Inside the Mind of an Analytical Transport Benchmark Theorist

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Concerning a new solution in diffusion theory:

TITLE: The Boundary Element Formulation of the One Group, 1D Nodal Equations

Submitted to last ANS Meeting

Reviewer's Objection:

The methodology used …. is not new. It can be found in nuclear engineering textbooks or PDE literature. The concept of solving multislab problems analytically in each slab, …., is well-known.

Reviewer’s Objection:

The significance of this reformulation (via the Green’s function) for the treatment of 1-d (compared to a cell-by-cell formulation, for example) <u>is not clear</u>.

In contrast:

The reformulation of the problem involving Green's functions is different from the presentation in these references, and yields, <u>admittedly</u>, a concise methodology.

Reviewer’s Objection:

The authors indicate that this work …. will be used to assess multidimensional Pebble Bed Reactor (PBR) production codes." The paper does not adequately support this and advantages of this approach to multi-d problems should be clearly explained. In the absence of this information, the merit of the paper is not sufficient to justify its publication.

Concerning a new DVM solution in transport theory:

The McCormack Model for Channel Flow of a Binary Gas Mixture: The Simple Way

Submitted to the European Journal of Mechanics

C.E. Siewert Review

…. I can see no reason to publish an algorithm that requires hours of computer time to (almost) reproduce results that required less than a second of computer time. This author claims his algorithm can be applied to more difficult problems …. if that were done, I could (perhaps) support that work for publication in a serious journal; but in regard to this current work, for me the answer is NO.

Another Reviewer's Objection:

+ In general , the manuscript does not provide any new physical results.

+ However, an acceleration [DSA] proposed in Ref 5…is more efficient.

My concerns:

+ Am I not understanding my audience?

+ Is my concept of transport research outdated and of minimal interest?

+ Am I not communicating my ideas properly?

+ Have my colleagues (reviewers) become less familiar with analytical methods?

+ Are the mathematical concepts I use too sophisticated?

+ Am I too far ahead of most colleagues?

+ Am I at the end of my run?

My Mission Statement:

To analytically and numerically solve the particle transport equation for increasingly comprehensive scenarios and provide the solutions to the nuclear and Earth science communities

My Vision:

Someday all routinely used numerical transport algorithms will incorporate automatic benchmarking for quality control

Guiding beliefs for success:

+ Education makes each of us a better person
+ <u>Always present a unique perspective</u>
+ Listen and learn
+ Share knowledge
+ <u>Have a sense of humor</u>
+ Don’t get too fat
+ Respect age and all life
+ <u>Don’t upset your boss or significant other</u>
+ Be passionate about transport and diffusion theory

My unique research perspective:

+ First and foremost an educator
+ Strong mathematical interests
  - Theory
  - Application
+ Passion for solving neutron transport and radiative transfer equations
  - Benchmarks (LANL/INL/ORNL?)
  - RT in leaf canopies
+ Make a difference at some level

Today:

Share my research perspective on

+ analytical investigations

I want you to get inside my head to see why I do what I do

+ future benchmarks

Analytical Transport (Diffusion) Benchmarks

+ Generation and evaluation of analytical solutions to the transport (diffusion) equation

+ Numerical evaluation to 5 or more places

+ Requires mathematical and numerical skills

The appeal

+ Continues the great tradition of analytical thinking

+ Beneficial to community

+ A challenging activity

+ Sometimes very frustrating however

Part 1

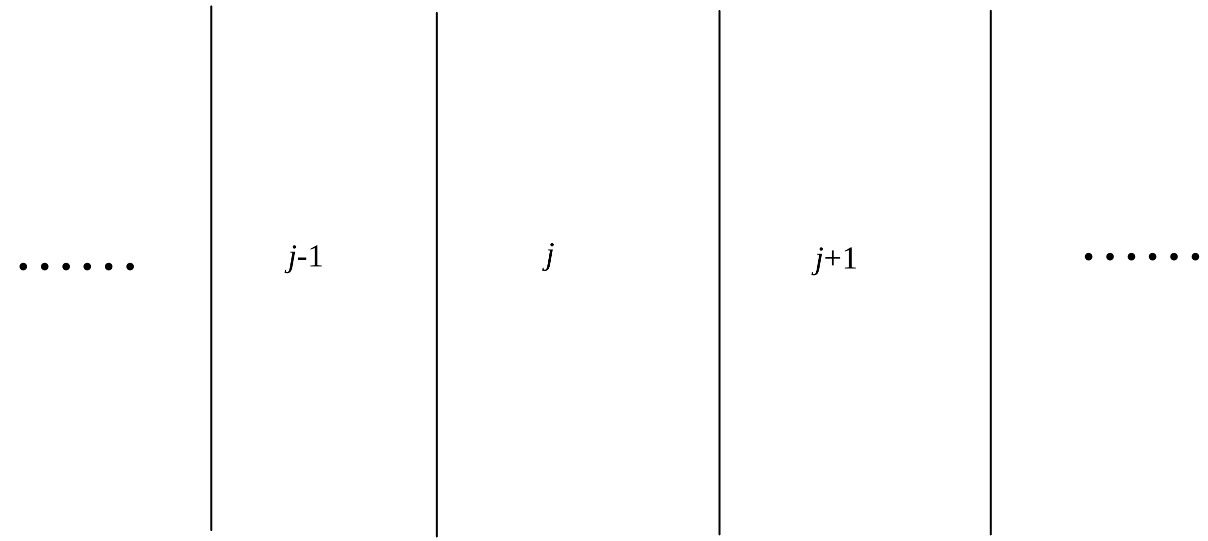
Boundary Element Formulation of the One Group, 1D Nodal Diffusion Equations

