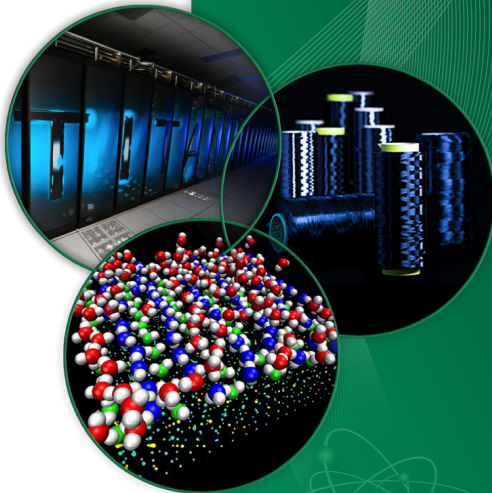


Parallel Algorithms for Monte Carlo Linear Solvers

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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

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

- Monte Carlo Linear Solvers
- Domain Decomposition and Replication
- Scaling Studies
- Matrix-Free and Stochastic Approximate Inverse Algorithms

Monte Carlo Methods

Monte Carlo for Linear Systems

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

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

- 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

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

Solving the Heat Equation: Forward Method

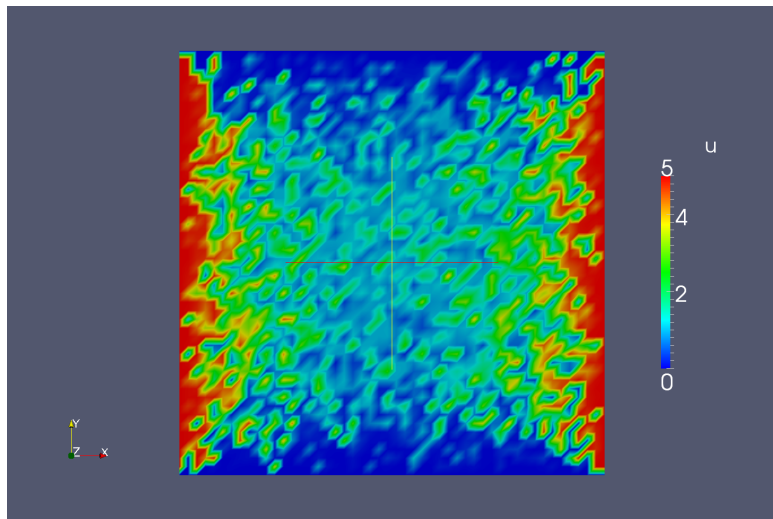


Figure : **Forward solution.** 2.5×10^3 *total histories.*

Solving the Heat Equation: Forward Method

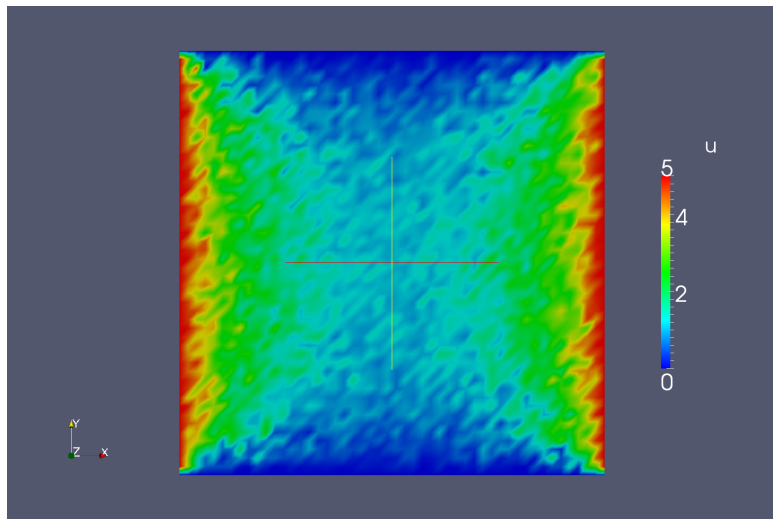


Figure : **Forward solution.** 2.5×10^4 *total histories.*

Solving the Heat Equation: Forward Method

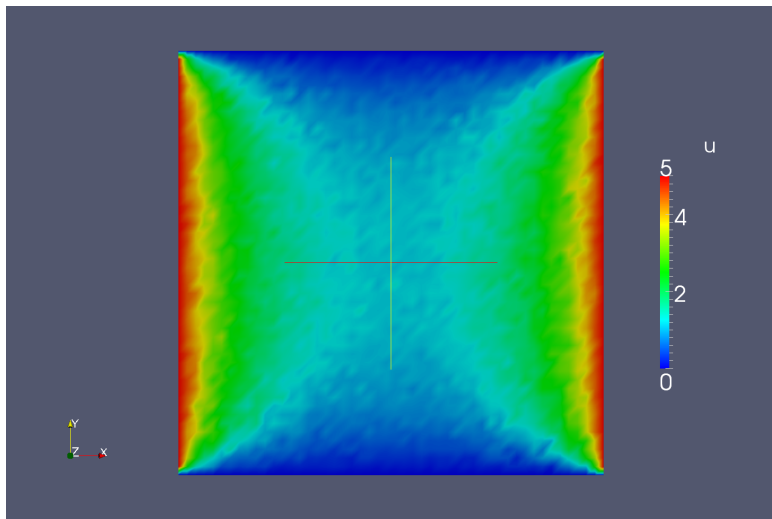


