# Algorithms for numerical simulation of non-stationary neutron diffusion problems

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#### Introduction

The physical processes occuring in a nuclear reactor, depend on the distribution of neutron flux, a mathematical description of which is based on neutron transport equation [Stacey 2007]. This equation is integro-differential and the neutron flux distribution is a function of time, energy, spatial and angular variables.

The multi-group diffusion approximation [Sutton 1996] is most widely used to analyze the reactor. This approach is used in the majority of engineering neutronic codes.

To increase calculational accuracy, nodal methods are widely used [Lawrence 1986]. These methods allow modelling on a rather coarse mesh. Nodal methods can be connected, in some respect, to the special variants of finite-element approximation [Grossman 2007].

We can note that it is more appropriate to use the standard procedures of increasing accuracy of the finite-element approximation for boundary problem solution with mesh refinement and using high-order finite elements.

#### Introduction

The most attention should be payed to two-level weighted schemes  $(\theta\text{-method})$  [Ascher 2008], also the Runge-Kutta and Rosenbrok schemes are used [Hairer 2010]. Note a special class of methods for modelling non-stationary neutron transport within the multi-group diffusion approach. It is based on multiplicative performance of the solution as space-time factorization or quasi-static method [Goluoglu 2001].

To characterize the reactor dynamic nature, a spectral parameter  $\alpha$  is used. It is defined as the fundamental eigenvalue of the spectral problem (time-eigenvalue or  $\alpha$ -eigenvalue problem), related to non-stationary diffusion equations [Bell 1970].

Analogously to ordinary problems of heat transfer [Luikov 2012] we can define a regular reactor mode. At large times a neutron flux behaviour is asymptotic. Then we can state space-time factorization of the solution with  $\exp(\alpha t)$ , as amplitude, and the shape function as the eigenfunction of the spectral problem.

### Problem definition

Let's consider modelling neutron flux in a multi-group diffusion approximation. Neutron flux dynamics is considered within limited 2D or 3D domain  $\Omega$  with a convex boundary  $\partial\Omega$ . Neutron transport is described by the set of equations without taking into account delayed neutron source:

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

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

Boundary and initial condition:

$$D_g \frac{\partial \phi_g}{\partial n} + \gamma_g \phi_g = 0, \quad g = 1, 2, ..., G,$$
  
$$\phi_g(\mathbf{x}, 0) = \phi_g^0(\mathbf{x}), \quad g = 1, 2, ..., G.$$

## Operator notation

Let's write the boundary problem in operator notation. Designations:

$$\phi = \{\phi_1, \phi_2, ..., \phi_G\}, \quad \phi^0 = \{\phi_1^0, \phi_2^0, ..., \phi_G^0\},$$

$$V = (v_{gg'}), \quad v_{gg'} = \delta_{gg'} v_g^{-1},$$

$$D = (d_{gg'}), \quad d_{gg'} = -\delta_{gg'} \nabla \cdot D_g \nabla,$$

$$S = (s_{gg'}), \quad s_{gg'} = \delta_{gg'} \Sigma_g - \Sigma_{s,g' \to g},$$

$$R = (r_{gg'}), \quad r_{gg'} = ((1 - \beta)\chi_g + \beta \widetilde{\chi}_g) \nu \Sigma_{fg'},$$

$$L = (l_{gg'}), \quad l_{gg'} = \delta_{gg'} \gamma_g, \quad g, g' = 1, 2, ..., G,$$

Cauchy problem:

$$V\frac{d\phi}{dt} + (D+S)\phi = R\phi.$$
$$D\frac{d\phi}{dn} + L\phi = 0, \quad \phi(0) = \phi^{0}.$$

#### Time discretization

Define uniform grid  $\omega=\{t^n=n\tau,\quad n=0,1,...,N,\quad \tau N=T\}$  and use notations  $\phi^n=\phi(x,t^n)$ . Fully implicit scheme:

$$V\frac{\phi^{n+1} - \phi^n}{\tau} + (D+S)\phi^{n+1} = R\phi^{n+1}.$$

Explicit-implicit scheme:

$$V\frac{\phi^{n+1} - \phi^n}{\tau} + (D+S)\phi^{n+1} = R\phi^n.$$

Crank-Nicolson scheme:

$$V\frac{\phi^{n+1} - \phi^n}{\tau} + (D+S)\frac{\phi^{n+1} + \phi^n}{2} = R\frac{\phi^{n+1} + \phi^n}{2}.$$