Question: Can the solution to the 1D diffusion equation be improved upon with regard to derivation and numerical accuracy?

+ Motivation:
    - Improve upon an old problem
+ Considerations:
    - Heterogeneous media
    - MG
    - 1D curvilinear
    - Time dependence

+ Begin with one group plane heterogeneous geometry and seek a unifying derivation

One group diffusion in a heterogeneous medium



$$\left[\frac{d^2}{dx^2}+B_j^2\right]\Phi_j(x)=-\frac{S_j}{D_j}=-q_j$$

Uniform source

$$B_j^2\equiv\left[\frac{\nu\Sigma_{fj}-\Sigma_{aj}}{D_j}\right]$$

$$J_j(x)\equiv-D_j\frac{d}{dx}\Phi_j(x)$$

Extend each region to $\pm\infty$

$$\rho_j(x) \equiv \Theta(x - x_{j-1}) - \Theta(x - x_j)$$

$$\Psi_j(x) \equiv \rho_j(x)\Phi_j(x)$$

$$\left[\frac{d^2}{dx^2} + B_j^2\right]\Psi_j(x) \equiv \left[\frac{d\delta}{dx}(x - x_{j-1}) - \frac{d\delta}{dx}(x - x_j)\right]\Phi_j(x) +$$

$$+2\left[\delta(x - x_{j-1}) - \delta(x - x_j)\right]\frac{d}{dx}\Phi_j(x) - \rho_j(x)q_j$$

Seek Green's Function in region *j*

$$\left[\frac{d^2}{dx^2}+B_j^2\right]G_j\left(x,x'\right)=-\delta\left(x-x'\right)$$

\+ Fourier transform solution

$$G_j\left(x,x'\right)=-\frac{1}{2B_j}\sin\left(B_j\left|x-x'\right|\right)$$

Integrate extended flux equation against Green' function

$$\Psi_j(x)=\frac{1}{2}\left\{\begin{array}{l}-\dfrac{1}{D_jB_j}\left[\begin{array}{l}J_j(x_{j-1})\sin\left(B_j\left|x_{j-1}-x\right|\right)-\\ -J_j(x_j)\sin\left(B_j\left|x_j-x\right|\right)\end{array}\right]+\\ +\left[\begin{array}{l}\Phi_j(x_j)\cos\left(B_j\left|x_j-x\right|\right)\operatorname{sgn}(x_j-x)-\\ -\Phi_j(x_{j-1})\cos\left(B_j\left|x_{j-1}-x\right|\right)\operatorname{sgn}(x_{j-1}-x)\end{array}\right]\end{array}\right\}+Q_j$$

