Parallel Monte Carlo Synthetic Acceleration Methods for Discrete Transport Problems

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Acknowledgments

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Outline

- **Introduction**
- 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 $O(1 \times 10^9)$ 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

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 the SP_N equations 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 the Navier-Stokes equations 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

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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

$$\mathbf{Ax} = \mathbf{b} \quad \rightarrow \quad \mathbf{x} = \mathbf{Hx} + \mathbf{b}$$

$$\mathbf{H} = \mathbf{I} - \mathbf{A}$$

- 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

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

- Define a sequence of state transitions

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

- Use the adjoint Neumann-Ulam decomposition

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

$$p_{ij} = \frac{|h_{ji}|}{\sum_j |h_{ji}|}, \;\; w_{ij} = \frac{h_{ji}}{p_{ij}}$$

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

Evolution of a Solution

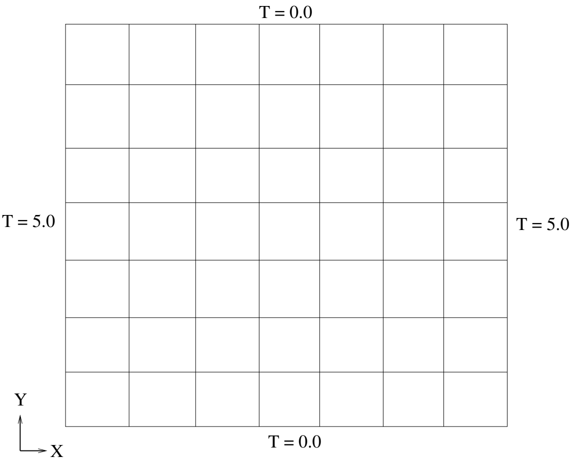

Figure: **Poisson Problem.** *Distributed source of 1.0 in the domain.*

Evolution of a Solution

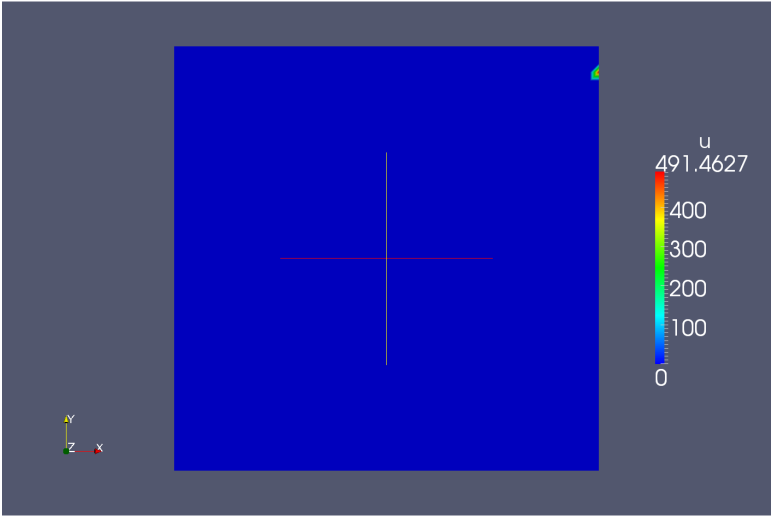

Figure: **Adjoint solution to Poisson Equation.** 1×10^0 *total histories, 0.286 seconds CPU time.*

Evolution of a Solution

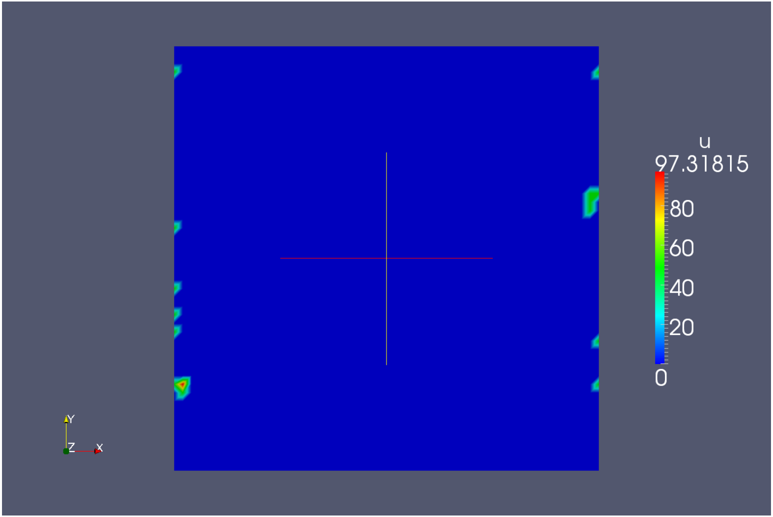

Figure: **Adjoint solution to Poisson Equation.** 1×10^1 *total histories, 0.278 seconds CPU time.*

