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Fourier Analysis of Fokker-Planck Synthetic Acceleration for S_N Equations with Highly Forward-Peaked Scattering in Slab Geometry

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Outline

- Introduction and Motivation
- Fourier Analysis
  - Continuous-in-Angle
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- Examples
  - Screened Rutherford
  - Henyey-Greenstein Kernel
  - P_L-Equivalent Kernel
- Conclusion/Future Work

Forward-Peaked Transport in Slabs

- Physical Characteristics
  - Extremely small mean free path and energy loss, near singular differential scattering cross-section in forward direction ($\mu_0 \sim 1$)
  - $\sigma_t \sim \sigma_{s,0}$
- Applications
  - Radiation shielding, astrophysics, medical physics, plasma physics etc.
- Representative Equation

$$\mu \frac{\partial \psi}{\partial x} + \sigma_t(x)\psi(x,\mu) = \int_{-1}^{1} d\mu' \sigma_s(\mu_0)\psi(x,\mu') + Q(x,\mu)$$

- S_N Discretization

$$\mu_n \frac{\partial \psi}{\partial x} + \sigma_t(x)\psi(x,\mu_n) = \sum_{l=0}^{L} \frac{(2l+1)}{2} P_l(\mu_n)\sigma_{s,l}\phi_l(x) + Q(x,\mu_n)$$

$$n = 0,1,2 \ldots N$$

$$\phi_l(x) = \int_{-1}^{1} d\mu P_l(\mu)\psi(x,\mu) \approx \sum_{n=1}^{N} w_n P_l(\mu_n)\psi(x,\mu_n)$$

Standard Solution

- Source Iteration (SI)

$$R\psi^{m+1} = T\psi^{m} + Q$$

$$R = \mu\frac{\partial}{\partial x} + \sigma_t, \text{ and } T = \sum_{l=0}^{L}\frac{(2l+1)}{2}P_l\sigma_{s,l}\int_{-1}^{1}d\mu P_l(\mu)$$

Eigenvalues of iteration matrix for SI are $\frac{\sigma_{s,l}}{\sigma_t}$ $(l = 0,1,2 \dots L)$

- Synthetic acceleration usually follows a "Predict-Correct-Iterate" structure
  - **Predict**: $R\psi^{m+\frac{1}{2}} = T\phi_l^m + q$, where, m is the iteration index
  - **Correct**: $\psi^{m+1} = \psi^{m+\frac{1}{2}} + F^{-1}T(\psi^{m+\frac{1}{2}} - \psi^m)$
  - **Iterate**: if $\| \phi_l^{m+1} - \phi_l^m \|_\infty > tolerence$
  - Equivalent to preconditioning
- Different choices of F return different synthetic acceleration schemes. For example, the choosing diffusion returns DSA.

Problem Statement and Train of Thought

- Want to solve forward peaked transport problems efficiently
- Do standard methods work?
  - Standard iterative methods? NO!
    - Why? Because eigenvalues for source iteration get arbitrarily close to unity
  - How about standard acceleration/preconditioning methods?
    - DSA? NO! Error no longer linear in angle.
    - NDA? NO! Can't attenuate higher order moments of angular flux.
- Well then, what could?
  - Correcting angular flux itself (or at least sufficiently high number of moments)
  - What approximates transport angular flux for highly forward peaked problems? Fokker-Planck Angular Flux

Fokker-Planck Synthetic Acceleration

- We know we need a corrector for synthetic acceleration. What could we try that?
    - Why not try Fokker-Planck?
        - FP solves themselves are inefficient using standard techniques!
        - Can an efficient solver for FP be developed in future? Maybe, yes?
    - Choosing F as FP in

$$\psi^{m+1} = \psi^{m+\frac{1}{2}} + F^{-1}T(\psi^{m+\frac{1}{2}} - \psi^{m})$$

returns FPSA

- What have others done?
    - Angular Multigrid (Morel, 1991), (Pautz et al., 1998), (Trucksin et al., 2012)
    - P_L acceleration (Valougeorgis et al., 1988)
    - Modified-PL acceleration (Khattab et al., 1991)

So What Will We talk About Today?

- We decided to look at FPSA for efficient solution of forward-peaked problems. So now what?
  - First, what is the simplest forward-peaked problem which is also general enough that the methods applied to it can eventually be applied to more complicated forward-peaked problems?
    - Monoenergetic, slab geometry problem with highly forward-peaked elastic scattering. So then, we test FPSA on this problem.
- What do we need to do to test FPSA on such problems?
  - Fourier Analysis – with an eye on the corresponding discretization!
  - Numerically Implement FPSA
  - Compare Fourier Analysis and Numerical Implementation
  - Test Method on Different Kernels
- We will primarily look at Fourier analysis today. Due to lack of time, however, a lot of details will be skipped.

