Neutronic-Thermohydraulic-Thermomechanic Coupling for the Modeling of Accidents in Nuclear Systems

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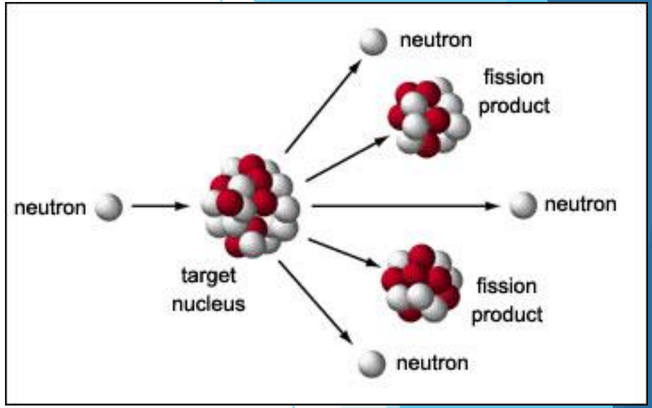
Outline

1. Criticality and Basics of Nuclear Physics
2. Thesis Subject
3. Multi-Physics Coupling
4. Results
5. Conclusions

1. Criticality Accidents

A criticality accident is an involuntary and uncontrolled fission chain reaction



The "Tickling the Tail of the Dragon" accident (Los Alamos, 1945) – Source Atomic Heritage Foundation

It can occur in nuclear systems involving very different

- **Geometric configurations**
- **Phases**
- **Phenomena**

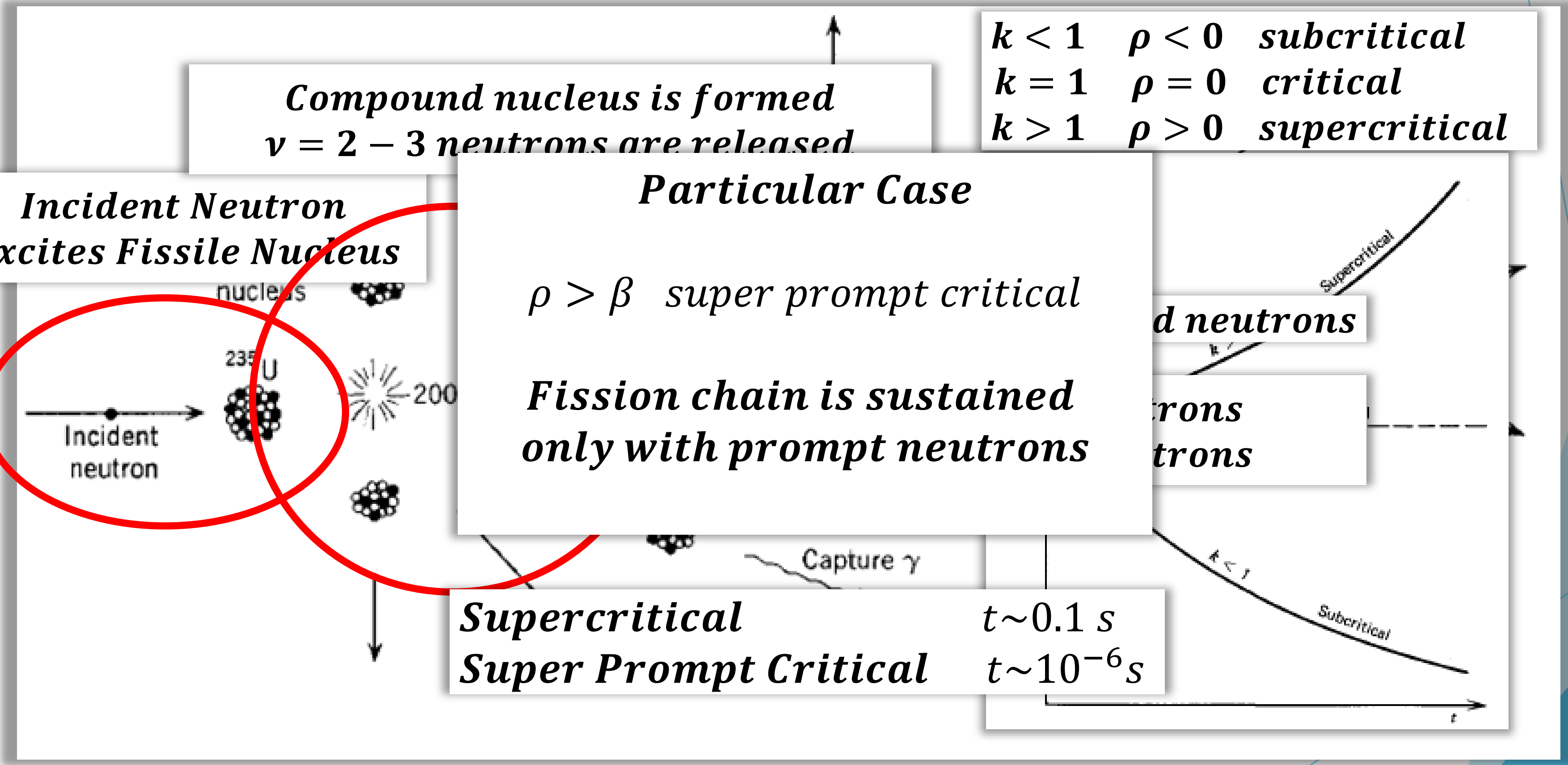
Recent accidents: Tokaï-Mura (Japan 1999, 3 deads), etc.

1. Nuclear Physics: Basic concepts

$$k_p \equiv \textbf{Prompt}\ Multiplication\ Factor \equiv \frac{Number\ of\ \textbf{prompt}\ neutrons\ in\ one\ generation}{Number\ of\ neutrons\ in\ preceding\ generation}$$

$$k \equiv Multiplication\ Factor \equiv \frac{Number\ of\ neutrons\ in\ one\ generation}{Number\ of\ neutrons\ in\ preceding\ generation}$$

$$\rho \equiv Reactivity \equiv \frac{k-1}{k}$$



Compound nucleus is formed
$\boldsymbol{\nu = 2 - 3}$ ***neutrons are released***

Incident Neutron excites Fissile Nucleus

$k < 1$	$\rho < 0$	***subcritical***
$k = 1$	$\rho = 0$	***critical***
$k > 1$	$\rho > 0$	***supercritical***

Particular Case

$\rho > \beta$ *super prompt critical*

Fission chain is sustained only with prompt neutrons

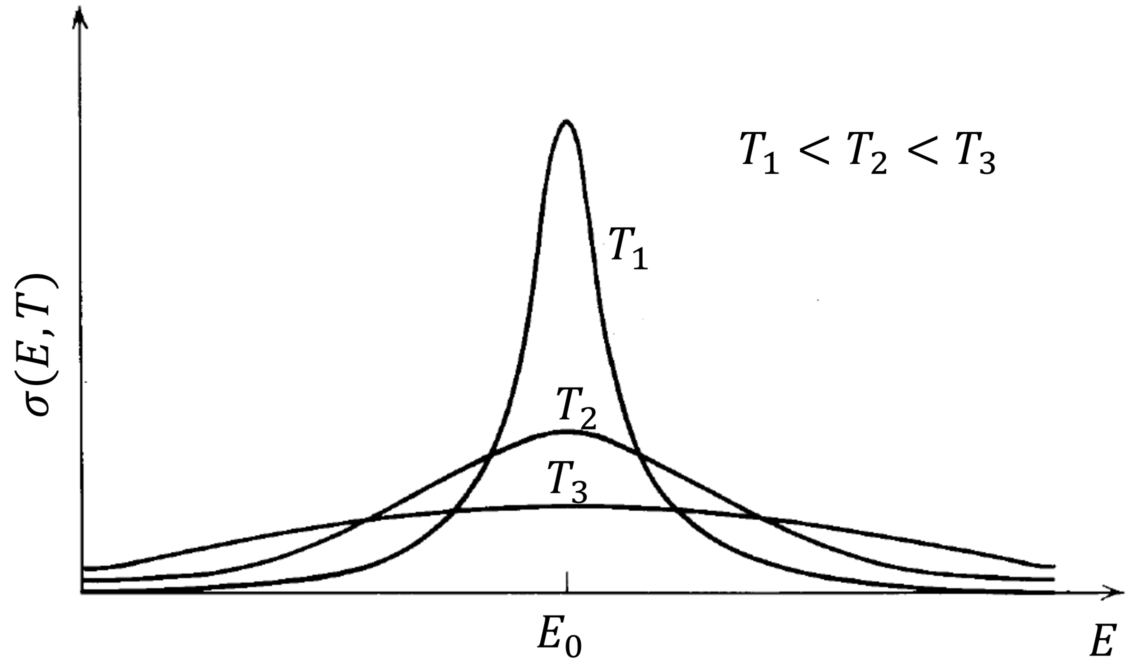
d neutrons

rons
trons

Supercritical $t{\sim}0.1\ s$
Super Prompt Critical $t{\sim}10^{-6}s$

Fission Chain Reaction

1. Nuclear Physics: Basic concepts



Doppler Broadening

- Dependence of neutron cross sections on the relative velocity between **neutron** and **nucleus**
- Target nuclei are in **continual motion** due to their **thermal energy**
- With increasing temperature the nuclei vibrate more rapidly within their lattice structures
- **Broadening** of the energy range of neutrons that may be resonantly absorbed in the fissile