Evolution of a Solution

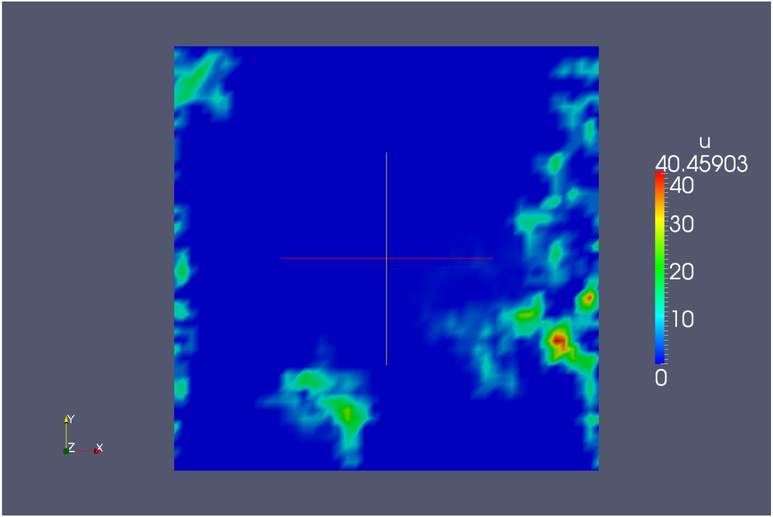

Figure: **Adjoint solution to Poisson Equation.** 1×10^2 *total histories, 0.275 seconds CPU time.*

Evolution of a Solution

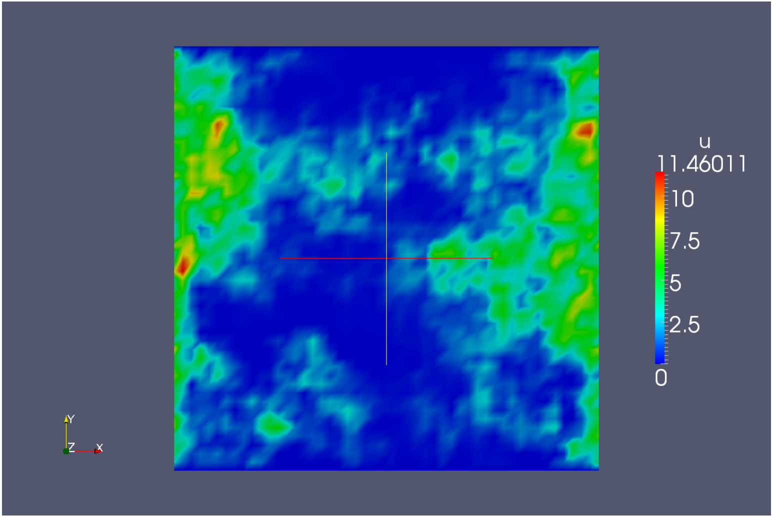

Figure: **Adjoint solution to Poisson Equation.** 1×10^3 *total histories, 0.291 seconds CPU time.*

Evolution of a Solution

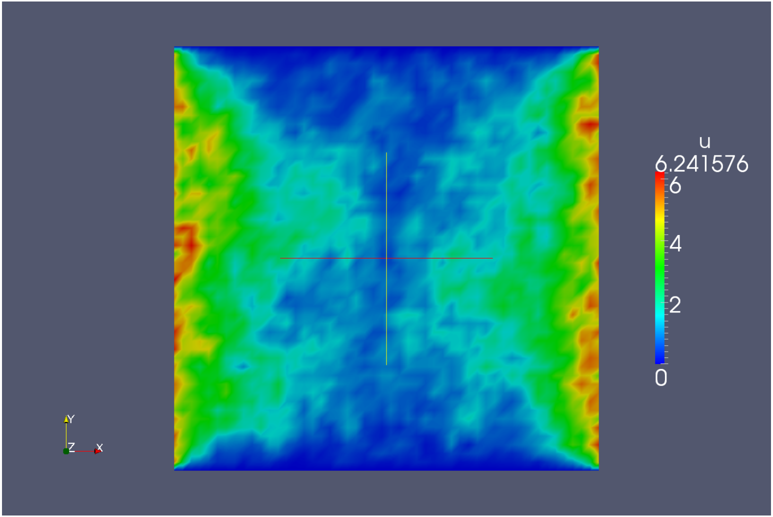

Figure: **Adjoint solution to Poisson Equation.** 1×10^4 *total histories, 0.428 seconds CPU time.*

