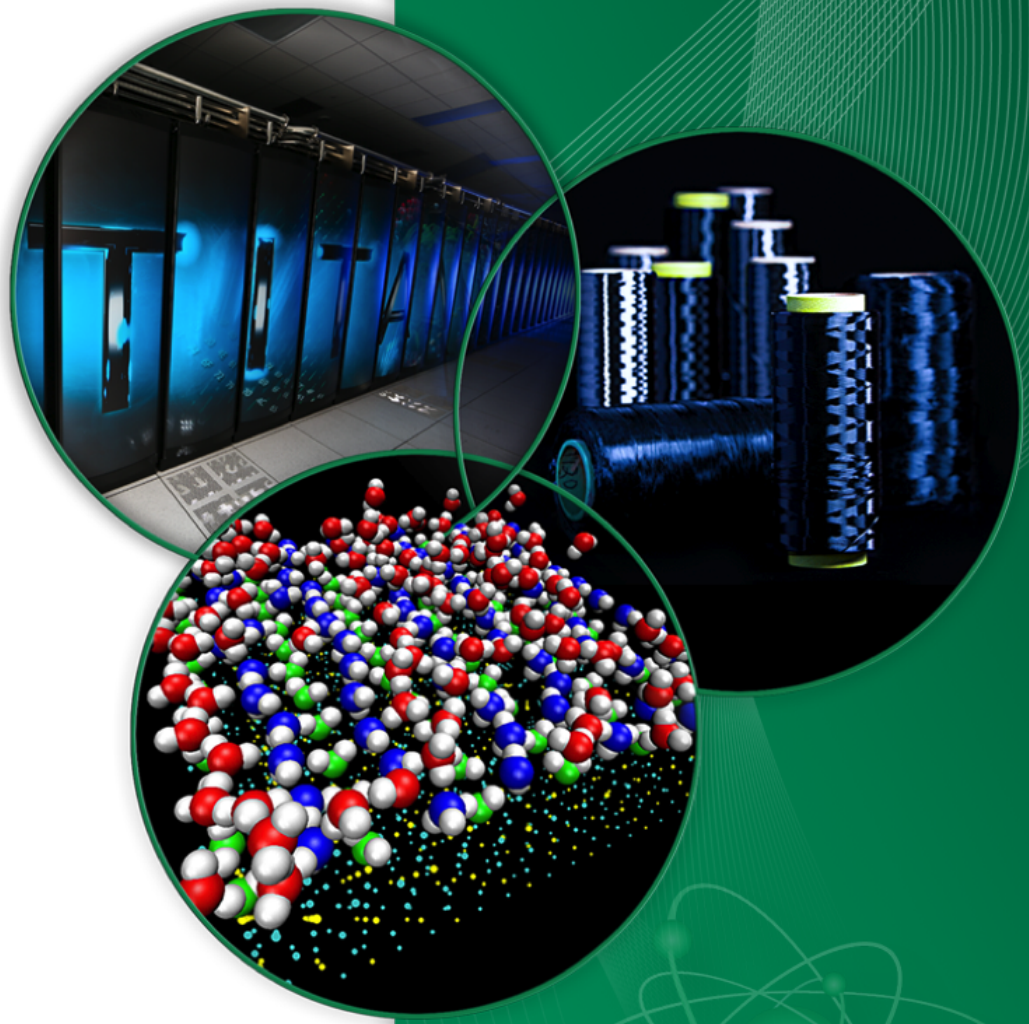
Monte Carlo Linear Solvers



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Emory Seminar
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U.S. DEPARTMENT OF ENERGY

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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

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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
   - One possibility: Monte Carlo methods

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Monte Carlo for Linear Systems

- Suppose we want to solve $\mathbf{A}\mathbf{x} = \mathbf{b}$
- 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 Richardson iteration matrix

- Traverse the Neumann series stochastically

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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

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Adjoint Monte Carlo

- Choose $\mathbf{P}$ and $\mathbf{W}$ such that $\mathbf{H}^T = \mathbf{P} \circ \mathbf{W}$
- Typical choice (Monte Carlo Almost-Optimal):

$$\mathbf{P}_{ij} = \frac{|\mathbf{H}_{ji}|}{\sum_{i=1}^{N} |\mathbf{H}_{ji}|}$$

- To estimate solution:
  - Start a history in random state i by sampling from distribution determined by $\mathbf{b}$
  - 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 $\mathbf{x}_j$ based on current history weight
- A given random walk can contribute to many different components of the solution vector

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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

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Solving Heat Equation: Forward Method

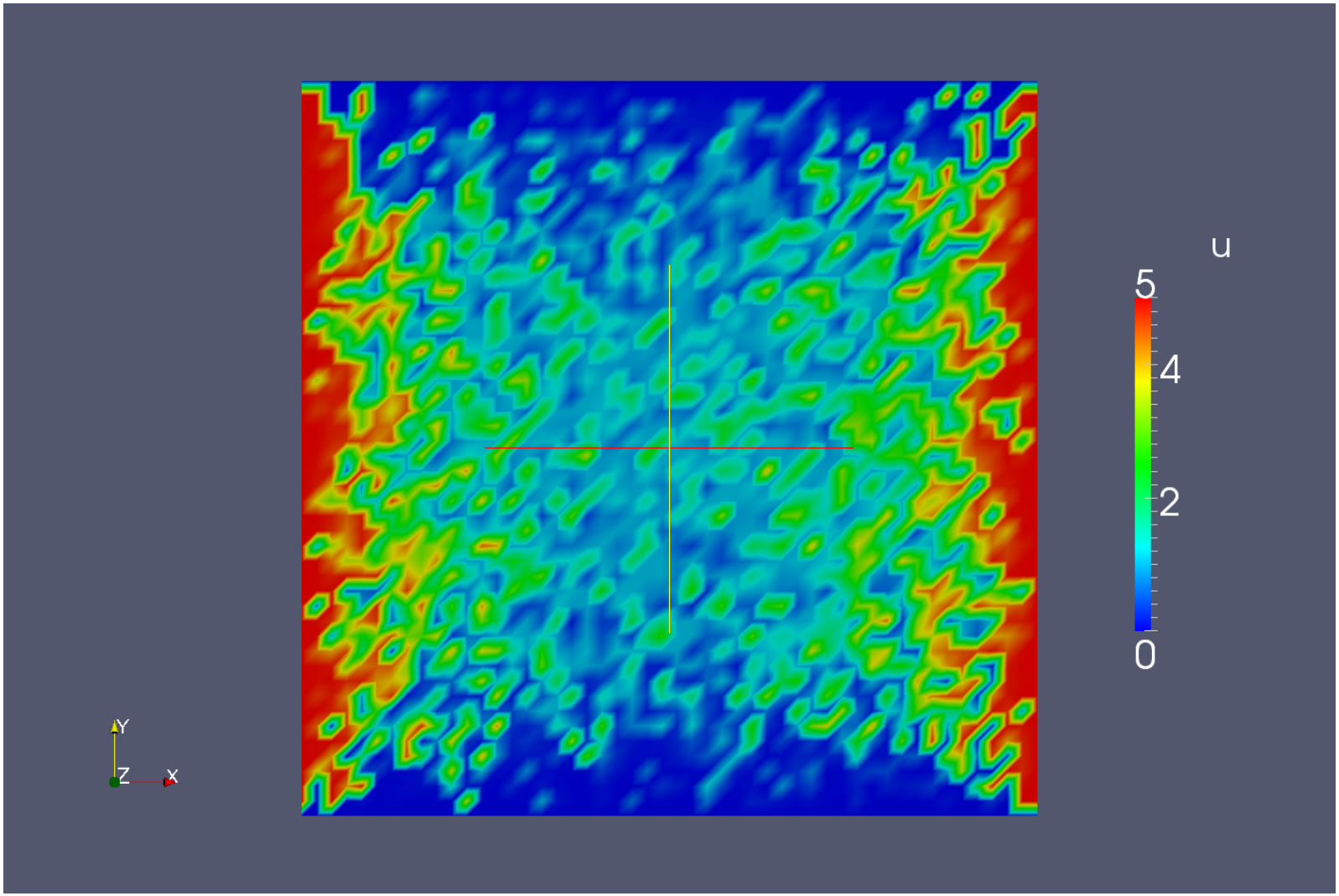

Figure : **Forward solution.** 2.5×10^3 *total histories.*

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Solving Heat Equation: Forward Method