Other Feedbacks exists like density change and geometry expansion (Leakage)

1. Criticality Accidents and Experiments

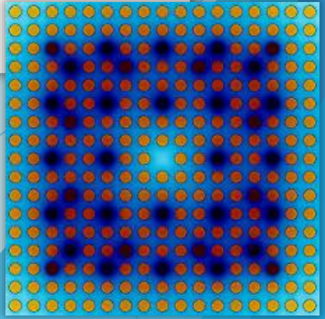
- Variety of accidents and experiments were **reviewed**
- Goal: select cases to cover a wide range of phenomena

Available Data

Solid Media:
- **GODIVA** I, II, III, IV
- Flattop

Liquid Media:
- **SILENE**
- CRAC (diphasic)
- Passed accidents (Tokai-mura…)

Heterogeneous Media (Solid-Liquid)
- **Spent Fuels Pools**
- CABRI



2.Thesis Subject

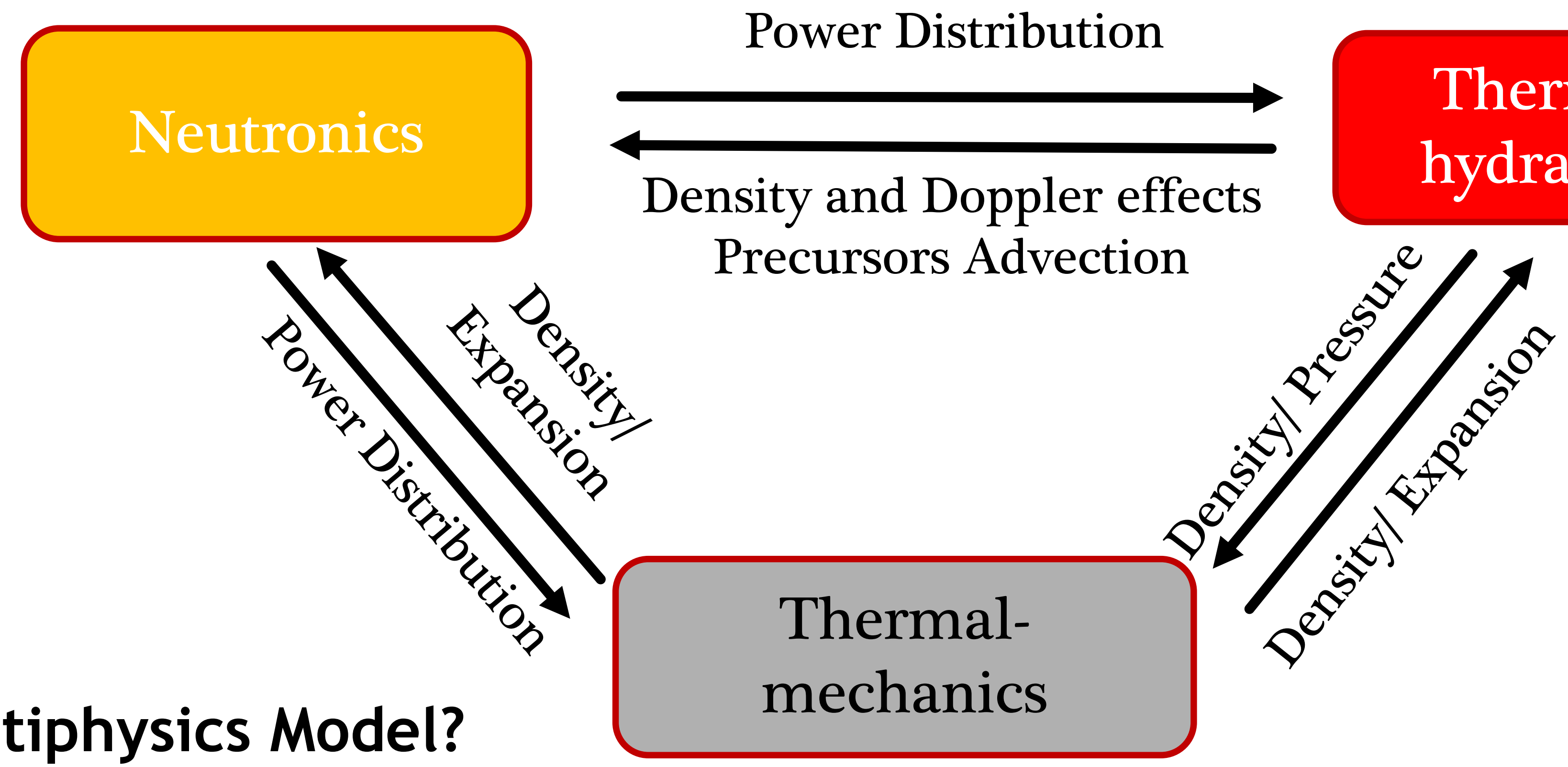
2.1 State of Art

- **Current numerical models used by the safety authority limited for criticality accidents in:**
  - Geometry modelling
  - Transient simulated time

2.2 Objective

- **Develop a more general transient multi-physics multiscale tool with:**
  - Detailed phenomena modelling
  - Higher space/time scale flexibility
  - Best-estimate (Not conservative)

3. Transient Multi-physics Multiscale Tool



Why Multiphysics Model?

- Mechanistic model
- Account for all relevant phenomena
- High time/space scale flexibility

3. Multi-physics Tool: the Bricks/Codes

CFD C++ Library

Open∇FOAM

- **OpenFOAM** is an open source software based in C++ for numerical resolution of the continuum mechanics including CFD

Monte Carlo Code (Serpent)

- **Serpent 2** is a 3D continue in energy Monte Carlo code for reactor physics and irradiation calculus (burnup)

