Serpent and multiphysics workshop
LPSC, Grenoble, France,
26-27 February 2015

Serpent-OpenFOAM coupling for criticality accidents modelling – Definition of a benchamrk for MSRs multiphysics modelling

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Serpent-OpenFOAM coupling for criticality accidents

- Validation against Godiva burst experimental data
- Application to the MSFR transient simulation

Definition of a benchamrk for MSRs multiphysics modelling

SERPENT/OpenFOAM internal coupling in transient mode

OpenFOAM libraries dynamically linked to Serpent-2 at source code level

- Neutron transport via standard SERPENT Monte Carlo routines
- Other physics are solved with standard OpenFOAM Finite-Volumes methods
- Coupling is performed at runtime
- Code-to-code coupling & complex I/O files are avoided
- Fast and flexible mesh handling and deformation
- Preliminary validation on Godiva super prompt critical transients

Assessment and verification: Godiva super prompt-critical burst

Godiva: spherical assembly $\sim$ 50 kg of metallic U

- Experimental results from LA-2029 (1960, public release 1995?)
- Effective prompt lifetime = few ns
- Rapid power excursion
- Thermal expansion feedbacks (no Doppler)
- In fast transients (T$\sim$10μs) speed of sound (few km/s) is relatively small: thermal-expansion is not in equilibrium with temperature fields

Modelling conditions "close" to MSFR super prompt-critical transients

Assessment and verification: Godiva super prompt-critical burst

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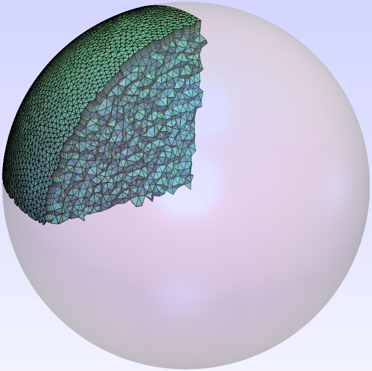

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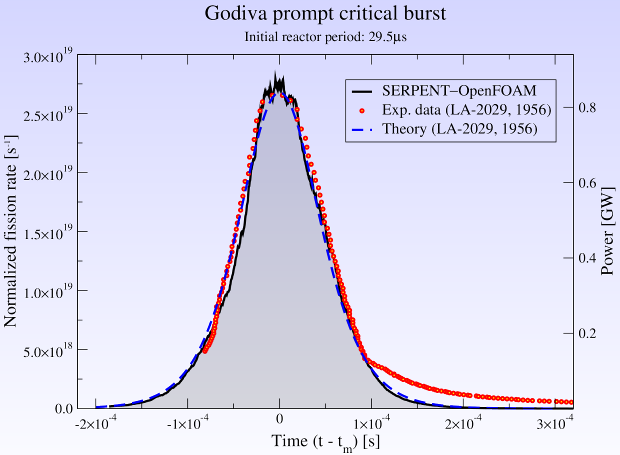
Modelling conditions "close" to MSFR super prompt-critical transients

Godiva super prompt-critical burst

Initial reactor periods: 11.6 and 29.5 μs

Validation against Los Alamos experimental data



Godiva super prompt-critical burst

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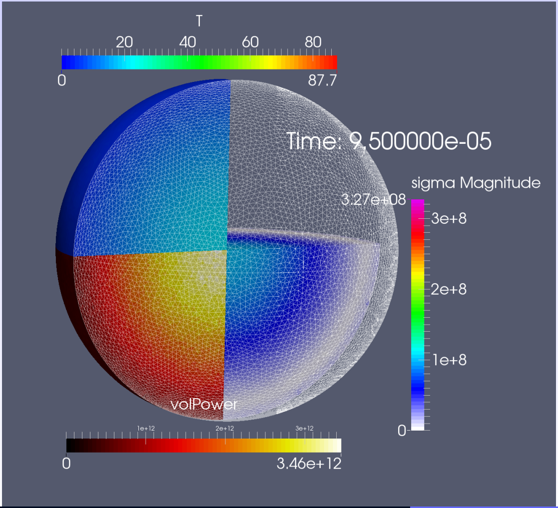

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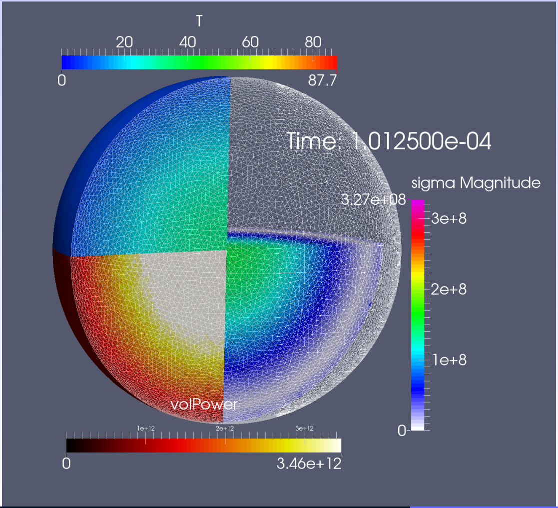

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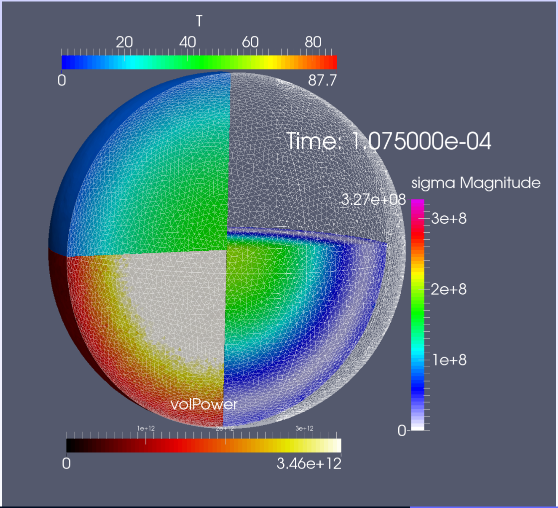

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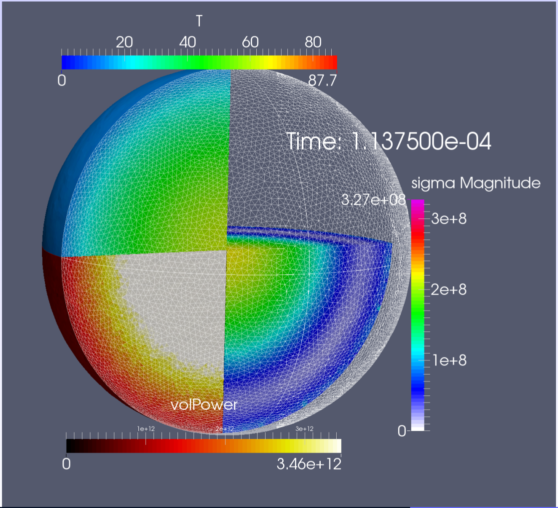

