Krylov Linear Solvers and Quasi Monte Carlo Methods for Transport Simulations

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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 ψ is

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

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

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

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

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

where

$$\vec{\psi} = (\psi_1, \psi_2, \ldots, \psi_G)^{\mathrm{T}}, \qquad \vec{q} = (q_1, q_2, \ldots, q_G)^{\mathrm{T}}, \tag{4}$$

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

and

$$\underline{\Sigma}_s(x) = \begin{pmatrix} \Sigma_{s,1\to1}(x) & \Sigma_{s,2\to1}(x) & \dots & \Sigma_{s,G\to1}(x) \\ \Sigma_{s,2\to1}(x) & \Sigma_{s,2\to1}(x) & \dots & \Sigma_{s,G\to2}(x) \\ \vdots & \vdots & & \vdots \\ \Sigma_{s,G\to1}(x) & \Sigma_{s,G\to1}(x) & \dots & \Sigma_{s,G\to G}(x) \end{pmatrix}, . \tag{6}$$

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.

For each example, we use two Krylov methods [6], GMRES [7] and Bi-CGSTAB [8].

II.C.1. Garcia-Siewert

We solve the QMC linear problem with N=2048 and Nx= 100. Figures 1 and 2 show that the Krylov iterations take fewer than half of the number of transport sweeps that Picard iteration required.

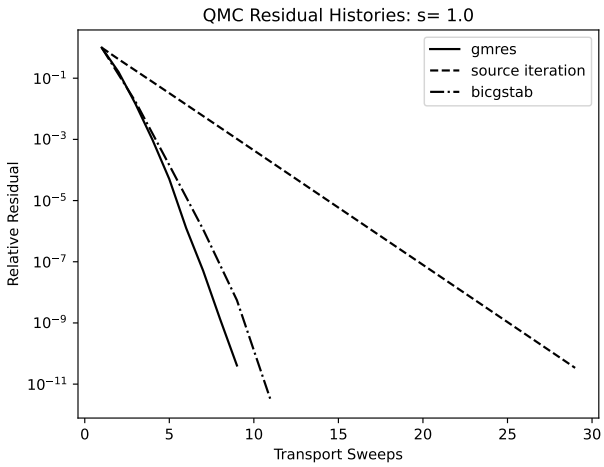

Fig. 1. $s = 1$

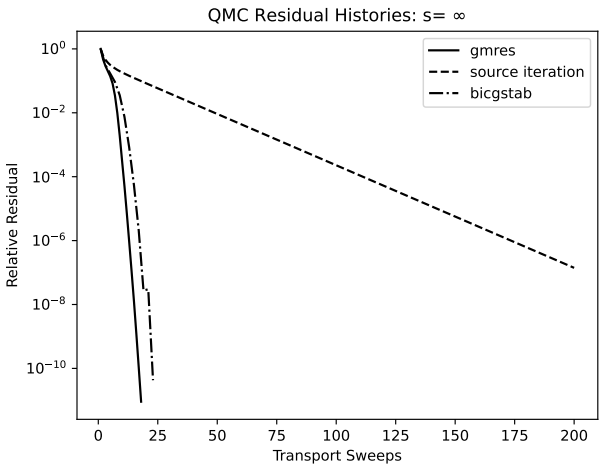
QMC Residual Histories: s= ∞
gmres
source iteration
bicgstab
Relative Residual
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
0
25
50
75
100
125
150
175
200
Transport Sweeps

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 $N = 2048$ 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	
μ	$\psi(0,-\mu)$	$\psi(\tau,\mu)$	$\psi(0,-\mu)$	$\psi(\tau,\mu)$
0.05	5.89664e-01	6.07488e-06	6.07035e-01	5.91908e-06
0.10	5.31120e-01	6.92516e-06	5.47466e-01	6.74075e-06
0.20	4.43280e-01	9.64232e-06	4.57064e-01	9.35453e-06
0.30	3.80306e-01	1.62339e-05	3.92223e-01	1.56108e-05
0.40	3.32964e-01	4.38580e-05	3.43481e-01	4.13721e-05
0.50	2.96090e-01	1.69372e-04	3.05510e-01	1.58622e-04
0.60	2.66563e-01	5.73465e-04	2.75098e-01	5.39514e-04
0.70	2.42390e-01	1.51282e-03	2.50192e-01	1.43257e-03
0.80	2.22235e-01	3.24369e-03	2.29422e-01	3.08975e-03
0.90	2.05174e-01	5.96036e-03	2.11837e-01	5.70555e-03
1.00	1.90546e-01	9.77123e-03	1.96756e-01	9.39189e-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: $s = \infty$

	Garcia/Siewert		QMC	
μ	$\psi(0,-\mu)$	$\psi(\tau,\mu)$	$\psi(0,-\mu)$	$\psi(\tau,\mu)$
0.05	8.97798e-01	1.02202e-01	9.06050e-01	1.03680e-01
0.10	8.87836e-01	1.12164e-01	8.95849e-01	1.13695e-01
0.20	8.69581e-01	1.30419e-01	8.76487e-01	1.31907e-01
0.30	8.52299e-01	1.47701e-01	8.58937e-01	1.49245e-01
0.40	8.35503e-01	1.64497e-01	8.42195e-01	1.66128e-01
0.50	8.18996e-01	1.81004e-01	8.25870e-01	1.82734e-01
0.60	8.02676e-01	1.97324e-01	8.09780e-01	1.99151e-01
0.70	7.86493e-01	2.13507e-01	7.93834e-01	2.15421e-01
0.80	7.70429e-01	2.29571e-01	7.77997e-01	2.31558e-01
0.90	7.54496e-01	2.45504e-01	7.62269e-01	2.47547e-01
1.00	7.38721e-01	2.61279e-01	7.46673e-01	2.63362e-01

