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A New Method for the Treatment of Local Strong Heterogeneities and its Application to the Phebus Experimental Facility

Enrico Girardi[1], Jean-Michel Ruggieri[*1], Patricia Sireta[1] and Guillaume Ritter[1]
[1]*Commissariat à l'Energie Atomique, Cadarache, 13108 - St-Paul Lez Durance, France*

This paper describes an application of our recently-developed decomposition method (Multi-method/multi-domain), showing its benefits, in terms of accuracy and computational time. The chosen application is a benchmark model of the PHEBUS experimental facility at CEA Cadarache. This benchmark is presented and we explain why it is relevant to problems with strong local heterogeneities. The discretization method is described and the results are presented and discussed. The main result is that this method allows us to reduce the CPU time by a factor of 3, while preserving the accuracy of the neutronic indicators: 50 pcm for reactivity, $\leq 1\%$ for the flux relative error and ≤ 0.1 % for the core-to-bundle power coupling coefficient.

KEYWORDS : Transport Calculation, Heterogeneities, Local refinement, Domain Decomposition, Multi-Method/Multi-Domain, Phebus Reactor

1. Introduction

Classical techniques for solving the neutron transport equation consist of separating the neutronic calculation in several successive steps. First, very detailed (in energy and space) transport calculations are performed for a small region (usually one or a few assemblies); then, the results are condensed in energy and space to yield few groups homogenized cross sections. These collapsed cross-sections are then used in coarse mesh full core diffusion or simplified transport calculations to yield fluxes and reaction rates. Finally, detailed pin-by-pin fluxes and reaction rates are reconstructed from the coarse mesh results, using an interpolation scheme. Every step in this procedure involves approximations with a limited validity domain. Of particular concern is the treatment of strong localized heterogeneities such as experimental bundles in a reactor, which, in the classical approach, are smeared with the surrounding fuel and moderator regions. This homogenization treatment usually introduces non negligible errors in the neutronic calculations, which might not be compatible with expected experimental accuracy goals.

In this work, we apply a new calculation scheme to a benchmark model of the PHEBUS experimental reactor, to quantify the improvements in terms of accuracy on the neutronic quantities of interest and computing time. This new recently-developed approach [1] uses domain decomposition techniques and two kinds of transport methods. The first one, based on the first order transport equation, is a discrete ordinates (S_n) nodal and characteristics method (SNM) [2, 3] whereas the second one, based on the second order transport equation, is the Variational Nodal Method (VNM) developed by E.E. Lewis [4]. These coupled methods give us the capability to employ a very fine mesh in describing a particular fuel bundle with an appropriate numerical method (SNM), while using a much large mesh size in the rest of the core, in conjunction with a coarse-mesh method (VNM).

In the next section, our new calculation method and its properties are briefly presented. In Section 3, the benchmark problem is described. Finally, in the last two sections (Secs. 4, 5), the discretization is presented and the results are discussed.

[*] Corresponding author, Tel. (33) 4 4225 7052, FAX (33) 4 4225 7009, E-mail: jmruggieri@cea.fr

2. Multi-Method/Multi-Domain Method

Our domain decomposition method, named Multi-Method/Multi-Domain (MM/MD), is intended for full core calculations, with provisions for local changes in the solution technique. Many past studies on domain decomposition and mesh refinement techniques have focused on only one resolution method [5, 6, 7]. The present technique is base on two very different methods within the same domain decomposition algorithm. This is an original way to take advantage of different method properties within the same calculation.