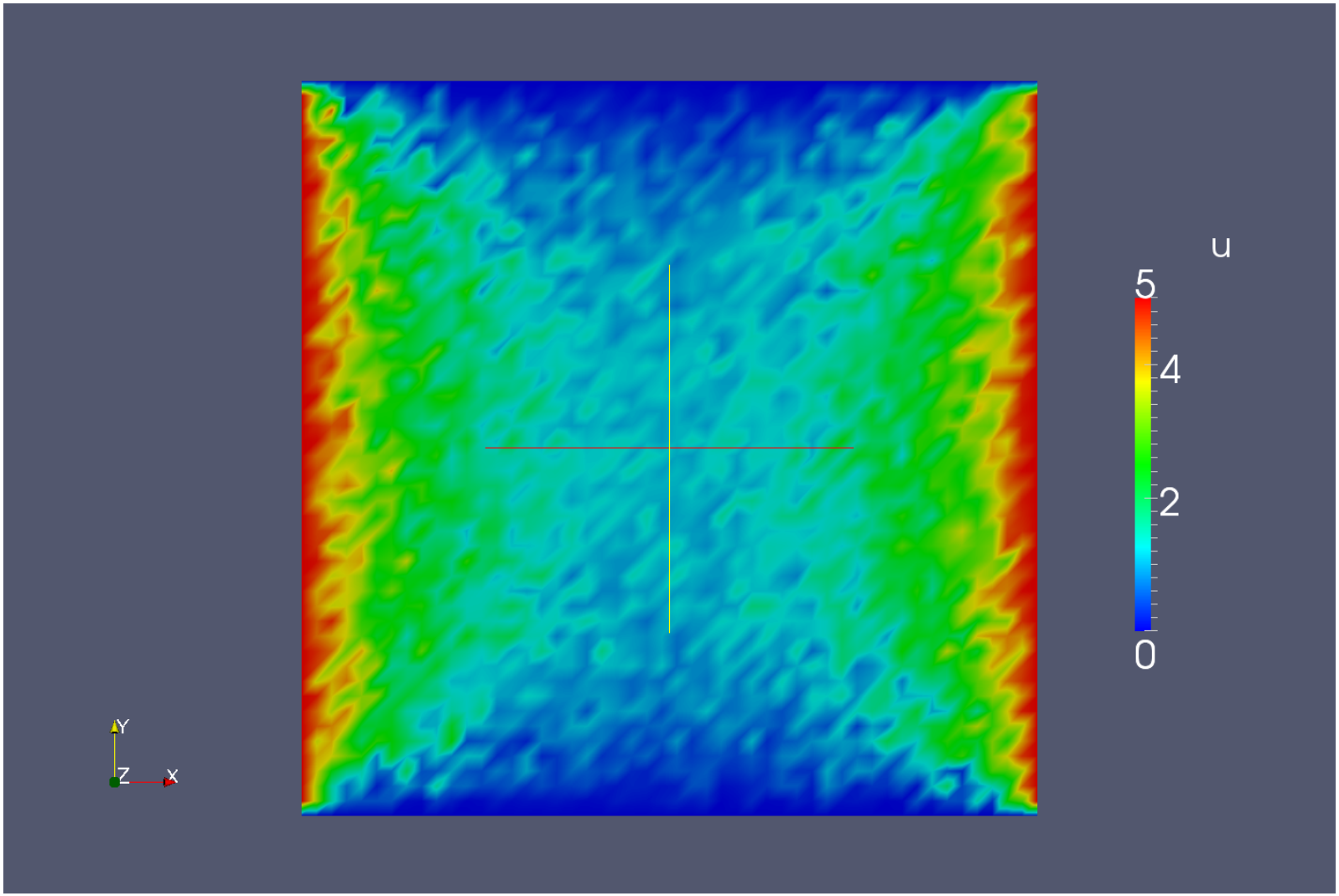

Figure : **Forward solution.** 2.5×10^4 *total histories.*

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Solving Heat Equation: Forward Method

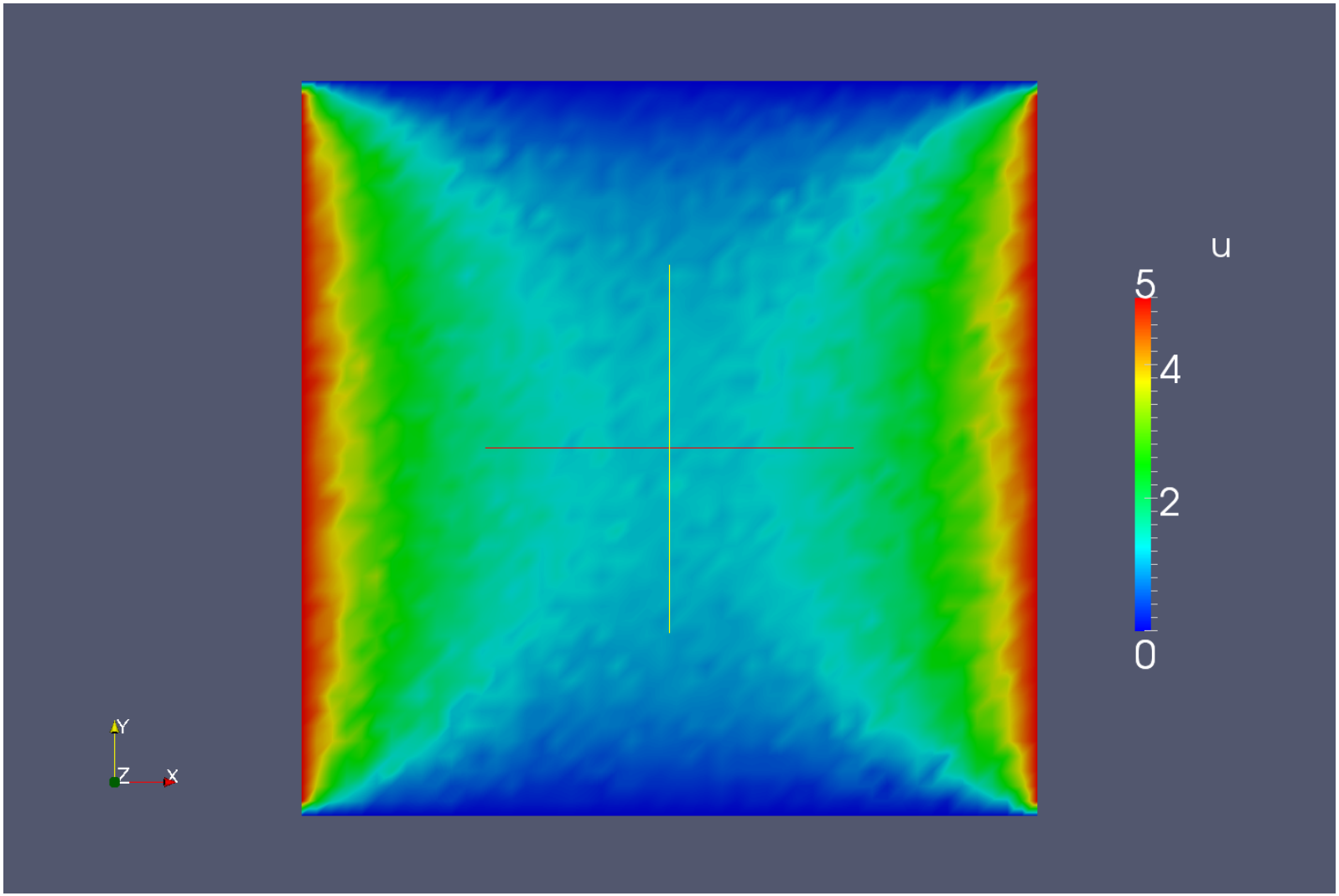

Figure : **Forward solution.** 2.5×10^5 *total histories.*

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Solving Heat Equation: Forward Method

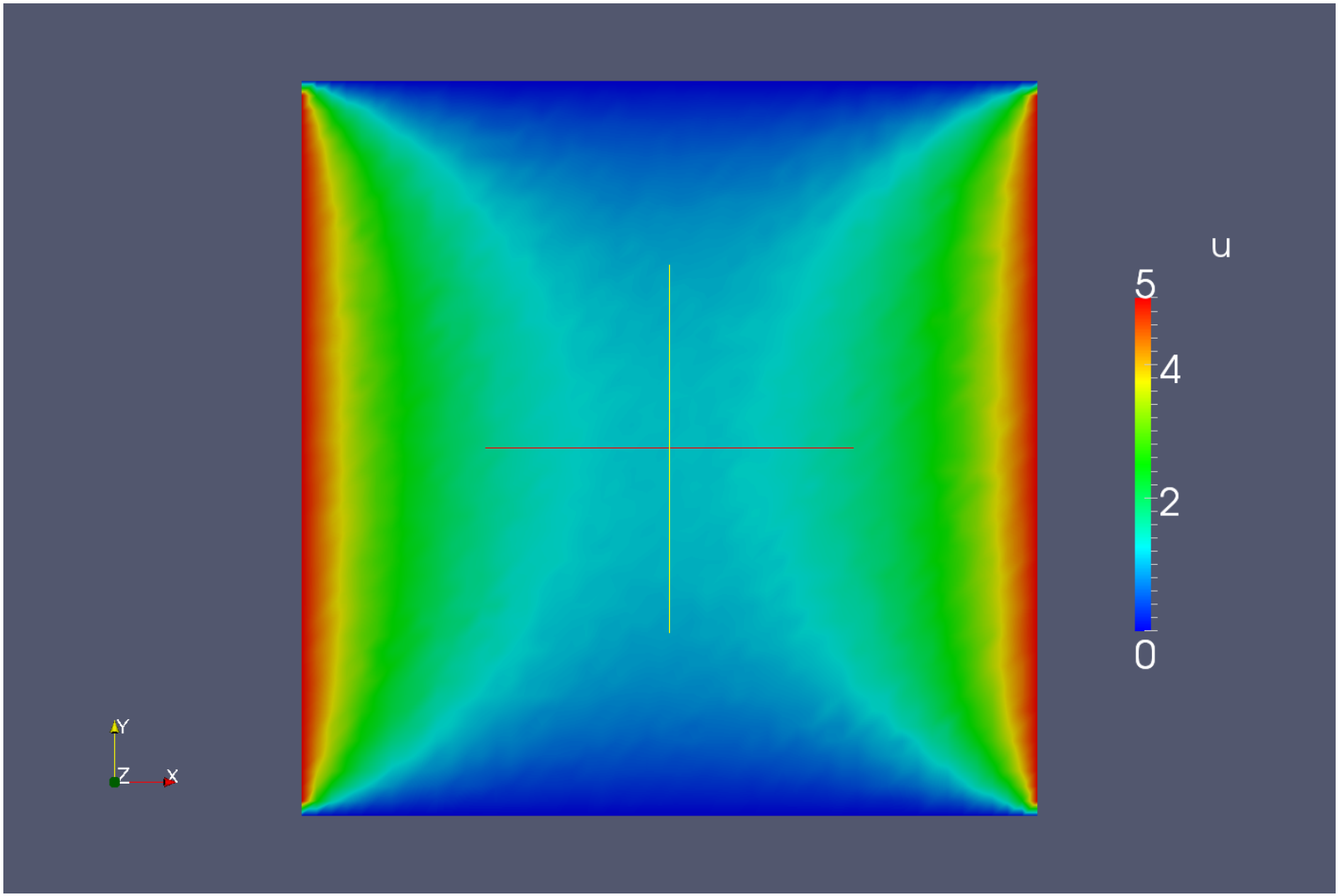

Figure : **Forward solution.** 2.5×10^6 *total histories.*

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Solving Heat Equation: Adjoint Method

