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NEUTRONIC MODELING STRATEGIES FOR A LIQUID FUEL TRANSIENT CALCULATION

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Abstract

Framework

- A detailed and highly flexible numerical tool to study criticality accidents has been developed
- The tool implements a Multi-Physics coupling using neutronics, thermal-hydraulics and thermal-mechanics models based on OpenFOAM and SERPENT codes
- Two neutronics models: Quasi-Static Monte Carlo and SPN

Objective:

In this work a system composed by a **2D square liquid fuel cavity** filled with a fuel molten salt has been used to:

- Investigate the performance of the tool's thermal-hydraulics and neutronics solvers coupling numerical scheme
- Evaluate possible strategies for the implementation of the Quasi-Static (QS) method with the Monte Carlo (MC) neutronics code
- Compare the QS-MC approach precision and computational cost against the Simplified P3 (**SP3**) method

Study Case: 2D Square Liquid Fuel Cavity

- The nuclear system: a critical 2 m x 2 m 2-D square cavity filled with a FLiBe molten fuel salt. Natural and/or forced convection conditions could be set in the cavity depending on the chosen boundary conditions as shown in Figure 1
- The fission power is removed from the cavity by a uniform heat exchange sink: $q'''(r) = h_{sink}\left(T(r) - T_{ref}\right)$
- Thermal-hydraulics modeling:
  - ❑ Laminar and incompressible formulation of the Navier-Stokes equations
  - ❑ Thermal expansion effects: Boussinesq approximation
- Neutronics modeling:
  - ❑ Neutronics feedback effects: (i) Doppler effect correction is not made (to decrease uncertainties in the comparison), (ii) Only fuel density effect is taken into account in the calculation of the macroscopic cross-sections
  - ❑ An 8 groups effective delayed neutron precursors and JEFF-3.1 data library are used. Six energy groups for the SP3 model
- Three Phases:

2D Square Liquid Fuel Cavity CNRS Benchmark		
Phase 1	Steady	Single physic and one-way coupling: hydraulics, thermal and neutronics
Phase 2	Steady	Full multi-physics and two way coupling
Phase 3	Transient	Determination of the Bode diagram from a small periodic perturbation

Table I. CNRS Multi-Physics Coupling Benchmark.

