

## Non-linear time-dependent modelling of heterogeneous nuclear reactors

Applications to Xenon oscillations in pressurized water reactors

Master's thesis in Physics

FREDRIK ÖHRLUND

# Master's thesis presentation:

## *Non-linear time-dependent modelling of heterogeneous nuclear reactors* *Applications to **Xenon oscillations** in pressurized water reactors*

### Awarded the 2024 SKC Sigvard Eklund price for best master's thesis

## Fredrik Öhrlund, MSc

# Outline of Presentation

- My Master Thesis 5 min
- Simulating a reactor 3 min
- Xenon-135 7 min

# Thesis background



From  
Page 1

- In thermal nuclear reactors, there is a fission product called Xenon-135
- Its well known in reactor physics that Xe-135 can cause "xenon oscillations"
- Xenon oscillations are expected to be a more frequent problem in the future
- The DREAM group at Chalmers is currently developing methods for predicting xenon-oscillations
- "This master thesis project aims at developing modelling capabilities that allow for the calculation of the three-dimensional time-dependence of the neutron flux in a nuclear reactor for the specific purpose of studying the xenon effect."
- Unlike proprietary software, will have full access to the source code

# Problem definition



From  
Page 2

$$\begin{aligned} \frac{1}{v_1} \frac{\partial}{\partial t} \phi_1(\vec{\mathbf{r}}, t) = & \left[ \vec{\nabla} \cdot D_1(\vec{\mathbf{r}}, t) \vec{\nabla} + \nu \Sigma'_{f,1}(\vec{\mathbf{r}}, t) - \Sigma_{a,1}(\vec{\mathbf{r}}, t) - \Sigma_r(\vec{\mathbf{r}}, t) \right] \phi_1(\vec{\mathbf{r}}, t) \\ & + \nu \Sigma'_{f,2}(\vec{\mathbf{r}}, t) \phi_2(\vec{\mathbf{r}}, t) \\ & + \alpha_{1 \rightarrow 1}(\vec{\mathbf{r}}) (\phi_1(\vec{\mathbf{r}}, t) - \phi_{eq,1}(\vec{\mathbf{r}})) + \alpha_{2 \rightarrow 1}(\vec{\mathbf{r}}) (\phi_2(\vec{\mathbf{r}}, t) - \phi_{eq,2}(\vec{\mathbf{r}})) \end{aligned}$$



To summarize the remaining 5 pages of the project description:

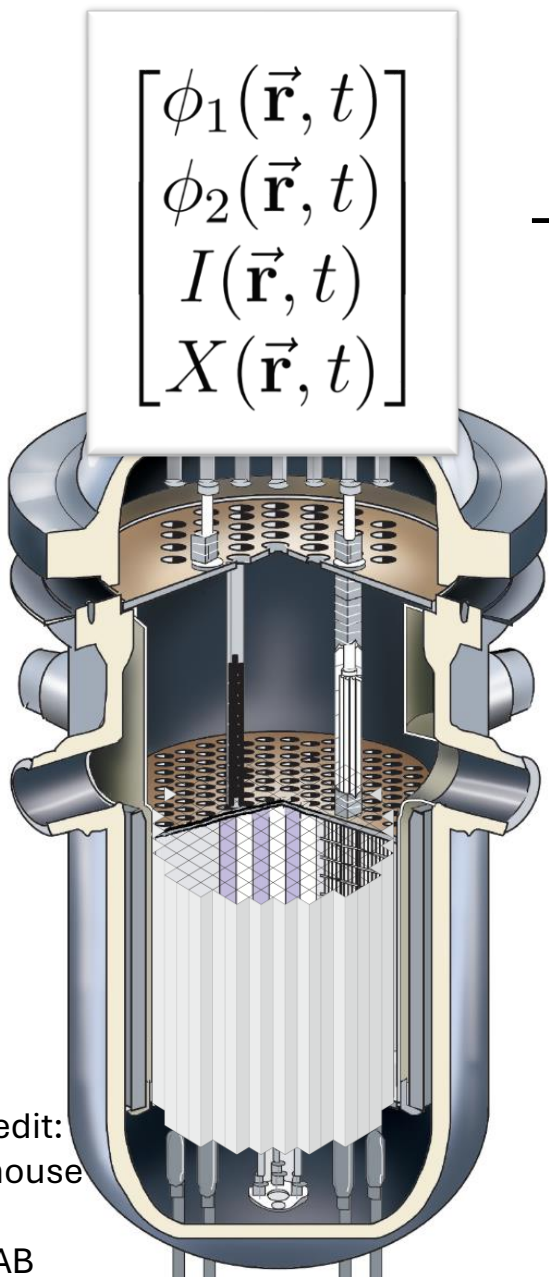
”Here is a long list of constraints and requirements...

... please solve these equations, using a computer...

... then...

... somehow perturb the system to generate xenon oscillations”

# Problem definition



$\begin{bmatrix} \phi_1(\vec{r}, t) \\ \phi_2(\vec{r}, t) \\ I(\vec{r}, t) \\ X(\vec{r}, t) \end{bmatrix}$

$$\frac{1}{v_1} \frac{\partial}{\partial t} \phi_1(\vec{r}, t) = \left[ \vec{\nabla} \cdot D_1(\vec{r}, t) \vec{\nabla} + \nu \Sigma'_{f,1}(\vec{r}, t) - \Sigma_{a,1}(\vec{r}, t) - \Sigma_r(\vec{r}, t) \right] \phi_1(\vec{r}, t)$$

$$+ \nu \Sigma'_{f,2}(\vec{r}, t) \phi_2(\vec{r}, t)$$

$$+ \alpha_{1 \rightarrow 1}(\vec{r}) (\phi_1(\vec{r}, t) - \phi_{eq,1}(\vec{r})) + \alpha_{2 \rightarrow 1}(\vec{r}) (\phi_2(\vec{r}, t) - \phi_{eq,2}(\vec{r}))$$

$$\frac{1}{v_2} \frac{\partial}{\partial t} \phi_2(\vec{r}, t) = \Sigma_r(\vec{r}, t) \phi_1(\vec{r}, t) + \left[ \vec{\nabla} \cdot D_2(\vec{r}, t) \vec{\nabla} - \Sigma_{a,2,wox}(\vec{r}, t) \right] \phi_2(\vec{r}, t)$$

$$+ \alpha_{1 \rightarrow 2}(\vec{r}) (\phi_1(\vec{r}, t) - \phi_{eq,1}(\vec{r})) + \alpha_{2 \rightarrow 2}(\vec{r}) (\phi_2(\vec{r}, t) - \phi_{eq,2}(\vec{r}))$$

$$- \sigma_X X(\vec{r}, t) \phi_2(\vec{r}, t)$$

$$\frac{\partial}{\partial t} I(\vec{r}, t) = \gamma_I \Sigma'_{f,1}(\vec{r}, t) \phi_1(\vec{r}, t) + \gamma_I \Sigma'_{f,2}(\vec{r}, t) \phi_2(\vec{r}, t) - \lambda_I I(\vec{r}, t)$$

$$\frac{\partial}{\partial t} X(\vec{r}, t) = \gamma_X \Sigma'_{f,1}(\vec{r}, t) \phi_1(\vec{r}, t) + \gamma_X \Sigma'_{f,2}(\vec{r}, t) \phi_2(\vec{r}, t) + \lambda_I I(\vec{r}, t) - \lambda_X X(\vec{r}, t) - \sigma_X X(\vec{r}, t) \phi_2(\vec{r}, t).$$

## XS INPUT DATA

$$\begin{array}{cc}
 D_1(\vec{r}) & D_2(\vec{r}) \\
 \nu \Sigma_{f,1}(\vec{r}) & \nu \Sigma_{f,2}(\vec{r}) \\
 \Sigma_{a,1}(\vec{r}) & \Sigma_{a,2}(\vec{r}) \\
 & \Sigma_r(\vec{r})
 \end{array}$$

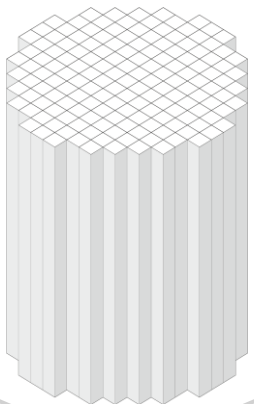
## CONSTRAINTS

Minimum solver capability ~50h sims  
 Marshak Boundary Conditions  
 Mesh-centered Finite Differences  
 Compatibility with CORE SIM  
 Etc etc etc etc...