Evolution of a Solution

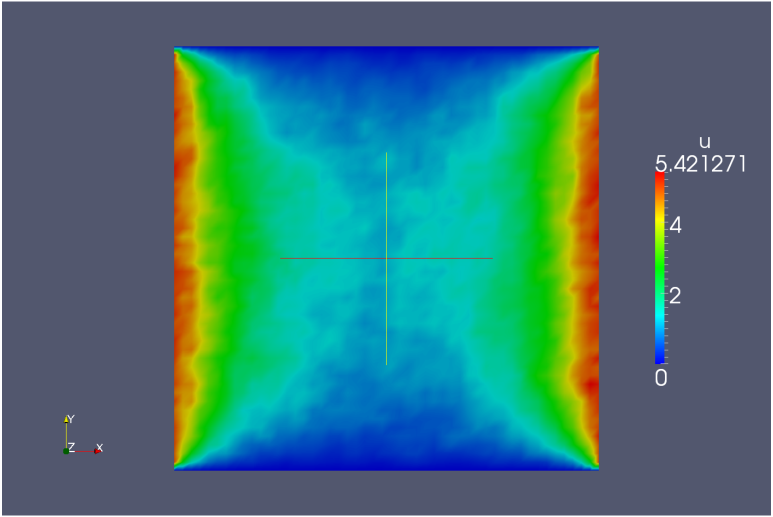

Figure: **Adjoint solution to Poisson Equation.** 1×10^5 *total histories, 1.76 seconds CPU time.*

Evolution of a Solution

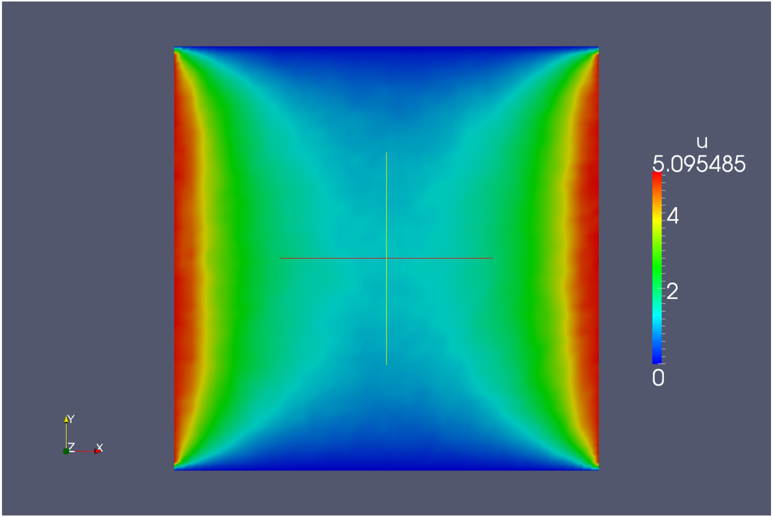

Figure: **Adjoint solution to Poisson Equation.** 1×10^6 *total histories, 15.1 seconds CPU time.*

Evolution of a Solution

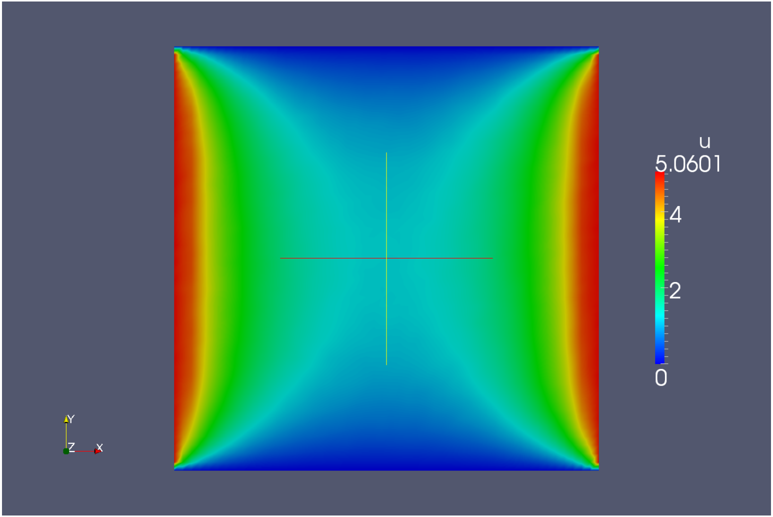

Figure: **Adjoint solution to Poisson Equation.** 1×10^7 *total histories, 149 seconds CPU time.*