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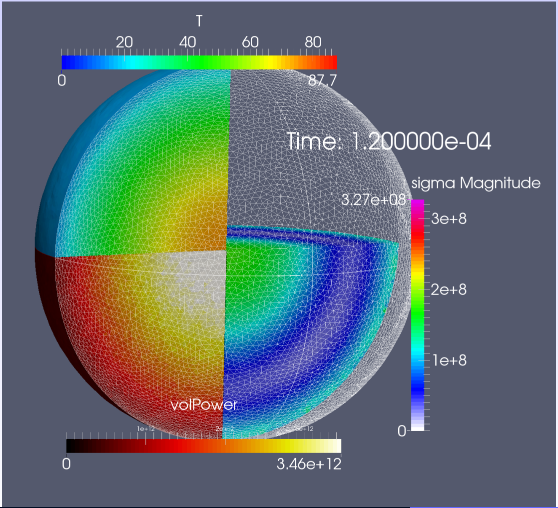

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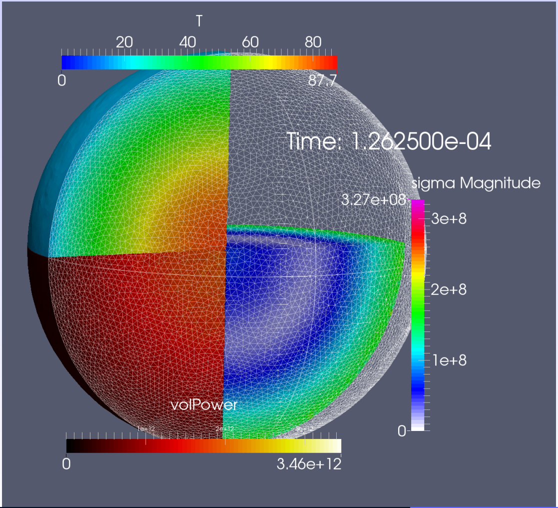


Serpent-OpenFOAM couplig... how does it work?

Linear elasticity

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

$$\mu = \frac{E}{2(1+\nu)}; \; \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \quad (2)$$

Energy equation

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c} \nabla^2 T + \frac{q'''_{\mathrm{fission}}}{\rho c} \quad (3)$$

Serpent-OpenFOAM couplig... how does it work?

Score fission energy deposition

Code snippet – OpenFOAMScoreFissionEnergy.cpp

```
void OFScoreFissE(long mat, long part, ... , indexedOctree<treeDataCell>& ioc)
{
    ...
    if (mat > VALID_PTR)
    {
        if ((rea = (long)RDB[mat + MATERIAL_PTR_FISSE]) > VALID_PTR)
        {
            if ((fissE = MacroXS(rea, E, id)*flx*g*wgt) > 0.0)
            {
                point sample(x/100.0, y/100.0, z/100.0);
                sampleCellIndex = ioc.findInside(sample);
                volPowerBuffer.internalField()[sampleCellIndex] += fissE;
            }
        }
    }
}
```

Serpent-OpenFOAM couplig... how does it work?

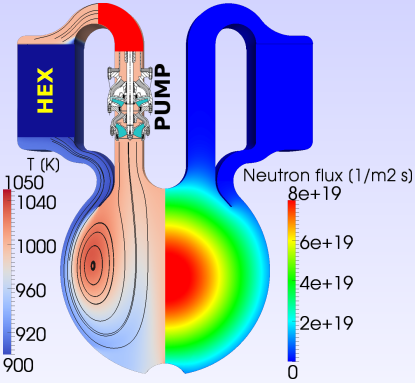
Material density at collision points

Code snippet – OpenFOAMDensityFactor.cpp

```
double OFDensityFactor(..., volScalarField& rhok, indexedOctree<treeDataCell>&
     ioc)
{
    double f;
    Foam::label sampleCellIndex;

    ...

    point sample(x/100.0, y/100.0, z/100.0);
    sampleCellIndex = ioc.findInside(sample);

    if (sampleCellIndex != -1)
        f = rhok.internalField()[sampleCellIndex];
    else
        f = 0.0;

    ...

    return f;
}
```

Application: MSFR reactivity insertion

Investigate the effect of fluid compressibility



- Fuel salt expansion is the main reactivity feedback
- Doppler is also important
- Density change is limited by the speed of sound
- 1300 m/s (pure liquid)
  600 m/s (Gas bubbles)
- In fast transients speed of sound is relatively small: thermal-expansion is not in equilibrium with temperature fields

Modelling conditions “close” to GODIVA super prompt-critical transients

Compressible sonic solver

Linearized momentum equation and continuity equation

$$\rho \frac{\partial \mathbf{U}}{\partial t} = \nabla \left(\rho \mathbf{U} \cdot \mathbf{U} \right) + \mu \nabla^2 \mathbf{U} = -\nabla p \tag{4}$$

```
fvm::ddt(rho,U) + fvm::div(phi,U) + fvm::laplacian(mu,U) = - fvc::grad(p)
```

$$\frac{\rho}{\partial t} = -\nabla \left(\rho \mathbf{U} \right) \tag{5}$$

```
fvm::ddt(rho) = + fvc::div(phi)
```

Linearized equation of state

$$\rho = \rho_0 + \psi \left(p - p_0 \right) - \rho_0 \beta \left(T - T_0 \right) \tag{6}$$

Compressible sonic solver

Pressure equation

$$\psi \frac{\partial p}{\partial t} + \nabla (\rho \mathbf{U}) = \rho_0 \beta \frac{\partial T}{\partial t} + \dots \quad (7)$$

```
fvm::ddt(psi, p) + fvc::div(phi) = fvc::ddt(rho_0 * beta, T) + ...
```

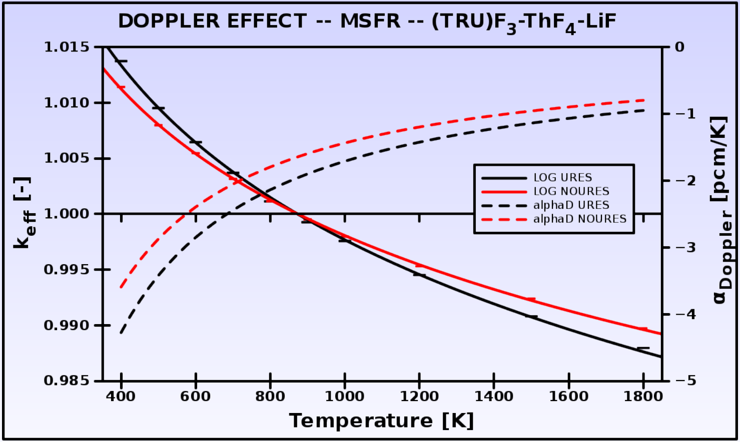
Energy equation

$$\rho c_p \frac{\partial p}{\partial t} + \rho c_p \nabla (\rho T) - \rho c_p \alpha \nabla^2 T = q''' \quad (8)$$

```
fvm::ddt(rho * c_p, T) + fvm::div(phi * c_p, T) - fvm::laplacian(rho * c_p *
    alpha, T) = volPower
```