# Problem definition

$$\begin{bmatrix} \phi_1(\vec{\mathbf{r}}, t) \\ \phi_2(\vec{\mathbf{r}}, t) \\ I(\vec{\mathbf{r}}, t) \\ X(\vec{\mathbf{r}}, t) \end{bmatrix}$$

Xenon oscillations

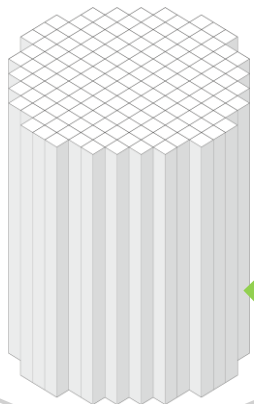


# My workflow

$$\begin{bmatrix} \phi_1(\vec{\mathbf{r}}, t) \\ \phi_2(\vec{\mathbf{r}}, t) \\ I(\vec{\mathbf{r}}, t) \\ X(\vec{\mathbf{r}}, t) \end{bmatrix}$$



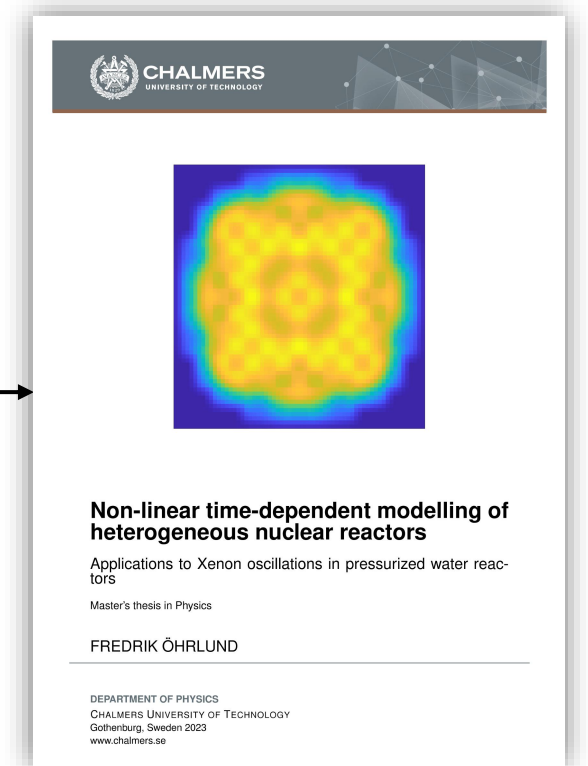
Xenon oscillations



## My workflow

- Significant time studying/preparing
- Wrote a steady-state solver
- Wrote a time-integration solver
- Implemented CRB perturbations
- Generated some xenon oscillations

Lines of code  
3328



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# Simulating a reactor

Figure Credit: Westinghouse Electric Sweden AB

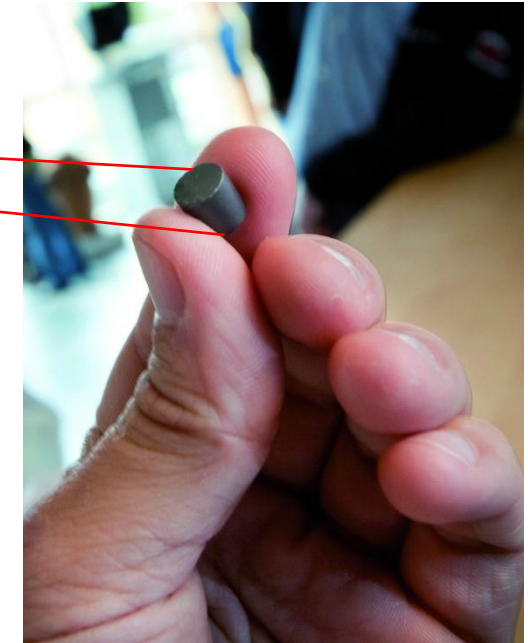
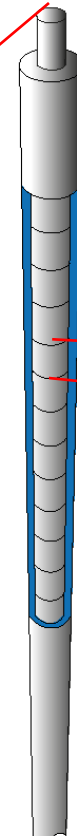
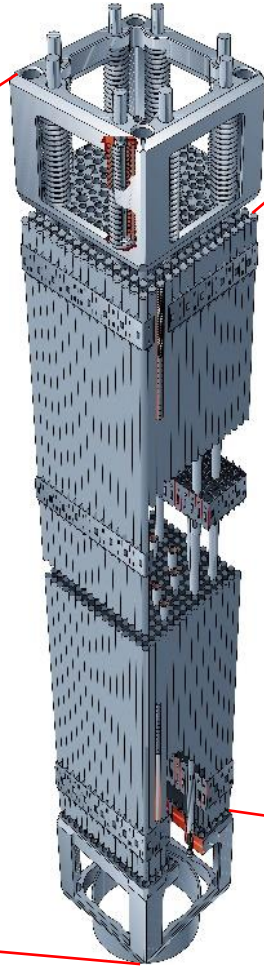
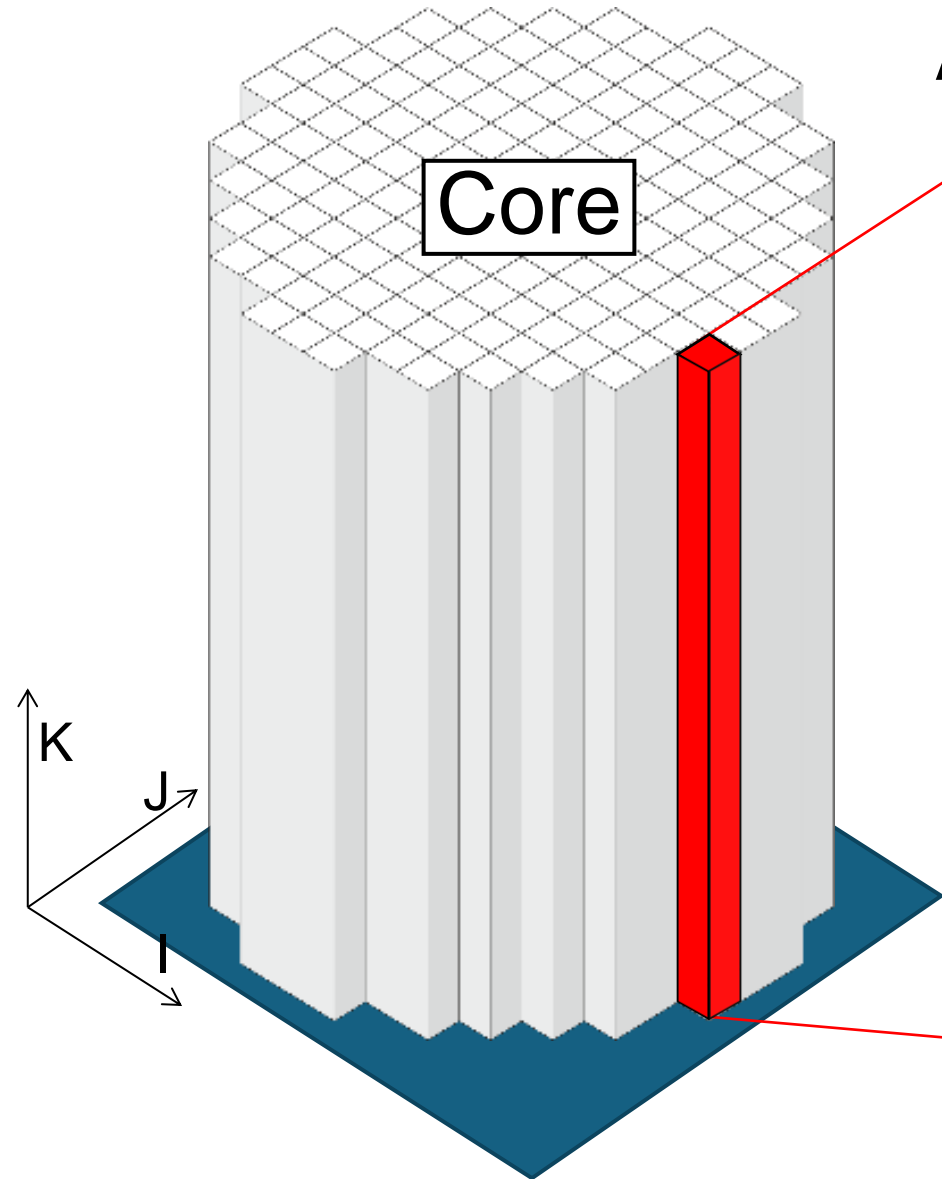
Fuel Assemblies

Figure Credit: Swedish Academic Initiative in radiation and Nuclear Technology research and development

