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Acceleration of the Method of Characteristics in the CRX Lattice Calculation Code for Anisotropic Scattering Problems

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Abstract

The method of characteristics used in the CRX lattice calculation code is accelerated with the coarse mesh rebalance (CMR) method for inner iteration and the coarse mesh/coarse group rebalance (CGR) method for outer iteration involved with the eigenvalue search. The CRX code with these two acceleration methods was applied to two multigroup eigenvalue problems with isotropic scattering and one multigroup eigenvalue problem with anisotropic scattering to show the effectiveness of the acceleration methods. The numerical results show that the acceleration is effective in reducing the number of iterations and the computing time in both isotropic and anisotropic scattering cases.

I. INTRODUCTION

The method of characteristics (MOC)([3],[4],[5],[6],[7],[8]) which combines desirable features of the integral transport and S_N methods have been considered as an effective methodology in the lattice calculation. This method gives accurate solutions in complex geometries, strong absorber problems, strong anisotropic problems and so on, while its calculation preserves the simplicity of the S_N method. It divides directions like in S_N and for each direction performs transport calculation like the collision probability method by integrating the differential form of the within-group transport equation along its parallel characteristic lines. For better accuracy, it needs many rays and fine angle divisions. Like most of the transport methods, MOC also requires long computing times for scattering dominant problems and problems with significant upscattering. Therefore to reduce computing time, it needs to be accelerated. Although there are many acceleration techniques([11],[12],[13],[14]) in the discrete ordinates transport calculation, these methods cannot be applied directly to or used effectively in the method of characteristics.

In this paper, the coarse mesh rebalance (CMR) method which uses the fact that converged solution must satisfy the neutron balance equation and can be easily implemented for various methods in general geometry was used for accelerating the inner iteration involved with the scattering source iteration. For eigenvalue problems, there are several ways to apply the coarse mesh rebalance method (e.g., whole-system group-wise, coarse mesh all-group-collapsed, and coarse mesh group-wise rebalance methods[1]). In this paper, a coarse mesh/coarse group

rebalance method including the coarse mesh group-wise rebalance as a particular case was used to accelerate the outer iteration. With this coarse mesh/coarse group rebalance method, the rebalance equation leads to an equation that resembles a multigroup finite-differenced eigenvalue problem. Therefore, this equation can be solved with two iteration schemes (i.e., inner and outer iterations).

The numerical tests of the acceleration method for multigroup eigenvalue problems including anisotropic scattering problems show that the coarse mesh group-wise rebalance method is best in terms of the reduction of the number of iterations and the computing time.

II. THEORY AND METHODOLOGY

II.1 The Methodology of the CRX Code

To describe the method of characteristics, the starting equation is the within-group transport equation in discrete ordinate form :

$$\left[\hat{\Omega}_n \cdot \vec{\nabla} + \sigma_g(\vec{r})\right] \psi_g(\vec{r}, \hat{\Omega}_n) = \sum_{g'=1}^{G} \sum_{l=0}^{L} \sum_{m=-l}^{l} Y_{ml}(\hat{\Omega}_n) \sigma_{slgg'}(\vec{r}) \phi_{lg'}^m(\vec{r}) + \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} (\nu\sigma_f)_{g'} \phi_{g'} = q_n, \tag{1}$$

where w_n is weight for direction $\hat{\Omega}_n$ (θ_n : polar angle, ϕ_n : azimuthal angle), L is the order of anisotropy of scattering (up to L=3 in the current version of CRX) and the moment ϕ_{lg}^m is given by

$$\phi_{lg}^m(\vec{r}) = \sum_{n=1}^{N} w_n Y_{ml}^*(\hat{\Omega}_n) \psi_g(\vec{r}, \hat{\Omega}_n), \tag{2}$$

where N is the number of directions. Eq.(1) can be rewritten in the following differential form :

$$\sin\theta_n \frac{d\psi_{g,n}}{dp} + \sigma_g \psi_{g,n} = q_{g,n}, \tag{3}$$

where p is the projected coordinate on $x-y$ plane of the coordinate along the neutron trajectory for direction $\hat{\Omega}_n$. The equation for the outgoing flux along a ray in computational mesh (i,j) with the flat source approximation is obtained by analytically integrating Eq.(3) :