Doppler effect: RESOLVED and UNRESOLVED resonances broadening

Logarithmic material interpolation

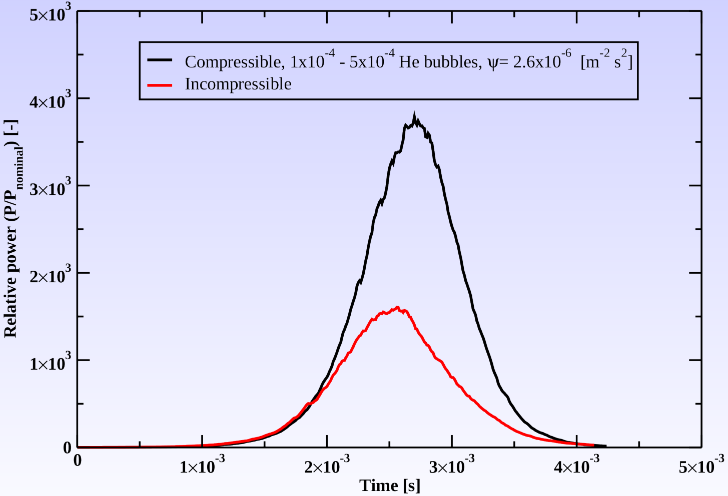


MSFR super prompt-critical burst

Effect of fluid compressibility – TRU started MSFR

Prompt reactivity insertion from zero power: ~230 pcm

$\beta_{eff,\ static}$ ~ 300 pcm $\beta_{eff,\ circ}$ ~ 145 pcm



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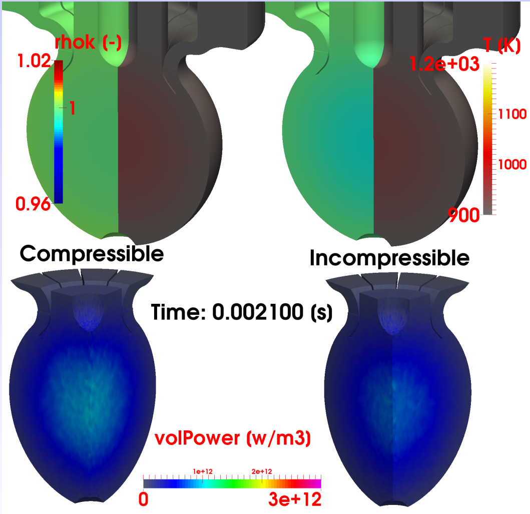

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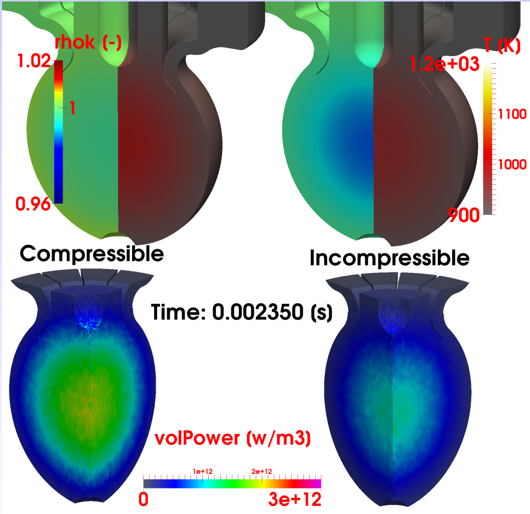

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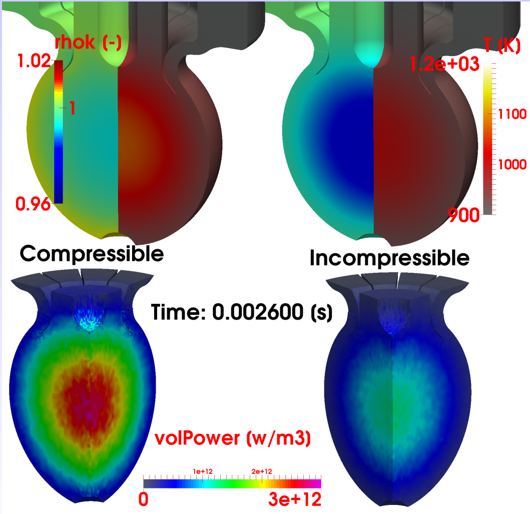

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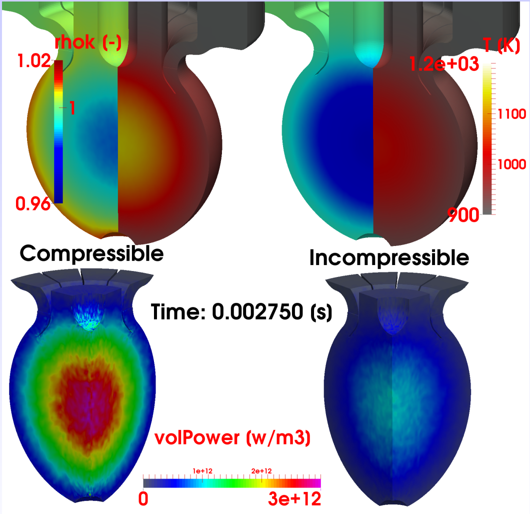

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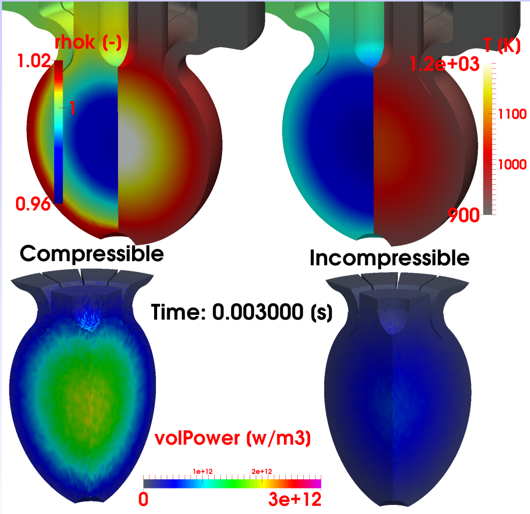

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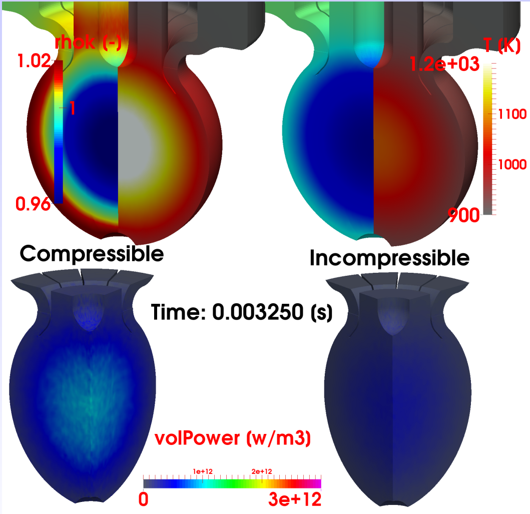

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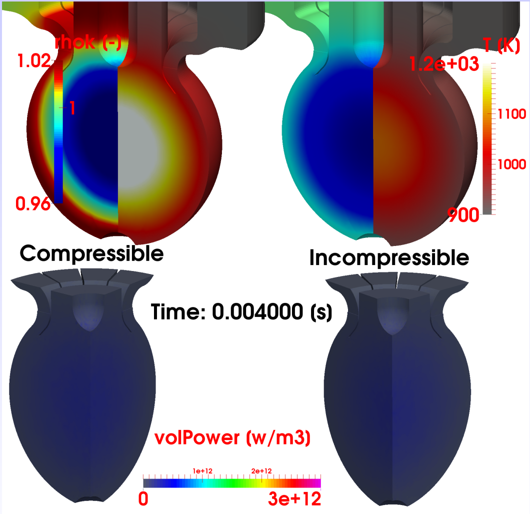

