

# Krylov Linear Solvers and Quasi Monte Carlo Methods for Transport Simulations

Sam Pasmann,<sup>a</sup> C. T. Kelley,<sup>b</sup> and Ryan McClarren<sup>\*,a</sup>

*<sup>a</sup>Department of Aerospace and Mechanical Engineering  
University of Notre Dame  
Fitzpatrick Hall, Notre Dame, IN 46556*

*<sup>b</sup>North Carolina State University, Department of Mathematics  
3234 SAS Hall, Box 8205  
Raleigh NC 27695-8205*

\*Email: [rmcclarr@nd.edu](mailto:rmcclarr@nd.edu)

Number of pages: 11

Number of tables: 4

Number of figures: 2

## **Abstract**

QMC + Krylov

**Keywords** — Quasi Monte Carlo Methods, Krylov Linear Solvers

## I. INTRODUCTION

## II. COMPUTATIONAL RESULTS

In this section we consider an example from [1]. The formulation of the transport problem is taken from [2]. The equation for the angular flux  $\psi$  is

$$\mu \frac{\partial \psi}{\partial x}(x, \mu) + \Sigma_t(x) \psi(x, \mu) = \frac{1}{2} \left[ \Sigma_s(x) \int_{-1}^1 \psi(x, \mu') d\mu' + q(x) \right] \text{ for } 0 \leq x \leq \tau \quad (1)$$

The boundary conditions are

$$\psi(0, \mu) = \psi_l(\mu), \mu > 0; \psi(\tau, \mu) = \psi_r(\mu), \mu < 0.$$

### II.A. Multigroup Equations

In general geometry the multigroup equations are

$$\mu \frac{\partial \psi_g}{\partial x}(x, \mu) + \Sigma_{t,g}(x) \psi_g(x, \mu) = \frac{1}{2} \sum_{g'=1}^G \Sigma_{s,g' \rightarrow g}(x) \int_{-1}^1 \psi_{g'}(x, \mu') d\mu' + \frac{q_g(x)}{2} \quad g = 1, \dots, G. \quad (2)$$

The boundary conditions are

$$\psi_g(0, \mu) = \psi_{l,g}(\mu), \mu > 0; \psi_g(\tau, \mu) = \psi_{r,g}(\mu), \mu < 0.$$

In matrix form, these equations are

$$\mu \frac{\partial \vec{\psi}}{\partial x}(x, \mu) + \underline{\Sigma}_t(x) \vec{\psi}(x, \mu) = \frac{1}{2} \underline{\Sigma}_s(x) \int_{-1}^1 \vec{\psi}(x, \mu') d\mu' + \frac{\vec{q}(x)}{2}, \quad (3)$$

where

$$\vec{\psi} = (\psi_1, \psi_2, \dots, \psi_G)^T, \quad \vec{q} = (q_1, q_2, \dots, q_G)^T, \quad (4)$$

$$\underline{\Sigma}_t(x) = \begin{pmatrix} \Sigma_{t,1}(x) & 0 & \dots \\ 0 & \Sigma_{t,2}(x) & 0 \dots \\ \vdots & & \ddots \\ 0 & \dots & 0 & \Sigma_{t,G}(x) \end{pmatrix}, \quad (5)$$

and

$$\underline{\Sigma}_s(x) = \begin{pmatrix} \Sigma_{s,1 \rightarrow 1}(x) & \Sigma_{s,2 \rightarrow 1}(x) & \dots & \Sigma_{s,G \rightarrow 1}(x) \\ \Sigma_{s,2 \rightarrow 1}(x) & \Sigma_{s,2 \rightarrow 1}(x) & \dots & \Sigma_{s,G \rightarrow 2}(x) \\ \vdots & \vdots & & \vdots \\ \Sigma_{s,G \rightarrow 1}(x) & \Sigma_{s,G \rightarrow 1}(x) & \dots & \Sigma_{s,G \rightarrow G}(x) \end{pmatrix}, \quad (6)$$

## II.B. Source Iteration and Linear Solvers

Source iteration is Picard iteration for the fixed point problem

$$\phi = \mathcal{S}(\phi, q, \psi_l, \psi_r)$$

To use other solvers we must convert to a linear system via

$$\mathcal{K}(\phi) = \mathcal{S}(\phi, 0, 0, 0) \text{ and } f = \mathcal{S}(0, q, \psi_l, \psi_r)$$

to get

$$A\phi \equiv (I - \mathcal{K})\phi = f,$$

which we can send to a linear solver.