Example of nodal equations

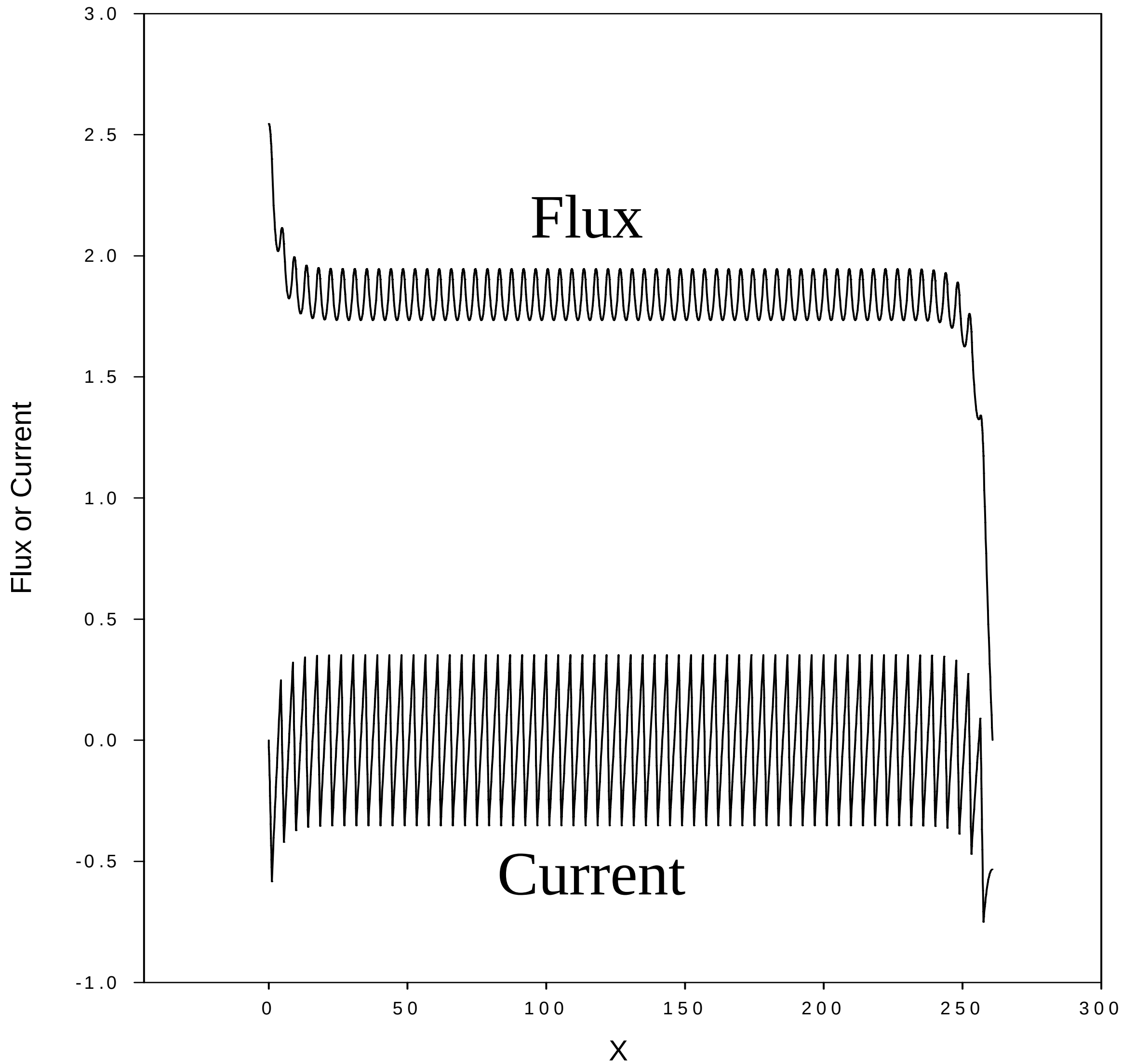
$$\Phi_j(x) = \left[\Phi_j - Q_j^+\right]\boxed{\left[\frac{\sin\left(B_j\left(x - x_{j-1}\right)\right)}{S_j}\right]} + \left[\Phi_{j-1} - Q_j^-\right]\boxed{\left[\frac{\sin\left(B_j\left(x_j - x\right)\right)}{S_j}\right]} + Q_j$$

$$\Phi_j + b_j\Phi_{j-1} + \gamma_j\Phi_{j-2} = f_j$$

$$\Phi_j(x) = \frac{1}{D_jB_j}\left[J_j + D_jB_jQ_{cj}^+\right]\boxed{\left[\frac{\cos\left(B_j\left(x - x_{j-1}\right)\right)}{S_j}\right]} - \frac{1}{D_jB_j}\left[J_{j-1} + D_jB_jQ_{cj}^-\right]\boxed{\left[\frac{\cos\left(B_j\left(x_j - x\right)\right)}{S_j}\right]} + Q_j$$

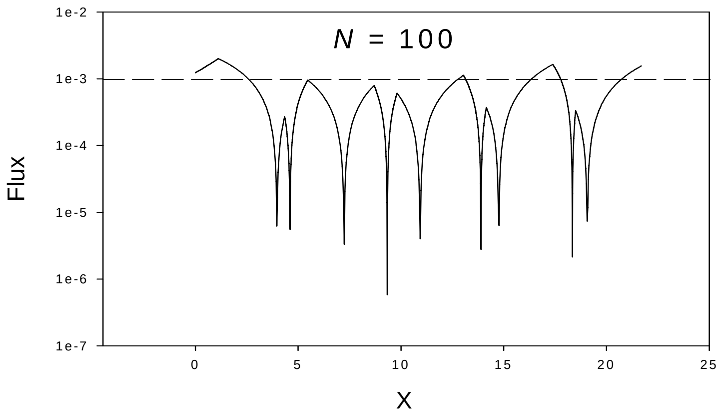
$$J_j + \hat{b}_jJ_{j-1} + \hat{\gamma}_jJ_{j-2} = \hat{f}_j$$