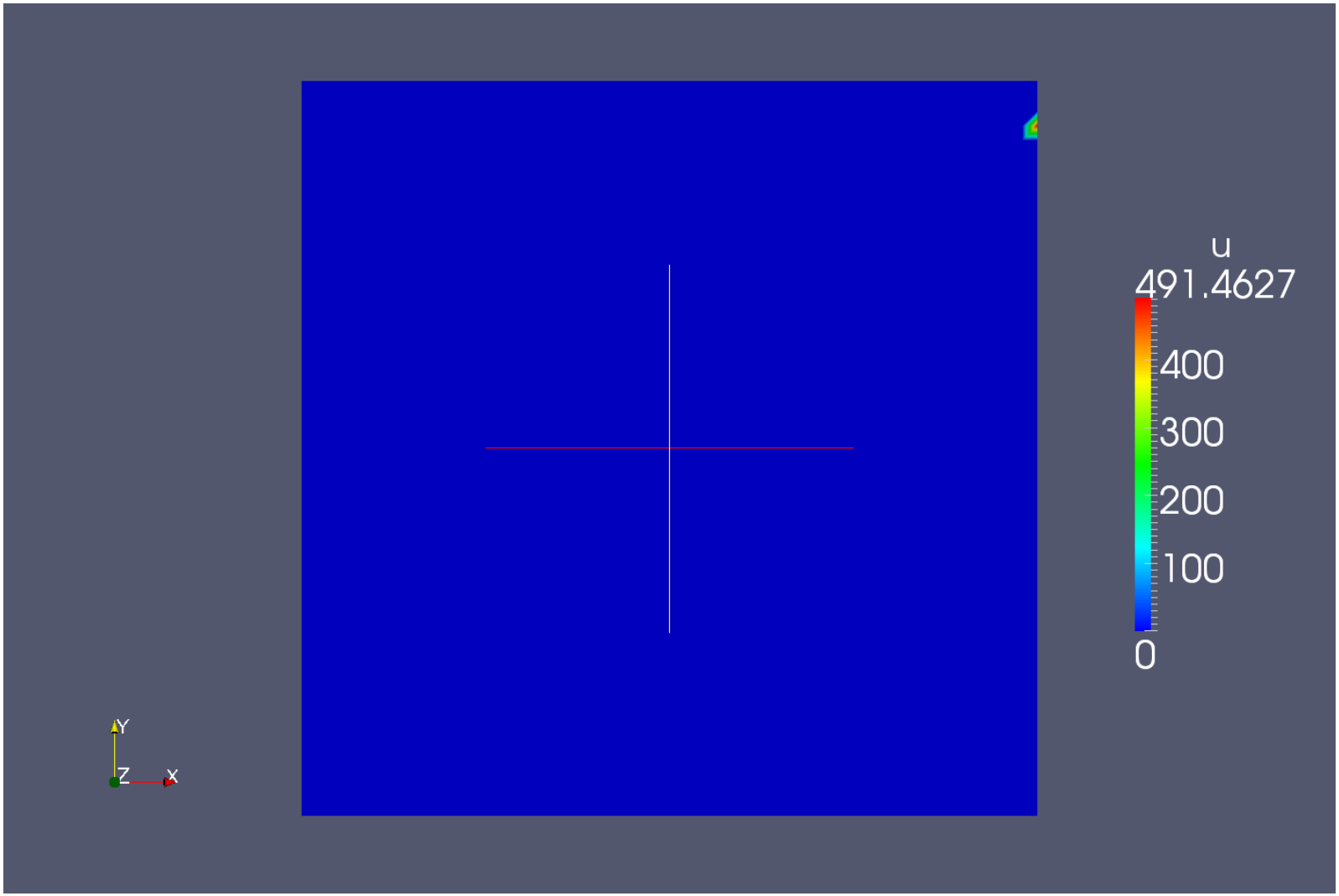

Figure : **Adjoint solution.** 1×10^0 *total histories.*

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Solving Heat Equation: Adjoint Method

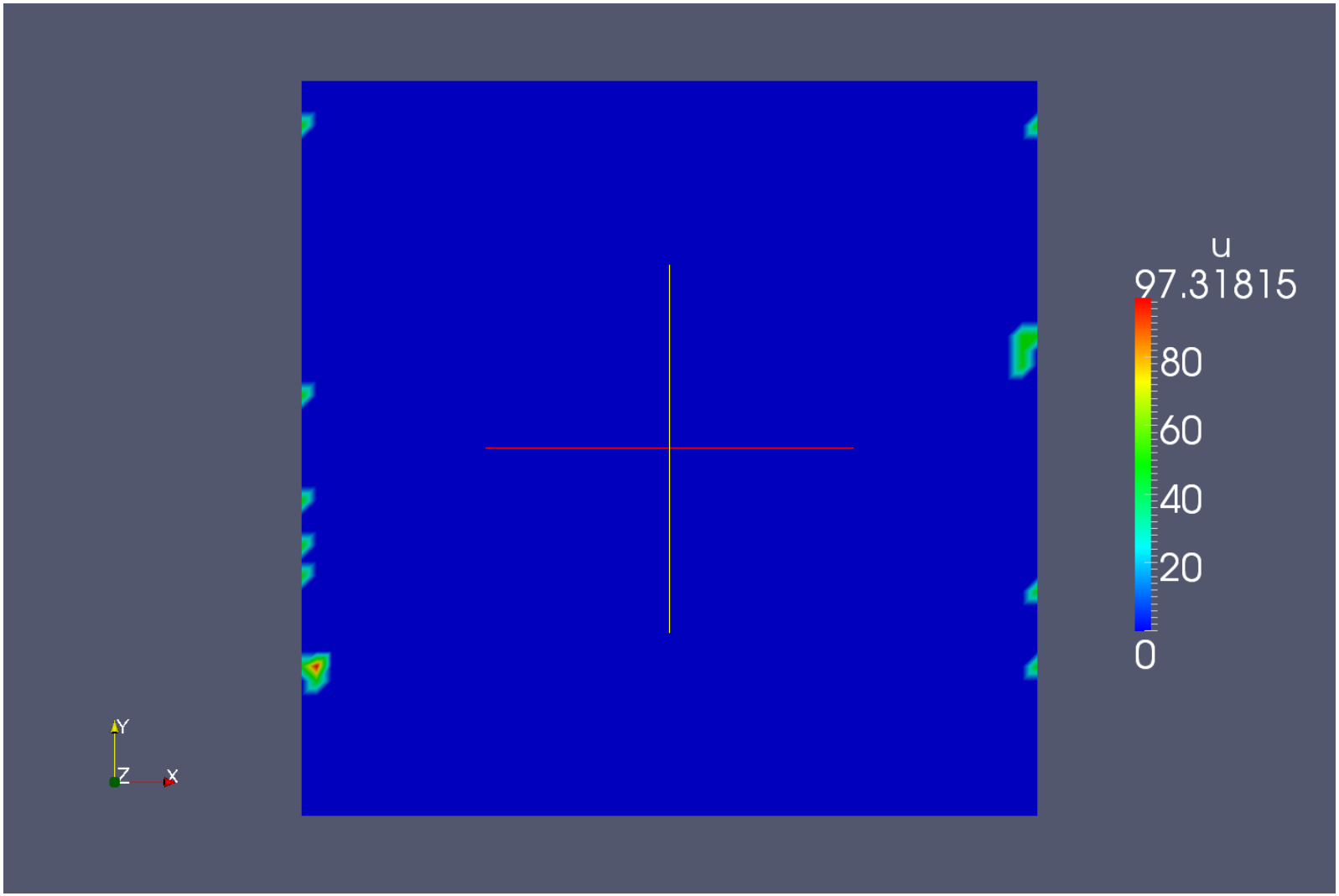

Figure : **Adjoint solution.** 1×10^1 *total histories.*

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Solving Heat Equation: Adjoint Method