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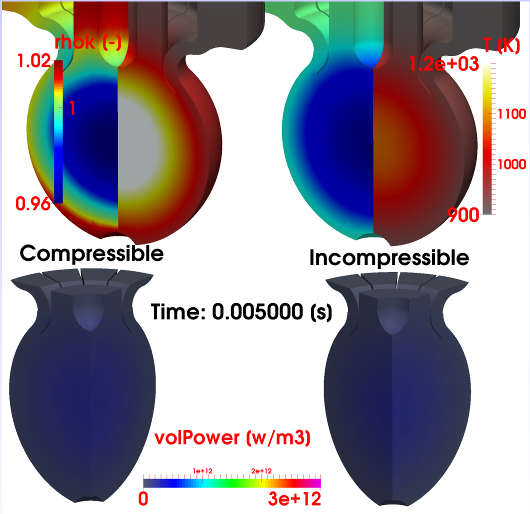
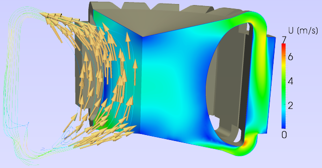
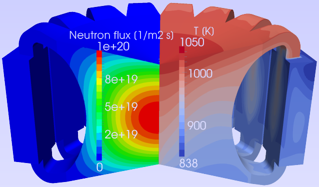


Simulation tools for the MSFR





- Legacy reactor physics codes are not suitable for MSFR steady-state and transient analysis
- (Unfortunately) the development of new tools is required
- These new tools should be tested/verified/compared

Code development in the EVOL project

Several multiphysics tools have been developed, adopting a variety of approaches:

- Neutronics
  - Deterministic (mainly few-group diffusion)
  - Monte Carlo
  - Hybrid (e.g., fission matrix)
- Spatial-discretization
  - Finite-volume
  - Finite-element
  - ...
- Time-integration/coupling
  - Explicit
  - Implicit (Euler, BDF, RK, ...)

Code development in the EVOL project

- Code availability
  - Open source-based (e.g., OpenFOAM, SERPENT, ...)
  - In-house (POLIMI, TUDelft, KIT Karlsruhe, ...)
  - Commercial (COMSOL, FLUENT, ...)

  - 2D $(r, z,)$ codes
  - Fully 3D codes
  - Parallel computing capabilities ?

How should we test/verify/compare the different tools?

How should we test/verify/compare the different tools?

The problem

Results of the EVOL CFD benchmark and comparisons among the partners highlighted differences for steady-state and transient simulations.

Several suspects have been identified:

- Nuclear data libraries
- Delayed neutrons data
- Turbulence models
- Geometrical domain approximations
- Coarse mesh discretization
- ...

Impossible to verify the consistency of the results of the different tools!

Simplified benchmark for MSFR simulation tools

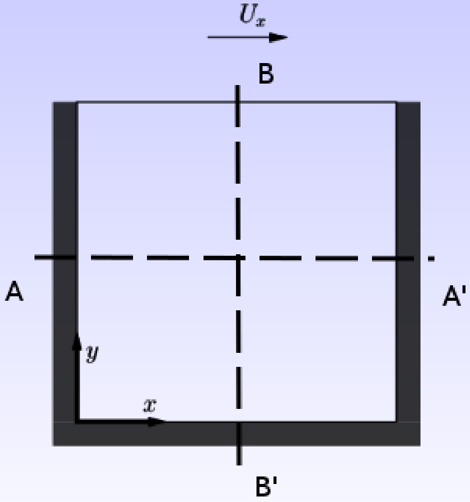
Focus only on multiphysics coupling

Let's get rid of any OTHER source of discrepancies:

- Simple 2D geometry
- No turbulence (laminar solution)
- Cartesian spatial discretization

Simplified benchmark for the MSFR simulation tools

Simple geometry



Simplified benchmark for the MSFR simulation tools

Material composition:

- Flibe (LiF + BeF_2 at 2:1). Natural Li enrichment
- ^{235}U as fissile

High neutronics similarity with the MSFR in terms of:

- Reaction rates ratios (similar neutron spectrum)
- k_{inf}, dominance ratio

Simplified benchmark for MSFR simulation tools

Phase-0 Single-physics verification

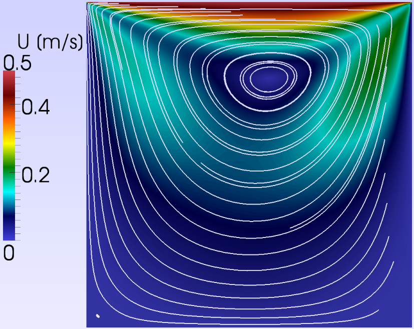
- Step-0.1 Velocity field
- Step-0.2 Neutronics
- Step-0.3 Temperature field

Phase-1 Steady-state coupling

- Step-1.1 Circulating fuel
- Step-1.3 Power coupling
- Step-1.5 Buoyancy
- Step-1.7 Full coupling

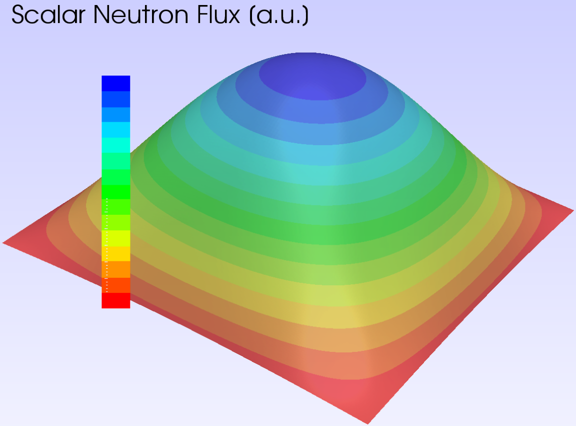
Phase-2 Transient simulations

Step-0.1 Velocity field



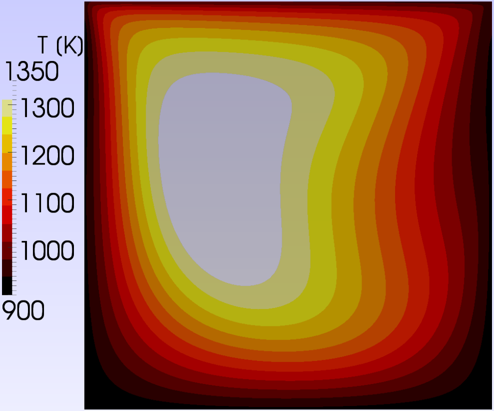
Velocity U_x imposed at the top boundary of the square 2D cavity.
Viscosity increased to have stable laminar solution.

Step-0.2 Scalar neutron flux distribution



Vacuum boundary conditions.
Very small spectrum change from the center to the boundaries.

Step-0.3 Temperature field



Heat source distribution from Step-0.1.

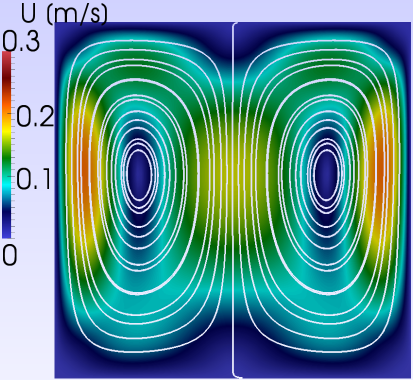
Velocity field from Step-0.2.

