

COARSE MESH REBALANCE  
ACCELERATION OF POWER  
ITERATION IN ADJOINT  
DIFFUSION CALCULATIONS

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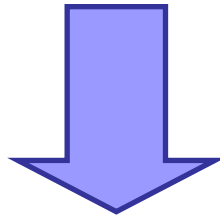
# I. INTRODUCTION

- Determination of the effective multiplication factor of nuclear systems by diffusion or transport theories





Solution of an eigenvalue-eigenvector problem for the largest eigenvalue by the power iteration method, well known in applied mathematics.


- When the dominance ratio (ratio of the magnitude of the second largest eigenvalue to the largest one) is close to unity



- The convergence rate of the power iteration method becomes slow and acceleration methods are required.

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- One of the prominent acceleration methods is the so called coarse mesh rebalance (CMR) method.
  - CMR is used in the acceleration of both inner and outer iterations of transport theory.
  - It is also used in the acceleration of outer iterations in neutron diffusion theory.
  - In multidimensional diffusion problems, it can also be used for the acceleration of the iterative methods of inner iterations.

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- CMR is based on the idea of the division of the problem domain into regions which are called coarse mesh regions.
  - Coarse mesh regions, in general, contain many fine mesh regions which are used for the spatial discretization of the problem domain.
  - In transport ( $S_N$ ), CMR is based on the principle of the requirement that the angular fluxes satisfy the neutron continuity equation over each coarse mesh region.
  - In diffusion theory, CMR is based on a variational principle involving fluxes in each coarse mesh region as trial vectors.

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- In this study, we investigate the performance of CMR in the acceleration of power iteration in multigroup adjoint diffusion calculations.
  - Direct calculations are also carried out for comparison with the adjoint case.
  - The geometry is chosen as spherical geometry and a cell centered finite difference approximation with zero outgoing adjoint current vacuum boundary condition is employed.

## II. THEORY

### II A. Discretization of the Within-Group Adjoint Diffusion Equation

$$-\frac{1}{\rho^2} \frac{d}{d\rho} \left[ \rho^2 D_g \frac{d\varphi_g^{+(p+1)}}{d\rho} \right] + \sum_{r,g} \varphi_g^{+(p+1)} = \mathbf{s}_g^{+(p+1)}(\rho) \quad (1)$$

$$\mathbf{s}_g^{+(p+1)} = \sum_{g'=g+1}^G \sum_s^{g' \leftarrow g} \varphi_{g'}^{+(p+1)} + \frac{v \sum_{f,g}}{\mathbf{k}^{(v)}} \sum_{g'=1}^G \chi_{g'} \varphi_{g'}^{+(p)} \quad (2)$$

- Omitting both the group index,  $g$  and the iteration number,  $p$ :

$$-\frac{1}{\rho^2} \frac{d}{d\rho} \left[ \rho^2 D(\rho) \frac{d\varphi^+}{d\rho} \right] + \Sigma_r(\rho) \varphi^+(\rho) = s^+(\rho) \quad (3)$$

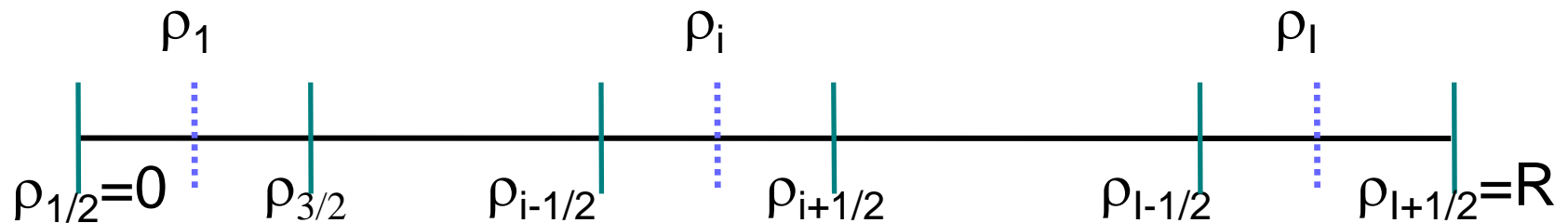
- subjected to either the zero outgoing adjoint current vacuum boundart condition

$$\frac{\varphi^+(R)}{4} + \frac{D(R)}{2} \frac{d\varphi^+}{d\rho} \Big|_{\rho=R} = 0 \quad (4)$$