The two methods coupled in the MM/MD method have the following characteristics :

1) the Discrete Ordinates Nodal Method (SNM) deals with :

   – the **Integro-differential** neutron transport equation :

$$[\hat{\Omega}\cdot\vec{\nabla} + \sigma(\vec{r})]\ \psi(\vec{r},\hat{\Omega}) = \left[K + \frac{1}{k_{\mathit{eff}}}F\right]\psi(\vec{r},\hat{\Omega})$$

   – the main unknown is the **angular flux** : ψ ;

   – spatial discretization is performed by expansion with Legendre polynomial basis ;

   – angular discretization is based on **discrete ordinates method** ;

2) the Variational Nodal Method (VNM) deals with :

   – the **Second-order** neutron transport equation :

$$\left[\hat{\Omega}\cdot\vec{\nabla}(-\frac{1}{\sigma(\vec{r})}\,\hat{\Omega}\cdot\vec{\nabla}) + \sigma(\vec{r})\right]\ \psi^{+}(\vec{r},\hat{\Omega}) = \left[\tilde{K} + \frac{1}{k_{\mathit{eff}}}F\right]\psi^{+}(\vec{r},\hat{\Omega})$$

   – the main unknowns are the **even-parity flux**, ψ^{+}, within each node, and the **odd-parity flux**, ψ^{-}, on the interfaces ;

   – spatial discretization is performed by expansion with Legendre polynomial basis ;

   – angular discretization is based on **spherical harmonics** expansion.

The first method, SNM, is very useful to obtain a very good local accuracy [2, 3, 8] because the spatial convergence criterion is the size of the mesh, it is a h-type convergence method: the smaller the mesh is, the more accurate the result is. This method is commonly used for assembly transport calculations. The second method, VNM, is a very powerful method for coarse mesh transport calculation [9, 10, 11]. The convergence criterion is the order of the polynomial basis we used for the expansion of the flux, it is a p-order convergence method: the higher the polynomial expansion is, the more accurate the result is. This method is usually employed in full core transport calculations.

The global MM/MD algorithm requires the solution of an eigenvalue problem with multigroup approximation. This algorithm imposes to solve, for each iteration of the power method, a one-speed equation for each group. The presence of several sub-domains doesn't affect the multigroup iterator; only the fission rate contribution for each sub-domain have to be collapsed to build the total fission rate and calculate the global eigenvalue. In order to solve the one-speed problem over the whole domain, iterations are done over the sub-domains [12]. The boundary conditions that represent the connection between sub-domains are computed by specific coupling operators [1].

3. PHEBUS' Benchmark Description

PHEBUS is a small, water cooled, experimental power reactor dedicated to the study of accidental transients [13]. An experimental fuel bundle is located in a dedicated separate loop in the middle of the core. In the PHEBUS-FP experiments, this central bundle is first irradiated for 9 days in a high water cooling flow; then it is heated up for 5 hrs in a monitored low rate steam flow environment (the water cooling circuit is turned off) until fuel meltdown. During this latter phase, the experimental fuel releases FP's in the form of gases and aerosols. The evaluation of this radiological source term is the goal of the PHEBUS-FP program. As a consequence, the power produced by the experimental bundle is an important normalization factor both for thermal degradation and chiefly for fission products release.

The neutronic characterization of PHEBUS is a major challenge that require a specific computation scheme as well as a dedicated validation case. The main features to be evaluated are reactivity parameters and power monitoring indicators. Integral and local power indicators are required with a very good accuracy in order to define the conduct of test strategy and also to allow an interpretation of the experiment.

Apart the central fuel element, the PHEBUS core does not present any major difficulty for modern neutronic tools. On the contrary, the neutronic characterization of the experimental bundle is very complicated. Indeed there are numerous heterogeneities among which vapor/fuel interfaces, absorbing material in the control rod, but also the experimental fuel burn up and eventually the experimental bundle geometrical evolution during the heat up phase. This is why a mixed calculation scheme seems appropriate, with a refined computation scheme for the bundle and a coarser model for the rest of the core.

To be able to analyse the benefit of the MM/MD method for the treatment of the local heterogeneities in the PHEBUS experiments, a benchmark of one configuration has been defined. In this benchmark, a horizontal 2D section has been considered, in which the bundle and the core are approximated in Cartesian geometry. The original geometry is presented with the benchmark model in figure 1. The benchmark model is defined by 13 homogeneous materials. Three regions correspond to the moderator, the reflector and the vessel. The pin cells in the core have been homogenized so that there are only two core regions. Finally, the bundle is described with eight different homogeneous regions.

