



Student Conference 2021

North Carolina State University

ENLIGHTEN / EMBRACE / EMPOWER



Nuclear
Engineering



Adjoint Solution of Time-dependent Multigroup Diffusion Model with Generalized Temporal and Spatial Boundary Conditions

Tao Liu and Zeyun Wu

Department of Mechanical and Nuclear Engineering
Virginia Commonwealth University, Richmond, Virginia

Paper ID: 34685



VCU

College of Engineering

Outline

- **Motivation**
- **Governing Equations**
- **Numerical Methods**
- **Test Problem and Numerical Results**
- **Conclusions and Future work**

Motivation

- The understanding of **time-dependent behavior** of neutron population in a nuclear reactor is of critical importance to the safe operation of nuclear reactors.
- The neutron **adjoint diffusion equation** could be used for kinetics parameter calculations or in perturbation theory for the sensitivity analysis.
- However, partly due to exaggerated **computation cost**, the time-dependent adjoint equation is **rarely solved**.
- The typical practice is to solve the **steady state** adjoint equation and use the fundamental mode adjoint function as an **approximation** for all other dynamic states.
- A **generalized temporal and spatial boundary conditions** for the adjoint models are considered.

Time-dependent Two-Group Diffusion Equations

$$\left\{ \begin{array}{l} \frac{1}{v_1} \frac{\partial \phi_1}{\partial t} - \frac{\partial}{\partial x} \left[D_1(x, t) \frac{\partial \phi_1}{\partial x} \right] + \Sigma_{r,1} \phi_1(x, t) = (1 - \beta) [v \Sigma_{f,1} \phi_1(x, t) + v \Sigma_{f,2} \phi_2(x, t)] + \sum_{k=1}^K \lambda_k C_k(x, t) \\ \frac{1}{v_2} \frac{\partial \phi_2}{\partial t} - \frac{\partial}{\partial x} \left[D_2(x, t) \frac{\partial \phi_2}{\partial x} \right] + \Sigma_{a,2} \phi_2(x, t) = \Sigma_{s,1 \rightarrow 2}(x, t) \phi_1(x, t) \\ \frac{\partial C_k(x, t)}{\partial t} = \beta_k [v \Sigma_{f,1} \phi_1 + v \Sigma_{f,2} \phi_2] - \lambda_k C_k(x, t) \quad k = 1, \dots, K. \end{array} \right.$$

- The reflective boundary conditions (B.C.) and a prescribed initial condition (I.C.) :

$$\text{B.C.:} \quad \left. \frac{\partial \phi_g(x, t)}{\partial x} \right|_{x=0} = 0, \quad \text{and} \quad \left. \frac{\partial \phi_g(x, t)}{\partial x} \right|_{x=L} = 0$$

$$\text{I.C.:} \quad \phi_g(x, 0) = \phi_{g0}(x)$$

- For the delayed neutron precursor (DNP) equations, the initial conditions can be defined similarly :

$$C_k(x, 0) = C_{k0}(x), \quad k = 1, \dots, K.$$

Adjoint Diffusion Equations

$$\left\{ \begin{array}{l} -\frac{1}{v_1} \frac{\partial \phi_1^*}{\partial t} - \frac{\partial}{\partial x} \left[D_1(x, t) \frac{\partial \phi_1^*}{\partial x} \right] + \Sigma_{r,1} \phi_1^*(x, t) = (1 - \beta) \nu \Sigma_{f,1} \phi_1^*(x, t) + \Sigma_{s,1 \rightarrow 2} \phi_2^*(x, t) + \beta_k \nu \Sigma_{f1} C_k^*(x, t) \\ -\frac{1}{v_2} \frac{\partial \phi_2^*}{\partial t} - \frac{\partial}{\partial x} \left[D_2(x, t) \frac{\partial \phi_2^*}{\partial x} \right] + \Sigma_{a,2}(x, t) \phi_2^* = (1 - \beta) \nu \Sigma_{f,2} \phi_1^*(x, t) + \beta_k \nu \Sigma_{f2} C_k^*(x, t) \\ -\frac{\partial C_k^*(x, t)}{\partial t} = \left(\sum_{k=1}^K \lambda_k \right) \phi_1^*(x, t) - \lambda_k C_k^*(x, t) \quad k = 1, \dots, K. \end{array} \right.$$