- or the reflective boundary condition:

$$\left. \frac{d\phi^+}{d\rho} \right|_{\rho=R} = 0 \quad (5)$$

- For the discretization of (3), we introduce a finite difference mesh



- Each mesh interval is assumed to be homogeneous:
- $D(\rho) = D_i$  ,  $\Sigma_r(\rho) = \Sigma_{r,i}$  and  $s^+(\rho) = s_i^+$   
 $\rho_{i-1/2} < \rho < \rho_{i+1/2}$ .
- Integration of (3) over the  $i$ 'th spherical shell yields:

$$-A_{i+1/2} \left( D \frac{d\phi^+}{d\rho} \right) \Big|_{\rho=\rho_{i+1/2}} + A_{i-1/2} \left( D \frac{d\phi^+}{d\rho} \right) \Big|_{\rho=\rho_{i-1/2}} + \Sigma_{r,i} V_i \phi_i^+ = V_i s_i^+ \quad (6)$$

- Due to continuity of adjoint current

$$\left( D(\rho) \frac{d\varphi^+}{d\rho} \right) \Big|_{\rho=\rho_{i+1/2}^-} = D_i \frac{d\varphi^+}{d\rho} \Big|_{\rho=\rho_{i+1/2}^-} = D_{i+1} \frac{d\varphi^+}{d\rho} \Big|_{\rho_{i+1/2}^+} \quad (7)$$

- Using the backward

$$\frac{d\varphi^+}{d\rho} \Big|_{\rho_{i+1/2}^-} \cong \frac{\varphi_{i+1/2}^+ - \varphi_i^+}{\rho_{i+1/2} - \rho_i} \quad (8)$$

- and the forward

$$\frac{d\varphi^+}{d\rho} \Big|_{\rho_{i+1/2}^+} \cong \frac{\varphi_{i+1}^+ - \varphi_{i+1/2}^+}{\rho_{i+1} - \rho_{i+1/2}} \quad (9)$$

- finite difference approximations in (7):

$$D_i \frac{\varphi_{i+1/2}^+ - \varphi_i^+}{\rho_{i+1/2} - \rho_i} = D_{i+1} \frac{\varphi_{i+1}^+ - \varphi_{i+1/2}^+}{\rho_{i+1} - \rho_{i+1/2}} \quad (10)$$

- Solving for  $\varphi_{i+1/2}^+$  :

$$\varphi_{i+1/2}^+ = \frac{(\rho_{i+1} - \rho_{i+1/2})D_i \varphi_i^+ + (\rho_{i+1/2} - \rho_i)D_{i+1} \varphi_{i+1}^+}{(\rho_{i+1} - \rho_{i+1/2})D_i + (\rho_{i+1/2} - \rho_i)D_{i+1}} \quad (11)$$

- Using (11) first in (8) and substituting the result in (7):

$$\left( D(\rho) \frac{d\varphi^+}{d\rho} \right) \Big|_{\rho=\rho_{i+1/2}} = \frac{\tilde{D}_{i+1/2}}{\rho_{i+1} - \rho_i} (\varphi_{i+1}^+ - \varphi_i^+) \quad (12)$$

■ where

$$\tilde{D}_{i+1/2} = \frac{(\rho_{i+1} - \rho_i) D_i D_{i+1}}{(\rho_{i+1} - \rho_{i+1/2}) D_i + (\rho_{i+1/2} - \rho_i) D_{i+1}} \quad (13)$$

■ When we substitute (12) into (6), we obtain the tridiagonal linear system:

$$a_{i,j-1} \varphi_{i-1}^+ + a_{i,j} \varphi_i^+ + a_{i,j+1} \varphi_{i+1}^+ = S_i^+ \quad (14)$$

■ where

$$a_{i,j-1} = -\frac{A_{i-1/2} \tilde{D}_{i-1/2}}{\rho_i - \rho_{i-1}} \quad (15)$$

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

$$a_{i,j} = V_i \Sigma_{r,i} - a_{i,j-1} - a_{i,j+1} \quad (16)$$

$$S_i^+ = V_i s_i^+$$

■  $a_{1,0} = a_{l,l+1} = 0$

- We note from (6), (14), (15) and (16),

$$a_{l,l-1}\varphi_{l-1}^+ + (\sum_{r,l} V_l - a_{l,l-1})\varphi_l^+ = S_l^+ + A_{l+1/2} D_l \frac{d\varphi^+}{d\rho} \Big|_{\rho=\rho_{l+1/2}} \quad (17)$$