Fourier Analysis – Intro and Foreshadowing

- Discretization?
  - Transport
    - S_N (Lewis and Miller, 1993) in angle
    - LD in space (Warsa, 2014)
  - Fokker-Planck
    - S_N in angle
    - LD in space
    - Weighted Finite Difference (Morel, 1985) and Moment Preserving Discretization (Warsa et al., 2012) for the angular Laplacian

Why the phrase "with an eye on the corresponding discretization"?

- Angularly-continuous Fourier analysis is inconsistent with numerical implementation of WFD discretization
    - WFD only preserves 0^{th} and 1^{st} moment while angularly-continuous analysis preserves all L+1 moments of FP angular flux.
- Expect angularly-continuous analysis to be inconsistent with numerical implementation when N and L are low.
    - Discrete and continuous representations of an equation are not the same. We must converge the solution of discrete equation in N and L to get to the solution of the continuous equation.
    - Difficult to do angularly-continuous analysis for anything beyond $L = 15$

Fourier Analysis – Error Equation

- Recall corrector equation

$$\psi^{m+1} = \psi^{m+\frac{1}{2}} + F^{-1}T(\psi^{m+\frac{1}{2}} - \psi^{m})$$

- Now, subtract exact angular flux, ψ, from both sides and add and subtract ψ inside the argument of scattering operator:

$$\psi^{m+1} - \psi = \psi^{m+\frac{1}{2}} - \psi + F^{-1}T(\psi^{m+\frac{1}{2}} - \psi + \psi - \psi^{m})$$

- Upon defining error in m^{th} iterate, $\epsilon^{m} = \psi - \psi^{m}$ (and so on), we get

$$\epsilon^{m+1} = \epsilon^{m+\frac{1}{2}} - F^{-1}T\left(\epsilon^{m} - \epsilon^{m+\frac{1}{2}}\right)$$

Fourier Analysis – Error-Moment Equation

Recall, $T=\sum_{l=0}^{L}\frac{(2l+1)}{2}P_l\sigma_{s,l}\int_{-1}^{1}d\mu P_l(\mu)$

- Defining $S=\sum_{l=0}^{L}\frac{(2l+1)}{2}P_l\sigma_{s,l}$, and introducing error iterate moment, $\epsilon_l^m=\int_{-1}^{1}d\mu P_m(\mu)\epsilon^m$, we have:

$$\epsilon^{m+1}=\epsilon^{m+\frac{1}{2}}-F^{-1}S\left(\epsilon_l^m-\epsilon_l^{m+\frac{1}{2}}\right)$$

- Taking l^{th} Legendre moment to the above equation returns:

$$\epsilon_l^{m+1}=\epsilon_l^{m+\frac{1}{2}}-M\left(\epsilon_l^m-\epsilon_l^{m+\frac{1}{2}}\right)$$

$$M=\int_{-1}^{1}d\mu P_m(\mu)F^{-1}S$$

Fourier Analysis – General Strategy

- For Fourier analysis, eventually, we want to find an iteration matrix, IM, such that we have

$$\hat{\epsilon}_l^{m+1} = [IM]\hat{\epsilon}_l^m$$

- Where, $\hat{\epsilon}_l^m$ comes from introduction of Fourier mode ansatz:

$$\epsilon^m = \hat{\epsilon}^m e^{i\omega x}, \epsilon_l^m = \hat{\epsilon}_l^m e^{i\omega x}$$

- The error-moments equation is

$$\epsilon_l^{m+1} = \epsilon_l^{m+\frac{1}{2}} - M\left(\epsilon_l^m - \epsilon_l^{m+\frac{1}{2}}\right)$$

- The introduction of Fourier mode ansatz transforms the above equation into the following ansatz-moment equation

$$\hat{\epsilon}_l^{m+1} = \hat{\epsilon}_l^{m+\frac{1}{2}} - \widehat{M}\left(\hat{\epsilon}_l^m - \hat{\epsilon}_l^{m+\frac{1}{2}}\right)$$

$\widehat{M}$ is the operator M transforms into when we introduce of Fourier mode ansatz.

- Now, in order to get to $\hat{\epsilon}_l^{m+1} = [IM]\hat{\epsilon}_l^{m}$, first, we introduce a dummy operator $[A]$ such that

$$\hat{\epsilon}_l^{m+\frac{1}{2}} = [A]\hat{\epsilon}_l^{m}$$

- Introduction of the above relation in ansatz-moment equation, upon simplification returns:

$$\epsilon_l^{m+1} = \left[A - \widehat{M}(I - A)\right]\epsilon_l^{m}$$

- Therefore, our iteration matrix becomes

$$[IM] = \left[A - \widehat{M}(I - A)\right]$$

- Here, I is the identity matrix
- Upon inspection of the ansatz-moments equation and our iteration scheme, we realize that A is the iteration matrix obtained from Fourier analysis of the predictor step. In other words A is the iteration matrix of source iteration source iteration.