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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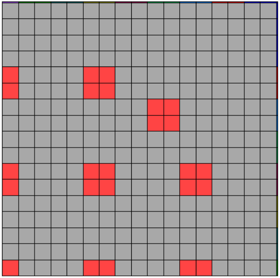
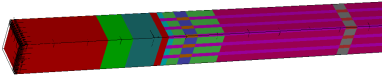
Fuel Assembly Criticality Calculations





- CASL Problem 3: 17×17 quarter symmetry HZP LWR fuel assembly
- Multigroup SP_N discretization
- MCLS leveraged by the Exnihilo code base (ORNL)
- Emphasize algorithm development for iterative performance

Parameter	Value
Power Level	0 MW
Inlet Temperature	326.85C
Fuel Temperature	600C
Boron Concentration	1300 ppm
Moderator Density	0.743 g/cc
Helium Density	1.79×10^{-4} 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

SP_N Equations

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

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

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

k-eigenvalue Solutions with MCSA

Algorithm 1 Power Iteration MCSA Scheme

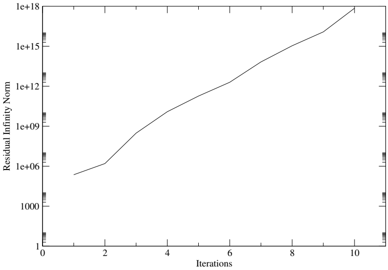
k_0 = initial guess
$\mathbf{\Phi}_0$ = initial guess
$n = 0$
while $|\frac{k^n - k^{n-1}}{k^n}| < \epsilon$ **do**
  $\mathbf{M}\mathbf{\Phi}^{n+1} = \frac{1}{k^n}\mathbf{F}\mathbf{\Phi}^n$ {Solve for the new flux state with MCSA}
  $k^{n+1} = k^n \frac{\int \mathbf{F}\mathbf{\Phi}^{n+1} d\mathbf{r}}{\int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

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

Block Jacobi Preconditioned Calculations

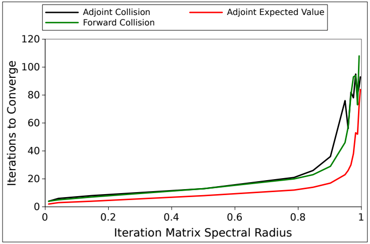
		SP_N Order			
		1	**3**	**5**	**7**
	0	0.0647	0.1275	0.1449	0.1514
	1	0.0686	0.1338	0.1484	0.1547
P_N Order	**3**	0.0687	0.1399	0.1582	0.1625
	5	0.0692	0.1399	0.1582	0.1657
	7	0.0678	0.1393	0.1624	0.166

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

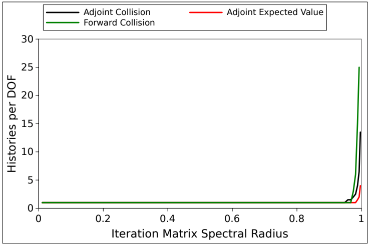


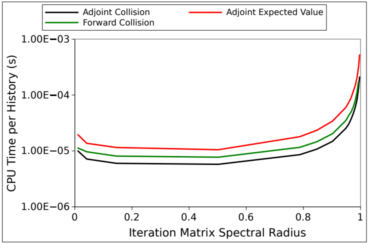
- Rapidly divergent results
- Light water moderator creates a lot of scattering and $\rho(\mathbf{H}) \approx 1$
- Convergence not achieved with 50 histories per DOF and 90 minutes compute time

MCSA Breakdown



- As $\rho(\mathbf{H}) \rightarrow 1$ terrible things happen...
- A more robust set of preconditioners is required for the SP_N equations





Explicit Preconditioning

$$\mathbf{M}_L^{-1}\mathbf{A}\mathbf{M}_R^{-1}\mathbf{M}_R\mathbf{x} = \mathbf{M}_L^{-1}\mathbf{b} \quad \rightarrow \quad \mathbf{M}_L^{-1}\mathbf{A}\mathbf{M}_R^{-1}\mathbf{u} = \mathbf{M}_L^{-1}\mathbf{b}$$

$$\mathbf{x} = \mathbf{M}_R^{-1}\mathbf{u}$$

Left/Right Preconditioned MCSA Iteration

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

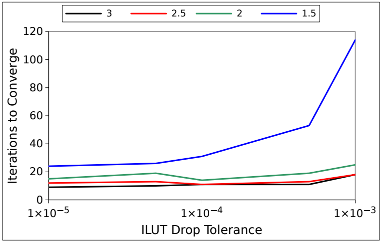
$$\mathbf{u}^{k+1/2} = \mathbf{u}^k + \mathbf{r}^k$$