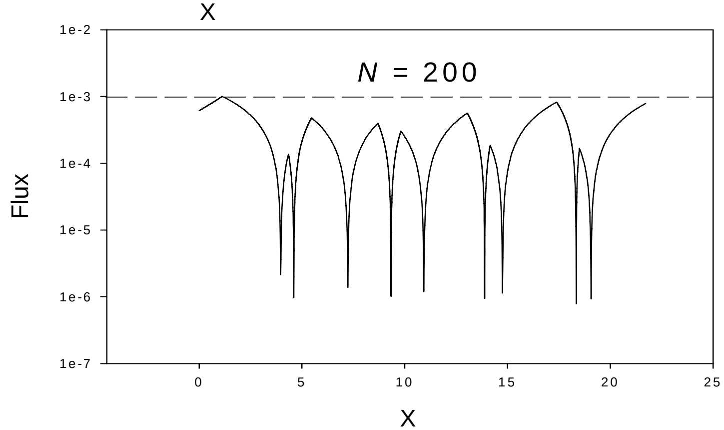
Benchmark Application: 120 Fuel Pins

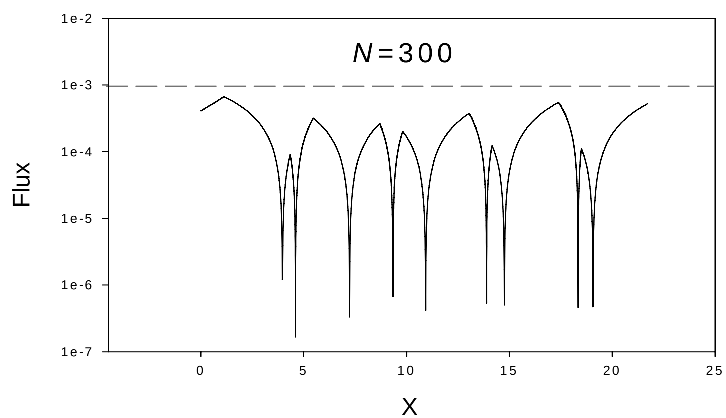


Error for FD Scheme

(3-point recurrence)







What has been accomplished?

+ Entirely new formulation for heterogeneous media not found in the literature

+ Continuity equations can be solved analytically (not shown)

+ Eliminated need for a numerical FD or FE solution

+ New criticality condition (not shown)

+ New solution strategy successfully applied to an old problem

+ Provides a basis for more complicated problems

Multigroup formulation:

$$\Phi_j(x) = \boxed{\left[\alpha_j h_j^{+}(x)\alpha_j^{-1}\right]}\Phi_j + \boxed{\left[\alpha_j h_j^{-}(x)\alpha_j^{-1}\right]}\Phi_{j-1}$$

One Group Cylindrical Geometry:

$$\Phi_j(r) = X_j^{+}(r)\left(\Phi_j - \Phi_{p,j+}\right) + X_j^{-}(r)\left(\Phi_{j-1} - \Phi_{p,j-}\right) + \Phi_{p,j}(r)$$

Time Dependence:

$$\bar{\Phi}_j(r,s) = X_j^{+}(r,s)\left(\bar{\Phi}_j(s) - \bar{\Phi}_{p,j}(s)\right) + X_j^{-}(r,s)\left(\bar{\Phi}_{j-1}(s) - \bar{\Phi}_{p,j}(s)\right) + \bar{\Phi}_{p,j}(s)$$

$$\Phi_j(r,t) = \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} ds\, e^{st}\bar{\Phi}_j(r,s)$$

Objection:

The significance of this reformulation for the treatment of 1-d ….. is not clear.

Objection:

The methodology used …. is not new.

Part 2

Mining the Multigroup-Discrete Ordinates Algorithm for High Quality Solutions

- Recent advances in **1D neutron transport semi-analytical Benchmarks**
  + Greens Function Method (GFM)
  + Analytical Discrete Ordinates (ADO-CES)
    - Discretize in angle
    - Solve resulting ODEs for eigenvalues and eigenfunctions

Question: Why develop semi-analytical benchmarks at all?

Answer: To avoid the numerical error of discretization

+ Development of semi-analytical benchmarks requires
  - special mathematical techniques
  - special programming
+ Limited to idealized scenarios
+ Not accessible to all

+ Reasonable to ask:
  - Can vast knowledge of analytical methods be applied to produce a more simple/accessible scheme?

  -Can discretization be used to theoretical advantage?

  -Can low order solutions be “mined” to generate high order solutions?

