Solution of the 3D Neutron Diffusion Benchmark by FEM

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11^{th} International Conference on
"Large-Scale Scientific Computations"
June 5-9, 2017, Sozopol, Bulgaria

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Introduction

- neutron-transport equation (time, energy, spatial and angular variables)
- simplified forms, multigroup diffusion approximation
- stationary state, critical state of the reactor (local balance between the neutron generation and apbsortion)
- spectral problem (Lambda Modes problem, λ-eigenvalue problem), provided that the k-effective is equal to unity, stationary neutron flux is a corresponding eigenfunction
- This work is focused on the solution of the 3D benchmark problem of a VVER-1000 core in steady state. Convergence of the benchmark solution is under investigation.

Multigroup diffusion approximation

Neutron flux dynamics is considered within a bounded 2D or 3D domain Ω ($\boldsymbol{x} = \{x_1, ..., x_d\} \in \Omega,\ d = 2, 3$) with a convex boundary $\partial\Omega$. The neutron transport is described by the following set of equations without taking into account delayed neutron sources:

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} - \nabla \cdot D_g \nabla \phi_g + \Sigma_{rg}\phi_g - \sum_{g \neq g'=1}^{G} \Sigma_{s,g' \to g}\phi_{g'} =$$

$$= ((1-\beta)\chi_g + \beta\widetilde{\chi}_g)\sum_{g'=1}^{G} \nu\Sigma_{fg'}\phi_{g'}, \quad g = 1, 2, ..., G.$$

Here $\phi_g(\boldsymbol{x}, t)$ is the neutron flux, v_g is the effective neutron velocity, $D_g(\boldsymbol{x})$ is diffusion coefficient, $\Sigma_{rg}(\boldsymbol{x}, t)$ is removal cross-section, $\Sigma_{s,g' \to g}(\boldsymbol{x}, t)$ is scattering cross-section, $\nu\Sigma_{fg}(\boldsymbol{x}, t)$ is generation cross-section, β is the effective fraction of delayed neutrons, χ_g, $\widetilde{\chi}_g$ is the spectra of instantaneous and delayed neutrons.

Initial and boundary conditions

The conditions so-called albedo-type are set at the boundary $\partial\Omega$:

$$D_g \frac{\partial \phi_g}{\partial n} + \gamma_g \phi_g = 0, \qquad g = 1, 2, ..., G,$$

where n is the outer normal to the boundary $\partial\Omega$.
Let's consider problem with albedo boundary conditions and initial conditions

$$\phi_g(\boldsymbol{x}, 0) = \phi_g^0(\boldsymbol{x}), \quad g = 1, 2, ..., G.$$

Operator formulation

Let's write the boundary problem in operator form. We define the vector $\phi = \{\phi_1, \phi_2, ..., \phi_G\}$ and the matrices

$$V = (v_{gg'}), \quad v_{gg'} = \delta_{gg'} v_g^{-1}, \quad D = (d_{gg'}), \quad d_{gg'} = -\delta_{gg'} \nabla \cdot D_g \nabla,$$

$$S = (s_{gg'}), \quad s_{gg'} = \delta_{gg'} \Sigma_{rg} - \Sigma_{s,g' \to g}, \quad R = (r_{gg'}), \quad r_{gg'} = ((1-\beta)\chi_g + \beta\widetilde{\chi}_g)\nu$$

$$g, g' = 1, 2, ..., G.$$

Using the set definitions, we get boundary problem in operator formulation:

$$V\frac{d\phi}{dt} + (D+S)\phi = R\phi.$$

We solve the Cauchy problem, when $\phi(0) = \phi^0$, where $\phi^0 = \{\phi_1^0, \phi_2^0, ..., \phi_G^0\}$.

To characterize the dynamic processes in a nuclear reactor, which are described by the Cauchy problem, solutions of some spectral problems (see avvakumov2017*). Let's consider the solution of the spectral problem, called Lambda Modes problem:

$$(D + S)\varphi = \lambda^{(k)} R\varphi.$$

This problem is known as the Lambda modes problem for a given configuration of the reactor core. The minimal eigenvalue is used for characterization of neutron flux, thus

$$k = \frac{1}{\lambda_1^{(k)}}$$

is the effective multiplication factor.