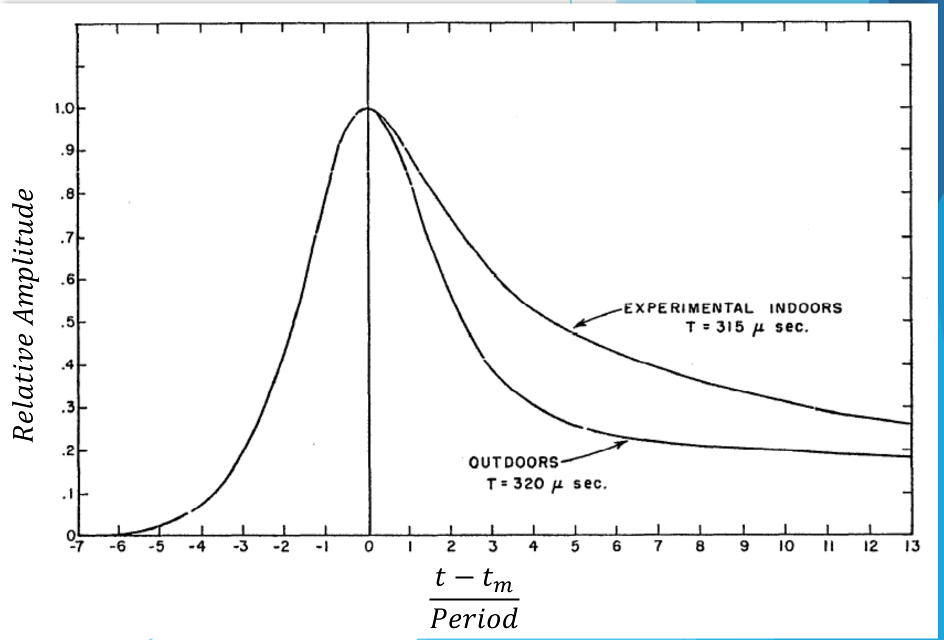
Multi-physics Coupling

- Godiva Experiment
- Neutronics
- Thermomechanics

3. Multi-physics Coupling

Godiva Experiment

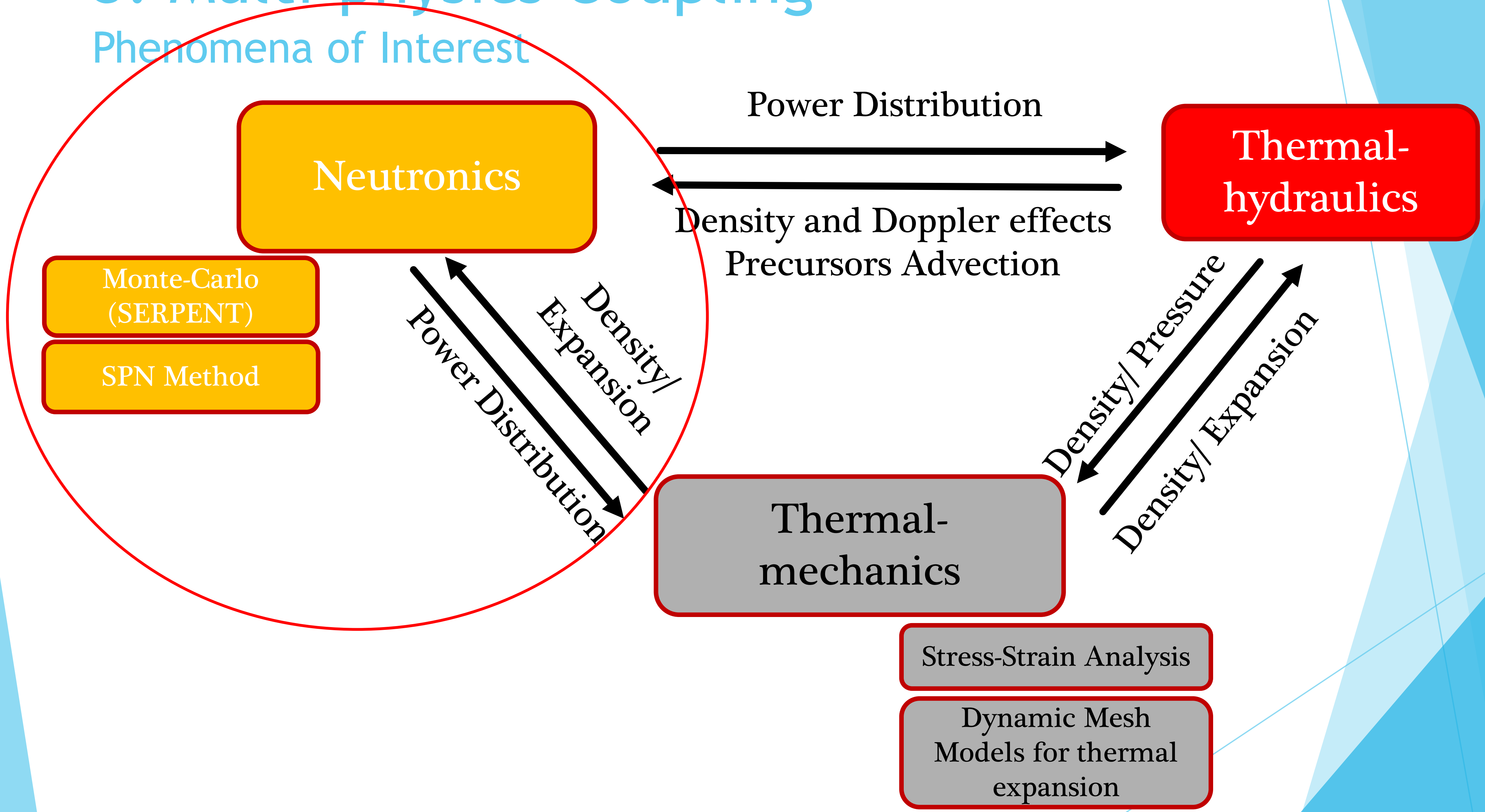
- Experiment description:
  - **Geometry:** sphere
  - **Size:** ~ 8.85 cm radius
  - **Fuel:** enriched Uranium (95%)
  - **Mass:** $\sim 54\ kg$
  - **Reactivity control mechanisms:** none
    - $\Longrightarrow$ only neutronics feedback effects
- Key phenomena to be modeled:
  - Super prompt critical transient (ρ>β)
  - Thermal expansion (density and leakage feedback)
  - Doppler effect (temperature feedback)



$$\frac{t - t_m}{Period}$$

3. Multi-physics Coupling

Phenomena of Interest



Neutronics

Monte-Carlo (SERPENT)

SPN Method

Thermal-hydraulics

Thermal-mechanics

Stress-Strain Analysis

Dynamic Mesh Models for thermal expansion

Power Distribution

Density and Doppler effects
Precursors Advection

Density/ Expansion

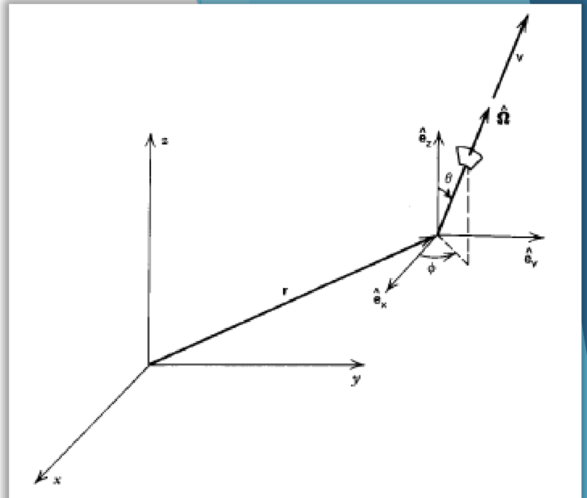
Power Distribution

Density/ Pressure

Density/ Expansion

3. Multi-physics Coupling

Neutronics



The position and direction variables characterizing a neutron.

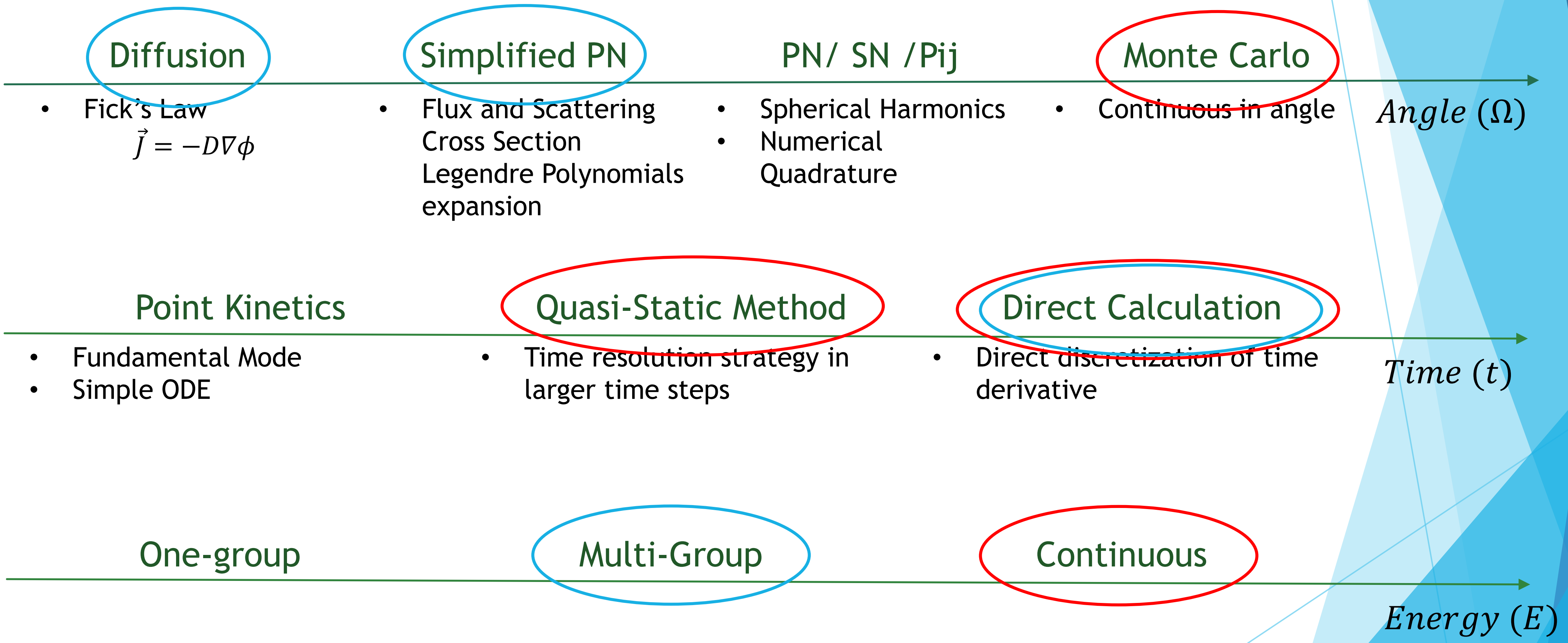
- Neutron population described by Boltzmann equation and a balance of precursors with an advection term is used (in case of liquid fuels)

$$\left\{\begin{aligned}
&\underbrace{\frac{1}{v(E)}\frac{\partial\psi}{\partial t}(\vec{r},\vec{\Omega},E,t)}_{\text{Rate of change}} = \underbrace{\left[-\mathcal{L}-\mathcal{T}+\mathcal{S}+\frac{\chi_p(E)}{4\pi}(1-\beta)F\right]\psi(\vec{r},\vec{\Omega},E,t)}_{\text{Streaming + Disappearance + Scattering + Fissions}} + \underbrace{\sum_{d=1}^{G_d}\frac{\chi_d(E)}{4\pi}\lambda_d C_d(\vec{r},t)}_{\text{Delayed Neutrons source}}\\
&\underbrace{\frac{\partial C_d}{\partial t}(\vec{r},t)}_{\text{Local rate of change}} = \underbrace{\beta_d F\psi(\vec{r},\vec{\Omega},E,t)}_{\text{Production}} - \underbrace{\lambda_d C_d(\vec{r},t)}_{\text{Destruction}} - \underbrace{\underbrace{\vec{u}\cdot\nabla C_d(\vec{r},t)}_{\text{Convection}} + \underbrace{D_d\nabla^2 C_d(\vec{r},t)}_{\text{Diffusion}}}_{\text{Liquid Media}} \qquad \text{for } d = 1\ to\ G_d
\end{aligned}\right.$$