## Finite element method

Let  $H^1(\Omega)$  – sobolev space,  $v \in H^1$ :  $v^2$  and  $|\nabla v|^2$  have a finite integral in  $\Omega$ . For  $v = \{v_1, v_2, ..., v_d\}$  define  $V^d = [H^1(\Omega)]^d$ . For test functions use  $\boldsymbol{\xi} = \{\xi_1, \xi_2, ..., \xi_G\}$ ,  $\boldsymbol{\zeta} = \{\zeta_1, \zeta_2, ..., \zeta_M\}$ . In variation formulation, find  $\boldsymbol{\phi} \in V^D$ ,  $\boldsymbol{c} \in V^M$ :

$$\begin{split} \int_{\Omega} \left( V \frac{\boldsymbol{\phi}^{n+1} - \boldsymbol{\phi}^{n}}{\tau} + S \boldsymbol{\phi}^{n+1} \right) \boldsymbol{\xi} d\boldsymbol{x} + \int_{\Omega} \sum_{g=1}^{G} D_{G} \nabla \phi_{g}^{n+1} \nabla \xi_{g} d\boldsymbol{x} + \\ + \int_{\partial \Omega} \sum_{g=1}^{G} \gamma_{g} \phi_{g}^{n+1} \xi_{g} d\boldsymbol{x} = \int_{\Omega} R \boldsymbol{\phi}^{n+1} \boldsymbol{\xi} d\boldsymbol{x}, \end{split}$$

 $\forall \pmb{\xi} \in V^D, \quad \forall \pmb{\zeta} \in V^M.$ 

## Spectral problem

Characterisation of dynamic processes in reactor involve solution of spectral problems.  $\lambda$ -spectral problem, connected with stationary condition of reactor, is usually considered:

$$(D+S)\varphi = \mu R\varphi.$$

The fundamental eigenvalue  $k=1/\mu^{(1)}$  is multiplication factor. The value k is associated with the critical condition of the reactor.

 $\lambda$ -spectral problem can not be directly attributed to the dynamic processes in a reactor. At best, we can only identify stationary critical state. More than acceptable spectral characteristic for a non-stationary equation is associated with  $\alpha$ -spectral problem.

## Spectral problem

Let's consider the solution of the spectral problem, called alpha modes problem:

$$A\varphi = \lambda^{(\alpha)}V\varphi, \quad A = D + S - R.$$

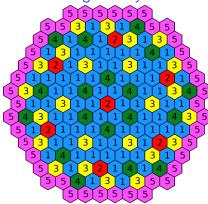
The fundamental eigenvalue

$$\alpha = \lambda_1^{(\alpha)}$$

is called  $\alpha$ -eigenvalues or period eigenvalues. The asymptotic behaviour (at large times) of the solution of Cauchy problem can be connected with the  $\alpha$ -eigenvalue. In this regular regime, the reactor behaviour is described by the function  $e^{-\alpha t} \varphi_{\alpha}(x)$ .

## Test problem

## VVER-1000 geometry



#### **Parameters**

The number of triangles per one assembly "k" varies from 6 to 96:



The standard Lagrangian finite elements of degree  $p=1,\,2,\,3$  are used:







## Results of spectral problem

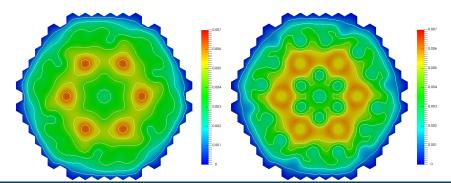
Table: The eigenvalues  $\alpha_n = \lambda_n^{(\alpha)}, \ n = 1, 2, ..., 5$ 

$\kappa$	p	$lpha_1$	$\alpha_2, \alpha_3$	$\alpha_4, \alpha_5$
6	1	-105.032	$159.802\pm0.025510i$	$659.109 \pm 0.034667i$
	2	-139.090	$115.793 \pm 0.029186i$	$591.782 \pm 0.034667i$
	3	-140.223	$114.035 \pm 0.033814i$	$588.762 \pm 0.069025i$
24	1	-130.422	$126.984 \pm 0.034409i$	$608.734 \pm 0.070724i$
	2	-140.187	$114.089 \pm 0.033512i$	$588.849 \pm 0.068555i$
	3	-140.281	$113.887 \pm 0.033604i$	$588.415 \pm 0.068695i$
96	1	-137.704	$117.345\pm0.033823i$	$593.818 \pm 0.069254i$
	2	-140.284	$113.886 \pm 0.033599i$	$588.419 \pm 0.068687i$
	3	-140.308	$113.842 \pm 0.033603i$	$588.336 \pm 0.068690i$

The eigenvalues  $\alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_9, \alpha_{10}$  are the complex values with small imaginary parts, and the eigenvalues  $\alpha_1, \alpha_6, \alpha_7, \alpha_8$  are the real values.