+Demonstration: SN applied to MG neutron transport

Multigroup Transport Equation: *Isotropic Scattering*

$$\left[\mu \underline{I}\frac{\partial}{\partial x}+\underline{\underline{\Sigma}}\right]\vec{\phi}(x,\mu)=\frac{1}{2}\left[\underline{\underline{\Sigma}}_S+\vec{\chi}\,\underline{\underline{\Sigma}}_f^T\,\underline{\nu}\right]\vec{\phi}(x)+\vec{Q}(x,\mu)$$

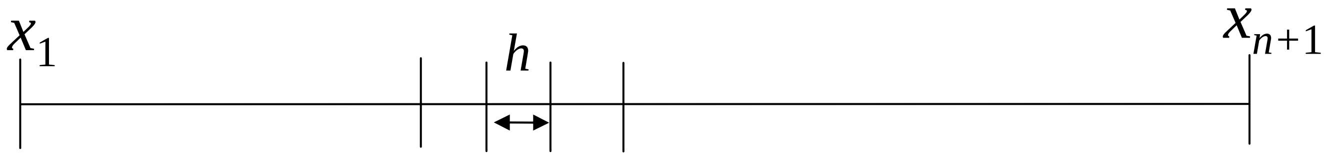
For Collided Component:

$$\left[\mu \underline{I}\frac{\partial}{\partial x}+\underline{\underline{\Sigma}}\right]\vec{\phi}_C(x,\mu)=\frac{1}{2}\left[\underline{\underline{\Sigma}}_S+\vec{\chi}\,\underline{\underline{\Sigma}}_f^T\,\underline{\nu}\right]\vec{\phi}_C(x)+\vec{Q}(x,\mu)+\vec{q}_1\left(x\right)$$

$$\vec{\phi}_C\left(0,\mu\right)=a_i\vec{e}_t \qquad \mu>0$$

$$\vec{\phi}_C(a,\mu)=\vec{0} \qquad \mu<0$$

Integrate over spatial interval h: $j = 1,n+1$



$$\mu_m\left[\vec{\phi}_{cm,j+1}-\vec{\phi}_{cm,j}\right]+\underline{\underline{\Sigma}}\int_h dx\vec{\phi}_{cm}(x)=$$

$$=\frac{1}{2}\left[\underline{\underline{\Sigma}}_S+\vec{\chi}\,\underline{\Sigma}_f^T\,\underline{\nu}\right]\sum_{m'=1}^{2N}\omega_{m'}\int_h dx\vec{\phi}_{cm'}(x)+\int_h dx\left[\vec{q}_1(x)+\vec{Q}_m(x)\right]$$

Angular Discretization

$$\mu\equiv\left\{\pm\mu_m;P_N\left(2\left|\mu_m\right|-1\right)=0,\ \ m=1,\ldots,N\right\}$$

Assume trapezoidal rule

$$\int_h dx\vec{\phi}_{cm}(x)=\vec{\bar{\bar{I}}}\left(h\right)+K_1h^3+K_2h^5+K_3h^7+\ldots$$

$$\vec{\bar{\bar{I}}}\left(h\right)\equiv\frac{h}{2}\left[\vec{\phi}_{cm,j+1}+\vec{\phi}_{cm,j}\right]$$

Reflectance and Transmittance

$$\vec{R}_f \equiv \int_0^1 d\mu\,\mu\vec{\phi}(0,-\mu) \cong \sum_{m=1}^{N} \omega_m |\mu_m| \vec{\phi}_{cm,1}$$

$$\vec{T}_n \equiv \int_0^1 d\mu\,\mu\vec{\phi}(a,\mu) \cong \sum_{m=N+1}^{2N} \omega_m \mu_m \vec{\phi}_{cm,n+1}$$

Solution via Inner Iterations (*k*)

$\mu \geq 0 \quad (m = N+1,\ldots,2N)$

$$\vec{\phi}^{(k)}_{cm,j+1} = \left[\underline{T}^{+}_{m}\right]^{-1} \underline{T}^{-}_{m} \vec{\phi}^{(k)}_{cm,j} +$$

$$+\frac{h}{4}\left[\underline{T}^{+}_{m}\right]^{-1}\left[\underline{\Sigma}_S + \vec{\chi}\underline{\Sigma}^T_f \underline{\nu}\right] \sum_{m'=1}^{2N} \omega_{m'} \left[\vec{\phi}^{(k-1)}_{cm',j+1} + \vec{\phi}^{(k-1)}_{cm',j}\right] + \left[\underline{T}^{+}_{m}\right]^{-1} \vec{U}_{js}$$

Convergence Acceleration

Romberg Acceleration: Form Tableau

$$\vec{\phi}_{cm,j} = \tilde{\vec{\phi}}_{cm,j} + \alpha_1 h^2 + \alpha_2 h^4 + \alpha_3 h^6 + ...$$

Wynn-Epsilon Acceleration

$$\varepsilon_{-1}^{(k)} = 0, \quad \varepsilon_0^{(k)} = q_k$$

$$\varepsilon_{s+1}^{(k)} = \varepsilon_s^{(k+1)} + \left[\varepsilon_s^{(k+1)} - \varepsilon_s^{(k)}\right]^{-1}$$

s=0	s=1	s=2	s=3	s=4	s=5
q1					
	e1				
q2		e1			
	e2		e1		
q3		e2		e1	
	e3		e2		e1
q4		e3		e2	
	e4		e3		
q5		e4			
	e5				
q6					