Angularly-Continuous Fourier Analysis for FPSA

- Upon carrying out relevant mathematical exercise, we note that

$$[\mathrm{A}] = \left[\sum_{l=0}^{L} \frac{(2l+1)}{2} \sigma_{s,l} \int_{-1}^{1} d\mu \, \frac{P_l P_m}{i\omega\mu + 1}\right]$$

$$\widehat{M} = B^{-1} X$$

with

$$X_{ll} = \sigma_{s,l}$$

$$B_{ll} = \sigma_a + \frac{\sigma_{tr}}{2} l(l+1), \; B_{l-1,l} = \frac{l}{2l+1} i\omega, B_{l+1,l} = \frac{l+1}{2l+1} i\omega$$

$$l = 0,1,2 \dots L$$

- Our overall iteration matrix, therefore becomes

$$[IM] = [A - B^{-1} X (I - A)]$$

Angularly-Continuous Fourier Analysis for P$_L$-Acceleration

- Carrying out a similar mathematical exercise for P$_L$ acceleration results in an iteration matrix that is exactly the same as the one we got for FPSA but for one difference:

$$B_{l,l}^{FPSA} = \sigma_a + \frac{\sigma_{s,o}-\sigma_{s,1}}{2} l(l+1), \text{ while}$$

$$B_{l,l}^{P_L} = \sigma_a + \sigma_{s,0} - \sigma_{s,l}$$

- Equating the two, we realize that FPSA and P$_L$ acceleration are equivalent when

$$\sigma_{s,l} = \sigma_{s,o} - \frac{\sigma_{s,o} - \sigma_{s,1}}{2} l(l+1)$$

- This is consistent with (Morel, 1981) where he came up with a way of using modified scattering cross-section moments with transport equation to obtain the Fokker-Planck.

Angularly-Discrete Fourier Analysis for FPSA-WFD

- We follow the same exact procedure as we did for continuous-in-angle case except, here, all moments and moment-integrals are written in terms of finite weighted sums using Gauss quadrature (S_N).
- So here, we will try to obtain the iteration matrix such that

$$\hat{\epsilon}^{m+1} = [IM]\hat{\epsilon}^{m}$$

- We begin with

$$\epsilon^{m+1} = \epsilon^{m+\frac{1}{2}} - F^{-1}T\left(\epsilon^{m} - \epsilon^{m+\frac{1}{2}}\right)$$

- Introduce Fourier-mode ansatz, just like before to get

$$\epsilon^{m+1} = \epsilon^{m+\frac{1}{2}} - \hat{F}\left(\epsilon^{m} - \epsilon^{m+\frac{1}{2}}\right)$$

Where, $\hat{F}$ is the operator $F^{-1}T$ transforms into when we introduce of Fourier mode ansatz.

- Following similar steps as before, our iteration matrix becomes

$$[IM] = \left[A_d - \hat{F}(I - A_d)\right]$$

- Here, A comes from angularly-discrete treatment of moments and moment integrals and is, therefore, a discrete representation of A that we got during our continuous analysis.
- We do angularly-discrete analysis for two different discretizations of the angular Laplacian in the FP equation – WFD and MPD.

Analysis with WFD

- Upon carrying out the relevant mathematical exercise, we find that

$$A_d = P^{-1}Q$$

$$P_{ln} = P_l(\mu_n)w_n\big(i\omega\sigma_t\mu_n + \sigma_t(x)\big)$$

$$Q_{ln} = \sigma_{s,l}(x)P_l(\mu_n)w_n$$

$$\hat{F} = B^{-1}C$$

$$B = B1 + B2 + B3$$

$$B1_{ln} = P_l(\mu_n)w_n\left\{i\omega\sigma_t\mu_n + \sigma_a + \frac{\sigma_{tr}}{2}b_n\right\}$$

$$B2_{ln+1} = -\frac{\sigma_{tr}}{2}a_nP_l(\mu_n)w_n$$

$$B3_{ln-1} = -\frac{\sigma_{tr}}{2}c_nP_l(\mu_n)w_n$$

$$C_{ln} = \sigma_{s,l}P_l(\mu_n)w_n$$

$$[IM] = [A_d - B^{-1}C(I - A_d)]$$

Analysis with MPD

Again,

- Upon carrying out the relevant mathematical exercise, we find that

$$A_d = P^{-1}Q$$

$$P_{ln} = P_l(\mu_n)w_n\big(i\omega\sigma_t\mu_n + \sigma_t(x)\big)$$

$$Q_{ln} = \sigma_{s,l}(x)P_l(\mu_n)w_n$$

$$\hat{F} = B^{-1}C$$

$$B_{ln} = i\omega\sigma_t w_n P_l(\mu_n)\mu_n + \sigma_a w_n P_l(\mu_n) + l(l+1)\frac{\sigma_{tr}}{2}w_n P_l(\mu_n)$$

$$C_{ln} = \sigma_{s,l}P_l(\mu_n)w_n$$

$$[IM] = [A_d - B^{-1}C(I - A_d)]$$

Here, B is different from that for WFD. Otherwise everything is the same!