Figure : **Forward solution.** 2.5×10^5 *total histories.*

Solving the Heat Equation: Forward Method

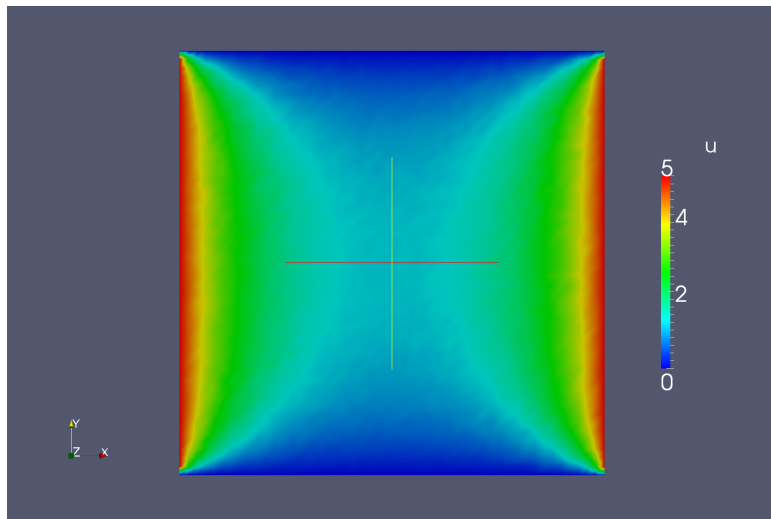


Figure : **Forward solution.** 2.5×10^6 *total histories.*

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, M_{MC}
- Combine with Richardson iteration as a “smoother” in between Monte Carlo steps:

$$\begin{aligned}\mathbf{r}^k &= \mathbf{b} - \mathbf{A}\mathbf{x}^k \\ \mathbf{x}^{k+1/2} &= \mathbf{x}^k + \mathbf{r}^k \\ \mathbf{r}^{k+1/2} &= \mathbf{b} - \mathbf{A}\mathbf{x}^{k+1/2} \\ \delta &= \mathbf{M}_{MC}\mathbf{r}^{k+1/2} \\ \mathbf{x}^{k+1} &= \mathbf{x}^{k+1/2} + \delta\end{aligned}$$

Domain Decomposition and Replication

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 straightforward for the forward method

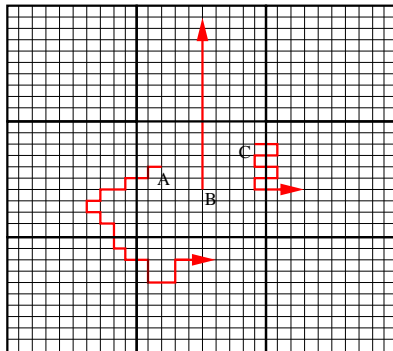
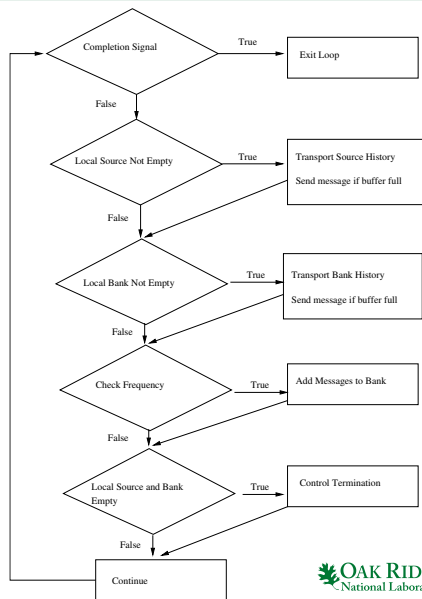
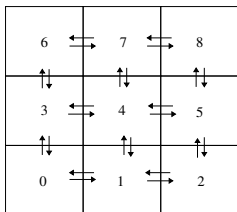


Figure : Domain decomposition example illustrating how domain-to-domain transport creates communication costs.