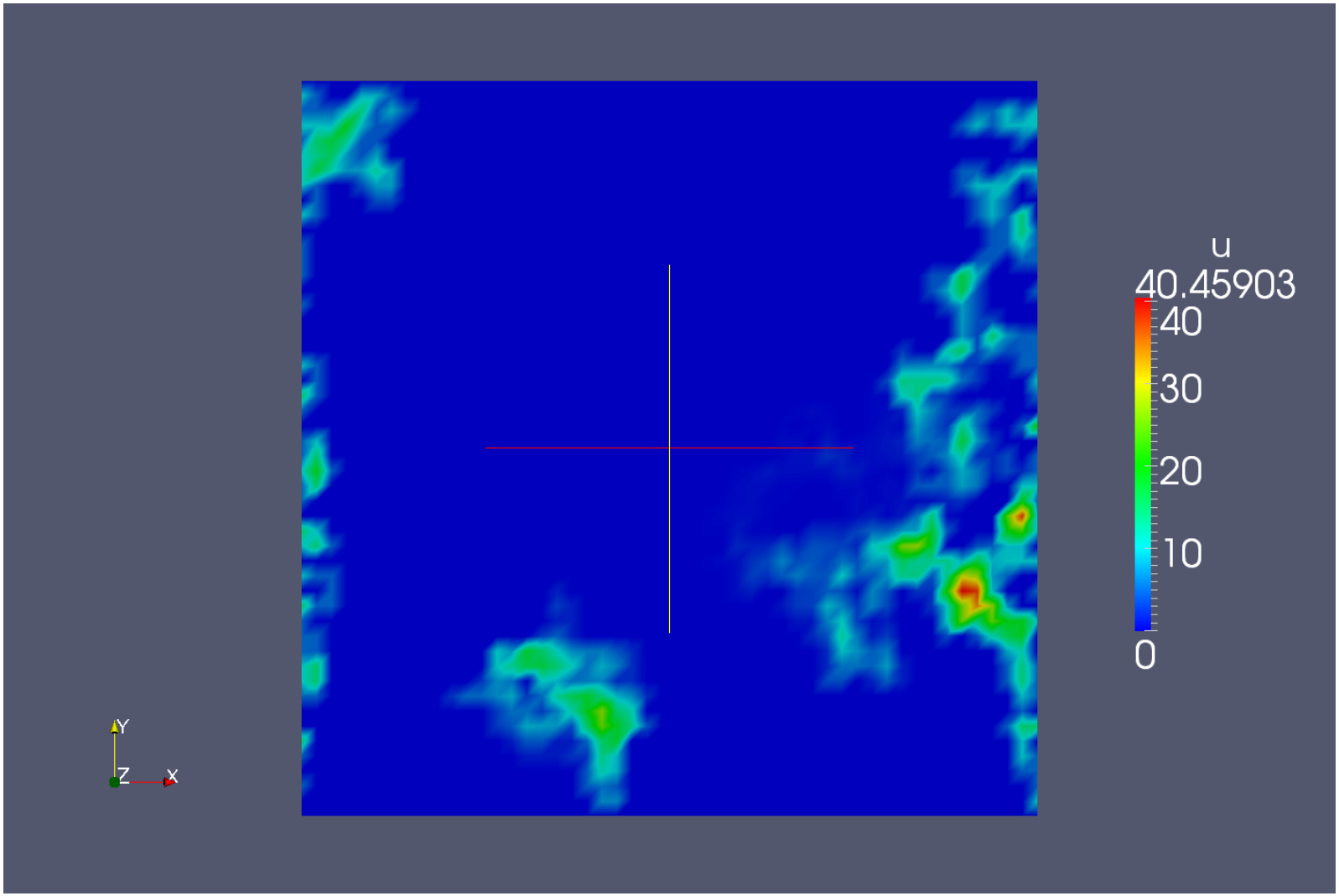

Figure : **Adjoint solution.** 1×10^2 *total histories.*

Solving Heat Equation: Adjoint Method

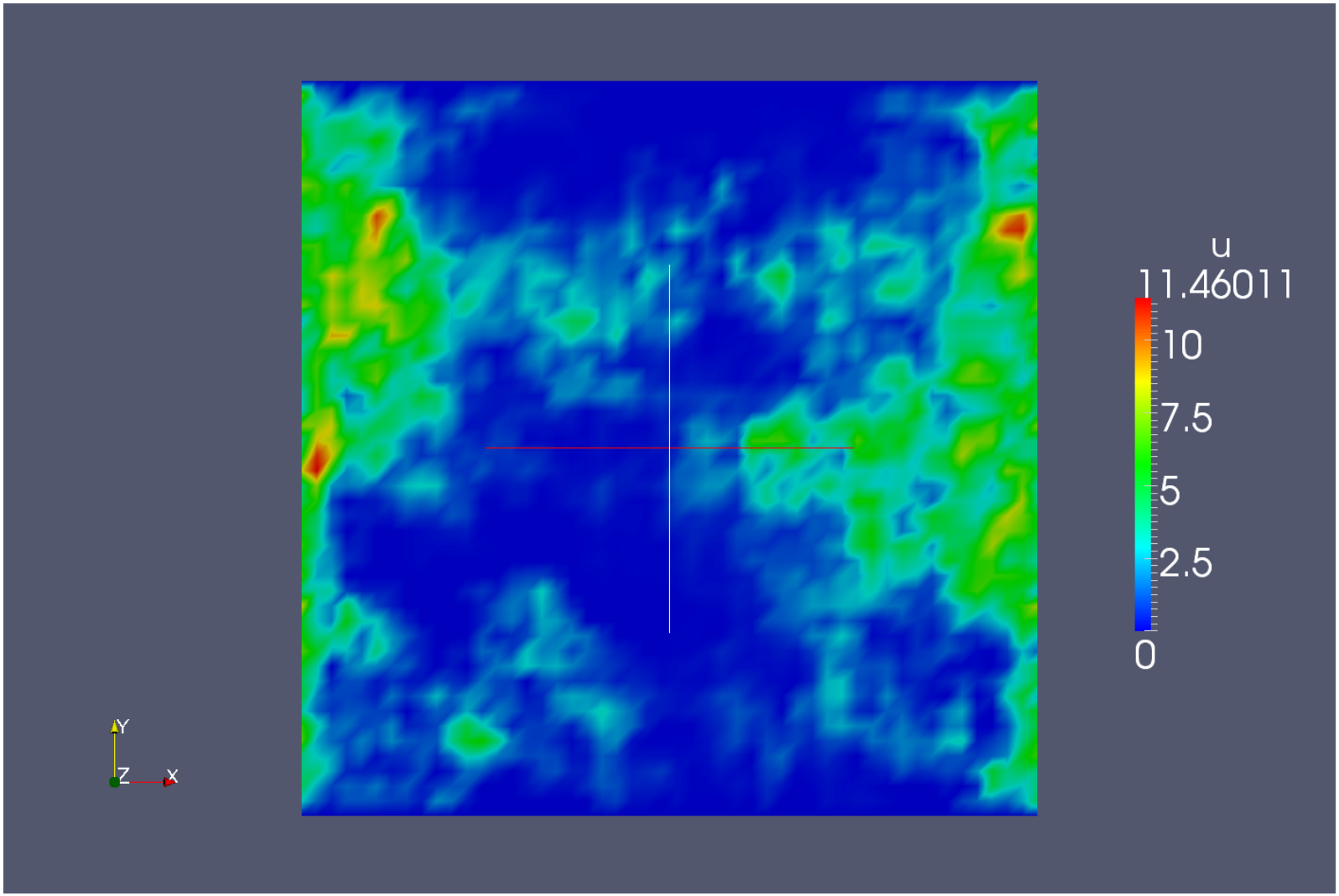

Figure : **Adjoint solution.** 1×10^3 *total histories.*

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Solving Heat Equation: Adjoint Method

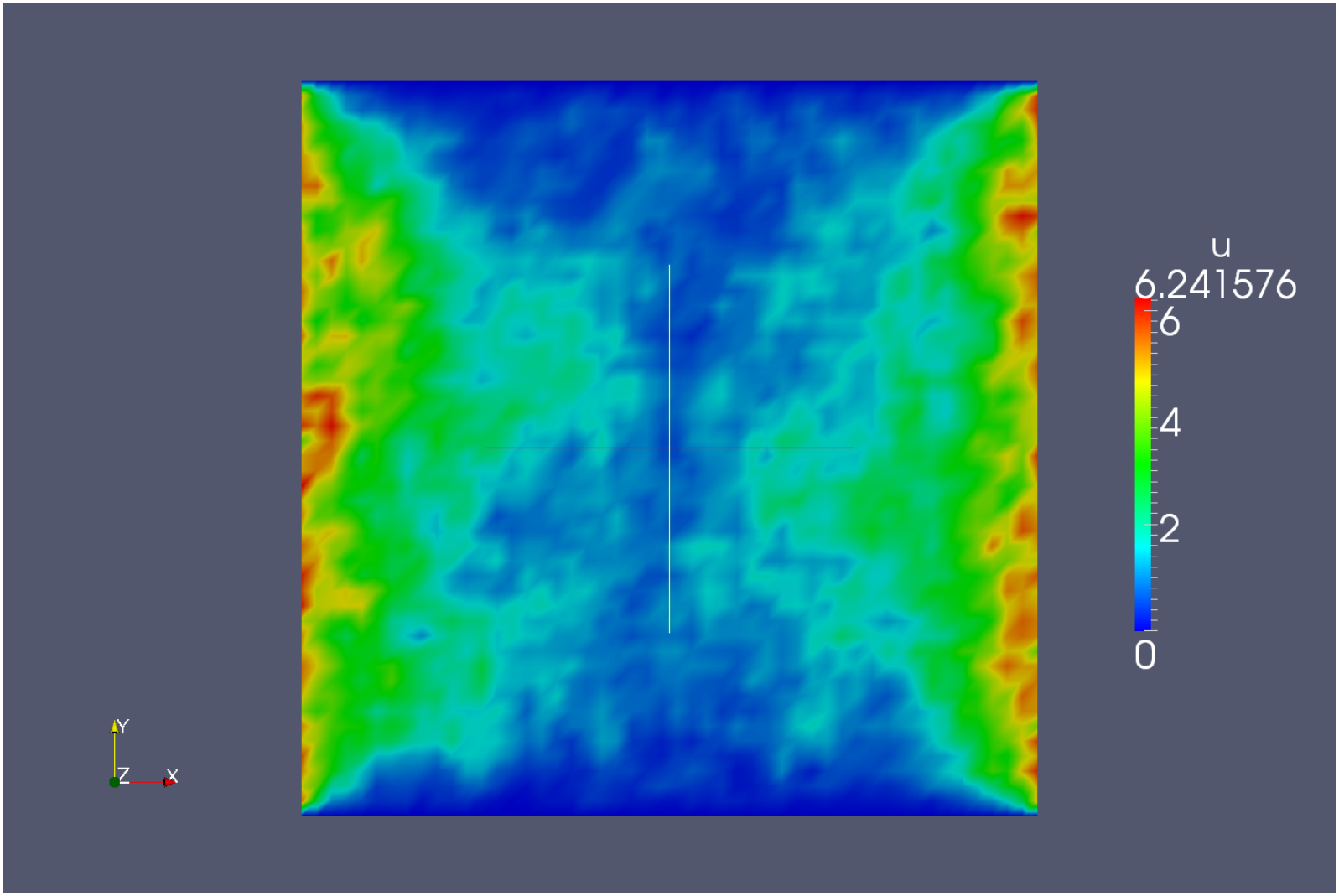

Figure : **Adjoint solution.** 1×10^4 *total histories.*

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Solving Heat Equation: Adjoint Method