Neutronics

3. Multi-physics Coupling

Neutronics methods and strategy



Diffusion

- Fick's Law

$\vec{J} = -D\nabla\phi$

Simplified PN

- Flux and Scattering Cross Section Legendre Polynomials expansion

PN/ SN /Pij

- Spherical Harmonics
- Numerical Quadrature

Monte Carlo

- Continuous in angle

$Angle\ (\Omega)$

Point Kinetics

- Fundamental Mode
- Simple ODE

Quasi-Static Method

- Time resolution strategy in larger time steps

Direct Calculation

- Direct discretization of time derivative

$Time\ (t)$

One-group

Multi-Group

Continuous

$Energy\ (E)$

Neutronics

3. Multi-physics Coupling

Neutronics: A) the Simplified PN

- The **transient multigroup SP3** equations consist in a set of two coupled PDEs
- The **order 0** is identical to diffusion approximation equation
- The **order 2** takes into account anisotropies in the scattering cross section with a **Legendre Polynomial Expansion**

$$\begin{cases} \frac{1}{V}\frac{\partial \hat{\phi}_0}{\partial t} = \nabla \frac{1}{3}\Sigma_1^{-1}\nabla \hat{\phi}_0 - \Sigma_0 \hat{\phi}_0 + \frac{F}{k}\left(\hat{\phi}_0 - 2\phi_2\right) + 2\Sigma_0\phi_2 + \frac{2}{V}\frac{\partial \phi_2}{\partial t} + S_d & \text{order 0} \\ \frac{3}{V}\frac{\partial \phi_2}{\partial t} = \nabla \frac{3}{7}\Sigma_3^{-1}\nabla \phi_2 - \left(\frac{5}{3}\Sigma_2 + \frac{4}{3}\Sigma_0\right)\phi_2 - \frac{2}{3}\frac{F}{k}\left(\hat{\phi}_0 - 2\phi_2\right) + \frac{2}{3}\Sigma_0\hat{\phi}_0 + \frac{2}{3V}\frac{\partial \hat{\phi}_0}{\partial t} - \frac{2}{3}S_d & \text{order 2} \end{cases}$$

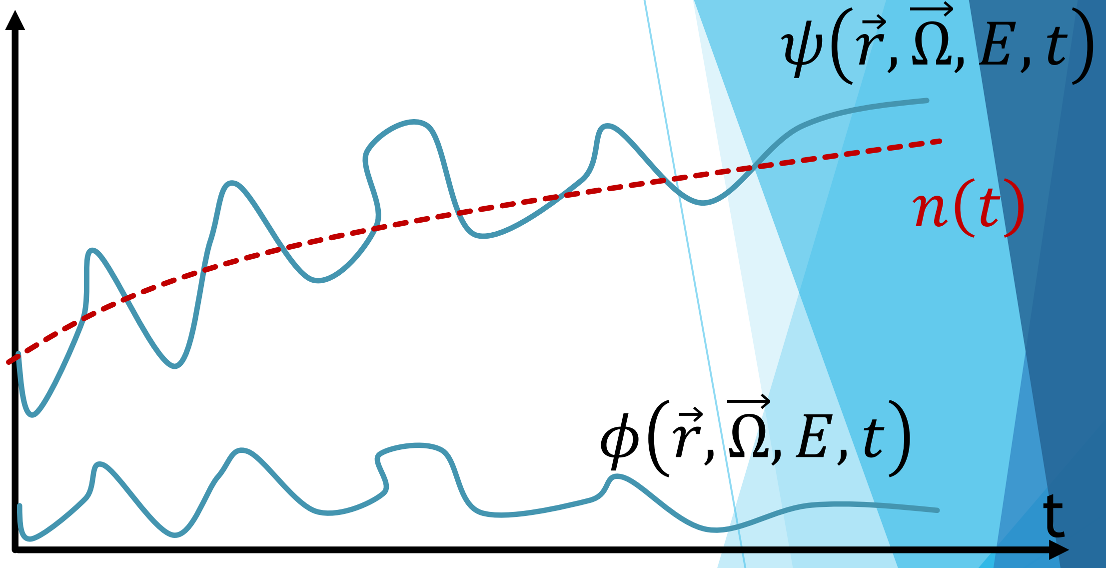
Neutronics

3. Multi-physics Coupling

Neutronics: B) the Quasi-Static Method

Key hypothesis:

$$\begin{cases} \psi(\vec{r},\vec{\Omega},E,t) = n(t)\phi(\vec{r},\vec{\Omega},E,t) \\ \left\langle \frac{1}{V(E)}\phi(\vec{r},\vec{\Omega},E,t) \middle| W_0(\vec{r},\vec{\Omega},E) \right\rangle = constant \end{cases}$$



- **First hypothesis**: separation of the neutron angular flux into an amplitude function $n(t)$ and a shape function $\phi(\vec{r},\vec{\Omega},E,t)$
- **Second hypothesis**: makes the two separated functions unique

Neutronics

3. Multi-physics Coupling

Neutronics: the Quasi-Static Method

Transport Equations

$$\frac{1}{v}\frac{\partial\psi}{\partial t} = \mathcal{L}\psi + \sum_{d=1}^{G_d}\frac{\chi_d}{4\pi}\lambda_d C_d$$

$$\frac{\partial C_d}{\partial t} = \beta_d \mathrm{F}\psi - \lambda_d C_d$$

The QS method allows splitting the neutron transport equation in two sets of equations:

- ➢ Neutron flux **shape (PDE)** and
- ➢ Neutron flux **amplitude (ODE)**

Neu x quat

$$\frac{\partial\phi}{\partial t} = 0$$

$$\frac{dn}{dt} = 0$$

$$\mathit{Improved\ Quasi\ Static}$$

$$\cancel{\frac{1}{v}\frac{\partial\phi}{\partial t}} = \left[\mathcal{L} - \frac{1}{v}\frac{\cancel{dn(t)/dt}}{n(t)}\right]\phi + \frac{1}{n(t)}\sum_{d=1}^{G_d}\frac{\chi_d}{4\pi}\lambda_d C_d$$

$$\frac{\partial C_d}{\partial t} = \beta_d F\phi\, n(t) - \lambda_d C_d$$

Neutron flux Amplitude Equations

$$\frac{\mathrm{dn}(t)}{\mathrm{dt}} = \left[\frac{\rho - \beta_d^{eff}}{\Lambda}\right]n(t) + \sum_{d=1}^{G_d}\lambda_d\bar{c}_d\,(t)$$

$$\frac{d\bar{c}_d(t)}{dt} = \frac{\beta_d^{eff}}{\Lambda}n(t) - \lambda_d\bar{c}_d(t)$$