- The reflective boundary conditions (B.C.) and the final condition (F.C.) :

$$\text{B.C.:} \quad \left. \frac{\partial \phi_g^*(x, t)}{\partial x} \right|_{x=0} = 0, \quad \text{and} \quad \left. \frac{\partial \phi_g^*(x, t)}{\partial x} \right|_{x=L} = 0,$$

$$\text{F.C.:} \quad \phi_g^*(x, T) = \phi_{g0}^*(x) \frac{\phi_{g0}(x)}{\phi_g(x, T)}$$

- For the delayed neutron precursor (DNP) equations, the final conditions can be defined similarly:

$$C_k^*(x, T) = C_k^*(x, 0) \frac{C_k(x, 0)}{C_k(x, T)} = C_{k0}^*(x) \frac{C_{k0}(x)}{C_k(x, T)}, \quad k = 1, \dots, K.$$

Summary of the Governing Equations

- Forward Diffusion Equations

$$\left\{ \begin{aligned} \frac{1}{v_1} \frac{\partial \phi_1}{\partial t} - \frac{\partial}{\partial x} \left[D_1(x, t) \frac{\partial \phi_1}{\partial x} \right] + \Sigma_{r,1} \phi_1(x, t) &= (1 - \beta) [v \Sigma_{f,1} \phi_1(x, t) + v \Sigma_{f,2} \phi_2(x, t)] + \sum_{k=1}^K \lambda_k C_k(x, t) \\ \frac{1}{v_2} \frac{\partial \phi_2}{\partial t} - \frac{\partial}{\partial x} \left[D_2(x, t) \frac{\partial \phi_2}{\partial x} \right] + \Sigma_{a,2} \phi_2(x, t) &= \Sigma_{s,1 \rightarrow 2}(x, t) \phi_1(x, t) \\ \frac{\partial C_k(x, t)}{\partial t} &= \beta_k [v \Sigma_{f,1} \phi_1 + v \Sigma_{f,2} \phi_2] - \lambda_k C_k(x, t) \quad k = 1, \dots, K. \end{aligned} \right.$$

- Adjoint Diffusion Equations

$$\left\{ \begin{aligned} -\frac{1}{v_1} \frac{\partial \phi_1^*}{\partial t} - \frac{\partial}{\partial x} \left[D_1(x, t) \frac{\partial \phi_1^*}{\partial x} \right] + \Sigma_{r,1} \phi_1^*(x, t) &= (1 - \beta) v \Sigma_{f,1} \phi_1^*(x, t) + \Sigma_{s,1 \rightarrow 2} \phi_2^*(x, t) + \beta_k v \Sigma_{f,1} C_k^*(x, t) \\ -\frac{1}{v_2} \frac{\partial \phi_2^*}{\partial t} - \frac{\partial}{\partial x} \left[D_2(x, t) \frac{\partial \phi_2^*}{\partial x} \right] + \Sigma_{a,2}(x, t) \phi_2^* &= (1 - \beta) v \Sigma_{f,2} \phi_1^*(x, t) + \beta_k v \Sigma_{f,2} C_k^*(x, t) \\ -\frac{\partial C_k^*(x, t)}{\partial t} &= \left(\sum_{k=1}^K \lambda_k \right) \phi_1^*(x, t) - \lambda_k C_k^*(x, t) \quad k = 1, \dots, K. \end{aligned} \right.$$

Numerical Methods

- **Time** Discretization (Semi-implicit Method)
 - Uniform time step: 0.5 s.
- **Space** Discretization (Finite Difference Method)
 - Mesh size: 1 cm.
- Iterative approach for the flux solver

