AN ASSESSMENT OF ACCELERATTON TECHNIQUES IN SCATTERING SOURCE ITERATIONS

Bilge OZGENER
Istanbul Technical University, Energy Institute
TURKEY

15th International Conference on Emerging Nuclear Energy Systems

OUTLINE

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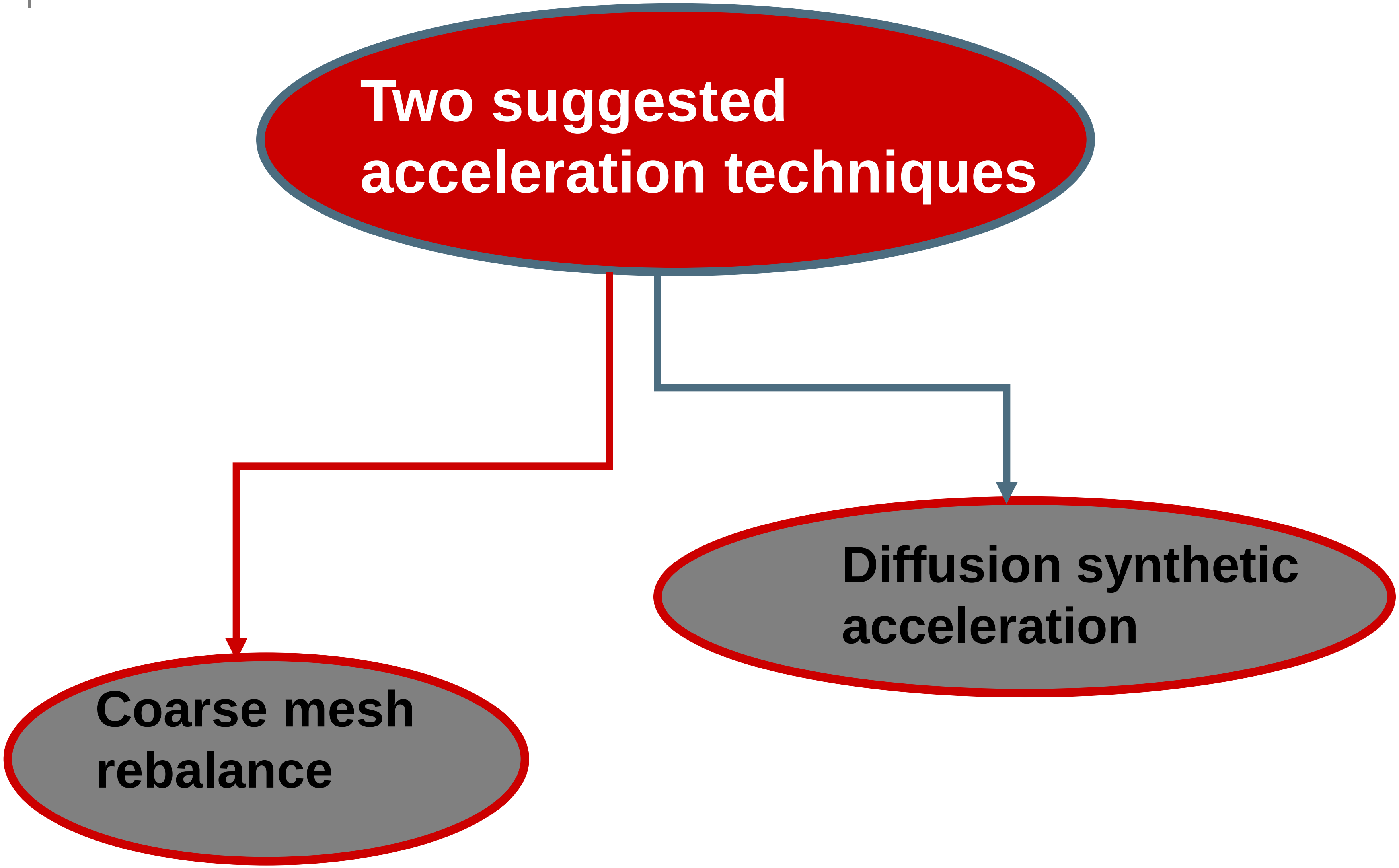
- Numerical Applications

INTRODUCTION

- In problems with optically thick and highly scattering regions, the convergence of scattering source iterations (SI) of the S_N method becomes very slow.
- Acceleration of the SI becomes necessary in such problems.