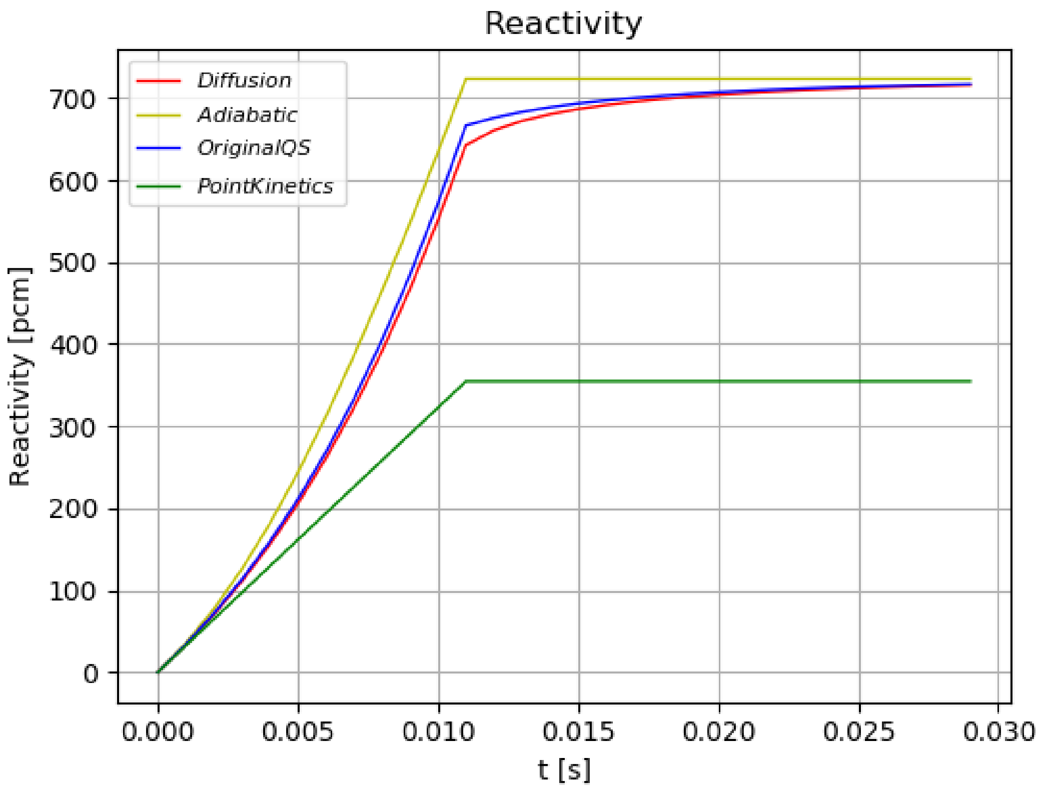
Neutronics

3. Multi-physics Coupling

Neutronics: the Quasi-Static Method variants

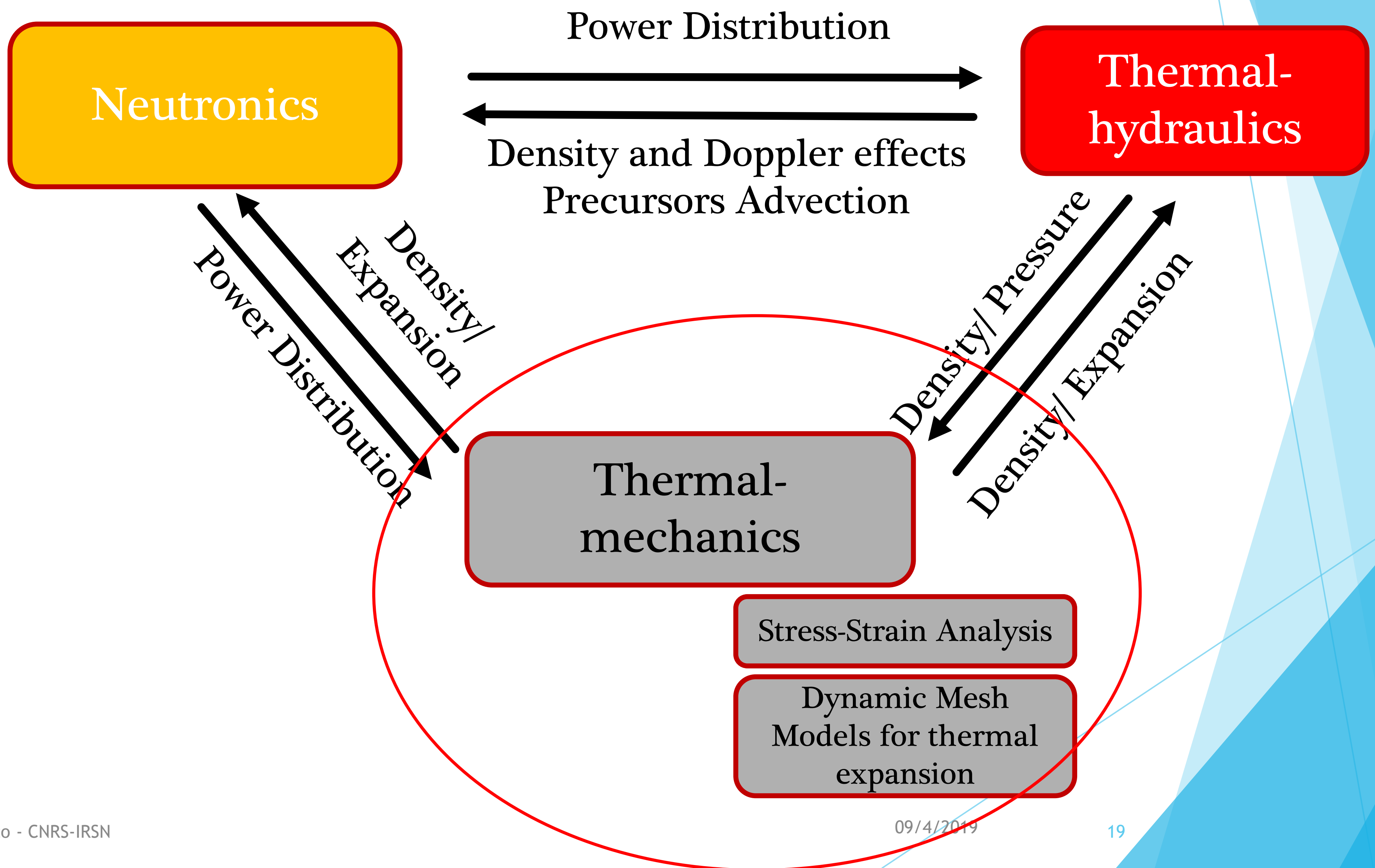
$$\begin{cases} \dfrac{\partial\phi}{\partial t} \neq 0 \quad \dfrac{dn(t)}{dt} \neq 0 \quad \textit{Improved Quasi Static} \\ \dfrac{\partial\phi}{\partial t} = 0 \quad \dfrac{dn(t)}{dt} \neq 0 \quad \textit{Original Quasi Static} \\ \dfrac{\partial\phi}{\partial t} = 0 \quad \dfrac{dn(t)}{dt} = 0 \quad \textit{Adiabatic Quasi Static} \end{cases}$$

- Sensibility study for 90$/s (ρ/β) reactivity increase was made using diffusion theory
- Adiabatic case (yellow) seems to be the less accurate but it is still better than point kinetics (**green**) alone
- Adiabatic case will be used for Monte Carlo calculations



Neutronics

3. Multi-physics Coupling



Neutronics

Power Distribution

Thermal-hydraulics

Density and Doppler effects
Precursors Advection

Power Distribution

Density/ Expansion

Density/ Pressure

Density/ Expansion

Thermal-mechanics

Stress-Strain Analysis

Dynamic Mesh Models for thermal expansion

3. Multi-physics Coupling

Thermal-Mechanics Model

- A linear elastic solid model with thermal expansion was used to calculate the displacement field D
- The governing equation are obtained from the force balance for the solid body element

$$\frac{\partial^2(\rho D)}{\partial t^2} = \nabla[\mu\nabla D + \mu(\nabla D)^T + \lambda I tr(\nabla D)] + \nabla\left(\frac{E}{1-2\nu}\alpha T\right)$$

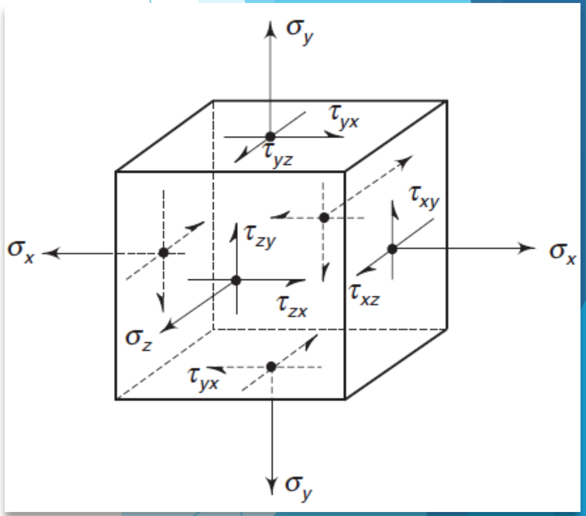
- The temperature field T is calculated via the heat transfer equation

Coupling term

$$\frac{\partial(\rho c T)}{\partial t} = \nabla(k\nabla T) + q'''_{fission}$$

- **Important for thermal expansion and density feedback**

$$\sigma = 2\mu\epsilon + \lambda tr(\epsilon)I$$
$$\epsilon = \frac{1}{2}(\nabla D + \nabla D^T)$$

