# Parallel Monte Carlo Synthetic Acceleration Methods for Discrete Transport Problems

Stuart R. Slattery University of Wisconsin - Madison

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# Acknowledgments



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### Outline



- Monte Carlo Synthetic Acceleration Methods
- Application to Neutron Transport
- Application to Fluid Flow
- Parallelization of MCSA
- Summary

#### Hardware-Based Motivation



- Modern hardware is moving in two directions (Kogge, 2011):
  - Lightweight machines
  - Heterogeneous machines
  - Both characterized by low power and high concurrency
- Some issues:
  - Higher potential for both soft and hard failures (DOE,2012)
  - 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 mitigated by replication
  - Memory savings over conventional methods

### Physics-Based Motivation



- New algorithms required to leverage new computational resources
  - Tremendous computational resources are required with  $O(1\times10^9)$  element meshes and O(100,000)+ cores used today for neutronics and fluid problems (Evans,2010)(Pawlowski,2012)
- Necessary to determine applicability to reactor physics and potential performance improvements before moving forward with other work
- Physics-driven development
  - Research applicability and potential improvements to neutronics and fluid flow
  - Offer solutions or a potential path forward for the observed issues
  - Work to improve iterative and parallel performance where possible

#### Statement of Work



The goal of this work is to improve the iterative performance and parallel scalability of solutions to discrete linear and nonlinear transport problems by researching and developing a new set of domain decomposed Monte Carlo Synthetic Acceleration methods.

#### Research Outline



- Development of a linear scheme for discrete systems leveraging Monte Carlo Synthetic Acceleration
  - Application to neutron transport
  - Research is required to study MCSA preconditioning
  - Iterative performance is of concern
- Development of a nonlinear scheme for discrete systems leveraging Monte Carlo Synthetic Acceleration
  - Monte Carlo is a more natural fit
  - Application to fluid flow
  - Convergence of the linear model is of concern
- Parallelization of Monte Carlo Synthetic Acceleration
  - Parallel strategies taken from modern reactor physics methods
  - Research is required to explore varying parallel strategies
  - Parallel scalability is of concern

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### 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

Thomas Evans and Scott Mosher, "A Monte Carlo Synthetic Acceleration method for the non-linear, time-dependent diffusion equation", American Nuclear Society - International Conference on Mathematics, Computational Methods and Reactor Physics, 2009.

### Monte Carlo Linear Solver Preliminaries



Split the linear operator

$$\mathbf{A}\mathbf{x} = \mathbf{b} \quad \rightarrow \quad \mathbf{x} = \mathbf{H}\mathbf{x} + \mathbf{b}$$

$$H = I - A$$

• 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 Neumann series

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

Define a sequence of state transitions

$$\nu = i \rightarrow i_1 \rightarrow \cdots \rightarrow i_{k-1} \rightarrow i_k$$

• Use the adjoint Neumann-Ulam decomposition

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

$$p_{ij} = \frac{|h_{ji}|}{\sum_{i} |h_{ji}|}, \ w_{ij} = \frac{h_{ji}}{p_{ij}}$$

The Hadamard product  $\mathbf{A} = \mathbf{B} \circ \mathbf{C}$  is defined element-wise as  $a_{ij} = b_{ij}c_{ij}$ .



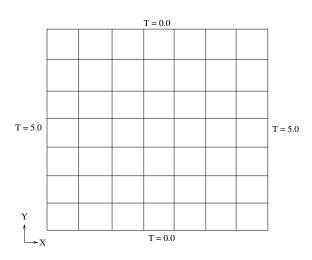


Figure: Poisson Problem. Distributed source of 1.0 in the domain.



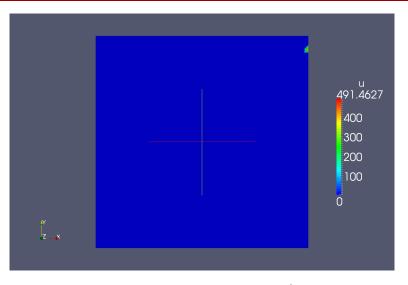


Figure: Adjoint solution to Poisson Equation.  $1 \times 10^0$  total histories, 0.286 seconds CPU time.