$$\psi_{g,n,l}^{out} = \psi_{g,n,l}^{in} e^{-\sigma_g L_{n,l}/\sin\theta_n} + \frac{q_{g,n}}{\sigma_g}(1 - e^{-\sigma_g L_{n,l}/\sin\theta_n}), \tag{4}$$

where $L_{n,l}$ is track length of the l'th ray for direction $\hat{\Omega}_n$ in mesh (i,j). The average flux along the ray included in mesh (i,j) for direction $\hat{\Omega}_n$ is obtained by integrating Eq.(3). The equation is given as follows :

$$\bar{\psi}_{g,n,l} = \frac{q_{g,n}}{\sigma_g} + \sin\theta_n \frac{(\psi_{g,n,l}^{in} - \psi_{g,n,l}^{out})}{\sigma_g L_{n,l}}. \tag{5}$$

However, to perform the scattering source iteration, the average angular flux over the computational mesh is required for generation of the source. The equation for the average flux over the computational mesh is obtained by summing the average fluxes (Eq.(5)) over the rays passing through the mesh. The equation is given as follows :

$$\bar{\psi}_{g,n} = \frac{q_{g,n}}{\sigma_g} + \frac{\sin\theta_n}{A\sigma_g} \sum_{l \in \text{mesh}(i,j)} \delta_n \left(\psi^{in}_{g,n,l} - \psi^{out}_{g,n,l} \right), \tag{6}$$

where δ_n represents spacing between adjacent rays for direction $\hat{\Omega}_n$, and A is the area of mesh (i,j). The mesh indices i,j were omitted in the above equations. In the method of characteristics, Eqs.(4) and (6) with a general tracking module are complete for transport calculation.

II.2 Coarse Mesh/Coarse Group Rebalance Method

The balance equation obtained by integrating Eq.(1) is given by

$$\vec{\nabla} \cdot \vec{J}_g(\vec{r}) + \sigma_{rg}(\vec{r})\phi_g(\vec{r}) = S_g(\vec{r}), \tag{7}$$

where $\sigma_{rg} = \sigma_g - \sigma_{s0gg}$, $\vec{J}_g$ is the current vector and $S_g(\vec{r})$ is the integration of the sum of the scattering source from other energy groups, fission source and anisotropic scattering source. The odd order terms of the anisotropic scattering source in $S_g(\vec{r})$ vanish by integration over all directions but the even order terms remain depending on the chosen angular sets. In the second order anisotropy, the following two terms remain :

$$S_{g,anisotropic} = \sum_{g'=1}^{G} \frac{5}{4}\sigma_{s2gg'} \sum_{n=1}^{N} w_n \left\{ (3\mu_n^2 - 1)\phi_{g',a} + (\mu_n^2 + 2\eta_n^2 - 1)\phi_{g',b} \right\}, \tag{8}$$

$$\begin{aligned} \phi_{g',a} &= \sum_{n'=1}^{N} w_{n'}(3\mu_{n'}^2 - 1)\psi_{g',n'}, \\ \phi_{g',b} &= \sum_{n'=1}^{N} w_{n'}(\mu_{n'}^2 + 2\eta_{n'}^2 - 1)\psi_{g',n'}, \end{aligned}$$

where μ_n and η_n are the direction cosines of $\hat{\Omega}_n$ with respect to x and y coordinates, respectively. If using S_N quadrature sets, integration of the even order terms of the anisotropic scattering source over all directions will become zero. But CRX does not use S_N quadrature sets. Thus the above anisotropic scattering source term must be considered. Then by integrating this equation over coarse mesh $\tilde{V}_m$ (in this paper, a cell is taken as the coarse mesh) and applying divergence theorem, we can rewrite this equation as follows :

$$\sum_{m'} \int_{\Gamma_{mm'}} d\Gamma \hat{n} \cdot \vec{J}_g + \int_{\tilde{V}_m} dV \sigma_{rg}\phi_g = \int_{\tilde{V}_m} dV S_g, \tag{9}$$