*Avvakumov, A.V., Strizhov, V.F., Vabishchevich, P.N., Vasilev, A.O.: Spectral properties of dynamic processes in a nuclear reactor. Annals of Nuclear Energy, vol. 99, pp. 68–79 (2017)

Finite element method

Let $H^1(\Omega)$ – Sobolev space, $v \in H^1$: v^2 and $|\nabla v|^2$ have a finite integral in Ω. For $\boldsymbol{v} = \{v_1, v_2, ..., v_d\}$ define $V^d = [H^1(\Omega)]^d$. For test functions use notations $\boldsymbol{\xi} = \{\xi_1, \xi_2, ..., \xi_G\}$.
In variation formulation we are looking for $\boldsymbol{\phi} \in V^D$ such that:

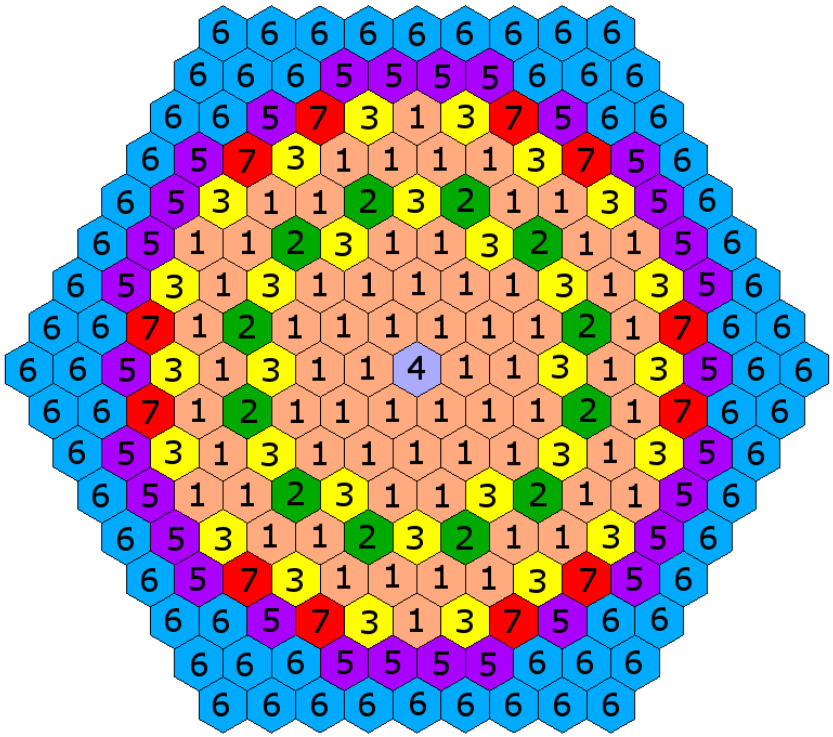
$$\int_\Omega \sum_{g=1}^{G} D_G \nabla \phi_g \nabla \xi_g d\boldsymbol{x} + \int_{\partial\Omega} \sum_{g=1}^{G} \gamma_g \phi_g \xi_g d\boldsymbol{x} + \int_\Omega S\boldsymbol{\phi}\boldsymbol{\xi} d\boldsymbol{x} = \lambda^{(k)} \int_\Omega R\boldsymbol{\phi}\boldsymbol{\xi} d\boldsymbol{x},$$

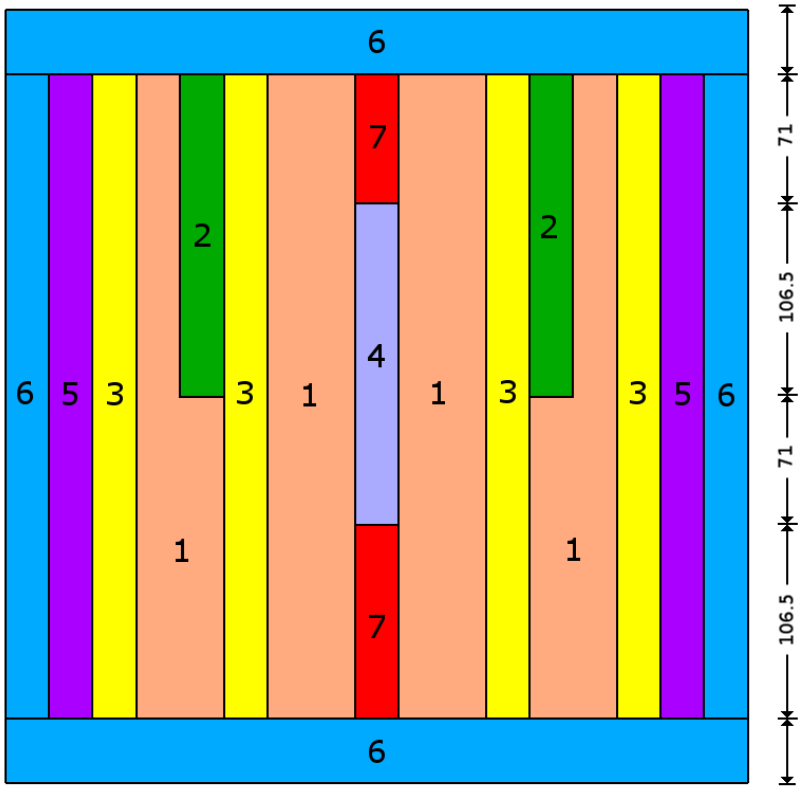
for all $\boldsymbol{\xi} \in V^D$.
Let introduce a discrete function spaces $V_h^D \subset V^D$ and define discrete variational problem.
The standard Lagrangian finite elements of degree p = 1, 2 and 3 are used.