❍ Solution Strategy

+ Solution based on spatial and angular discretizations *n* and *N*

  - Never certain if converged or not

+ Consider solution as a sequence in *n* and *N*

+ Accelerate sequence through Romberg and Wynn-epsilon convergence accelerators

+ Also accelerate inner iterations

Example of Wε convergence acceleration

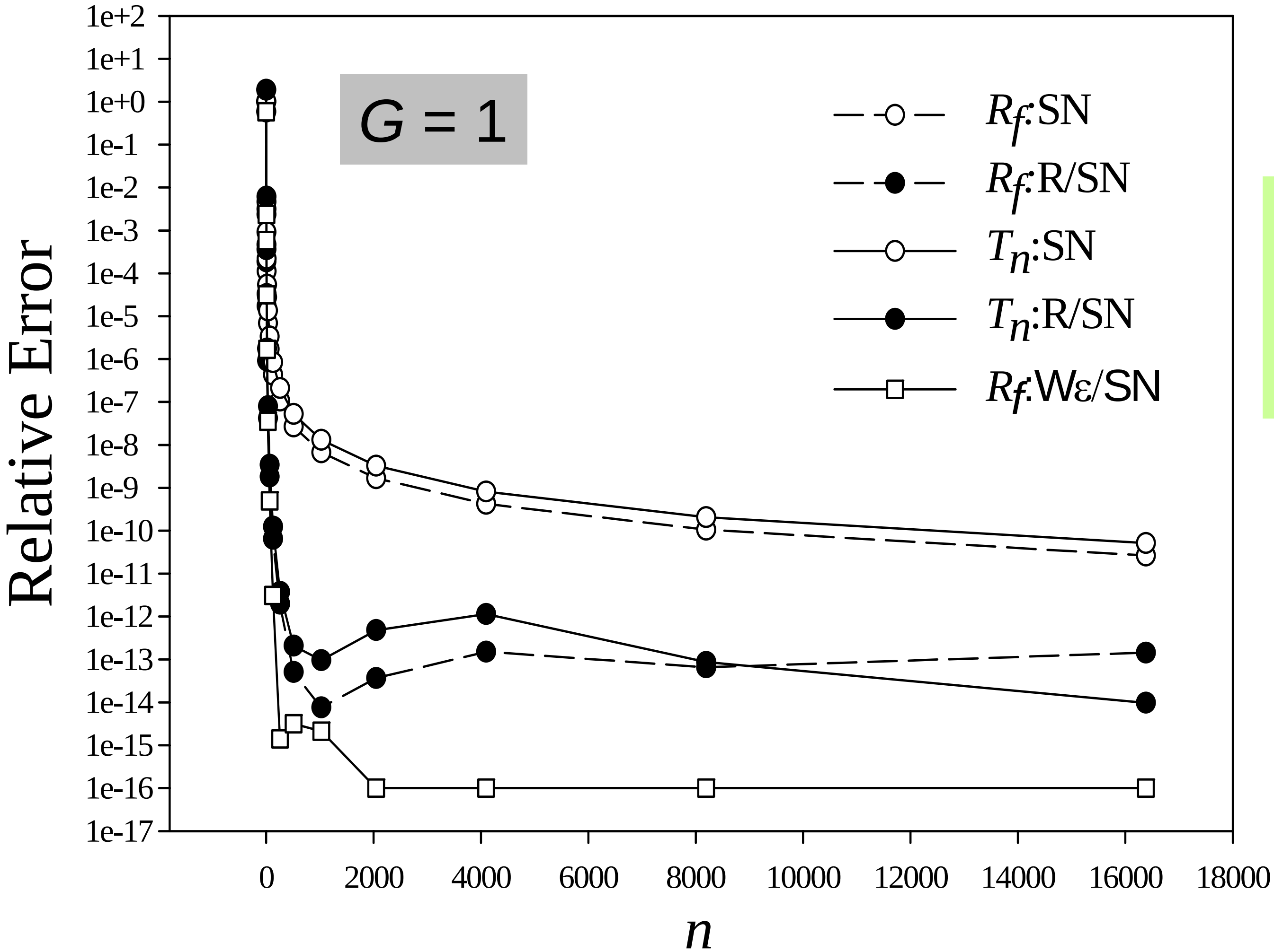
$$S_l(\mu_0) = \frac{1}{2}\sum_{k=0}^{l}(2k+1)g^k P_k(\mu_0)$$

