

COARSE MESH REBALANCE ACCELERATION REVISITED : KRYLOV PRECONDITIONING

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ABSTRACT

Coarse mesh rebalance (CMR) considers neutron balance over the coarse-mesh cell and thus it is easy to apply it to unstructured fine meshes by overlaying simple orthogonal coarse meshes. However, CMR method is unstable or ineffective with scattering ratio c close to unity for optically thin or thick cells. By coupling CMR with Krylov subspace method, we expected that this deficiency of CMR can be removed as the consistent discretization requirement relaxed in DSA if it is used as a preconditioner for Krylov method. In 1-D slab geometry, the test results indicate that Krylov methods with linear CMR preconditioner can be much more effective than source iteration accelerated by traditional CMR or Krylov method without preconditioner. However, in 2-D test problems, preconditioned Krylov method was not always more effective than pure Krylov method although both are better than source iteration (SI).

Key Words: Coarse mesh rebalance, Krylov subspace method, Preconditioner, Acceleration

1. INTRODUCTION

Coarse mesh rebalance (CMR) acceleration method for neutron transport calculation was once the most popular acceleration method since the mid-1960s and was implemented in many neutron transport codes. The CMR method is versatile, which can be applied to a wide range of problems in various geometries with any S_N differencing scheme. However, it is known that CMR is unstable or ineffective with scattering ratio c close to unity for optically thin or thick cells by experience, and Cefus and Larsen [1] showed this analytically by using Fourier analysis. Due to this deficiency and development of the unconditionally stable diffusion synthetic acceleration (DSA) method, CMR was replaced by DSA in modern transport codes. However, DSA requires consistency in spatial discretization of high and low order equations for unconditional stability and thus DSA has its own limitations in its applicability. The recent work, e.g. [2, 3], indicate that the consistent discretization requirement can be relaxed in DSA if it is used as a preconditioner for Krylov iterative methods.

In this paper, we revisit the CMR method. Because CMR considers neutron balance over the coarse-mesh cell, it is easy to apply it to other than S_N methods such as method of characteristics (MOC) and treat unstructured meshes overlaid by simple orthogonal coarse meshes. These aspects are very attractive. For these reasons, we discuss performance of a form of CMR methods by coupling CMR with Krylov subspace method. The test results indicate that Krylov methods, even with relatively simple preconditioners, can be much more effective than source

iteration (SI) accelerated by traditional CMR. By applying CMR to Krylov methods as a preconditioner, we expect more effective acceleration behavior in a wider range of problems.

2. LINEAR CMR PRECONDITIONED KRYLOV METHOD

2.1. 1-D Linear CMR Formulation

In the slab geometry, the neutron transport equation is written as follows:

$$\mu \frac{d}{dx} \psi^{l+1/2}(x, \mu) + \sigma(x) \psi^{l+1/2}(x, \mu) = \sigma_s(x) \phi^l + q(x), \quad (1)$$

with boundary conditions :

$$\psi_{1/2,n} = 0, \quad n = 1, \dots, N/2 \quad (\text{vacuum at left boundary}), \quad (2)$$

$$\psi_{1/2,n} = \psi_{1/2,N+1-n}, \quad n = N/2+1, \dots, N \quad (\text{reflective at right boundary}), \quad (3)$$

where all notations are standard and l denotes the iteration index.

To derive linear CMR equation, let us consider a system of coarse meshes in which each coarse mesh cell contains several fine mesh cells [4].