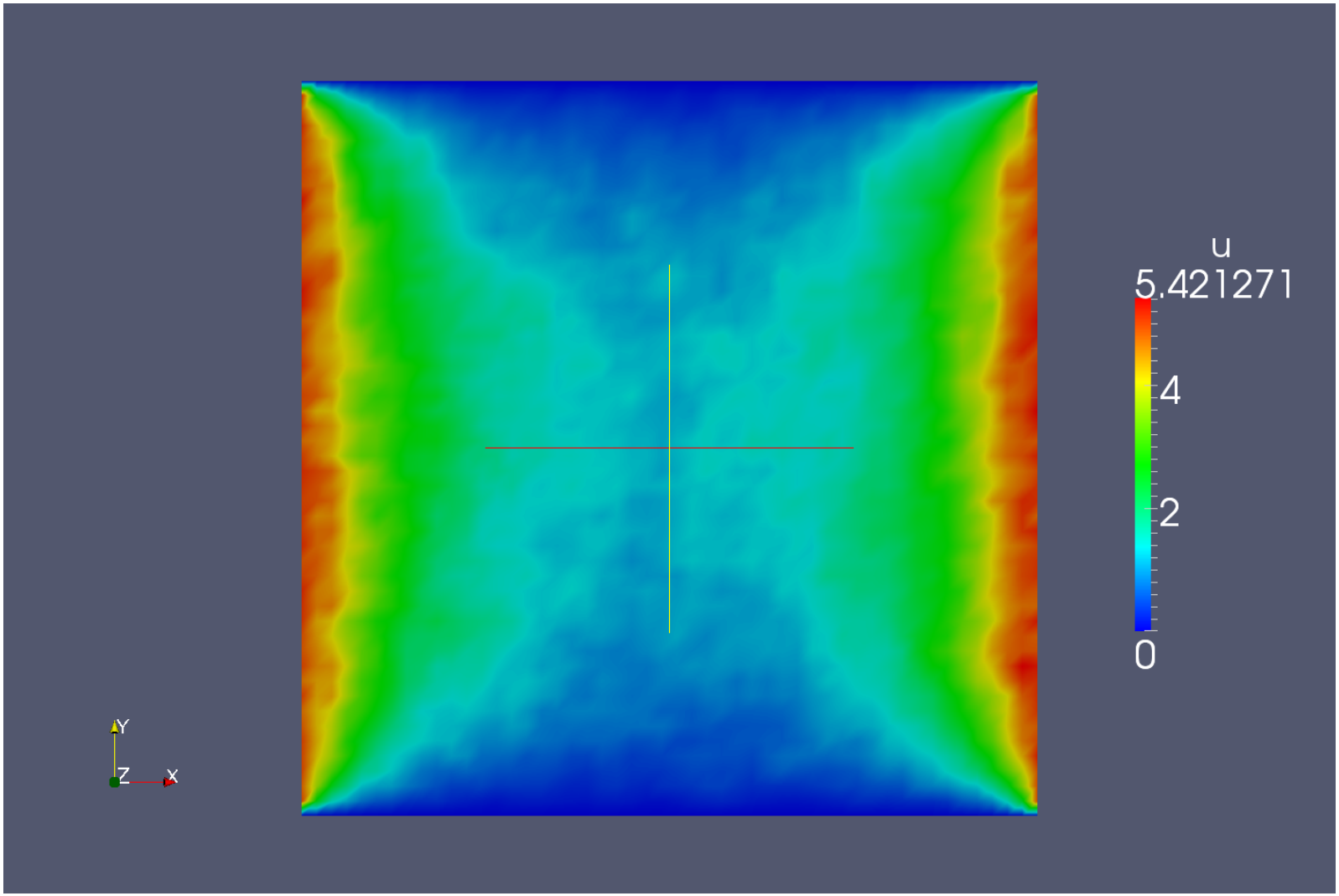

Figure : **Adjoint solution.** 1×10^5 *total histories.*

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Solving Heat Equation: Adjoint Method

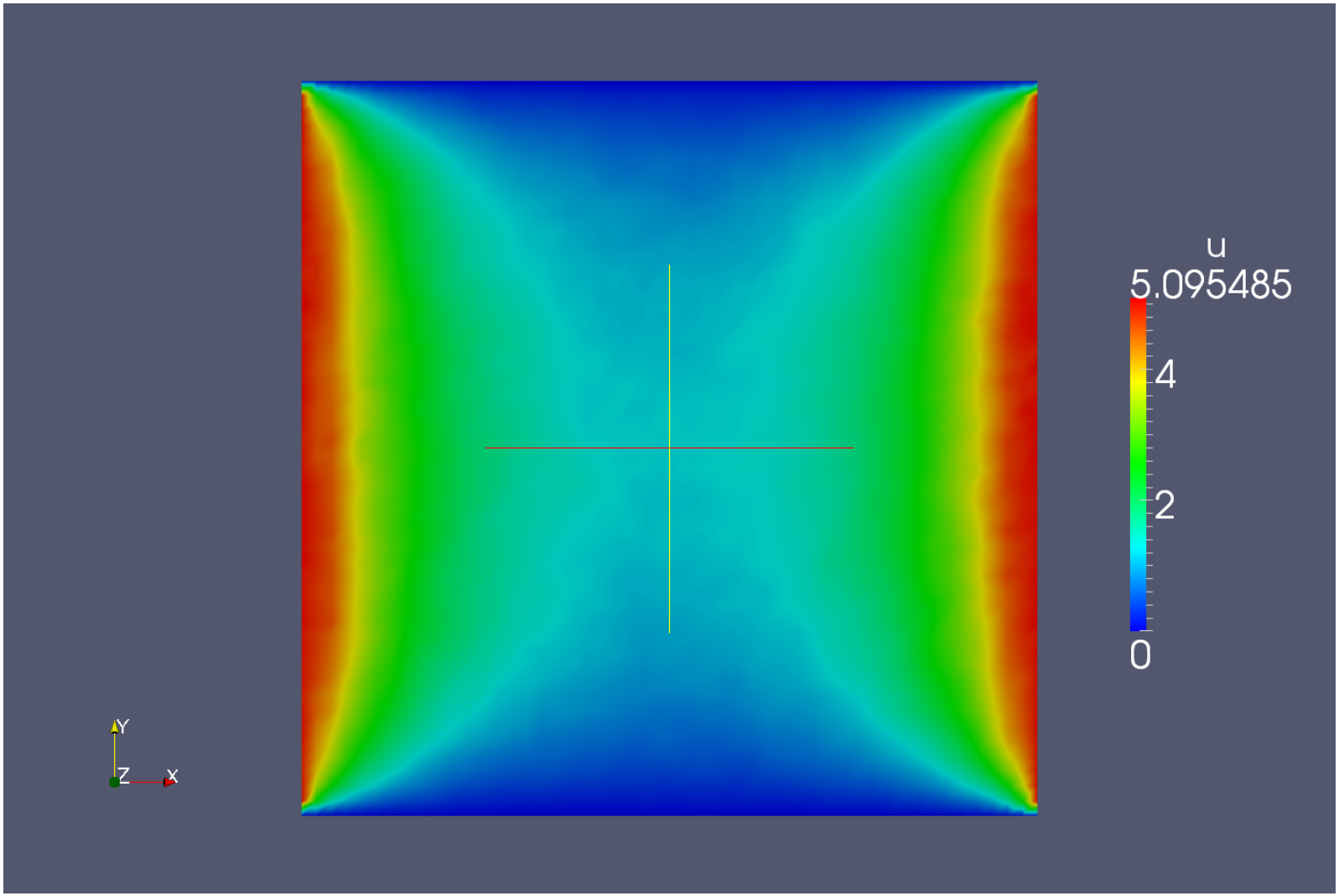

Figure : **Adjoint solution.** 1×10^6 *total histories.*

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Solving Heat Equation: Adjoint Method

