International Conference on Advances in Nuclear Science and Engineering in Conjunction with LKSTN 2007 (403-406)

# *Development of Cell Homogenization Code Using General Geometry Approach*

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***Abstract***

*DEVELOPMENT OF CELL HOMOGENIZATION CODE USING GENERAL GEOMETRY APPROACH Cell homogenization is one of the most complicated steps in the reactor physics calculations. It is employed to get representative group constants over an assembly or pin cell. In the previous study we have developed cell calculation for simple annular cylindrical cell of fast reactors. Element of general geometry modules have been developed also. In this study we focus on performing parallel computation using socket programming method. Using socket programming we build a tree structure with one computer as a master and 2,3 up to 5 computers as slaves. The master processor is dividing the job into several parts and distributes it according to each slave and collecting the data from the slaves and combining them. Initial results shows that the parallelization is effective thanks to the nature of multi region and multi energy group of the problem so that it can be distributed to many computer easily.*

***Keywords*** *: Cell homogenization, general geometry, parallel computation*

## I. Introduction

Cell homogenization calculation of fuel assembly or pin cell in reactor physics and reactor design to get representative group constants is important. One of the most complicated step in order to estimate neutronic parameters is to solve neutron transport equation in nuclear reactor core. For the reason, the development of advanced reactor core designs required that followed by computer power allowed more accurate solution of neutron transport equation. One of the most commonly used techniques for solutions to the transport equation is that of collision probabilities (Su'ud et.al, 2002). However, computer codes based on the exact collision probability formalism have historically been limited to a single assembly analysis. A few numerical methods to solve neutron transport equation have been developed, but the problems are limited by time consuming to convergent, and memory or computer power. The great alternative to help the restriction of the computer perform is parallel computing (Zao and Maldonado, 2006).

In this paper we focus on performing parallel computation using socket programming method. Using socket programming we build a tree structure with one computer as a master and 2,3 up to 5 computers as slaves. The master processor is dividing the job into several parts and distributes it according to each slave and collecting the data from the slaves and combining them.

## II. Theory

To perform cell homogenization we start with multigroup integral transport equation as shown in the following equation

$$\Psi_g(\bar{r},\overset{\rho}{\Omega}) = \int_V \frac{d\bar{r}'}{|\bar{r}-\bar{r}'|^2}\delta(\overset{\rho}{\Omega},\overset{\rho}{\Omega}_R)Q_g(\bar{r}',\overset{\rho}{\Omega}) \exp\left(-\int_0^{|\bar{r}-\bar{r}'|}\Sigma_{t,g}(\bar{r}-R')\frac{\bar{r}-\bar{r}'}{|\bar{r}-\bar{r}'|}dR'\right) \quad (1)$$

where $r$ variable of position, $g$ energy group, $\overline{\Omega}$ solid angel vector, $\Psi_g(\bar{r},\overline{\Omega})$ angular neutron flux, $Q_g(\bar{r},\overline{\Omega})$ neutron source, and $\Sigma_{t,g}$ macroscopic cross section. If Eq. (1) is integrated over all solid angels, then we obtained scalar flux angular

$$\phi_g(\vec{r},\vec{\Omega}) = \int_V d\vec{r}' \left( Q(\vec{r}',\vec{\Omega}) \frac{\exp\left(-\lambda_g(\vec{r},\vec{r}_s)\right)}{|\vec{r}-\vec{r}'|^2} \right), \tag{2}$$

where $\lambda_g(\bar{r},\bar{r}') = \int_0^{|\bar{r}-\bar{r}'|} \Sigma_{t,g}(\bar{r}-R') \frac{\bar{r}-\bar{r}'}{|\bar{r}-\bar{r}'|} dR'$

is optical path length.