Two suggested acceleration techniques

Coarse mesh rebalance

Diffusion synthetic acceleration

Coarse Mesh Rebalance (CMR)

- System is divided into so-called coarse mesh regions (cmr).
- A cmr in general includes many fine mesh regions (fmr) used for the spatial discretization in the S_N method.
- Angular flux iterates are then forced to satisfy the neutron continuity equation integrated over each cmr.
- This results in the determination of rebalance factors which accelerate the base iteration.

Diffusion Synthetic Acceleration (DSA)

- After the transport sweep (base SI iteration) is competed, if a low order solution is obtained to make an additive correction, the technique is called SA.
- If the low order solution is diffusion theory, the method is called DSA.

- CMR is a nonlinear method; theorerical attempts to quantitatively predict the stability properties have been limited.
- In planar geometry applications, DSA is found to be rapidly convergent for sufficiently fine meshes.
- In coarser meshes divergence has been observed and certain remedies have been suggested.

- The application of DSA and CMR to curvilinear geometries has not been extensively studied in the literature.
- In this work,
  - DSA and CMR techniques have been implemented in a diamond-difference S_N code, SNSP, which has been developed for spherical geometry.
  - The examples studied are one-group external source problems.
  - The effects of c, the mesh size and the degree of anisotropy on convergence are studied.
  - The effect of the ratio of the # of fmr to cmr (p) on convergence is also studied for CMR.

THEORY

- <u>SCATTERING SOURCE ITERATION</u> (SI)

$$H_0\psi^{(m+1)} = H_1\psi^{(m)} + s$$ (unaccelarated algorithm)

$$H_0 = \vec{\Omega}\cdot\vec{\nabla} + \sigma$$ streaming and collision operator

$$H_1 = \int d\Omega' \sigma_s\left(\vec{\Omega}'\cdot\vec{\Omega}\right)$$ scattering operator

CMR

$$H_0\tilde{\psi}^{(m)} = H_1\psi^{(m)} + s \qquad \text{(base iteration)}$$

Multiplicative correction:

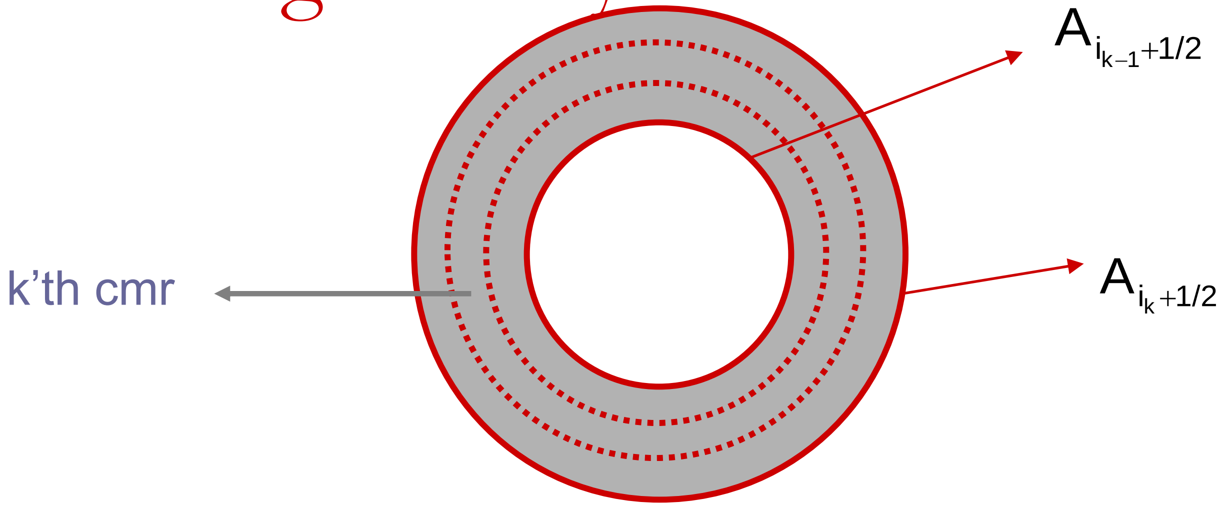
$$\psi^{(m+1)}\left(\vec{r},\vec{\Omega}\right) = f_k\ \tilde{\psi}^{(m)}\left(\vec{r},\vec{\Omega}\right), \qquad \vec{r} \in \tilde{V}_k\ ,\ k=1,\ldots,K$$