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

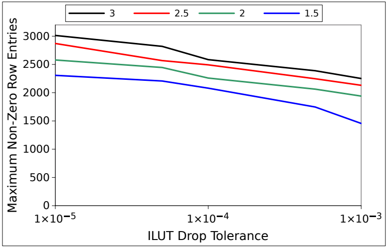
$$\mathbf{M}_L^{-1}\mathbf{A}\mathbf{M}_R^{-1}\delta\mathbf{u}^{k+1/2} = \mathbf{r}^{k+1/2}$$

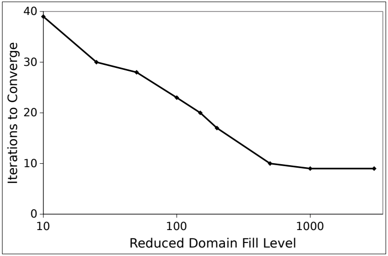
$$\mathbf{u}^{k+1} = \mathbf{u}^{k+1/2} + \delta\mathbf{u}^{k+1/2}$$

ILUT Preconditioning



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

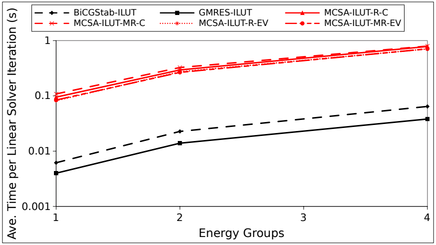




Fuel Assembly Results

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 verified for the k-eigenvalue and neutron flux in all groups
- 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

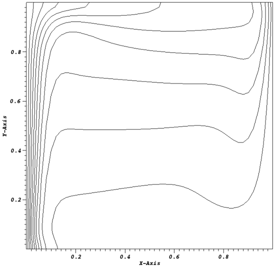
$$\rho \mathbf{u} \cdot \nabla \mathbf{u} - \nabla \cdot \mathbf{T} - \rho \mathbf{g} = \mathbf{0}$$

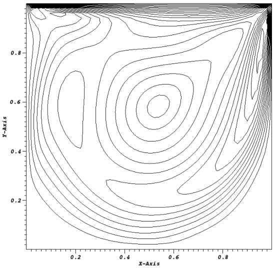
$$\nabla \cdot \mathbf{u} = 0$$

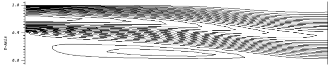
$$\rho C_p \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = 0$$

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

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







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
  - Simple implementation
  - 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

$$\mathbf{F}(\mathbf{u}) = \mathbf{0}$$
$$\mathbf{u} \in \mathbb{R}^n,\ \mathbf{F} : \mathbb{R}^N \to \mathbb{R}^N$$

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

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

- Form Newton's method

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

The FANM Method

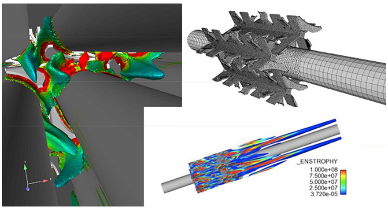
Forward-Automated Newton-MCSA

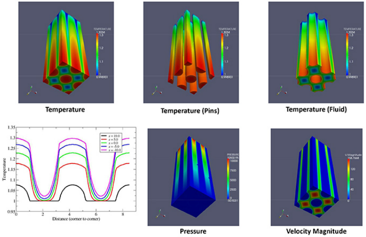
Algorithm 2 FANM

$k := 0$
while $||\mathbf{F}(\mathbf{u}^k)|| > \epsilon ||\mathbf{F}(\mathbf{u}^0)||$ **do**
    $\mathbf{J}(\mathbf{u}^k) \leftarrow AD(\mathbf{F}(\mathbf{u}^k))$ {Automatic differentiation}
    $\mathbf{J}(\mathbf{u}^k)\delta\mathbf{u}^k = -\mathbf{F}(\mathbf{u}^k)$ {Solve for the Newton correction with MCSA}
    $\mathbf{u}^{k+1} \leftarrow \mathbf{u}^k + \delta\mathbf{u}^k$
    $k \leftarrow k + 1$
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

Thermal Convection Cavity Results

Benchmark	NK	FANM	NR
Ra=1×10^3	5	5	5
Ra=1×10^4	7	7	7
Ra=1×10^5	9	10	9
Ra=1×10^6	11	11	11

Table: Nonlinear iterations.

