Solution of the multigroup neutron diffusion equations by the finite element method

Misfeldt, I.

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Solution of the Multigroup Neutron Diffusion Equations by the Finite Element Method

by

Ib Misfeldt

Abstract

The finite element method is applied to the multigroup neutron diffusion equations. General formulas are given for Lagrange type elements. Description of some 2D- and one 3D computer code is given. Several investigations are described and the results are presented. The capability of the 3D code is demonstrated on the 3D IAEA Benchmark problem. Suggestions for further work are given.

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3rd order FEM calculation
1. SHORT ABOUT THE ELEMENT METHOD

1.1 General

I have worked on the solution of the multigroup diffusion theory equation by the finite element method.

The inhomogeneous equation for one energy group is

\[-\nabla(D(r)\nabla\phi(r)) + E_r^*(r)\phi(r) - S_r(r) = 0 \quad \text{in} \quad \Omega \]  

and

\[ D(r) \frac{\partial \phi(r)}{\partial n} + \gamma(r)\phi(r) + q(r) = 0 \quad \text{on} \quad \Gamma \]

on the boundary \( \Gamma \) of \( \Omega \).

In the finite element method the domain \( \Omega \) is divided into a number of subdomains, \( \Omega_e \) each corresponding to an element, \( e \).

Within each element the flux, \( \phi(r) \) is approximated by a polynomial, \( \Theta(r) \). The coefficients in the polynomial are connected with the flux or the derivative of the flux, at corner points and other fixed points (called nodes or flux-points) in the element.

The flux in these fixed points (or derivative) is collected in a vector, \( \delta^e \) and the element interpolation function, \( N(r) \) is defined by the equation

\[ \phi(r) = N^T(r) \cdot \delta^e. \]

A characteristic for the element interpolation function is

\[ N_1(r_i) = 1 \quad \text{and} \quad N_j(r_i) = 0, \ j \neq i \]

where \( r_i \) is the flux-point with flux (or derivative of the flux) corresponding to \( \delta_1^e \).

It is shown (ref. 1) that the one group diffusion equation (1) is the Euler equation for the functional

\[ J[\phi] = \frac{1}{2} \int_\Omega (D \nabla \phi \nabla \phi^T - \Sigma_r^2 \phi^2 - 2q) \, d\Omega \]

\[ + \frac{1}{2} \int_\Gamma (\psi^2 + 2q) \, d\Gamma. \]  

(3)
The term $S(r)$ gives the coupling between the groups.

In variational calculation it is shown that the best approximation to the solution of the equations (1) + (2) within a given class of functions is the function which minimizes the functional (3). With the finite element approximation this minimum requirement leads to the equations

$$
\mathbf{K} \mathbf{A} + \mathbf{F} = \mathbf{0}
$$

where

$$(E)_{rs} = \sum_{e} (E^e)_{rs} \quad r,s = 1, 2, \ldots, M$$

$$(F)^e = \sum_{e} (F^e)^{T} \quad r = 1, 2, \ldots, M$$

the summations run over all elements in $\Omega$, $N$ is the total number of nodes (flux-points),

$$
\mathbf{E}^e = B^e \int_{\Omega^e} (\mathbf{V}^T \mathbf{W})^T (\mathbf{VW}) \, d\Omega + E^e \int_{\Omega^e} (\mathbf{W}^T \mathbf{W}) \, d\Omega + \gamma^e \int_{\Omega^e} (\mathbf{N}^T \mathbf{N}) \, d\Omega,
$$

$$
F^e = - \int_{\Omega} H^e \, d\Omega + q^e \int_{\Omega} M \, d\Omega
$$

$$
= \sum_{g=1}^{G} (S_{g^e \to g} \int_{\Omega} (\mathbf{N}^T \mathbf{N}_{g^e}) \, d\Omega + q^e \int_{\Omega} M_{g^e})
$$

$G$ = total number of groups

$$
S_{g^e \to g} = \left( \chi_{g^e \to g} + \gamma_{g^e \to g} \right),
$$

$\Omega^e$ is the external boundary for the element $e$. This is shown in details in ref. 2.