$\downarrow$

rebalance factors

K: Total number of cmr

Determination of rebalance factors in spherical geometry



Coarse mesh shell k containing fine mesh shells $i_{k-1}+1$ to i_k

Area of the inner spherical surface: $A_{i_{k-1}+1/2}$

Area of the outer spherical surface: $A_{i_k+1/2}$

Volume of the fine mesh shell i: V_i

- Requirement of neutron balance over the coarse mesh shell k:

$$A_{i_k+1/2}J_{i_k+1/2}^{(m+1)} - A_{i_{k-1}+1/2}J_{i_{k-1}+1/2}^{(m+1)} + \sum_{i=i_{k-1}+1}^{i_k}\sigma_{r,i}\varphi_i^{(m+1)}V_i = \sum_{i=i_{k-1}+1}^{i_k}S_iV_i$$

- Separating the currents into partial currents:

$$J_{i_k+1/2}^{(m+1)} = J_{+,i_k+1/2}^{(m+1)} - J_{-,i_k+1/2}^{(m+1)}$$

- to obtain:

$$- A_{i_{k-1}+1/2} J^{(m+1)}_{+,i_{k-1}+1/2} + \left(A_{i_{k-1}+1/2} J^{(m+1)}_{-,i_{k-1}+1/2} + A_{i_k+1/2} J^{(m+1)}_{+,i_k+1/2} + \sum_{i=i_{k-1}+1}^{i_k} \sigma_{r,i} \varphi_i^{(m+1)} V_i \right) - A_{i_k+1/2} J^{(m+1)}_{-,i_k+1/2} = \sum_{i=i_{k-1}+1}^{i_k} S_i V_i$$

- In terms of rebalance factors:

$$\varphi_i^{(m-1)} = f_k \tilde{\varphi}_i^{(m-1)} = f_k \frac{1}{2} \sum_{n=1}^{N} w_n \tilde{\psi}_{n,i}^{(m)} , \quad V_i \in \tilde{V}_K$$

$$J^{(m+1)}_{+,i_{k-1}+1/2} = f_{k-1} \tilde{J}^{(m)}_{+,i_{k-1}+1/2} = f_{k-1} \frac{1}{2} \sum_{n=N/2+1}^{N} \mu_n w_n \tilde{\psi}^{(m)}_{n,i_{k-1}+1/2}$$

$$J_{-,i_k+1/2}^{(m+1)} = f_{k+1}\tilde{J}_{-,i_k+1/2}^{(m)} = f_{k+1}\frac{1}{2}\sum_{n=1}^{N/2}\mu_n w_n \tilde{\psi}_{n,i_k+1/2}^{(m)}$$

$$J_{-,i_{k-1}+1/2}^{(m+1)} = f_k \tilde{J}_{-,i_{k-1}+1/2}^{(m)} = f_k \frac{1}{2}\sum_{n=1}^{N/2}\mu_n w_n \tilde{\psi}_{n,i_{k-1}+1/2}^{(m)}$$

$$J_{+,i_k+1/2}^{(m+1)} = f_k \tilde{J}_{+,i_k+1/2}^{(m)} = f_k \frac{1}{2}\sum_{n=N/2+1}^{N}\mu_n w_n \tilde{\psi}_{n,i_k+1/2}^{(m)}$$