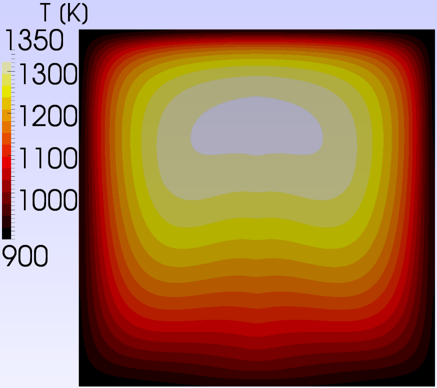
$q'' = h \cdot (T - T_{cold})$ $T_{cold} = 900K$.

Thermal conductivity 1 $W/m \cdot K$.

Step-1.1 "Buoyancy" (two-way coupling)

Temperature and velocity fields



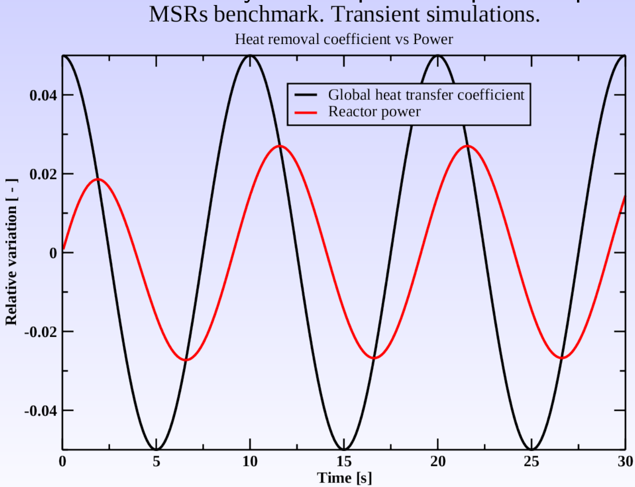


Constant fuel volumetric expansion coefficient $(2 \cdot 10^{-4} K^{-1})$.

Phase-2 Transient simulation

Still under definition

Verification of the system response to periodic perturbations.



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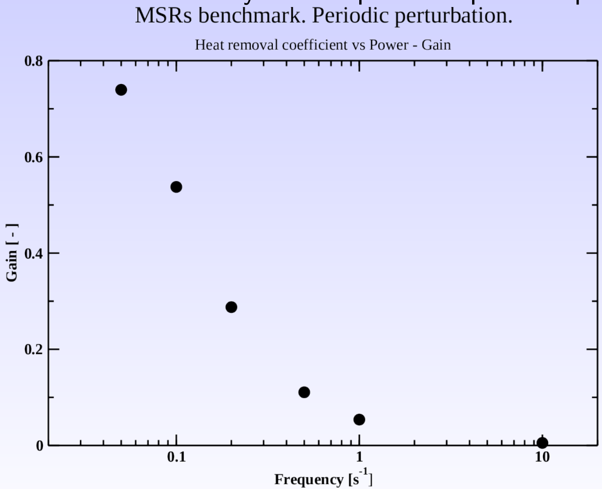

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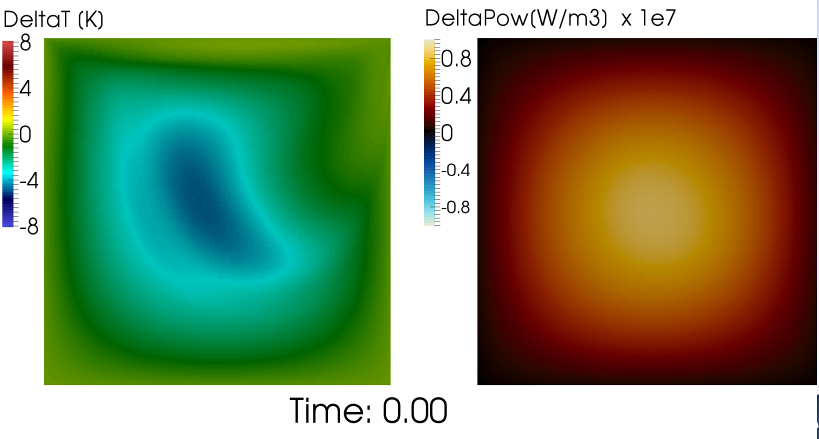

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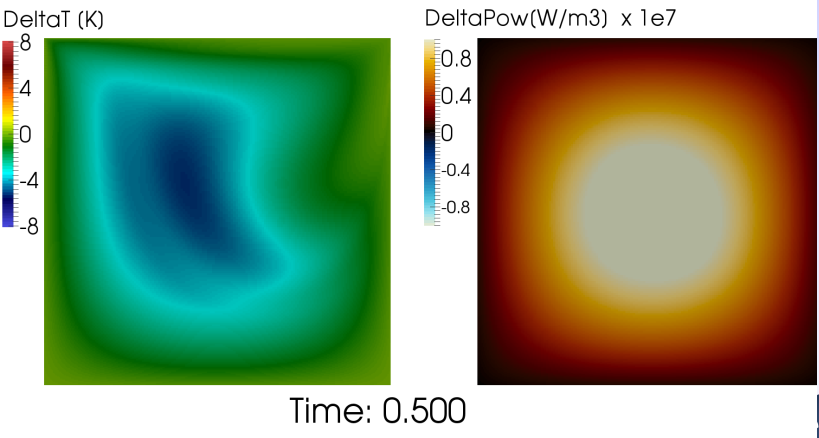

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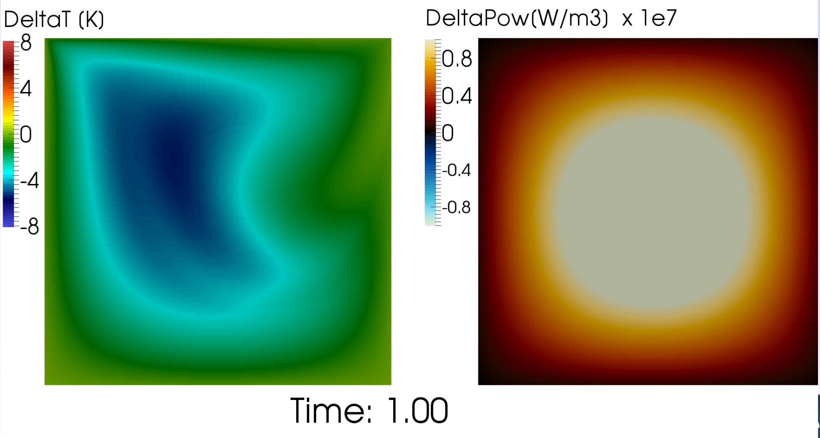