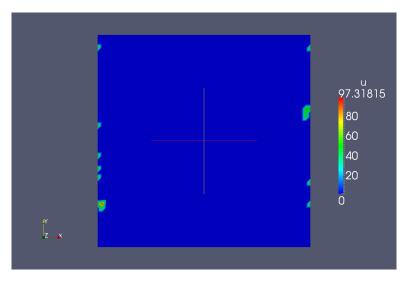


Figure: Adjoint solution to Poisson Equation.  $1 \times 10^1$  total histories, 0.278 seconds CPU time.



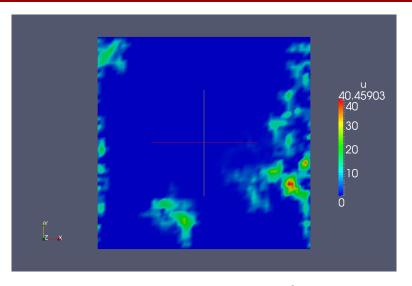


Figure: Adjoint solution to Poisson Equation.  $1 \times 10^2$  total histories, 0.275 seconds CPU time.



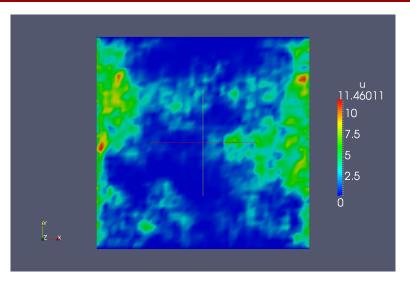


Figure: Adjoint solution to Poisson Equation.  $1 \times 10^3$  total histories, 0.291 seconds CPU time.



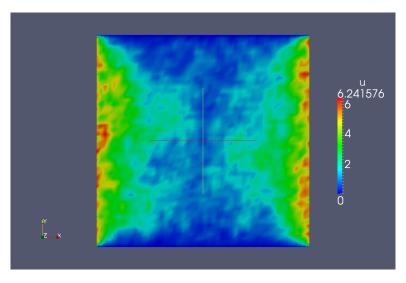


Figure: Adjoint solution to Poisson Equation.  $1 \times 10^4$  total histories, 0.428 seconds CPU time.



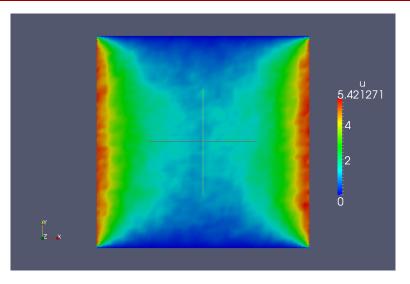


Figure: Adjoint solution to Poisson Equation.  $1\times10^5$  total histories, 1.76 seconds CPU time.



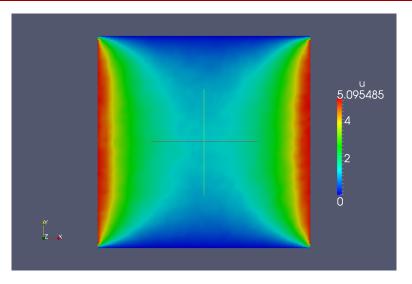


Figure: Adjoint solution to Poisson Equation.  $1 \times 10^6$  total histories, 15.1 seconds CPU time.



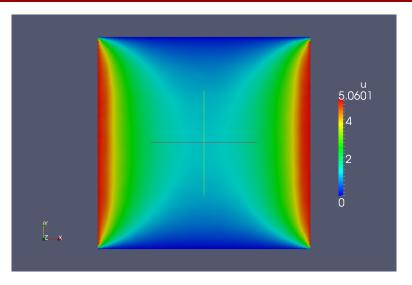


Figure: Adjoint solution to Poisson Equation.  $1 \times 10^7$  total histories, 149 seconds CPU time.

