LA-UR-13-26459

Approved for public release; distribution is unlimited.

Title: Linear-Multi-Frequency-Grey Preconditioning for Radiative Transfer SN Calculations

Author(s): Till, Andrew T.

Intended for: Informal presentation at university in US; presentation to my advisor at said university.

Issued: 2013-08-15

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

70 YEARS OF CREATING TOMORROW

Los Alamos
NATIONAL LABORATORY

Linear Multi-Frequency-Grey Preconditioning for Radiative Transfer S_n Calculations

Andrew T. Till
James S. Warsa

SAS
08/15/2013
UNCLASSIFIED

Introduction and Theory

- The radiative transfer equations

- Linear multi-frequency grey acceleration

- Operator notation

- Scalar flux and absorption rate formulations

Results

- The Yang problem (no scattering)

- The Yang problem (with scattering)

- The CRASH-like problem

- The Tophat problem

Results and Conclusions

- Observations

- Obligations

UNCLASSIFIED

The radiative transfer equations describe the dynamic interplay and transport of radiation and material energies

- They couple **thermal radiation transport** to **internal material energy**, ignoring material motion and thermal conduction

$$\left(\frac{1}{c} \frac{\partial}{\partial t} + \nabla \cdot \Omega + \sigma_t(T, E) \right) \psi(r, E, \Omega, t) = \frac{\sigma_s(T, E)}{4\pi} \phi(r, E, t) + \sigma_a(T, E) B(T, E), \quad (1a)$$

$$C_v(T) \frac{\partial}{\partial t} T(r, t) = a T^4 \int dE (\sigma_a [\phi - 4\pi B]) + q(r, t), \quad (1b)$$

$$\text{Scalar flux} \quad \phi(r, E, t) = \int d\Omega \psi, \quad (1c)$$

$$\text{Absorption rate density} \quad \rho(r, t) = \int dE \sigma_a \phi. \quad (1d)$$

UNCLASSIFIED

We time-, angle- and energy-discretize the system and apply a linearization in temperature on the Planckian

- m is the S_n angular discretization index,
 g is the **multigroup** energy discretization index, and
 n is the **backward Euler** time discretization index:

$$(\nabla \cdot \Omega_m + \sigma_{t,g}^n(r) + \tau) \psi_{m,g}^{n+1}(r) = \frac{\sigma_{s,g}^n(r)}{4\pi} \phi_g^{n+1}(r) + \frac{\nu^n(r) \chi_g^n(r)}{4\pi} \rho^{n+1}(r) + \xi_{m,g}^n(r), \quad (2a)$$

Scalar flux $\phi_g^{n+1}(r) = \langle w_m \psi_{m,g}^{n+1} \rangle_m,$ (2b)

Absorption rate density $\rho^{n+1}(r) = \langle \sigma_{a,g}^n \phi_g^{n+1} \rangle_g,$ (2c)

Reemission rate density $f^{n+1}(r) = \nu^n(r) \rho^{n+1}(r),$ (2d)

$$\nu^n(r) = \frac{\langle \sigma_a \partial_T B \rangle_g^n \Delta t}{C_v^n + \langle \sigma_a \partial_T B \rangle_g^n \Delta t} \in (0, 1), \quad \chi_g^n(r) = \frac{4\pi \sigma_{a,g}^n \partial_T B_g^n}{\langle \sigma_a \partial_T B \rangle_g^n}.$$

UNCLASSIFIED

Linear-Multi-Frequency-Grey (LMFG) acceleration is used to accelerate the **absorption-reemission**

- ▶ If using **source iteration** (SI): approximate error in solution using grey diffusion solve
- ▶ If using **Krylov methods** (e.g., GMRES): precondition with grey diffusion solve
- ▶ In either case, the process is the same:

$$(\nabla \cdot \Omega_m + \sigma_{t,g}^n + \tau) \psi_{m,g}^{l+1/2} = \frac{\sigma_{s,g}^n}{4\pi} \phi_g^{l+1/2} + \frac{\chi_g^n}{4\pi} f^l + \xi_{m,g}^n, \quad (3a)$$

$$(\nabla \cdot \Omega_m + \sigma_{t,g}^n + \tau) \left(\psi_{m,g}^{n+1} - \psi_{m,g}^{l+1/2} \right) = \frac{\sigma_{s,g}^n}{4\pi} \left(\phi_g^{n+1} - \phi_g^{l+1/2} \right) + \frac{\chi_g^n}{4\pi} \left(f^{n+1} - f^l \right), \quad (3b)$$

$$(-\nabla \cdot D \nabla + \tau + (1 - \nu) \langle \sigma_a \rangle) \delta = f^{l+1/2} - f^l, \quad (3c)$$

$$f^{n+1} \simeq f^{l+1} = f^{l+1/2} + \nu \langle \sigma_a \rangle \delta. \quad (3d)$$