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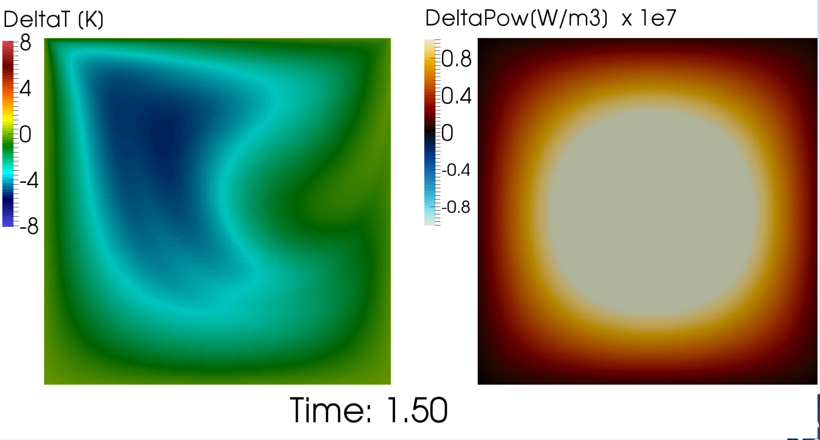

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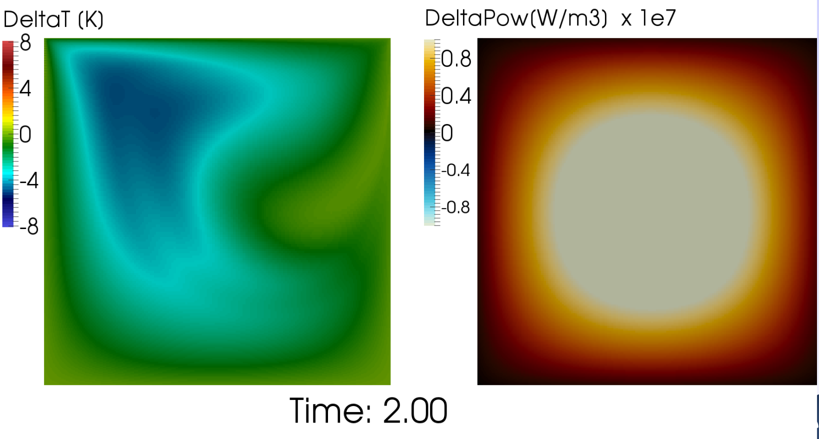

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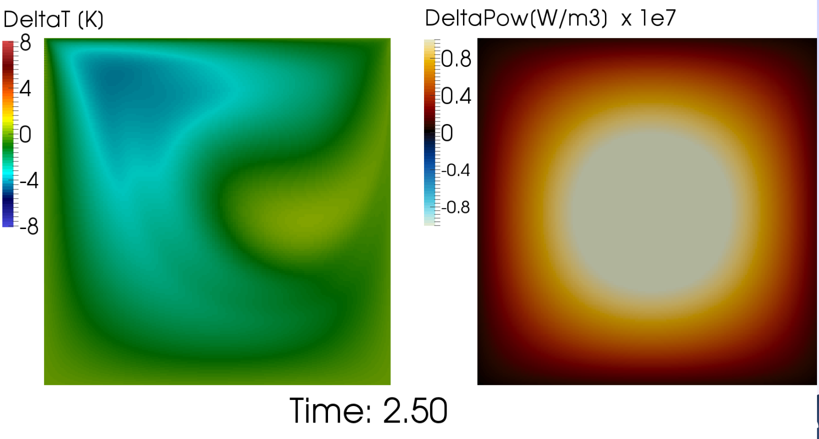

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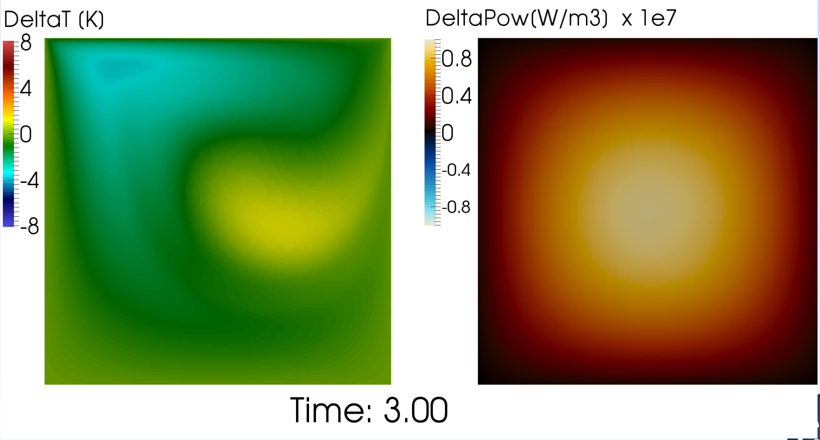

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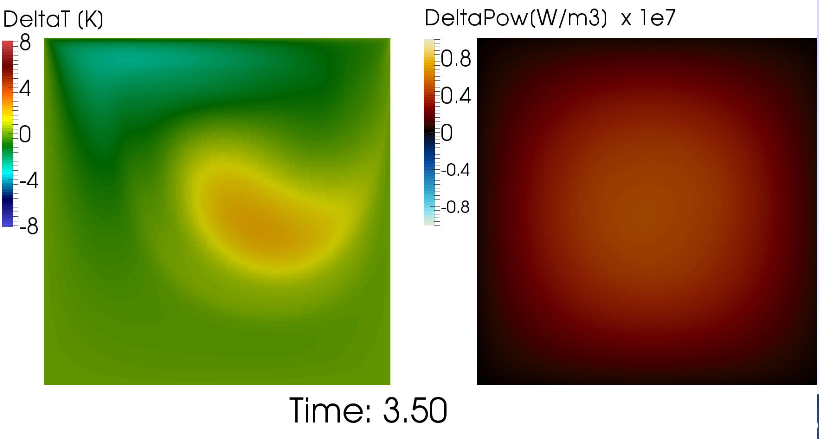

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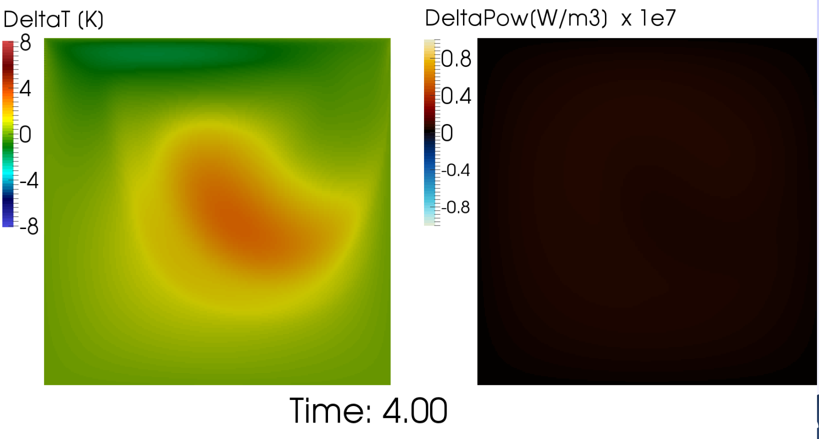