We than define collision probability from region *i* to region *j* (the probability that neutron born in region *i* experienced first collision/reaction in region *j*) as follows

$$P_{ij} = \frac{1}{4\pi V_i} \int_{V_i} d\bar{r} \int_{V_j} \left( \frac{\Sigma_t(\bar{r}')}{|\bar{r}-\bar{r}'|^2} \exp[-\lambda_g(\bar{r},\bar{r}')] \right) d\bar{r}' \tag{3}$$

After some mathematical simplification we get simpler eigen value equation as follows (Stacey, 2001)

$$\Sigma_{tj} V_j \phi_{g,j} = \frac{1}{k_{eff}} \sum_k V_k P_{kj} Q_k \tag{4}$$

We consider the infinitely long cylinder which is divided into several annular shells. The outer radius of the shell *i* is $r_i$. Suppose neutron emitted at point P in the shell *i* has its collision at the point Q in the shell *j*. The line PQ makes an angel $\theta$ with the vertical line. In the cylindrical coordinat system as shown in Fig.1a, the collision probability $P_{ij}$ is

$$P_{ij} = \frac{2}{V_i} \int_{r_i-1} r dr \int_0^{\pi} d\beta \int_0^{\pi/2} \sin\theta \, d\theta \int_{R_{j-}}^{R_{j+}} dR \frac{\Sigma_j}{\sin\theta} \exp\left( -\int_0^R \frac{\Sigma_s(s)}{\sin\theta} ds \right) \tag{5}$$

where $V_i = \pi(r_i^2 - r_{i-1}^2)$.

We transform the variable *r*, $\beta$ and *R* into new ones $\rho, x$ and $x'$ as illustrated in Fig.1b. There are three relations among variables :

$$r^2 = \rho^2 + x^2;$$
$$r\sin\beta = \rho;$$
$$R = x' - x;$$

Using these relations we get the Jacobian

$$\frac{\partial(r,\beta,r)}{\partial(\rho,x,x')} = \frac{1}{r}$$

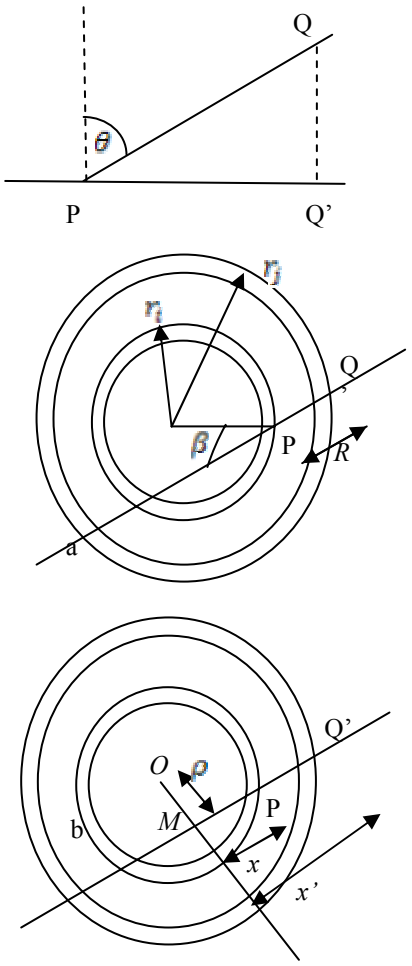


**Figure 1**. Cylindrical coordinate

Using new variables we can rewrite Eq. (5) by

$$P_{ij} = \frac{2}{V_i} \int_0^{r_i} dr \int_0^{\pi} d\theta \int_{x_{i-1}}^{x_i} dx \int_{x'_{j-1}}^{x'_j} dx' \left( \exp\left( -\int_x^{x'} \frac{\Sigma_s(t)}{\sin\theta} dt \right) + \exp\left( -\int_{-x}^{x'} \frac{\Sigma_s(t)}{\sin\theta} dt \right) \right) \tag{6}$$

where $x_i = \sqrt{r_i^2 - \rho^2}$ for $r_i > \rho$ and $x_i = 0$ for $r_i < \rho$.

