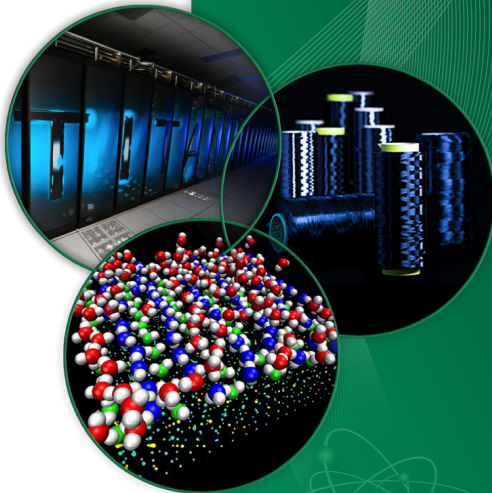


Parallel Algorithms for Monte Carlo Linear Solvers

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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

Outline

- Monte Carlo Linear Solvers
- Domain Decomposition and Replication
- Scaling Studies
- Algorithm Variations
- Conclusions and Future Work

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 with $\mathbf{x} \approx \mathbf{M}_{\text{MC}} \mathbf{b}$

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

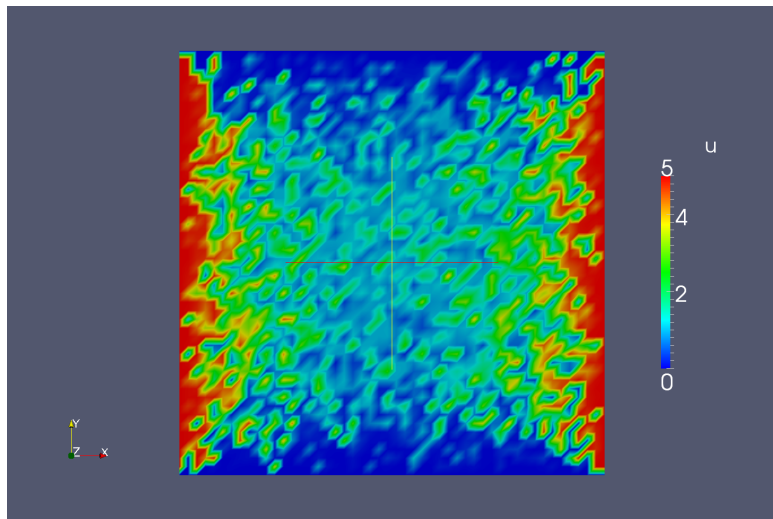


Figure : **Forward solution.** 2.5×10^3 *total histories.*

Solving the Heat Equation: Forward Method