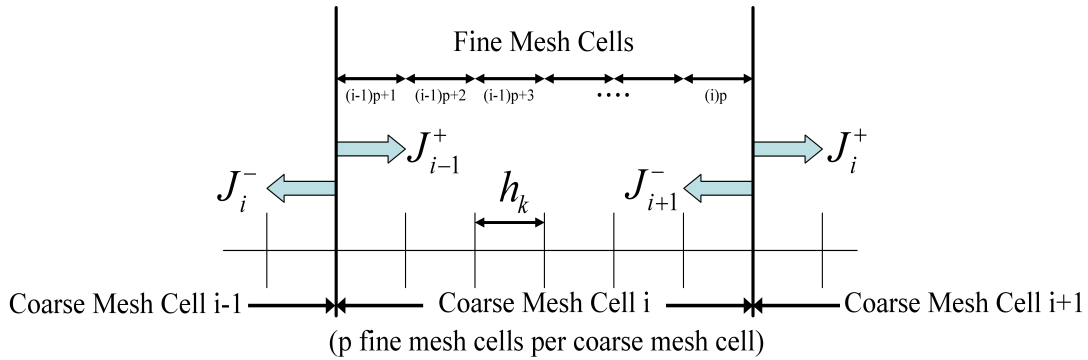


Figure 1. Configuration of coarse meshes and fine meshes in slab geometry.

When angular iteration and spatial integration over the coarse mesh cell are performed, we obtain the following equation:

$$\left(J_i^{+,l+1/2} + J_i^{-,l+1/2} + \sum_k h_k (\sigma_{ki} - \sigma_{s,ki}) \phi_{ki}^{l+1/2} \right) - J_{i-1}^{+,l+1/2} - J_{i+1}^{-,l+1/2} = \sum_k h_k q_{ki}, \quad (4)$$

where

$$J_i^{+,l+1/2} = \frac{1}{2} \sum_{n=1}^{N/2} w_n |\mu_n| \psi_{n,i+1/2}^{l+1/2}, \quad \mu_n > 0, \quad (5)$$

$$J_i^{-,l+1/2} = \frac{1}{2} \sum_{n=N/2+1}^N w_n |\mu_n| \psi_{n,i-1/2}^{l+1/2}, \quad \mu_n < 0, \quad (6)$$

and i denotes coarse mesh cell and k fine mesh cell, and $(\mu_n, w_n), n = 1, 2, \dots, N$, are the discrete ordinates quadrature set.

Now we define rebalance factor f_i for each coarse mesh cell as follows:

$$\psi_{n,i}^{l+1} = \psi_{n,i}^{l+1/2} + f_i^{l+1} \quad (7)$$

$$\psi_{n,i+1/2}^{l+1} = \psi_{n,i+1/2}^{l+1/2} + f_i^{l+1}, \quad \mu_n > 0, \quad (8)$$

$$\psi_{n,i-1/2}^{l+1} = \psi_{n,i-1/2}^{l+1/2} + f_i^{l+1}, \quad \mu_n < 0. \quad (9)$$

Using Eqs. (5), (6), and (7) in Eq. (2), we can derive equations for linear CMR:

$$-\gamma f_{i-1}^{l+1} + 2 \left(\gamma + \sum_k \sigma_{a,k} h_k \right) f_i^{l+1} - \gamma f_{i+1}^{l+1} = \sum_k \left[\phi_{ki}^{l+1/2} - \phi_{ki}^l \right] \sigma_{s,k} h_k, \quad (10)$$

where

$$\gamma = \sum_{\mu_n > 0} w_n \mu_n, \quad (11)$$

with boundary conditions:

$$f_0 = 0 \quad (\text{vacuum at left boundary}), \quad (12)$$

$$f_{I+1} = f_I \quad (\text{reflective at right boundary}). \quad (13)$$

Now, we are prepared to solve the problem by CMR since all coefficients in front of the rebalance factors (f_i) are already known from previous transport sweep. After we get the rebalance factors, we can update the flux by the following equation:

$$\phi_{ki}^{l+1} = \phi_{ki}^{l+1/2} + 2 f_i^{l+1}. \quad (14)$$

With this simple linear CMR equation, whenever we do transport sweep in a Krylov solver (such as BiCGSTAB), we update the flux by linear CMR. This is the basic scheme of linear CMR-Krylov method. In other words, CMR-Krylov method is a Krylov solver which can be “wrapped around” the source iteration code based on transport sweep, including the CMR step that plays the role of a preconditioner.