Fuel Pins

Figure Credit: Fredrik Ekenborg, Analysgruppen vid KSU

Fuel Pellets



193

264

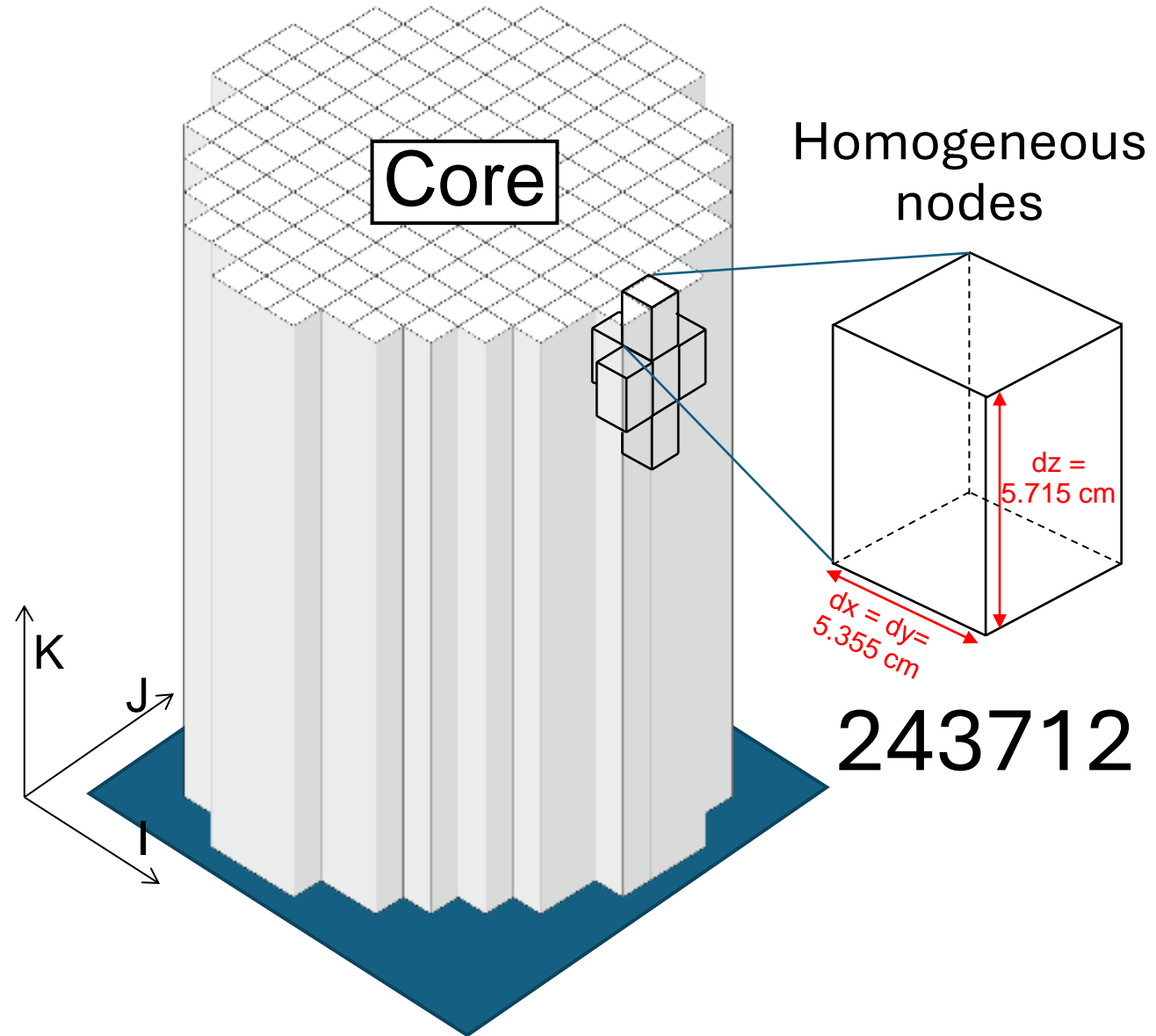
**Serpent**

*a Continuous-energy Monte Carlo neutron and photon transport code*

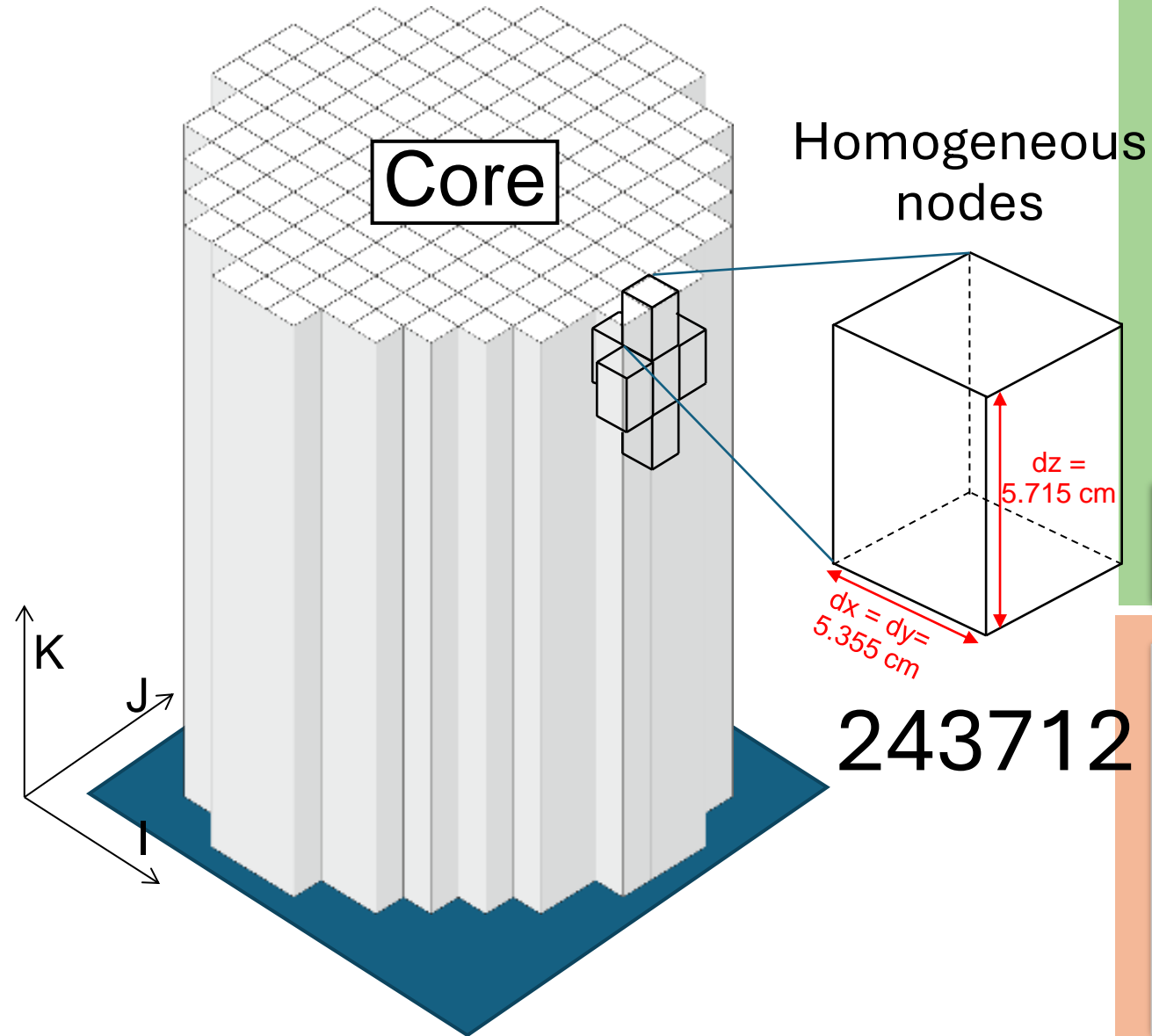
~17 million



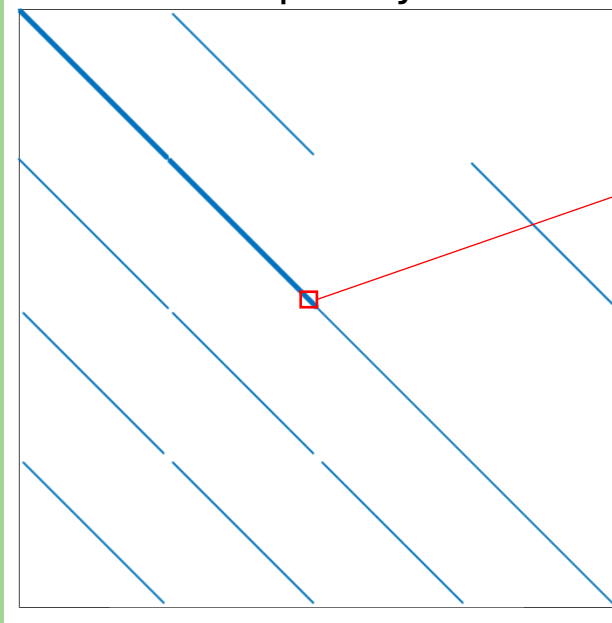
# Simulating a reactor



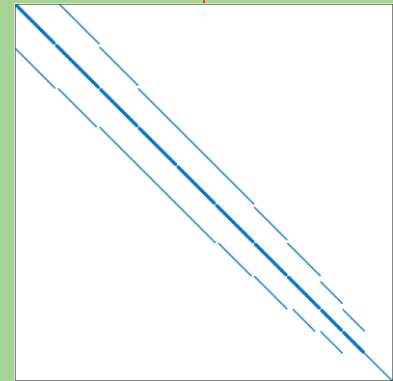
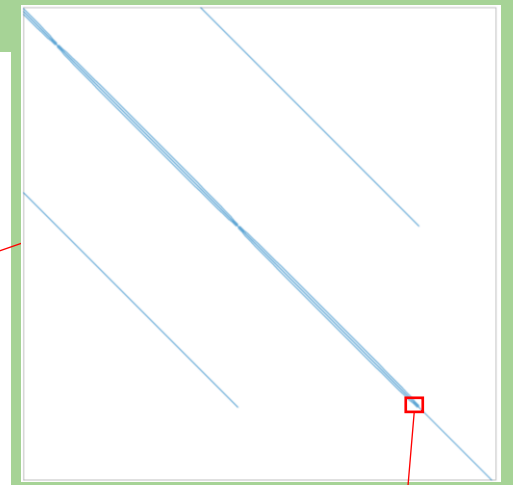
# Simulating a reactor