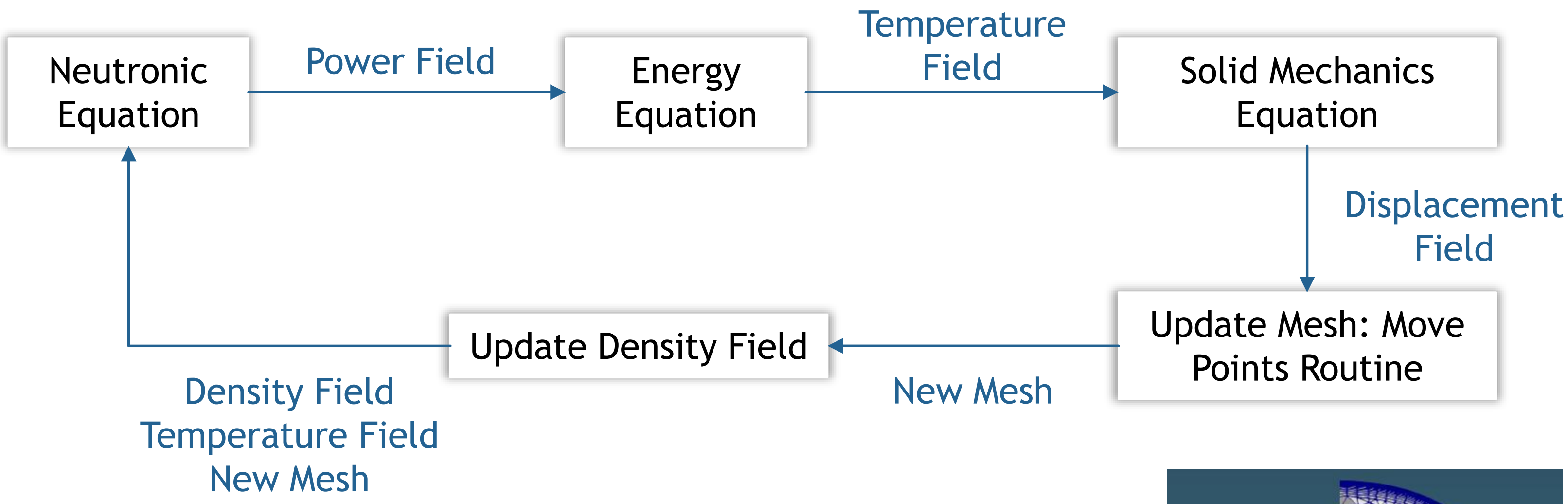


Differential Element Force Balance

Thermal-mechanics

3. Multi-physics Coupling

Implementation of the example for the Godiva Experiment



Neutronic Equation

Power Field

Energy Equation

Temperature Field

Solid Mechanics Equation

Displacement Field

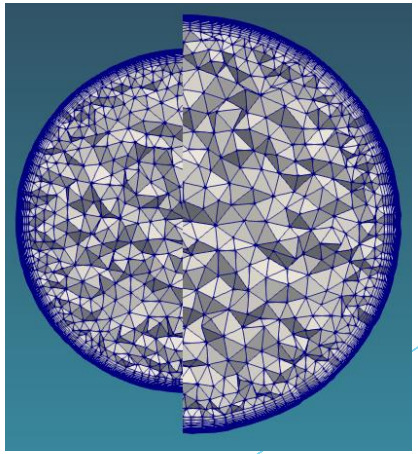
Update Mesh: Move Points Routine

New Mesh

Update Density Field

Density Field
Temperature Field
New Mesh

- Mesh discretization (~100000 cells)
- Adaptive mesh for thermal expansion implemented in OpenFOAM
- Density fields updated for accounting geometry changes



Results

- Monte Carlo Quasi Static
- SPN

4. Results

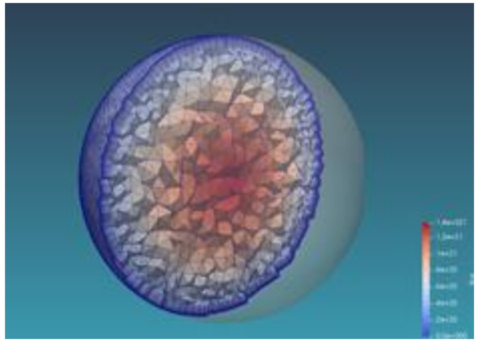
Serpent Quasi-Static Stochastic Approach

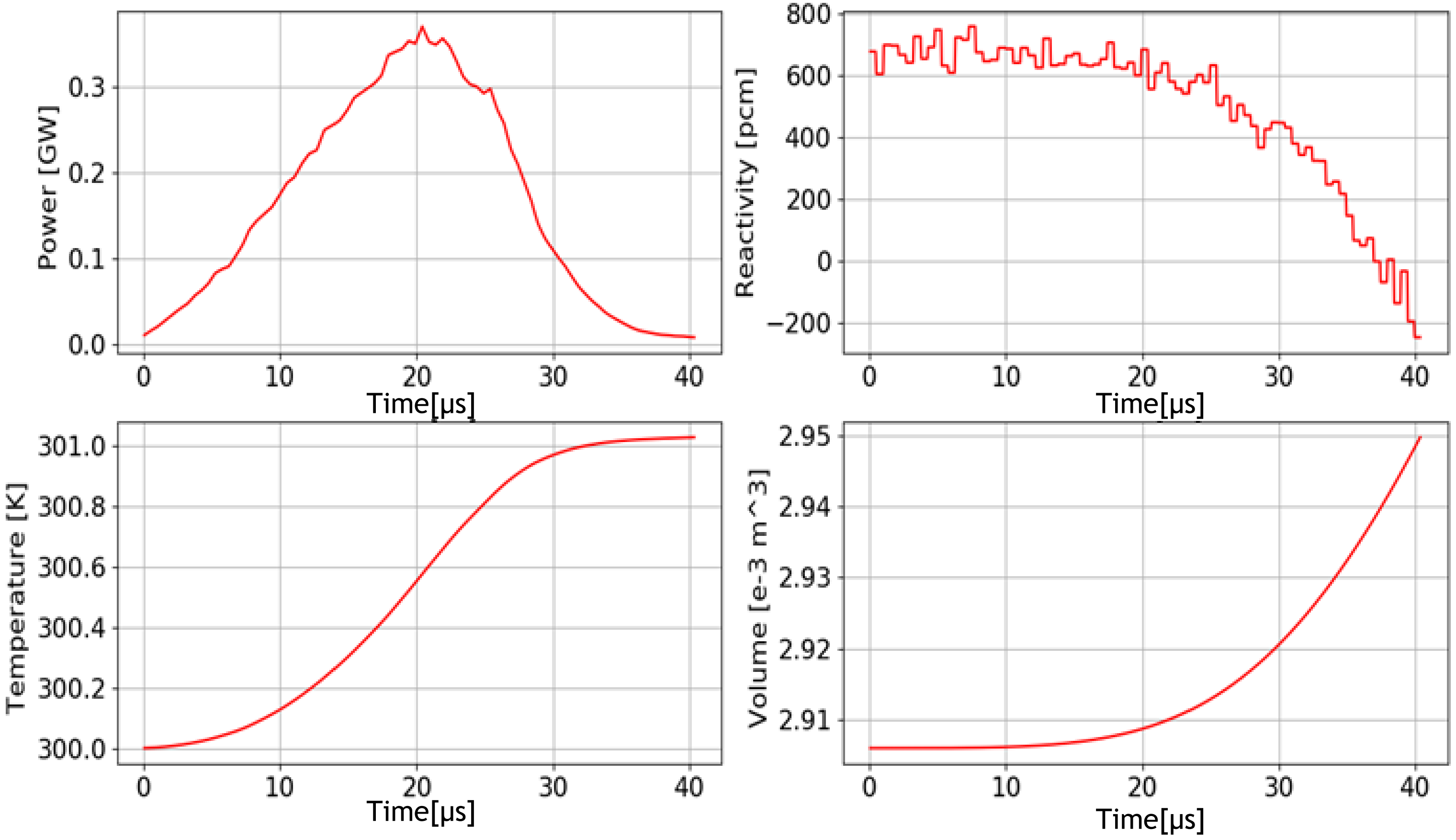
Godiva Experiment

- $\frac{\rho}{\beta} \sim \mathbf{1.06\ \$}$
- $\boldsymbol{r \sim 8.85\ cm}$
- $\boldsymbol{ExecutionTime\ = 4.1h}$
- $\boldsymbol{1\ processor\ 1.7Ghz}$

  $\boldsymbol{(OpenFOAM)}$
- $\boldsymbol{10\ processors\ 1.7Ghz}$ $\boldsymbol{(Serpent)}$

Flux



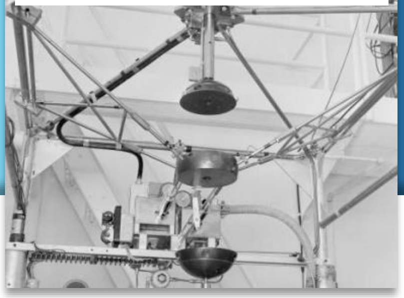


4. Results

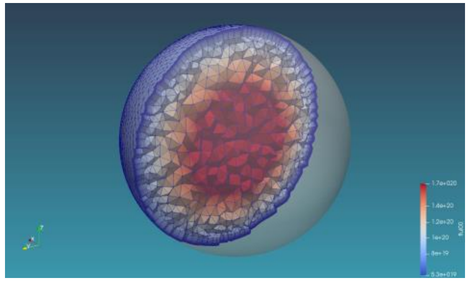
SPN Deterministic Approach

- $\frac{\rho}{\beta} \sim 1.015\ \$$
- $r \sim 8.4\ cm$
- $ExecutionTime\ = 2.1h$
- $1\ processor\ 1.7Ghz$