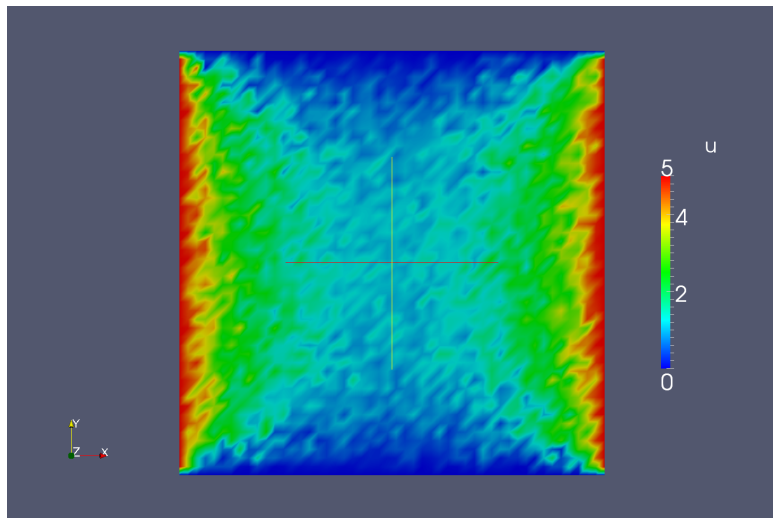


Figure : **Forward solution.** 2.5×10^4 *total histories.*

Solving the Heat Equation: Forward Method

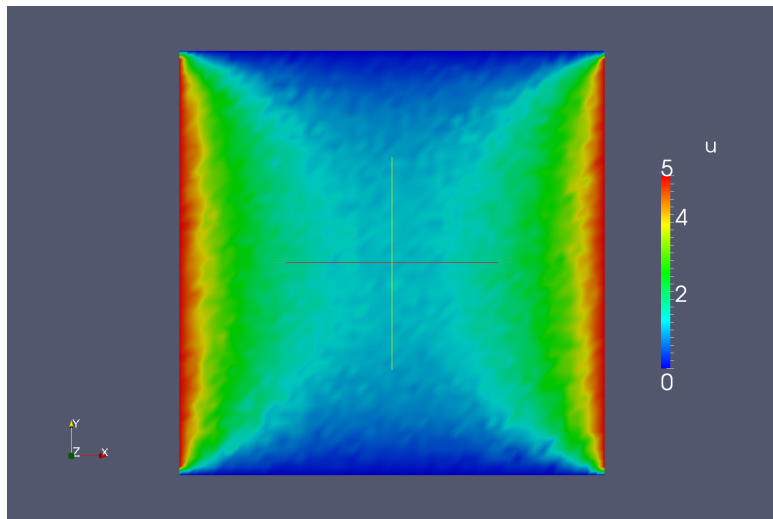


Figure : **Forward solution.** 2.5×10^5 *total histories.*

Solving the Heat Equation: Forward Method

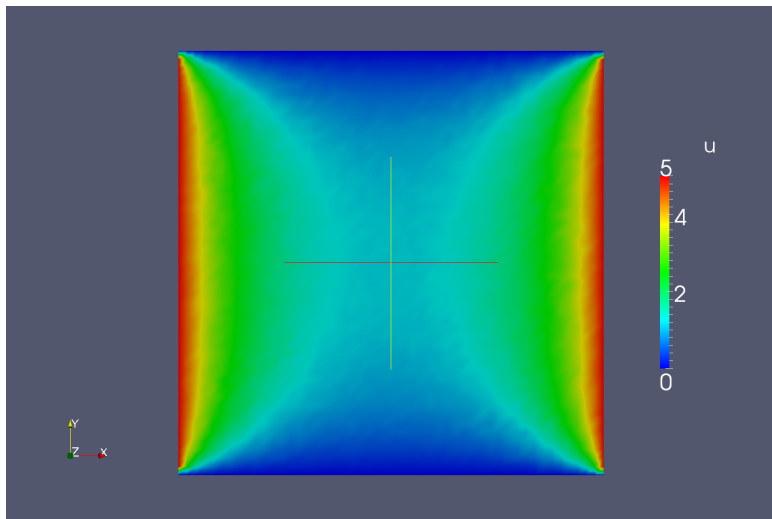


Figure : **Forward solution.** 2.5×10^6 *total histories.*

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 not yet addressed

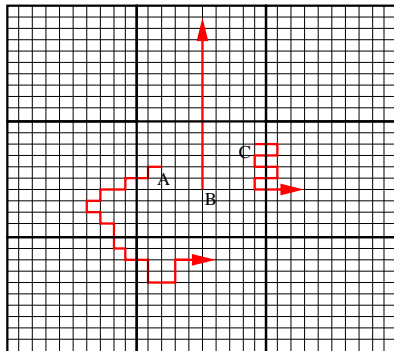
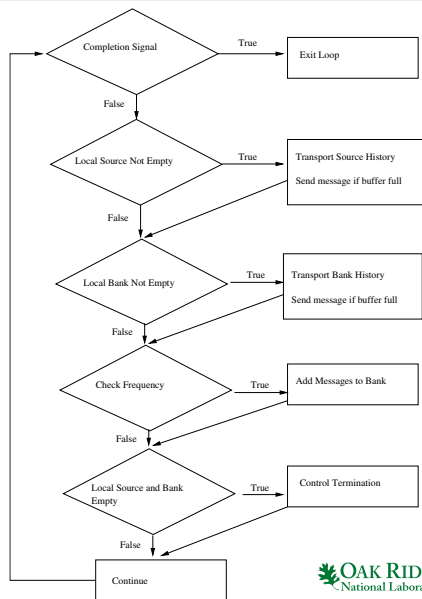
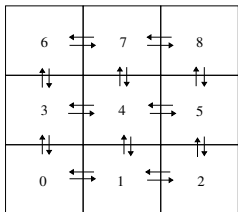


Figure : Domain decomposition example illustrating how domain-to-domain transport creates communication costs.