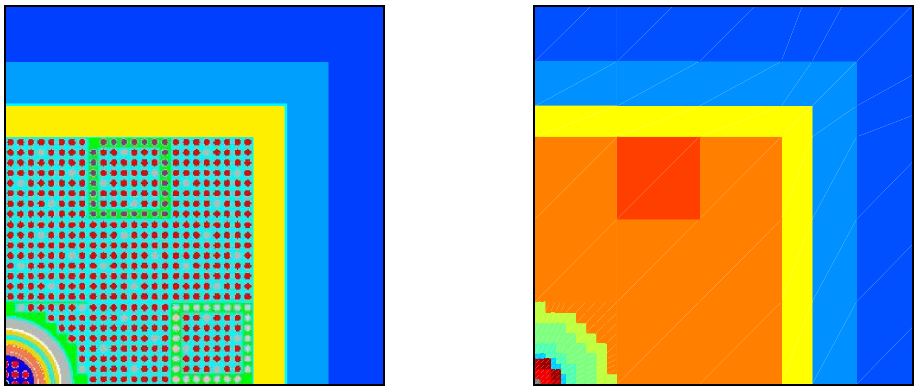


Figure 1: Original geometry and corresponding benchmark model for the PHEBUS core

The core-to-bundle power coupling coefficient is defined as the ratio of the energies released in both the core and the bundle. This coupling coefficient is obtained from a calculation which requires a good prediction of the core overall power and an even better prediction of the bundle integral power. The expected overall accuracy in this parameter is between 5% and 10%.

To obtain the neutronic characteristics of this model, a classical calculation scheme has been used: a 172 energy groups and detailed collision probability transport calculation has been performed for each sub-assembly. The results are, then, condensed in 4 energy groups and homogenized, to yield the 13 materials cross sections. These sections have been calculated with the APOLLO 2 cell code [14].

The neutronic quantities to be evaluated are : the reactivity, the flux shape in each energy group in the bundle and the core-to-bundle power coupling coefficient.

4. Problem Discretization

In order to compare all calculations performed in this study, we first produce a reference solution for the benchmark problem. This reference scheme is obtained with a fine mesh, high order S_n calculation (S_8), in order to take into account spatial and angular flux dependency. A particular attention is needed for thermal group which present the characteristic peak at the interface core-moderator (see Fig.5). The reference mesh (see Fig.2) is 1 mesh per cell for the core, 2 cm square mesh for the moderator, 2 meshes in the reflector thickness and 2 in the aluminum vessel.

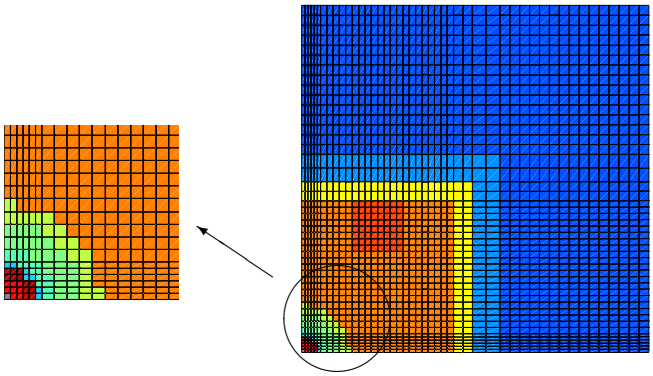


Figure 2: One-domain, conformal computational mesh : reference grid

This choice gives a good reactivity and flux prediction, with a reasonable computational time in 2D calculations. This reference discretization represents a standard PHEBUS calculation mesh in the case that no local refinement method is available.

Let us consider the discretization strategy that has been adopted to combine the two types of methods in the same calculation. For that, let us define a 2-subdomain partition for the MM/MD method: the first one is located in the SW corner, containing the bundle and the second one contains the surrounding core. This allows us to independently define the computational mesh for each subdomain. Indeed, this partition has been done to keep in the bundle zone the very fine description of the reference mesh and a relatively coarse mesh discretization in the other sub-domain. So, a good local accuracy can be expected for the experimental bundle with SNM, while accurate global core predictions should be obtained with VNM.

