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IMPLEMENTATION OF A DOMINANT MODES SOLVER IN DRAGON

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Abstract

Solution of the k-eigenvalue transport problem has been limited in lattice codes to the fundamental mode corresponding to the largest eigenvalue. Despite the fact that the higher order modes have no physical meaning, they can have significant uses in different applications. While the fundamental mode represents the asymptotic behaviour of the neutron flux, higher modes describe the small perturbations about it; hence, they can be employed in perturbation studies. Another important application of the higher modes is flux synthesis or mapping. Starting with a reference solution of the neutron flux at a coarse level and a number of modes at a finer level, detailed flux distribution can be reconstructed from a coarse solution. In this work, an implementation of a neutron flux modes solver in DRAGON is described. The solver is based on the QZ decomposition algorithm. The approach is described and results are presented.

1. Introduction

Nuclear reactor design and analysis rely on finding a solution for the neutron transport equation or one of its approximations. In neutron multiplying media, this equation becomes an eigenvalue problem which means that it admits an infinite number of mathematical solutions. The eigenvalue describes the neutron multiplication factor and the corresponding eigenfunction or eigenvector represents the neutron flux. Ideally, the general solution of the problem can be represented by a series summation of the eigensolutions; however, many difficulties render finding the general solution to the transport equation unfeasible. In practice, the physical nature of the problem as well as the boundary conditions (ex. positive solution, outward or inward flux, etc.) impose some restrictions on the solution. It is found that the fundamental mode corresponding to the largest multiplication factor satisfies all the conditions and is widely accepted as the asymptotic solution for the neutron flux. Higher order modes which are solutions corresponding to smaller multiplication factors have no physical meaning when considered independently. Hence, practice in computational reactor physics has been to limit the solution in transport codes to the fundamental mode; calculation of the high order modes has been considered only in diffusion codes [1]. In spite of this, higher order modes can be found useful in many different applications, namely perturbation studies [2] and flux synthesis [3].

Driven by the possible and important applications of the high order solutions of the transport equation, an implementation of a modes solver in the DRAGON lattice code is presented. The implementation is based on the QZ decomposition method applied to the discretised collision probability approximation of the integral transport equation. In the next section, the transport equation and collision probabilities are reviewed. Section 3 describes the QZ decomposition method for solving generalised eigenvalue problems. In section 4, verification of the modes solver is presented along with some example results. The work is concluded by a brief description of possible applications of the high order modes of the transport equation.

2. The transport equation and collision probabilities

The conservation of neutrons in the phase space at steady state conditions can be translated mathematically by the multigroup integro-differential transport equation [4]:

$$\left[\vec{\Omega}\vec{\nabla}+\Sigma_t^g(\vec{r})\right]\phi^g(\vec{r},\vec{\Omega})=Q_s^g(\vec{r},\vec{\Omega})+\frac{1}{k}Q_f^g(\vec{r}) \quad (1)$$

where $\phi^g(\vec{r},\vec{\Omega})$ is the neutron flux density at location $\vec{r}$ in the direction of solid angle $\vec{\Omega}$ in energy group g,

$$Q_s^g=\sum_{h=1}^{G}\int d^2\,\Omega'\,\Sigma_s^{g\leftarrow h}(\vec{r},\vec{\Omega}\leftarrow\overrightarrow{\Omega'})\phi^h(\vec{r},\overrightarrow{\Omega'}) \quad (2)$$

is the scattering source into energy group g, k is the multiplication factor and

$$Q_f^g=\chi^g(\vec{r})\sum_{h=1}^{G}\nu\,\Sigma_f^h(\vec{r})\int d^2\,\Omega'\phi^h\left(\vec{r},\overrightarrow{\Omega'}\right) \quad (3)$$

is the fission source in energy group g respectively, with G being the number of energy groups, χ^g the fission spectrum in energy group g, Σ_t^g, $\Sigma_s^{g\leftarrow h}$, and $\nu\Sigma_f^h$ are the total, scattering and fission production macroscopic cross sections respectively. Perhaps, the most commonly solved form of the transport equation in lattice codes is the integral form:

$$\phi^g(\vec{r},\vec{\Omega})=\int_0^{R_s}e^{-\tau\left(R',\vec{\Omega},\Sigma_t^g\right)}\left[Q_s^g(\vec{r}-R'\vec{\Omega},\vec{\Omega})+\frac{1}{k}Q_f(\vec{r}-R'\vec{\Omega})\right]\mathrm{dR}' \quad (4)$$

where $\tau\left(R',\vec{\Omega},\Sigma_t^g\right)=\int_0^{R'}\Sigma_t^g\left(\vec{r}-R''\vec{\Omega}\right)dR''$ is the neutron optical path in the direction $\vec{\Omega}$. Equation 2 can be further simplified if scattering is assumed to be independent of the direction, i.e. isotropic; in this case integration over $\vec{\Omega}$ yields:

$$\phi^g(\vec{r})=\frac{1}{4\pi}\int_0^{R_s}d^3\,r'\,\frac{e^{-\tau^g(R)}}{R^2}\left[Q_s^g(\overrightarrow{r'})+\frac{1}{k}Q_f^g(\overrightarrow{r'})\right] \quad (5)$$

with $\overrightarrow{r'}=\vec{r}-R\vec{\Omega}$, $R=\left|\vec{r}-\overrightarrow{r'}\right|$ and $d^3r'=R^2d^2\Omega dR$.