2.2. 2-D Linear CMR Formulation

Neutron balance equation for a coarse-mesh cell in 2-D is written as follows:

$$\mu_n \Delta y_J [\phi_{I+1/2,J,n} - \phi_{I-1/2,J,n}] + \eta_n \Delta x_I [\phi_{I,J+1/2,n} - \phi_{I,J-1/2,n}] + A_{I,J} \sigma_{I,J} \phi_{I,J,n} = A_{I,J} \sigma_{I,J,s} \phi_{I,J} + A_{I,J} q_{I,J,n}, \quad (15)$$

where

$$A_{I,J} = \Delta x_I \Delta y_J, \quad (16)$$

$$\sum_{n=1}^N w_n = 1, \quad (17)$$

$$\phi_{I,J} = \sum_{i,j \in I,J} \sum_{n=1}^N w_n \phi_{i,j,n}, \quad (18)$$

$$A_{I,J} \sigma_{I,J} \phi_{I,J,n} = \sum_{i,j \in I,J} A_{i,j} \sigma_{i,j} \phi_{i,j,n}, \quad (19)$$

$$A_{I,J} s_{I,J,n} = \sum_{i,j \in I,J} A_{i,j} q_{i,j,n}. \quad (20)$$

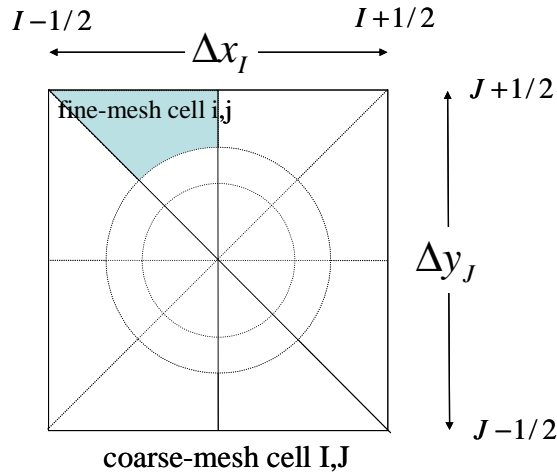


Figure 2. Configuration of coarse mesh and fine meshes

Multiplying Eq. (15) by w_n and summing over n , we obtain:

$$\sum_n w_n [\mu_n \Delta y_J [\phi_{I+1/2,J,n}^{j+1/2} - \phi_{I-1/2,J,n}^{j+1/2}] + \eta_n \Delta x_I [\phi_{I,J+1/2,n}^{i+1/2} - \phi_{I,J-1/2,n}^{i+1/2}] + A_{I,J} \sigma_{I,J} \phi_{I,J,n}^{i+1/2} = A_{I,J} \sigma_{I,J,s} \phi_{I,J}^i + A_{I,J} q_{I,J,n}]. \quad (21)$$

For linear CMR, we define ϕ^{l+1} by setting:

$$\phi_{I+1/2,J,n}^{l+1} = \phi_{I+1/2,J,n}^{l+1/2} + f_{I,J,n}^{l+1}, \quad \mu_n > 0 \quad (22)$$

$$\phi_{I-1/2,J,n}^{l+1} = \phi_{I-1/2,J,n}^{l+1/2} + f_{I-1,J,n}^{l+1}, \quad \mu_n < 0 \quad (23)$$

$$\phi_{I,J-1/2,n}^{l+1} = \phi_{I,J-1/2,n}^{l+1/2} + f_{I,J-1,n}^{l+1}, \quad \eta_n < 0 \quad (24)$$

$$\phi_{I,J+1/2,n}^{l+1} = \phi_{I,J+1/2,n}^{l+1/2} + f_{I,J,n}^{l+1}, \quad \eta_n > 0 \quad (25)$$