Jacobian Sparsity Pattern



nonzeros = 5,477,373



1. Invert Jacobian 1000-10000 times per simulation

$$\begin{bmatrix} \phi_1(\vec{r}, t) \\ \phi_2(\vec{r}, t) \\ I(\vec{r}, t) \\ X(\vec{r}, t) \end{bmatrix}$$

Characteristic Time-scales:

$\sim 10 \text{ ns}$

$\sim 1 \text{ ms}$

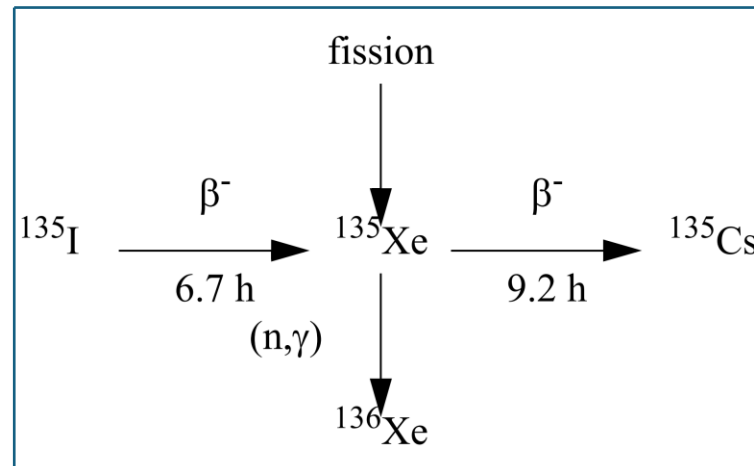
$\sim 1 \text{ h}$

Time-scales spanning  $\sim 10^{11}$

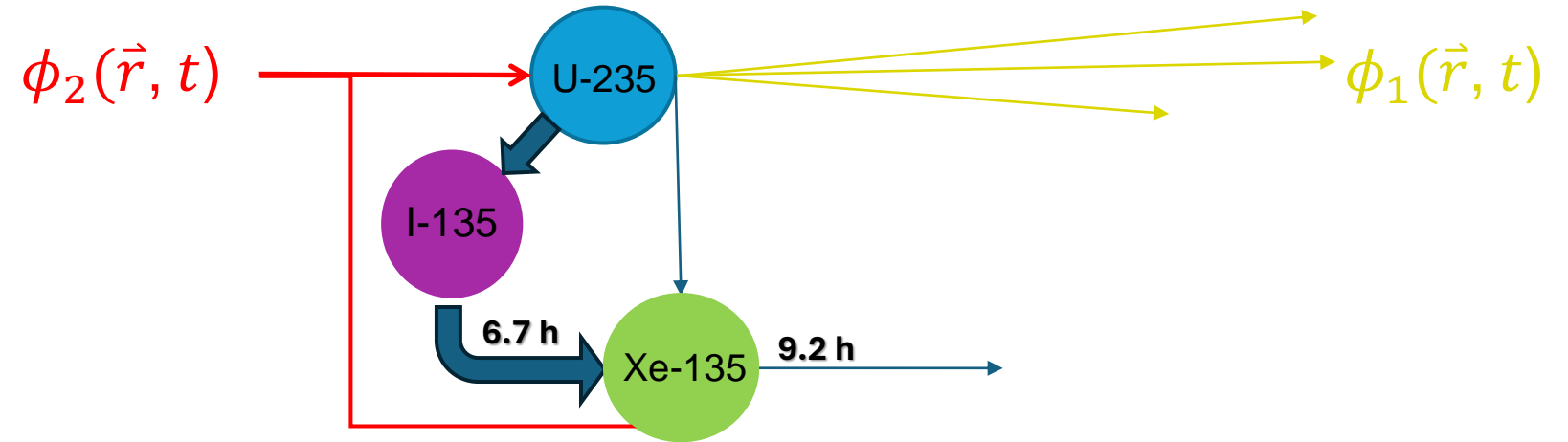
2. Extremely stiff dynamics -> -> Numerical oscillations

# Xenon poisoning

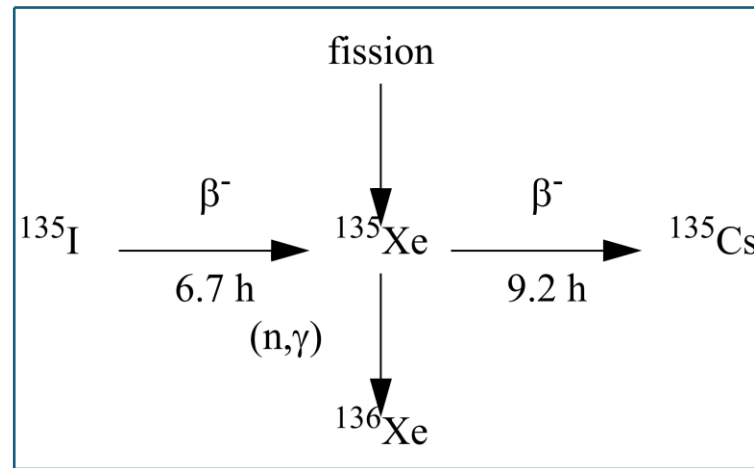
Evolution chain of Xenon-135



# Xenon poisoning

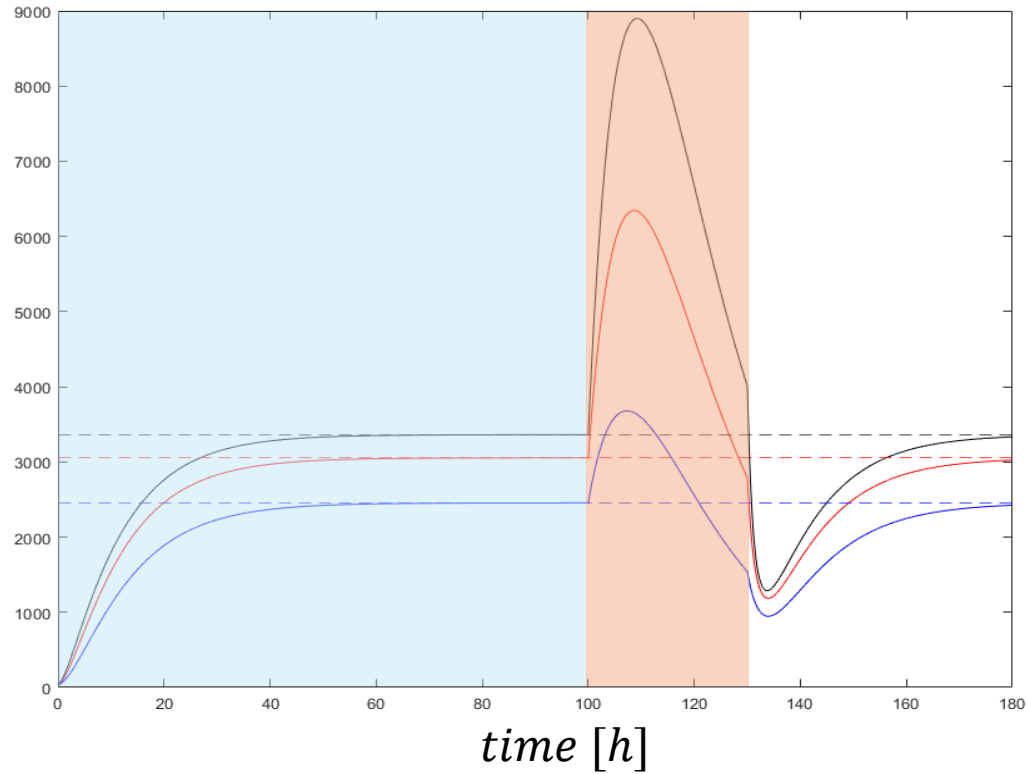


Evolution chain of Xenon-135



*time [h]*

# Xenon poisoning



$\phi_2(\vec{r}, t)$

$$\frac{d}{dt} \begin{bmatrix} I(t) \\ X(t) \end{bmatrix} = \begin{bmatrix} -\lambda_I & \\ \lambda_I & -\lambda_X \end{bmatrix} \begin{bmatrix} I(t) \\ X(t) \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} I(t) \\ X(t) \end{bmatrix} = \exp \left( \begin{bmatrix} -\lambda_I & \\ \lambda_I & -\lambda_X \end{bmatrix} t \right) \begin{bmatrix} I_0 \\ X_0 \end{bmatrix}$$

$$\Rightarrow X(t) = \frac{\lambda_I}{\lambda_I - \lambda_X} (e^{-\lambda_X t} - e^{-\lambda_I t}) I_0 + e^{-\lambda_X t} X_0$$