# Monte Carlo Synthetic-Acceleration



#### MCSA Iteration

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

- Neumann-Ulam methods bound by the Central Limit Theorem
- Build on Halton's 1962 Sequential Monte Carlo method
- Neumann-Ulam Monte Carlo solver computes the correction
- Decouples MC error from solution error, exponential convergence

# Monte Carlo Linear Solvers Library (MCLS)



- Designed to be easily incorporated with production physics codes
- General asynchronous MSOD MCSA implementation
  - Forward and adjoint Monte Carlo with method of expected values
  - Parallel row matrix/vector interface
  - General fixed point iteration strategy
  - Explicit algebraic preconditioner suite
- Implemented in C++
- Heavy use of the Trilinos scientific computing libraries
- Open-source BSD 3-clause license
- https://github.com/sslattery/MCLS

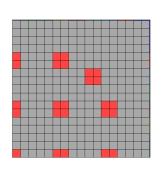
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# Fuel Assembly Criticality Calculations





- CASL Problem 3:  $17 \times 17$  quarter symmetry HZP LWR fuel assembly
- Multigroup SP<sub>N</sub> discretization
- MCLS leveraged by the Exnihilo code base (ORNL)
- Emphasize algorithm development for iterative performance

Value

0 1 11 1

Power Level	U IVIVV
Inlet Temperature	326.85C
Fuel Temperature	600C
Boron Concentration	1300 ppm
Moderator Density	0.743 g/cc
Helium Density	$1.79 \times 10^{-4} \text{ g/cc}$
Zirconium Density	6.56 g/cc
Stainless Steel Density	8.0 g/cc
Inconel Density	8.19 g/cc
UO2 Density	10.257 g/cc
Fuel Pin Radius (w/o clad)	0.4096 cm

Parameter



# $SP_N$ Equations



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

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

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

### k-eigenvalue Solutions with MCSA



#### **Algorithm 1** Power Iteration MCSA Scheme

```
k_0= initial guess oldsymbol{\Phi}_0= initial guess n=0 while |rac{k^n-k^{n-1}}{k^n}|<\epsilon do oldsymbol{\mathsf{M}}oldsymbol{\Phi}^{n+1}=rac{1}{k^n}oldsymbol{\mathsf{F}}oldsymbol{\Phi}^n {Solve for the new flux state with MCSA} k^{n+1}=k^nrac{\int \mathbf{F}oldsymbol{\Phi}^{n+1}d\mathbf{r}}{\int \mathbf{F}oldsymbol{\Phi}^nd\mathbf{r}} n=n+1 end while
```

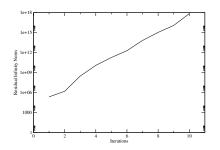
- Inject MCSA as the solver at each eigenvalue operation
- Transport operator is static one time cost for MCSA setup
- Current Exnihilo implementation gives the full operator

### Block Jacobi Preconditioned Calculations



	SP <sub>N</sub> Order						
		1	3 N Older	5	7		
	0	0.0647	0.1275	0.1449	0.1514		
	1	0.0686	0.1338	0.1484	0.1547		
P <sub>N</sub> Order	3	0.0687	0.1399	0.1582	0.1625		
	5	0.0692	0.1399	0.1582	0.1657		
	7	0.0678	0.1393	0.1624	0.166		

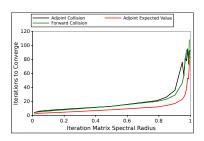
Table: Spectral radius results for the block Jacobi preconditioned iteration matrix with 10 energy groups and full downscatter for sample problem.