- Substituting into partial currents balance equation, we obtain the tridiagonal, nonsymmetric linear system yielding the rebalance factors as solution:

$$a_{k,k-1}f_{k-1} + a_{k,k}f_k + a_{k,k+1}f_{k+1} = \tilde{S}_k$$

$$a_{k,k\text{-}1} = - \quad A_{i_{k-1}+1/2}\tilde{J}^{(m)}_{+,i_{k-1}+1/2}$$

$$a_{k,k+1} = \quad -A_{i_k+1/2}\tilde{J}^{(m)}_{-,i_k+1/2}$$

$$a_{k,k} = A_{i_{k-1}+1/2}\tilde{J}^{(m)}_{-,i_{k-1}+1/2} + A_{i_k+1/2}\tilde{J}^{(m)}_{+,i_k+1/2} + \sum_{i=i_{k\ 1}+1}^{i_k} \sigma_{r,i}\tilde{\varphi}_i^{(m+1)} V_i$$

$$\tilde{S}_k = \sum_{i=i_{k\ 1}+1}^{i_k} S_i V_i$$

DSA

$$H_0\psi^{(m+1)} = H_1\psi^{(m)} + s$$ (unaccelarated algorithm)

$$\psi^{(m+1)} = M_U\psi^{(m)} + H_0^{-1}s$$

$$M_U = H_0^{-1}H_1$$ (iteration operator of the unaccelerated algorithm)

- Low order solution (diffusion theory)

$$H_L \varphi_L = S$$

$$H_L = -\vec{\nabla} \cdot D \vec{\nabla} + \sigma_r$$

$$S = \int d\Omega \, s$$

$$D = \frac{1}{3\left(\sigma - \sigma_{s,1}\right)}$$

$$\sigma_r = \sigma - \sigma_s$$

- DSA algorithm based on additive correction:

$$\psi^{(m+1)} = \tilde{\psi}^{(m)} + H_L^{-1} H_1 \tilde{R}^{(m)} \qquad (1)$$

$$\tilde{R}^{(m)} = \tilde{\psi}^{(m)} - \psi^{(m)} \qquad (2)$$

$$\tilde{\psi}^{(m)} = M_U \psi^{(m)} + H_0^{-1} s \qquad (3)$$

- Using (2) and (3) in (1):

$$\psi^{(m+1)} = M_A \psi^{(m)} + \left(I + H_L^{-1} H_1 \right) H_0^{-1} s$$

- The iteration operator for the DSA algorithm:

$$M_A = M_U + H_L^{-1} H_1 \left(M_U - I \right)$$

- We note:

$$\begin{aligned} M_A &= M_U + H_L^{-1} \left(H\, H^{-1} \right) H_1 \left(M_U - I \right) \\ &= M_U + H_L^{-1} H \left(H_0 - H_1 \right)^{-1} H_1 \left(M_U - I \right) \\ &= M_U + H_L^{-1} H \left[H_0 \left(I - H_0^{-1} H_1 \right) \right]^{-1} H_1 \left(M_U - I \right) \\ &= M_U - H_L^{-1} H \left(I - M_U \right)^{-1} M_U \left(I - M_U \right) \end{aligned}$$

$$M_A = \left(I - H_L^{-1} H \right) M_U$$

- If the operators H_L and H are close in some sense then the spectral radius of M_A would be expected to be considerably smaller than the spectral radius of M_U.
- Thus, DSA would be expected to have a better convergence rate relative to the unaccelerated algorithm.
- Practical application of DSA:
    - premultiplying (1) by H_L,
    - integrating over all directions,
    - assuming scattering is isotropic,

$$H_L R^{(m+1)} = H_1 \tilde{R}^{(m)} \qquad (4)$$

- where

$$R^{(m+1)} = \varphi^{(m+1)} - \tilde{\varphi}^{(m)}$$

- (4) represents the solution of the equivalent of an external source problem in diffusion theory which must be solved numerically in each SI iteration.
- Once (4) is solved the fluxes are updated according to:

$$\varphi^{(m+1)} = \tilde{\varphi}^{(m)} + R^{(m+1)}$$

- We have used a cell-centered finite difference formulation for the numerical solution of (4).
- This yields a tridiagonal, symmetric linear system