To solve the equations (4) one must know the element interpolation function, $N(r)$. When the interpolation function is fixed the integrals can be evaluated and the system of linear equations can be solved.

1.2 Element interpolation functions

I have decided only to consider element interpolation function of Lagrange type. They use only the flux and not the derivatives as parameters, which for me seems more reasonable than involving derivatives leading to difficulties at corner points between materials with different diffusion coefficients, though this difficulties have been treated (e.g. in ref. 6), it is only possible for rectangular mesh and I did not want to exclude the improvement obtainable by triangular mesh.

Fig. 1 shows Lagrange triangles and rectangles of dimension $m = 1, 2$, and $3$. 

Fig. 1. Lagrange triangles and rectangles of order 1, 2, and 3.
If we consider a triangle in the barycentric coordinate system, defined in fig. 2, we can easily show that \( N(L_1, L_2, L_3) \) for a Lagrange triangle of order \( m \) is defined by

\[
N_{p,q,r} = \frac{1}{p!q!r!} \cdot \prod_{s=0}^{p-1} \prod_{t=0}^{q-1} \prod_{u=0}^{r-1} s^p t^q u^r,
\]

where \( s(1) \) is the Stirling number of the first kind.

\( P_1 = (p, 0, 0) \) is the fixed fluxpoint corresponding to \( N_{p,q,r} \), the point with the flux \( \delta_1 \). This is shown in details in ref. 2.

For a rectangle of order \( m \) the used coordinate system is natural coordinates as defined on fig. 3.

The interpolation function \( N_j(\frac{1}{4}, \frac{3}{4}) \) is defined by

\[
N_j = N_{p,q} (\frac{1}{4}, \frac{3}{4}) = f_p (\frac{1}{4}) \cdot f_q (\frac{3}{4})
\]

\[
f_p (x) = \frac{(-1)^{m-p}}{p!(m-p)!} \sum_{j=0}^{m} s^j_{m,p} (mx)^j
\]

where

\[
s^j_{m,p} = s^j_{m+1,p+1} + p \cdot s^j_{m+1,p} + 1
\]

with these interpolation functions the equation (4) is easily set up.

**Fig. 2. Barycentric coordinates.**

**Fig. 3. Natural coordinates**
2. THE DEVELOPED PROGRAMS

During my work with the solution of the multigroup diffusion theory equation I have developed several programs. In the following chapter I will give a short description of the most important versions.

2.1 FEME

The program uses Lagrange triangles of arbitrary order, the group equations are solved by direct methods taking advantages of the sparsity in the matrices involved.

This method seemed very effective until the number of unknowns exceeded 1000 then the execution times rose drastically, in fact I could not exceed 1400 unknowns in a night's calculation.

The program is described in details in ref. 2.

2.2 Problems to be solved before the extension to 3D.

The number of unknowns for a realistic 3D calculation was expected to be 10 000 - 30 000 or even more, therefore it was clear that new solution techniques had to be found.

Another problem was the element shape, if I continued with the triangular shape (tetrahedron) in three dimensions the input-preparation would become very complicated unless the program could automatically divide box-formed meshes into tetrahedrons.

A third problem was the very large matrices that arise from the finite-element approximation in 3D calculations, as an example the matrix (H) for a 3rd order calculation with about 10 000 unknowns per group contains about 10^6 elements ≠ 0 per group.

2.3 FEMB

The solution of the problems was carried through in 2 dimensions, leading to the program FEMB.

The direct solution of the group equations was replaced by a pointwise successive overrelaxation. This method was found to be superior to the direct solution in most cases; only in very small unrealistic examples, the direct solution was faster. I can refer to a calculation which I and O.K. Kristiansen performed on a German Benchmark problem, representing a reactor where one control rod was accidentally removed, leading to a very high local reactivity. On this example the second eigenvalue was very near 1 which made it practically impossible for the direct method to converge (more than 1000 outer iterations were needed even though extrapolation was used).

With a good overrelaxation factor the iterative solution converged on less than 100 outer iterations with one inner per outer iteration. If I performed many (5 - 20) inner iterations per outer the same difficulty as with the direct solution arose.

I decided to use box-formed elements in the 3D program instead of tetrahedrons, this leads to a loss in flexibility, but the program became much easier to use.