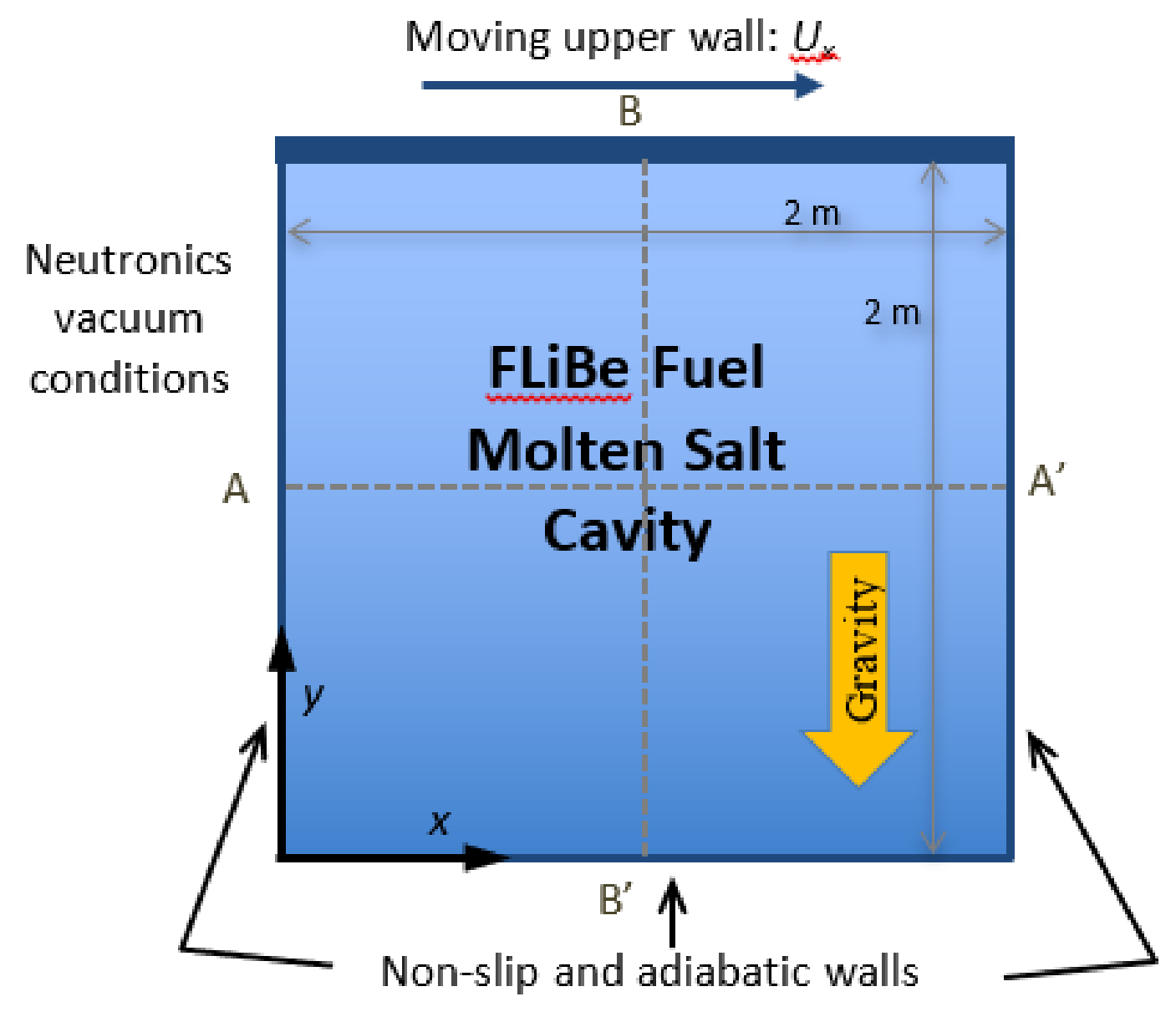
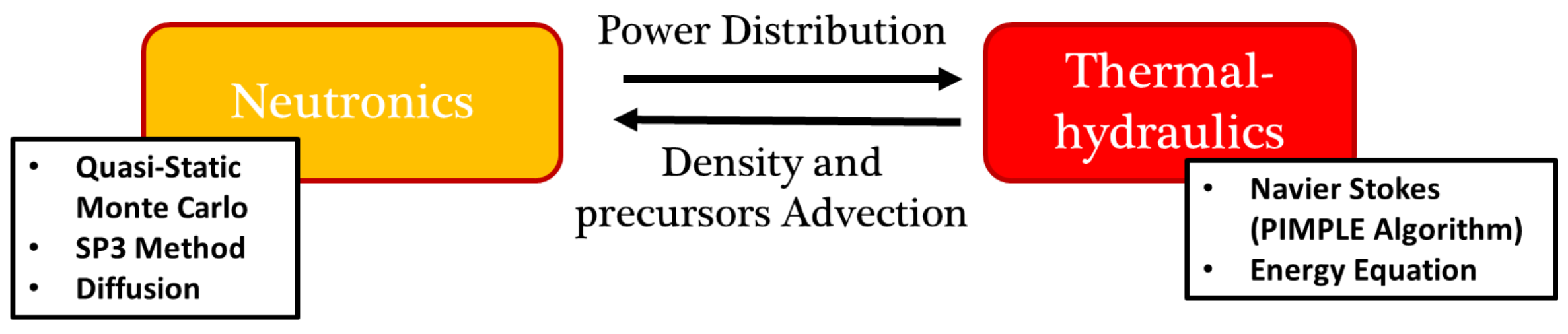


Figure 1. CNRS multi-physics benchmark: lid-driven Cavity Scheme.

Model

Neutronics and Thermal-Hydraulics Coupling Scheme


Neutronics

- Quasi-Static Monte Carlo
- SP3 Method
- Diffusion

Power Distribution

Density and precursors Advection

Thermal-hydraulics

- Navier Stokes (PIMPLE Algorithm)
- Energy Equation

Figure 2. Coupling scheme for neutronics and thermal-hydraulics cases.