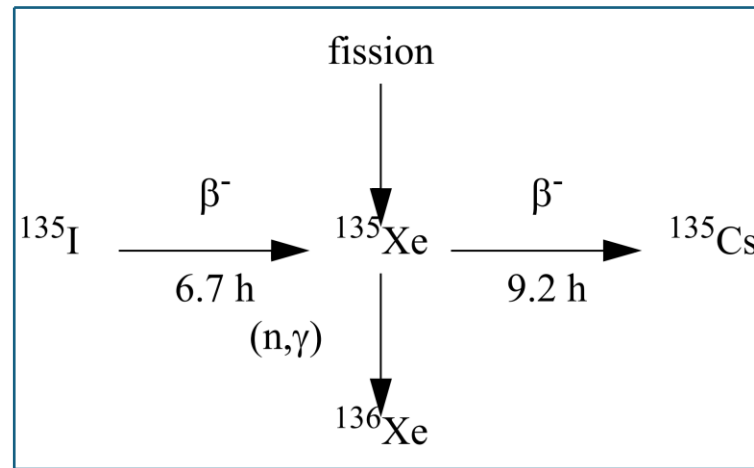
I-135

6.7 h

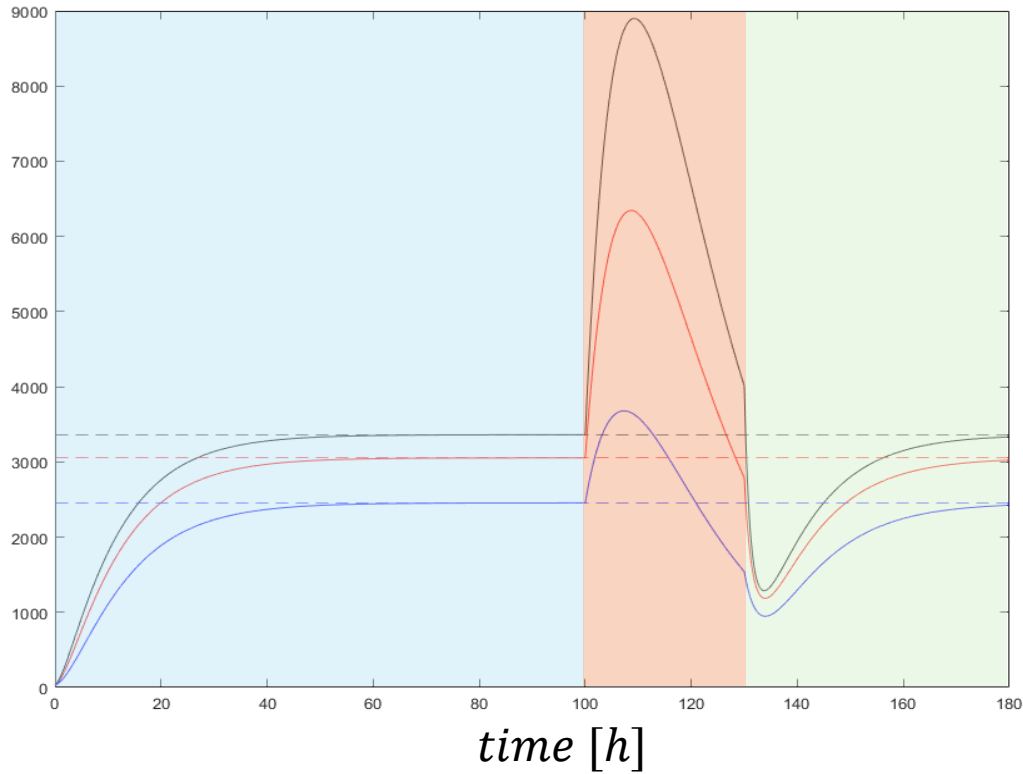
Xe-135

9.2 h

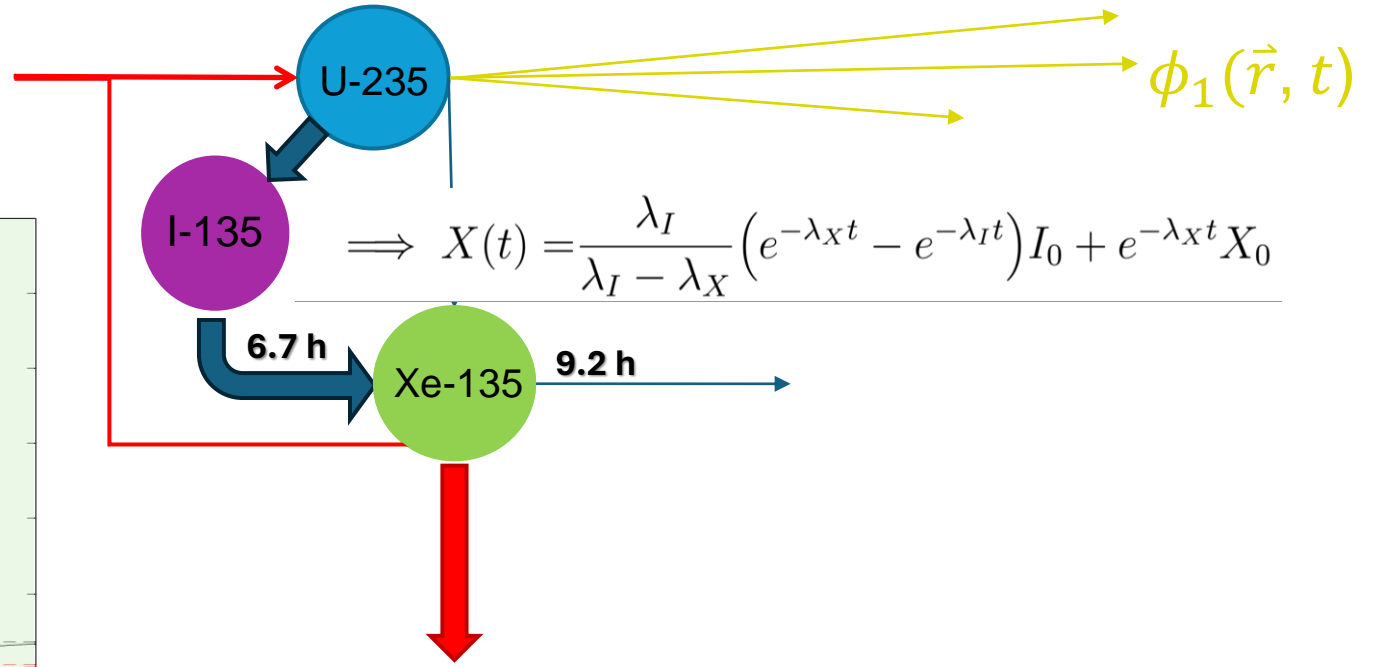
Evolution chain of Xenon-135



# Xenon poisoning

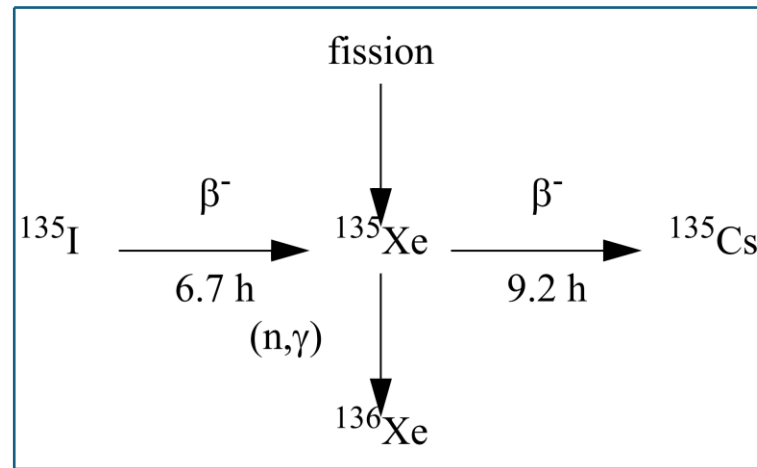


$\phi_2(\vec{r}, t)$



$$\Rightarrow X(t) = \frac{\lambda_I}{\lambda_I - \lambda_X} (e^{-\lambda_X t} - e^{-\lambda_I t}) I_0 + e^{-\lambda_X t} X_0$$