- Weaker preconditioning at 1×10^{-5} case
- Forcing term method adapts to nonlinear convergence
- Constant forcing term for 1×10^{-6} case

Benchmark	GMRES	MCSA	Richardson
Ra=1×10^3	32	18	38
Ra=1×10^4	23	17	34
Ra=1×10^5	25	20	34
Ra=1×10^6	39	25	48

Table: Total linear solver iterations.

Benchmark	NK Speedup
Ra=1×10^3	338
Ra=1×10^4	336
Ra=1×10^5	346
Ra=1×10^6	465

Table: Newton-Krylov speedup over FANM.

Lid Driven Cavity Results

Benchmark	NK	FANM	NR
Re=100	6	6	7
Re=300	9	9	9
Re=500	11	11	11
Re=700	14	10	12

Table: Nonlinear iterations.

- Forcing term selection can significantly modify nonlinear convergence
- $\eta_k = \gamma \left(\frac{||\mathbf{F}(\mathbf{u}_k)||}{||\mathbf{F}(\mathbf{u}_{k-1})||} \right)^{\alpha}$

Benchmark	GMRES	MCSA	Richardson
Re=100	27	42	151
Re=300	35	52	133
Re=500	41	56	154
Re=700	21	14	32

Table: Total linear solver iterations.

Benchmark	NK Speedup
Re=100	299
Re=300	322
Re=500	288
Re=700	488

Table: Newton-Krylov speedup over FANM.

Backward Facing Step Results

Benchmark	NK	FANM	NR
Re=200	10	9	10
Re=300	15	14	15
Re=400	10	10	10
Re=500	19	20	21

Table: Nonlinear iterations.

- Significantly more ill-conditioned than cavity problems
- Forcing terms are not the culprit
- Multigrid is doing significantly more work

Benchmark	GMRES	MCSA	Richardson
Re=200	24	13	21
Re=300	23	17	21
Re=400	18	12	14
Re=500	30	52	98

Table: Total linear solver iterations.

Benchmark	NK Speedup
Re=200	400
Re=300	593
Re=400	825
Re=500	1057

Table: Newton-Krylov speedup over FANM.

Iterative Performance Summary

Benchmark	Newton-Krylov	FANM
Convection, Ra=1 $\times$ 10^3	$\times$	$\times$
Convection, Ra=1 $\times$ 10^4	$\times$	$\times$
Convection, Ra=1 $\times$ 10^5	$\times$	
Convection, Ra=1 $\times$ 10^6	$\times$	$\times$
Lid Driven, Re=100	$\times$	$\times$
Lid Driven, Re=300	$\times$	$\times$
Lid Driven, Re=500	$\times$	$\times$
Lid Driven, Re=700		$\times$
Backward Step, Re=200		$\times$
Backward Step, Re=300		$\times$
Backward Step, Re=400	$\times$	$\times$
Backward Step, Re=500	$\times$	

Table: Navier-Stokes benchmark comparison for nonlinear iterations.

Benchmark	Newton-Krylov	FANM
Convection, Ra=1 $\times$ 10^3		$\times$
Convection, Ra=1 $\times$ 10^4		$\times$
Convection, Ra=1 $\times$ 10^5		$\times$
Convection, Ra=1 $\times$ 10^6		$\times$
Lid Driven, Re=100	$\times$	
Lid Driven, Re=300	$\times$	
Lid Driven, Re=500	$\times$	
Lid Driven, Re=700		$\times$
Backward Step, Re=200		$\times$
Backward Step, Re=300		$\times$
Backward Step, Re=400		$\times$
Backward Step, Re=500	$\times$	

Table: Navier-Stokes benchmark comparison for total linear solver iterations.

- Over all benchmarks, FANM performed better in terms of nonlinear iterations for 1 more case than the Newton-Krylov method
- Over all benchmarks, FANM performed better in terms of linear solver iterations for twice as many cases as the Newton-Krylov method

Outline

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

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

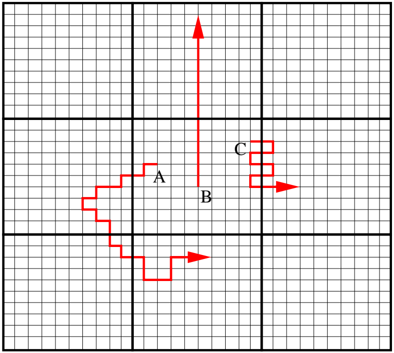
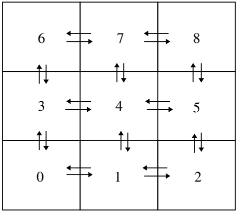