- From the vacuum boundary condition (4):

$$D_l \frac{d\varphi^+}{d\rho} \Big|_{\rho=\rho_{l+1/2}} = -\frac{\varphi_{l+1/2}}{2} \quad (18)$$

- Using (18) in (17):

$$a_{l,l-1}\varphi_{l-1}^+ + (\sum_{r,l} V_l - a_{l,l-1})\varphi_l^+ = S_l^+ - \frac{A_{l+1/2}}{2} \varphi_{l+1/2}^+ \quad (19)$$

- Using the backward finite difference approximation (8) in the vacuum boundary expression (4) and solving for  $\varphi_{l+1/2}^+$  :

$$\varphi_{l+1/2}^+ = \frac{2D_l}{2D_l + (\rho_{l+1/2} - \rho_l)} \varphi_l^+ \quad (20)$$

- Substituting (20) into (19)

$$a_{l,l-1} \varphi_{l-1}^+ + a_{l,l} \varphi_l^+ = S_l^+ \quad (21)$$

- where

$$a_{l,l} = \sum_{r,l} V_l - a_{l,l-1} + \frac{A_{l+1/2} D_l}{2D_l + (\rho_{l+1/2} - \rho_l)}$$

## II B. Coarse Mesh Rebalance Acceleration

- Discretized direct criticality eigenvalue problem:
- G: Number of energy groups
- I: Number of fine mesh points

$$\mathbf{M} \boldsymbol{\varphi} = \frac{1}{k_{\text{eff}}} \mathbf{F} \boldsymbol{\varphi} \quad (22)$$

- $\boldsymbol{\varphi}$ : (GxI) dimensional vector of pointwise group fluxes.
- $\mathbf{M}$ : (GxI) dimensional square matrix representing leakage, interaction and scattering couplings.
- $\mathbf{F}$ : (GxI) dimensional square matrix representing fission couplings.

- Discretized adjoint criticality eigenvalue problem

$$\mathbf{M}^T \boldsymbol{\varphi}^+ = \frac{1}{k_{\text{eff}}} \mathbf{F}^T \boldsymbol{\varphi}^+ \quad (23)$$

- $\boldsymbol{\varphi}^+$ : (GxI) dimensional vector of pointwise group adjoint fluxes.

- Variational Principle

- The stationary point of the bilinear functional

$$F[\mathbf{x}^+, \mathbf{x}] = \mathbf{x}^{+T} \mathbf{M} \mathbf{x} - \frac{1}{k_{\text{eff}}} \mathbf{x}^{+T} \mathbf{F} \mathbf{x} \quad (24)$$


- satisfies the direct, (22) and adjoint, (23) problems.

- Thus, finding the stationary point of the bilinear functional is equivalent to solving the direct and adjoint eigenvalue problems.
- Hence this variational principle could be used to design a method for the acceleration of the power iteration.
- Assume at the end of an iteration we have obtained an estimate for the adjoint flux vector  $\tilde{\Phi}^+$ .
- We want to obtain  $\tilde{\Phi}_{\text{cor}}^+$ , a corrected estimate for the adjoint flux vector which is presumably a better estimate  $\Phi^+$  using the above variational principle.

- For this purpose, the system is divided into N coarse mesh regions each containing  $I_n$  fine mesh points.
- We order the adjoint flux vector estimate coming from power iteration by partitioning it into subvectors of dimension  $(G \times I_n)$  each of which contains the group pointwise adjoint fluxes belonging to coarse mesh region n:

$$\tilde{\boldsymbol{\Phi}}^{+T} = \left[ \tilde{\boldsymbol{\Phi}}_1^{+T} \quad \dots \quad \tilde{\boldsymbol{\Phi}}_n^{+T} \quad \dots \quad \tilde{\boldsymbol{\Phi}}_N^{+T} \right] \quad (25)$$