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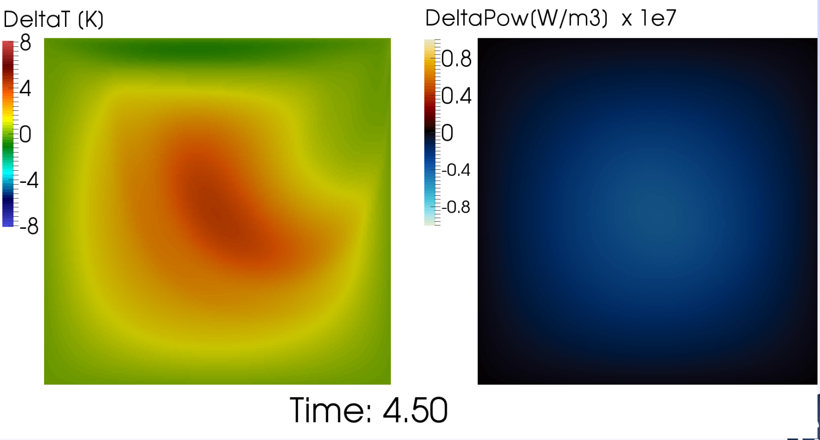

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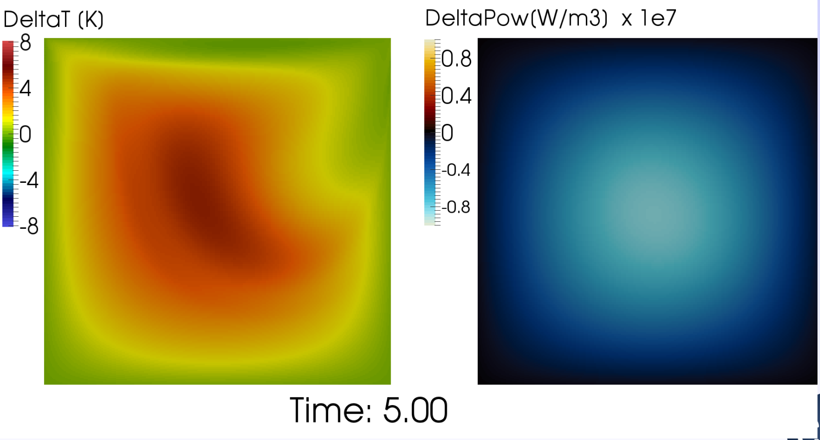

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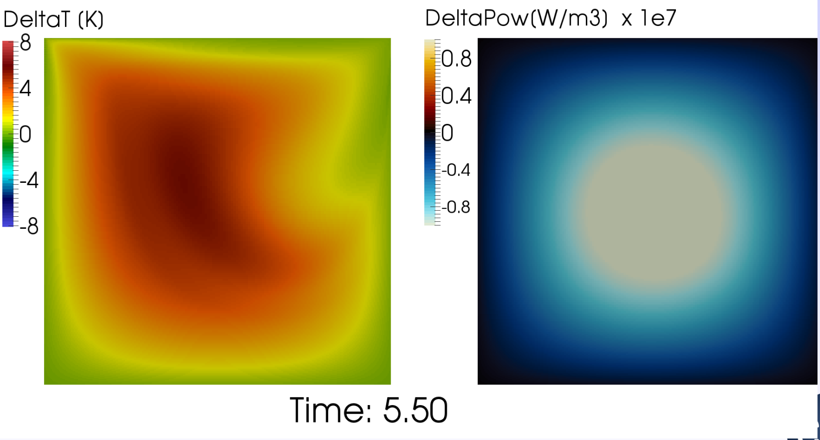

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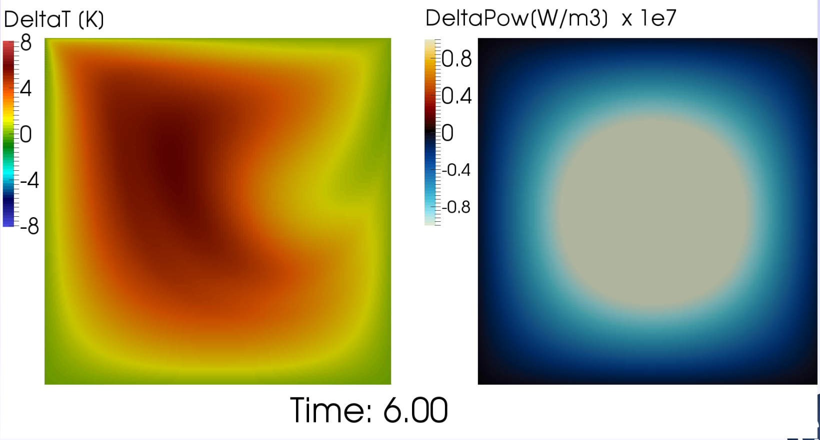

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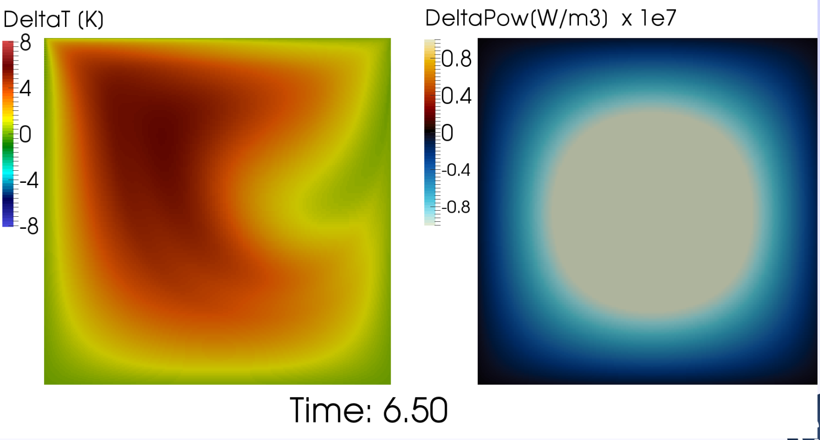

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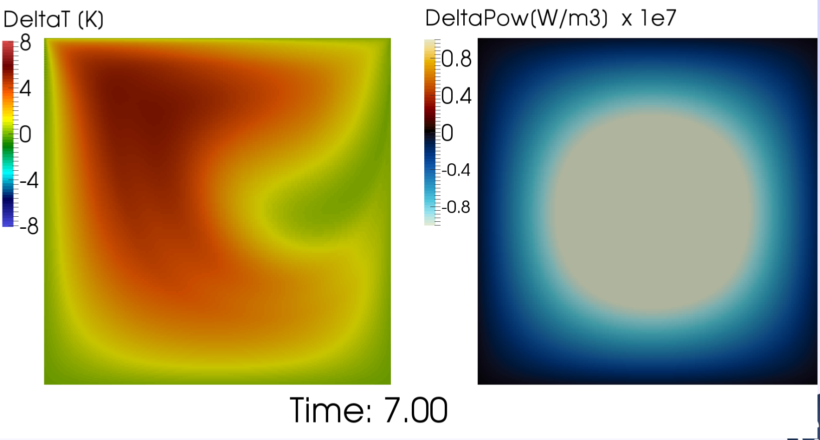