We have the final form of $P_{ij}$ for the case $r_i < r_j$, as follows

$$P_{ij} = \frac{2}{\Sigma_i V_i} \int_0^{\pi/2} d\theta \left\{ K_{i3}(\lambda_{ij}^1) - K_{i3}(\lambda_{ij}^1 + \lambda_i) - K_{i3}(\lambda_{ij}^1 + \lambda_j) + K_{i3}(\lambda_{ij}^1 + \lambda_i + \lambda_j) + K_{i3}(\lambda_{ij}^2) - K_{i3}(\lambda_{ij}^2 + \lambda_i) - K_{i3}(\lambda_{ij}^2 + \lambda_j) + K_{i3}(\lambda_{ij}^2 + \lambda_i + \lambda_j) \right\} \tag{7}$$

where $\lambda_{ij}^{1} = \sum_{k=i+1}^{j-1} \lambda_k$ and

$\lambda_{ij}^{2} = \sum_{k=1}^{i-1} \lambda_k + \sum_{k=1}^{j-1} \lambda_k$ and

$K_{in} = \int_0^{\pi/2} d\theta \ \sin^{n-1}\theta \ \exp\left(-\frac{x}{\sin\theta}\right)$

is introduced as a Bickley-Naylor function.

For the case $r_i \ll r_j$, the optical path length become to $\lambda_{ij}^{1} = \sum_{k=j-1}^{i-1} \lambda_k$ and $\lambda_{ij}^{2} = \sum_{k=1}^{i-1} \lambda_k + \sum_{k=1}^{j-1} \lambda_k$.

For the case $i = j$, Eq. (7) is reduce to

$$P_{ii} = \frac{2}{\Sigma_i V_i}\int_0^{r_{i-1}} d\rho\{2\lambda_i - 2K_{i3}(0) + 2K_{i3}(\lambda_i) + K_{i3}(\lambda_{ii}) \quad (8) - 2K_{i3}(\lambda_{ii}+\lambda_i)\} + \frac{2}{\Sigma_i V_i}\int_{i-1}^{r_i} d\rho\{2\lambda_i - K_{i3}(0) + K_{i3}(2\lambda_i)\} \tag{8}$$

where $\lambda_{ii} = 2\sum_{k=1}^{i-1} \lambda_k$.

If we substitute total reflection boundary condition on the outer cylindrical cell, Eq. (7) must be added with terms like those as follows (Okumura et.al., 2007)

$$K_{i3}(\lambda_{ij}^{3}) - K_{i3}(\lambda_{ij}^{3} + \lambda_i) - K_{i3}(\lambda_{ij}^{3} + \lambda_j) + K_{i3}(\lambda_{ij}^{3} + \lambda_i + \lambda_j)$$

$$+K_{i3}(\lambda_{ij}^{4}) - K_{i3}(\lambda_{ij}^{4} + \lambda_i) - K_{i3}(\lambda_{ij}^{4} + \lambda_j) + K_{i3}(\lambda_{ij}^{4} + \lambda_i + \lambda_j) \tag{9}$$

$$+K_{i3}(\lambda_{ij}^{n}) - K_{i3}(\lambda_{ij}^{n} + \lambda_i) - K_{i3}(\lambda_{ij}^{n} + \lambda_j) + K_{i3}(\lambda_{ij}^{n} + \lambda_i + \lambda_j)$$

Background cross section calculation process was started with atomic density calculation for each nucleus in each region. Furthermore, background cross section was calculated for each nucleus roughly as follow

$$\sigma_0^n = \sum_{m \neq n} N_m \sigma_t^m / N_n \tag{10}$$

The calculation result from Eq. (10) is used once again to calculate total cross section. In addition, heterogeneity correction has been carried out by inserting Dancoff and Bell factor

$$\sigma_{0,k}^{n} = \sigma_{0,k}^{n*} + \frac{S_k}{4N_k^n V_k}\frac{a(1-C)}{1+a(1-C)} \tag{11}$$

where mark * denote the value of homogeny model, $S_k$ is element of surface area at $k$, $V_k$ is volume element at $k$, $N_k^n$ is atomic density $n$ in the element $k$, $a$ is a Bell factor and $C$ is Dankoff factor (Sugimura and Yamamoto, 2006). We can recalculate cross section for each nucleus for the type of reaction by using Eq. (11). From Eq.(10) and (11), iteration continued to convergent.

Collision probability matrix was evaluated by using Eq.(6) to (9), after that, from Eq. (4) we compute neutron transport. From the result of neutron spectrum, we can process the calculation of cross section effective for each nucleus by using this spectrum as a weighting.

