Krylov Linear Solvers and Quasi Monte Carlo Methods for Transport Simulations

Sam Pasmann, a C. T. Kelley, b and Ryan McClarren*, a

^aDepartment of Aerospace and Mechanical Engineering University of Notre Dame Fitzpatrick Hall, Notre Dame, IN 46556

^bNorth Carolina State University, Department of Mathematics 3234 SAS Hall, Box 8205 Raleigh NC 27695-8205

*Email: rmcclarr@nd.edu

Number of pages: 6 Number of tables: 0 Number of figures: 0

Abstract

 $\mathrm{QMC}\,+\,\mathrm{Krylov}$

 $\mathbf{Keywords}$ — 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

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

The boundary conditions are

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

The notation is

- ψ is intensity of radiation or angular flux at point x at angle $\cos^{-1}(\mu)$
- $\phi = \phi(x) = \int_{-1}^{1} \psi(x, \mu) \ d\mu$ is the scalar flux, the 0^{th} angular moment of the angular flux. - $\tau < \infty$, length of the spatial domain. - $\Sigma_s \in C([0, \tau])$ is the scattering cross section at x- $\Sigma_t \in C([0, \tau])$ is the total cross section at $x - \psi_l$ and ψ_r are incoming intensities at the bounds - $q \in C([0, \tau])$ is the fixed source

II.A. The Garcia-Siewert Example

In this example

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

II.B. Solvers

The linear and nonlinear solvers come from the Julia package SIAMFANLEQ.jl [3]. The documentation for these codes is in the Julia notebooks that accompany the package [4]. These are part of a book project [5].

II.C. Source Iteration and Krylov Methods

We use two krylov methods [6], GMRES [7] and Bi-CGSTAB [8].

II.D. QMC

II.E. Validation and calibration study

I'll compare the results from the SN computation to what I get from Sam's QMC code. My SN results are for a very fine spatial mesh and fine enough angular mesh. They are good to at least six figures and I will regard them as exact for this study.

I will use the SN results for the table in the Garcia-Siewert paper and get results from QMC in the following way

- For a give N and Nx I will get cell average fluxes from Sam's code.
- I will use the same code to generate the tables that I used for the SN fluxes. That code is src/sn_tabulate.jl
- \bullet I will take the two 11 x 2 arrays of results DataSN and DataQMC and compoute componentwise relative error with

Derr = (DataSN-DataQMC)./DataSN

II.F. QMC and Krylov Linear Solvers

I can solve the QMC linear problem with both Krylov methods now and, just like the classical case, I'm seeing fewer than half of the number of transport sweeps. Herewith the results for N=1000 and Nx=100.

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).