The rectangular elements were examined in two dimensions and I found about the same accuracy as if the rectangles were divided into two triangles.

The third problem, the large matrices, was handled in the following manner. I did naturally take full advantage of the sparsity of the matrices, furthermore their elements are stored on backing storage and accessed absolutely sequentially during the iterations, but during the set up of the matrices I access the element unordered. This did run very well even for very large 2D problems and on the basis of this 2D program I decided to develop the 3D version.

During the 3D calculations I soon ran into problems because of the large matrices, during the set up of the matrices. I did solve these problems in a rather untraditional way, but on computers with more backing storage these problems could easily be solved in a more efficient way.

3. INVESTIGATIONS CARRIED THROUGH

The goal for my investigations with finite element methods was, if possible, to develop a fast and accurate 3D-flux-calculation program.

There had already been done a lot of work in this field with 2D-codes, for example the investigations described in ref. 3, ref. 5 and ref. 6. What I missed in these investigations was realistic
examples on light water reactors, which mainly is the field in which we are working at Rise. An other lack was flux comparisons, I do not believe that a high precision on the eigenvalue necessarily means a high precision on the calculated flux.

3.1 First investigation

The first investigation, carried through with FEM, is described in details in ref. 2. The goal was to complete the investigations found in the literature with respect to our interests. On basis on this we should decide whether or not we would work on a 3D program.

I only examined the accuracy of the solution as function of meshsize for a rectangular division because of the expected difficulties with tetrahedrons in a 3D calculation.

The investigation included 2 realistic examples, a 2 group calculation on the midplane of the Connecticut Yankee reactor and a 2D version of the 3D IAEA Benchmark. Further I included 3 smaller examples with varying discontinuities caused by different diffusion coefficients in core and reflector.

The result of this investigation was:

1) On "nice" problems (small difference in diffusion coefficients) the high order finite element approximations provide a more accurate solution within the same execution time, but with increasing discontinuities the accuracy of the high order methods decrease faster than for the low order methods (FDT as well as FEM 1st order).

2) The realistic problems seemed to be "nice" enough for the high order method to converge faster (as function of meshsize) than the low order methods when considering calculation times, but the improvements were less than expected at the beginning of the investigation.

All in all I did from my first investigation conclude that the finite element method does not constitute an alternative to the fast nodal methods, but the method is superior to the low order FDT program with respect to calculation time when high precision is wanted.

3.2 Second investigation

The next phase in my work was the development of the program FEMB as described in chapter 2.

With this program I performed some calculations on planes in the 3D IAEA Benchmark problem in order to estimate the precision of a calculation on the 3D IAEA Benchmark problem.

One of the considered planes was the core midplane, where I naturally used the 2D IAEA specification as published in ref. 7. As reference solution I used an extrapolated FDT solution performed by G.K. Kristiansen. The results from this calculation are described in appendix A.

This investigation showed that my first investigation was too optimistic in its conclusions considering FEM, but still the FEM program seemed to be a good deal faster than the FDT programs, so I continued the work with the 3D version based on the program FEMB.

3.3 Third investigation

After the development and testing of the 3D program I had planned some calculations on the 3D IAEA Benchmark problem. The goal of these calculations was to provide a reliable reference solution to the problem. In order to get a good estimate of the errors in the flux distribution I had performed the described 2D calculations.

The largest calculation on the 3D IAEA Benchmark problem is described in appendix B, it is a calculation with 16 x 16 x 13 mesh and a second order approximation. The mesh used in the directions is chosen so that the max. error in the planes considered (in 2D calculations), was about 3.5% (relative to $\frac{\text{max}}{\text{max}}$ in the group). According to the 2D calculations I assume the max. error to be less than 5% on the 3D calculation described in appendix B.

This calculation is until now the most accurate calculation performed on this problem. Naturally there will be some doubt about this result, because the program is new, including risk for errors, and the method is not too well known considering accuracy for realistic examples, especially not in three dimensions. I hope that a large FDT calculation with comparable accuracy will soon be available and support my results and estimations.

I performed two further calculations on the problem, a 2nd
order and a 3rd order coarse mesh calculation, the result from the 3rd order calculation is shown in appendix C.