where $\Gamma_{mm'}$ is the surface between $\tilde{V}_m$ and $\tilde{V}_{m'}$,and $\hat{n}$ represents unit normal vector of $\Gamma_{mm'}$. Coarse mesh rebalance method requires that the new iterate $\psi_g^{t+1}(\vec{r}, \hat{\Omega}_n)$ must satisfy this

balance equation for each cell, and this is accomplished by multiplying the unaccelerated iterate $\tilde{\psi}_g^t$ by a factor $f_{m,g}$ for each coarse mesh $\tilde{V}_m$:

$$\begin{aligned}
\psi_g^{t+1}(\vec{r},\hat{\Omega}_n) &= f_{m,g}\tilde{\psi}_g^t(\vec{r},\hat{\Omega}_n), && \vec{r}\in\tilde{V}_m,\\
\psi_g^{t+1}(\vec{r},\hat{\Omega}_n) &= f_{m,g}\tilde{\psi}_g^t(\vec{r},\hat{\Omega}_n), && \vec{r}\in\Gamma_{mm'},\quad \hat{n}\cdot\hat{\Omega}_n>0,\\
\psi_g^{t+1}(\vec{r},\hat{\Omega}_n) &= f_{m',g}\tilde{\psi}_g^t(\vec{r},\hat{\Omega}_n), && \vec{r}\in\Gamma_{mm'},\quad \hat{n}\cdot\hat{\Omega}_n<0.
\end{aligned} \tag{10}$$

We can rewrite Eq.(9) using Eq.(10) as follows :

$$\begin{aligned}
\left[\int_{\tilde{V}_m} dV\sigma_{rg}\tilde{\phi}_g^t + \sum_{m'}\int_{\Gamma_{mm'}} d\Gamma\tilde{J}_{g+}^t - \text{S.A}\right] f_{m,g} - \sum_{m'}\int_{\Gamma_{mm'}} d\Gamma\tilde{J}_{g-}^t f_{m',g}\\
= \int_{\tilde{V}_m} dV\left[\frac{\chi_g}{k_{eff}}\text{F.S} + \text{I.S} + \text{A.S}\right],
\end{aligned} \tag{11}$$

$$\tilde{\phi}_g^t = \sum_n w_n\tilde{\psi}_g^t(\vec{r},\hat{\Omega}_n), \tag{12}$$

$$\tilde{J}_{g+}^t = \sum_{\hat{\Omega}_n\cdot\hat{n}>0} w_n\hat{\Omega}_n\cdot\hat{n}\tilde{\psi}_g^t(\vec{r},\hat{\Omega}_n), \tag{13}$$

$$\tilde{J}_{g-}^t = \sum_{\hat{\Omega}_n\cdot\hat{n}<0} w_n|\hat{\Omega}_n\cdot\hat{n}|\tilde{\psi}_g^t(\vec{r},\hat{\Omega}_n), \tag{14}$$

$$\begin{aligned}
\text{F.S} &= \sum_{g'=1}^{G}(\nu\sigma_f)_{g'}\tilde{\phi}_{g'}^t,\\
\text{I.S} &= \sum_{g'=1,g'\neq g}^{G}\sigma_{s0gg'}\tilde{\phi}_{g'}^t,\\
\text{S.A} &= \sum_{\substack{l=2\\ l=\text{even}}}^{L}\sum_{m=-l}^{l}\left\{\sum_{n=1}^{N}w_nY_{ml}(\hat{\Omega}_n)\right\}\sigma_{slgg}\tilde{\phi}_{lg}^{m,t},\\
\text{A.S} &= \sum_{g'=1,g'\neq g}^{G}\sum_{\substack{l=2\\ l=\text{even}}}^{L}\sum_{m=-l}^{l}\left\{\sum_{n=1}^{N}w_nY_{ml}(\hat{\Omega}_n)\right\}\sigma_{slgg'}\tilde{\phi}_{lg'}^{m,t},
\end{aligned}$$

where F.S represents fission source, I.S represents isotropic scattering source from other energy groups, S.A represents self group anisotropic scattering source and A.S represents anisotropic scattering source from other energy groups.