Ryan, for large Nx 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: $s = 1.0$

Nx \N	1024	2048	4096	8192	16384
50	1.31716e-01	1.34260e-01	1.35123e-01	1.35328e-01	1.35242e-01
100	6.09631e-02	6.35764e-02	6.46191e-02	6.48898e-02	6.48536e-02
200	3.77223e-02	3.12496e-02	3.12005e-02	3.17337e-02	3.16710e-02
400	2.63214e-02	1.45106e-02	1.52355e-02	1.56636e-02	1.56854e-02
800	2.39486e-02	9.94925e-03	7.24627e-03	8.86212e-03	7.84063e-03
1600	4.16277e-02	9.95048e-03	5.11618e-03	8.02709e-03	4.44021e-03
3200	4.60905e-02	1.07345e-02	4.45922e-03	7.49522e-03	3.76179e-03

II.D.1. Multigroup Problems

These are preliminary results with $N_x = 40$ and $N = 2^{10}$. We may want to make these larger and/or make tables like Table III and Table III.

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

Nx \N	1024	2048	4096	8192	16384
50	1.31716e-01	1.34260e-01	1.35123e-01	1.35328e-01	1.35242e-01
100	6.09631e-02	6.35764e-02	6.46191e-02	6.48898e-02	6.48536e-02
200	3.77223e-02	3.12496e-02	3.12005e-02	3.17337e-02	3.16710e-02
400	2.63214e-02	1.45106e-02	1.52355e-02	1.56636e-02	1.56854e-02
800	2.39486e-02	9.94925e-03	7.24627e-03	8.86212e-03	7.84063e-03
1600	4.16277e-02	9.95048e-03	5.11618e-03	8.02709e-03	4.44021e-03
3200	4.60905e-02	1.07345e-02	4.45922e-03	7.49522e-03	3.76179e-03

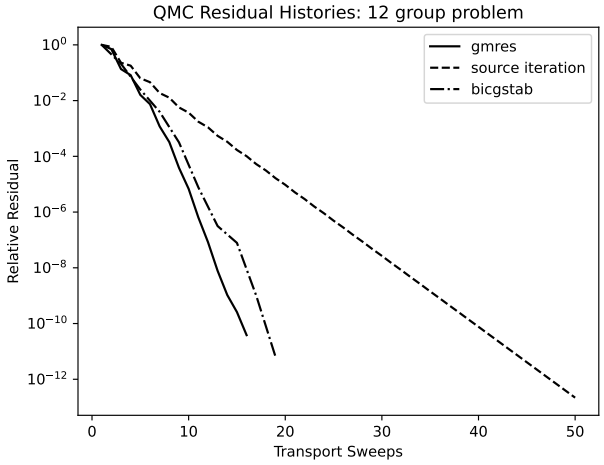

Fig. 3

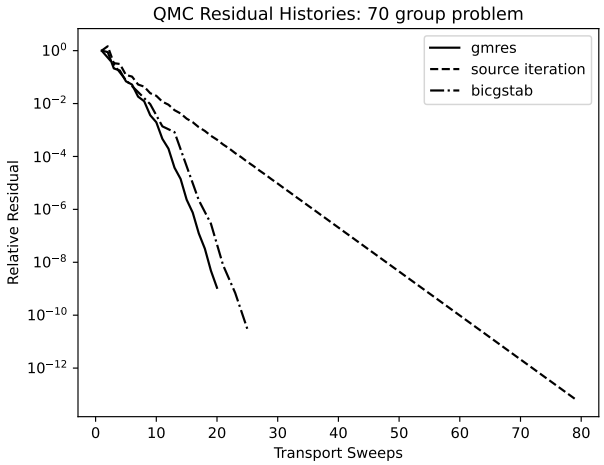

Fig. 4

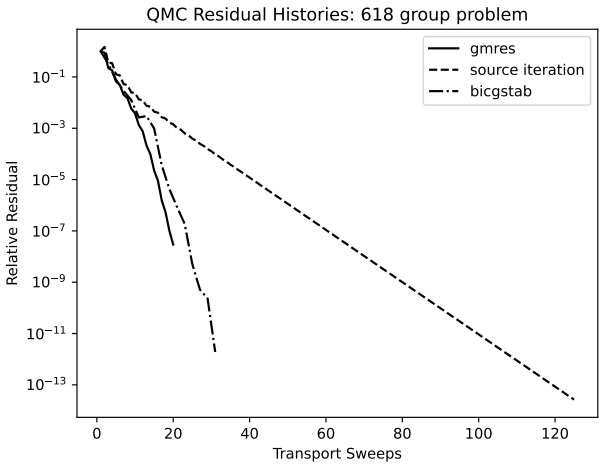
QMC Residual Histories: 618 group problem
gmres
source iteration
bicgstab
Relative Residual
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^{-9}
10^{-11}
10^{-13}
0
20
40
60
80
100
120
Transport Sweeps

Fig. 5

III. CONCLUSION

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