3.4 Comparative study on the way

A comparative study of different methods, FDT-cornerpoint, FDT-midpoint and FEM is at the moment carried out by Mr. G.K. Kristiansen, Risø. The results of this work will soon be available.

4. FUTURE WORK

In the future work with FEM programs we will concentrate on programs suitable for 3D-overall calculations.

Until now we have in no way taken advantage of improvements, which can be achieved by the flexible division of the reactor with a triangular mesh. The gain obtained by this seems to be quite large (see f. ex. ref. 3 and ref. 5).

We have planned to develop a 3D-code using prism-formed elements (triangles in the xy-plane, rectangles in the xz- and the yz-plane). This should at the expense of some manual work be able to reduce the calculation time.

The last part of the work with the 3D-codes is planned to be an optimisation of the code.

There are several ways which can lead to a faster code, I will mention some.

Most of the calculation time is spent during the iterations, here the solving of the equations and the calculation of the right side ($F$) takes almost all the time. The calculation of $F$ can be accelerated sacrificing some generality (scattering from all groups to all groups, fission neutrons born in all groups). If the order of approximation is fixed, a lot of calculation can be saved, I have tried this for 1st order approximation, leading to a saving of about 80% cpu-time. The gain will be less in higher order calculations, I expect about 50% for 2nd order calculation etc.

An other way to accelerate the calculation of $F$ is at the expense of more storage, here the gain should be about 50%, but at the moment this would not be advisable at our computer.

The total number of iterations might be reduced by introduction of more efficient iteration techniques. But as long as the simple pointwise successive overrelaxation is able to finish within about 100 iterations, it will probably be difficult to find a much faster method.
REFERENCES

2. I. Misfeldt, Master thesis.

APPENDIX A

Danish Atomic Energy Commission
Research Establishment Risø
Department of Reactor Technology
Reactor Physics Section

This is an internal report. It may contain results or conclusions that are only preliminary and should therefore be treated accordingly. It is not to be reproduced nor quoted in publications or forwarded to persons unauthorized to receive it.
In connection with the calculation on the 3D Benchmark problem we have performed some 3D-calculations. The 3D problem is the one specified in ref. 1 from which fig. 1 is copied.

To get a reasonably accurate independent reference solution Mr. G.K. Kristiansen has performed a series of FDT-calculations and from them obtained a solution by Richardson-extrapolation in each power assembly.

Table 1 shows the results from these calculations. In table 1 are further shown some calculations with FEMB, a twodimensional finite element flux calculation program using a rectangular mesh. From ref. 1 are taken two calculations with FEM2D, a finite element flux calculation program using a triangular mesh. The errors shown in Table 1 are defined:

\[ \varepsilon_P = \max_i \left( \frac{P_i - P_{i,\text{ref}}}{P_{i,\text{ref}}} \right) \times 100 \]

\[ \varepsilon_{\text{flux}} = \max_i \left( \frac{\phi_i - \phi_{i,\text{ref}}}{\phi_{i,\text{ref}}} \right) \times 100 \]

(P, in the assembly power, and i denotes the assembly)

The error in the flux, defined as:

\[ \varepsilon = \max_i \left( \frac{\phi_i - \phi_{i,\text{ref}}}{\phi_{i,\text{ref}}} \right) \times 100 \]

(i denotes the meshpoint, \( \rho \) in a group-index) is typically found to be twice as big as \( \varepsilon_{\text{flux}} \) in the power.

In fig. 1 the error as function of the mesh is shown for the different calculations.

---

**Solution No** | description | cpu-time
---|---|---
1 | tvsedim 17 x 17 | 1.4 min.
2 | " 34 x 34 | 7.1 "
3 | " 68 x 68 | 30 "
4 | " 136 x 136 | 110 "
5 | " 170 x 170 | 145 "
6 | extrapolated value | "
7 | FEMB 2. order 9 x 9 (19 x 19) \(^n\) | 4.4 "
8 | " 2. order 18 x 18 (37 x 37) \(^n\) | 23.3 "
9 | " 2. order 36 x 36 (73 x 73) \(^n\) | 98.5 "
10 | FEM2D 2. order 182 fluxpoints 1/8 core | 18.9 "
11 | " 2. order 606 fluxpoints 1/8 core | 90.6 "
12 | " 3. order 9 x 9 (28 x 28) \(^n\) | 18.9 "
13 | " 3. order 18 x 18 (55 x 55) \(^n\) | 90.6 "