UNCLASSIFIED

We introduce an operator notation and our two formulations

- ▶ Operator notation:

$$L\psi = MSD\psi + MHXD\psi + q, \quad (4a)$$

- ▶ Scalar flux formulation (SFF):

$$\begin{aligned} L\psi &= M(S + HX)D\psi + q, \\ D\psi &= DL^{-1}M(S + HX)D\psi + DL^{-1}q, \\ \phi &= DL^{-1}M(S + HX)\phi + DL^{-1}q, \end{aligned} \quad (4b)$$

- ▶ Absorption rate formulation (ARF):

$$\begin{aligned} (L - MSD)\psi &= MHXD\psi + q, \\ XD\psi &= XD(L - MSD)^{-1}MHXD\psi + XD(L - MSD)^{-1}q, \\ f &= XD(L - MSD)^{-1}MHf + XD(L - MSD)^{-1}q. \end{aligned} \quad (4c)$$

UNCLASSIFIED

When scattering is present, our two formulations become three methods

- ▶ “Modern” SFF (no inner iterations):

$$\phi = DL^{-1}M(S + HX)\phi + DL^{-1}q, \quad (5a)$$

- ▶ “Traditional” SFF (inner iterations):

$$\phi = D(L - MSD)^{-1}MHX\phi + D(L - MSD)^{-1}q, \quad (5b)$$

- ▶ “Traditional” ARF (inner iterations):

$$f = XD(L - MSD)^{-1}MHf + XD(L - MSD)^{-1}q. \quad (5c)$$

- ▶ We employ a changing tolerance on the inner iterations

UNCLASSIFIED

When no scattering is present, our two formulations become two methods

- ▶ SFF (no inner iterations):

$$\phi = DL^{-1}MHX\phi + DL^{-1}q, \quad (6a)$$

- ▶ ARF (no inner iterations):

$$f = XDL^{-1}MHf + XDL^{-1}q. \quad (6b)$$

UNCLASSIFIED

We cast our equations in residual form, ignoring scattering for simplicity

- ▶ SFF (no LMFG):

$$F(\phi) = (I - DL^{-1}MHX) \phi - DL^{-1}q = 0, \quad (7a)$$

- ▶ SFF (with LMFG):

$$F(\phi) = (I + \Gamma) (I - DL^{-1}MHX) \phi - (I + \Gamma) DL^{-1}q = 0, \quad (7b)$$

- ▶ ARF (no LMFG):

$$F(f) = (I - XDL^{-1}MH) f - XDL^{-1}q = 0. \quad (7c)$$

- ▶ ARF (with LMFG):

$$F(f) = (I + \Gamma) (I - XDL^{-1}MH) f - (I + \Gamma) XDL^{-1}q = 0. \quad (7d)$$

UNCLASSIFIED

We tested the Yang problem

- ▶ Developed by Warsa, Morel and Yang in their 2007 J. Comp. paper “Linear multifrequency-grey acceleration recast for preconditioned Krylov iterations”
- ▶ Analytic opacities in the form $\sigma \propto T^{-1/2} E^{-3} \rho$; constant specific heats and ramping external heat source
- ▶ Marshak-like in center channel surrounded by thick, cool material
- ▶ Logarithmic zoning between center and thick material
- ▶ For simplicity, no reflecting boundaries and 2D Cartesian geometry (for Capsaicin devs: no augments)

We tested the Yang problem without scattering

Δt (sh)	Solver	LMFG	Formulation	Avg. outers	Avg. sweeps
0.2	GMRES	Yes	ARF	7.50	12.50
			SFF	7.30	12.30
		No	ARF	11.90	16.90
			SFF	11.30	16.30
	SI	Yes	ARF	17.10	20.10
			SFF	16.20	19.20
0.1	GMRES	Yes	ARF	6.85	11.85
			SFF	6.45	11.45
		No	ARF	10.15	15.15
			SFF	9.85	14.85
	SI	Yes	ARF	14.40	17.40
			SFF	13.60	16.60
0.01	GMRES	Yes	ARF	4.23	9.23
			SFF	4.22	9.22
		No	ARF	5.09	10.09
			SFF	5.01	10.01
	SI	Yes	ARF	6.80	9.80
			SFF	6.49	9.49