$$\boldsymbol{Au} = \lambda^{(k)} \boldsymbol{Bu}$$

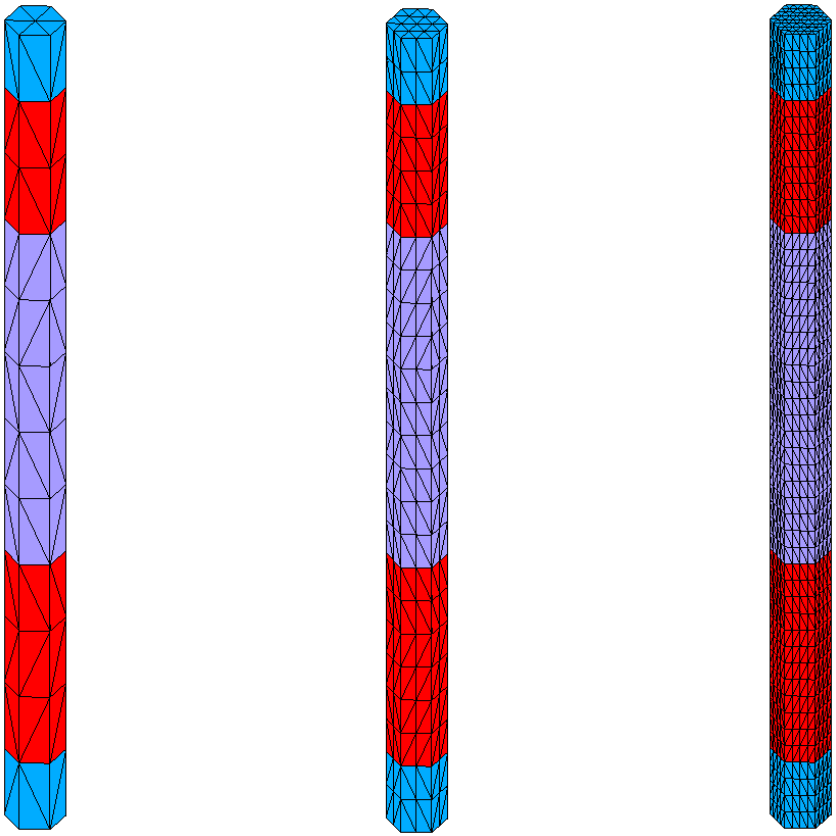
AER benchmark

Three-dimensional and two-group approximation, assemblies are homogeneous. There are seven material compositions including





mesh and parameters



In the computations the following parameters are varied:

- κ from 6 to 96
- z from 12 to 48
- p from 1 to 3

The following parameters were calculated:

- the effective multiplication factor k;
- the power distribution P per assembly:

$$P = a(\Sigma_{f1}\varphi_1 + \Sigma_{f2}\varphi_2)$$

Computation parameters

The results are compared with those, obtained using the diffusion program CRONOS.
Let's consider the following variations in the calculated parameters:

- for the effective multiplication factor, absolute deviation from the reference value k_{ref}: $\Delta k = |k - k_{ref}|$, expressed in *pcm* (percent-milli, i.e. 10^{-5});
- for power distribution per assembly P_i calculated relative deviation ε_i (expressed in %):

$$\varepsilon_i = \frac{P_i - P_i^{ref}}{P_i^{ref}},$$

  where P_i^{ref} — reference value of power per assembly i ($i = 1, ..., N_e$).
- by deviations ε_i calculated integral deviation:

$$\mathrm{RMS} = \sqrt{\frac{1}{N_e}\sum_{i=1}^{N_e}\varepsilon_i^2}, \quad \mathrm{AVR} = \frac{1}{N_e}\sum_{i=1}^{N_e}|\varepsilon_i|, \quad \mathrm{MAX} = \max_i |\varepsilon_i|.$$

Hardware

CPU:

- 160 nodes (1920 cores)
- 23.5 TFLOPS (peak), 20.21 TFLOPS (Linpack)

GPU:

- 15 nodes (45 gpu)
- 22.5 TFLOPS (peak), 11.12 TFLOPS (Linpack)

Software

Code section	Software	Description
Geometry and mesh	Gmsh 3.0.2	a three-dimensional finite element mesh generator
Eigenvalue	SLEPc 3.7	the scalable library for eigenvalue problem computations
FEM library	FEniCS 1.6	a popular computing platform for partial differential equations
Programming	Python 2.7	a programming language
Visualization	ParaView 5.4	a multi-platform data analysis and visualization application

Eigenvalues for p=1

Table: k_1 results for the Schulz benchmark.