g = 0.9999

l	***Partial Sum Original***	***Partial Sum Accelerated***	***Relative Error***
1	9.69700E-01	1.00000E+00	1.00000E+00
2	-1.52903E+00	9.69700E-01	3.12468E-02
3	-1.42302E+00	1.00037E+00	3.06605E-02
4	1.94718E+00	-1.42734E+00	1.70087E+00
5	1.73905E+00	-6.47730E-02	2.10360E+01
6	-2.31231E+00	-6.07241E-02	6.66772E-02
7	-1.98141E+00	-6.49686E-02	6.53320E-02
8	2.64626E+00	2.95109E-02	3.20152E+00
9	2.17509E+00	-1.15740E-03	2.64975E+01
----	-----	-----	-----
23	-2.78688E+00	6.96306E-05	1.18331E-04
24	4.85207E+00	6.96642E-05	4.83440E-04
25	2.80419E+00	6.96588E-05	7.74507E-05
26	-5.09681E+00	6.96591E-05	3.12922E-06
27	-2.80798E+00	6.96588E-05	4.22008E-06
28	5.33715E+00	6.96598E-05	1.43532E-05
39	-2.59184E+00	6.96596E-05	5.28799E-09
40	6.68810E+00	6.96596E-05	3.12727E-09
41	2.52072E+00	6.96596E-05	1.84265E-09
42	-6.89855E+00	6.96596E-05	1.75157E-09
43	-2.44029E+00	6.96596E-05	8.53647E-10
44	7.10509E+00	6.96596E-05	7.52985E-10

Acceleration of Spatial Discretization

Romberg $D_k^{l+1} = D_k^l + \left[\frac{D_k^l - D_{k-1}^l}{4^{k+1}-1}\right]$ Interrogate $\left[D_0^0, D_1^1, \ldots D_l^l\right]$



a = 1.853722cm
Pu^{239}
Σ = 0.248006986cm^{-1}
c = 0.95

$$n = 2^{l-1} N_e$$

Comparison of SN and CSN

SN

n	*Rf*	*Tn*
1	1.11861466956E+00	6.78957930002E-01
2	1.15327669420E+00	6.19839302224E-01
4	1.16316241561E+00	6.07910137691E-01
8	1.16569131974E+00	6.04814881906E-01
16	1.16632520874E+00	6.04030089243E-01
32	1.16648370128E+00	6.03833097036E-01
64	1.16652332129E+00	6.03783790439E-01
128	1.16653322568E+00	6.03771458922E-01
256	1.16653570185E+00	6.03768376052E-01
512	1.16653632089E+00	6.03767605335E-01
1024	1.166536**47565**E+00	6.03767**412656**E-01

N = 60

G = 1

CSN

N	*Rf*	*Tn*
20	1.16653649998E+00	6.03767342886E-01
22	1.16653651192E+00	6.03767343361E-01
24	1.16653652348E+00	6.03767342658E-01
26	1.16653652635E+00	6.03767318239E-01
28	1.16653652681E+00	6.03767345381E-01
30	1.16653652670E+00	6.03767347942E-01
32	1.16653652676E+00	6.03767348259E-01
34	1.16653652655E+00	6.03767348352E-01
36	1.16653652720E+00	6.03767348388E-01
38	1.16653652719E+00	6.03767348407E-01
40	1.16653652732E+00	6.03767348353E-01
42	1.16653652720E+00	6.03767348450E-01
44	1.16653652705E+00	6.03767348447E-01
46	1.16653652728E+00	6.03767348431E-01
48	1.16653652727E+00	6.03767348435E-01
50	1.16653652727E+00	6.03767348439E-01
52	1.16653652727E+00	6.03767348450E-01
54	1.16653652728E+00	6.03767348439E-01
56	1.16653652727E+00	6.03767348440E-01
58	1.16653652727E+00	6.03767348440E-01
60	1.16653652728E+00	6.03767348442E-01

MG/One-Group Comparison

$$\Sigma_g \equiv \Sigma \qquad \Sigma_{g,g'} \equiv \Sigma_{g,g',random} \qquad \sum_{g=1}^{G} \Sigma_{g,g'} = \Sigma_s \qquad \Sigma_{fg} \equiv \Sigma_f$$

$\Sigma, \Sigma_s, \Sigma_f$ Set to one group values

$$\phi(0,\mu) = \sum_{g=1}^{G} \phi_g(0,\mu) = 1 \qquad \mu > 0$$

$$a = 1 \qquad \Rightarrow \phi(x,\mu) = \sum_{g=1}^{G} \phi_g(x,\mu)$$

$$\mu_0 = 1$$

			One	Group
G	***R_fx10***	***T_nx10***	***R_f x10***	***T_nx10***
2	1.2832453401	3.4950923023	1.2832453400	3.4950923024
3	1.2832453401	3.4950923023		
4	1.2832453401	3.4950923023		

Comparison of scalar flux for MGCSN and BLUE

$G = 1$

x/Scalar Flux	MGCSN	BLUE	SN
0.0000E+00	1.32981011E+00	1.3298101**4**E+00	1.32981011E+00
4.5974E-02	1.23534502E+00	1.23534502E+00	1.2353450**1**E+00
9.1947E-02	1.16034430E+00	1.16034430E+00	1.1603442**9**E+00
1.3792E-01	1.09121992E+00	1.0912199**3**E+00	1.09121992E+00
1.8389E-01	1.02519657E+00	1.0251965**8**E+00	1.02519657E+00
2.2987E-01	9.60879383E-01	9.6087938**5**E-01	9.60879383E-01
2.7584E-01	8.97286872E-01	8.9728687**4**E-01	8.97286872E-01
3.2182E-01	8.33492083E-01	8.3349208**4**E-01	8.3349208**4**E-01
3.6779E-01	7.68298912E-01	7.6829891**4**E-01	7.6829891**4**E-01
4.1376E-01	6.99461727E-01	6.9946172**9**E-01	6.9946173**0**E-01
4.5974E-01	6.16214882E-01	6.162148**75**E-01	6.1621488**1**E-01