Changing iteration index from l to $l+1$ in Eq. (21),

$$\sum_n w_n \left[\mu_n \Delta y_J [\phi_{I+1/2,J,n}^{l+1} - \phi_{I-1/2,J,n}^{l+1}] + \eta_n \Delta x_I [\phi_{I,J+1/2,n}^{l+1} - \phi_{I,J-1/2,n}^{l+1}] + A_{I,J} \sigma_{I,J} \phi_{I,J,n}^{l+1} = A_{I,J} \sigma_{I,J,s} \phi_{I,J}^{l+1} + A_{I,J} s_{I,J,n} \right]. \quad (26)$$

Subtract Eq. (21) from Eq. (26), and obtain:

$$\begin{aligned} & \sum_{\mu_n > 0} w_n \mu_n \Delta y_J [f_{I,J,n}^{l+1} - f_{I-1,J,n}^{l+1}] + \sum_{\mu_n < 0} w_n \mu_n \Delta y_J [f_{I+1,J,n}^{l+1} - f_{I,J,n}^{l+1}] + \sum_{\eta_n > 0} w_n \eta_n \Delta x_I [f_{I,J,n}^{l+1} - f_{I,J-1,n}^{l+1}] \\ & + \sum_{\eta_n < 0} w_n \eta_n \Delta x_I [f_{I,J+1,n}^{l+1} - f_{I,J,n}^{l+1}] + \sum_n w_n A_{I,J} \sigma_{I,J,a} f_{I,J,n}^{l+1} = \sum_n w_n A_{I,J} \sigma_{I,J,s} [\phi_{I,J,n}^{l+1/2} - \phi_{I,J,n}^l]. \end{aligned} \quad (27)$$

By defining $\gamma = \sum_{\mu_n > 0} \mu_n \omega_n$, $\nu = \sum_{\eta_n > 0} \eta_n \omega_n$, linear CMR equation is written as:

$$\begin{aligned} & -\gamma \Delta y_J f_{I-1,J,n}^{l+1} - \nu \Delta x_I f_{I,J-1,n}^{l+1} - \gamma \Delta y_J f_{I+1,J,n}^{l+1} - \nu \Delta x_I f_{I,J+1,n}^{l+1} \\ & + [2(\gamma \Delta y_J + \nu \Delta x_I) + A_{I,J} \sigma_{I,J,a}] f_{I,J,n}^{l+1} = A_{I,J} \sigma_{I,J,s} [\phi_{I,J,n}^{l+1/2} - \phi_{I,J,n}^l], \end{aligned} \quad (28)$$

with boundary conditions:

$$f_{I-1} = 0 \quad (\text{vacuum at left boundary}), \quad (29)$$

$$f_{I+1} = f_I \quad (\text{reflective at right boundary}), \quad (30)$$

$$f_{J+1} = 0 \quad (\text{vacuum at top boundary}), \quad (31)$$

$$f_{J-1} = f_J \quad (\text{reflective at bottom boundary}). \quad (32)$$

After solving Eq. (28) for f^{l+1} , average scalar flux in fine-mesh cell is updated by

$$\phi_{i,j,n}^{l+1} = \phi_{i,j,n}^{l+1/2} + f_{I,J,n}^{l+1}. \quad (33)$$

In the same way as in 1-D case, now this CMR method can be used as a preconditioner within Krylov solver.

3. NUMERICAL RESULTS

3.1. 1-D Numerical Results

Several numerical tests were done using the CMR-Krylov solver. First, we tested if the CMR-Krylov method solution converges to the original source iteration solution. Then, we checked whether the deficiency of the linear CMR method (nonconvergent in optically thin and thick mesh sizes) disappears. Fig. 3 shows configuration of an example problem. Fig. 4 and Table I show the computational results of several methods, using diamond difference (DD) scheme in the discrete ordinates (S_8) method, with fine mesh size of 0.2cm and initial guess of $\phi_{ki} = 1$.