To reach our goal, four computational grids have been chosen (see Figs. 3 and 4). The four grids have the same fine reference mesh to discretize the bundle in sub-domain 1. So, the only difference, between them, is the mesh discretization of the core in sub-domain 2.

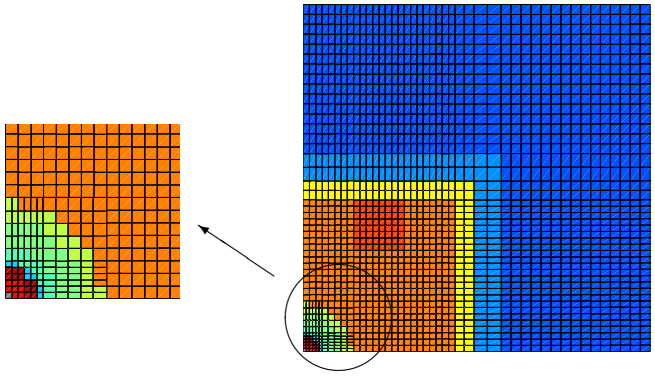
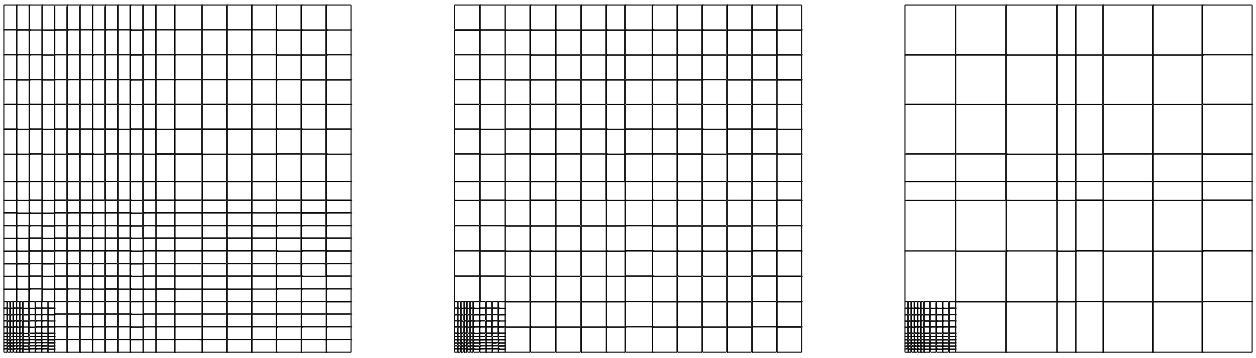


Figure 3: Two-domains, non-conformal computational mesh : Grid 1

The first grid (Fig.3) looks closely like the reference mesh (Fig.2), with one fundamental difference, permitted by the MM/MD method: a non conformal mesh is used at the interface between the two sub-domains. The mesh in the core corresponds to 1 mesh per cell in the core, 15 meshes in the moderator region, 2 in the reflector and 2 in the aluminum box.

The second grid, Grid 2, and third grid, Grid 3, have coarser meshes in the core: 4 by 4 meshes for (Grid 2) and 2 by 2 for (Grid 3), but they both have 6 meshes in the moderator region, one in the reflector and the aluminum box. Finally, the last computational mesh, Grid 4, has 1 coarse mesh per assembly in the core and 3 meshes in the moderator.



Grid 2 Grid 3 Grid 4

Figure 4: Coarse computational mesh grids employed in PHEBUS calculations

In all calculations, to enforce accuracy, the reference S_8 angular discretization of SNM is kept in the sub-domain containing the bundle. With these four grids, the analysis of MM/MD calculations, in terms of accuracy and computing time, is presented below for different approximations of the VNM or SNM methods in the second subdomain.