The collision probability approximation is a direct result of spatial discretisation; assuming that the domain can be decomposed into a number of regions *N*, each of volume V_i, over which the neutron cross sections can be taken uniform, equation 5 is multiplied by $\Sigma_t^g(r)$ and then integrated over V_i to obtain:

$$V_j\Sigma_{t,j}^g\phi_j^g=\sum_{i=1}^{N}\sum_{h=1}^{G}\left[\Sigma_{s,i}^{g\leftarrow h}+\frac{1}{k}\chi_i^g\nu\Sigma_{f,i}\right]\phi_i^hV_iP_{ij}^g \quad (6)$$

where

$$\phi_j^g=\frac{1}{V_j}\int_{V_j}d^3\,r\phi^g(\vec{r}) \quad (7)$$

is the average flux in the *j-th* region,

$$\Sigma_{x,j}^{g} = \frac{1}{V_j \phi_j^g} \int_{V_j} d^3 r \Sigma_x^g(\vec{r}) \phi^g(\vec{r}) \quad (8)$$

is the homogenised neutron cross section in the *j-th* region for reaction of type *x* and

$$P_{ij}^{g} = \frac{1}{4\pi V_i} \int_{V_i} d^3 r' \int_{V_j} d^3 r \Sigma_t^g(\vec{r}) \frac{e^{-\tau^g(R)}}{R^2} \quad (9)$$

is the probability that a neutron born in region *i* will make its first collision in region *j*, i.e. the collision probability. Here, calculation of collision probabilities is not discussed and interested readers are referred to the literature [4] [5].

Equation 4 can be written in matrix notation:

$$(I - PS_c)\Phi = \frac{1}{k} PF\Phi \quad (10)$$

where Φ is a column vector of dimension $N \times G$, P is a block diagonal matrix of order $N \times G$ whose block diagonals are collision probability matrices in each energy group, I is the identity matrix, S_c is the scattering matrix and F is the fission production matrix. Equation 10 is an eigenvalue problem that takes the form:

$$A\Phi = \lambda B\Phi \quad (11)$$

where $A = (I - PS_c)$ and $B = PF$ with $\lambda = \frac{1}{k}$ eigenvalue and Φ eigenvector. This equation admits $N \times G$ distinct eigenpairs as solutions; the eigenpair (λ_1, Φ_1) corresponding to the smallest eigenvalue is the fundamental neutron flux and those with larger eigenvalues represent high order modes.

3. Neutron flux modes solver in DRAGON

Different methods exist for finding the high order flux modes of the transport equation. The subspace iteration method is a generalisation of the power iteration method for finding the fundamental mode [6]. This method is characterised by poor convergence and unreliability especially when large number of eigenpairs are required. Deflation techniques can be also used to extract high order modes one at a time [7]. These techniques also suffer from slow convergence in addition to instability and error accumulation problems. One of the most stable and reliable approaches for finding the eigensolutions of matrix eigenvalue problems is the QZ decomposition method [8]. This method is implemented in DRAGON for finding the modal solutions of the transport equation in the collision probability approximation.

The generalised Schur decomposition or QZ decomposition method is a stable and reliable method for finding the full spectrum, i.e. eigenpairs, of the eigenvalue problem in equation 11. A drawback of QZ decomposition is the large demand for computer resources as the system matrices, which are dense in most cases, need to be built explicitly. In this method, matrices *A* and *B* are written in the form:

$$A = QSZ^T \text{ and } B = QTZ^T \quad (12)$$

where matrices *S* and *T* are two unitary matrices giving the Schur forms of *A* and *B* respectively and matrices *Q* and *Z* are two upper triangular matrices. The *i-th* eigenvalue of equation 11 is calculated from the diagonal elements of *S* and *T*:

$$\lambda_i = \frac{1}{k_i} = \frac{S_{ii}}{T_{ii}} \tag{13}$$

In order to arrive at the forms described in equation 12, the algorithm proceeds in two steps. A first factorisation of matrices *A* and *B* is performed:

$$A = Q_1 H Z_1^T \text{ and } B = Q_1 K Z_1^T \tag{14}$$

where *H* is an upper Hessenberg matrix, matrices Q_1 and Z_1 are two unitary matrices and *K* is an upper triangular. Then, a second factorisation of matrices *H* and *K* is performed:

$$H = Q_2 U Z_2^T \text{ and } K = Q_2 V Z_2^T \tag{15}$$

where Q_2 and Z_2 are two unitary matrices and *U* and *V* are two upper triangular matrices. The eigenvalue problem of equation 11 can be rewritten by orthogonal transformation into:

$$H\Phi_i' = \frac{1}{k_i} K\Phi_i' \tag{16}$$

where Φ_i' is an eigenvector in the transformation subspace. Equation 16 is simple to solve for any eigenvector since matrices *H* and *K* are upper Hessenberg and upper triangular respectively. In order to retrieve the eigenvectors of the original problem, a back transformation is performed by pre-multiplying the eigenvectors Φ_i' by $Z_1 Z_2$:

$$\Phi_i = Z_1 Z_2 \Phi_i' \tag{17}$$

4. Verification and example results

In order to verify the modes solver, two case studies are evaluated. The first case study is a PWR 17x17 fuel assembly and the second is a CANDU6 super-cell. The neutron flux modes are calculated in two energy groups: a thermal group corresponding to neutrons with less than 0.625eV and a fast group of neutrons having higher energies. The solution of the flux modes in both cases is verified by considering the residual vector *R* defined as:

$$R = A\Phi_i - \lambda_i B\Phi_i \tag{18}$$

Convergence of the solution to the flux modes is assured when the residual vector is close to zero. Verification and results are presented in the next subsections.

4.1 Case study 1: PWR fuel assembly

A PWR fuel assembly consisting of 17×17 cells with dimensions of 21.42×21.42cm^2 is considered. The assembly comprises 264 fuel square cells, each with dimensions of 1.26×1.26cm^2, with three regions. The central region is a 3% enrichment uranium dioxide pellet with a radius of 0.41cm; the second region is a zircaloy cladding with outer radius of 0.475cm. The outer region is water moderator. The remaining 25 cells represent guide tubes for control mechanism and instrumentation. These cells are also 1.26×1.26cm^2 in dimension with three regions. The central region is water filled with a radius of 0.56cm. The second region is zircaloy cladding with an outer radius of 0.62cm. The outer region is water moderator. The configuration is shown in figure 1 where black regions are fuel pellets, red regions are cladding, yellow regions are moderator and white regions are moderator filled guide tubes.

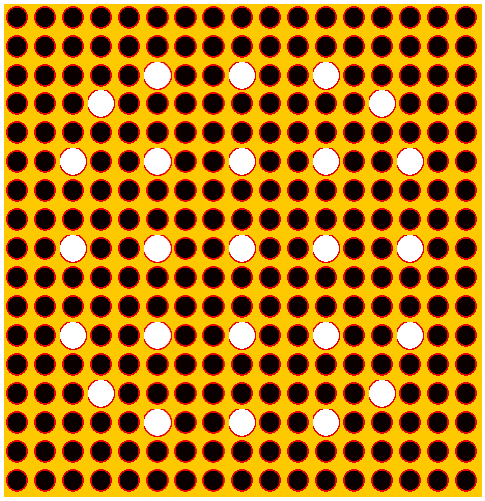


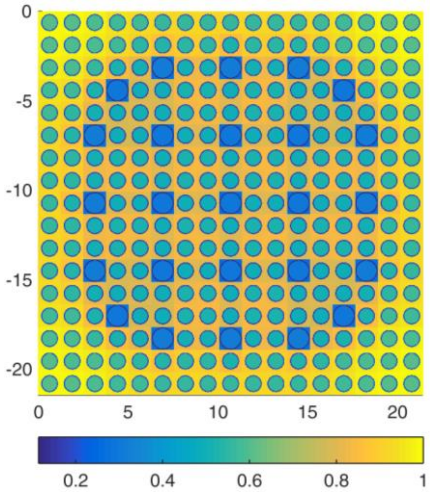
Figure 1 Configuration of a 17x17 PWR assembly

Experience with this case shows slight sensitivity to the mesh size with insignificant changes in the eigenvalues observed when using very fine spatial mesh. The described configuration contains a total of 867 regions which means that 1734 flux solutions can be found using this QZ decomposition. The first 50 modes, those with the largest *k*-eigenvalue, are calculated. In Table 1, the multiplication factors and the euclidean norm of the residual vector for calculated eigenpairs are presented. The norm of the residual is of the order 10^{-14} which means that the solver succeeds in calculating the eigensolutions of the collision probability approximation. Furthermore, the eigenvalue of the fundamental mode compares well to a reference value estimated by the flux solver of DRAGON which is 1.072501. The eigenvalues presented in Table 1 show that a number of modes have relatively large multiplication factors which might indicate that their excitation amplitudes in the general solution could be relatively large. In addition, their contribution to the contamination of the fundamental solution obtained by power iterations in transport codes might be considerable.

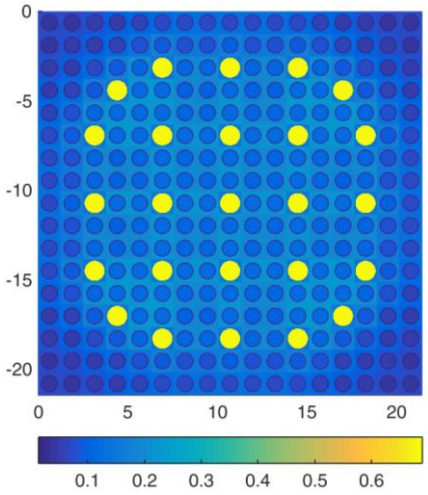
Among the calculated 10 dominant modes, only the fundamental mode is positive, hence satisfies all the conditions of the problem. The first 6 modes are plotted in figures 2 and 3. The normalisation of the modes is performed such that the largest element of each mode Φ_i has an absolute value of 1.