**TVSEDIM** is a FDT flux calculation program using corner mesh points.

**FEMB** is a finite-element flux calculation program using Lagrange interpolation in a rectangular mesh.

**FEM 2D** is a finite-element flux calculation program using Lagrange interpolation in a triangular mesh. See ref. 1.

\[ 9 \times 9 (19 \times 19) \] means 9 mesh in each direction and 19 fluxpoints because of the second order approximation etc.
REFERENCES

1. Proceedings of the Conference on COMPUTATIONAL METHODS IN NUCLEAR ENGINEERING
   April 15 - 17, 1975
   SESSION I

### Group Constants for 30 IAEA Benchmark Problem

<table>
<thead>
<tr>
<th>Region</th>
<th>( D_0 )</th>
<th>( D_2 )</th>
<th>( \Sigma_{1+2} )</th>
<th>( \Sigma_{a1} )</th>
<th>( \Sigma_{a2} )</th>
<th>( V_{E_1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.5</td>
<td>0.4</td>
<td>0.02</td>
<td>0.01</td>
<td>0.01</td>
<td>0.15</td>
</tr>
<tr>
<td>2</td>
<td>1.5</td>
<td>0.4</td>
<td>0.02</td>
<td>0.01</td>
<td>0.01</td>
<td>0.15</td>
</tr>
<tr>
<td>3</td>
<td>1.5</td>
<td>0.4</td>
<td>0.02</td>
<td>0.01</td>
<td>0.01</td>
<td>0.15</td>
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<tr>
<td>4</td>
<td>1.5</td>
<td>0.3</td>
<td>0.04</td>
<td>0</td>
<td>0</td>
<td>0.05</td>
</tr>
<tr>
<td>5</td>
<td>1.5</td>
<td>0.3</td>
<td>0.04</td>
<td>0</td>
<td>0</td>
<td>0.05</td>
</tr>
</tbody>
</table>

**Notes:**
- \( X_1 = 1.0 \), \( X_2 = 0.0 \), \( V_{E_II} = 0 \) all regions
- The 30 IAEA Benchmark Problem represents a 150 cm with constant axial height \( L = 0.8 \times 10^{-4} \) for all regions and energy groups.

**Fig. 1** 30 IAEA Benchmark Problem Specification
### Table 1

**2D IAEA BENCHMARK PROBLEM**

Comparison of finite element- and finite difference-methods.

Average assembly powers.
This is an internal report. It may contain results or conclusions that are only preliminary and should therefore be treated accordingly. It is not to be reproduced nor quoted in publications or forwarded to persons unauthorized to receive it.
3. Calculation description (simplifications, meshes, iterations, problems, etc.) (max. 15 lines):

This solution is performed with 2. order interpolation. The mesh size is $16 \times 16 \times 13$ ($33 \times 33 \times 27$ flux points) and 2 energy groups are used.

The result scheme is filled in after 7 iterations and the local error is assumed to be less than 0.1% of $\phi_{\text{max}}$ in each group.

4. Computer type: Burroughs 6700
Calculation time: 23 hours cpu

Computer speed relative to one or two well-known computer types:
1 hour on CDC 6600 ~ 10 hours on B 6700.

An extra page A4 with information may be added if necessary.
**3D Benchmark Problem**

**Results Scheme 2: k\text{eff} and flux points**

\[ k_{\text{eff}} = 1.0232 \]