5. Results and Discussions

Two series of calculations are discussed. In the first one, we explore the capability of the MM/MD algorithm of providing local refinements in space and angle with SNM in both sub-domains. In the second part, the mixed SNM/VNM method with local mesh refinement is tested, using VNM in the second sub-domain.

5.1 Phebus benchmark: $\mathbf{S_8 - S_n}$ coupled calculations

In this part, we present local refinement calculations for SNM with :

- S_8 in the sub-domain 1 containing the bundle
- S_n for $n = 4, 6, 8$ in sub-domain 2.

As the SNM method could have trouble with meshes having a too important optical thickness, the calculations are performed only with Grid 1, 2 and 3. Results are reported in Tab.1.

In this table, the interesting parameters of the benchmark are given. On the one hand, reactivity ρ, core-to-bundle power coupling coefficient C and the flux error in the bundle subdomain, give a global indication of calculation accuracy compared to the reference calculation. On the other hand, the computational time is presented with S_2-Boundary Projection Acceleration [15] of inner iterations (t_{BPA}) or without acceleration (t_{noAcc}).

Mesh Grid	Bundle	Core	ρ	err_ρ	flux err	C	err_C	t_{BPA} (s)	t_{noAcc} (s)
Reference	S_8		6763	-	-	50.95	-	18.06	196.3
Grid 1	S_8	S_8	6764	1	0.02 %	50.98	0.05 %	41.69	189.2
	S_8	S_6	6746	17	0.04 %	50.57	0.75 %	35.72	121.2
	S_8	S_4	6709	55	0.24 %	49.55	2.76 %	30.65	67.3
Grid 2	S_8	S_8	6762	1	0.06 %	50.99	0.07 %	11.76	48.4
	S_8	S_6	6749	14	0.05 %	50.60	0.69 %	10.21	34.0
	S_8	S_4	6711	51	0.25 %	49.58	2.69 %	9.19	22.0
Grid 3	S_8	S_8	6622	140	0.57 %	50.71	0.47 %	6.97	30.0
	S_8	S_6	6603	159	0.57 %	50.32	1.24 %	6.55	25.4
	S_8	S_4	6563	200	0.81 %	49.30	3.24 %	5.44	16.1

Table 1: Phebus calculation $S_n - S_m$ coupling

Reference calculation results are contained in the first line of the table and reference flux shapes for the four groups are given in figure 5. These flux shapes show the difficulty to calculate the neutronic parameters of this benchmark while keeping CPU time reasonable.

First, neutronic parameters are analysed. The error made in the flux in the bundle subdomain never exceed 1%, so the solution in subdomain 1 is very accurate. Therefore, in this case, it is not a discriminant parameter for the method.

Reactivity and power coupling coefficient are more discriminant. From the reactivity point of view, a discrepancy of less than 100 pcm is assumed to be in good agreement with the reference calculation. None of the solution obtained on grid 3 meet this criterion. This is not surprising as we expected that this grid would not be appropriate for the SNM method ($O(h)$ type of convergence).

For the coefficient C, the expected target of 5% accuracy, translate into a maximum error of about 1% vs the reference calculation. So, the solutions based on $S_8 - S_4$ angular discretization are not accurate enough.

The conclusion of this first part is that, for this benchmark, the most interesting calculation performed by the MM/MD with SNM $S_8 - S_n$ coupled calculation, with local refinement method, is the $S_8 - S_6$ discretization on Grid 2. Indeed, compared to the reference calculation, the numerical results for all parameters are very good and the computing time is reduced by a factor of about 2.

5.2 Phebus benchmark: $\mathbf{S_8 - P_n}$ coupled calculations

In this section, the coupled SNM/VNM method and local mesh refinement are tested using MM/MD with VNM in the second sub-domain, keeping the S_8 method in sub-domain 1.

In contrast to the preceding case, we don't expect any problem with the mesh size thickness, by using an appropriate high order polynomial expansion for the even parity flux for VNM. The calculation on Grid 1 has not been performed, our analysis focusing on Grids 2, 3 and 4. For each grid, the following angular expansions have been performed : P_1, SP_3, SP_5, and P_3. The results are reported in table 2.