In the computations we use the problem from [1]

$$\tau = 5, \Sigma_s(x) = \omega_0 e^{-x/s}, \Sigma_t(x) = 1, q(x) = 0, \psi_l(\mu) = 1, \psi_r(\mu) = 0,$$

and consider two cases  $s = 1$  and  $s = \infty$

## II.C. QMC and Krylov Linear Solvers

The linear and nonlinear solvers come from the Julia package [SIAMFANLEQ.jl](#) [3]. The documentation for these codes is in the [Juila notebooks](#) [4] and the book [5] that accompany the package.

We solve the QMC linear problem with  $N=1000$  and  $N_x=100$ . We use two krylov methods [6], GMRES [7] and Bi-CGSTAB [8]. Figures 1 and 2 show that the Krylov iterations take fewer than half of the number of transport sweeps that Picard iteration required.

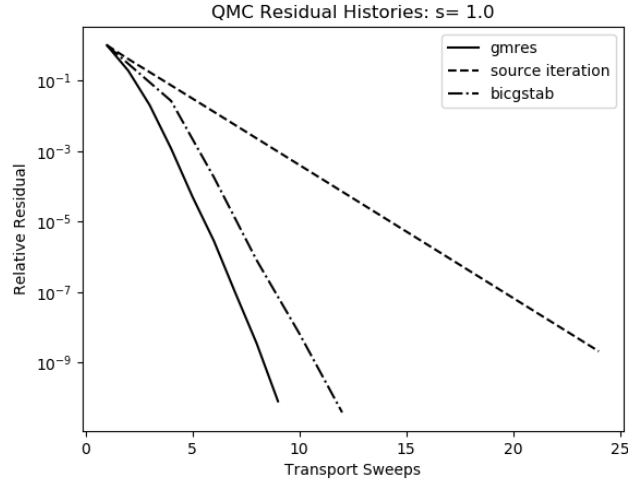


Fig. 1.  $s = 1$

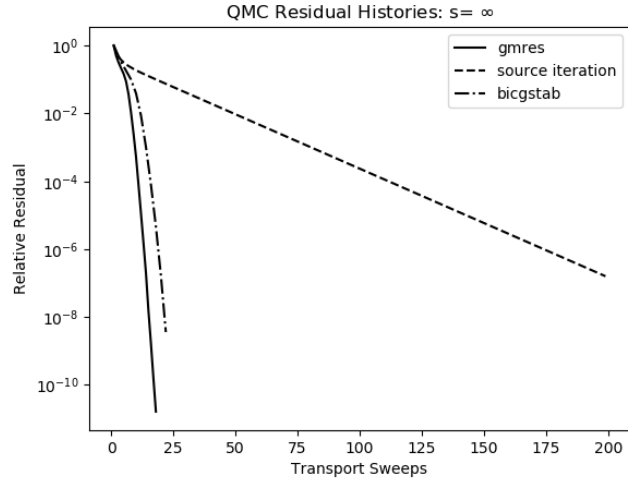


Fig. 2.  $s = \infty$

## II.D. Validation and calibration study

We conclude this section with a validation study. We compare the QMC results with the results from [1]. The results in [1] are exit distributions and are accurate to six figures. We have duplicated those results with an  $Sn$  computation on a fine angular and spatial mesh.

**Sam, Ryan, should we use more or different values of  $N$  and  $Nx$ ?**

For  $N = 1000$  and  $Nx = 100$  we obtain the cell-average fluxes from the QMC approximation. We then use a single  $Sn$  transport sweep to recover the exit distributions from the QMC cell-average fluxes. We report the results and the corresponding results from [1] in Tables I and II.

The exit distributions, as is clear from Table I can vary by five orders of magnitude. Even so, the results from QMC agree with the benchmarks to roughly two figures.

