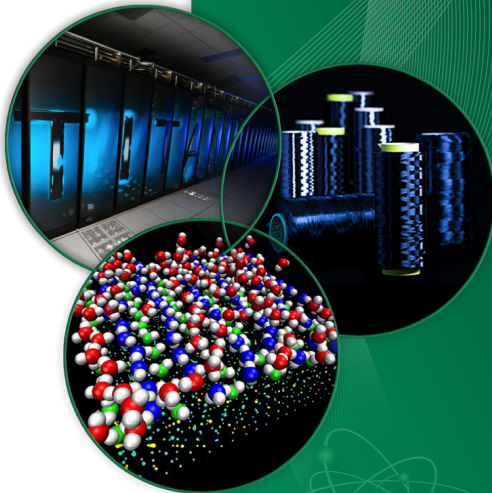


Parallel Algorithms for Monte Carlo Linear Solvers

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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

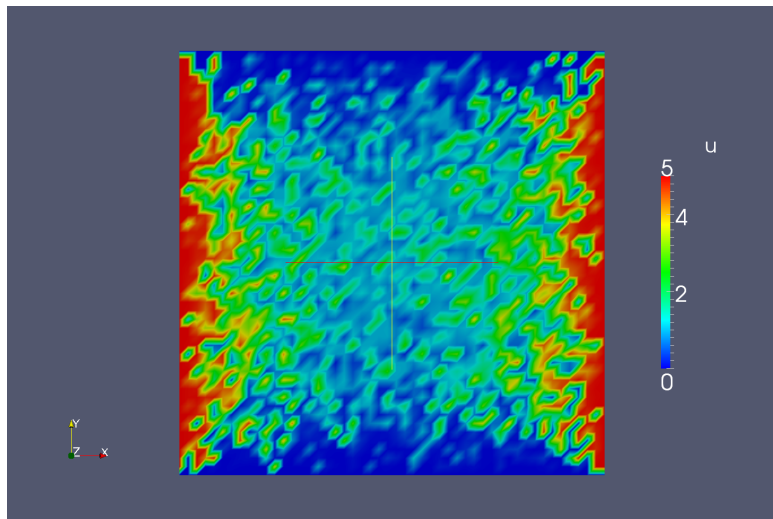


Figure : **Forward solution.** 2.5×10^3 *total histories.*

Solving the Heat Equation: Forward Method

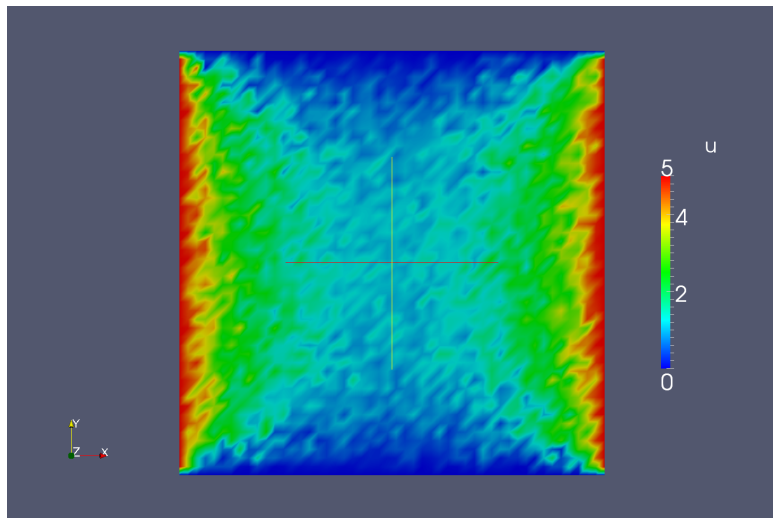


Figure : **Forward solution.** 2.5×10^4 *total histories.*

Solving the Heat Equation: Forward Method

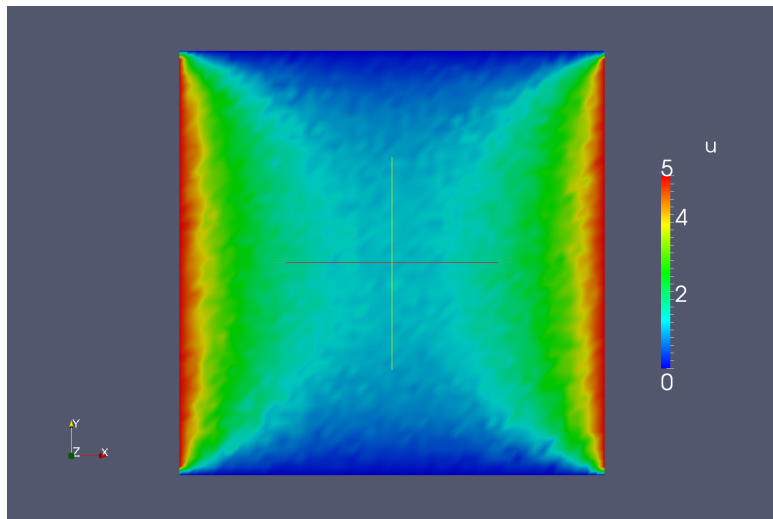


Figure : **Forward solution.** 2.5×10^5 *total histories.*

Solving the Heat Equation: Forward Method

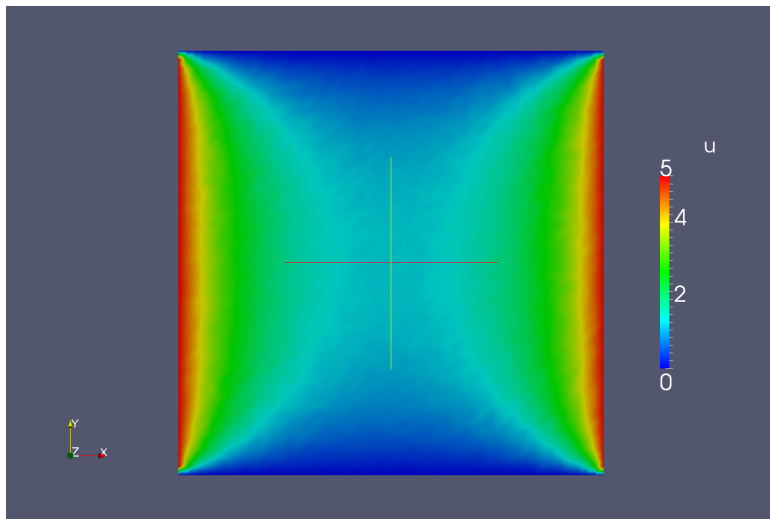


Figure : **Forward solution.** 2.5×10^6 *total histories.*

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

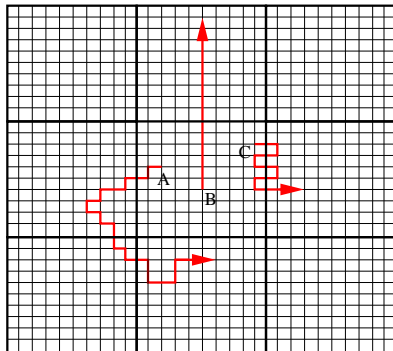
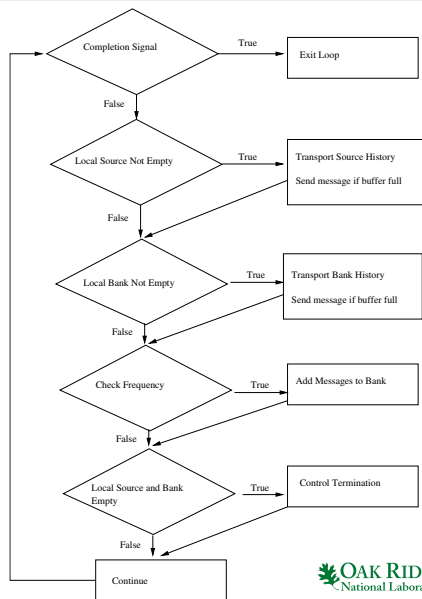
