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

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9th April 2019
Grenoble, France
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.

It can occur in nuclear systems involving very different:

- Geometric configurations
- Phases
- Phenomena

Recent accidents: Tokai-Mura (Japan 1999, 3 deads), etc.
1. Nuclear Physics: Basic concepts

\[ k \equiv \text{Prompt Multiplication Factor} \equiv \frac{\text{Number of } \text{prompt} \text{ neutrons in one generation}}{\text{Number of neutrons in preceding generation}} \]

\[ \rho \equiv \text{Reactivity} \equiv \frac{k - 1}{k} \]

- \( k < 1 \)  \( \rho < 0 \) subcritical
- \( k = 1 \)  \( \rho = 0 \) critical
- \( k > 1 \)  \( \rho > 0 \) supercritical

Compound nucleus is formed
\( \nu = 2 - 3 \) neutrons are released

Incident Neutron excites Fissile Nucleus

\[ v > 2 \quad \text{super prompt critical} \]

Fission chain is sustained only with prompt neutrons

Supercritical Super Prompt Critical
\[ t \sim 0.1 \text{ s} \quad t \sim 10^{-6} \text{ s} \]
1. Nuclear Physics: Basic concepts

- 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

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

- **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
Experiment description:
- **Geometry:** sphere
- **Size:** ~8.85 cm radius
- **Fuel:** enriched Uranium (95%)
- **Mass:** ~54 kg
- **Reactivity control mechanisms:** none
  ⇒ only neutronics feedback effects

Key phenomena to be modeled:
- Super prompt critical transient ($\rho > \beta$)
- Thermal expansion (density and leakage feedback)
- Doppler effect (temperature feedback)
3. Multi-physics Coupling

Phenomena of Interest

Neutronics

- Monte-Carlo (SERPENT)
- SPN Method

Power Distribution

Density and Doppler effects
Precursors Advection

Thermal-hydraulics

Power Distribution

Density/Expansion

Thermal-mechanics

- Stress-Strain Analysis
- Dynamic Mesh Models for thermal expansion

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3. Multi-physics Coupling

Neutronics

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

\[
\frac{1}{v(E)} \frac{\partial \psi}{\partial t}(\vec{r}, \Omega, E, t) = \left[ -\mathcal{L} - \mathcal{T} + S + \frac{\chi_p(E)}{4\pi} (1 - \beta) F \right] \psi(\vec{r}, \Omega, E, t) + \sum_{d=1}^{G_d} \frac{\chi_d(E)}{4\pi} \lambda_d C_d(\vec{r}, t)
\]

Rate of change
Streaming + Disappearance + Scattering + Fissions
Delayed Neutrons source

\[
\frac{\partial C_d}{\partial t}(\vec{r}, t) = \beta_d F \psi(\vec{r}, \Omega, E, t) - \lambda_d C_d(\vec{r}, t) - \vec{u} \cdot \nabla C_d(\vec{r}, t) + D_d \nabla^2 C_d(\vec{r}, t)
\]

for \( d = 1 \) to \( G_d \)

Local rate of change
Production
Destruction
Convection
Diffusion

Liquid Media
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

Point Kinetics
- Fundamental Mode
- Simple ODE

Quasi-Static Method
- Time Resolution strategy in
- larger time steps

Direct Calculation
- Direct discretization of time
- derivative

One-group

Multi-Group

Continuous

Angle (\(\Omega\))

Time (\(t\))

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

\[
\begin{align*}
\frac{1}{V} \frac{\partial \phi_0}{\partial t} &= \nabla \left( \frac{1}{3} \Sigma_1^{-1} \nabla \phi_0 - \Sigma_0 \phi_0 + \frac{F}{k} (\phi_0 - 2\phi_2) + 2\Sigma_0 \phi_2 + \frac{2}{V} \frac{\partial \phi_2}{\partial t} \right) + S_d \quad \text{order 0} \\
\frac{3}{V} \frac{\partial \phi_2}{\partial t} &= \nabla \left( \frac{3}{7} \Sigma_3^{-1} \nabla \phi_2 - \left( \frac{5}{3} \Sigma_2 + \frac{4}{3} \Sigma_0 \right) \phi_2 - \frac{2F}{3k} (\phi_0 - 2\phi_2) + \frac{2}{3} \Sigma_0 \phi_0 + \frac{2}{3V} \frac{\partial \phi_0}{\partial t} \right) - \frac{2}{3} S_d \quad \text{order 2}
\end{align*}
\]
3. Multi-physics Coupling
Neutronics: B) the Quasi-Static Method

**Key hypothesis:**

\[
\begin{align*}
\psi(\vec{r}, \Omega, E, t) &= n(t)\phi(\vec{r}, \Omega, E, t) \\
\left\langle \frac{1}{V(E)} \phi(\vec{r}, \Omega, E, t) \middle| W_0(\vec{r}, \Omega, E) \right\rangle &= \text{constant}
\end{align*}
\]

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

Neutronics: the Quasi-Static Method

Transport Equations

\[
\frac{1}{v} \frac{\partial \psi}{\partial t} = \mathcal{L} \psi + \sum_{d=1}^{G_d} \frac{\chi_d}{4\pi} \lambda_d C_d \\
\frac{\partial C_d}{\partial t} = \beta_d F \phi - \lambda_d C_d
\]

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

- Neutron flux shape (PDE) and
- Neutron flux amplitude (ODE)
3. Multi-physics Coupling

Neutronics: the Quasi-Static Method variants

\[
\begin{align*}
\frac{\partial \phi}{\partial t} &\neq 0 & \frac{dn(t)}{dt} &\neq 0 & \text{Improved Quasi Static} \\
\frac{\partial \phi}{\partial t} &= 0 & \frac{dn(t)}{dt} &\neq 0 & \text{Original Quasi Static} \\
\frac{\partial \phi}{\partial t} &= 0 & \frac{dn(t)}{dt} &= 0 & \text{Adiabatic Quasi Static}
\end{align*}
\]

- Sensibility study for 90$/s (\rho/B)$ 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
3. Multi-physics Coupling

Neutronics

Power Distribution

Density and Doppler effects
Precursors Advection

Thermal-hydraulics

Power Distribution

Density/Pressure

Density/Expansion

Thermal-mechanics

Stress-Strain Analysis

Dynamic Mesh Models for thermal expansion

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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

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

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

\[
\frac{\partial (\rho c T)}{\partial t} = \nabla (k \nabla T) + q_{\text{fission}}
\]

- Important for thermal expansion and density feedback

\[\sigma = 2\mu \varepsilon + \lambda \text{tr}(\varepsilon) I\]
\[\varepsilon = \frac{1}{2} (\nabla D + \nabla D^T)\]
3. Multi-Physics Coupling

Implementation of the example for the Godiva Experiment

- 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

- $\frac{p}{\bar{p}} \sim 1.06$
- $r \sim 8.85 \text{ cm}$
- ExecutionTime = 4.1h
- 1 processor 1.7Ghz
  (OpenFOAM)
- 10 processors 1.7Ghz
  (Serpent)

Flux

Godiva Experiment

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4. Results

SPN Deterministic Approach

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

Flux Field Order 0 Energy Group 1/8

Density Field

Godiva Experiment
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

Density and Doppler effects
Precursors Advection

Thermal-mechanics

Thermal-hydraulics

Two-phase flow
Radyolisis Models
Compressible Model
Porous Media

Neutronics

Power Distribution

Density/Expansion

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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
Thank you