Mass and momentum Conservation

Incompressible laminar flow Navier-Stokes with the Boussinesq approximation:

$$\nabla \cdot \vec{u} = 0$$

$$\frac{\partial \vec{u}}{\partial t} + \nabla \cdot (\vec{u}\vec{u}) = \nabla \cdot (\nu \nabla \vec{u}) - \frac{\nabla p}{\rho_0} + \left(1 - \beta_{exp}(T - T_{ref})\right)\vec{g}$$

Energy Conservation

Boussinesq approximation with the fission source and the heat sink:

$$\frac{\partial T}{\partial t} + \nabla \cdot (\vec{u}T) = \nabla \cdot (\alpha \nabla T) + \frac{Q_{fission}}{\rho C_p} - \frac{h_{sink}}{\rho C_p}(T - T_{ref})$$

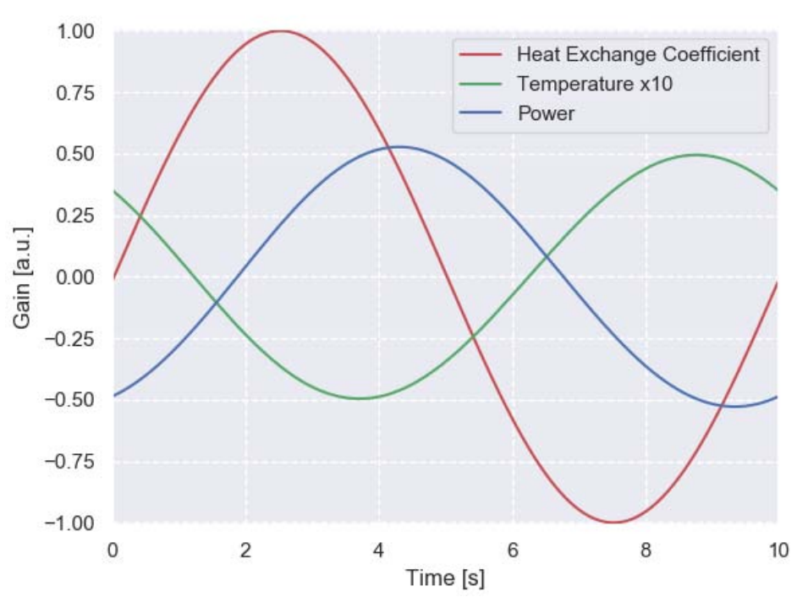


Figure 3. Key system parameters during transient (Phase 2).

Neutronics modeling

Quasi-static Method

The Quasi-Static (QS) method allows decreasing the computational cost of a transient Monte Carlo code analysis. The QS method separates the neutron angular flow as $\psi(\vec{r},\vec{\Omega},E,t) = n(t)\phi(\vec{r},\vec{\Omega},E,t)$ with n being the amplitude and ϕ the shape.

$$\begin{cases} \frac{1}{V(E)}\frac{\partial \phi}{\partial t}(\vec{r},\vec{\Omega},E,t) = \frac{1}{n(t)}\sum_{d=1}^{G_d}\frac{\chi_d(E)}{4\pi}\lambda_d C_d(\vec{r},t) + \left(-\mathcal{L} - T + S + \frac{\chi_p(E)}{4\pi}(1-\beta)F - \frac{1}{V(E)}\frac{1}{n(t)}\frac{\partial n(t)}{\partial t}\right)\phi(\vec{r},\vec{\Omega},E,t) \\ \frac{\partial C_d}{\partial t}(\vec{r},t) + \vec{u}\cdot\nabla C_d(\vec{r},t) = \nabla\cdot(D_d \nabla C_d) + \beta_d F \psi(\vec{r},\vec{\Omega},E,t) - \lambda_d C_d(\vec{r},t) \end{cases}$$

$$\begin{cases} \frac{\partial n(t)}{\partial t} = \left[\frac{\rho - \beta^{eff}}{\Lambda}\right] n(t) + \sum_{d=1}^{G_d}\lambda_d \bar{c}_d(t) \\ \frac{d\bar{c}_d(t)}{dt} = \frac{\beta_d^{eff}}{\Lambda} n(t) - \lambda_d \bar{c}_d(t) \end{cases}$$