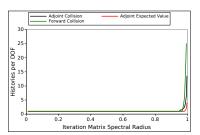


- Rapidly divergent results
- Light water moderator creates a lot of scattering and  $\rho(\mathbf{H}) \approx 1$
- Convergence not achieved with 50 histories per DOF and 90 minutes compute time

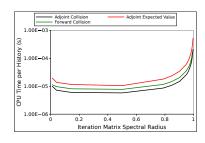
#### MCSA Breakdown







- As  $\rho(\mathbf{H}) \to 1$  terrible things happen...
- A more robust set of preconditioners is required for the SP<sub>N</sub> equations



# **Explicit Preconditioning**



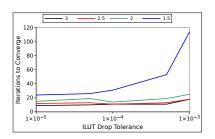
$$\begin{aligned} \mathbf{M}_L^{-1}\mathbf{A}\mathbf{M}_R^{-1}\mathbf{M}_R\mathbf{x} &= \mathbf{M}_L^{-1}\mathbf{b} &\to & \mathbf{M}_L^{-1}\mathbf{A}\mathbf{M}_R^{-1}\mathbf{u} &= \mathbf{M}_L^{-1}\mathbf{b} \\ \\ \mathbf{x} &= \mathbf{M}_R^{-1}\mathbf{u} \end{aligned}$$

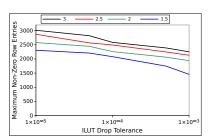
#### Left/Right Preconditioned MCSA Iteration

$$\mathbf{r}^k = \mathbf{M}_L^{-1} (\mathbf{b} - \mathbf{A} \mathbf{M}_R^{-1} \mathbf{u}^k)$$
 $\mathbf{u}^{k+1/2} = \mathbf{u}^k + \mathbf{r}^k$ 
 $\mathbf{r}^{k+1/2} = \mathbf{M}_L^{-1} (\mathbf{b} - \mathbf{A} \mathbf{M}_R^{-1} \mathbf{u}^{k+1/2})$ 
 $\mathbf{M}_L^{-1} \mathbf{A} \mathbf{M}_R^{-1} \delta \mathbf{u}^{k+1/2} = \mathbf{r}^{k+1/2}$ 
 $\mathbf{u}^{k+1} = \mathbf{u}^{k+1/2} + \delta \mathbf{u}^{k+1/2}$ 

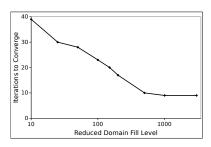
## **ILUT** Preconditioning







- Factor transport operator into upper and lower triangular parts
  - R = LU M
- Control factorization content with level-of-fill and drop tolerance
- Use the reduced domain approximation to recover sparsity

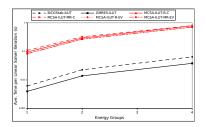


### Fuel Assembly Results



Solver	1 Group	2 Groups	4 Groups
BiCGStab-ILUT	11.6	11.6	12.4
GMRES-ILUT	18.1	17.9	18.9
MCSA-ILUT-R-C	14.6	15.4	17.6
MCSA-ILUT-MR-C	16.0	17.1	23.7
MCSA-ILUT-R-EV	18.3	19.4	16.8
MCSA-ILUT-MR-EV	19.6	22.4	17.5
Richardson-ILUT	60.9	60.4	63.4

Table: Average number of linear solver iterations per eigenvalue iteration.



- Comparison to Trilinos Aztec Krylov solvers with ILUT
- MCLS generates the same k-eigenvalue and neutron flux in all groups and spatial locations
- MCSA converged in fewer iterations than GMRES, more iterations than BiCGStab
- Explicit preconditioning strategy destroys sparsity and elevates CPU times (Ifpack ILUT)
- Spectral radius and memory limitations combine to prevent solutions at finer discretizations

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#### Navier-Stokes Benchmark Problems



- Sequence of Navier-Stokes benchmarks
  - Thermal convection cavity problem (De Vahl Davis, 1983)
  - Lid driven cavity problem (Ghia et al., 1982)
  - Backward-Facing step problem (Gartling, 1990)
- Tuning benchmark parameters varies the strength of nonlinearities