- Consistently with this ordering, the matrix  $\mathbf{M}$  consists of  $(I_n \times G)$  by  $(I_{n'} \times G)$  dimensional rectangular submatrices,  $\mathbf{M}_{n,n'}$  containing the couplings between the fine mesh points in the  $n^{\text{th}}$  coarse mesh region to those in the  $n'^{\text{th}}$  coarse mesh region
- In a similar way  $\mathbf{F}$  consists of the submatrices  $\mathbf{F}_{n,n'}$ .
- We consider a subspace of the  $(I \times G)$  dimensional vector space with basis vectors  $\hat{\boldsymbol{\psi}}_n$ ,  $n=1, \dots, N$


$$\hat{\boldsymbol{\phi}}_n^{+\text{T}} = \left[ \mathbf{0} \quad \dots \quad \mathbf{0} \quad \tilde{\boldsymbol{\phi}}_n^{+\text{T}} \quad \mathbf{0} \quad \dots \quad \mathbf{0} \right] \quad (26)$$

- Any vector  $\mathbf{x}^+$  or  $\mathbf{x}$  in the subspace could be expressed in terms of these basis vectors as:

$$\mathbf{x}^+ = \sum_{n=1}^N a_n^+ \hat{\boldsymbol{\phi}}_n^+ \quad (27)$$

$$\mathbf{x} = \sum_{n=1}^N a_n \hat{\boldsymbol{\phi}}_n^+ \quad (28)$$

- Now we seek the stationary point of the functional (24) in this vector subspace.

- Substituting (27) and (28) into (24):

$$F[\mathbf{a}_1^+ \dots \mathbf{a}_N^+ \mathbf{a}_1 \dots \mathbf{a}_N] = \sum_{n=1}^N \sum_{n'=1}^N \mathbf{a}_n^+ \mathbf{g}_{n,n'} \mathbf{a}_{n'} - \frac{1}{k} \sum_{n=1}^N \sum_{n'=1}^N \mathbf{a}_n^+ \mathbf{d}_{n,n'} \mathbf{a}_{n'} \quad (29)$$

- where

$$\mathbf{g}_{n,n'} = \hat{\boldsymbol{\phi}}_n^{+\text{T}} \mathbf{M}_{n,n'} \hat{\boldsymbol{\phi}}_{n'}^+ \quad (30)$$

- and

$$\mathbf{d}_{n,n'} = \hat{\boldsymbol{\phi}}_n^{+\text{T}} \mathbf{F}_{n,n'} \hat{\boldsymbol{\phi}}_{n'}^+ \quad (31)$$

- Defining the N dimensional vectors

$$\mathbf{a}^{+\text{T}} = [\mathbf{a}_1^+ \quad \dots \quad \mathbf{a}_n^+ \quad \dots \quad \mathbf{a}_N^+] \quad (32)$$

- and

$$\mathbf{a}^T = [\mathbf{a}_1 \quad \cdots \quad \mathbf{a}_n \quad \cdots \quad \mathbf{a}_N] \quad (33)$$

- we can write the reduced functional as:

$$F[\mathbf{a}^+, \mathbf{a}] = \mathbf{a}^{+\top} \mathbf{G} \mathbf{a} - \frac{1}{k} \mathbf{a}^{+\top} \mathbf{D} \mathbf{a} \quad (34)$$

- The stationary point of the functional, (34) gives:


$$\mathbf{G} \mathbf{a} = \frac{1}{k} \mathbf{D} \mathbf{a} \quad (35)$$

- and

$$\mathbf{G}^T \mathbf{a}^+ = \frac{1}{k} \mathbf{D}^T \mathbf{a}^+ \quad (36)$$

- In adjoint calculations, we solve the eigenvalue-eigenvector problem, (36).
- $k$  becomes the new  $k_{\text{eff}}$  estimate of the accelerated power iteration.
- The corrected adjoint flux estimate is then:

$$\tilde{\boldsymbol{\Phi}}_{\text{cor}}^+ = \sum_{n=1}^N \mathbf{a}_n^+ \hat{\boldsymbol{\Phi}}_n^+ \quad (37)$$

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- In spherical geometry applications coarse mesh regions are spherical shells which have only their inner and outer shells as neighbors.
  - Since there is coupling only between the neighboring coarse mesh shells, the matrix  $\mathbf{G}$  assumes a tridiagonal but unsymmetric form.
  - With the cell-centered finite difference discretization,  $\mathbf{D}$  is a diagonal matrix.
  - The eigenvalue-eigenvector problem of (36) is in general solved by the power method.