## Evolution chain of Xenon-135



# Xenon poisoning

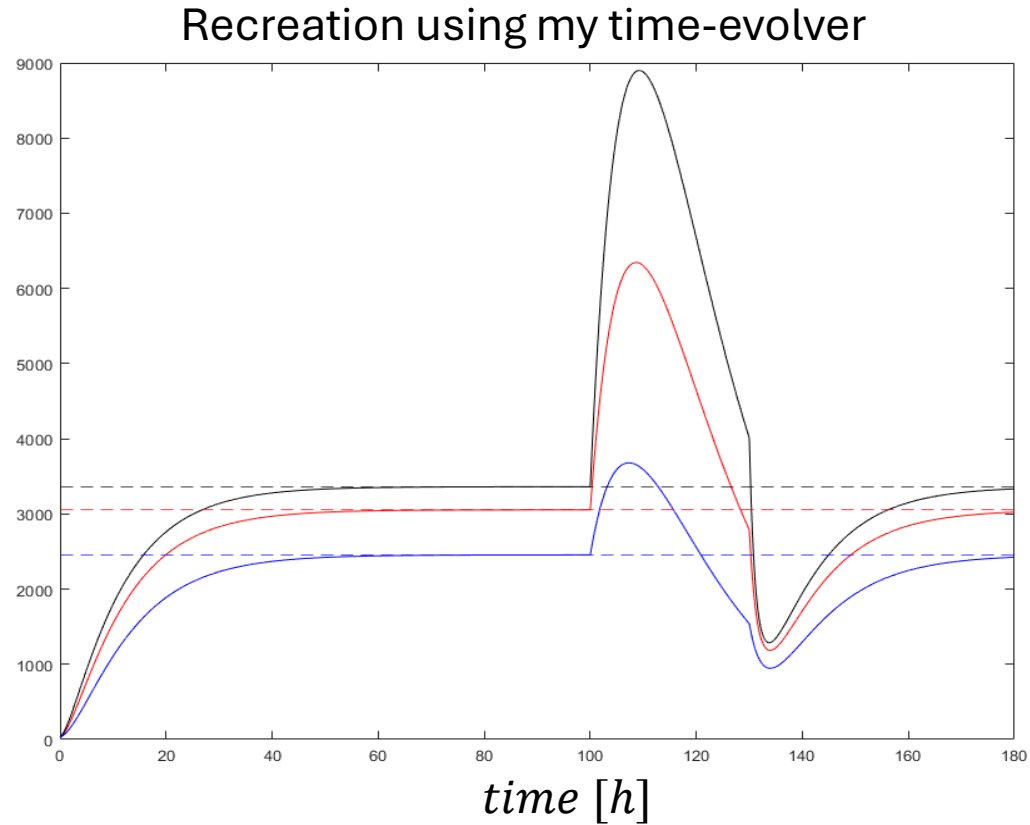


Figure Credit:  
C. Demaziere, "Physics of Nuclear Reactors", p. 179

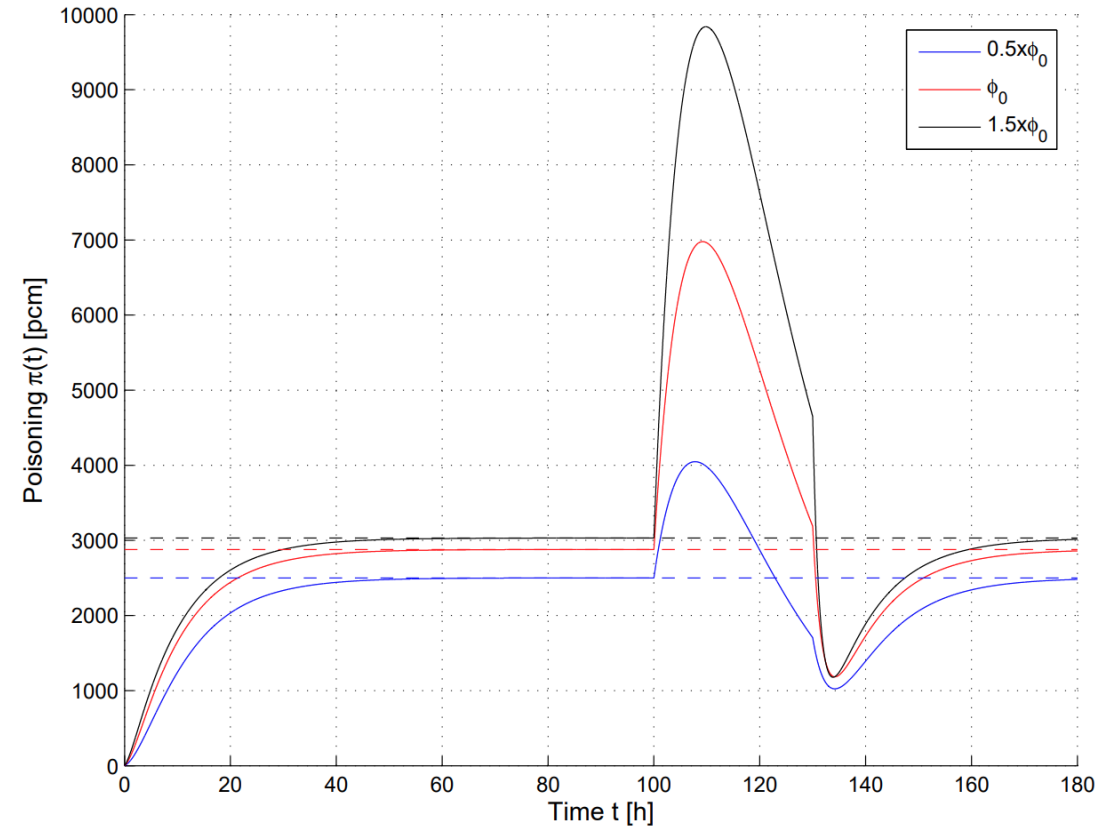
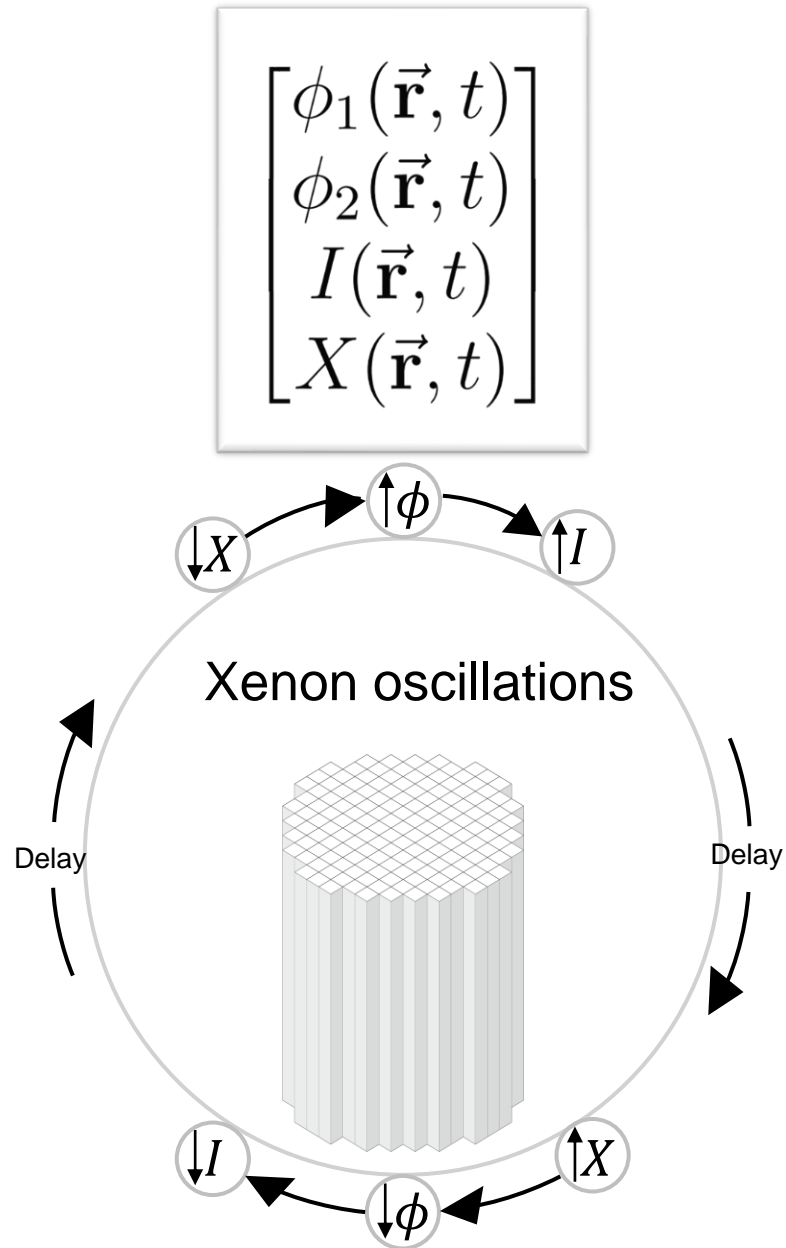
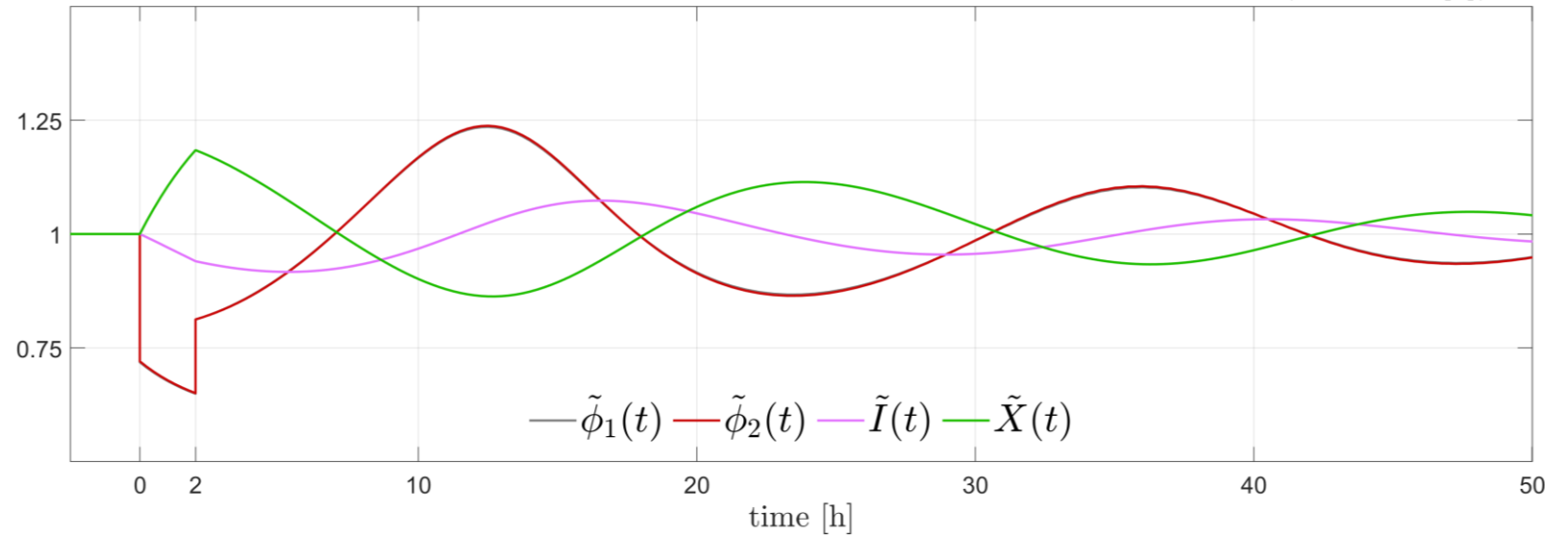