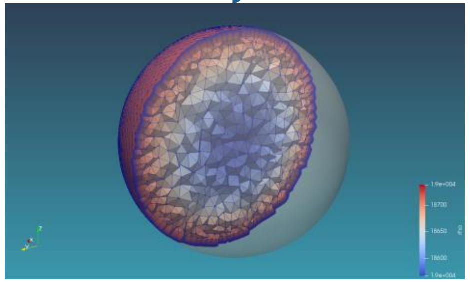
Godiva Experiment

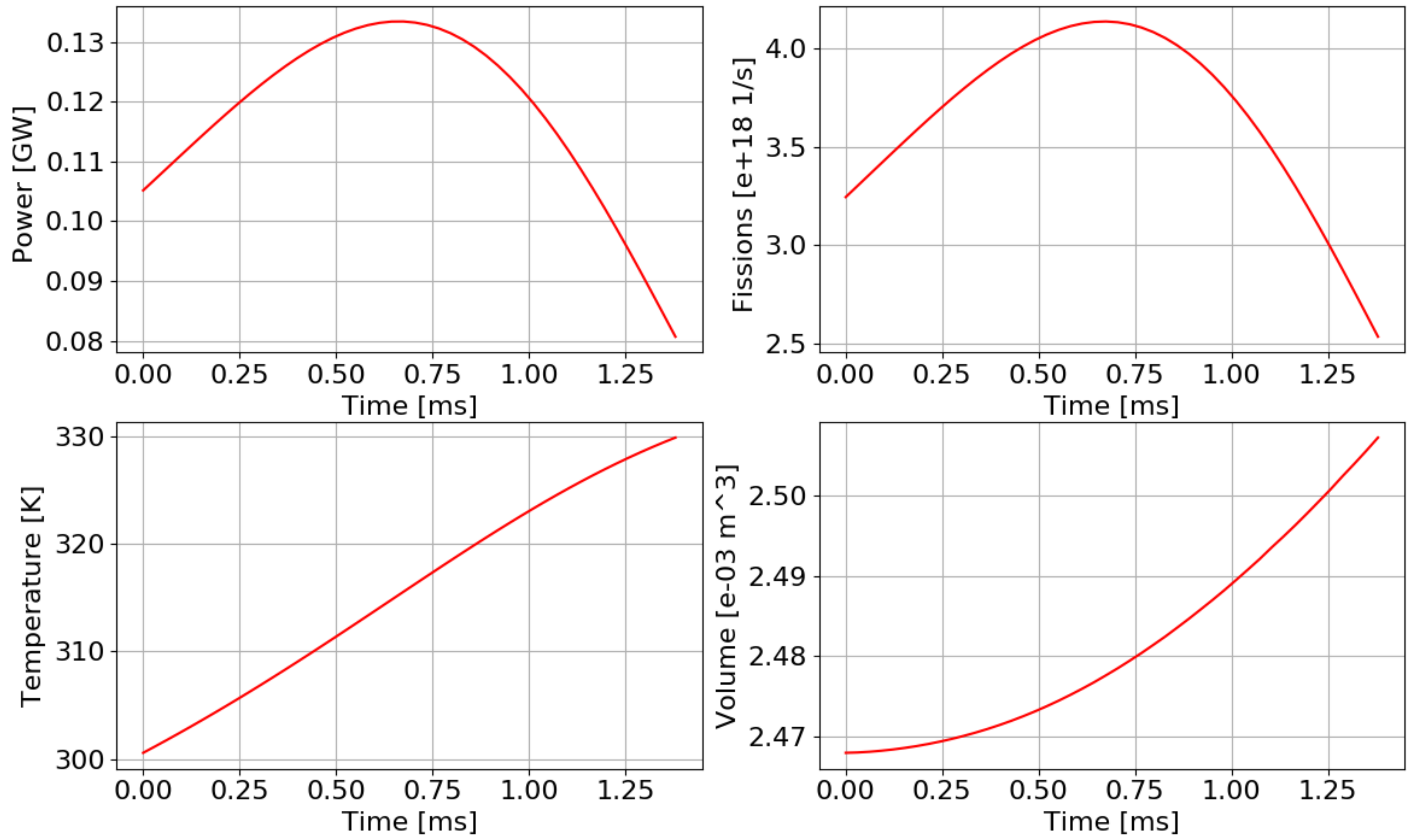


Flux Field Order 0 Energy Group 1/8



Density Field





4. Results

Discussion for the Godiva Experiment

- Both SP3 and Serpent QS provide consistent simulation results to experimental data
  - The initial reactivity (k-eff) obtained by the SP3 and Serpent methods were not the same in these preliminary results due to the approximations made by each method
  - A more precisely evaluation is currently underway to obtain closer initial conditions
- Calculation Time: SP3 is quicker than Quasi-Static serpent but the latter is more precise
- Advantage SP3: useful for quicker testing of other parts of the coupling (TM or TH)
- Cross Section data for SP3: condensed in Serpent taking into account Legendre polynomial expansion. This step is time consuming and has to be added to the total calculation time

Conclusions

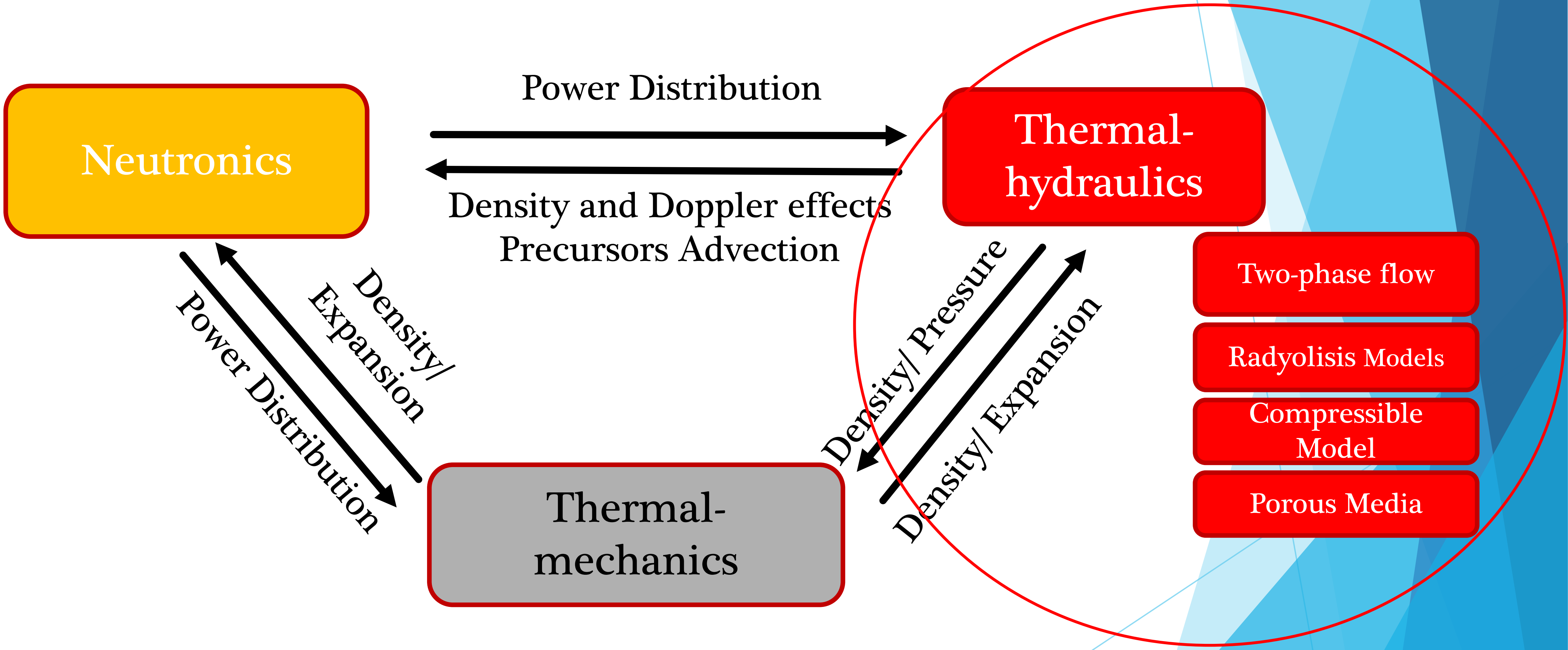
- Godiva
- On-going Work

5. Conclusions

- Good agreement for Godiva transient was obtained
- The adiabatic method is inaccurate for extreme transients (90$/s). Still it is a better estimation than point kinetics alone
- Three neutronics method have been implemented in the multiphysics tool allowing covering:
  - Larger spectrum of sizes, times and energy