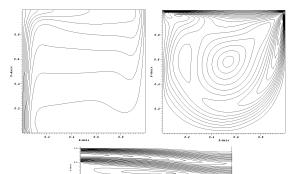
$$\rho \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \mathbf{T} - \rho \mathbf{g} = \mathbf{0}$$

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho C_{\rho} \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = 0$$

$$\mathbf{T} = -P\mathbf{I} + \mu [\nabla \mathbf{u} + \nabla \mathbf{u}^{T}]$$

$$\mathbf{q} = -k \nabla T$$



## MCSA for the Navier-Stokes Equations



- Need a nonlinear solution scheme for the Navier-Stokes equations
- Significant research on Newton methods since the 1980's
- Newton methods often leverage Krylov solvers
  - Robust implementations
  - No operator required
- Monte Carlo methods need the full operator
- Automatic construction of the linear model is available
  - Operator overloading for nonlinear residual differentiation
  - Ideal for Monte Carlo
  - Similar framework properties to matrix-free methods

### Newton's Method



• Seek solutions of the general nonlinear problem

$$\begin{aligned} & F(u) = 0 \\ & u \in \mathbb{R}^n, \ F: \mathbb{R}^N \rightarrow \mathbb{R}^N \end{aligned}$$

• Interpret the exact solution  $\mathbf{u}$  to be the roots of  $\mathbf{F}(\mathbf{u})$ 

$$F(u^{k+1}) = F(u^k) + F'(u^k)(u^{k+1} - u^k) + \frac{F''(u^k)}{2}(u^{k+1} - u^k)^2 + \cdots$$

Form Newton's method

$$J(\mathbf{u})\delta\mathbf{u}^k = -\mathbf{F}(\mathbf{u}^k)$$
$$\mathbf{u}^{k+1} = \mathbf{u}^k + \delta\mathbf{u}^k$$

### The FANM Method



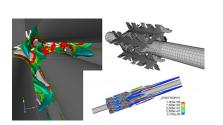
#### Forward-Automated Newton-MCSA

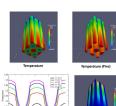
#### **Algorithm 2** FANM

- 1: k := 0
- 2: while  $||\mathbf{F}(\mathbf{u}^k)|| > \epsilon ||\mathbf{F}(\mathbf{u}^0)||$  do
- 3:  $J(\mathbf{u}^k) \leftarrow AD(\mathbf{F}(\mathbf{u}^k))$  {Automatic differentiation}
- 4:  $\mathbf{J}(\mathbf{u}^k)\delta\mathbf{u}^k = -\mathbf{F}(\mathbf{u}^k)$  {Solve for the Newton correction with MCSA}
- 5:  $\mathbf{u}^{k+1} \leftarrow \mathbf{u}^k + \delta \mathbf{u}^k$
- 6:  $k \leftarrow k + 1$
- 7: end while
  - Robustness of Newton's method (inexact)
  - · Accuracy and convenience of FAD
  - Potential parallelism, and resiliency benefits of MCSA
  - Requires only nonlinear function evaluations
  - Can utilize globalization and forcing term selection methods

### FANM Numerical Experiments











- Drekar is a production fluid base using Newton methods with FAD
- MCLS incorporated into Drekar nonlinear scheme to implement FANM
- Newton-Krylov method with Aztec GMRES used for benchmark comparisons
- All problems preconditioned with explicit scheme using algebraic multigrid (ML) and leveraged some kind of globalization (e.g. backtracking)

Images source: www.casl.gov

#### FANM Nonlinear Iteration Results



Benchmark	NK	NK FANM	
Convection, Ra= $1 \times 10^3$	5	5	5
Convection, Ra $=1  imes 10^4$	7 7		7
Convection, Ra $=1  imes 10^5$	9 10		9
Convection, Ra $=1  imes 10^6$	11 11		11
Lid Driven, Re=100	6	6	7
Lid Driven, Re=300	9	9	9
Lid Driven, Re=500	11 11		11
Lid Driven, Re=700	14 10		12
Backward Step, Re=200	10	9	10
Backward Step, Re=300	15 14		15
Backward Step, Re=400	10 10 10		10
Backward Step, Re=500	19	20	21

Table: Navier-Stokes benchmark comparison for nonlinear iterations. Over all benchmarks, FANM performed better in terms of nonlinear iterations for 1 more case than the Newton-Krylov method.