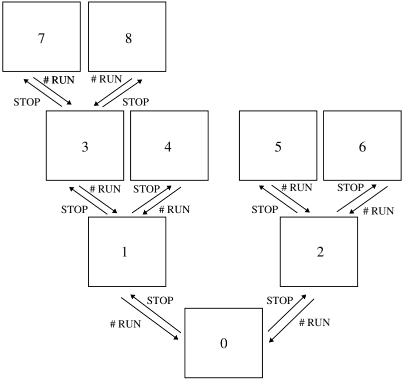
Figure: *Domain decomposition example illustrating how domain-to-domain transport creates communication costs.*

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)



Thomas A. Brunner and Patrick S. Brantley, "An efficient, robust, domain-decomposition algorithm for particle Monte Carlo", Journal of Computational Physics, vol. 228, pp.3882-3890, 2009.

Multiple-Set Overlapping-Domain Decomposition

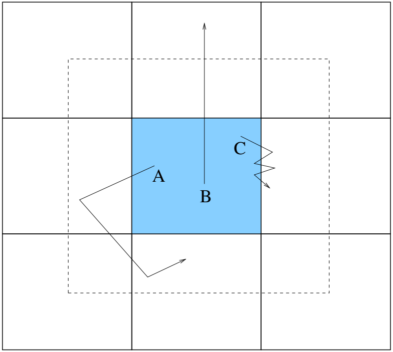


Figure: *Overlapping domain example illustrating how domain overlap can reduce communication costs.*

- 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

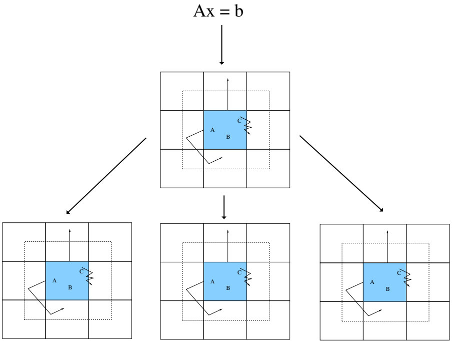


Figure: *MSOD construction.*

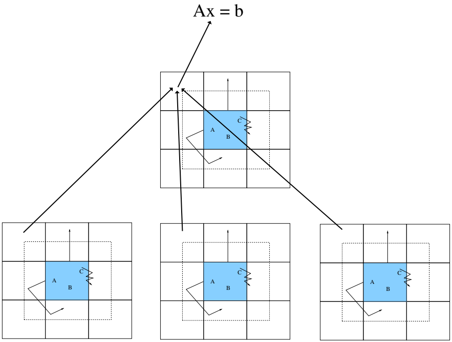


Figure: *MSOD tally reduction.*

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

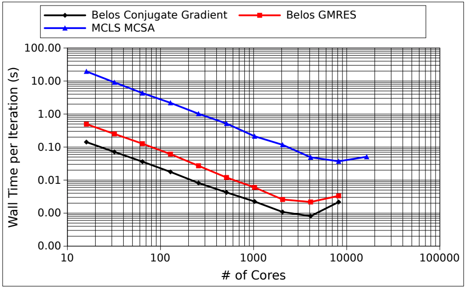


Figure: Wall time.

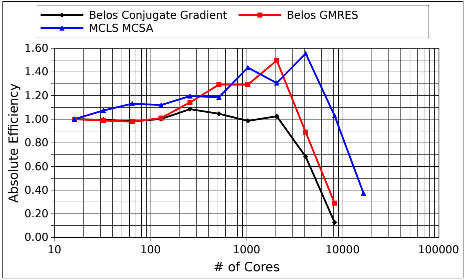
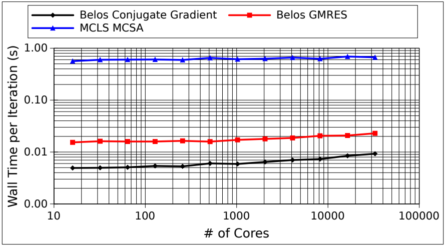
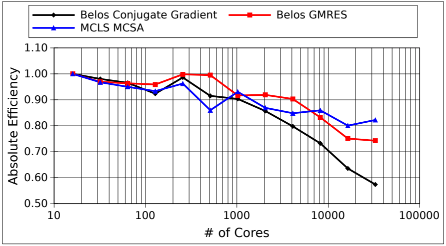


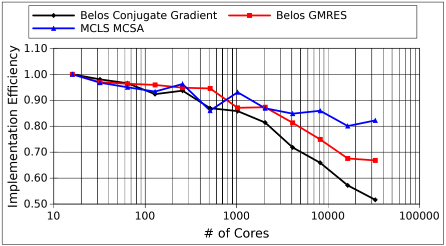
Figure: Absolute efficiency.