Asynchronous Monte Carlo Transport Kernel

- General extension of the Milagro algorithm (LANL)
- Asynchronous nearest neighbor communication of histories
- System-tunable communication parameters of buffer size and check frequency (performance impact)
- Need an asynchronous strategy for exiting the transport loop without a collective



Stopping the Asynchronous Kernel

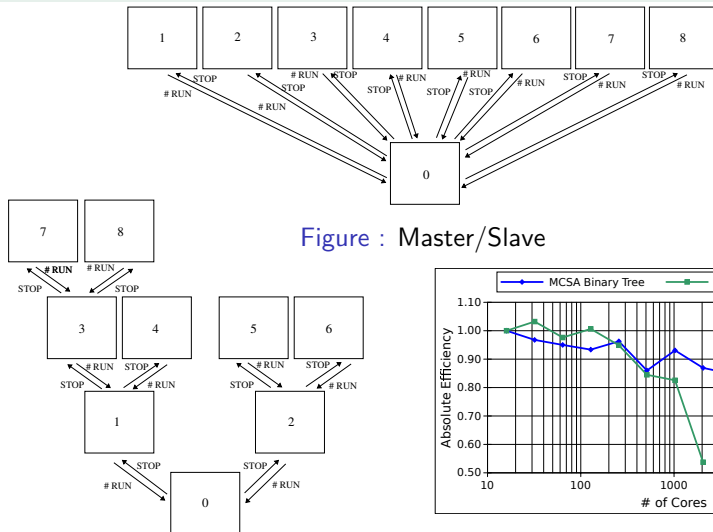


Figure : Master/Slave

Figure : Binary Tree

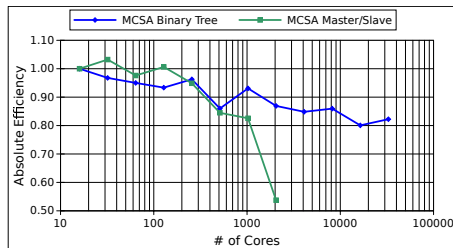


Figure : Weak scaling absolute efficiency


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:

$$\mathbf{M}_{\text{MC}}\mathbf{x} = \frac{1}{2}(\mathbf{M}_1 + \mathbf{M}_2)\mathbf{x}$$

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:

$$\mathbf{M}_{\text{MC}} = \frac{1}{N_S} \sum_{n=1}^{N_S} \mathbf{M}_n$$

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. 

Scaling Studies

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

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

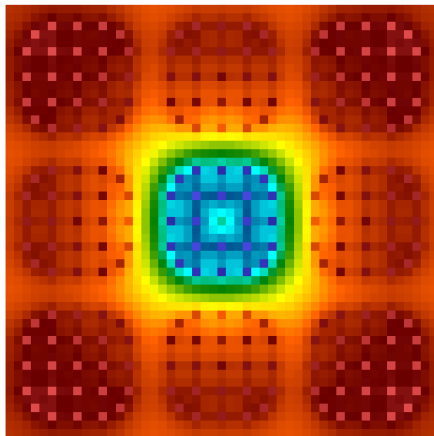
$$\begin{aligned} -\nabla \cdot \left[\frac{n}{2n+1} \frac{1}{\Sigma_{n-1}} \nabla \left(\frac{n-1}{2n-1} \phi_{n-2} + \frac{n}{2n-1} \phi_n \right) \right. \\ \left. + \frac{n+1}{2n+1} \frac{1}{\Sigma_{n+1}} \nabla \left(\frac{n+1}{2n+3} \phi_n + \frac{n+2}{2n+3} \phi_{n+2} \right) \right] \\ + \Sigma_n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

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

SP_N Assembly Problem

Test problem – 3×3 array of fuel assemblies with control rod in center location (Profugus)

- 23 energy groups, 2 angular moments, 25M degrees of freedom
- 1,000 computational cores via domain decomposition
- We are interested in solving generalized eigenvalue problem, for this study we use Arnoldi as the eigensolver and compare different methods for solving linear systems



Parallel SP_N Results

Method	Total Linear Iteration	Setup Time (s)	Solve Time (s)
GMRES-ILUT	1675	0.7	18.4
GMRES-AMG	626	0.7	46.0
GMRES-MGE	498	1.5	33.7
Richardson-AINV	5208	20.6	52.0
MCSA-AINV	1268	25.5	46.6

- ILUT preconditioning is winner here, but known to have issues with parallel scaling on large core counts
- Solve times for MCSA are competitive, but setup times are very large due to construction of sparse approximate inverse

Matrix-Free and Stochastic Approximate Inverse Algorithms

Alternative Parallelism – Additive Schwarz

- Instead of performing Monte Carlo on full problem, another possibility is to apply Monte Carlo as an additive Schwarz approach
- Decompose problem into (possibly overlapping) domains
- Perform Monte Carlo on individual subdomains
 - No communication costs in Monte Carlo problem!
- With domain decomposed Monte Carlo, iteration counts are effectively independent of the number of processors
- In an additive Schwarz approach, the preconditioner will become less effective as processor counts grow – algorithmic scalability may be an issue
- **Replication for resiliency and performance**

More Parallelism – Threading

- Within a Monte Carlo solve, every history is independent of other histories – great potential for highly concurrent hardware (GPU, Xeon Phi)
- Polynomial formulation enables a priori determination of operation counts per thread
- Memory locality an issue due to random access via random walks (block formulation?)
- Early experiments using the Trilinos Kokkos library show promising performance for multi-core CPUs
- Team members recently took part in OLCF “Hackathon” in late October to begin implementing computation kernels in OpenACC to allow for GPU capability on Titan with early results indicating **1.3-9.4x** speedup for MCSA (largely dependent on random number generation)

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