5. Conclusions

On-going Work: SILENE


Power Distribution

Neutronics

Density and Doppler effects
Precursors Advection

Thermal-hydraulics

Two-phase flow

Radyolisis Models

Compressible Model

Porous Media

Density/ Expansion

Power Distribution

Density/ Pressure

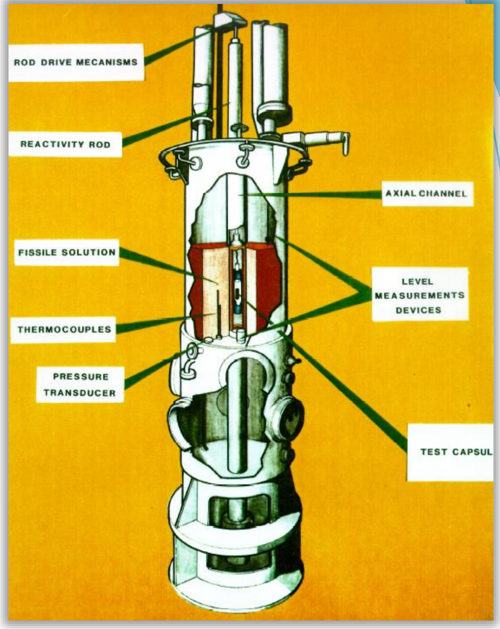
Density/ Expansion

Thermal-mechanics

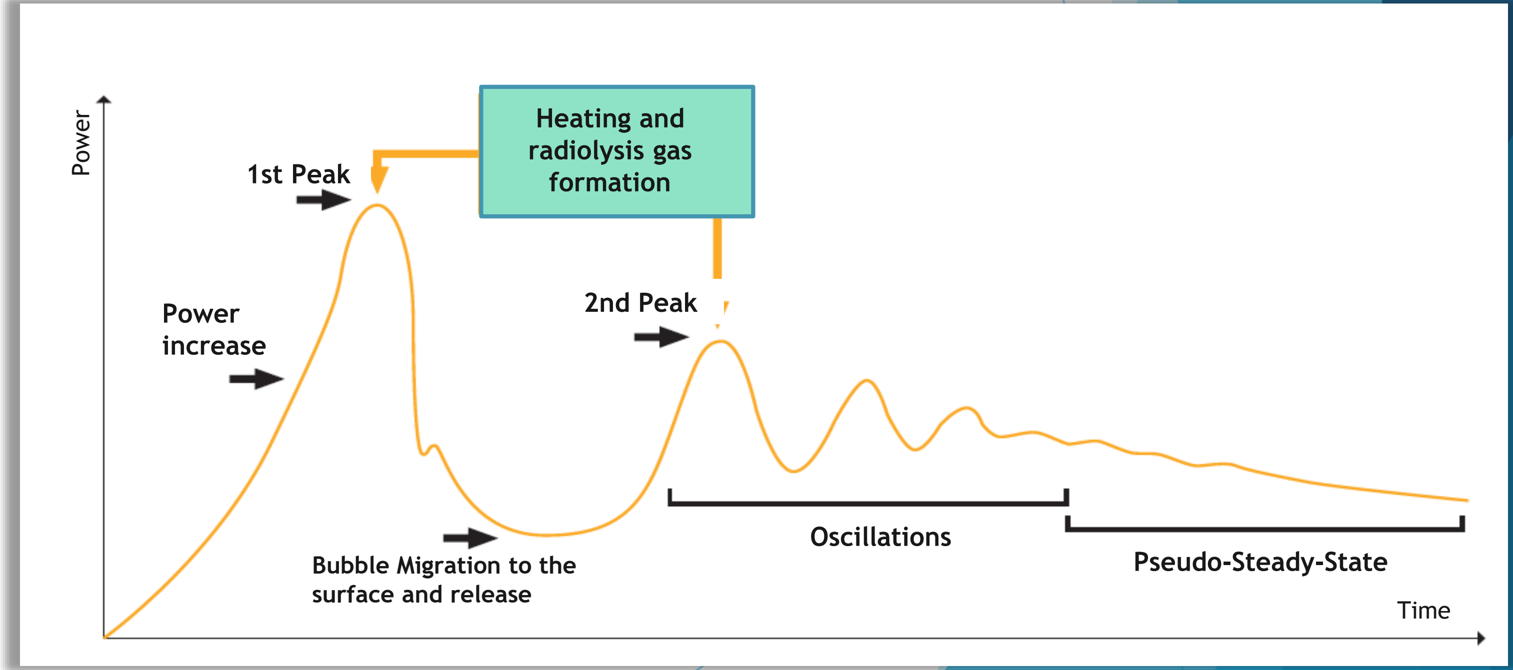
5. Conclusions

On-going Work: Liquid Media -> SILENE

- Experiment description:
  - **Geometry:** Annular cylinder
  - **Size:** 36 cm diameter and ~23 cm height
  - **Fuel:** solution of enriched uranyl nitrate (~93%)
  - **Reactivity control mechanisms:**
    - Control rod
    - Liquid fuel level

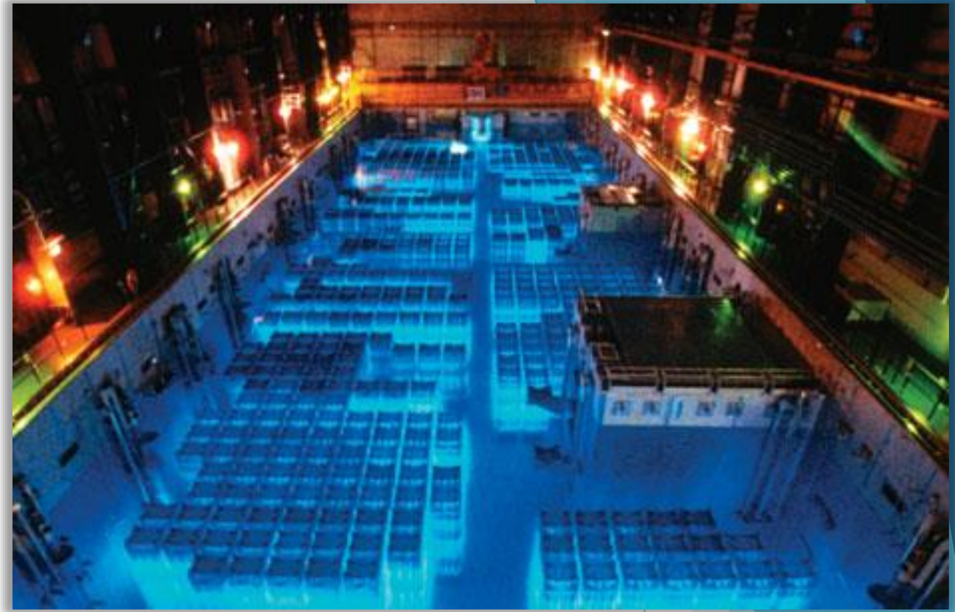


- Principal Phenomena
  - Super prompt critical transient ($\rho > \beta$)
  - Precursors transport
  - Radiolysis: gas phase production
  - Pressure waves
  - Free surface sloshing

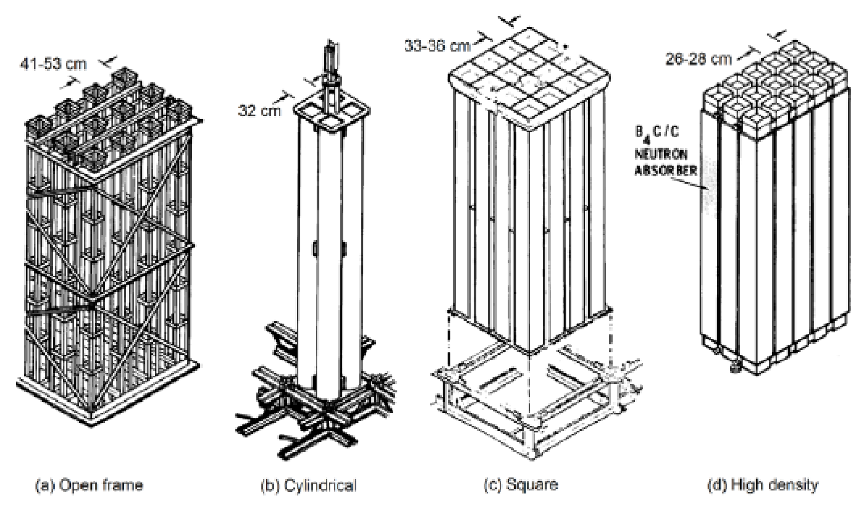


5. Conclusions

On-going Work:
Heterogeneous Media -> Spent Fuel Pools

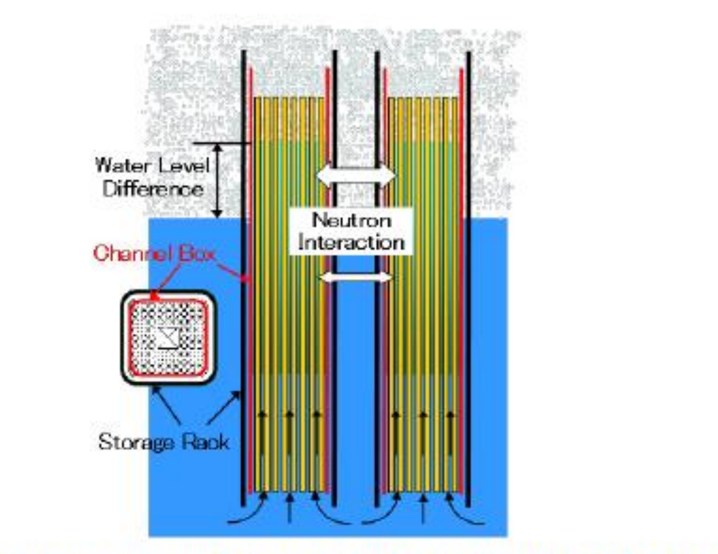


- Experiment description:
  - **Geometry:** Assemblies grouped in racks
  - **Fuel:** PWR/BWR Assemblies
  - **Reactivity control mechanisms:**
    - Neutron Poisons
- Principal Phenomena
  - Biphasic Porous Media
  - Criticality Margins



(a) Open frame (b) Cylindrical (c) Square (d) High density

Spent fuel storage racks used in PWRs



Fuel uncovering and onset of water level difference for BWR fuel.

Thank you