Iterative Strategy for the Flux Solver

The power iteration method is used to solve for the time-dependent diffusion equations. Here we take the forward equation as example to illustrate the iterative procedures:

$$\begin{cases} -\frac{\partial}{\partial x} \left[D_1^n(x) \frac{\partial \phi_1^n}{\partial x} \right] + \left[\Sigma_{r,1}^n(x) + \frac{1}{v_1 \Delta t_n} - (1 - \beta + \gamma_n) v \Sigma_{f,1}^n(x) \right] \phi_1^n = (1 - \beta + \gamma_n) v \Sigma_{f,2}^n(x) \phi_2^n + \frac{1}{\Delta t_n} \sum_{k=1}^K C_k^{n-1}(x) (1 - e^{-\lambda_k \Delta t_n}) + S_1^n(x) \\ -\frac{\partial}{\partial x} \left[D_2^n(x) \frac{\partial \phi_2^n}{\partial x} \right] + \left[\Sigma_{a,2}^n(x) + \frac{1}{v_2 \Delta t_n} \right] \phi_2^n = \Sigma_{s,1 \rightarrow 2}^n(x) \phi_1^n + S_2^n(x) \end{cases}$$

Where

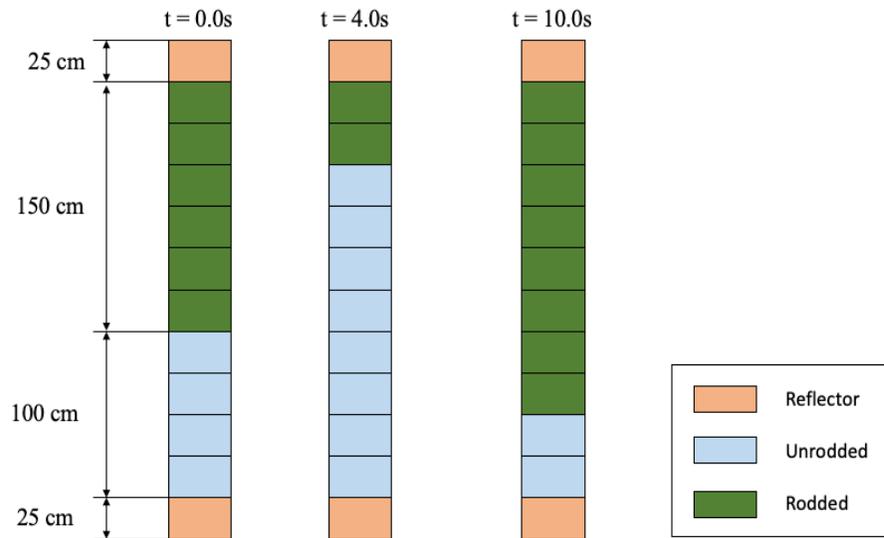
$$\begin{cases} S_1^n(x) = \frac{\phi_1^{n-1}}{v_1 \Delta t_n} \\ S_2^n(x) = \frac{\phi_2^{n-1}}{v_2 \Delta t_n} \end{cases} \quad \text{and} \quad \gamma_n = \sum_{k=1}^K \beta_k \left[1 - \frac{1 - e^{-\lambda_k \Delta t_n}}{\Delta t_n \lambda_k} \right]$$

The DNP concentration at time step n :

$$C_k^n(x) = C_k^{n-1}(x) e^{-\lambda_k \Delta t_n} + \frac{\beta_k (1 - e^{-\lambda_k \Delta t_n})}{\lambda_k} [v \Sigma_{f,1}^n(x) \phi_1^n + v \Sigma_{f,2}^n(x) \phi_2^n]$$

Rod-ejection Test Problem

A rod-ejection accident in a one-dimensional reactor problem is considered as a test problem to demonstrate the applicability and validation of the presented method [5].



Geometry of the one-dimensional reactor

- **Three** regions: reflector, unrodded fuel, and rodded fuel.
- During the rod-ejection accident, the control rod is assumed to be **withdrawn** from **0 s to 4.0 s** with a speed of 25cm/s.
- Later the control rod is **inserted** from **4.0 s to 10.0 s** with the same constant speed. Uniform time step which is 0.5s are considered in this problem.

Rod-ejection Test Problem

Table 1. Material Properties [5].