p	κ	z	k_1	Δk	MAX	AVR	RMS	N
1	6	12	1.0476057	192.03	7.9382	2.5145	2.7918	18,278
1	6	24	1.0484070	111.90	7.6614	2.3465	2.5983	35,150
1	6	48	1.0486511	87.49	7.6793	2.3643	2.6092	68,894
1	24	12	1.0482940	123.20	2.2234	0.5665	0.7041	70,382
1	24	24	1.0487937	73.23	1.9377	0.4050	0.4774	135,350
1	24	48	1.0493645	16.15	1.9823	0.3980	0.4612	265,286
1	96	12	1.0483122	121.38	1.2015	0.3780	0.4857	276,146
1	96	24	1.0490651	46.09	0.2647	0.1129	0.1389	531,050
1	96	48	1.0493997	12.63	0.4554	0.1019	0.1243	1,040,858

Eigenvalues for p=2

Table: k_1 results for the Schulz benchmark.

p	κ	z	k_1	Δk	MAX	AVR	RMS	N
2	6	12	1.0496463	-12.03	0.9739	0.4801	0.5581	135,350
2	6	24	1.0497290	-20.30	0.9576	0.4504	0.5314	265,286
2	6	48	1.0497379	-21.19	0.9576	0.4501	0.5307	525,158
2	24	12	1.0494978	2.82	0.3246	0.1577	0.1861	531,050
2	24	24	1.0495665	-4.05	0.2597	0.1176	0.1414	1,040,858
2	24	48	1.0495858	-5.98	0.2435	0.1117	0.1335	2,060,474
2	96	12	1.0494551	7.09	0.1786	0.0662	0.0771	2,103,650
2	96	24	1.0495265	-0.05	0.0844	0.0309	0.0377	4,123,154
2	96	48	1.0495471	-2.11	0.0573	0.0256	0.0298	8,162,162

Eigenvalues for p=3

Table: k_1 results for the Schulz benchmark.

p	κ	z	k_1	Δk	MAX	AVR	RMS	N
3	6	12	1.0495750	-4.90	0.2149	0.0956	0.1153	444,962
3	6	24	1.0495782	-5.22	0.2110	0.0931	0.1125	877,898
3	6	48	1.0495771	-5.11	0.2005	0.0900	0.1082	1,743,770
3	24	12	1.0495406	-1.46	0.0430	0.0177	0.0216	1,756,982
3	24	24	1.0495382	-1.22	0.0317	0.0123	0.0146	3,466,478
3	24	48	1.0495381	-1.21	0.0286	0.0102	0.0126	6,885,470
3	96	12	1.0495357	-0.97	0.0317	0.0106	0.0137	6,982,418
3	96	24	1.0495338	-0.78	0.0211	0.0092	0.0110	13,776,122
3	96	48	1.0495336	-0.76	0.0162	0.0080	0.0100	27,363,530

Comparison with reference(CRONOS)