$$b_{i,i-1} R_{i-1}^{(m+1)} + b_{i,i} R_i^{(m+1)} + b_{i,i+1} R_{i+1}^{(m+1)} = g_i$$

$$b_{i,i-1} = -\frac{A_{i-1/2} \tilde{D}_{i-1/2}}{\rho_i - \rho_{i-1}}$$

$$b_{i,i+1} = -\frac{A_{i+1/2}\tilde{D}_{i+1/2}}{\rho_{i+1} - \rho_i}$$

$$b_{i,i} = -b_{i,i-1} - b_{i,i+1} + V_i \sigma_{r,i}$$

$$g_i = V_i \sigma_{s,i} \tilde{R}_i^{(m)}$$

$$\tilde{D}_{i+1/2} = \frac{(\rho_{i+1} - \rho_i)\, D_i D_{i+1}}{(\rho_{i+1} - \rho_{i+1/2})\, D_i + (\rho_{i+1/2} - \rho_i)\, D_{i+1}}$$

NUMERICAL APPLICATONS

- Since the objective of the present study is the assesement of SI iterations, only one group external source problems are considered.
- In all problems the convergence criterion is 10^{-4} for the maximum absolute fractional difference in pointwise flux.
- The scattering is assumed to be isotropic unless otherwise stated.
- If an external source exists, it is isotropic and is equal to 1 $cm^{-3}s^{-1}$.

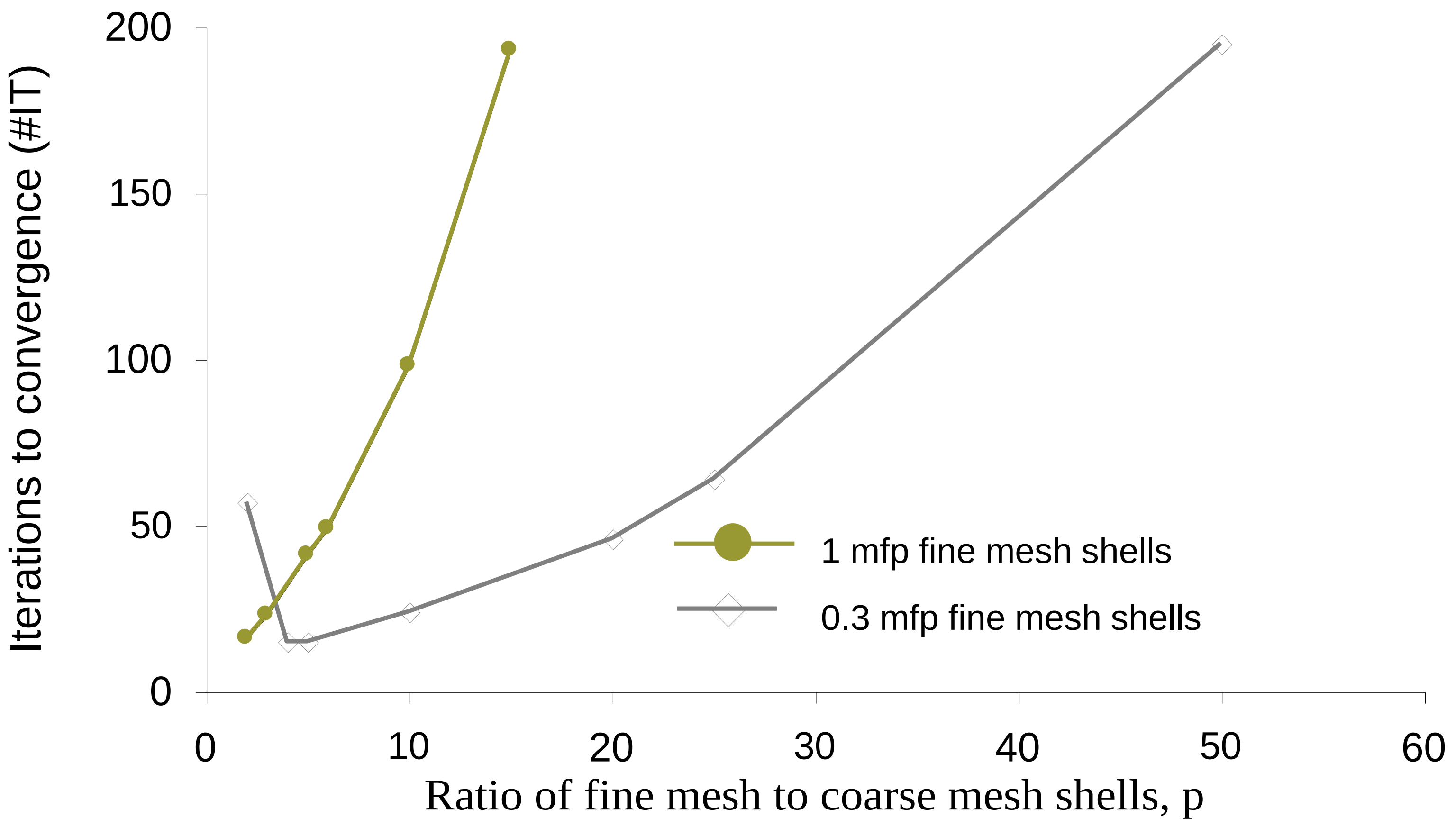
I. Purely Scattering Bare Sphere with Uniform Source