TABLE I  
Exit Distributions:  $s = 1$

| Garcia/Siewert |                 |                   | QMC             |                   |
|----------------|-----------------|-------------------|-----------------|-------------------|
| $\mu$          | $\psi(0, -\mu)$ | $\psi(\tau, \mu)$ | $\psi(0, -\mu)$ | $\psi(\tau, \mu)$ |
| 5.00e-02       | 5.89664e-01     | 6.07488e-06       | 5.71197e-01     | 5.85487e-06       |
| 1.00e-01       | 5.31120e-01     | 6.92516e-06       | 5.22137e-01     | 6.66741e-06       |
| 2.00e-01       | 4.43280e-01     | 9.64232e-06       | 4.41567e-01     | 9.25261e-06       |
| 3.00e-01       | 3.80306e-01     | 1.62339e-05       | 3.81029e-01     | 1.54416e-05       |
| 4.00e-01       | 3.32964e-01     | 4.38580e-05       | 3.34673e-01     | 4.09691e-05       |
| 5.00e-01       | 2.96090e-01     | 1.69372e-04       | 2.98224e-01     | 1.57373e-04       |
| 6.00e-01       | 2.66563e-01     | 5.73465e-04       | 2.68871e-01     | 5.35989e-04       |
| 7.00e-01       | 2.42390e-01     | 1.51282e-03       | 2.44749e-01     | 1.42448e-03       |
| 8.00e-01       | 2.22235e-01     | 3.24369e-03       | 2.24583e-01     | 3.07431e-03       |
| 9.00e-01       | 2.05174e-01     | 5.96036e-03       | 2.07478e-01     | 5.67991e-03       |
| 1.00e+00       | 1.90546e-01     | 9.77123e-03       | 1.92789e-01     | 9.35351e-03       |

In Tables III and IV we look at the relative errors in the QMC exit distributions as compared to a highly accurate SN result. We compensate for the widely varying scales by tabulating, for each value of  $N$  and  $Nx$

$$R = \max(R^0, R^\tau)$$

where

$$R^0 = \max_{\mu} \frac{|\psi^{SN}(0, -\mu) - \psi^{QMC}(0, -\mu)|}{\psi^{SN}(0, -\mu)}$$

and

$$R^\tau = \max_{\mu} \frac{|\psi^{SN}(\tau, \mu) - \psi^{QMC}(\tau, \mu)|}{\psi^{SN}(\tau, \mu)}.$$

TABLE II  
Exit Distributions:  $s = \infty$

| $\mu$    | Garcia/Siewert  |                   | QMC             |                   |
|----------|-----------------|-------------------|-----------------|-------------------|
|          | $\psi(0, -\mu)$ | $\psi(\tau, \mu)$ | $\psi(0, -\mu)$ | $\psi(\tau, \mu)$ |
| 5.00e-02 | 8.97798e-01     | 1.02202e-01       | 8.47454e-01     | 1.00663e-01       |
| 1.00e-01 | 8.87836e-01     | 1.12164e-01       | 8.52822e-01     | 1.10325e-01       |
| 2.00e-01 | 8.69581e-01     | 1.30419e-01       | 8.47710e-01     | 1.29064e-01       |
| 3.00e-01 | 8.52299e-01     | 1.47701e-01       | 8.35879e-01     | 1.46849e-01       |
| 4.00e-01 | 8.35503e-01     | 1.64497e-01       | 8.22291e-01     | 1.64034e-01       |
| 5.00e-01 | 8.18996e-01     | 1.81004e-01       | 8.08044e-01     | 1.80827e-01       |
| 6.00e-01 | 8.02676e-01     | 1.97324e-01       | 7.93459e-01     | 1.97336e-01       |
| 7.00e-01 | 7.86493e-01     | 2.13507e-01       | 7.78672e-01     | 2.13625e-01       |
| 8.00e-01 | 7.70429e-01     | 2.29571e-01       | 7.63768e-01     | 2.29725e-01       |
| 9.00e-01 | 7.54496e-01     | 2.45504e-01       | 7.48818e-01     | 2.45642e-01       |
| 1.00e+00 | 7.38721e-01     | 2.61279e-01       | 7.33889e-01     | 2.61361e-01       |

Ryan, for large  $N_x$  I see convergence as  $N$  increases. Is it clearly  $1/N$ ? Am I missing something? Am I tabulating the wrong thing?