#### FANM Linear Solver Iteration Results



Benchmark	GMRES	MCSA	Richardson
Convection, Ra= $1 \times 10^3$	32	18	38
Convection, Ra= $1 \times 10^4$	23	17	34
Convection, Ra $=1  imes 10^5$	25	20	34
Convection, Ra= $1 \times 10^6$	39	25	48
Lid Driven, Re=100	27	42	151
Lid Driven, Re=300	35	52	133
Lid Driven, Re=500	41	56	154
Lid Driven, Re=700	21	14	32
Backward Step, Re=200	24	13	21
Backward Step, Re=300	23	17	21
Backward Step, Re=400	18	12	14
Backward Step, Re=500	30	52	98

Table: Navier-Stokes benchmark comparison for total linear solver iterations. Over all benchmarks, FANM performed better in terms of linear solver iterations for twice as many cases as the Newton-Krylov method.

#### FANM CPU Time Results



NK Speedup	
338	
336	
346	
465	
299	
322	
en, Re=500 288	
488	
400	
593	
825	
1057	

Table: **Newton-Krylov speedup over FANM.** For all benchmarks the explicit MCSA preconditioning strategy caused significantly larger CPU times for FANM when compared to the Newton-Krylov solutions.

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#### Parallelization of Monte Carlo Methods



- No literature observed for parallel Neumann-Ulam solvers beyond history-level parallelism
- Numerous references for modern parallel Monte Carlo methods in reactor physics
- Build a strategy for applying modern methods to the Neumann-Ulam method
- MCSA iteration-level parallelism comes from parallel matrix/vector operations

### 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

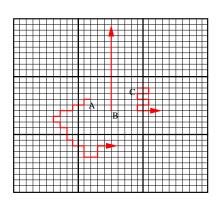
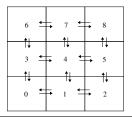


Figure: Domain decomposition example illustrating how domain-to-domain transport creates communication costs.

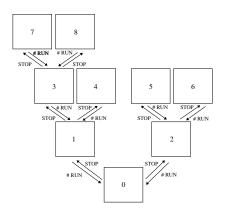
### Asynchronous Monte Carlo Transport Kernel



- Developed by Brunner and Brantley in 2009
- Asynchronous nearest neighbor communication of histories
- Binary asynchronous communication tree for completing transport



 Extensible to problems where histories may be created (i.e. variance reduction)



### Multiple-Set Overlapping-Domain Decomposition



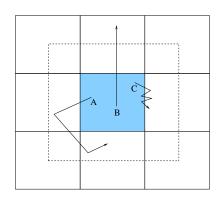


Figure: Overlapping domain example illustrating how domain overlap can reduce communication costs.

- Developed by Wagner and colleagues in 2010
- Each set contains the full domain
- Multiple sets replicate the domain
- Domains overlap within a set
- Redundancy for resiliency (and useful work)

Wagner et. al., "Hybrid and parallel domain-decomposition methods development to enable Monte Carlo for reactor analysis", Joint International Conference on Supercomputing in Nuclear Applications and Monte Carl (SNA+MC 2010), 2010.

### Multiple-Set Overlapping-Domain Decomposition



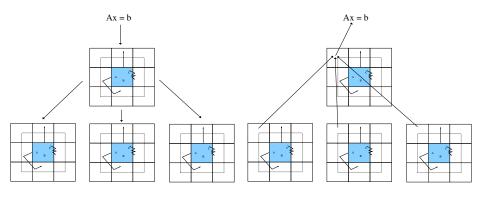


Figure: MSOD construction.