- Sphere of radius 30 cm.
- $\sigma=\sigma_s=1\ \text{cm}^{-1}$
- S_2 approximation

A. <u>Optimization of p in CMR</u>

- p= #of fine mesh shells(I)/#of coarse mesh shells(K)
- p=1 (fine mesh rebalance)
- p=I (system rebalance)
- Two different fine meshes:
  - Fine fine mesh: 100 fine mesh shells with Δ=0.3 mfp.
  - Coarse fine mesh: 30 fine mesh shells with Δ=1 mfp.

Iterations to convergence versus p

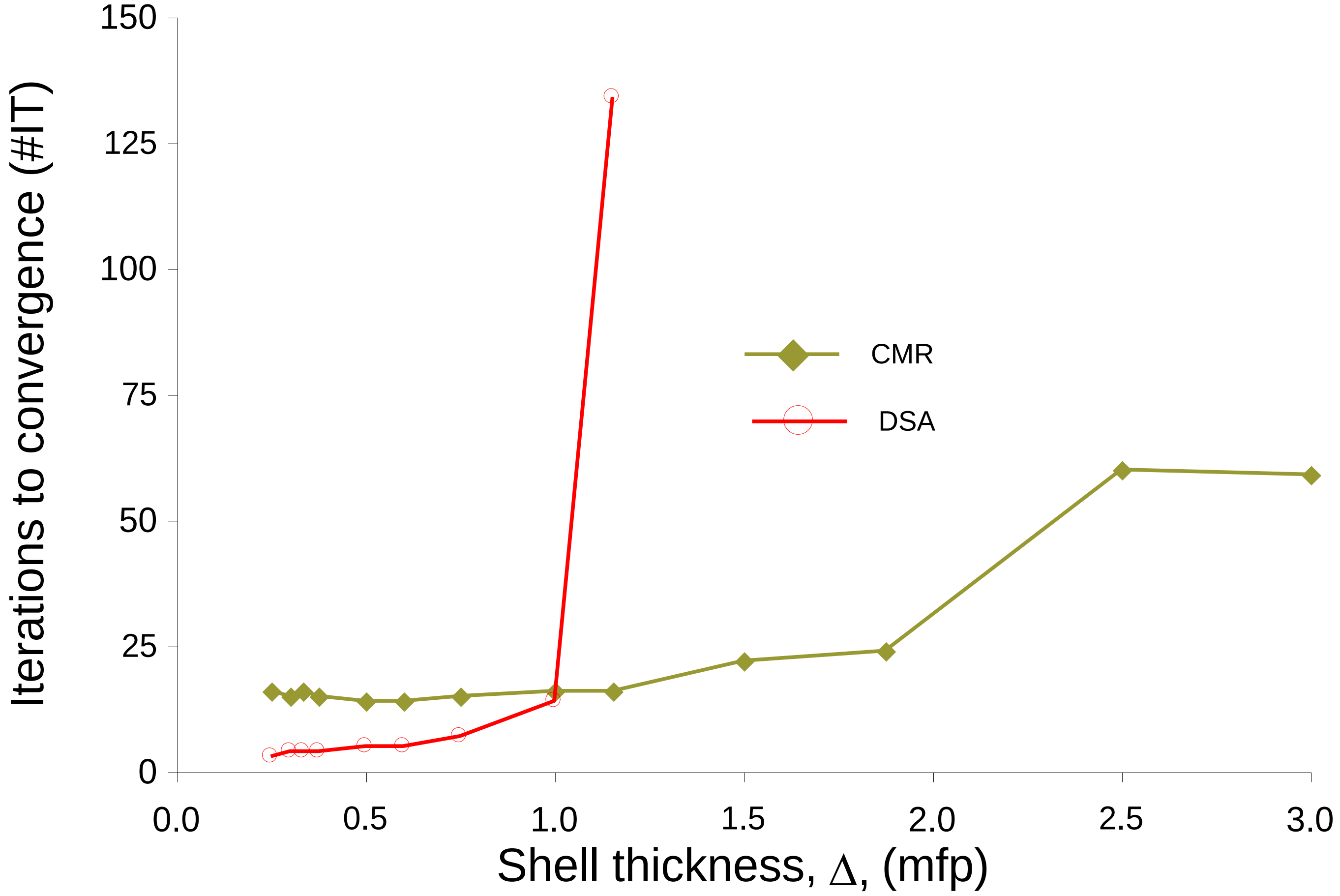


- For the coarse fine mesh, #IT decreases monotonically as the coarse mesh is refined from system rebalance to fine mesh rebalance. Minimum #IT is 16 which is obtained for p=2.
- For the fine fine mesh, as p is decreased starting from system rebalance, #IT decreases and reaches a minimum for p=4 and 5 where #IT=15 and then increases when p is further decreased.

B. Variation of iterations to convergence with fine mesh size

- In unaccelerated runs, #IT is independent of fine mesh size, Δ, and is equal to 1090.
- CMR runs are made with the p values yielding the minimum #IT.
- For Δ¤0.5, $p=2$; $\Delta<0.5$, $p=4$.
- DSA diverges for Δ¤1.5

Iterations to Convergence versus Δ



- For Δ<1 mfp DSA requires less iterations to convergence than CMR.
- In this Δ range #IT for CMR is approximately constant at 15.