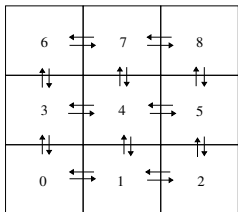


Figure : Domain decomposition example illustrating how domain-to-domain transport creates communication costs.

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

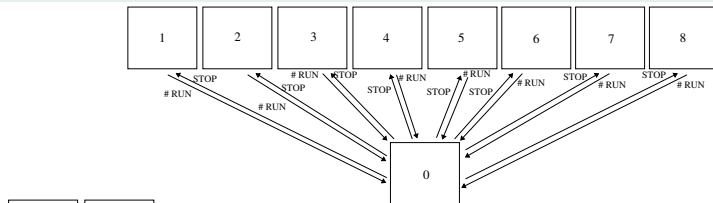


Figure : Master/Slave

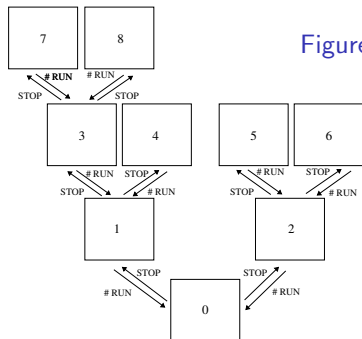


Figure : Binary Tree

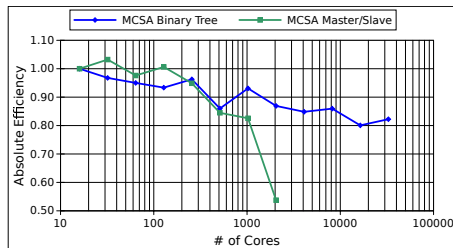


Figure : Weak scaling absolute efficiency


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 - Simplified P_N (SP_N) Assembly Problem

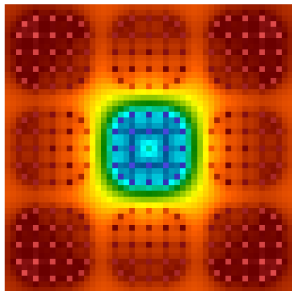


Figure : SP_N solution example

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	DOFs	DOFs/Core	Time Min (s)	Time Max (s)	Time Ave (s)	Efficiency
1	6 473 600	25 288	6.493	6.493	6.493	1.00
2	6 473 600	25 288				1.00
3	6 473 600	25 288				1.00
4	6 473 600	25 288				1.00

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