Figure: MSOD tally reduction.

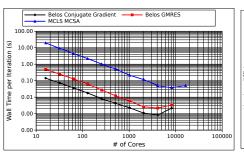
## Leadership-Class Parallel Scaling Studies



- Simple 2D neutron diffusion problem for control spectral radius is maintained as global problem size grows
- Comparison to Trilinos Belos Krylov solvers with Jacobi preconditioning - conjugate gradient and GMRES
- Strong scaling Global size fixed at 1.6E7 DOFs
- Weak scaling Local size fixed at 4.0E4 DOFs
- Calculations performed on the Titan Cray XK7 machine at ORNL (MPI only)
- Limited MCLS arithmetic optimization artificially inflates efficiencies

# Strong Scaling Results





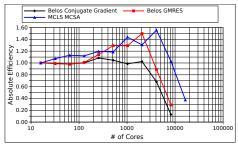


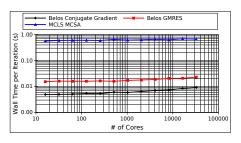
Figure: Wall time.

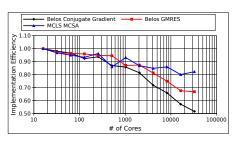
Figure: Absolute efficiency.

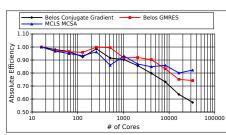
- MCLS is an order of magnitude slower arithmetically.
- Super-linear speed-up from memory thrashing in base case.
- CG demonstrates poor scaling due to the cheaper iteration sequence

# Weak Scaling Results









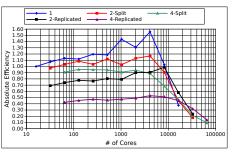
- Krylov implementation efficiencies drop with reduced iteration count
- MCSA maintained constant number of iterations

### Strong Scaling Results with Multiple Sets



**Splitting:** same global number of histories as the single set

**Replicating:** set-multiple of single set problem global histories



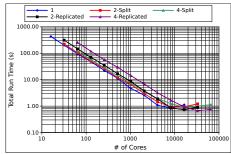


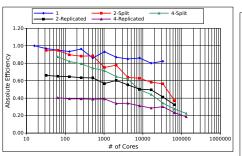
Figure: Absolute efficiency relative to 16-core 1-set base case.

Figure: Wall time

# Weak Scaling Results with Multiple Sets



- Need to consider adding sets is a strong scaling exercise
- Modify the weak scaling efficiency computation to account for these extra resources
- Superposition of Monte Carlo results enhances time to solution!



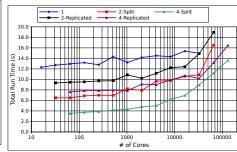


Figure: Absolute efficiency relative to 16-core 1-set base case.

Figure: Wall time.

# Scaling Results with Overlap



- Overlap values selected based on average 'diffusion length' of a history in the system of 2.6 discrete states
- Overlap eliminates communication in the Monte Carlo sequence but simply differs it to an overlapping tally vector reduction

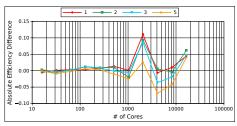


Figure: Strong scaling efficiency difference compared to the 0 overlap case.

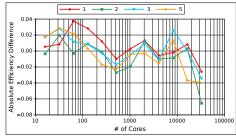
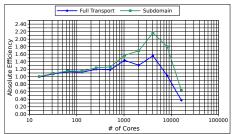


Figure: Weak scaling efficiency difference compared to the 0 overlap case.