- On the other hand, DSA requires 3 or 4 iterations to convergence when Δ<0.5
- For Δ barely exceeding 1, DSA requires more #IT than CMR.
- For larger values of Δ, DSA diverges.

C. The Effect of Linear Anistoropy on #IT

- We assume linear anisotropy in scattering of the form:

$$\sigma_s(\mu_0) = \sigma_s(1 + 3\bar{\mu}_0 \mu_0)$$

- where μ_0 is the cosine of the scattering angle and $\bar{\mu}_0$ is the average value of μ_0.
- We have used $\bar{\mu}_0$ values ranging from 0 (scattering from an infinitely massive nucleus) to 2/3 (scattering from H).

Effect of Anisotropy on Iterations

$\bar{\mu}_0$	#IT (Δ=1 mfp)			#IT (Δ=0.3 mfp)		
	UA	DSA	CMR (p=2)	UA	DSA	CMR (p=4)
0.	1090	14	16	1091	4	15
1/8	993	9	15	993	9	12
1/4	890	13	14	891	13	10
1/2	669	22	18	669	22	16
2/3	504	38	23	505	38	21

- If no acceleration is applied, #IT decreases as the scattering becomes more forward peaked, independent of the chosen mesh.
- If CMR is applied, as $\bar{\mu}_0$ is varied between 0 and 2/3, #IT first decreases passes through a minimum at $\bar{\mu}_0$ =1/4 and then starts to increase.
- If DSA is applied, a behavior similar to CMR is observed for the coarser one of the meshes.
- For the finer mesh #IT increases monotonically as scattering becomes more forward peaked.