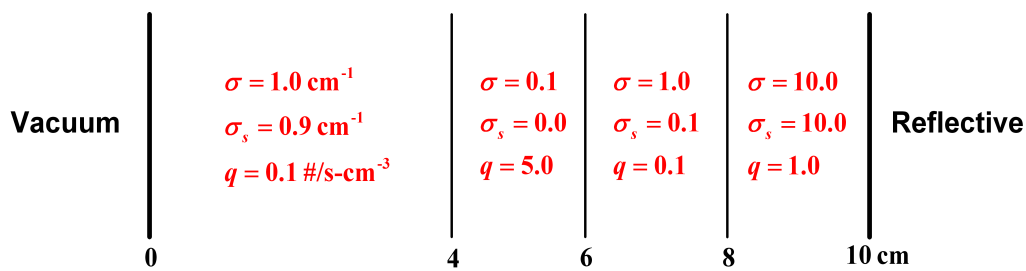


Figure 3. Configuration of an Example Problem.

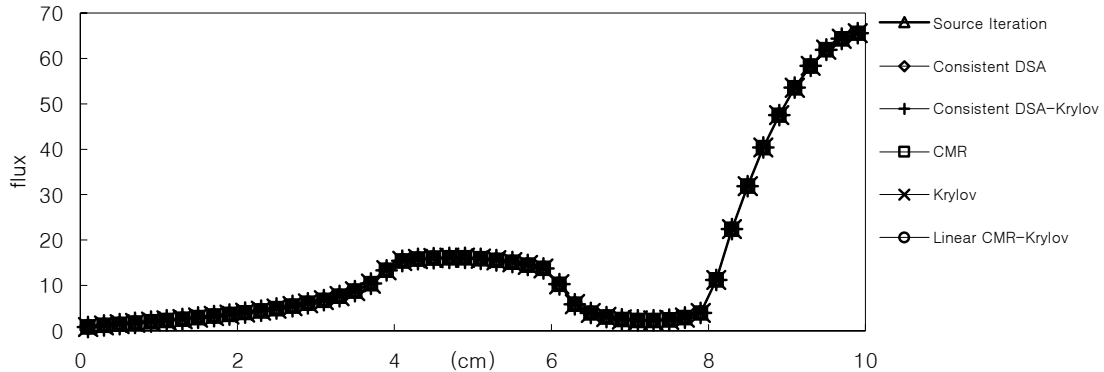


Figure 4. Flux Distribution of an Example Problem.

Table I. Performance of Various Acceleration Methods

	# of Iterations	CPU time(sec) ^a
Source Iteration	5158	0.181
Consistent DSA	10	0.001
Consistent DSA-Krylov	5	0.001
Nonlinear CMR	188	0.009
Krylov	22	0.001
Linear CMR-Krylov(p=4)	12	0.002

^a Pentium IV 3.06MHz

The solutions of the six methods have converged to the same flux distribution of the source iteration.

As mentioned earlier, CMR method is unstable in optically thin or thick problems and the stability also depends on the degree of the coarseness p . The example problem above has optically thick regions. Table II provides results for the same problem but with varying coarseness.

Table II. Results of an Example Problem vs Coarseness

p^a	Linear CMR		Nonlinear CMR		Linear CMR-Krylov	
	# of Iterations	CPU time(sec) ^b	# of Iterations	CPU time(sec)	# of Iterations	CPU time(sec)
1	5014	0.322	N.C. ^c		12	0.001
2	3536	0.214	58	0.004	13	0.002
3	4203	0.244	113	0.007	13	0.003
4	N.C.		188	0.010	12	0.002
8	N.C.		492	0.025	13	0.002
25	N.C.		786	0.041	22	0.003

^a Coarseness : Number of fine mesh cells per coarse mesh cell^b Pentium IV 3.06MHz^c N.C. : Not Converged.