UNCLASSIFIED

We tested the Yang problem without scattering

We tested the Yang problem with scattering

Los Alamos National Laboratory

Scat.	Solver	Formulation		LMFG	DSA	Outers	Inners	Sweeps
Low	GMRES	SFF	Modern	Yes	No	4.22	0.00	9.22
				No		5.01	0.00	10.01
			Trad.	Yes	Inner	4.22	13.85	45.80
				No	No	4.23	13.92	46.17
				No	Inner	5.02	15.46	49.81
					No	5.01	15.50	50.11
		ARF	Trad.	Yes	Inner	4.27	13.88	46.05
					No	4.26	13.89	46.21
				No	Inner	5.14	15.54	50.24
					No	5.13	15.60	50.56
		SI	SFF	Yes	No	6.49	0.00	9.49
				No		11.56	0.00	14.56
			Trad.	Yes	Inner	6.49	13.13	46.58
					No	6.49	13.25	46.71
				No	Inner	11.56	22.63	71.29
					No	11.56	22.81	71.47
High	GMRES	SFF	Modern	Yes	No	8.73	0.00	13.73
				No		12.11	0.00	17.11
			Trad.	Yes	Inner	4.44	71.09	113.13
					No	4.50	87.50	134.77
				No	Inner	5.44	80.47	125.41
					No	5.49	101.88	152.18
		ARF	Trad.	Yes	Inner	4.39	69.42	110.92
					No	4.40	85.91	132.57
				No	Inner	5.48	79.36	124.08
					No	5.46	100.33	150.08

UNCLASSIFIED | 3

We tested the Yang problem with scattering

We tested the radiation-only CRASH problem

- ▶ Developed at TAMU for the PSAAP Center for Radiative Shock Hydrodynamics (CRASH) project
- ▶ Realistic, low-Z opacities; constant specific heats and internal heat sources
- ▶ Pseudo shock-tube, radiation-only problem to study wall heating
- ▶ Logarithmic zoning in wall
- ▶ For simplicity, no reflecting boundaries and 2D Cartesian geometry (for Capsaicin devs: no augments)

UNCLASSIFIED

We tested the radiation-only CRASH problem without scattering

Δt (sh)	Solver	LMFG	Formulation	Avg. outers	Avg. sweeps
0.01	GMRES	Yes	ARF	14.75	19.75
			SFF	13.40	18.40
		No	ARF	32.60	38.35
			SFF	26.25	31.70
	SI	Yes	ARF	66.00	69.00
			SFF	57.45	60.45
0.003	GMRES	Yes	ARF	10.78	15.78
			SFF	10.97	15.97
		No	ARF	27.31	32.31
			SFF	26.49	31.49
	SI	Yes	ARF	30.49	33.49
			SFF	30.40	33.40
0.001	GMRES	Yes	ARF	9.05	14.05
			SFF	9.87	14.87
		No	ARF	21.81	26.81
			SFF	22.48	27.48
	SI	Yes	ARF	21.49	24.49
			SFF	22.95	25.95

UNCLASSIFIED

We tested the radiation-only CRASH problem without scattering

We tested the topHat / crooked-pipe problem

- ▶ Developed at LLNL for radiative transfer problems
- ▶ Constant opacities over entire problem; low-density turning path embedded in a high-density region; constant specific heats and boundary heat source
- ▶ Radiation-only problem known for its difficulty (teleportation for IMC, diffusing around bends with P_n / diffusion, ray effects with S_n)
- ▶ Linear but fine zoning at material interface
- ▶ RZ geometry with vacuum boundaries (for Capsaicin devs: no augments)

UNCLASSIFIED

We tested the topHat problem without scattering

Δt (sh)	Solver	LMFG	Formulation	Avg. outers	Avg. sweeps
0.2	GMRES	Yes	ARF	13.50	18.50
			SFF	12.60	17.60
		No	ARF	81.40	88.50
			SFF	56.60	62.90
0.1	GMRES	Yes	ARF	13.65	18.65
			SFF	12.95	17.95
		No	ARF	74.50	81.45
			SFF	54.90	61.30
0.01	GMRES	Yes	ARF	11.24	16.24
			SFF	10.58	15.58
		No	ARF	34.00	39.85
			SFF	27.42	32.46

UNCLASSIFIED

We tested the topHat problem without scattering

LMFG is an efficacious preconditioner for multigroup TRT problems

- ▶ LMFG provides effective acceleration in all cases tested and is especially powerful when combined with a Krylov method
- ▶ In the absence of (real) scattering, ARF and SFF perform similarly
- ▶ In the presence of (real) scattering, non-nested (“modern”) formulations vastly outperform nested (“traditional”) formulations
- ▶ We are investigating why on average SFF performs better than ARF

UNCLASSIFIED

Thank you to all who made this summer possible!

- ▶ My LANL mentor, **Jim Warsa**
- ▶ My TAMU advisor, **Jim Morel**
- ▶ My funding source, the **CSGF**
- ▶ CCS-2 staff and my fellow interns,
esp. **Allan Wollaber**, **Erin Fichtl**, and **Kelly Thompson**

Funded by the Department of Energy Computational Science Graduate Fellowship,
grant number DE-FG02-97ER25308.

UNCLASSIFIED