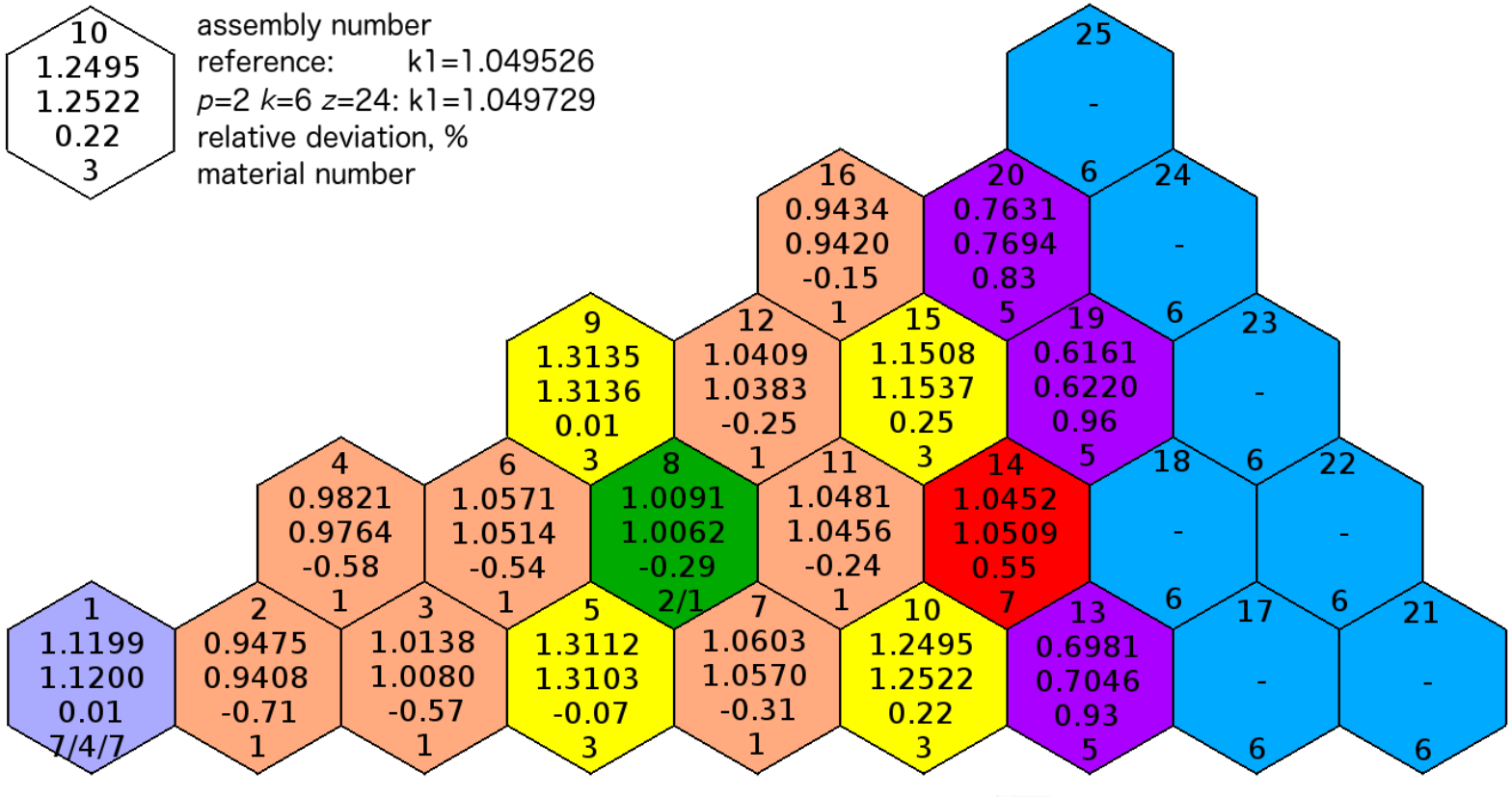


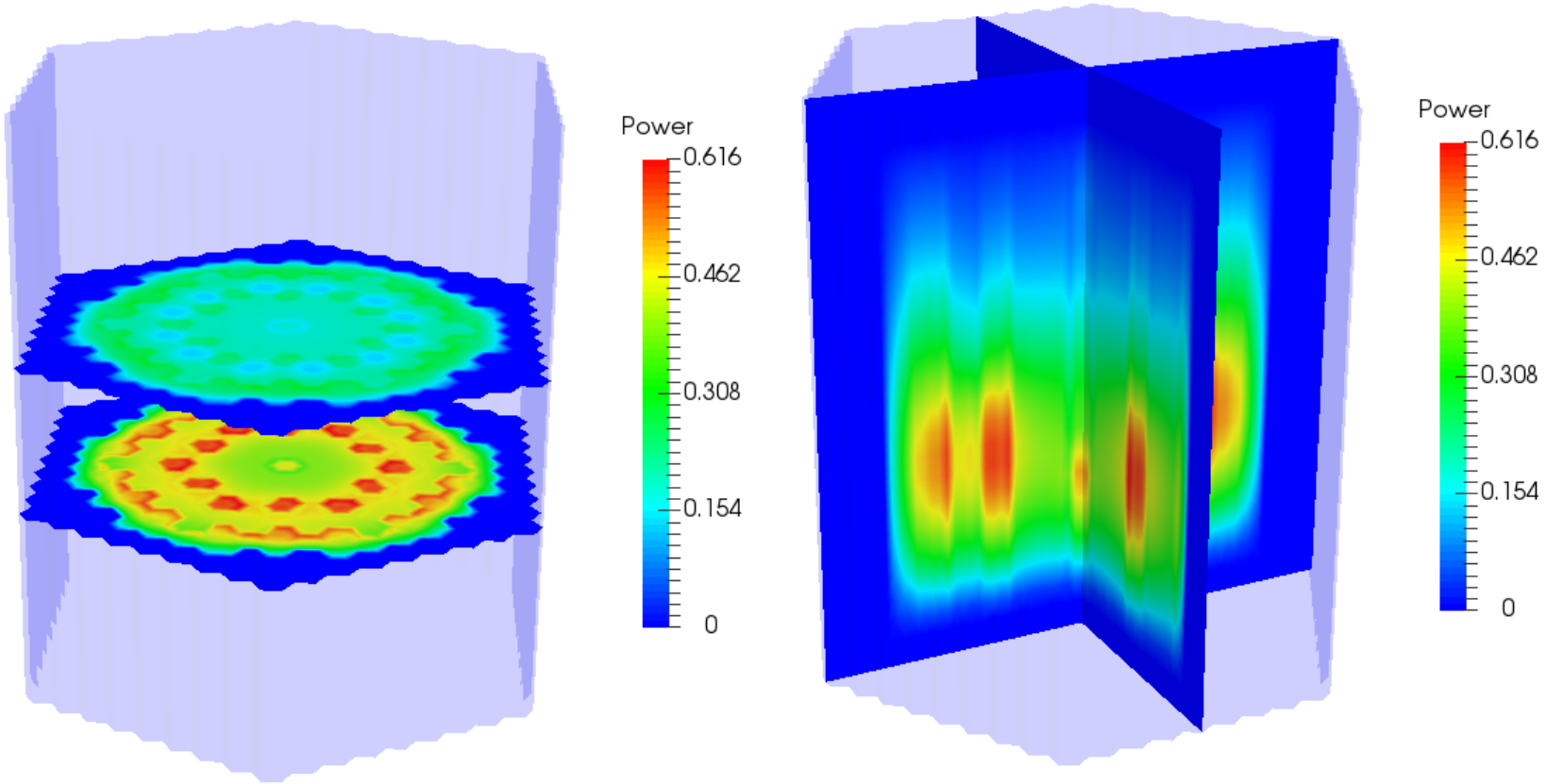
Figure: Power distribution at $p = 2, \kappa = 6, z = 24$.