#### MCSA as a Stochastic Additive Schwarz Method



- No domain-to-domain communication in Monte Carlo sequence
- Fixed point iteration acts as a smoother
- Observed to converge in the same number of iterations
- Can add overlap to preserve iterative performance for more ill-conditioned problems



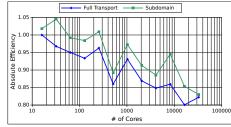


Figure: Strong scaling absolute efficiency relative to full transport base case.

Figure: Weak scaling absolute efficiency relative to full transport base case.

#### Outline



- Monte Carlo Synthetic Acceleration Methods
- Application to Neutron Transport
- Application to Fluid Flow
- Parallelization of MCSA
- Summary

### MCSA Application to Neutronics Summary



- MCSA has been incorporated into the Exnihilo neutronics production code base developed at Oak Ridge National Laboratory
- ullet MCSA can solve the asymmetric system generated by the  $SP_N$  equations
- Light water reactor problems are difficult to solve with MCSA as they have large spectral radii due to the neutron scattering in the moderator
- Advanced algebraic preconditioning strategies were applied to the SP<sub>N</sub> equations to obtain convergence with ILUT chosen for subsequent investigations
- MCSA with the reduced domain approximation was observed to converge in fewer iterations per eigenvalue iteration than GMRES for the fuel assembly criticality problem and more than Bi-CGStab using the same preconditioning

## MCSA Application to Fluid Flow Summary



- Forward-Automated Newton-MCSA (FANM) has been developed
- The FANM method has been incorporated into the Drekar multiphysics production code base developed at Sandia National Laboratories
- The FANM method has been verified to produce the same solutions as a production Newton-Krylov method for three difficult benchmark problems for the Navier-Stokes equations in different flow regimes and geometries
- The FANM method has better iterative performance than the Newton-Krylov method for convection dominated problems, converging in fewer linear solver iterations with the same preconditioning for high and low Rayleigh numbers
- The spectral radius convergence restriction on MCSA was observed to be a significant hindrance by preventing solutions to forced flow problems at high Reynolds numbers

### Parallelization of MCSA Summary



- The multiple-set overlapping-domain (MSOD) parallel algorithm for domain decomposed particle transport has been adapted to parallelize MCSA
- MCSA scales favorably compared to production Krylov methods for both strong and weak scaling cases
- Overlap in small quantities can provide parallel efficiency boosts of a few percent in strong scaling cases but is ineffective in weak scaling cases
- Multiple sets offers a means to reduce time to solution by solving multiple copies of the original problem and combining the solutions using superposition
- MCSA is most efficiently used in parallel as a stochastic realization of an additive Schwarz method

#### Future Work



- Shortcomings observed on real problems
  - Significant optimization required to determine production feasibility and true scalability
  - Explicit algebraic preconditioning methods not sufficient
  - Spectral radius limitation is severe
- Performance improvements
  - Random walk optimizations
  - Multiple set reduction analysis
  - FANM forcing term and MCSA history relationships
- Preconditioning improvements
  - Variance reduction based strategy
  - Reduced order physics/PDE models for acceleration
- Breaking away from  $ho(\mathbf{H}) < 1$ 
  - Monte Carlo methods of the second degree

#### **Publications**



- S.R. Slattery, T.M. Evans, P.P.H. Wilson, A Multiple-Set Overlapping-Domain Decomposed Monte Carlo Synthetic Acceleration Method for Linear Systems, Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2013 (SNA+MC 2013), Paris, France, October 27-31, 2013. Accepted for oral presentation.
- S.R. Slattery, T.M. Evans, P.P.H. Wilson, A Spectral Analysis of the Domain Decomposed Monte Carlo Method for Linear Systems, International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2013), American Nuclear Society, Sun Valley, ID, May 5-9, 2013.
- **3** T.M. Evans, S.W. Mosher, S.R. Slattery, S.P. Hamilton, **A Monte Carlo Synthetic-Acceleration Method for Solving the Thermal Radiation Diffusion Equation**, *Journal of Computational Physics, Submitted.*

#### Thank You



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