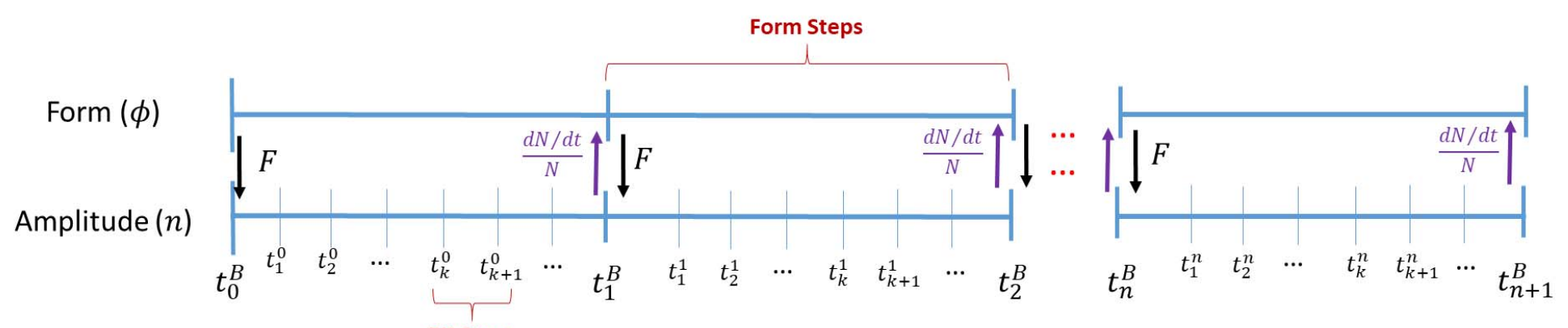


Figure 4. Shape and amplitude time steps discretization.

SP1 and SP3 Methods

The SPN deterministic method has also been implemented as an alternative neutronic model in the multi-physic tool. This method is a 3D extension of the plane-geometry PN equations and makes the following assumptions:

- It exists a local coordinate system where the flux varies slowly with x, y and φ,
- This coordinates system does not vary much or slowly enough in space,
- The flux expansion is truncated to order N.

By using these approximations, the following equations can be obtained for N equal to 3:

$$\frac{1}{v^g}\frac{d\phi_0^g}{dt} = \nabla\cdot\left(\frac{1}{3\Sigma_{r1}^g}\nabla\phi_0^g\right) - \Sigma_{r0}^g\phi_0^g + 2\Sigma_{r0}^g\phi_2^g + (1-\beta)\chi_p^g\sum_{g'}\nu\Sigma_f^{g'}\left(\phi_0^g - 2\phi_2^g\right) + \chi_d^g\sum_d\lambda_d C_d + \sum_{g'\neq g}\Sigma_{s0}^{gg'}\left(\phi_0^{g'} - 2\phi_2^{g'}\right) + \frac{2}{v^g}\frac{d\phi_2^g}{dt}$$

$$\frac{3}{v^g}\frac{d\phi_2^g}{dt} = \nabla\cdot\left(\frac{3}{7\Sigma_{r1}^g}\nabla\phi_2^g\right) - \left(\frac{5}{3}\Sigma_{r2}^g + \frac{4}{3}\Sigma_{r0}^g\right)\phi_2^g - \frac{2}{3}\left(\sum_{g'\neq g}\Sigma_{s0}^{gg'}\left(\phi_0^{g'} - 2\phi_2^{g'}\right) - \Sigma_{r0}^g\phi_0^g\right) - \frac{2}{3}(1-\beta)\chi_p^g\sum_{g'}\nu\Sigma_f^{g'}\left(\phi_0^g - 2\phi_2^g\right)$$
$$+ \frac{2}{3v^g}\frac{d\phi_0^g}{dt} + \frac{5}{3}\sum_{g'\neq g}\Sigma_{s2}^{gg'}\phi_2^{g'} - \frac{2}{3}\chi_d^g\sum_d\lambda_d C_d$$

Results

Phase 2: Steady-State Full Multi-Physics Coupling

- Velocity field: determined by the forced convection and the buoyancy effects
- Temperature field: determined by the power profile and less strongly by the advection effects
- Delayed neutrons/ precursors concentration fields:
  - Large impact of advection effect,
  - Contrary to solid fuels, the precursors distribution is not proportional to the fission source for long half-life precursors families.
- Coupling effect: large effect on reactivity. About -1200 pcm change between coupling and no coupling (**Table II**)
- Very good agreement between SP1, SP3 and QS-MC approaches due to the large system size

Model	K-eff [a.u.]	
	Stand-alone	Fully-coupled
Diffusion	1.00413	0.99212
SP3	1.00355	0.99155
QS-MC	1.00410	0.99214