- If we denote the iteration number in the solution of (36) by  $r$ , the convergence criterion we have used is:


$$\left| \max_n \left( \frac{a_n^{+(r)}}{a_n^{+(r-1)}} \right) \right| - \left| \min_n \left( \frac{a_n^{+(r)}}{a_n^{+(r-1)}} \right) \right| < \varepsilon \quad (38)$$

# III. NUMERICAL APPLICATIONS

- DIFSP: Multigroup diffusion theory program for direct and adjoint calculations developed in FORTRAN run under LINUX operating system.
- The outer iterations are optionally accelerated by the CMR technique.
- The convergence criterion:


$$\left| \frac{k^{(p+1)} - k^{(p)}}{k^{(p+1)}} \right| < \varepsilon = 10^{-6}$$

- The fluxes/adjoint fluxes are normalized by assigning a value of unity to the first group flux at the center of the sphere.
- Problem 1:
- Variation of the effectiveness of CMR with the theoretical dominance ratio ( $\sigma$ ):
- Bare sphere with one group data  $D=9.21$  cm,  $\Sigma_a=0.152149$  cm<sup>-1</sup>,  $\nu\Sigma_f=0.155952$  cm<sup>-1</sup>.
- Fine mesh with radial thickness of 0.2 cm.
- The theoretical dominance ratio is increased by increasing the radius of the sphere.

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- #UA and #CM represent the number of iterations to convergence for the unaccelerated and CMR cases respectively.
  - $p = \frac{\text{\# of fine mesh shells}}{\text{\# of coarse mesh shells}} = 2$  for this problem.
  - % iter: represents the savings in the number of outer iterations due to the use of CMR relative to the UA case.

## Variation of CMR performance with dominance ratio

R(cm)	50	100	150	300	500
$\sigma$	0.635	0.885	0.941	0.983	0.993
$k_{\text{eff}}$	0.9151	0.9844	1.004	1.019	1.023
#UA	26	64	108	244	359
#CM	7	8	8	14	25
% iter	73	88	93	94	93

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- CMR becomes more effective as the  $\sigma$  is increased.
  - The savings in the number of iterations to convergence passes 90% as the dominance ratio rises above 0.94
  - **Problem 2:**
  - Reflected reactor with one-group cross sections.
  - The geometry and the cross sections are given below.

Region	R (cm)	D (cm)	$\Sigma_a$ (cm <sup>-1</sup> )	$\nu\Sigma_f$ (cm <sup>-1</sup> )
Core	45	0.65	0.16	0.185
Reflector	125	0.84	0.00032	0.

- Analytical solution:
- $k_{\text{eff}}=1.145321$
- $\sigma=0.961182$
- $\bar{\Phi}_C = \bar{\Phi}_C^+ = 0.598395$
- $\bar{\Phi}_R = \bar{\Phi}_R^+ = 0.0648071$

- Numerical solution:
- 200 shell fine mesh with each region containing 100.

	#IT	$k_{\text{eff}}$	%error in $k_{\text{eff}}$
UA	115	1.145294	0.0024
CMR (p=5)	15	1.145320	0.00009

- With CMR:
- 87% savings in the number of iterations.
- ~60% savings in cpu time.