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 (running sum)



Exiting the Transport Loop without Collectives

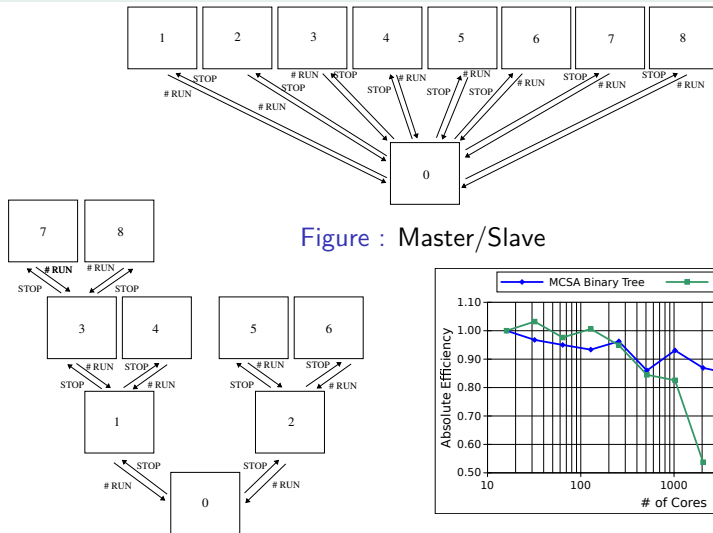


Figure : Master/Slave

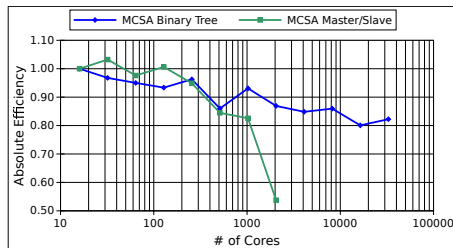


Figure : Weak scaling absolute efficiency


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 - Simplified P_N (SP_N) Assembly Problem

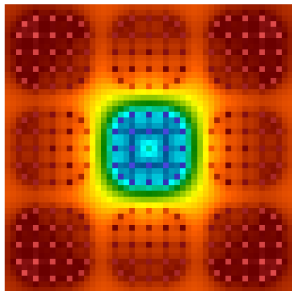


Figure : SP_N solution example

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

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

Scaling problem – 1×1 to 17×17 array of fuel assemblies with 289 pins each resolved by a 2×2 spatial mesh and 200 axial zones

- 7 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

Monte Carlo Communication Parameters

| | | Message Check Frequency | | | |
|---------------------|--------|-------------------------|-------|-------|-------|
| | | 128 | 256 | 512 | 1 024 |
| Message Buffer Size | 256 | 1.054 | 1.061 | 1.076 | 1.076 |
| | 512 | 1.103 | 1.146 | 1.211 | 1.270 |
| | 1 024 | 1.062 | 1.088 | 1.133 | 1.176 |
| | 2 048 | 1.030 | 1.042 | 1.072 | 1.107 |
| | 4 096 | 1.010 | 1.012 | 1.025 | 1.050 |
| | 8 192 | 1.001 | 1.000 | 1.008 | 1.018 |
| | 16 384 | 1.017 | 1.003 | 1.010 | 1.009 |

- OLCF Eos: 736-node Cray XC30, Intel Xeon E5-2670, 11,776 cores, 47 TB memory, Cray Aries interconnect
- 64 cores, 1.6M DOFs, history length of 15, 3 histories per DOF
- 27% decrease in runtime observed for bad parameter choices
- Worth the time to do this parameter study when running on new hardware

Monte Carlo Scaling

| Cores | DOFs | DOFs/Core | Time Min (s) | Time Max (s) | Time Ave (s) | Efficiency |
|--------|-------------|-----------|--------------|--------------|--------------|------------|
| 256 | 273 509 600 | 1 068 397 | 260.53 | 260.54 | 260.54 | 1.00 |
| 1 024 | 273 509 600 | 267 099 | | | | |
| 4 096 | 273 509 600 | 66 775 | | | | |
| 7 744 | 273 509 600 | 35 319 | | | | |
| 10 816 | 273 509 600 | 25 288 | | | | |

Table : Strong Scaling

| Cores | DOFs | DOFs/Core | Time Min (s) | Time Max (s) | Time Ave (s) | Efficiency |
|--------|-----------|-----------|--------------|--------------|--------------|------------|
| 64 | 1 618 400 | 25 288 | 6.432 | 6.432 | 6.432 | 1.00 |
| 256 | 6 473 600 | 25 288 | 6.493 | 6.493 | 6.493 | 0.99 |
| 1 024 | | 25 288 | | | | |
| 4 096 | | 25 288 | | | | |
| 7 744 | | 25 288 | | | | |
| 10 816 | | 25 288 | | | | |

Table : Weak Scaling

| Sets | Cores | DOFs | Time Min (s) | Time Max (s) | Time Ave (s) | Efficiency |
|------|-------|-----------|--------------|--------------|--------------|------------|
| 1 | 256 | 6 473 600 | 6.493 | 6.493 | 6.493 | 1.00 |
| 2 | 512 | 6 473 600 | | | | |
| 3 | 768 | 6 473 600 | | | | |
| 4 | 1 024 | 6 473 600 | | | | |

Table : Replication Scaling. 256 cores per set.