Table III and Table IV provide further results of an example problem whose configuration is almost the same with the previous problems except that the size is a hundred times larger with different coarseness. The problem size is 1000cm (10m) which is comparable to a PBMR core. The convergence dependency on mesh size with $p=2$ and $p=4$ has been examined.

Table III. Convergence Results vs. Mesh Size with Coarseness p=2

$\sigma_i h$	Linear CMR		Nonlinear CMR		Linear CMR-Krylov	
	Convergence	# of Iterations	Convergence	# of Iterations	Convergence	# of Iterations
0.1	N.C.		N.C.		Converged	204
1	Converged	2870257	N.C.		Converged	21
10	N.C.		N.C.		Converged	68
100	Converged	5413272	Converged	33554	Converged	113
1000	Converged	5067278	Converged	848776	Converged	13

*p (coarseness) = 2

Table IV. Convergence Results vs. Mesh Size with Coarseness p=4

$\sigma_i h$	Linear CMR		Nonlinear CMR		Linear CMR-Krylov	
	Convergence	# of Iterations	Convergence	# of Iterations	Convergence	# of Iterations
0.1	N.C.		N.C.		Converged	90
1	N.C.		N.C.		Converged	34
10	N.C.		N.C.		Converged	87
100	N.C.		Converged	101820	Converged	92
1000	N.C.		Converged	849251	Converged	12

*p (coarseness) = 4

3.2. 2-D Numerical Results

As in 1-D, several numerical tests have been done using CMR-Krylov solver in 2-D. However, in 2-D, MOC scheme is used to solve high order equation instead of the diamond difference schemes. Stopping criterion for iterative methods is difference between the fluxes of two consecutive iterations.

3.2.1. Test problem I

Fig. 5 shows configuration of test problem I. A small assembly of 7 by 7 configuration with two types of cells is composed of 3 kinds of materials. Only material 1 has source (fixed source) and each cell is divided into 24 regions (fine-mesh cells) by 2 concentric circles and 8 radial lines. Cross sections of each material are listed in Table VI.

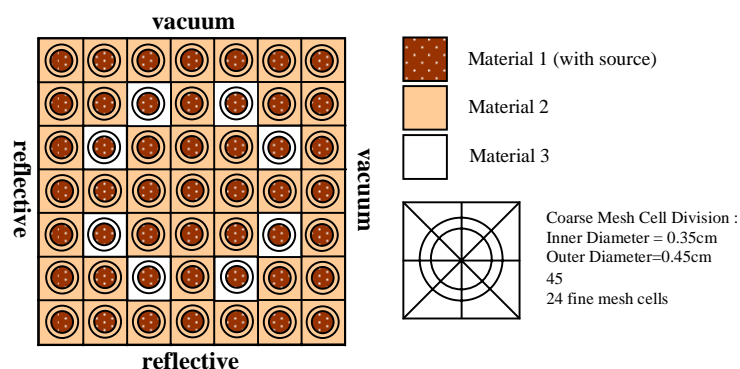


Figure 5. Configuration of Test Problem I

Table VI. Cross Sections of Materials in Test Problem I

	$\sigma (cm^{-1})$	$\sigma_s (cm^{-1})$
Material 1	1.250	1.242
Material 2	0.625	0.355
Material 3	14.00	0.000

Since convergence and performance of CMR method depends on σh (optical thickness) value, we checked several cases with different σh values. The results of the test problem I are given in Table VII. In this problem, there are three different materials and each material has different σh , only its minimum and maximum values are listed in the table. σh values are changed by multiplying 0.01, 0.1, 1.0, 10, 100 on original cross sections.