Table 1 Eigenvalues and Euclidean norm of residual for 10 dominant modes – PWR Assembly

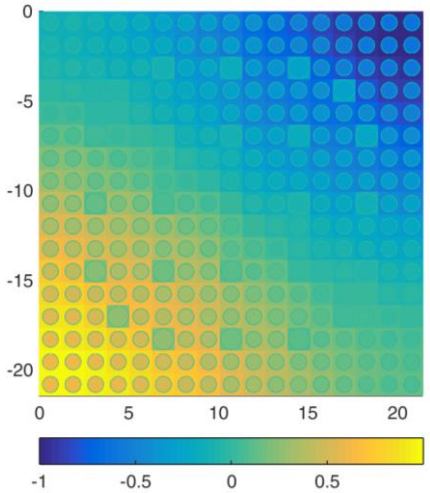
Mode	K-Eigenvalue	Norm of residual	Mode	K-Eigenvalue	Norm of residual
1	1.0725004054	3.48E-014	11	0.0956223218	2.70E-015
2	0.6221028818	1.30E-014	12	0.0881488218	2.54E-014
3	0.6221028395	1.30E-014	13	0.0700234113	3.34E-014
4	0.3811255801	7.91E-015	14	0.0573216769	1.81E-014
5	0.2484900721	5.70E-015	15	0.0573216765	1.17E-014
6	0.2216925267	5.51E-015	16	0.0503413277	1.79E-015
7	0.1674975662	8.65E-014	17	0.0493087525	2.79E-015
8	0.1674975551	6.25E-014	18	0.0443510717	2.07E-014
9	0.0970887507	1.15E-014	19	0.0443510703	9.95E-015
10	0.0970887489	1.46E-014	20	0.0403998017	1.14E-014