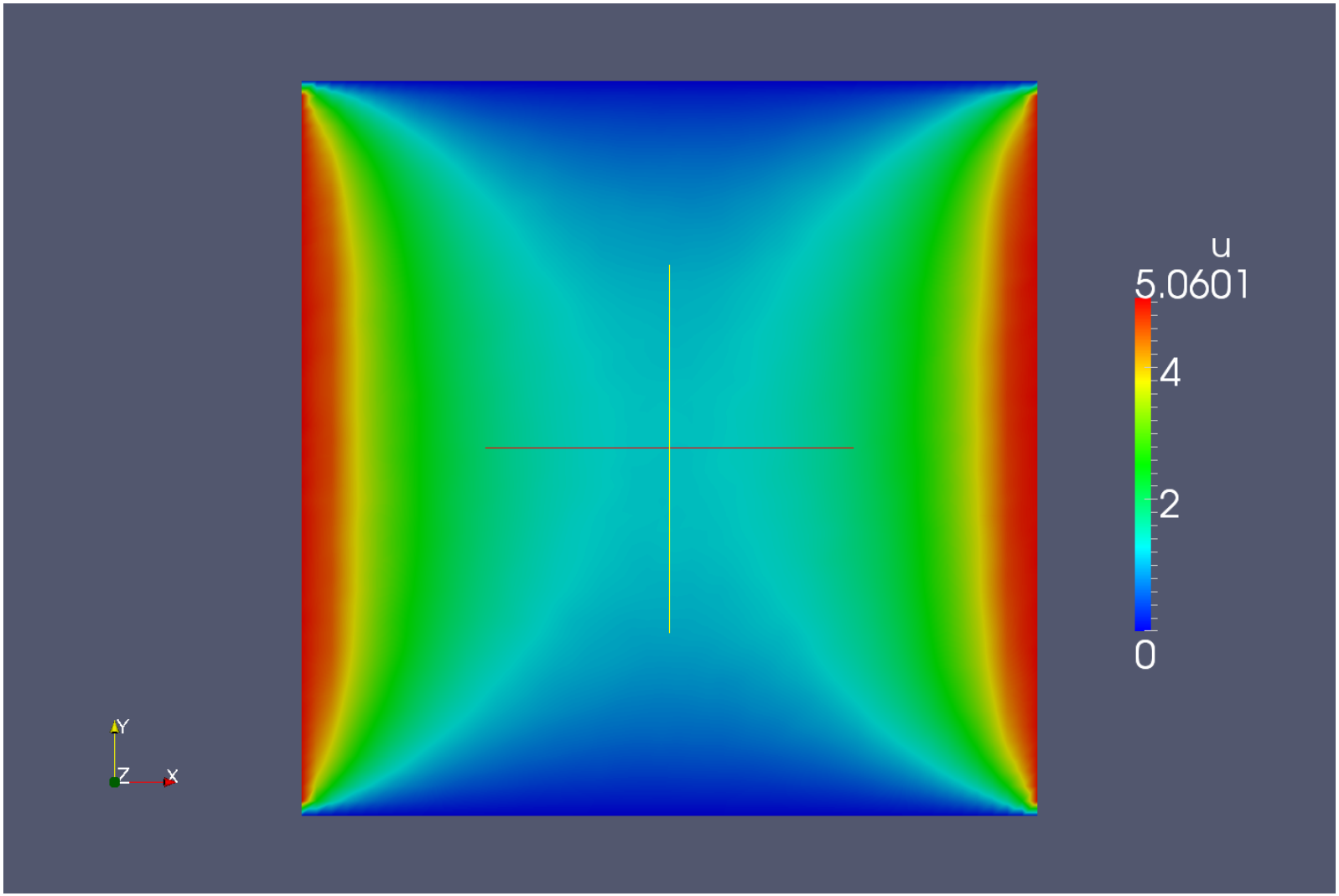

Figure : **Adjoint solution.** 1×10^7 *total histories.*

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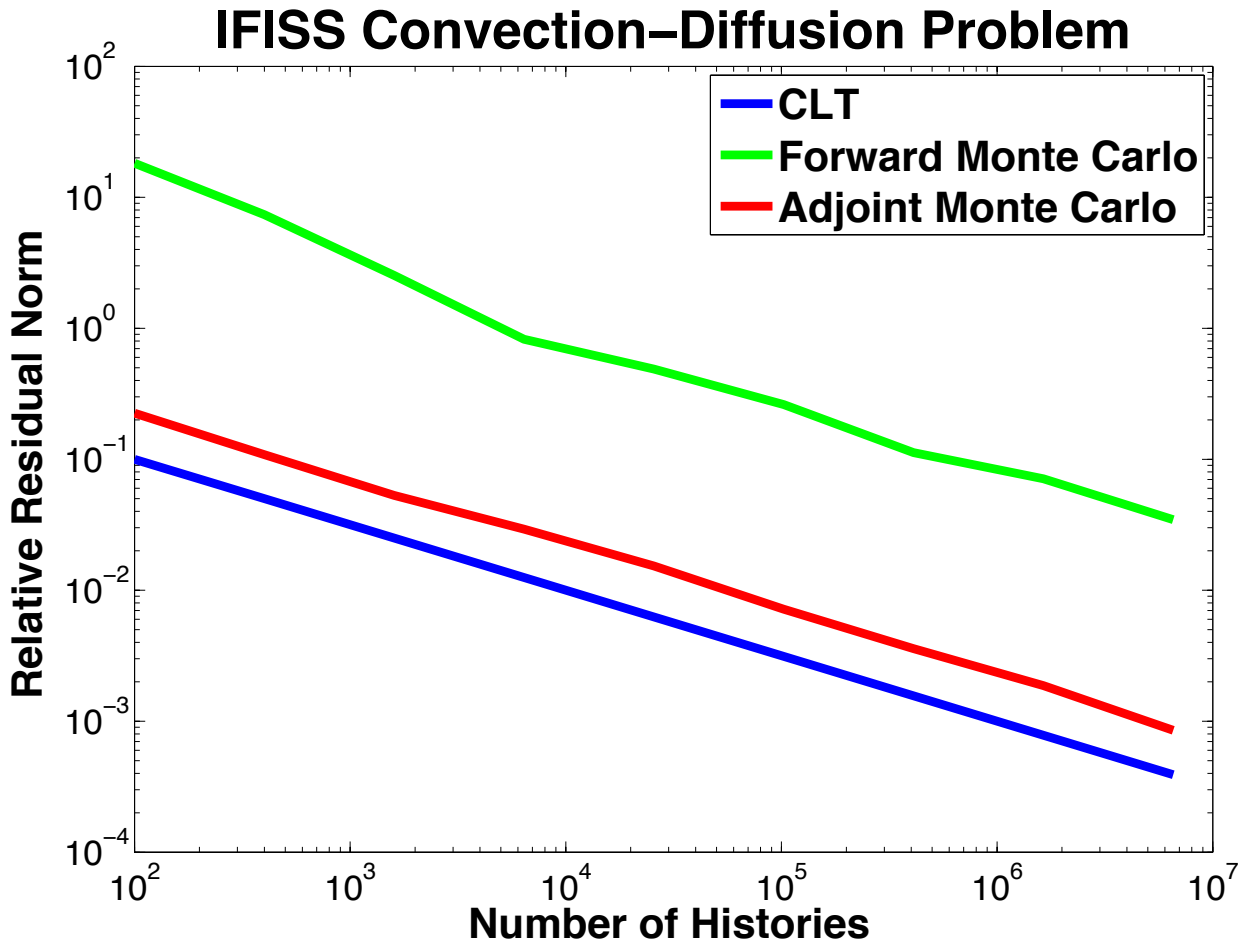
Limitations of Monte Carlo

- Solving linear systems of equations with "pure" Monte Carlo methods is generally intractable
  - Central limit theorem is barrier to accurate solutions



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Beyond the Central Limit Theorem

- Instead of directly solving $\mathbf{Ax} = \mathbf{b}$ with Monte Carlo, apply Monte Carlo to residual equation $\mathbf{A}\delta = \mathbf{r}$
- Preconditioned Richardson iteration using Monte carlo as preconditioner:

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

- This is the sequential Monte Carlo method devised by Halton

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Further Beyond the Central Limit Theorem

- Combine with Richardson iteration as a "smoother" in between Monte Carlo steps:

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

- We call this algorithm Monte Carlo Synthetic Acceleration (MCSA)

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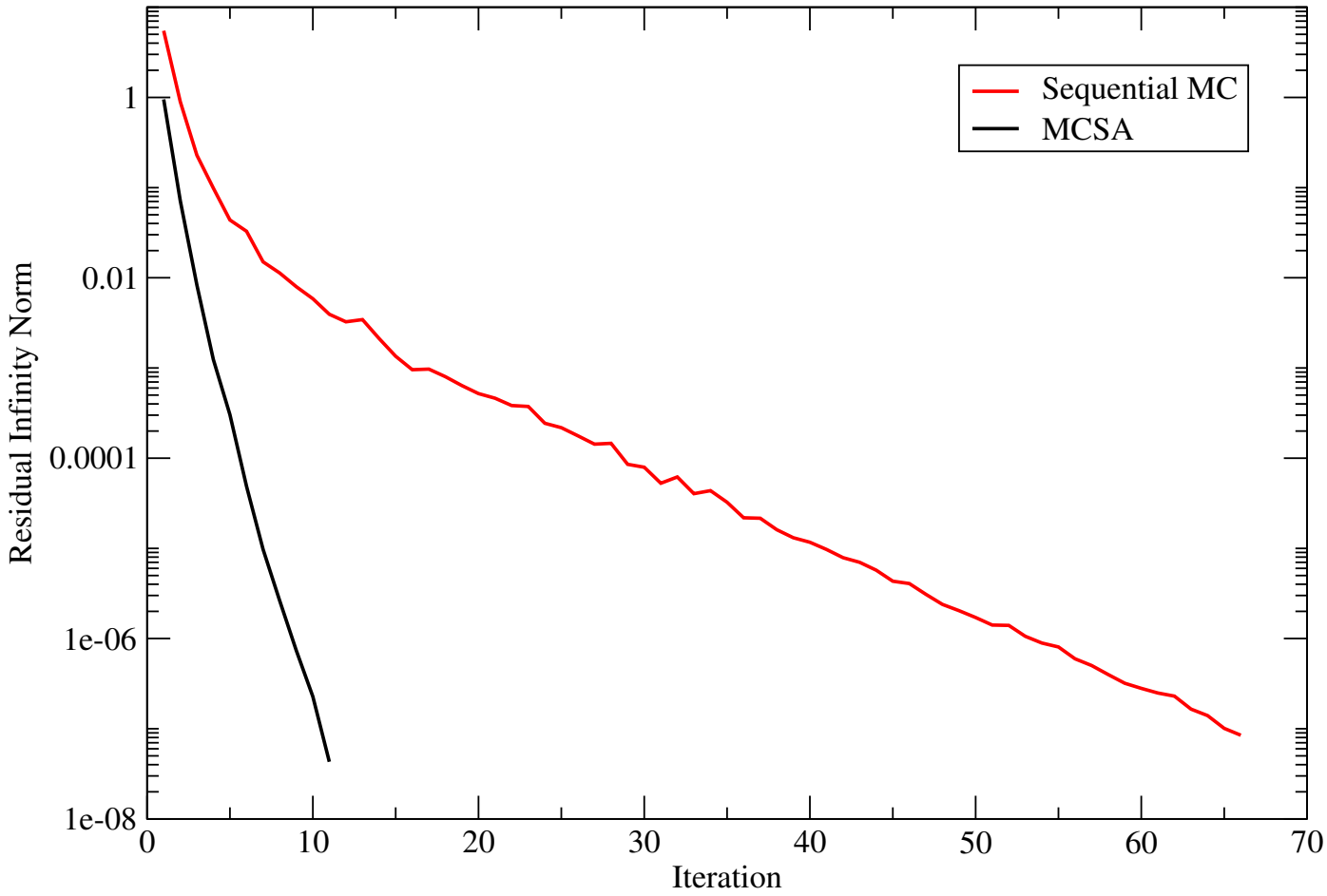
Algorithm Comparison