	Group 1				Group 2		
	D_1 (cm)	$\Sigma_{a,1}$ (cm ⁻¹)	$\nu\Sigma_{f,1}$ (cm ⁻¹)	$\Sigma_{s,1\rightarrow 2}$ (cm ⁻¹)	D_2 (cm)	$\Sigma_{a,2}$ (cm ⁻¹)	$\nu\Sigma_{f,2}$ (cm ⁻¹)
Unrodded fuel	1.40343	1.17659e-2	5.62285e-3	1.60795e-2	0.32886	1.07186e-1	1.45865e-1
Rodded fuel	1.40343	1.17659e-2	5.60285e-3	1.60795e-2	0.32886	1.07186e-1	1.45403e-1
Reflector	0.93344	2.81676e-3	0	1.08805e-2	0.95793	8.87200e-2	0

Table 2. Delayed Neutron Precursor Parameters [5].

	Group 1	Group 2	Group 3	Group 4	Group 5	Group 6
β_k (-)	0.000247	0.0013845	0.001222	0.026455	0.000832	0.000169
λ_k (1/s)	0.0127	0.0317	0.115	0.311	1.4	3.87
	$v_1 = 1.27 \times 10^7$ cm / s		$v_2 = 2.5 \times 10^5$ cm / s		$\beta_k = 0.0065$	

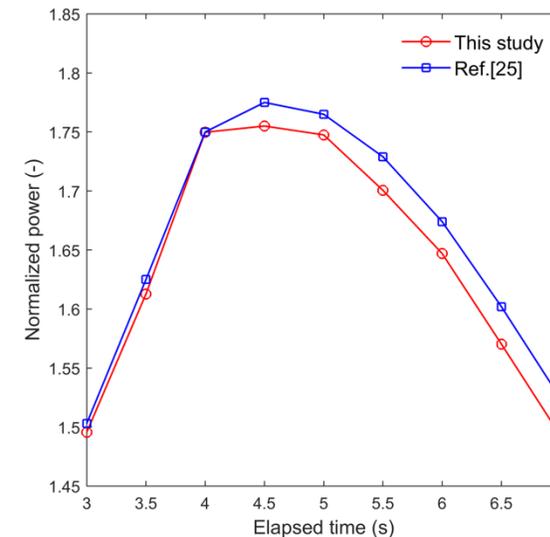
Numerical Result

Before performing the time-dependent analysis, the **steady state** condition was examined as a criticality calculation. The K_{eff} obtained at the initial time of the reactor is 0.978821. This value agrees well with the result for the test problem in Ref. [5]

For the **dynamics** behavior, the power changes of the slab reactor during the rod-ejection accident was calculated.

The **normalized mean power** was calculated by using the formula:

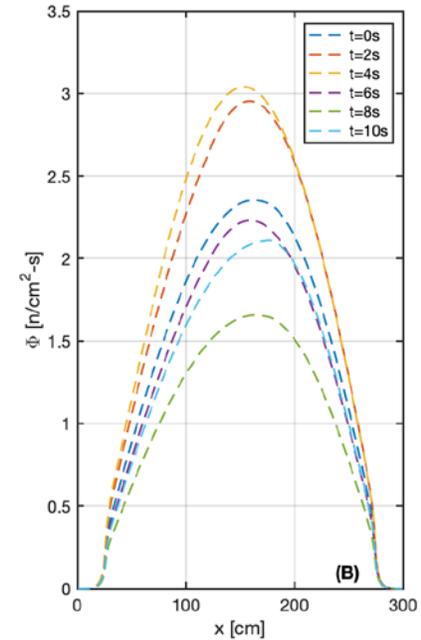
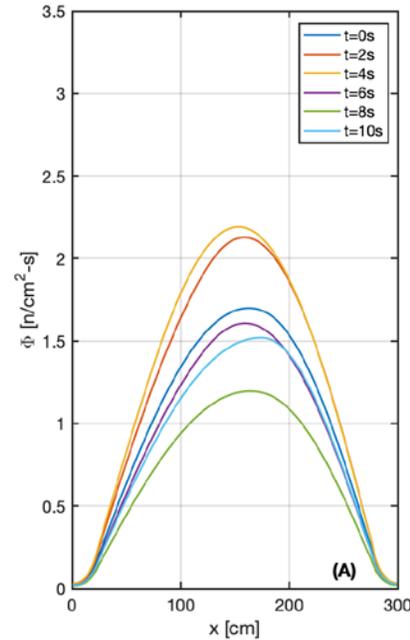
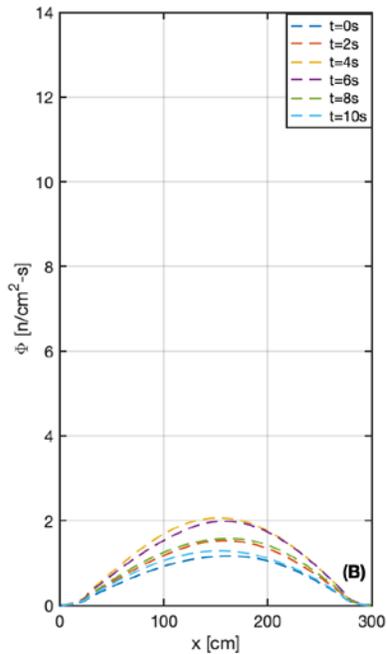
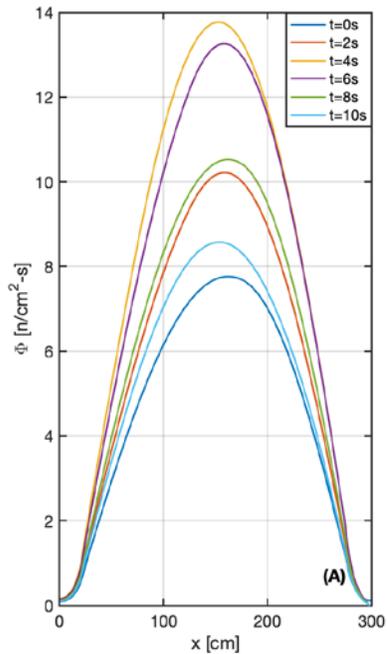
$$\bar{P}(t) = \frac{\int_{\Omega} \left(\Sigma_{f,1}(x)\phi_1(x,t) + \Sigma_{f,2}(x)\phi_2(x,t) \right) dV}{\int_{\Omega} \left(\Sigma_{f,1}(x)\phi_1(x,0) + \Sigma_{f,2}(x)\phi_2(x,0) \right) dV}$$



Normalized power evolution for the 1D reactor.

Numerical Result

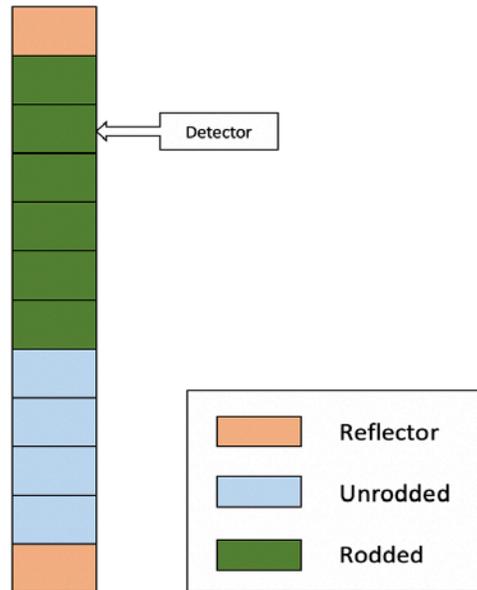
For **transient** behaviors, the following figures show the **neutron flux distributions** and **adjoint solutions** at various times during the rod-ejection accident.



Fast neutron flux (A) and thermal neutron flux (B). Fast adjoint solutions (A) and thermal adjoint solutions (B).

Numerical Result

To better understand the physical meaning of the adjoint neutron flux, we assume there is a **neutron detector** placed at the middle of the third cell of the reactor core.