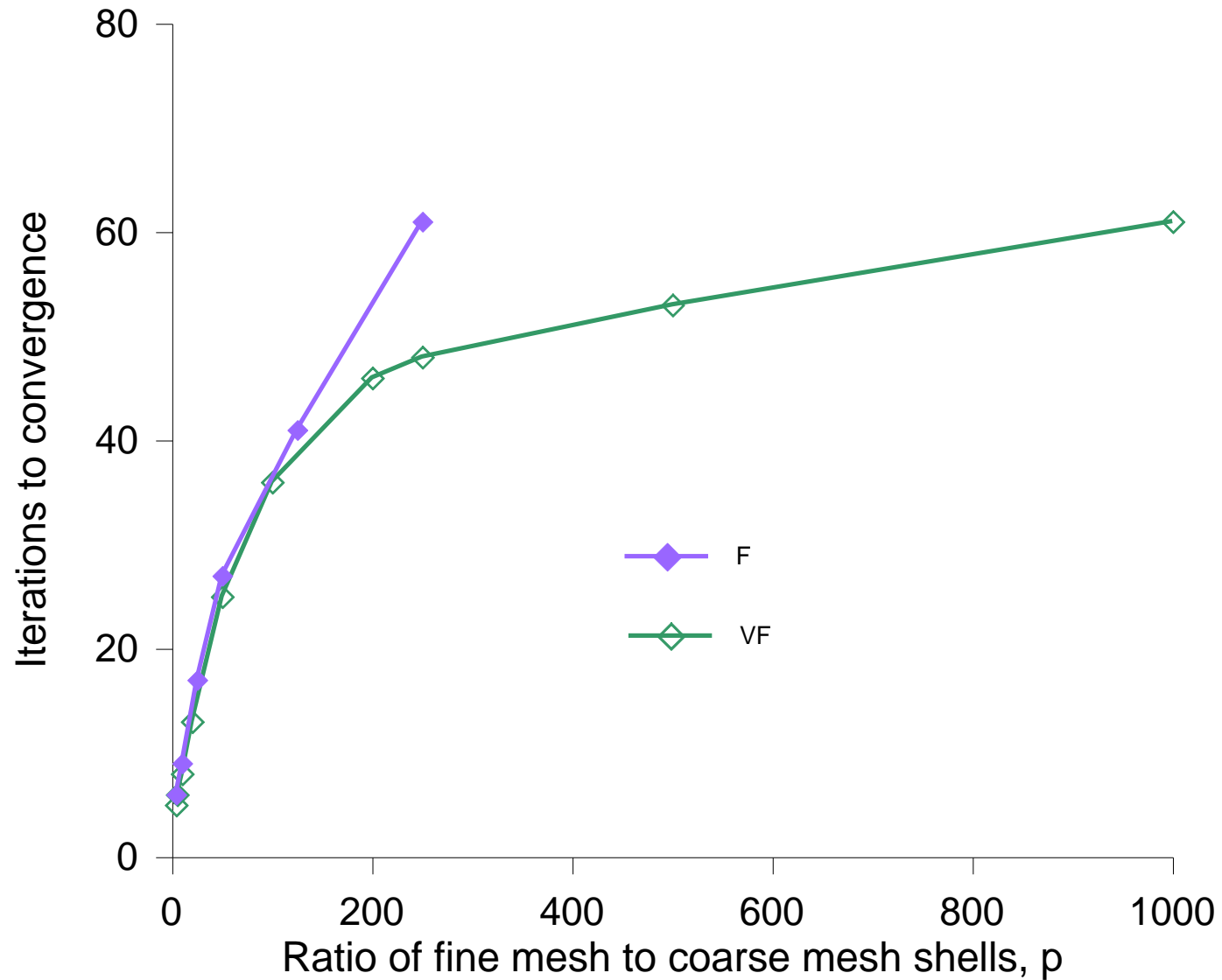
### ■ Problem 3:

- Bare reactor with two group cross sections:
- Sphere of radius 125 cm.

g	$D_g$ (cm)	$\Sigma_{r,g}$ (cm <sup>-1</sup> )	$\nu\Sigma_{f,g}$ (cm <sup>-1</sup> )	$\Sigma_{s,g\leftarrow g-1}$	$\chi_g$
1	1.267	0.0362	0.0085	-	1.
2	0.354	0.155	0.1851	0.0241	0.

- Dominance ratio= $\sigma=0.93819$
- Two meshes used for numerical solution:
  - VF (very fine mesh): 1000 shells of  $\Delta=1/8$  cm.
  - F (fine mesh): 250 shells of  $\Delta=1/2$  cm.

# Number of iterations versus $p$ for the adjoint problem



## Performance of CMR Relative to UA


	Adjoint				Direct			
	F		VF		F		VF	
	UA	CM (p=10)	UA	CM (p=4)	UA	CM (p=5)	UA	CM (p=2)
#IT	110	9 (92%)	110	5 (95%)	110	15 (86%)	110	8 (93%)
t	8	1 (88%)	35	10 (71%)	10	3 (70%)	32	17 (47%)

## Results of Two Group Adjoint Calculations

	$k_{\text{eff}}$ (% error)	$\bar{\varphi}_1^+$ (% error)	$\bar{\varphi}_2^+$ (% error)
Analytical	1.007302	0.32138	0.38088
UA (F)	1.007288 (0.00139)	0.32178 (0.124)	0.38056 (0.0840)
CM (F)	1.007303 (0.0001)	0.32222 (0.261)	0.38110 (0.0578)
UA (VF)	1.007288 (0.00139)	0.32177 (0.121)	0.38055 (0.0866)
CM (VF)	1.007302 (0.0)	0.32167 (0.0902)	0.38044 (0.116)