Algorithm Variations

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:

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

Matrix-Free Algorithm

- At each application of \mathbf{M}_{MC} , execute the Monte Carlo process
- Must perform Monte Carlo every time you want to apply with a better approximation requiring more time and more operations
- Variations in random number streams are amortized over iterations
- Vast majority of solve time spent doing Monte Carlo

| L | N_S | MC Time (s) | MC Fraction | MCSA Iters |
|-----|-------|-------------|-------------|------------|
| 3 | 1 | 30.885 | 0.96 | 266 |
| 3 | 2 | 60.869 | 0.98 | 261 |
| 5 | 1 | 27.422 | 0.97 | 180 |
| 5 | 2 | 54.319 | 0.98 | 175 |
| 10 | 1 | 23.871 | 0.98 | 102 |
| 10 | 2 | 45.551 | 0.99 | 97 |
| 15 | 1 | 50.395 | 0.98 | 164 |
| 15 | 2 | 42.951 | 0.99 | 69 |
| 15 | 3 | 65.292 | 0.99 | 68 |
| 25 | 1 | - | - | - |
| 25 | 2 | 70.505 | 0.99 | 78 |
| 25 | 3 | 63.677 | 1.00 | 47 |

Table : MCSA performance. A had 115 600 rows.

Stochastic Approximate Inverse Algorithm

- Construct \mathbf{M}_{MC} as a sparse matrix by executing the Monte Carlo process once and tallying the row entries
- Use this operator as a stochastic approximation to the inverse
- A better approximation to the inverse requires more setup time and more storage
- We will investigate a drop tolerance strategy to control sparsity

| L | N_S | NNZ | NNZ Ratio | MC Time (s) | Setup Time (s) | MCSA Iters |
|-----|-------|-----------|-------------|-------------|----------------|------------|
| 3 | 2 | 484 714 | 0.41 | 0.104 | 0.671 | 255 |
| 3 | 3 | 622 123 | 0.52 | 0.145 | 0.705 | 255 |
| 5 | 2 | 783 153 | 0.66 | 0.158 | 0.737 | 185 |
| 5 | 3 | 1 032 573 | 0.87 | 0.237 | 0.831 | 171 |
| 5 | 4 | 1 241 442 | 1.05 | 0.302 | 0.906 | 171 |
| 10 | 3 | 1 969 540 | 1.66 | 0.433 | 1.061 | 95 |
| 10 | 4 | 2 416 572 | 2.04 | 0.570 | 1.214 | 95 |
| 15 | 3 | 2 867 005 | 2.42 | 0.645 | 1.317 | 132 |
| 15 | 4 | 3 544 181 | 2.99 | 0.833 | 1.534 | 67 |
| 15 | 5 | 4 157 269 | 3.50 | 1.029 | 1.765 | 66 |

Table : MCSA Performance. A had 115 600 rows and 1 186 464 non-zero entries.

Unpreconditioned Algorithm Comparison

- No preconditioning, serial computation
- GMRES easier to preconditioner - performance here only indicates Monte Carlo potential
- These results indicate good stochastic approximate inverse performance for traditional CPU architectures
- Matrix-free approach may be more effective when vectorized for new architectures by favoring operations over storage - 95%+ of the runtime spent in Monte Carlo

| Solver | Iters | Time (s) | Time/Iter (s) |
|--------------------------|-------|----------|---------------|
| MCSA Matrix-Free | 102 | 24.414 | 0.239 |
| MCSA Approximate Inverse | 67 | 0.611 | 0.009 |
| Belos GMRES | 81 | 0.974 | 0.012 |

Table : A had 115 600 rows and 1 186 464 non-zero entries.

Conclusions and Future Work

Conclusions

- Monte Carlo methods offer great potential for both resilient and highly parallel solvers
- A fully asynchronous algorithm provides a scheme without collectives
- Good scaling demonstrated so far on reasonably load balanced problems
- Replication a potential resiliency strategy with some overhead
- Matrix-free and stochastic approximate inverse algorithms are complementary - trade operations for storage

Conclusions

- Vectorization an area of active research with a focus on heterogeneous architectures (Titan and Summit)
- Multiple threading models are being explored (Kokkos, HPX, etc.)
- Extending methods to broader problem areas is significant algorithmic challenge and an attractive area for continued research
- Performance modeling and resiliency simulations this FY