## Results of spectral problem

The eigenvalues  $\lambda_1^{(\alpha)} \leq \lambda_2^{(\alpha)} \leq \ldots$  are well separated. In our example, the fundamental eigenvalue is negative and therefore the main harmonic will increase, while all others will attenuate. The regular mode of the reactor is thereby defined. The value  $\alpha = \lambda_1^{(\alpha)}$  determines the amplitude of neutron flux development and connects directly with the reactor period in the regular regime. Fundamental eigenfunctions  $\varphi_1^{(1)}(\text{left}), \; \varphi_2^{(1)}(\text{right}).$ 



## The appearance of the regular regime

For all schemes initial conditions:

$$\phi_1^0 = 1.0, \quad \phi_2^0 = 0.25$$

and k=24, p=2. Let's  $T=5\times 10^{-3}$  and consider the fully implicit solution at  $\tau=1\times 10^{-5}$  as the reference one.

The appearance of the regular mode of neutron flux is controlled by the proximity of the normed solution of the non-stationary problem and the fundamental eigenfunction  $\phi$ . Let's define for g=1:

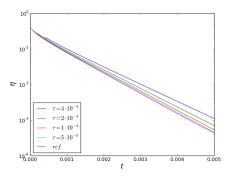
$$\eta(t) = \|\overline{\phi}_1(t) - \overline{\varphi}_1\|, \quad \overline{\phi}_1(t) = \frac{\phi_1(t)}{\|\phi_1(t)\|}, \quad \overline{\varphi}_1 = \frac{\varphi_1}{\|\varphi_1\|}.$$

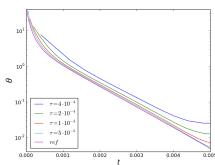
The appearance of the dynamic behaviour trend is evaluated by the value:

$$\theta(t) = \frac{1}{\sqrt{2} \|\alpha\|} \left( \left\| \frac{1}{\phi_1(t)} \frac{\partial \phi_1(t)}{\partial t} - \alpha \right\|^2 + \left\| \frac{1}{\phi_2(t)} \frac{\partial \phi_2(t)}{\partial t} - \alpha \right\|^2 \right)^{1/2}.$$

### Results

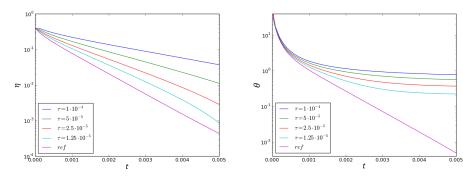
The fully implicit scheme,  $\eta(t)$  (left) and  $\theta(t)$  (right):





#### Results

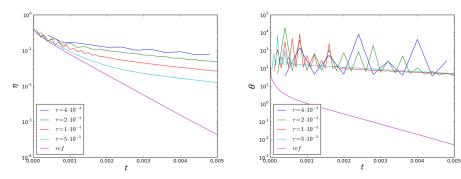
The explicit-implicit scheme,  $\eta(t)$  (left) and  $\theta(t)$  (right):



The fully implicit scheme has significantly higher accuracy than explicit-implicit scheme.

#### Results

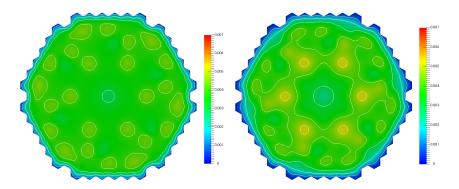
The Crank-Nicolson scheme,  $\eta(t)$ (left) and  $\theta(t)$ (right):



As expected, the Crank-Nicolson scheme is unsuitable for modelling regular regime as it has a poor property of asymptotic stability.

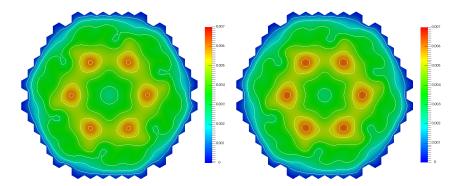
## **Evolution**

Eigenfunction  $\overline{\phi}_1$  in t = 0.0001(left) and t = 0.0004(right):



## **Evolution**

Eigenfunction  $\overline{\phi}_1$  in t = 0.0016(left) and t = 0.0064(right):



#### Conclusion

We consider non-stationary problem of neutron diffusion in a nuclear reactor using a multigroup approximation. Obtained  $\alpha$ -spectral problem, which characterizes the dynamic neutron nuclear reactor field at the asymptotic stage for large time — regular regime.

Non-stationary neutron diffusion problem with access to the regular regime. Test calculations are made in the two-dimensional approximation for the nuclear reactor model VVVER-1000 without reflector using two-group diffusion approximation.

It established a good separability of the eigenvalues in the  $\alpha$ -spectral problem. There is a good convergence of nonstationary problem by reducing the time step for fully implicit scheme. Explicit-implicit scheme converges much worse than fully implicit scheme.

Crank-Nicolson scheme, though a second-order approximation, almost unusable for regular simulation of a nuclear reactor regime.

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Thank you for your attention! Any questions?