Krylov Linear Solvers and Quasi Monte Carlo Methods for Transport Simulations

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Our Place in Project Roadmap

Model Problem

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

$$\equiv \frac{1}{2}(\phi(x) + q(x)),$$

where $0 \le x \le \tau$ and

$$\phi(x) = \int_{-1}^{1}\psi(x,\mu')\,d\mu'.$$

Subject to boundary conditions

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

Source Iteration

Given an iteration n and $\phi_n(x)$ Compute ϕ_{n+1} by solving the fixed source problem

$$\mu \frac{\partial \psi_{n+1}}{\partial x}(x, \mu) + \Sigma_t(x)\psi(x, \mu) = \frac{1}{2}\left[\Sigma_s(x)\phi_n(x) + q(x)\right],$$

and then compute

$$\phi_{n+1}(x) = \int_{-1}^{1} \psi_{n+1}(x, \mu')\, d\mu' \equiv \mathcal{S}(\phi_n, q, \psi_l, \psi_r)$$

Linear System

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.

Solving the problem

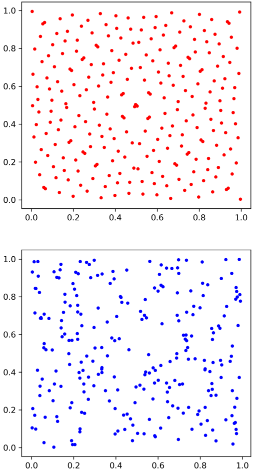
- Evaluating the Source iteration map
  - Conventional deterministic methods (SN ...)
  - Monte Carlo
  - Quasi Monte Carlo (this talk)
- Solving the linear problem
  - Source (Picard) iteration (in most codes)
  - Krylov methods: matrix-free
    - needs **CONSISTENT** evaluation of $\mathcal{S}$ to get $A\phi$
      MC has trouble with this
    - but no matrix assembly

Overview of Krylov Methods for $\mathbf{Ax} = \mathbf{b}$

- Initialization
  - $\mathbf{x}_0$: initial iterate
  - $\mathbf{r}_0 = \mathbf{b}_0 - \mathbf{A}\mathbf{x}_0$: initial residual
- Find iteration $\mathbf{x}_k$ in
  $\mathcal{K}_k = \text{ span } (\mathbf{r}_0, \mathbf{A}\mathbf{r}_0, \ldots, \mathbf{A}^{k-1}\mathbf{r}_0)$
- Example GMRES (Sadd/Schultz 1986): $\mathbf{x}_k$ minimizes $\|\mathbf{b} - \mathbf{A}\mathbf{x}\|$ over $\mathcal{K}_k$
- All is well if matrix-vector product is consistent.
  - $\mathbf{Ax}$ returns the same result with every call.
  - MC is not deterministic and hence not consistent.

QMC vs MC

QMC (red) and MC (blue)



A few facts

- MC and QMC are continuous in space/angle/energy
- With N samples/particles
  - QMC error $O(1/N)$
  - MC variance $O(1/\sqrt{N})$
- MC randomness
  - can break Krylov solvers
  - Willert et al 2013, 2014, 2015
  - Simoncini et al, 2003
- QMC gives consistent matrix-vector products

Preliminary Results

CEMENT

- All codes in Julia on github
  https://github.com/ctkelley/NDA_QMC.jl
- Model problem from Garcia/Siewert 1982

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

- Two cases: $s = 1$ (easy) and $s = \infty$ (hard)
- Evaluate source iteration map with QMC
- Compare GMRES and Bi-CGSTAB (van der Vorst 1992) to Picard
- Validation with with Garcia/Siewert exit distributions
  - QMC: N samples, Nx cells
  - Two figure accuracy with $N = 1000$ and $Nx = 100$

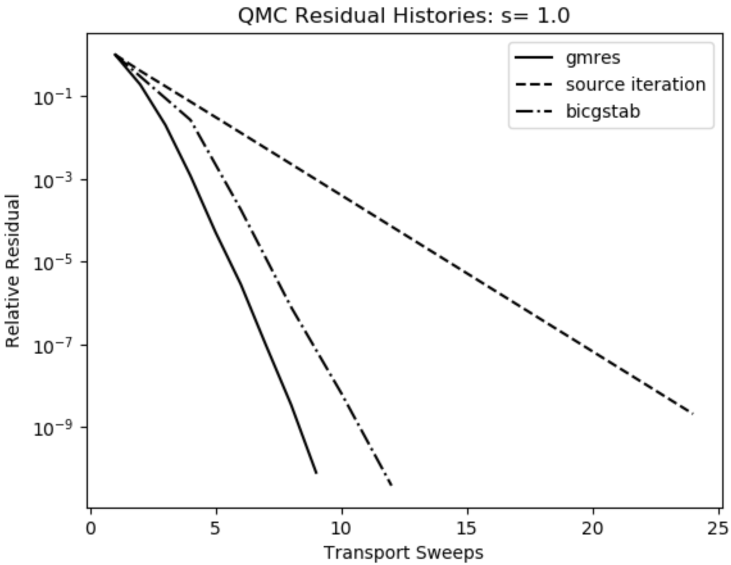
Validation: Easy case, $N = 1000$, $Nx = 100$

	Garcia/Siewert		QMC	
μ	$\psi(0,-\mu)$	$\psi(\tau,-\mu)$	$\psi(0,-\mu)$	$\psi(\tau,-\mu)$
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

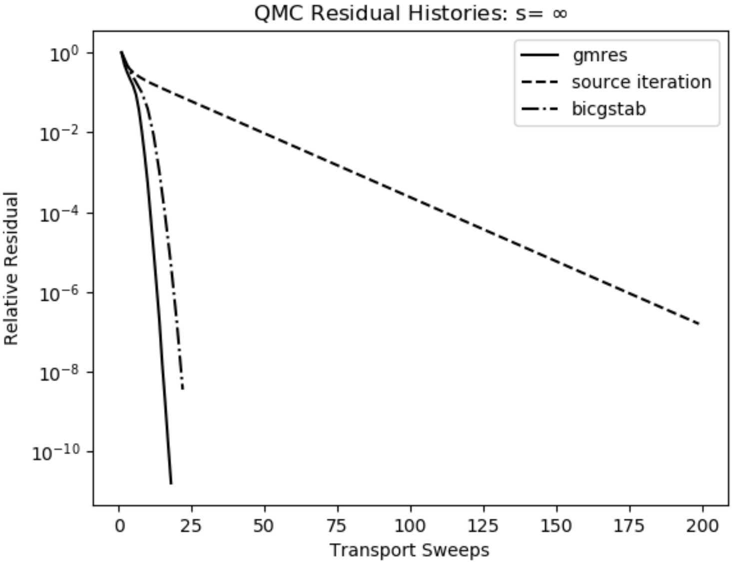
Validation: Hard case, $N = 1000$, $Nx = 100$

	Garcia/Siewert		QMC	
μ	$\psi(0,-\mu)$	$\psi(\tau,-\mu)$	$\psi(0,-\mu)$	$\psi(\tau,-\mu)$
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

Convergence: Easy Case



Convergence: Hard Case



Conclusions

- QMC for neutron transport simulations
  - Completely deterministic
  - Avoids problems with MC and Krylov methods
  - Krylov solvers very promising
- Test on benchmark problem
- Next up: NDA

Links

- Jupyter notebook draft of paper: https://github.com/ctkelley/NDA_QMC.jl
- Julia package: https://github.com/ctkelley/SIAMFANLEquations.jl
- Jupyter notebook draft of solver book: https://github.com/ctkelley/NotebookSIAMFANL

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