In the CRX code, the integrals over the top or bottom cell of Eq.(13) is calculated as follows :

$$\int_{\Gamma_{mm'}} d\Gamma\tilde{J}_{g+}^t = \sum_{l\in\Gamma_{mm'}}\sum_{\hat{\Omega}_n\cdot\hat{n}>0} w_n(\sin\theta_n\sin\phi_n)\tilde{\psi}_g^t(\delta_n/\sin\phi_n), \tag{15}$$

and over the left or right cell is calculated as follows :

$$\int_{\Gamma_{mm'}} d\Gamma \tilde{J}^t_{g+} = \sum_{l\in\Gamma_{mm'}} \sum_{\hat{\Omega}_n\cdot\hat{n}>0} w_n(\sin\theta_n\cos\phi_n)\tilde{\psi}^t_g(\delta_n/\cos\phi_n). \tag{16}$$

To close the rebalance equation (Eq.(11)), the current continuity relations are used to obtain incoming current.

For an eigenvalue problem, Eq.(11) can be expressed as follows :

$$\begin{aligned}
&\left[\int_{\tilde{V}_m} dV\sigma_{rg}\tilde{\phi}^k_g + \sum_{m'}\int_{\Gamma_{mm'}} d\Gamma\tilde{J}^k_{g+} - \mathrm{S.A_o}\right] f_{m,g} - \sum_{m'}\int_{\Gamma_{mm'}} d\Gamma\tilde{J}^k_{g-} f_{m',g} \\
&\qquad = \int_{\tilde{V}_m} dV\left[\frac{\chi_g}{k_{eff}}\mathrm{F.S_o} + \mathrm{I.S_o} + \mathrm{A.S_o}\right], \\
\mathrm{F.S_o} &= \sum_{g'=1}^{G}(\nu\sigma_f)_{g'}\tilde{\phi}^k_{g'} f_{m,g'}, \\
\mathrm{I.S_o} &= \sum_{g'=1,g'\neq g}^{G}\sigma_{s0gg'}\tilde{\phi}^k_{g'} f_{m,g'}, \\
\mathrm{S.A_o} &= \sum_{\substack{l=2\\ l=\text{even}}}^{L}\sum_{m=-l}^{l}\left\{\sum_{n=1}^{N} w_n Y_{ml}(\hat{\Omega}_n)\right\}\sigma_{slgg}\tilde{\phi}^{m,k}_{lg}, \\
\mathrm{A.S_o} &= \sum_{g'=1,g'\neq g}^{G}\sum_{\substack{l=2\\ l=\text{even}}}^{L}\sum_{m=-l}^{l}\left\{\sum_{n=1}^{N} w_n Y_{ml}(\hat{\Omega}_n)\right\}\sigma_{slgg'}\tilde{\phi}^{m,k}_{lg'} f_{m,g'},
\end{aligned} \tag{17}$$

where k is outer iteration index,

Summing Eq.(17) over a coarse energy group (g_c) with the assumption that the rebalance factor is common in the coarse energy group g_c gives the following equation :

$$\begin{aligned}
&\sum_{g\in g_c}\left[\int_{\tilde{V}_m} dV\left\{\sigma_g\tilde{\phi}^k_g - \sum_{g'\in g_c}\sigma_{s0gg'}\tilde{\phi}^k_{g'}\right\} + \sum_{m'}\int_{\Gamma_{mm'}} d\Gamma\tilde{J}^k_{g+} - \mathrm{S.A_c}\right] f_{m,g_c} \\
&- \sum_{g\in g_c}\sum_{m'}\int_{\Gamma_{mm'}} d\Gamma\tilde{J}^k_{g-} f_{m',g_c} = \sum_{g\in g_c}\left[\frac{\chi_g}{k_{eff}}\int_{\tilde{V}_m} dV(\mathrm{F.S}_c) + \int_{\tilde{V}_m} dV\,(\mathrm{I.S}_c + \mathrm{A.S}_c)\right],
\end{aligned} \tag{18}$$