II. Bare Sphere with Uniform Source

- Same as problem I with $\sigma=1$ cm^{-1}.
- $\Delta=1$ mfp.
- Absorption is introduced by choosing values of $c=\sigma_s/\sigma$ in the range $0<c<1$.
- For the unaccelerated case #IT increases dramatically for values of c close to unity.
- Acceleration becomes necessary for values of c exceeding approximately 0.7
- CMR runs are made for $p=2$.
- The acceleration provided by DSA and CMR are comparable.

The Effect of c on #IT

c	#IT		
	UA	DSA	CMR
0.1	3	2	3
0.4	9	4	4
0.7	22	7	6
0.9	65	10	9
0.94	103	12	10
0.98	250	13	13
0.99	395	14	14
1.0	1090	14	16

III. Two Concentric Spherical Regions Surrounded by Vacuum

- The inner and outer spherical regions have radii of 3.5 cm and 12 cm respectively.
- Both regions are made of the same material with cross sections:
- σ=1.796 cm^{-1} and σ_s=1.356 cm^{-1} (c=0.755).
- Inner region has uniform unit source while the outer region contains no source.
- Fine mesh involves 14 and 34 shells in the inner and outer regions respectively.

- $\Delta \cong$ 0.45 mfp.
- Runs are made in the S_{16} approximation.

	UA	CMR (p=2)	DSA
#IT	67	12	10

- Do to the relatively low value of c the acceleration provided is moderate.
- DSA and CMR shows comparable performance.

IV. Problem Three with Modified Radii and Cross Sections

i	$\sigma(cm^{-1})$	$\sigma_s(cm^{-1})$	Δ (mfp)	c	R (cm)
1	0.5	0.499	0.012	0.998	0.24
2	2	1.98	0.2	0.99	6.246

- The fine mesh consists of 10 and 60 shells for the inner and outer regions respectively.

	UA	CMR (p=5)	DSA
#IT	440	12	10

- Since c is near unity sizable acceleration is provided by both CMR and DSA.
- Despite considerable difference in the neutronic properties of the two regions, DSA performs as well as CMR.

V. Model Shielding Problem

- Four concentric spherical regions surrounded by vacuum R_1=12 cm, R_2=15 cm, R_3=21 cm and R_4=30 cm.
- The cross sections are chosen to model those of water in the first, second and fourth regions and those of iron in the third region.
- Scattering is linearly anisotropic.
- There is an uniform unit source only in the first (innermost) region.
- S_{16} approximation.

Cross Section Data

	σ (cm^{-1})	σ_s (cm^{-1})	$\sigma_{s,1}$ (cm^{-1})	c
Water	3.3333	3.3136	0.9256	0.994
Iron	1.3333	1.1077	0.0367	0.831

Number of Shells and Computed Average Fluxes

i	1	2	3	4
N_i	40	10	8	30
$\overline{\Phi}_i$ ($\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$)	34.50	8.127	0.2313	0.0001851

Number of Iterations to Convergence

	UA	CMR (p=2)	DSA
#IT	1213	16	36

- Since the values of c are high both acceleration methods perform well.
- CMR converges in less than half of the iterations of DSA ($\Delta \cong 1$mfp).
- Mesh refinement does not seem to change this situation appreciably.

Conclusion

- When the fine mesh is not too fine (Δ<<1 mfp) the #IT is at a minimum near fine mesh rebalance (p=2).
- For very fine fine meshes, #IT is at a minimum for p=4 or 5.
- When c=1, the SI algorithm results in excessively many iterations.
- Both CMR and DSA provide ample acceleration in this case.
- For Δ<1 mfp, DSA has better convergence rates than CMR.

- For Δ>1 mfp, DSA first becomes slower than CMR and then finally diverges.
- CMR provides adequate acceleration even for very large mesh sizes.
- In two and more region problems, both acceleration methods perform well compared to the unaccelerated case when c approaches unity.
- This is correct for both diffusive media and media in which transport effects are important.