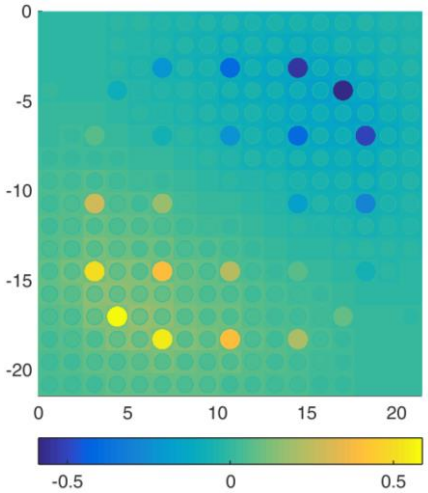
(i) Mode 1 – Fast group



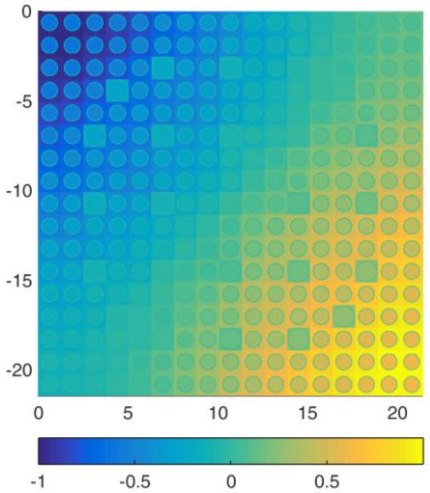
(ii) Mode 1 – Thermal group



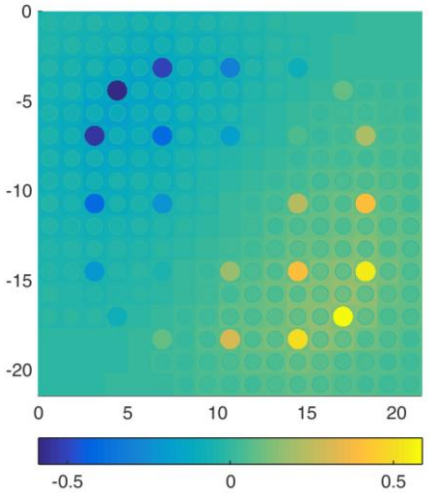
(iii) Mode 2 – Fast group



(iv) Mode 2 – Thermal group

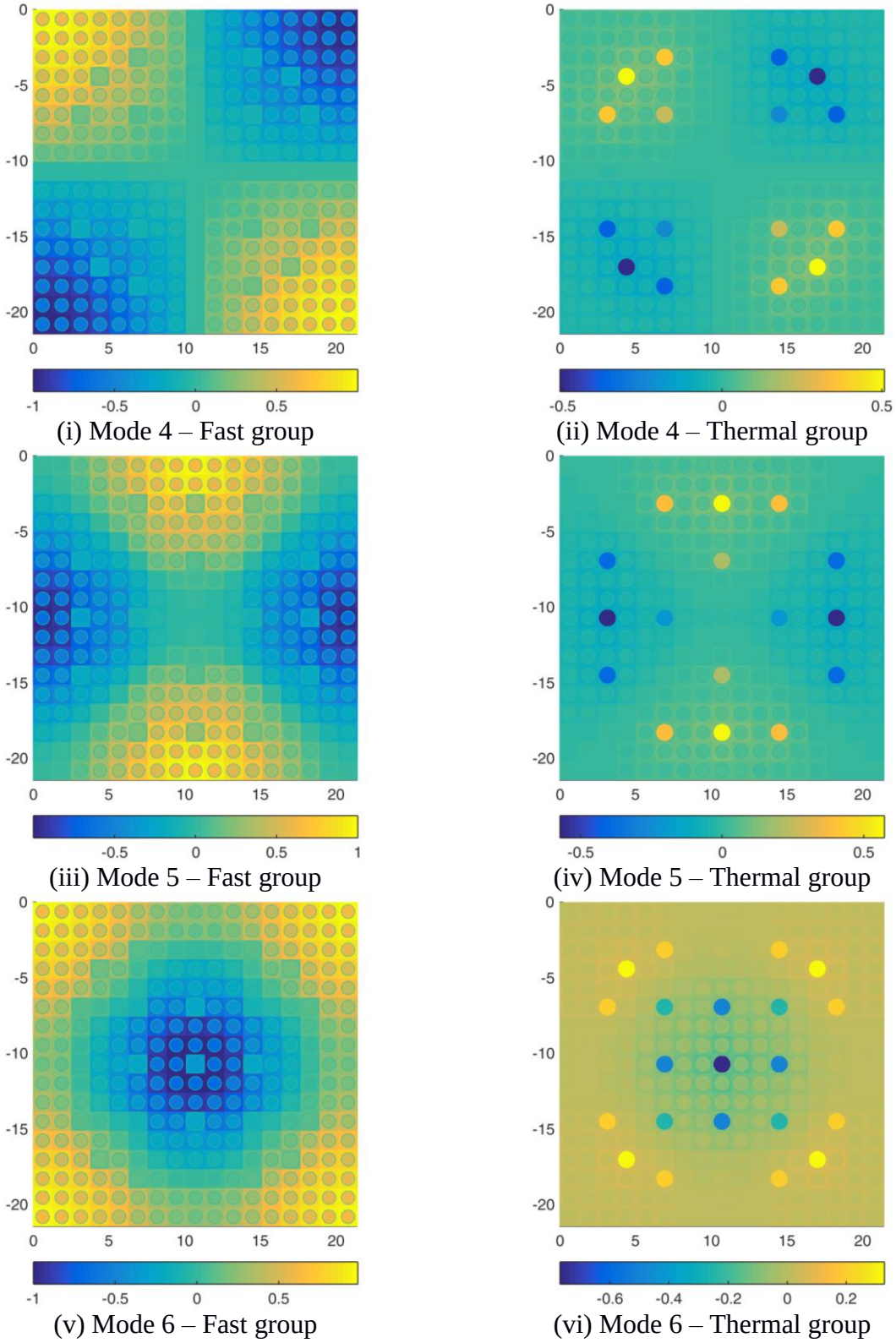


(v) Mode 3 – Fast group



(vi) Mode 3 – Thermal group

Figure 2 Modes 1, 2 and 3 in both energy groups – PWR Assembly



(i) Mode 4 – Fast group

(ii) Mode 4 – Thermal group

(iii) Mode 5 – Fast group

(iv) Mode 5 – Thermal group

(v) Mode 6 – Fast group

(vi) Mode 6 – Thermal group

Figure 3 Modes 4, 5 and 6 in both energy groups – PWR Assembly

4.2 Case study 2: CANDU-6 super-cell

The neutron flux modes of a CANDU-6 super-cell shown in figure 4 are studied. The super-cell comprises 4 unit cells each composed of a single fuel cluster of 37 natural enrichment fuel rods (dark blue) clad in zircaloy (light blue). The fuel rods are arranged in a pressure tube of zircaloy (yellow) and surrounded by heavy water coolant (light green). The pressure tube is placed at the centre of a calandria tube made of zirconium-niobium alloy (red) and is surrounded by thermal insulator of helium (orange). The outer space of the calandria tube is the heavy water moderator (dark red).