$$\begin{aligned}
\mathrm{F.S}_c &= \sum_{g'_c=1}^{G_c}\sum_{g'\in g'_c}(\nu\sigma_f)_{g'}\tilde{\phi}^k_{g'} f_{m,g'_c}, \\
\mathrm{I.S}_c &= \sum_{g'_c=1,g'_c\neq g_c}^{G_c}\sum_{g'\in g'_c}\sigma_{sgg'}\tilde{\phi}^k_{g'} f_{m,g'_c}, \\
\mathrm{S.A}_c &= \sum_{g'\in g_c}\sum_{\substack{l=2\\ l=\text{even}}}^{L}\sum_{m=-l}^{l}\left\{\sum_{n=1}^{N} w_n Y_{ml}(\hat{\Omega}_n)\right\}\sigma_{slgg'}\tilde{\phi}^{m,k}_{lg'}, \\
\mathrm{A.S}_c &= \sum_{g'_c=1,g'_c\neq g_c}^{G_c}\sum_{g'\in g'_c}\sum_{\substack{l=2\\ l=\text{even}}}^{L}\sum_{m=-l}^{l}\left\{\sum_{n=1}^{N} w_n Y_{ml}(\hat{\Omega}_n)\right\}\sigma_{slgg'}\tilde{\phi}^{m,k}_{lg'} f_{m,g'_c},
\end{aligned}$$

where G_c is the number of coarse energy groups and $f_{m,g} = f_{m,g_c}$ for $g \in g_c$. This equation looks like the finite differenced equation of the multigroup diffusion equation involved with the eigenvlaue. Therefore, this equation is solved iteratively.

II.3 Calculational Procedure

Prior to the start of the iteration, the CRX code calculates ray track lengths in each mesh by a general geometric tracking routine. Next, initial fission source, multiplication factor and incoming boundary fluxes are assumed to start the first outer iteration. The transport sweep is then performed to calculate the mesh averaged angular fluxes and the coarse mesh rebalance method is used for accelerating the scattering source iteration for each energy group. At this point, it must be noted that the coupling among the thermal groups by upscattering is stronger than the coupling via the fission source. Therefore, a distinction should be made in the eigenvalue iterations on the fission source and upscattering iterations[10]. Hence, before starting a new eigenvalue iteration, additional upscattering iterations are performed on the thermal groups. Next, after the upscattering iteration, the coarse group rebalance is performed to improve the fission source and the eigenvalue. In inner iterations, too strong a criterion may require many inner iterations in early phase of the outer iteration. So in this paper, the inner iteration criterion decreases gradually at every outer iteration step from a loose criterion (first 10^{-2} and then equal to the maximum flux error of the first energy group in the previous outer iteration step) to a strong criterion (10^{-6}). This procedure is shown in Figure 1.

III. NUMERICAL RESULTS

We solved several problems to test the CMR/CGR acceleration efficiency in CRX. In the following tables, speedup represents the ratio of the computing time without acceleration to the computing time with acceleration. The notation CRX(a, b, c) represents that the test was performed under a angular divisions in azimuthal direction, b angular divisions in polar direction and c rays in each direction over the problem domain.

To show the effectiveness of CMR for isotropic scattering, we chose NEACRP2 (Figure 2) and BWR 4x4 (Figure 3). We accelerated the outer iteration of these problems by applying CMR/CGR (all-group-collapsed), coarse group, and group-wise methods. In coarse group rebalance method, we grouped mutigroups into two coarse groups. The notation CGR$[1, g]$ in Tables 1 and 2 represents that the groups from group 1 to group $g-1$ were grouped into the first coarse group and the groups from group g to group G were grouped into the second coarse energy group.

For these problems, convergence criterion of 10^{-6} for eigenvalue and fission source were used. The results for NEACRP2 are given in Table 1. The results show that the number of iterations and the computing time are reduced as the number of coarse energy groups (i.e., g_c) increases. Therefore , the group-wise rebalance method is best in comparison with others. The reason is due to the fact that for problems with significant upscattering the group-wise rebalance method gives the most detailed description of the energy dependence of the rebalance factor and the computing time for solving the rebalance equation is relatively short compared to the total computing time.