All solutions obtained with $S_8 - P_1$ calculation present an important discrepancy in terms of reactivity and bundle flux error compared to the reference solution. These results can be easily explained by the fact that the VNM P_1 method is very close to diffusion theory, so that it accounts poorly for transport effects.

The other coupled $S_8 - (S)P_n$ calculations provide more interesting results. The flux error in the bundle subdmain, and power coupling coefficient error do not exceed 1%. From the reactivity point of view, the $S_8 - P_3$ calculation gives the best results ($\leq$ 50 pcm), compared to $S_8 - SP_n$ (100 $\div$ 125 pcm).

The most accurate calculation obtained with the mixed SNM/VNM method is the $S_8 - P_3$ discretization on Grid 4. This case produces results very close to the reference case. It is about three times faster than the reference case and about 1.5 times faster than the "best" $S_n - S_m$ calculation.

Mesh Grid	Bundle	Core	ρ	err_ρ	flux err	C	err_C	t_{BPA} (s)	t_{noAcc} (s)
Reference	S_8		6763	-	-	50.95	-	18.06	196.3
Grid 2	S_8	P_1	6279	483	2.16 %	50.08	1.72 %	6.45	11.7
	S_8	SP_3	6639	124	0.95 %	50.65	0.59 %	10.95	15.4
	S_8	SP_5	6644	118	0.97 %	50.66	0.57 %	15.88	20.0
	S_8	P_3	6710	52	0.53 %	50.90	0.11 %	24.55	27.7
Grid 3	S_8	P_1	6285	478	2.18 %	50.08	1.71 %	3.61	10.1
	S_8	SP_3	6643	119	0.94 %	50.65	0.59 %	4.69	11.6
	S_8	SP_5	6648	115	0.96 %	50.66	0.57 %	7.66	13.4
	S_8	P_3	6729	34	0.53 %	50.90	0.10 %	9.78	16.7
Grid 4	S_8	P_1	6298	465	1.86 %	50.13	1.62 %	2.82	12.7
	S_8	SP_3	6653	110	0.72 %	50.70	0.50 %	3.57	13.3
	S_8	SP_5	6658	104	0.73 %	50.71	0.48 %	4.49	14.1
	S_8	P_3	6747	16	0.66 %	50.96	0.02 %	6.20	15.6

Table 2: Phebus calculation $S_n - P_m$ coupling

6. Conclusion

In this work, a new approach to take into account strong localized heterogeneities in transport core calculations is presented. This technique allows to distinguish, within a full core calculation, the capability to define several sub-domains where appropriate transport balance equation and resolution techniques can be used. Moreover, in each sub-domain the mesh size is independently refined to take advantage of the selected solution method.

To treat correctly local heterogeneities, this MultiMethod/MultiDomain decomposition method relies on two kinds of transport methods. The first one, a discrete ordinates nodal and characteristics method (SNM), is employed with highly refined meshes for the treatment of strong local heterogeneities. The second one, the Variational Nodal Method (VNM), is a powerful method for the treatment of the surrounding core, with a very coarse mesh discretization.

To show the efficiency of these techniques, a benchmark model of the PHEBUS reactor, in which a central experimental fuel element require a finer mesh description than the surrounding core, has been defined.

The numerical results, show very good accuracy of the coupling method for the most important neutronic indicators. The analysis of these results show that the best way to use the method is to define 2 sub-domains with the following characteristics:

Sub-domain 1 : Containing the bundle, discretized with reference fine mesh and SNM method with S_8 angular approximation;

Sub-domain 2 : The whole domain without the bundle, discretized with a very coarse mesh and VNM method with P_3 angular approximation.

The numerical accuracy is $\leq$ 50 pcm for reactivity, $\leq$ 1% for the flux relative error and 0.02 % for the power coupling coefficient with a cpu time three times smaller with respect to a reference full S_8 calculation.