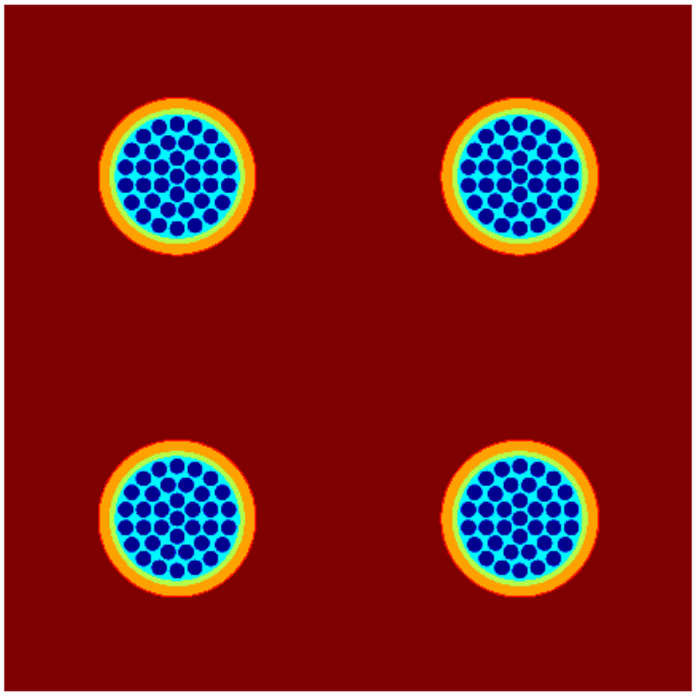


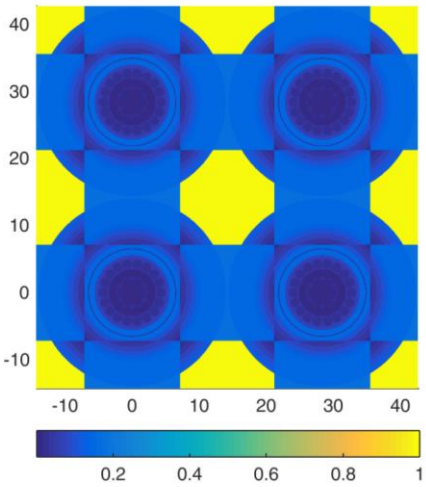
Figure 4 CANDU-6 Super-cell of four unit cells

Each unit cell has the dimensions of $28.575 \times 28.575 cm^2$. The fuel pellets have a radius of 0.6122cm and the cladding thickness is 0.0418cm. The pressure tube has an inner radius of 5.1689cm and an outer radius of 5.6032cm. The inner radius of the calandria tube is 6.4478cm and its outer radius is 6.5875cm. By using a trial and error approach, it is found that the modes calculation for the CANDU case is very sensitive to the level of details in the definition of the geometry and the phase space mesh. In each unit cell, the moderator is split radially into 10 regions, while the coolant is split into 6 radial regions. 37 fuel pins are defined explicitly in each fuel cell without taking advantage of geometrical symmetries. In addition, each unit cell is split into 4 sub-cells in the *x*-direction and 4 sub-cells in the *y*-direction. Hence, a total of 264 regions per unit cell are defined. With 2 energy groups and 984 regions for the super-cell, a total of 1968 neutron flux modes can be calculated. The eigenvalues and the Euclidean norm of the residual for the first 10 dominant modes are shown in table-2.

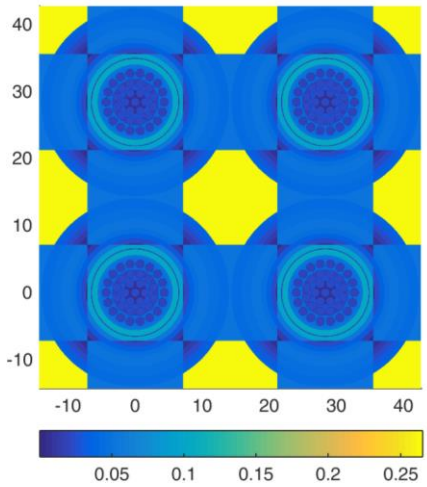
Table 2 Eigenvalues and euclidean norm of residual for 20 dominant modes – CANDU6 Super-cell

Mode	K-Eigenvalue	Norm of residual	Mode	K-Eigenvalue	Norm of residual
1	1.1164101843	7.68E-15	11	0.0323552471	2.90E-14
2	0.4258407851	3.47E-15	12	0.0308200276	1.51E-14
3	0.4256994184	3.74E-15	13	0.0177152045	4.14E-16
4	0.2630152439	2.23E-15	14	0.0172607333	1.09E-15
5	0.0374918420	8.80E-16	15	0.0172597910	2.32E-15
6	0.0370831366	8.58E-16	16	0.0169190832	2.62E-15
7	0.0346434974	1.15E-14	17	0.0154444790	2.00E-15
8	0.0342833386	3.03E-14	18	0.0153769528	9.72E-15
9	0.0326774822	6.73E-15	19	0.0153769301	1.02E-14
10	0.0324427165	2.39E-14	20	0.0153300121	2.61E-15