The results for a BWR 4x4 problem is given in Table 2. In this problem, the results show that the computing time with the group-wise rebalance method is reduced to 1/6 of that of

Table 1: Results of NEACRP2 (6 groups), CRX(8,4,250)

	# of outer iterations	Computing time* (sec)	Speedup
No acceleration	68	745.38	1.0
CMR/CGR (all-group-collapsed)	10	285.92	2.61
CMR/CGR[1,3]	9	268.01	2.78
CMR/CGR (group-wise)	7	198.22	3.76

* on Intel Celeron 300A CPU

Table 2: Results of BWR 4x4 (7 groups), CRX(8,3,600)

	# of outer iterations	Computing time (sec)	Speedup
No acceleration	112	3140.26	1.0
CMR/CGR (all-group-collapsed)	13	802.16	3.91
CMR/CGR[1,3]	11	597.56	5.26
CMR/CGR (group-wise)	10	516.93	6.07

no acceleration and that the number of iterations and computing time are reduced as the number of coarse energy groups increases. The coarse mesh group-wise rebalance method also shows the best results in this test problem.

To test efficiency in problems with anisotropic scattering, the 7x7 BWR fuel assembly problem in Ref. 15 (Figure 4) was selected and modified. The isotropic components of the cross section data are described in Table A1 of Ref. 15. We removed water gaps and assemlby walls in the original problem and added anisotropic scattering cross sections whose values are a tenth of the isotropic scattering cross sections.

Table 3: Results of BWR 7x7 (2 groups) with mesh division I, CRX(4,4,400)

order of anisotropy		# of outer iterations	Computing time (s)	Speedup
0	No acceleration	147	234.97	1.00
	CMR/CGR (all-group-collapsed)	12	44.56	5.27
	CMR/CGR (group-wise)	14	47.46	4.95
1	No acceleration	147	245.13	1.00
	CMR/CGR (all-group-collapsed)	13	44.93	5.46
	CMR/CGR (group-wise)	11	43.43	5.64
2	No acceleration	147	266.09	1.00
	CMR/CGR (all-group-collapsed)	13	49.44	5.38
	CMR/CGR (group-wise)	11	47.88	5.56
3	No acceleration	147	302.86	1.00
	CMR/CGR (all-group-collapsed)	11	54.17	5.59
	CMR/CGR (group-wise)	11	54.16	5.59

The results are shown in Tables 3 and 4. This problem does not have upscattering. Thus the significant difference in effieciency between accelerations of all-group-collapsed CGR and of

Table 4: Results of BWR 7x7 (2 groups) with mesh division II, CRX(4,4,400)

order of anisotropy		# of outer iterations	Computing time (s)	Speedup
0	No acceleration	147	402.64	1.00
	CMR/CGR (all-group-collapsed)	12	76.88	5.24
	CMR/CGR (group-wise)	15	81.70	4.93
1	No acceleration	147	420.94	1.00
	CMR/CGR (all-group-collapsed)	11	76.47	5.50
	CMR/CGR (group-wise)	11	75.22	5.60
2	No acceleration	147	457.97	1.00
	CMR/CGR (all-group-collapsed)	11	81.69	5.61
	CMR/CGR (group-wise)	11	81.67	5.61
3	No acceleration	147	522.07	1.00
	CMR/CGR (all-group-collapsed)	13	97.35	5.36
	CMR/CGR (group-wise)	11	92.68	5.63

group-wise CGR does not appear. The speedup is about $5 \sim 6$. Note that the speedup in anisotropic scattering problems is slightly better than that of isotropic scattering problems.