Table II. Steady-State reactivity

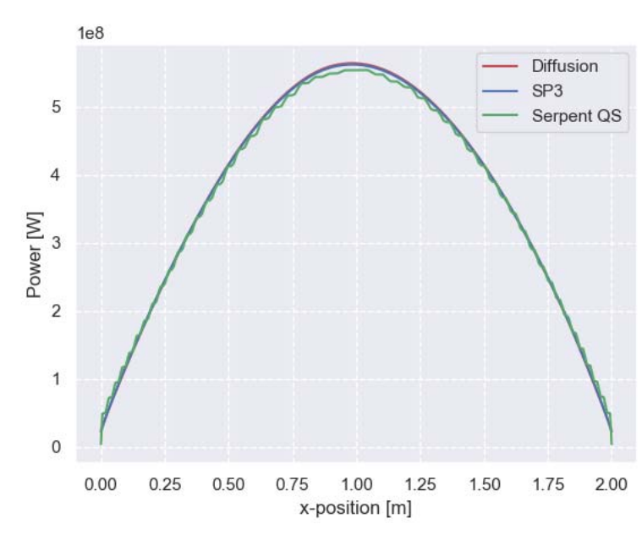


Figure 5. Steady-State Power Distribution

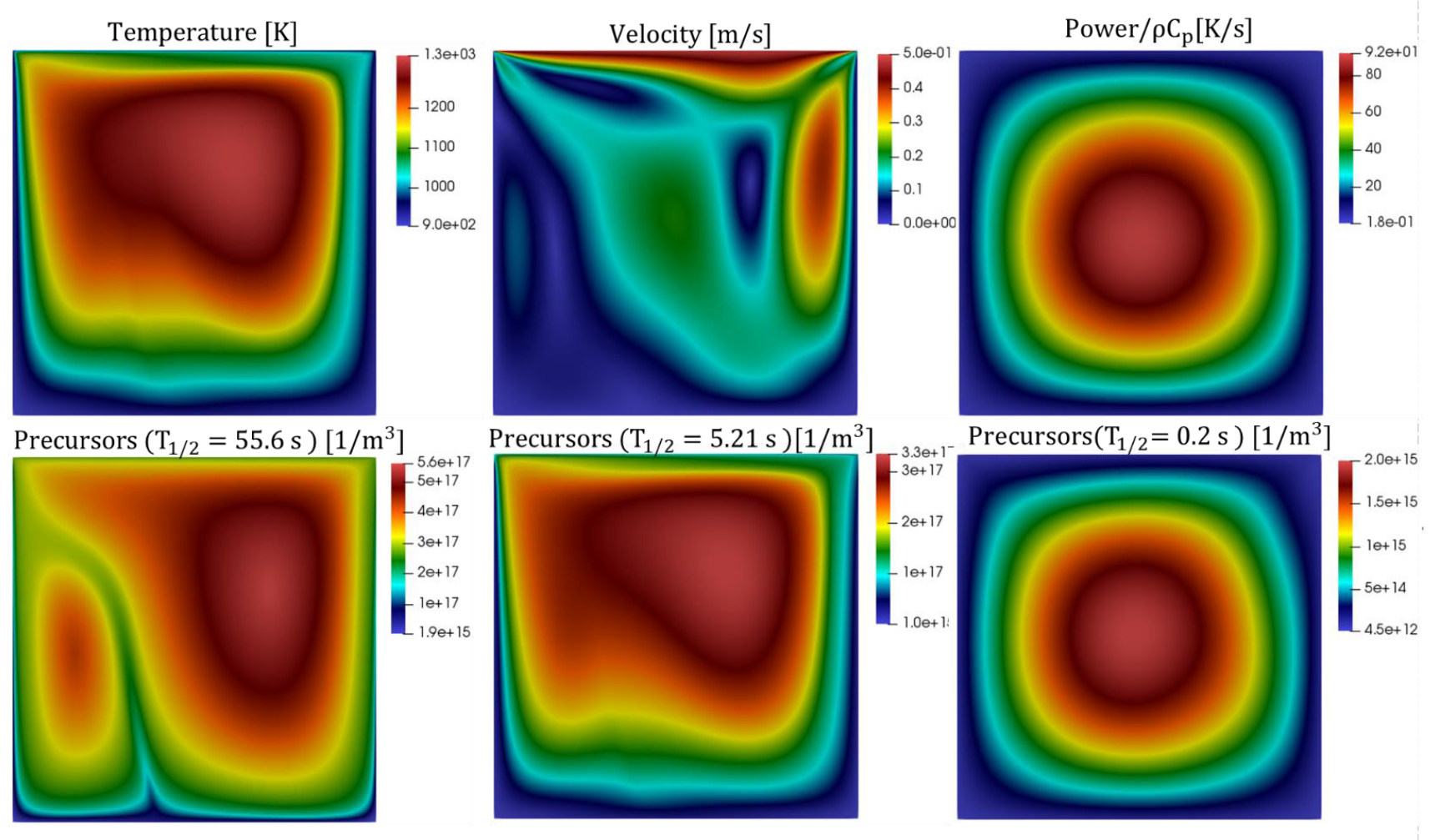


Figure 6. Cavity Temperature, Velocity, Power and Precursors Fields (Phase 2)

Phase 3: Transient Full Multi-Physics Coupling

- The system Bode Diagram was numerically determined by assuming a linear response for the following small periodic perturbation on the heat exchange coefficient: $\mathbf{h_{sink} = h_0(1 + A\sin(2\pi t/T))}$.
- **The transient was discretized with a fixed time step set to** 0.012 s in order to obtain a maximum **Courant number of 0.8**
- System response:
  - ❑ **At low frequencies** the system is able to "follow" the perturbation (i.e. little phase change) and the transfer function is close to unity
  - ❑ **At high frequencies** the system inertia damps and delays the perturbation due to the combine effects of convective transport and delayed neutrons emitted by long half-life precursors
- In all cases, there is a good agreement between SP1, SP3 and QS-MC models
- Comparison between computational costs: QS-MS computational cost found to be reasonable: about 3 times higher the one of SP1/SP3 (See **Table III**)

Model	Average Execution Time (s) per Cycle
Diffusion	21815
SP3	29355
Monte Carlo QS	95816

Table III. Transient Computational Cost per time step. Diffusion and SP3 methods were calculated with 20 processors. The QS-MC approach used 1 processor for the OpenFOAM calculations and 24 processors for SERPENT Monte Carlo.

