carlo Synthetic Acceleration

- Devised by Evans and Mosher in the 2000's as an acceleration scheme for radiation diffusion problems (LANL)

- Can be abstracted as a general linear solver with Monte Carlo as a preconditioner

- Combine with Richardson iteration as a "smoother" in between Monte Carlo steps:

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

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Unpreconditioned Algorithm Comparison

Conclusions and Future Work

Conclusions

- Monte Carlo methods offer great potential for both resilient and highly parallel solvers

- For certain classes of problems, Monte Carlo methods can be competitive with leading modern solvers

- Extending methods to broader problem areas is significant challenge and an attractive area for continued research

- Performance modeling and resiliency simulations this FY

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