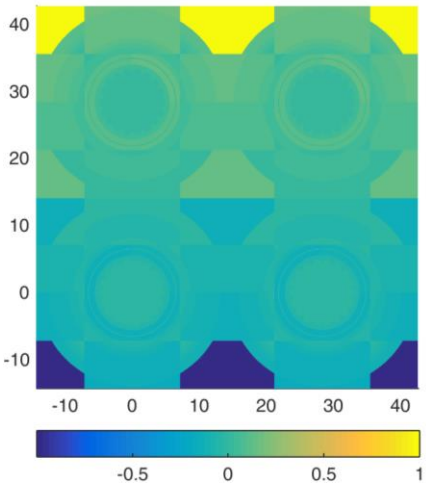
The Euclidean norm of the residual is in the order 10^{-14} which confirms the convergence of the solutions obtained to the neutron flux dominant modes. Furthermore, the eigenvalue of the fundamental modes agrees well with the reference value obtained by the DRAGON main flux solver which is 1.116393.
The CANDU-6 super-cell case shows that the eigenvalues of the dominant modes are well below that of the fundamental mode with a dominance ratio of 0.38. Perhaps, this might be attributed to the loose neutronic coupling between the elements of the CANDU lattice. Unlike the PWR case, the contribution of the dominant modes to the contamination of the fundamental mode obtained by power iterations can be assumed to be of less importance.
Again, only the fundamental mode among the calculated modes represents a positive distribution over the full phase space. The first 6 dominant modes for the CANDU-6 super-cell are shown in figure 5 and 6. The normalisation of the modes is performed such that the largest element of each mode Φ_i has an absolute value of 1.



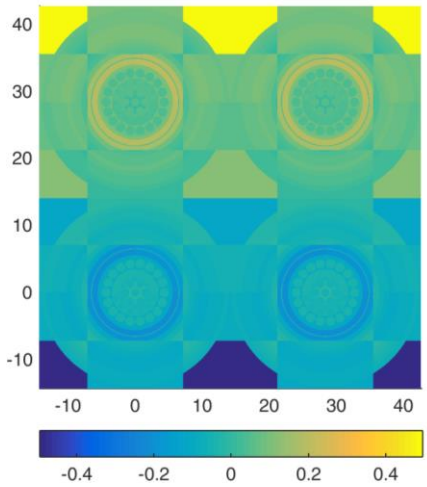
(i) Mode 1 – Fast group



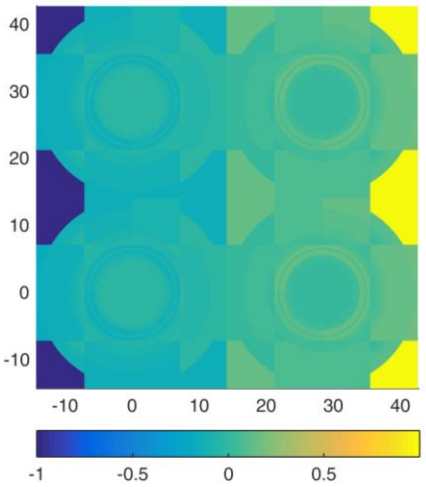
(ii) Mode 1 – Thermal group



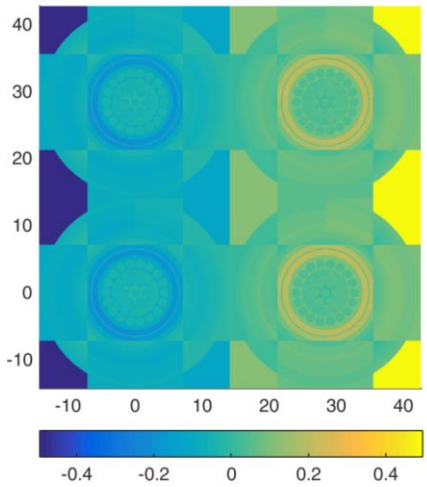
(iii) Mode 2 – Fast group



(iv) Mode 2 – Thermal group

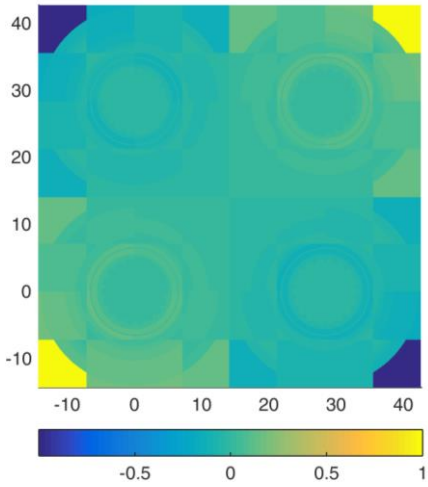


(v) Mode 3 – Fast group

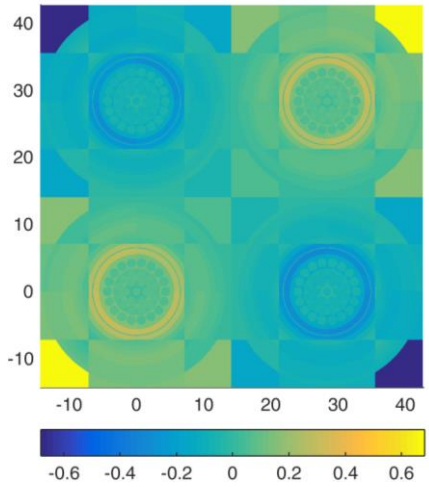


(vi) Mode 3 – Thermal group

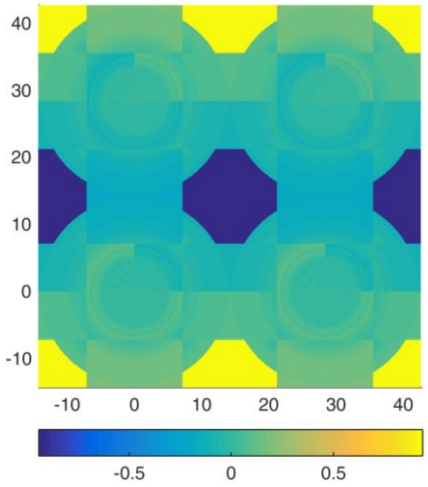
Figure 5 Modes 1, 2 and 3 in both energy groups – CANDU6 Super-cell