Write \( \phi_1 \) and \( \phi_2 \) relative to \( \phi_1 \), average, core

<table>
<thead>
<tr>
<th>Co-ordinates</th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
<th>( \phi_1 )</th>
<th>( \phi_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Core midplane</td>
<td>80</td>
<td>40</td>
<td>190</td>
<td>7.743</td>
<td>1.816</td>
</tr>
<tr>
<td></td>
<td>80</td>
<td>80</td>
<td>190</td>
<td>2.846</td>
<td>0.641</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>80</td>
<td>190</td>
<td>4.499</td>
<td>1.108</td>
</tr>
<tr>
<td></td>
<td>120</td>
<td>40</td>
<td>190</td>
<td>6.326</td>
<td>1.568</td>
</tr>
<tr>
<td>10 cm's up</td>
<td>0</td>
<td>0</td>
<td>290</td>
<td>2.656</td>
<td>0.444</td>
</tr>
<tr>
<td>the partially inserted control absorber</td>
<td>80</td>
<td>40</td>
<td>290</td>
<td>3.815</td>
<td>0.835</td>
</tr>
<tr>
<td></td>
<td>140</td>
<td>0</td>
<td>290</td>
<td>2.504</td>
<td>0.649</td>
</tr>
<tr>
<td></td>
<td>150</td>
<td>0</td>
<td>290</td>
<td>1.271</td>
<td>0.941</td>
</tr>
<tr>
<td>Core bottom</td>
<td>0</td>
<td>0</td>
<td>20</td>
<td>0.613</td>
<td>0.370</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>40</td>
<td>20</td>
<td>0.925</td>
<td>0.659</td>
</tr>
<tr>
<td>Power peak</td>
<td>130</td>
<td>56</td>
<td>178</td>
<td>3.291</td>
<td>2.426</td>
</tr>
<tr>
<td></td>
<td>32</td>
<td>32</td>
<td>174</td>
<td>9.805</td>
<td>2.298</td>
</tr>
</tbody>
</table>

Relative fluxes and position, where \( \phi_1 \) has its maximum in the core.
This is an internal report. It may contain results or conclusions that are only preliminary and should therefore be treated accordingly. It is not to be reproduced nor quoted in publications or forwarded to persons unauthorized to receive it.
FEM 3D is a three-dimensional finite-element flux calculation programme. The programme uses box-shaped elements with Lagrange interpolation. The order of the interpolation might be 1., 2., or 3. order. The programme uses an ordinary power iteration technique with one inner iteration per outer. The group equations are solved by SCR and the iterations are accelerated by extrapolation.

This calculation is performed with 3rd order interpolation. The mesh used was $9 \times 9 \times 4$ ($28 \times 28 \times 13$ flux points). The solution is not yet sufficiently converged so the local error is large, but less than 5%.

The mesh in the $z$ direction is too coarse so the precision will not be as high as predicted in RP-3-75 (6%) for the $xy$-plane.

These results do mostly serve the purpose to prove that 3rd order FEM calculation is possible on a realistic 3D-problem.

Computer type: Burroughs 6700
Calculation time: 9.5 hours

Computer speed relative to one or two well-known computer types:
1 hour on C-M 6600 $\approx$ 10 hours on B 6700.

An extra page A4 with information may be added if necessary.
Code name: FEM 3D
Organization: Risø DK

3D Benchmark Problem

Results include $k_{\text{eff}}$ and flux points

$k_{\text{eff}} = 1.0287$

Write $\phi_1$ and $\phi_2$ relative to $\phi_2, \text{average, core}$

<table>
<thead>
<tr>
<th>Co-ordinate cm</th>
<th>Relative Fluxes</th>
<th>( \phi_1 )</th>
<th>( \phi_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Core midplane</td>
<td>80 80 193</td>
<td>7.626</td>
<td>1.796</td>
</tr>
<tr>
<td></td>
<td>100 80 193</td>
<td>4.395</td>
<td>1.095</td>
</tr>
<tr>
<td></td>
<td>120 80 193</td>
<td>6.289</td>
<td>1.541</td>
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<tr>
<td>10 cm's up</td>
<td>0 0 293</td>
<td>2.760</td>
<td>0.426</td>
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<td>the partially</td>
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<td>control absorber</td>
<td>140 0 293</td>
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<td>Core bottom</td>
<td>0 0 20</td>
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<td>Core peak</td>
<td>130 56 175</td>
<td>3.229</td>
<td>2.389</td>
</tr>
<tr>
<td>Power peak</td>
<td>34 34 175</td>
<td>9.481</td>
<td>2.250</td>
</tr>
</tbody>
</table>

Relative fluxes and position, where $\phi_2$ has its maximum in the core.