IV. CONCLUDING REMARKS

The coarse mesh rebalance method for inner iteration and the coarse mesh/coarse group rebalance method for outer iteration were implemented in the CRX code of the method of characteristics and applied to two multigroup eigenvalue problems without anisotropic scattering and one multigroup eigenvalue problem with anisotropic scattering. The results show that the group-wise coarse mesh rebalance method is the most effective in problems having upscattering. This is due to the fact that for problems with significant upscattering as in the test problems the group-wise coarse mesh rebalance method provides the most detailed description of the energy dependence of the rebalance factor and the computing time for solving the rebalance equation is relatively short compared to the total computing time. The speedup achieved by the acceleration is typically about $3 \sim 6$.

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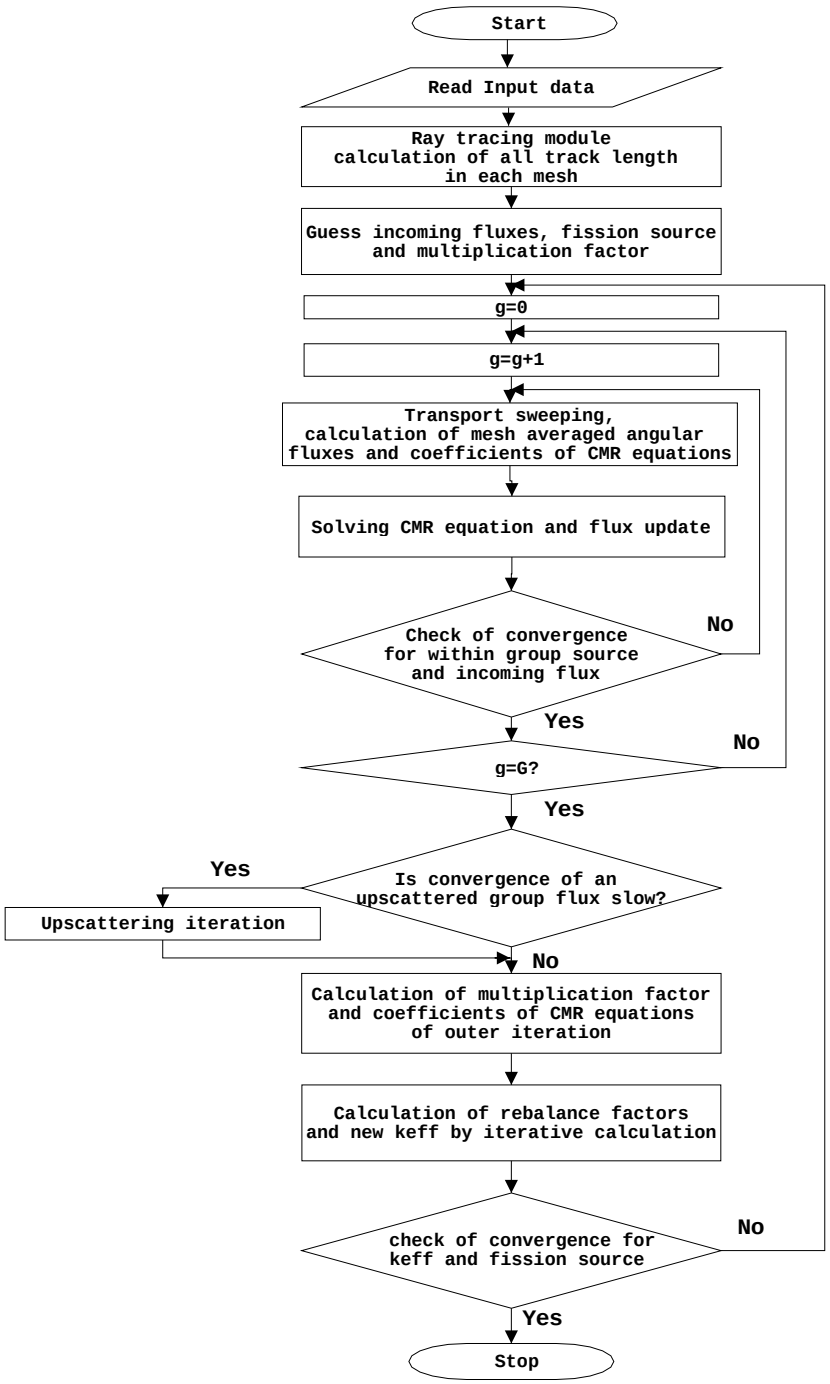