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Recent Success

- T. Evans, S. Mosher, S. Slattery, S. Hamilton, "A Monte Carlo synthetic-acceleration method for solving the thermal radiation diffusion equation," Journal of Computational Physics **258**, pp. 338–358 (2014).
- Applied MCSA to time-dependent thermal radiation diffusion equation

Solver	**Total Iterations**	**Relative Time Per Iteration**	**Relative Total Time**
CG (ML)	12150	74.7	2.7
GMRES (ILU)	40294	103.0	9.2
MCSA	98863	1.0	1.0

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Path to Harder Problems

- Experience with radiation diffusion suggests that for problems where spectral radius is low ($\lesssim 0.8$), MCSA can be competitive with leading methods
  - Very low cost per iteration to approximate Neumann series

- What about more challenging problems?
  - Neumann series converges more slowly, so histories last longer
  - More histories may be required
  - What if Neumann series is not convergent?

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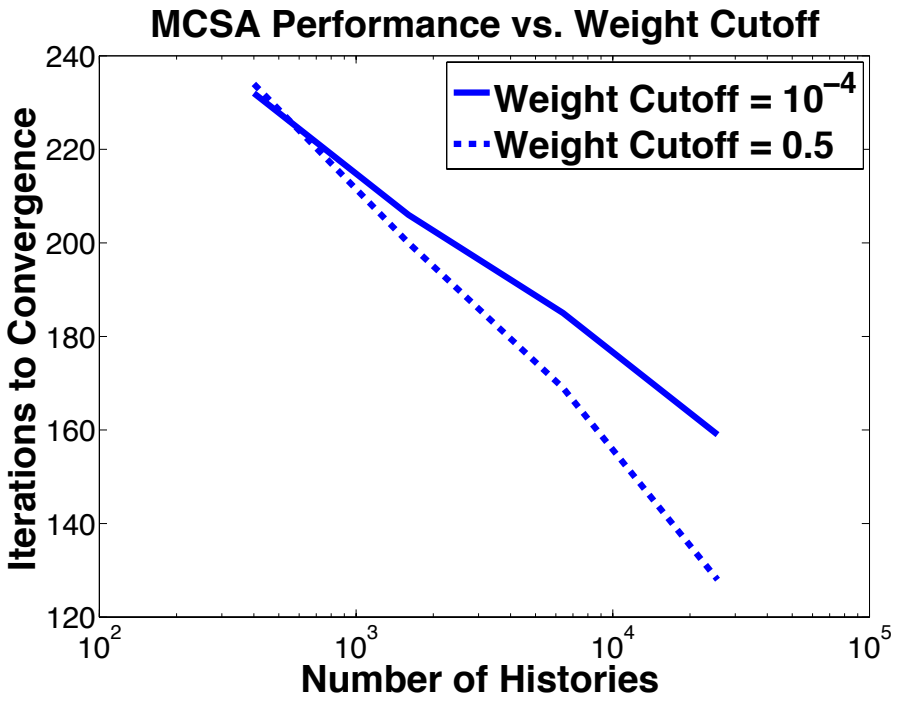
Stopping Criteria – Weight Cutoff

- Histories are usually terminated when the relative weight drops below a specified cutoff (i.e. $\frac{w}{w_0} < \tau$)
- Adjoint MCSA on JPWH_991 matrix with diagonal preconditioning ($\rho(\mathbf{I} - \mathbf{D}^{-1}\mathbf{A}) \approx 0.98$):



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Stopping Criteria – History Length Cutoff

- Somewhat counterintuitive result: using larger weight cutoff often results in better MCSA convergence
  - A good approximation to a few terms in the Neumann series performs better than a statistically noisy approximation to full series

- If statistical performance is better for large weight cutoff, what happens if we simply terminate histories after prescribed number of steps

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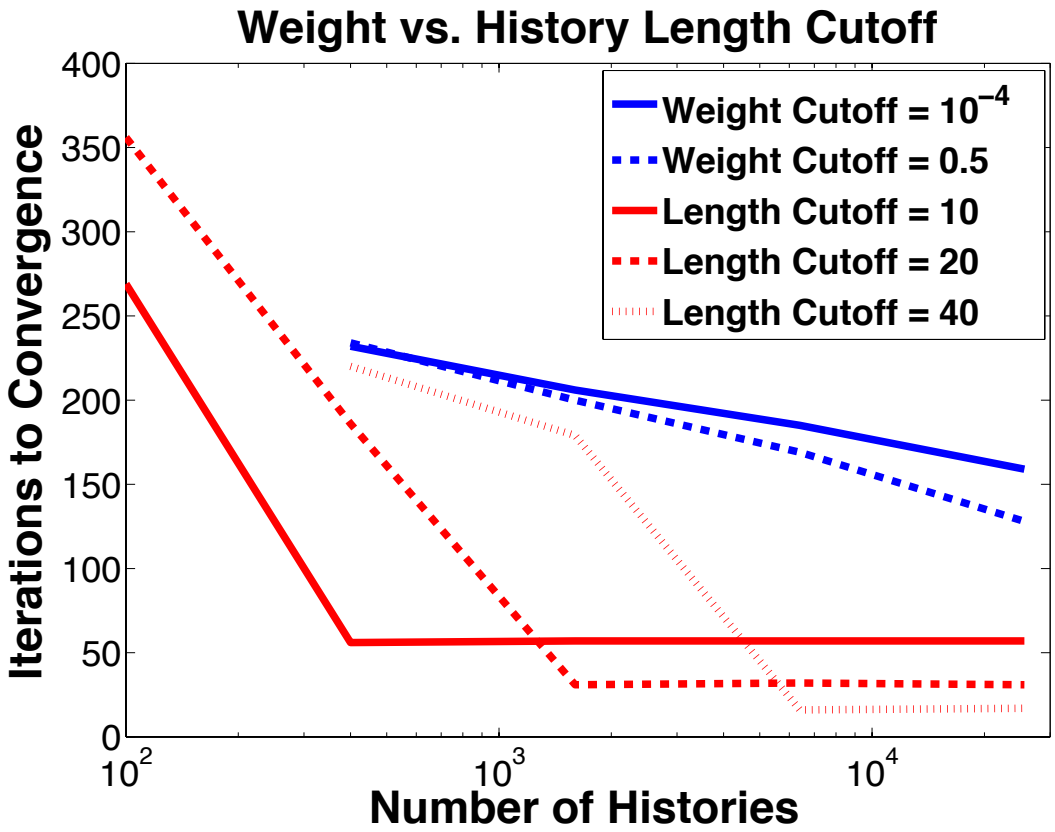
Weight vs. History Length Cutoff



- Unlike weight cutoff, history length cutoff "saturates" at some number of histories – fixed length Neumann series has been perfectly reproduced
- Saturation point is higher for longer history lengths

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Monte Carlo as Approximate Polynomial Preconditioning

- Using history length cutoff, Monte Carlo process is approximating a fixed length Neumann series polynomial
- As number of histories grows, iteration count becomes identical to using "true" polynomial
- Why limit ourselves to the Neumann series polynomial?
  - Chebyshev or GMRES polynomials are viable alternatives

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Neumann Series Polynomial

Table : Adjoint MCSA with Neumann Polynomial, 1000×1000 Shifted Laplacian Matrix. Values are MCSA iteration counts (timing in milliseconds)

Histories per Iteration	Polynomial Order		
	2	4	6
250	775(100)	651(96)	664(110)
500	725(122)	502(104)	394(95)
1000	707(174)	482(179)	366(144)
2000	703(280)	471(259)	356(251)
4000	698(494)	467(497)	350(458)
8000	697(923)	464(905)	350(873)
16000	695(1796)	462(1768)	347(1711)

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Chebyshev Polynomial

Table : Adjoint MCSA with Chebyshev Polynomial, 1000×1000 Shifted Laplacian Matrix. Values are MCSA iteration counts (timing in milliseconds)

Histories per Iteration	Polynomial Order		
	1	2	3
250	-	-	-
500	-	-	-
1000	-	-	-
2000	-	328(134)	-
4000	-	296(210)	-
8000	-	288(380)	262(423)
16000	1132(1866)	283(721)	175(550)

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GMRES Polynomial

Table : Adjoint MCSA with GMRES Polynomial, 1000×1000 Shifted Laplacian Matrix. Values are MCSA iteration counts (timing in milliseconds)

Histories per Iteration	Polynomial Order		
	2	4	6
250	2572(337)	-	-
500	616(105)	-	-
1000	566(142)	-	-
2000	557(222)	-	-
4000	554(412)	203(236)	-
8000	549(731)	184(423)	-
16000	548(1426)	247(965)	146(744)