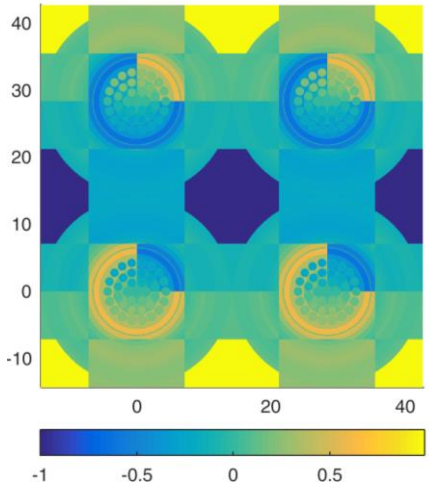
(i) Mode 4 – Fast group



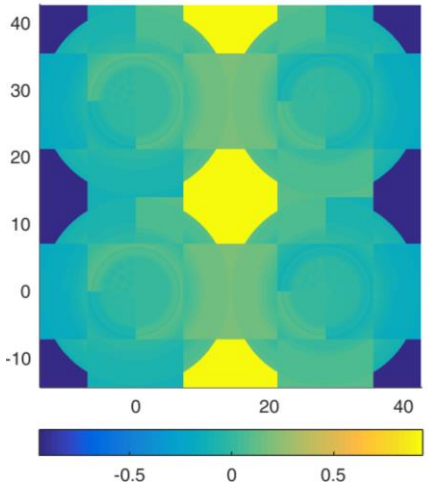
(ii) Mode 4 – Thermal group



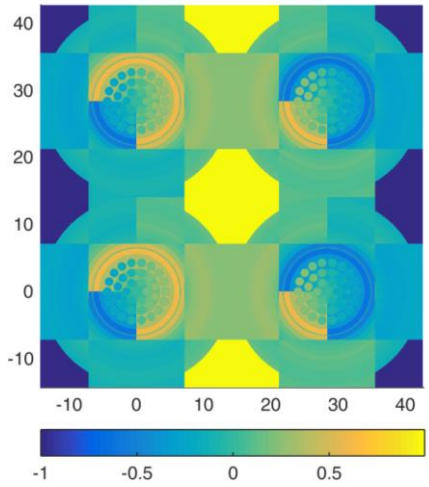
(iii) Mode 5 – Fast group



(iv) Mode 5 – Thermal group



(v) Mode 6 – Fast group



(vi) Mode 6 – Thermal group

Figure 6 Modes 4, 5 and 6 in both energy groups – CANDU6 Super-cell

5. Conclusions and future work

A new solver dedicated for finding the high order modes of the transport equation is implemented in DRAGON 5. The solver is based on a QZ decomposition approach for finding the eigensolutions of the collision probability approximation. The solver is tested successfully for finding the neutron flux harmonics in two case studies. Despite the lack of interest in the high order solutions of the transport equation, the work is motivated by possible important applications of these in perturbation studies and flux synthesis.

The fundamental mode describes the unperturbed shape of the neutron flux over the reactor domain. Under small perturbations, one or more of the higher order modes may become excited and perturbations around the fundamental mode are expected. Such perturbations can be mathematically described by changes in the amplitudes of the excited modes. Given the large number of possible perturbations that need to be considered during reactor design and analysis, it becomes impractical to perform independent analysis for each considered case. A more practical option is the study of the excitation of the higher order perturbation modes.

Another field where high order flux modes are found to be useful is flux synthesis or mapping. As mentioned before, the generalised solution of the transport equation can be written as a series summation of the modes. Assuming that a set of modes are already calculated on a fine mesh and a reference flux at a coarse mesh is available, it is possible to reconstruct the flux at a fine mesh to good accuracy using modal expansion. It is sufficient to calculate the modal amplitudes in order to map the flux distribution over the fine mesh without the need for performing an independent full calculation.

Note that the technique described here can also be used to evaluate the modes of the diffusion equation. However, while the transport modes are evaluated at the cell (or assembly) level, the modes of the diffusion equation are evaluated on the full reactor with a flat spatial variation inside each cell (or assembly). As a result, the transport modes give more flexibility for flux reconstruction in addition to providing the information required for pin power reconstruction.

Future work focuses on understanding the uses and implementing methods for utilisation of the high order neutron flux modes in perturbation studies and flux synthesis.

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7. References

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