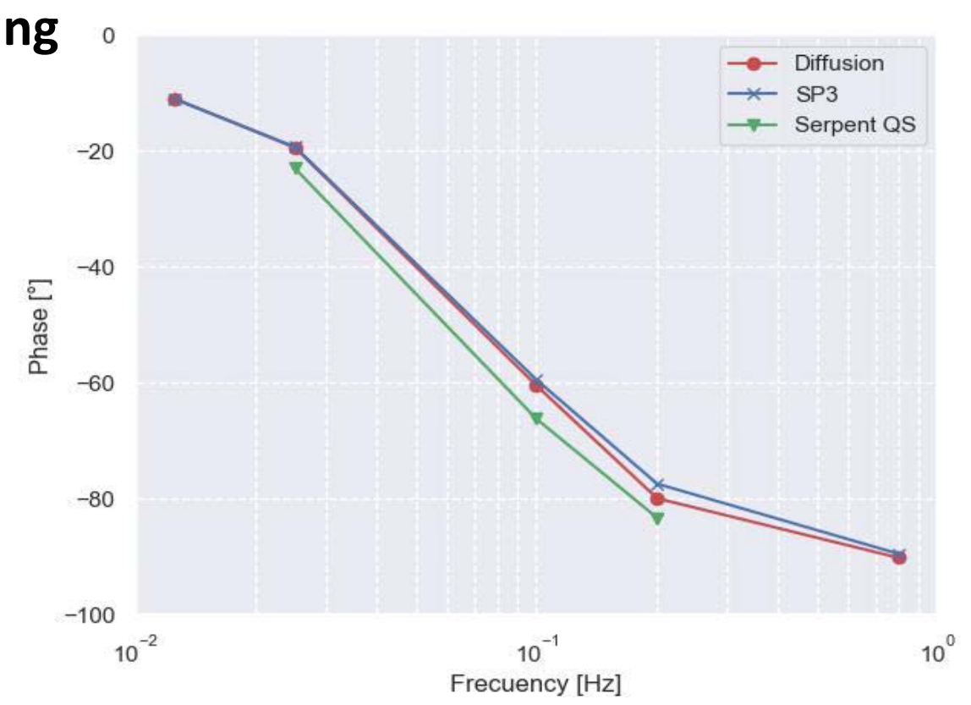


Figure 7. Phase Diagram of the cavity

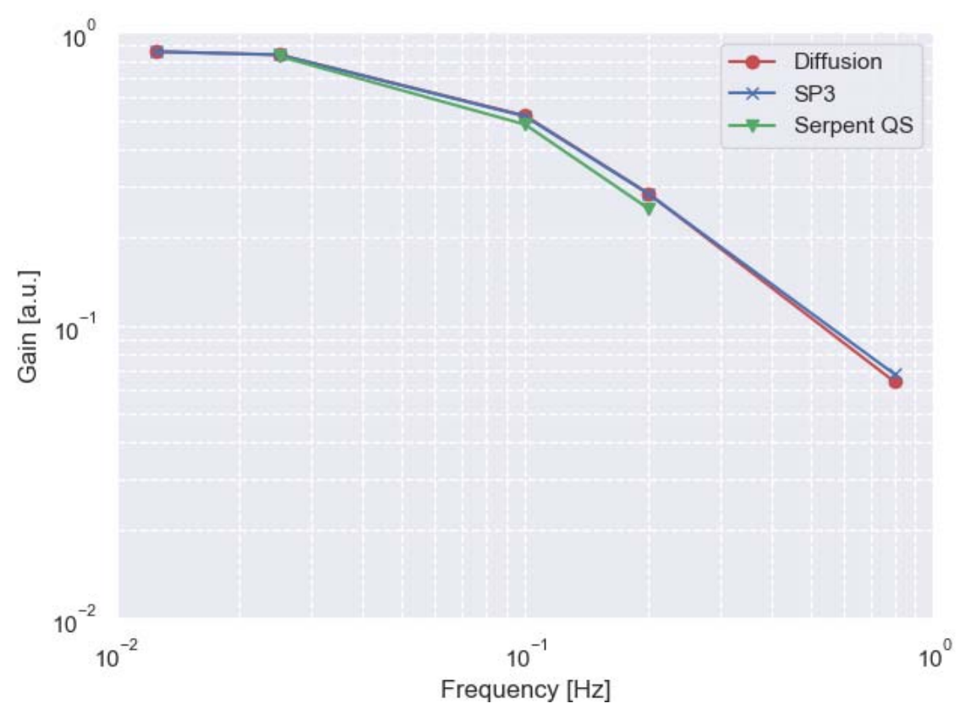


Figure 8. Gain Diagram of the cavity

Conclusions

- A transient Monte Carlo calculation has been implemented in a Multi-Physics tool through a Quasi-Static method (QS-MC approach),
- The implementation of the QS-MC approach in the Multi-Physics tool enables great flexibility on the modeling capabilities (in terms of characteristic time, model details, materials, geometries, etc.) of the tool that are mandatory for its use for the study of a broad range of criticality accidents,
- The performance of the QS-MC approach has been compared against a SP1 and SP3 neutronics models using a 2D Square Liquid Fuel Cavity system designed for evaluation of Multi-Physics coupling,
- The computational cost of the QS-MC approach appears to be very reasonable,
- The QS-MC would allow the higher precision in criticality accidents studies with a reasonable cost.

References

1. M. Aufiero, P. Rubiolo, "Testing and Verification of Multiphysics Tools for Fast-Spectrum MSRs: The CNRS Benchmark", Transactions of the American Nuclear Society, Vol. 118, Philadelphia, Pennsylvania, June 17–21, 2018.
2. M. Tiberga et al. "A coupled fluid-dynamics and neutronics numerical benchmark for multi-physics codes dedicated to fast molten salt reactors", to be submitted at Nuclear Science and Engineering.
3. Y. JO, B. CHO, N. Z. CHO, "Nuclear reactor transient analysis by continuous-energy Monte Carlo calculation based on predictor-corrector quasi-static method", Nuclear Science and Engineering, vol. 183 229-246 (2015).
4. U.S. ATOMIC ENERGY COMISSION, "Neutron kinetics", in Naval Reactor Physics Handbook, vol. 1, Washington, 64 855-864 (1958).
5. K. O. OTT & D. A. MENELEY, "Accuracy of the Quasistatic Treatment of Spatial Reactor Kinetics," Nuclear Science and Engineering, 36:3, 402-411 (1969).
6. HAMILTON, Steven P.; EVANS, Thomas M. Efficient solution of the simplified PN equations. Journal of Computational Physics, 2015, vol. 284, p. 155-170.