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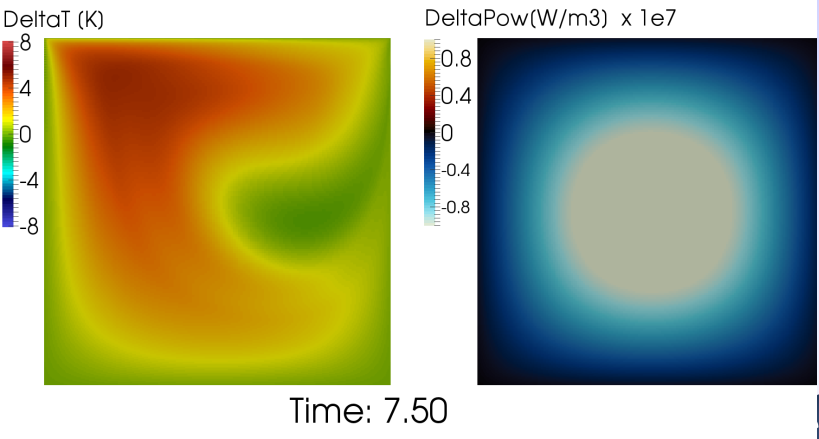

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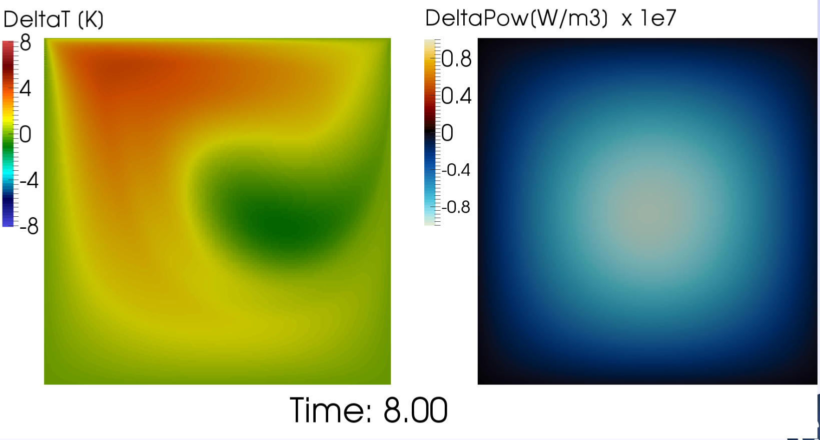
Still under definition

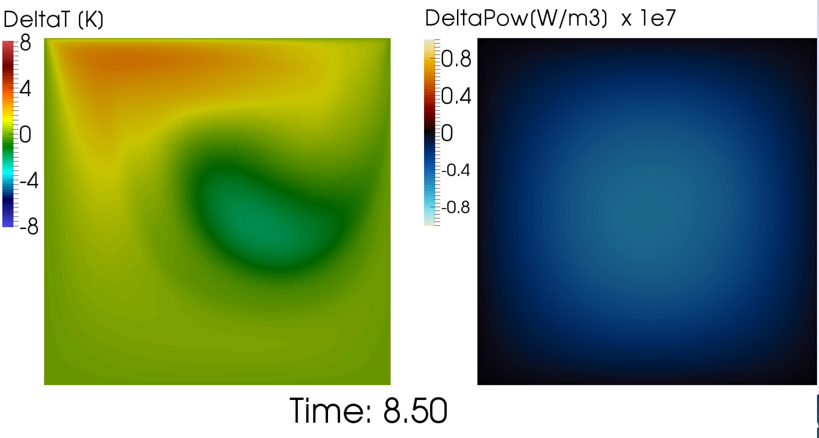
Verification of the system response to periodic perturbations.



Phase-2 Transient simulation

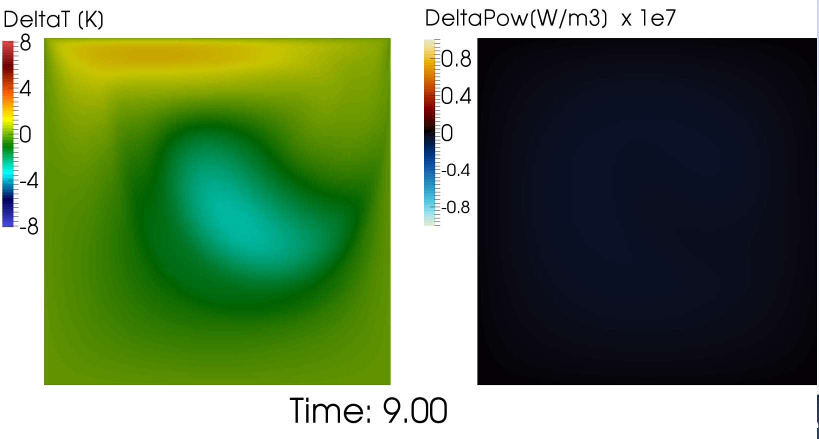
Still under definition

Verification of the system response to periodic perturbations.



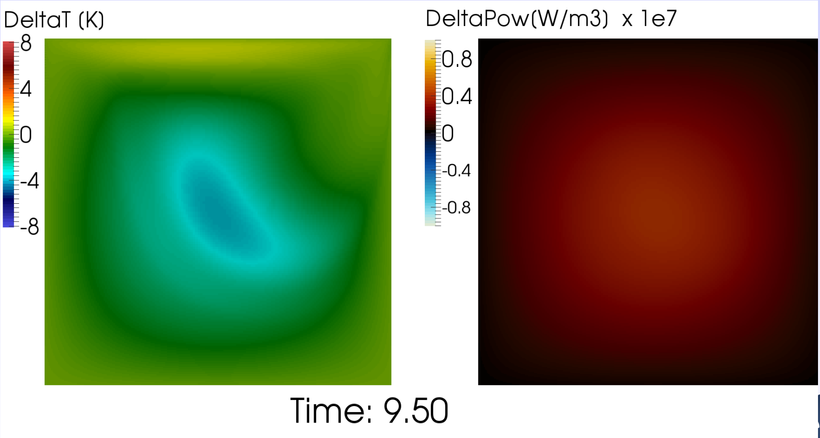
Phase-2 Transient simulation
Still under definition

Verification of the system response to periodic perturbations.



Phase-2 Transient simulation
Still under definition

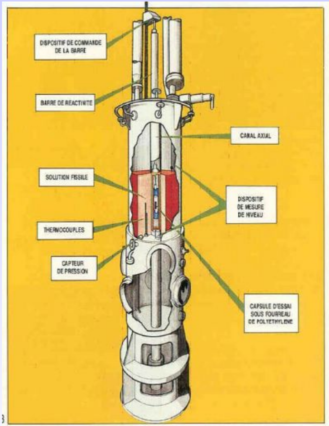
Verification of the system response to periodic perturbations.



Conclusions (Serpent–OpenFOAM)

- Serpent-OpenFOAM proved to be quite useful for criticality accident modelling
- We are considering other validations against experimental data (SILENE reactor)...
  any suggestions?

Silene reactor



Next steps (Serpent–OpenFOAM)

- Volume-integrate approach (analog/implicit) for delayed neutron precursors
- Extension of the approach to other physics and reactors
- Long term goal: uncertainty propagation with Generalized Perturbation theory in Serpent–OpenFOAM

Acknowledgement

- Mathieu Salanne (Université Pierre et Marie Curie)
  molecular dynamics calculation
  $LiF-ThF_4$ bulk modulus
- Serpent team

Conclusions (MSRs benchmark)

- A simplified benchmark is under definition
- Focused on multiphysics coupling
- Ideal for reduced order modelling tools
- Reference results from Serpent simulations
- Anyone interested?

THANK YOU FOR THE ATTENTION

QUESTIONS? SUGGESTIONS? NEW IDEAS?