Comparing Fourier Analyses

η	**MPD / WFD**	ρ_{SI}	ρ_{cts}	ρ_{dct}	$\rho_{measured}$
2.836×10^{-5}	MPD	0.9999	0.4706	0.4706	0.4706
2.836×10^{-6}	MPD	0.9999	0.4266	0.3906	0.3898
2.836×10^{-5}	WFD	0.9999	0.4706	0.2121	0.2120
2.836×10^{-6}	WFD	0.9999	0.4266	0.3215	0.3213

Spectral Radius Comparison with Screened Rutherford Scattering Kernel

We see how measured spectral radii match the discrete-in-angle analysis very well but not the standard angularly-continuous analysis as suspected before.

Screened Rutherford Kernel

L	**N**	**MPD**	**WFD**
1	2	1.268e-12	1.268e-12
15	16	0.4706	0.2123
31	32	0.5697	0.3676
63	64	0.5877	0.4972
127	128	0.5877	0.5622

Spectral Radius with $\eta = 2.84 \times 10^{-5}$

FP-Solve	**L/N**	**GMRES (150) iter/time**	**GMRES-MPD iter/time**	**GMRES-WFD iter/time**	**FPSA-MPD iter/time**	**FPSA-WFD iter/time**
GMRES	15/16	1487 26.6s	12 11.4 s	8 6.97s	21 9.69s	13 5.40s
Factorize (Davis, 2009)			12 2.547s	9 1.69s	21 0.447s	13 0.307s

Efficiency data – unit beam source at most forward angle

Henyey-Greenstein Kernel

L	N	MPD	WFD
1	2	1.869e-12	6.403e-12
15	16	0.8709	0.7466
31	32	0.9338	0.8671
63	64	0.9624	0.9291
127	128	0.9719	0.9579

Spectral Radius with $g = 0.9999$

FP-Solve	L/N	GMRES (150) iter/time	GMRES-MPD iter/time	GMRES-WFD iter/time	FPSA-MPD iter/time	FPSA-WFD iter/time
GMRES	15/16	597 42.29s	16 479.9s	12 331.2s	29 1040s	17 285.7s
Factorize			12 12.41s	9 6.795s	29 2.131s	17 1.316s

Efficiency data – unit beam source at most forward angle

P_L-Equivalence Kernel…Just for fun!

L	N	MPD	WFD
1	2	2.060e-12	7.275e-12
15	16	1.917e-11	0.4353
31	32	2.734e-11	0.3300
63	64	7.257e-11	0.7889
127	128	8.434e-11	1.263

Spectral Radius with $\sigma_{s,0} = 1$, $\sigma_{tr} = 1.059\text{e-}7$

- Note how the spectral radius reduces to pretty much zero with MPD but not with WFD. This is because WFD only preserves the first two moments.
- We see near-zero spectral radius for MPD because the crosssection moments were chosen according to the FPSA-P_L acceleration equivalence relation.

Conclusion

- Spectral radius of accelerated scheme is problem and discretization dependent.
- Significant improvement in the spectral radius as scattering kernel gets closer to having FP limit.
- Discrete Fourier analysis is more suitable for analysis of FPSA.
- Significant cut down in number of iterations compared to unaccelerated problem.
- Need to solve FP more efficiently.
- WFD can get unstable for P_L equivalence kernel.

More Questions?

- Is the FPSA solution as good as analytical solution?
  - No. Need to converge in N, L and space in order to get high precision answer. Spatially, at least, we get third order convergence. Yes, there is scope to use convergence acceleration especially in L and N!
- Does discrete-in-angle analysis approach continuous-in-angle analysis?
  - Yes, if we use MPD and sufficiently large L (it can be seen from numerical results).
- Is the method any good especially if FP is slow to converge?
  - It can potentially be a good method if we converge FP faster (some methods proposed but not tested). We saw that with a decent way of solving FP in 1D with Davis's Factorize (Davis, 2009), there was significant (at least an order of magnitude) saving in time.
- Detailed theory on relationship between eigenvalues and eigenfuncions of original equations (transport) and their asymptotic limits?
  - Would be very interesting to look at!

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