Figure 1: Flow chart of the CMR/CGR-accelerated CRX algorithm

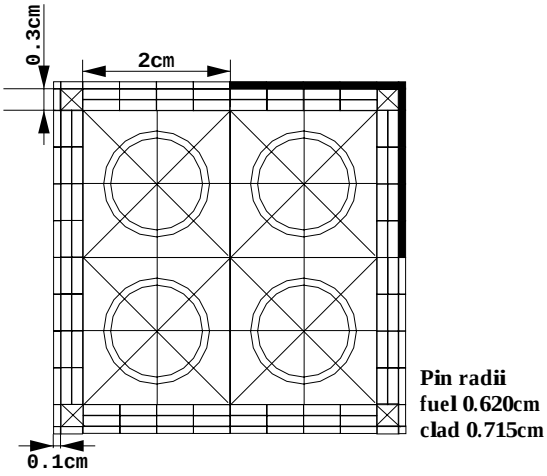

Figure 2: Configuration of NEACRP2

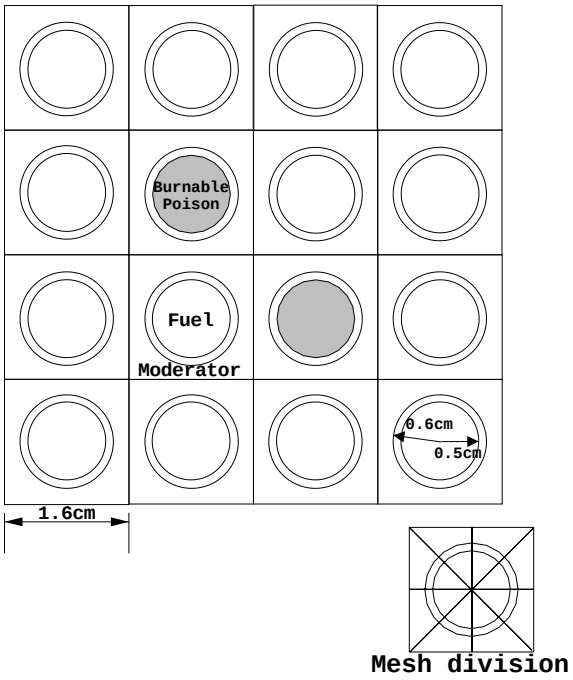

Figure 3: Configuration of 4x4 BWR

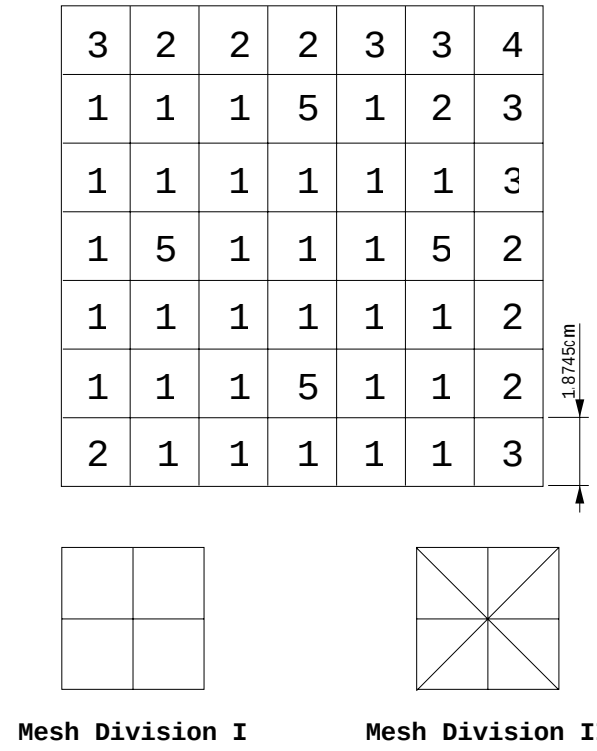

Figure 4: Configuration of 7x7 BWR Fuel Assembly