- 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

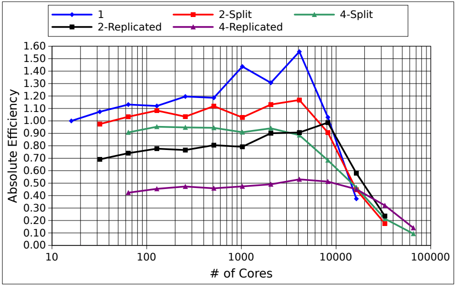


Figure: Absolute efficiency relative to 16-core 1-set base case.

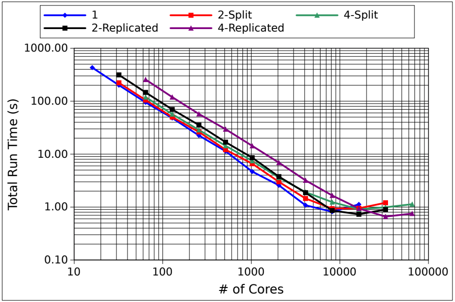


Figure: Wall time

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!

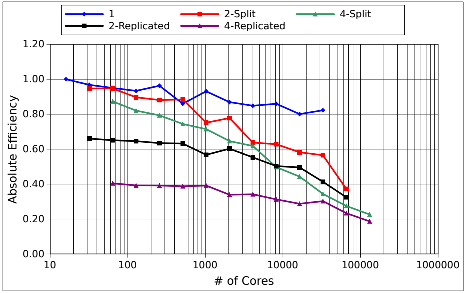


Figure: Absolute efficiency relative to 16-core 1-set base case.

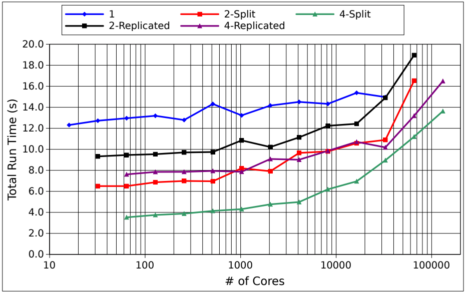


Figure: Wall time.

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

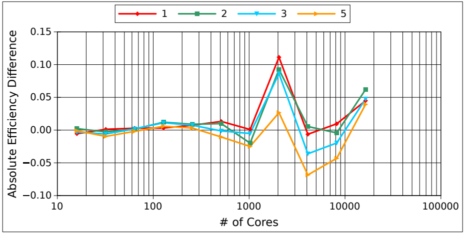


Figure: Strong scaling efficiency difference compared to the 0 overlap case.

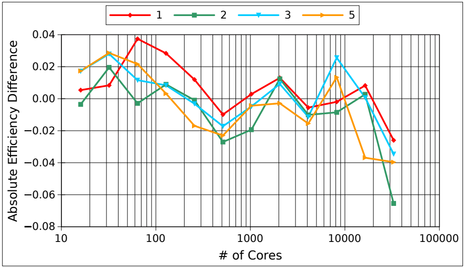


Figure: Weak scaling efficiency difference compared to the 0 overlap case.

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

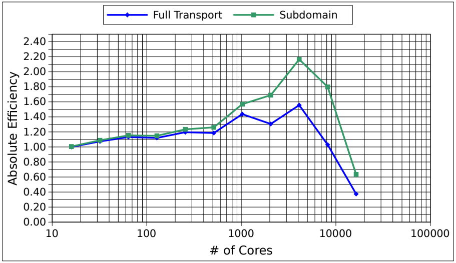


Figure: Strong scaling absolute efficiency relative to full transport base case.

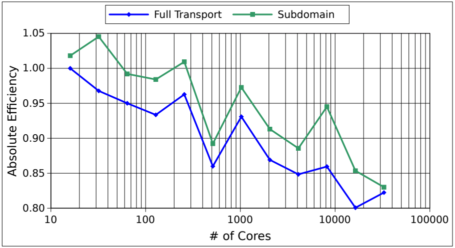


Figure: Weak scaling absolute efficiency relative to full transport base case.

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- 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
- 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_N 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 $\rho(\mathbf{H}) < 1$
  - Monte Carlo methods of the second degree

Publications

1. 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.*
2. 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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