Random Scattering Matrix

$a = 5$

			One	Group
G	$R_f x10$	$T_n x10$	Time (s)	$T_n x10$
2	0.524728607	0.127491020	5	0.127491016
12	0.524728607	0.127491020	35	
24	0.524728607	0.127491020	103	
46	0.524728607	0.127491020	381	
64	0.524728607	0.127491020	447	
96	0.524728608	0.127491020	3369	

Siewert Benchmarks

NSE: 78,315 (1981)

617s

g	R_f	T_n
1	6.6351E-02	5.1058E-06
2	4.2002E-02	4.4781E-06
3	3.2483E-02	4.9308E-06
4	2.7501E-02	5.4649E-06
5	2.4382E-02	6.0283E-06
6	2.2221E-02	6.6050E-06
7	2.0624E-02	7.1879E-06
8	1.9388E-02	7.7730E-06
9	1.8399E-02	8.3577E-06
10	1.7586E-02	8.9399E-06
11	1.6904E-02	9.5178E-06
12	1.6321E-02	1.0090E-05
13	1.5816E-02	1.0655E-05
14	1.5373E-02	1.1212E-05
15	1.7893E-05	2.3445E-09
16	8.1585E-03	2.2968E-06

$\Sigma_{15} = 10^4 cm^{-1}$

$\Sigma_{s15} = 0 cm^{-1}$

29s

g	R_f	T_n
1	1.3060E-02	2.4188E-03
2	2.6476E-02	3.9163E-04
3	2.0013E-02	2.9446E-04
4	2.0420E-02	3.0057E-04
5	2.1216E-02	3.1339E-04
6	2.2650E-02	3.3596E-04
7	1.6399E-02	2.4287E-04
8	1.8059E-02	2.6601E-04
9	2.0613E-02	2.9930E-04
10	2.4717E-02	3.4873E-04
11	3.1745E-02	4.2569E-04
12	4.4141E-02	5.5031E-04
13	1.8729E-02	3.1938E-04
14	1.7023E-02	2.8604E-04
15	1.2201E-02	1.9924E-04
16	3.5378E-03	5.9937E-05
17	9.0059E-04	1.4905E-05
18	6.2046E-05	1.0301E-06
19	9.1048E-06	1.5020E-07

What has been accomplished?

+ A fully discretized discrete ordinates algorithm has been adapted to give benchmark accuracy through "solution mining"

+ Not limited to constant scattering cross sections any longer

What is the disadvantage to CSN?

+ Requires considerably more computational time than SN

  - Justified for benchmark accuracy however

C.E. Siewert Review

…. I can see no reason to publish an algorithm that requires hours of computer time to (almost) reproduce results that required less than a second of computer time.

Professor's Siewert negative reaction to the CSN method could possibly have also resulted of the following comment:

With the CSN method, one can do all benchmarks that Professor Siewert has previously done or will ever do.

What's next in transport benchmarks?

+ CSN application to RT with anisotropic scattering
  - Reproduce a majority of CES results
  - Derivation of error term for SN (SC,DD,LD)

+ 1D criticality
  - Critical system with a source

+ 1D cylindrical geometry benchmark for PBMR (INL)
  - To be presented at Reno ANS
  - CIT (converged integral transport)

+ CSN in 2D cylindrical geometry (INL)

+ CSN in 1D Spherical geometry (INL)

+ CSN with time dependence

+ GFM and 2T benchmarks for LANL (CCS4/D2)

What's next in diffusion benchmarks?

+ Investigation of MG criticality condition

+ 1D 47 group benchmark for GaTech
  - MATLAB version

+ 2D converged finite difference diffusion

+ New LT inversion for time dependent diffusion

Semi-analytical Benchmarks in Nuclear Engineering

+ Slowing Down
+ MG slowing down
+ 1-D/1-gp
+ 1-D/MG
+ 2-D searchlight

To be Published

Canopy RT:

+ Enhance UAV capability with LCM2 (ACR)

+ CORMOD (NASA)

+ Polarization signatures (AFRL)

+ Mars water (LPL,NASA)

+ Earth’s oceans (NASA)

For ORNL: A Verification Strategy

+ Apply standard benchmarks during code development
+ Develop application-specific benchmarks
+ Embed benchmarks into code
+ <u>Designed accountability</u>

There’s lots left to do.