Next three eigenvalues

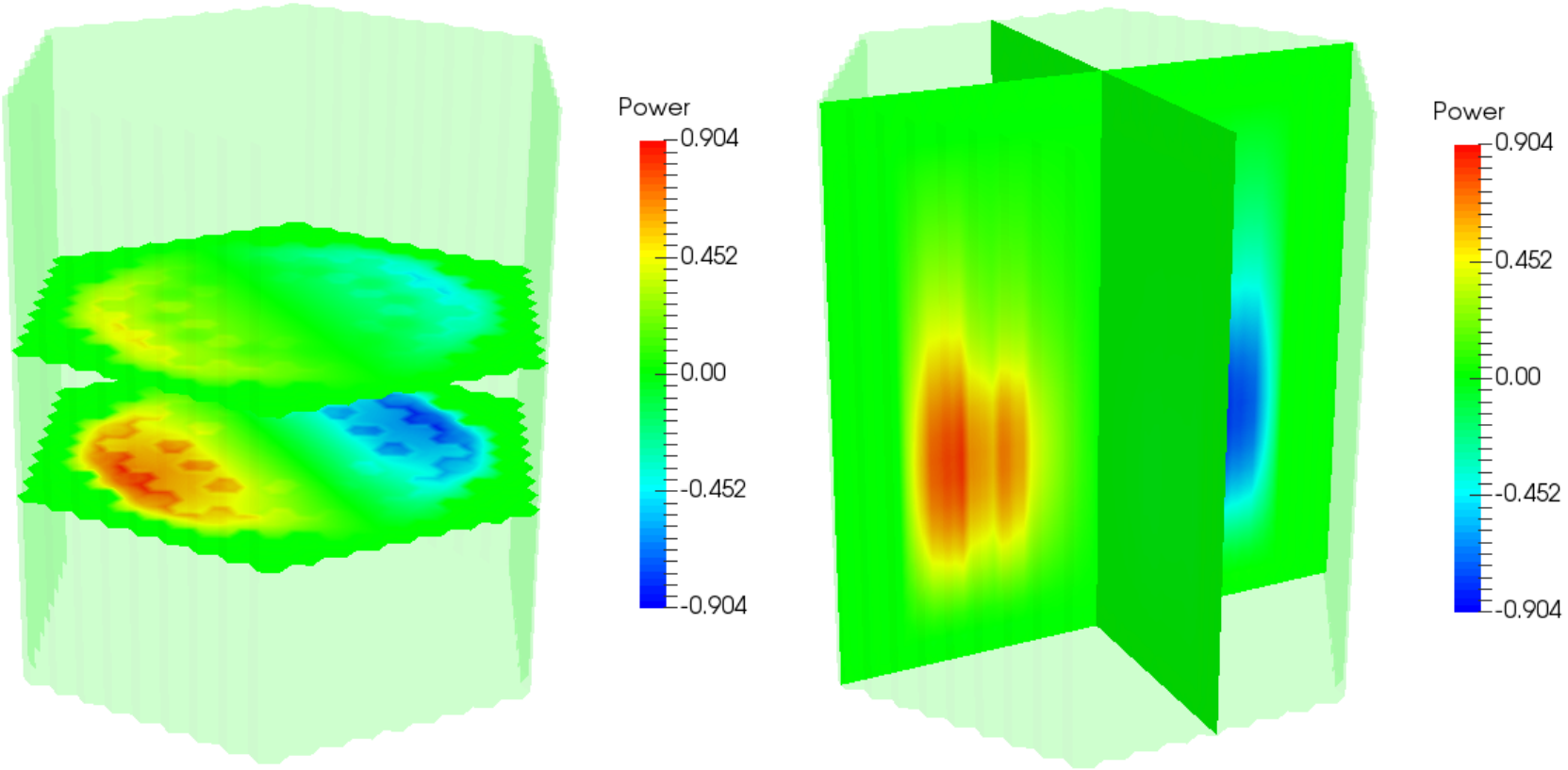
Table: The eigenvalues k_2, k_3 and k_4.