These results are very encouraging and show that the MM/MD algorithm could be an effective way to reduce computational time in Phebus-like problems. We expect even better performance in the case of a 3D calculations.

In the future, we intend to investigate an unstructured characteristics solver in the MM/MD method. This will allow us to eliminate the modeling errors due to the Cartesian description of the bundle.

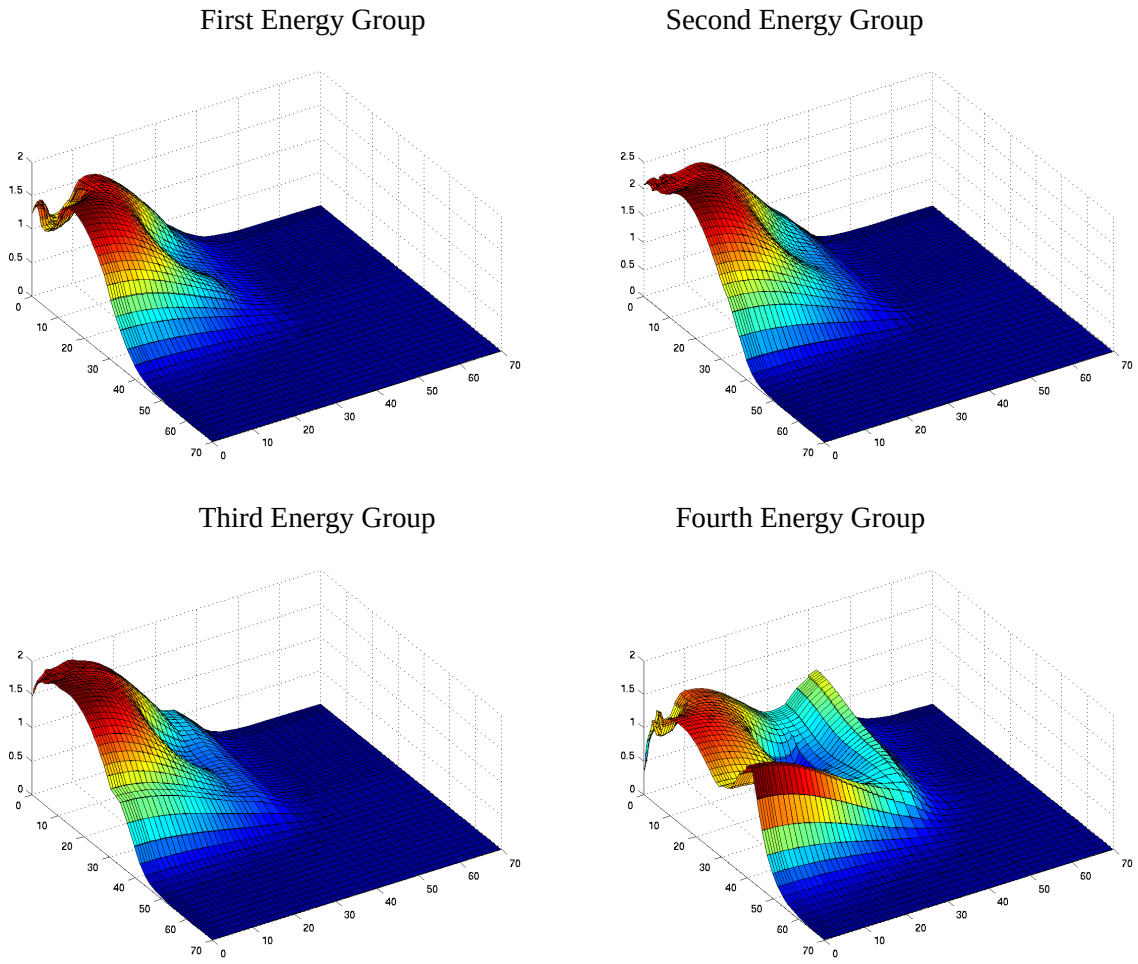


Figure 5: Flux shapes for the four energy group of PHEBUS benchmark

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