TABLE III  
Exit Distributions Errors:  $s = 1.0$

| $N_x \setminus N$ | 1000        | 2000        | 4000        | 8000        | 16000       |
|-------------------|-------------|-------------|-------------|-------------|-------------|
| 50                | 1.41162e-01 | 1.36428e-01 | 1.34747e-01 | 1.35736e-01 | 1.35577e-01 |
| 100               | 7.08438e-02 | 6.60744e-02 | 6.52017e-02 | 6.51605e-02 | 6.49914e-02 |
| 200               | 4.17171e-02 | 3.30480e-02 | 3.23088e-02 | 3.21432e-02 | 3.17467e-02 |
| 400               | 4.55590e-02 | 1.73115e-02 | 1.63072e-02 | 1.61542e-02 | 1.58469e-02 |
| 800               | 4.83754e-02 | 1.93087e-02 | 1.29178e-02 | 8.30117e-03 | 7.96562e-03 |
| 1600              | 5.07584e-02 | 2.03691e-02 | 1.44681e-02 | 4.52388e-03 | 4.11350e-03 |
| 3200              | 5.09694e-02 | 2.13418e-02 | 1.48086e-02 | 2.88667e-03 | 2.18194e-03 |

TABLE IV  
Exit Distributions Errors:  $s = \infty$

| $N_x \setminus N$ | 1000        | 2000        | 4000        | 8000        | 16000       |
|-------------------|-------------|-------------|-------------|-------------|-------------|
| 50                | 5.95648e-02 | 2.42755e-02 | 1.36521e-02 | 1.29509e-02 | 1.22769e-02 |
| 100               | 5.60749e-02 | 2.31030e-02 | 1.31680e-02 | 6.45949e-03 | 6.59550e-03 |
| 200               | 5.62864e-02 | 2.32524e-02 | 1.42149e-02 | 4.77319e-03 | 3.55246e-03 |
| 400               | 5.30954e-02 | 2.17854e-02 | 1.48225e-02 | 4.73260e-03 | 2.05558e-03 |
| 800               | 7.66264e-02 | 1.88155e-02 | 1.60082e-02 | 4.34610e-03 | 1.41402e-03 |
| 1600              | 5.99376e-02 | 2.15675e-02 | 1.56784e-02 | 4.21636e-03 | 1.29138e-03 |
| 3200              | 5.74319e-02 | 1.89482e-02 | 2.00195e-02 | 3.26688e-03 | 1.49649e-03 |



### III. CONCLUSION

## **ACKNOWLEDGMENTS**

The research of CTK was supported by Department of Energy grant DE-NA003967, and National Science Foundation Grants DMS-1745654, and DMS-1906446.

## REFERENCES

- [1] R. GARCIA and C. SIEWERT, “Radiative transfer in finite inhomogeneous plane-parallel atmospheres,” *J. Quant. Spectrosc. Radiat. Transfer*, **27**, 141 (1982).
- [2] J. WILLERT, C. T. KELLEY, D. A. KNOLL, and H. K. PARK, “Hybrid Deterministic/Monte Carlo Neutronics,” *SIAM J. Sci. Comp.*, **35**, S62 (2013).
- [3] C. T. KELLEY, “SIAMFANLEquations.jl,” <https://github.com/ctkelley/SIAMFANLEquations.jl> (2020); 10.5281/zenodo.4284807., URL <https://github.com/ctkelley/SIAMFANLEquations.jl>, julia Package.
- [4] C. T. KELLEY, “Notebook for Solving Nonlinear Equations with Iterative Methods: Solvers and Examples in Julia,” <https://github.com/ctkelley/NotebookSIAMFANL> (2020); 10.5281/zenodo.4284687., URL <https://github.com/ctkelley/NotebookSIAMFANL>, iJulia Notebook.
- [5] C. T. KELLEY, “Solving Nonlinear Equations with Iterative Methods: Solvers and Examples in Julia,” (2020) Unpublished book ms, under contract with SIAM.
- [6] C. T. KELLEY, *Iterative Methods for Linear and Nonlinear Equations*, no. 16 in Frontiers in Applied Mathematics, SIAM, Philadelphia (1995).
- [7] Y. SAAD and M. SCHULTZ, “GMRES a generalized minimal residual algorithm for solving nonsymmetric linear systems,” *SIAM J. Sci. Stat. Comp.*, **7**, 856 (1986).
- [8] H. A. VAN DER VORST, “Bi-CGSTAB: A fast and smoothly converging variant to Bi-CG for the solution of nonsymmetric systems,” *SIAM J. Sci. Statist. Comput.*, **13**, 631 (1992).