p	κ	z	k_2	k_3	k_4
1	6	12	1.0367578	1.0367505	1.0265919
1	6	24	1.0378381	1.0378355	1.0286801
1	6	48	1.0381457	1.0381434	1.0292950
1	24	12	1.0378816	1.0378762	1.0277542
1	24	24	1.0389665	1.0389631	1.0299569
1	24	48	1.0392872	1.0392857	1.0306072
1	96	12	1.0378388	1.0378365	1.0276575
1	96	24	1.0390329	1.0390303	1.0300412
1	96	48	1.0393812	1.0393798	1.0307428

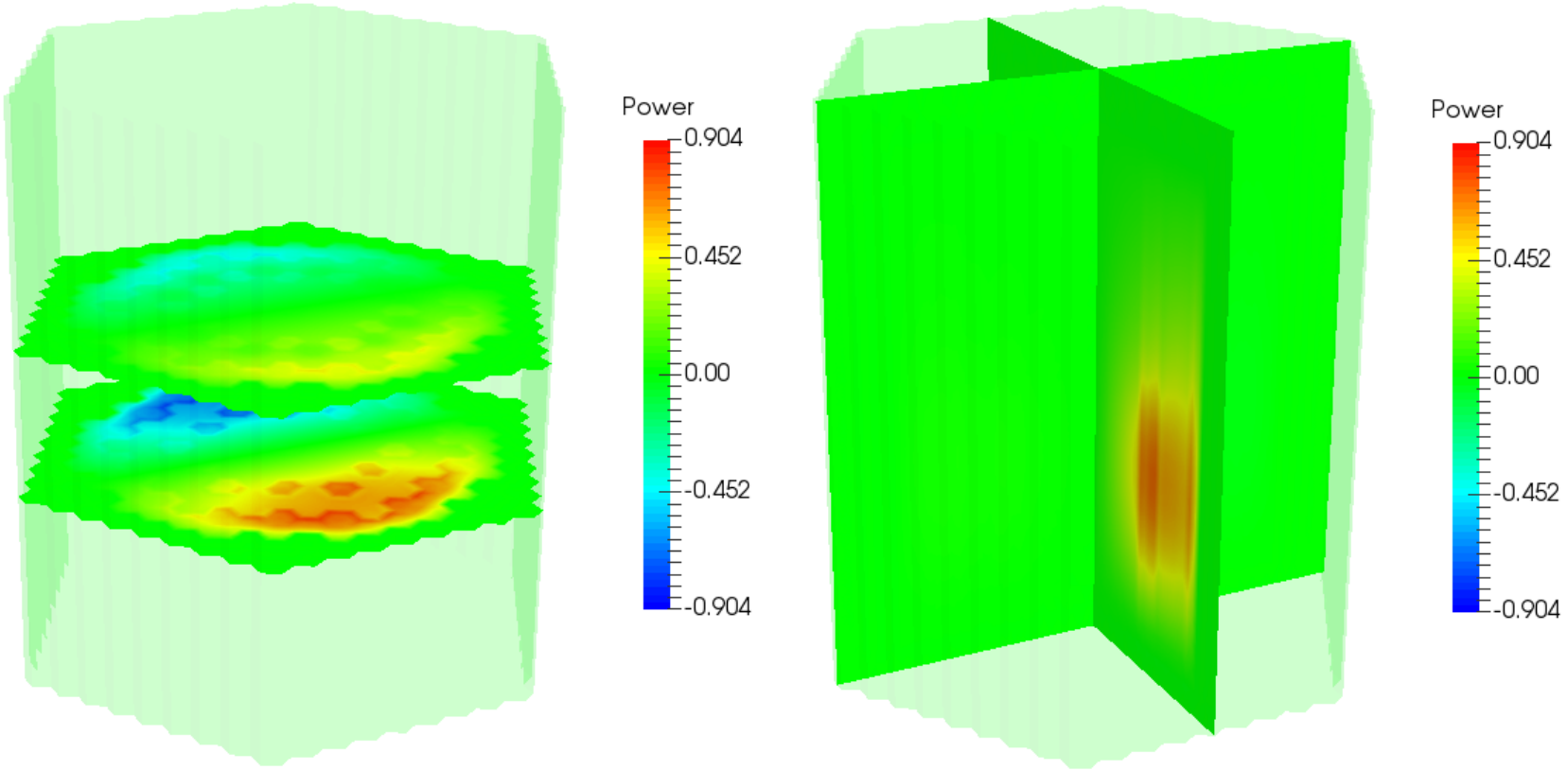
Vertical and horizontal cuts for k_1



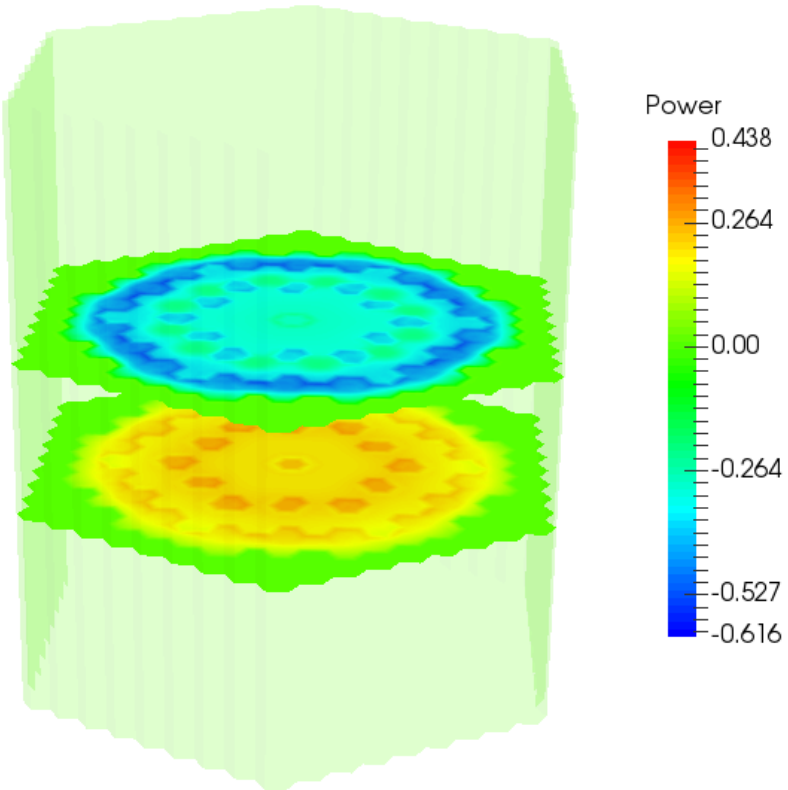
Vertical and horizontal cuts for k_2

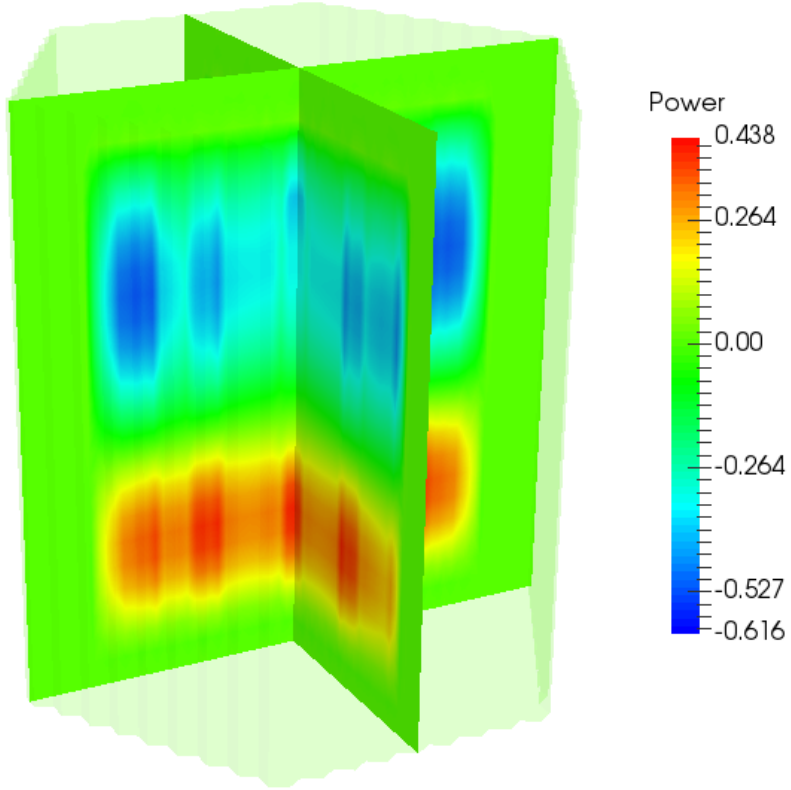


Vertical and horizontal cuts for k_3



Vertical and horizontal cuts for k_4





Conclusion

In this paper we have performed computational analysis of the 3D neutron diffusion benchmark of a VVER-1000 core. The software has been developed using the engineering and scientic library FEniCS and the matrix spectral problem is solved using the SLEPc package. The number of tetrahedrons per assembly κ varies from 6 to 96; the number of tetrahedrons in height z varies from 12 to 48. The finite elements of degree $p = 1, 2, 3$ are used. The results are compared with the extrapolated finite-element solution of the second-order CRONOS results recommended as the reference solution. An excellent agreement of the results was obtained for the maximum values of the parameters (κ=96, z=48 and p=3). There are deviations in the results at the rounding error level. In the practice of engineering calculations it is sufficient to use the following parameters: κ=6, z=24 and p=2. The results can be useful for the diffusion codes intercomparison.

Thank you for your attention!