## Results of Two Group Direct Calculations

	$k_{\text{eff}}$ (% error)	$\bar{\Phi}_1$ % error	$\bar{\Phi}_2$ (% error)
Analytical	1.007302	0.32138	0.049833
UA (F)	1.007287 (0.00149)	0.32178 (0.124)	0.049910 (0.00155)
CM (F)	1.007302 (0.0)	0.32375 (0.737)	0.050215 (0.767)
UA (VF)	1.007288 (0.00139)	0.32177 (0.121)	0.049910 (0.00155)
CM (VF)	1.007302 (0.0)	0.32224 (0.268)	0.049980 (0.295)

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- The CMR provide ample acceleration in both direct and adjoint calculations.
  - Nevertheless both the number of iterations and the relative cpu times are somewhat smaller in the adjoint calculations compared to the direct ones when CMR acceleration is applied.

## Problem 4

- Spherical geometry mockup of a BWR:
  - Core is modeled as an inner spherical region with a radius of 100 cm.
  - The reflector has a radial thickness of 20 cm.
  - Fine mesh:
    - 300 shells in the core
    - 150 shells in the reflector
- 450 shells total

## Three Group BWR Problem Cross Sections


g	1	2	3
$D_g^C$ (cm)	1.39217	0.70056	0.25016
$\Sigma_{r,g}^C$ (cm <sup>-1</sup> )	0.04832	0.10352	0.075056
$\Sigma_{s,g \leftarrow g-1}^C$ (cm <sup>-1</sup> )	-	0.04832	0.08225
$\nu \Sigma_{f,g}^C$ (cm <sup>-1</sup> )	0.	0.009671	0.095338
$\chi_g$	1.	0.	0.
$D_g^R$ (cm)	1.40513	0.59328	0.16321
$\Sigma_{r,g}^R$ (cm <sup>-1</sup> )	0.081038	0.14612	0.018938
$\Sigma_{s,g \leftarrow g-1}^R$ (cm <sup>-1</sup> )	-	0.081038	0.13661

	UA	CMR (p=3)
$k_{\text{eff}}$ (adjoint)	1.066899	1.066911
$k_{\text{eff}}$ (direct)	1.066808	1.066909
#IT (adjoint)	82	7 (91%)
#IT (direct)	82	12 (85%)
t (adjoint)	2.3	1.0 (55%)
t (direct)	2.4	1.2 (45%)
$\bar{\Phi}_{1,C}^+, \bar{\Phi}_{1,C}$	0.3654, 0.3649	0.3675, 0.3661
$\bar{\Phi}_{2,C}^+, \bar{\Phi}_{2,C}$	0.3740, 0.1695	0.3762, 0.1700
$\bar{\Phi}_{3,C}^+, \bar{\Phi}_{3,C}$	0.4334, 0.1874	0.4360, 0.1880
$\bar{\Phi}_{1,R}^+, \bar{\Phi}_{1,R}$	0.01767, 0.01082	0.01788, 0.01088
$\bar{\Phi}_{2,R}^+, \bar{\Phi}_{2,R}$	0.01098, 0.006815	0.01113, 0.006852
$\bar{\Phi}_{3,R}^+, \bar{\Phi}_{3,R}$	0.009346, 0.03925	0.009469, 0.03947



# CONCLUSIONS

- CMR provides sufficient acceleration in the power iteration of the adjoint and direct diffusion calculations.
- The effectiveness of the CMR acceleration increases as the dominance ratio approaches unity.
- The efficiency of the CMR acceleration depends on  $p$ .
- Although the value of  $p$  is problem dependent, a value of  $p \leq 5$  seems near optimal in the cases considered.

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- In the problems with high dominance ratio ( $>0.9$ ) CMR acceleration is capable of reducing the number of iterations to convergence by  $\sim 90\%$ .
  - In terms of execution time, the savings is somewhat smaller, usually in the range 50-60%.
  - CMR results in somewhat smaller iteration numbers and cpu times in adjoint calculations compared to the direct ones.