Fig. 4.10 Evolution of the poisoning due to  $^{135}\text{Xe}$  after the start of the reactor ( $t=0$ ), after a reactor scram ( $t=100$  h), and after a reactor restart ( $t=130$  h) (the horizontal dashed lines represent the equilibrium poisonings).

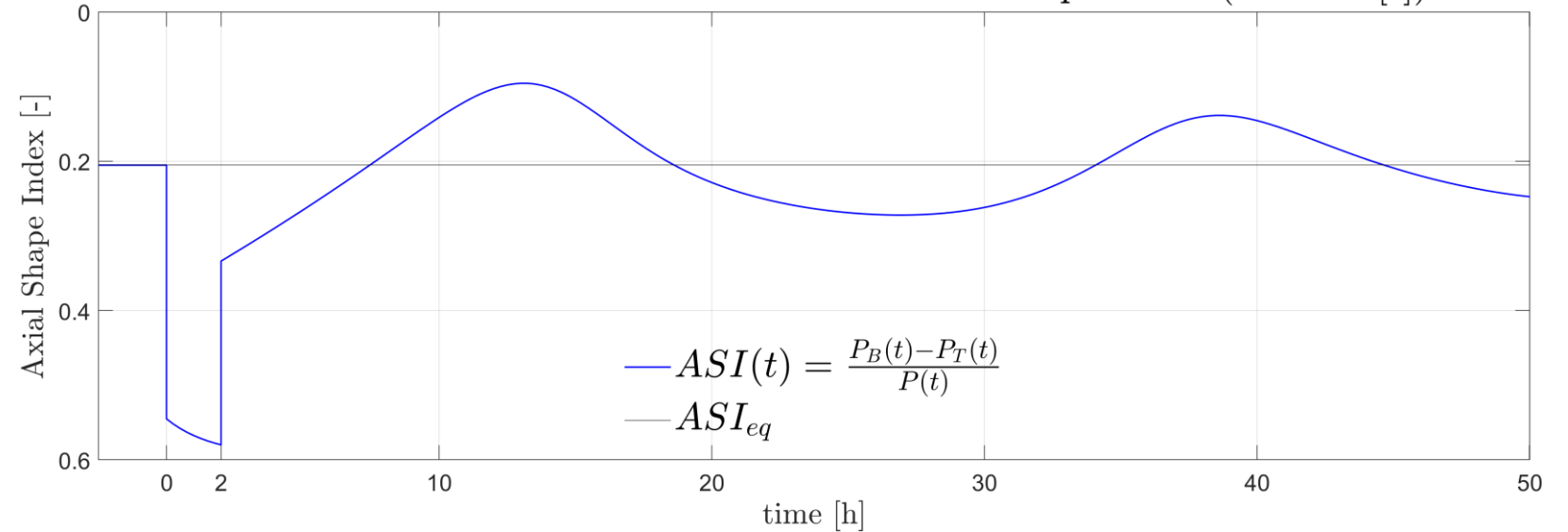
# Xenon oscillations



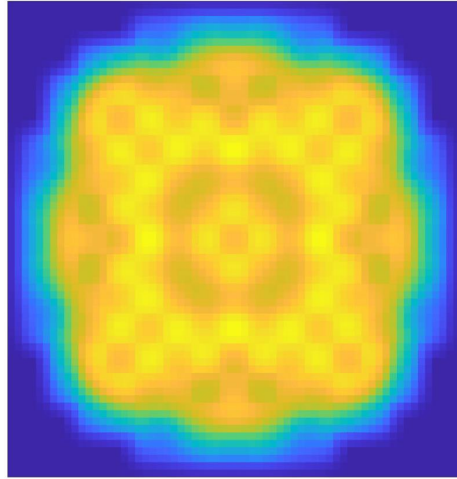
Simulation to induce Xenon oscillations: Core-Averaged Quantities ( $dt = 900[s]$ )



Simulation to induce Xenon oscillations: Axial Shape Index ( $dt = 900[s]$ )







## **Non-linear time-dependent modelling of heterogeneous nuclear reactors**

Applications to Xenon oscillations in pressurized water reactors

Master's thesis in Physics

FREDRIK ÖHRLUND

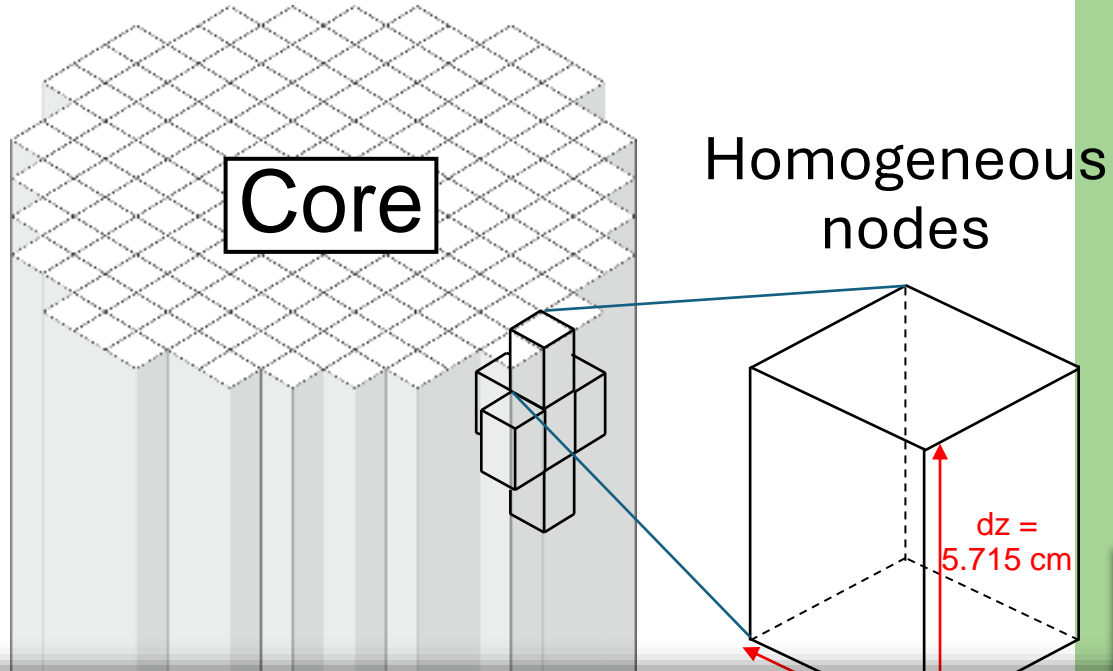
# Master's thesis presentation:

## *Non-linear time-dependent modelling of heterogeneous nuclear reactors*

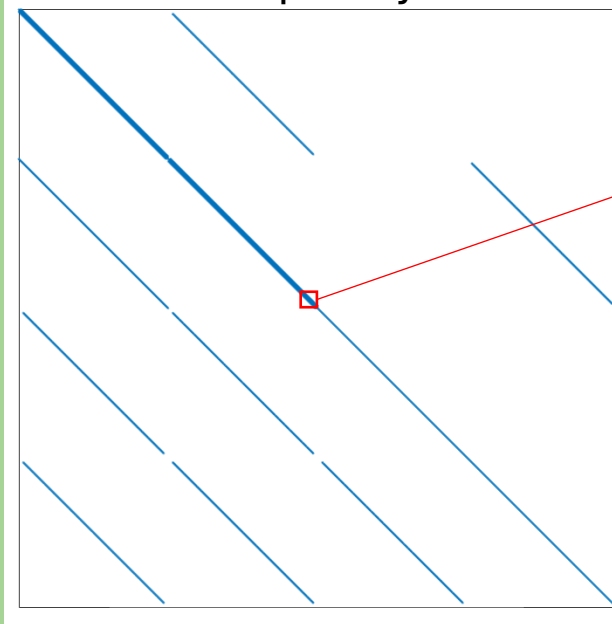
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**Fredrik Öhrlund, MSc**