Table VII. Results of Test Problem I

σh	SI		Krylov		Linear CMR		CMR-Krylov	
	# of iterations	CPU time(sec)	# of iterations	CPU time(sec)	# of iterations	CPU time(sec)	# of iterations	CPU time(sec)
0.0078/0.175	8	4.038	3	3.392	11	5.703	4	4.454
0.078/1.75	19	9.447	5	5.737	16	8.134	5	5.319
0.78/17.5	81	36.297	12	10.948	23	10.460	7	6.641
7.8/175	243	99.038	19	15.363	145	59.204	17	13.771
78.0/1750	949	396.521	25	20.853	714	303.194	35	29.473

3.3.3. Test problem II

Another test problem is calculated in the same procedure. In this problem, a cell is homogenized so only one material exists (Table VIII). Source is distributed in the inner part of the assembly. Coarse mesh cell division is same with the test problem I. The results are given in Table IX.

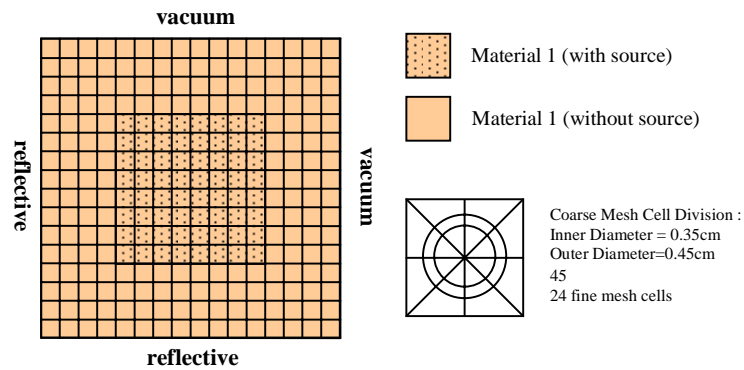


Figure 5. Configuration of Test Problem I

Table VIII. Cross Sections of Materials in Test Problem II

	$\sigma (cm^{-1})$	$\sigma_s (cm^{-1})$
Material 1	1.250	1.242

Table IX. Results of Test Problem II

σh	SI		Krylov		Linear CMR		CMR-Krylov	
	# of iterations	CPU time(sec)	# of iterations	CPU time(sec)	# of iterations	CPU time(sec)	# of iterations	CPU time(sec)
0.01	8	22.989	4	25.199	N.C.		5	32.601
0.10	30	85.962	7	41.696	N.C.		7	41.632
1.00	958	2565.25	28	133.249	52	169.292	7	41.363
10.0	5353	12214.1	94	425.053	137	345.496	26	131.021
100	13310	30059.2	59	285.400	822	1984.94	52	1350.56

4. CONCLUSIONS

The linear coarse mesh rebalance (CMR) method in transport calculation has been implemented as a preconditioner for Krylov solver. This linear CMR-Krylov method is proved to be a good acceleration method, that is, computer time and iteration number have greatly reduced compared to the source iteration. Also the well known deficiencies of the CMR method have disappeared in the problems tested. However, in 2-D test problems, the linear CMR-Krylov method do not necessarily always show better performance than Krylov alone (although both CMR-Krylov and Krylov alone are better than SI). This point should be further investigated.

REFERENCES

- [1] G..R. Ce fus and E.W. Larsen, “Stability Analysis of Coarse-Mesh Rebalance”, *Nuclear Science and Engineering*, **105**, 31 (1990)
- [2] J.S. Warsa, T.A. Wareing, and J.E. Morel, “Krylov Iterative Methods and the Degraded Effectiveness of Diffusion Synthetic Acceleration for Multidimensional SN Calculations in Problems with Material Discontinuities, *Nuclear Science and Engineering*, **147**, 218 (2004)
- [3] J.E. Morel, “Basic Krylov Methods with Application to Transport”, *Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, Avignon, France, September 12-15, 2005, on CD-ROM, American Nuclear Society, LaGrange Park , IL (2005)
- [4] N.Z. Cho and C.J. Park, “A Comparison of Coarse Mesh Rebalance and Coarse Mesh Finite Difference Accelerations for the Neutron Transport Calculations”, *Nuclear Mathematical and Computational Sciences : A Century in Review, A Century Anew*, Gatlinburg, TN, April 6-11, 2003, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2003)