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Polynomial Methods – Summary

- Using history length cutoff rather than weight cutoff can lead to large reductions in iteration counts

- Significant reduction in iteration counts are possible using alternate polynomials, but generally outweighed by increase in number of histories required
  - May be very beneficial from resiliency and parallel efficiency standpoints
  - Will be re-evaluated in future efforts

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Preconditioning

- If a non-trivial preconditioner is used, the Monte Carlo problem must be formed based on preconditioned iteration matrix, $\mathbf{H} = \mathbf{I} - \mathbf{M}^{-1}\mathbf{A}$
- Requires explicit construction of preconditioned matrix
  - This has generally limited preconditioner selection to diagonal, block diagonal, sparse approximate inverse approaches
- Sparsity in $\mathbf{A}$, $\mathbf{M}$, does not imply sparsity in $\mathbf{M}^{-1}\mathbf{A}$
- Need to investigate preconditoning strategies that lead to sparse preconditioned systems (Michele/Max)

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Multiple-Set Overlapping-Domain Decomposition

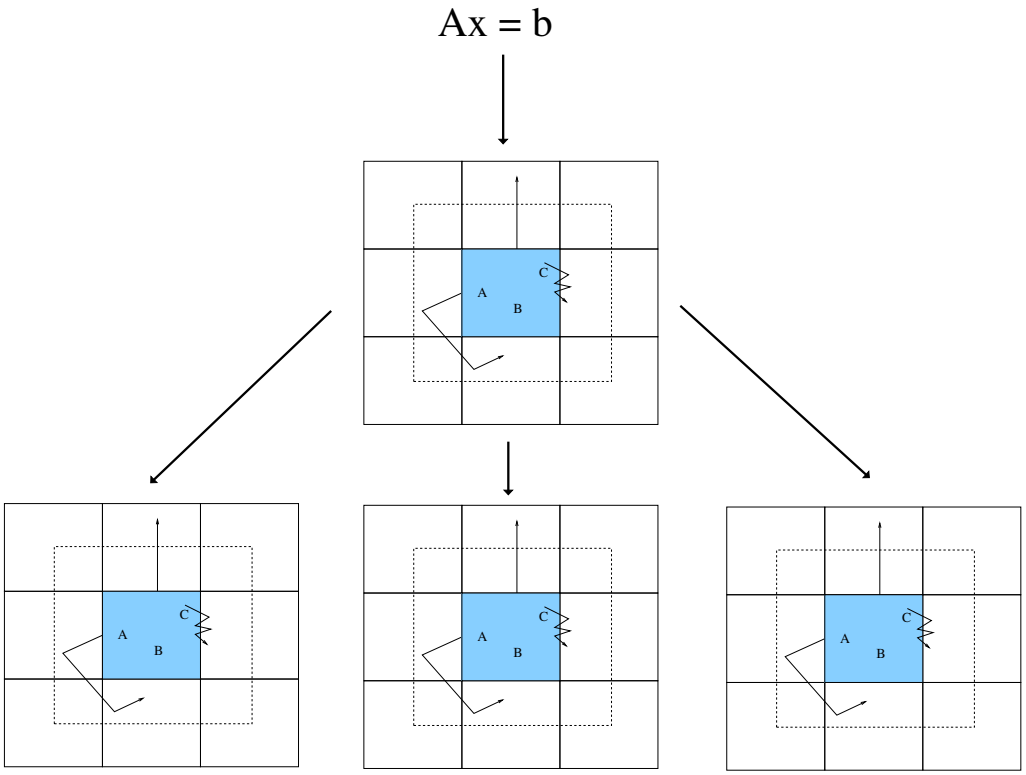

Figure : MSOD construction.

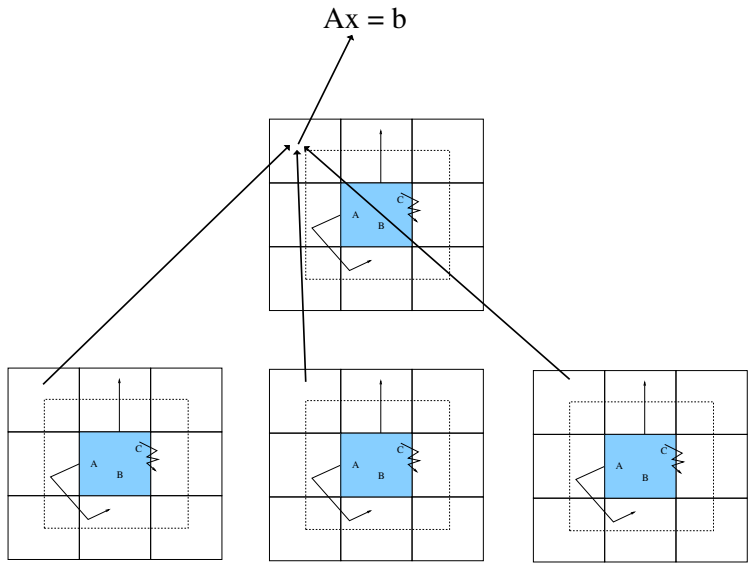

Figure : MSOD tally reduction.

- Multiple sets replicate the domain
- Domains overlap within a set
- Each set contains the full domain

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Alternative Parallelism – Additive Schwarz

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

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More Parallelism – Threading

- Within a Monte Carlo solve, every history is independent of other histories – great potential for highly concurrent hardware (GPU, Xeon Phi)
- Early experiments using the Trilinos Kokkos library show promising performance for multicore CPUs
- Will be taking part in OLCF "Hackathon" in late October to begin implementing computation kernels in OpenACC to allow GPU capability

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Application – Nuclear Reactor Analysis

- The simplified P_N (SP_N) equations are an approximation to the Boltzmann neutron transport equation used to simulate nuclear reactors
  - We are interested in solving generalized eigenvalue problem, for this study we use Arnoldi as the eigensolver and compare different methods for solving linear systems

- Test problem – 3×3 array of fuel assemblies with control rod in center location
  - 23 energy groups, 2 angular moments, 25M degrees of freedom
  - 1000 computational cores

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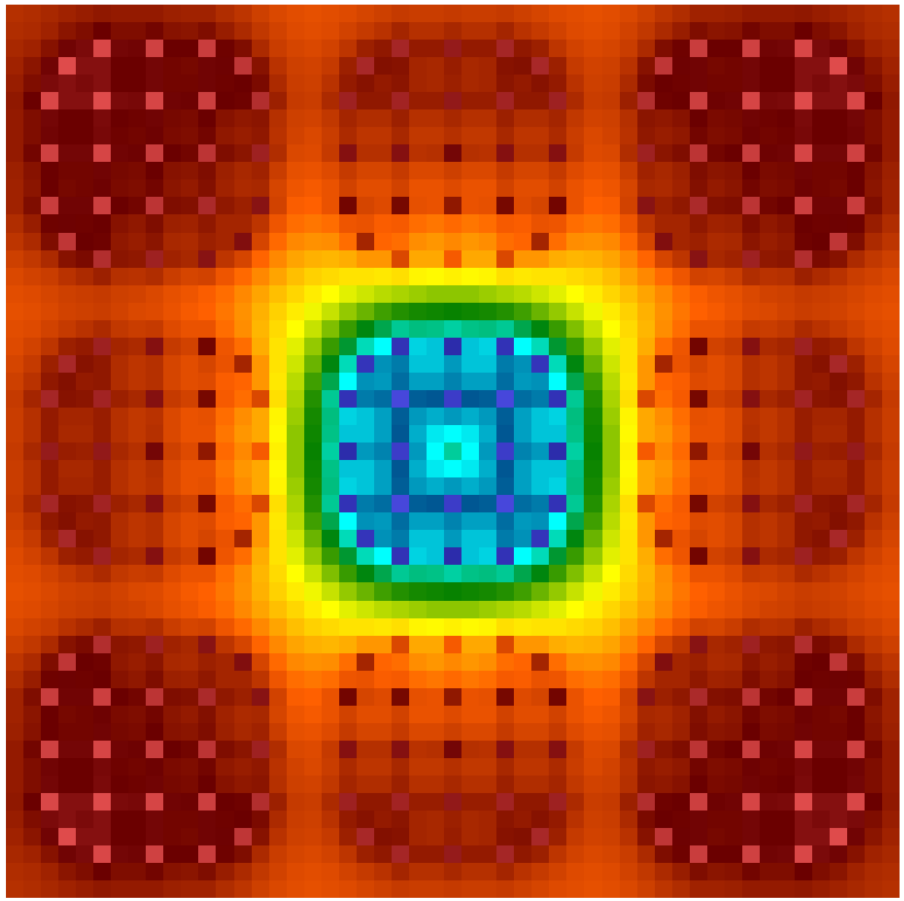
SPN Solution



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SPN Results

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

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

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Additional Thoughts

- Our current implementations rely on performing fixed number of histories per Monte Carlo solve
  - How can we dynamically select/adapt the number of histories that should be performed? Use variance-based stopping criteria?
- The "almost optimal" selection of the probability and weight matrices is arbitrary (as long as $\mathbf{H}/\mathbf{H}^T = \mathbf{P} \circ \mathbf{W}$)
  - If $\mathbf{P}$ is taken to have a uniform distribution within each row, then sampling from the distribution can be done in constant (rather than logarithmic) time
- Anderson acceleration of MCSA (Tim Kelly @ NCSU)

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Conclusions

- Monte Carlo methods offer great potential for both resilient and highly parallel solvers
- For certain classes of problems, Monte Carlo methods can be competitive with leading modern solvers
- Extending methods to broader problem areas is significant challenge and an attractive area for continued research

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