The typical **response** R chosen is the reading of detector which could be given by the reaction rate:

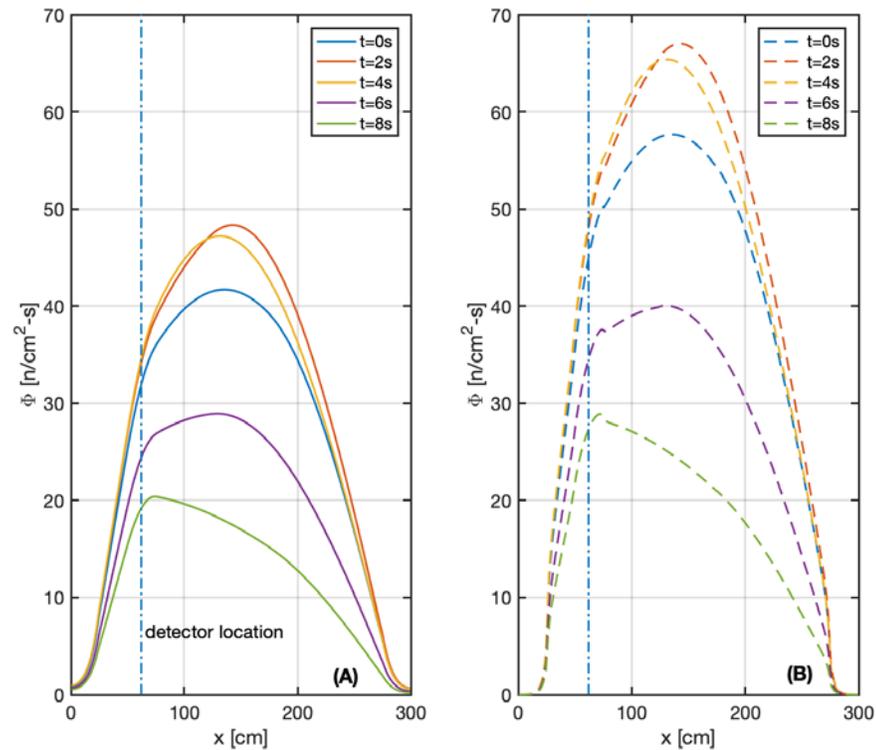
$$R = \sum_{g=1}^G \Sigma_{d,g} \phi_g(x, t), \quad G = 2$$

The adjoint source is defined as a **delta** function in this problem. Then the adjoint equation with adjoint source become:

$$-\frac{1}{v} \frac{\partial \phi_g^*}{\partial t} - \frac{\partial}{\partial x} \left[D_g(x, t) \frac{\partial \phi_g^*}{\partial x} \right] + \Sigma_{r,g} \phi_g^*(x, t) = S + \Sigma_{d,g}$$

Numerical Result

- The figure shows the adjoint solutions variation during the rod-ejection accident, which represents the neutron importance distribution for the designated detector response R.



Fast adjoint (A) and thermal adjoint (B) for R.

Conclusions and Future Work

- A numerical approach to obtain the **forward and adjoint solution** of the **time-dependent** one-dimensional two-group neutron diffusion model for the spatial reactor kinetics problems was presented.
- The **generalized temporal and spatial boundary conditions** for both the forward and adjoint models are derived for application purposes
- The numerical approaches are based on the **finite difference method** for the spatial discretization and **semi-implicit method** for the temporal discretization
- A **rod-ejection accident** in a one-dimensional model reactor problem is applied as a test example to demonstrate the applicability of the presented method. The computational results of the test problem demonstrate that the code is capable of outputting reasonably accurate solutions.
- In the future, the time-dependent adjoint solution will be used in the perturbation theory for dynamics **sensitivity analysis**.

References

- [1]. W.M. Stacey, Nuclear Reactor Physics, 3rd ed., Wiley VCH, Weinheim (2018).
- [2]. E.P. Wigner, “Effects of Small Perturbations on Pile Period,” CP-3048, Manhattan Project Report (1945).
- [3]. D.G. Cacuci. Sensitivity and Uncertainty Analysis, Chapman and Hall/CRC, Washington, D.C. (2003).
- [4]. G.I. Bell and S. Glasstone, Nuclear Reactor Theory, Van Nostrand Reinhold Company, New York (1970).
- [5]. A. Vidal-Ferràndiz., et al, “Moving meshes to solve the time-dependent neutron diffusion equation in hexagonal geometry,” Journal of Computational and Applied Mathematics, 291, 197–208 (2016).

Thank you!