# Simulating a reactor



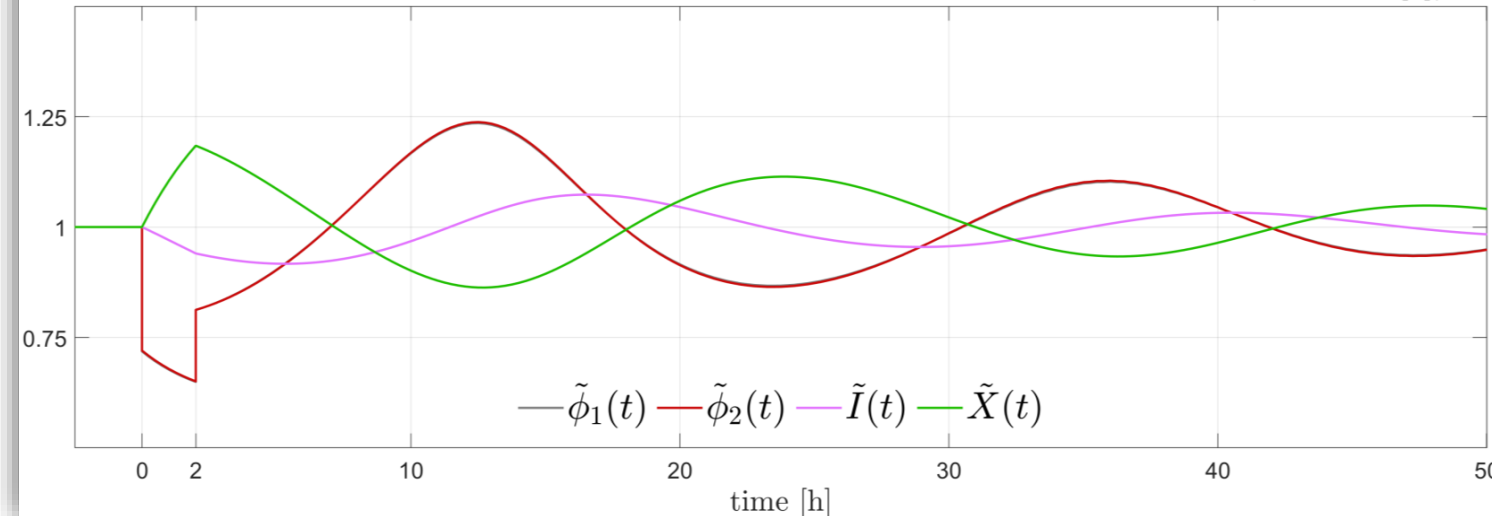
Jacobian Sparsity Pattern



nonzeros = 5,477,373

1. Invert Jacobian 1000-10000 times per simulation

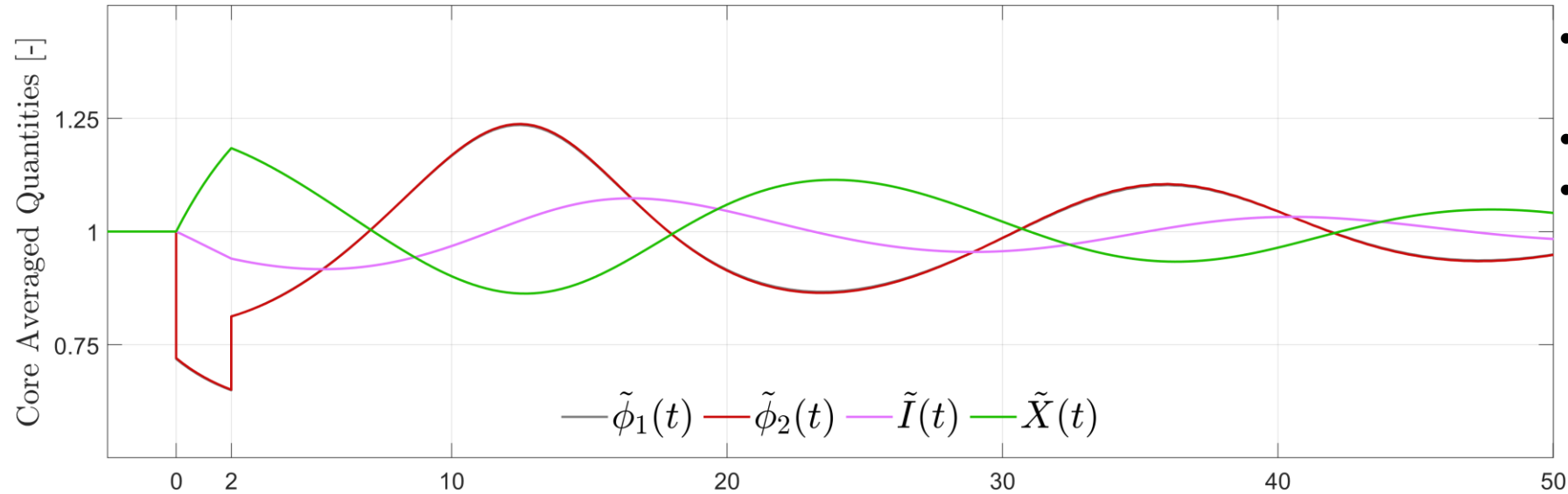
Simulation to induce Xenon oscillations: Core-Averaged Quantities ( $dt = 900[s]$ )



- Real example from my code: Solve  $Ax = b$
- $A \setminus b$  (MatLab): 125s
- $ILU(A) + GMRES(A,b)$  0.11s
- 1136x speedup
- The total run-time of a simulation becomes
- 2 days 6 hours
- 180s

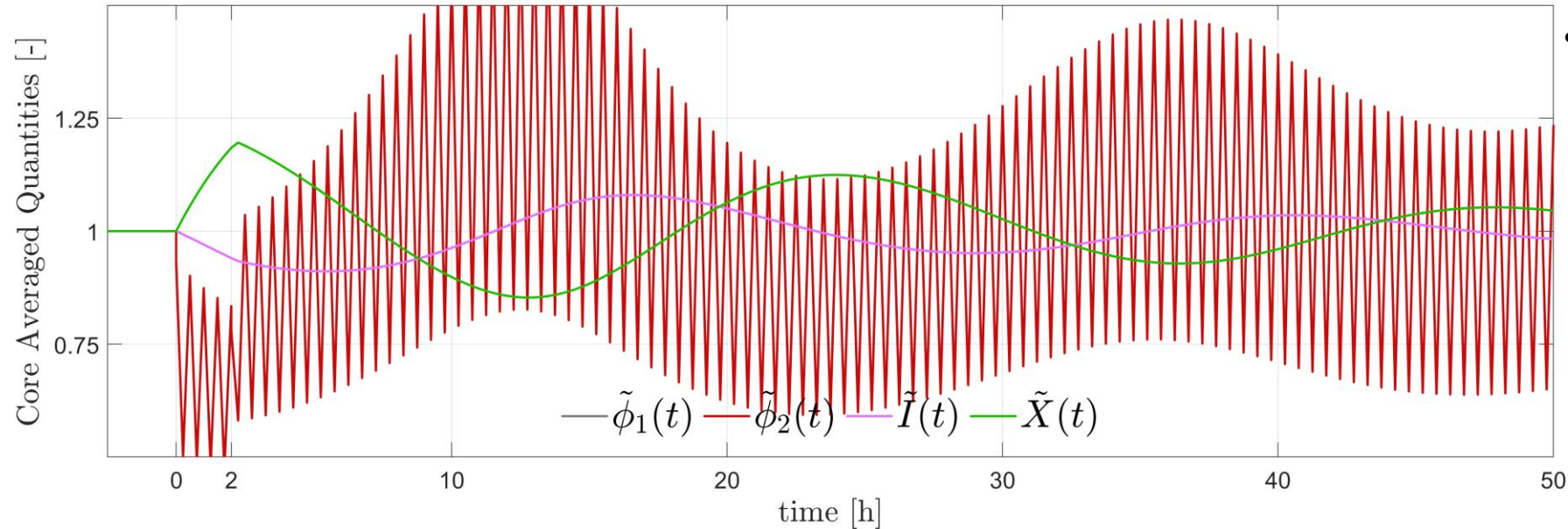
# Highlight from the development process

Simulation to induce Xenon oscillations: Core-Averaged Quantities ( $dt = 900[s]$ )



- Time-evolution is done with the Crank-Nicolson method,
- Asymptotically stable (A-stable)
- This means that the method is numerically stable for arbitrarily large time-steps...

Simulation to induce even worse Numerical oscillations ( $dt = 900[s]$ )



- From a certain perspective, this is not an error/mistake, but is in fact the correct solution according to Crank-Nicolson...

- When I handed in my thesis for grading and I had officially finished my work on the project, I still wasn't done with the problem.
  1. Numerical oscillations fascinated me, wanted to find general solution.
  2. Arbitrary XS-perturbation
  3. Adaptive time-stepping
- So after I finished my thesis, I completely rewrote my entire code from scratch, and fixed/implemented points 1-3.
- It turned out that this required roughly as much time and effort as the entire original master's thesis project.
- Lines of code: 4485
- I would happily tell you everything about this!