## III. Computational Method

To find out effective constant group from library, we have interpolated temperature variable and background cross section by Spline-cubic method. Bickley-Naylor function was considered with two ways, series expansion or interpolation from the table. Similar with the integration to compute collision probability matrix, the Gauss integration method was used with 40 order number. Solution of diffusion equation 2D in the process of collapsing constant group used successive over relaxation method in spite of power method approximation or used acceleration for outer iteration.

We write the program in Borland Delphi 7. Using socket programming we build a tree structure with one computer as a master and 2, 3 up to 5 computers as slaves. The master processor is dividing the job into several parts and distributes it according to each slave and collecting the data from the slaves and combining them.

## IV. Result and Discussion

As a sample of calculation, we were used a peace of fuel cell mixing of U-Pu with Pb and material structure HT9 as a coolant. The computation was carried out for two type of cell, which is in reactor core and the blanket. From previous calculation, it was resulted constant group in the 70 groups. The next step was considered the calculation of 2 dimension diffusion equations for reactor that consists of three region, inlet core, outlet core and reflector. This process has been done in 70 group energy using constant group as a result from those cell calculations. The neutron spectrum that was calculated at the previous step is

used as a weighted function to get collapsing for 7 group energy. Furthermore, the result of constant group of 8 group were applicated to calculate multiplication factor of reactor and the result were compared with FI-ITB-CH1 computer code (Su'ud, 1998).

The great difference of constant group value that counted by this program and FI-ITB-CH1 computer code is at the thermal region. However, while this reactor type is a fast reactor, then the influence of thermal region can be neglected. Notice that the behavior of thermal region in order to calculate constant group for fast reactor occasionally avoid the differentiation. If we want more precision, it must be considered discrete resonances in the ev order region to hundred ev regions. In addition, matrix transfer for elastic scattering is excluded in the library, for the reason in this program we build special procedure to execute one.

The result shows that the calculation of $k_{eff}$ from this program with FI-ITB-CH1 computer code not quite different, although at microscopic cross section level has a little differentiation. This is appreciated because of multiplication factor is a unit of integral, than the different of microscopic cross section value is not important.

| Computer Code | Multiplication Factor |
|---|---|
| This program | 1.06727 |
| FI-ITB-CH1 | 1.06726 |

Using socket programming, parallelization of collision probability matrix calculation reduced time consuming and shows the significant speed up process. However, the using of optimal weighted is absolutely needed if the velocity of processor were n In this case communication speed between processor is not quite critical to perform the final result.

## V. Conclusion

Development of computer code for fuel cell homogenization calculation in the fast reactor has been compared these result with the FI-ITB-CH1 computer code. The result show that both calculation very closely, especially on integral parameter. Using socket programming, parallelization of collision probability matrix calculation reduced time consuming and shows the significant speed up process.

## VI. Acknowledgment

The first author wishes to thank Mr. Pramuditha Syeilendra, Mrs. Yanti and Mr. Epung S. Bahrun for their assistance and were very helpful in this study.

## VII. References

1. Okumura, K., Kugo, T., Kaneko, K., and Tsuchihashi, K., 2007, *SRAC* 2006*: A Comprehensive Neutronics Calculation Code System*, Japan Atomic Energy Agency
2. Sugimura, N., and Yamamoto, A., 2006, Evaluation of Dancoff Factor in Complicated Geometry Using the Method of Characteristics, *J. Nucl. Sci. Technol.*, Vol.43, No.10
3. Stacey, W., M., 2001, *Nuclear Reactor Physics*, John Wiley & Son, NY
4. Su'ud, Z., 1998, *Kode Komputer Untuk Homogenisasi Sel Bahan Bakar Pada Reaktor Cepat*, Prosiding Lokakarya Komputasi dalam Sain dan Teknologi Nuklir, BATAN
5. Su'ud, Z., Rustandi, Y.K. dan Kurniadi, R., 2002, *Komputasi Paralel dalam Perhitungan Grup Konstan Nuklir*, Prosiding Seminar ke-7 Teknologi dan Keselamatan PLTN serta Fasilitas Nuklir, Bandung
6. Zhao, Z. and Maldonado, G.I., 2006, Speedup of Particle Transport Problems with a Beowulf Cluster, *Am. J. Appl. Sci,* 3(8)