Nuclear Reactors Group

An OpenFOAM Solver for Criticality Safety Assessment in Dynamic Compression Events

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INTRODUCTION:
A multiphysics simulation tool for nuclear criticality safety

The purpose of this work is to present a multiphysics simulation tool for numerical criticality safety evaluations.

Typical design-basis events that should be considered for impact on reactivity safety are [1]:

- Fires;
- Seismic events;
- Wind, tornado and hurricane events;
- External flood and precipitation events;
- Aircraft crash events;
- Strongly energetic events such as explosions.

In these conditions, materials exhibit a wide range of responses, requiring the development of different material response models for a correct simulation of all these accidents.

INTRODUCTION:
Features of the developed model

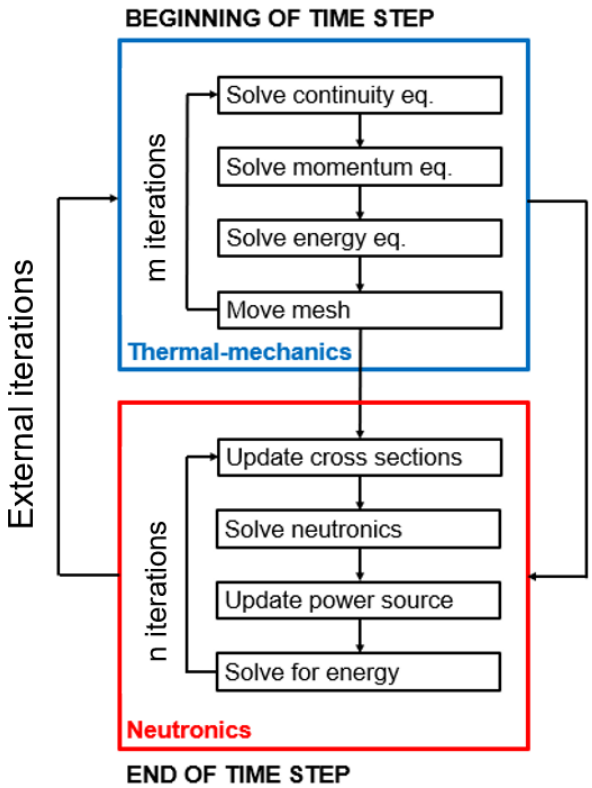
In this work, particular focus is devoted to criticality safety assessment in shockwave compression events (such as chemical explosions) of solid fissile materials.

- Accidental explosions in facilities;
- **Subcritical plutonium experiments.**

To this aim, a coupled neutronics and thermal-mechanics model has been developed in OpenFOAM (open-source CFD and multiphysics toolkit) [2].

This model includes:

- Multi-group SP3 neutron transport equations;
- A thermal-mechanics module, implementing a **dynamic mesh** and **different material response models**.
  - Linear thermo-elastic model for small deformations;
  - Hydrodynamic model for strong shockwave compression.



PART 1: MODELLING

Overview:

PART 1: MODELLING

PART 2: VERIFICATION

PART 3: COUPLED NEUTRONICS AND SHOCK PHYSICS

Presentation of the developed models:

- Thermal-mechanics module → Hydrodynamic model for shock physics problems;
- Neutronics module.

PART 1: MODELLING
The thermal-mechanics module

In the thermal-mechanics cycle, the mass, momentum and energy balance equations for a continuum medium are solved:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho(\boldsymbol{u} - \boldsymbol{w})] = 0$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot [\rho \boldsymbol{u}(\boldsymbol{u} - \boldsymbol{w})] = \nabla \cdot \underline{\underline{\boldsymbol{\tau}}} - \nabla p + \boldsymbol{b}$$

$$\frac{\partial (\rho h)}{\partial t} + \nabla \cdot [\rho h(\boldsymbol{u} - \boldsymbol{w})] = k\nabla^2 T + \frac{Dp}{Dt} + \dot{q}$$

The equations are written in an Arbitrary Lagrangian-Eulerian (ALE) form. The dynamic mesh can be moved with a velocity $\boldsymbol{w}$, arbitrarily chosen to preserve the mesh quality in case of strong mesh distortions.

If $\boldsymbol{w} = 0$ ⟶ purely Eulerian approach

If $\boldsymbol{w} = \boldsymbol{u}$ ⟶ purely Lagrangian approach

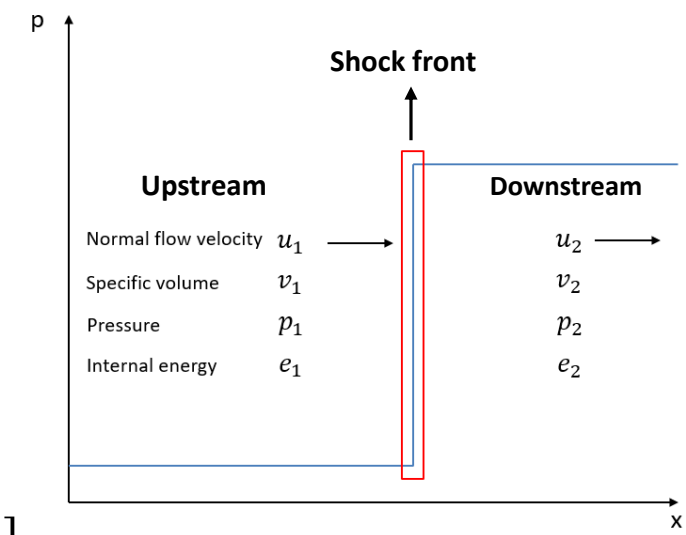
An equation of state is required to close the problem. To this aim, a hydrodynamic material response model is implemented.

PART 1: MODELLING

The hydrodynamic model - An introduction to shockwaves

A shockwave is a very thin region of rapid state variation across which there is a flow of matter [3].

For strong shockwaves (5-10 GPa or above), the shear stresses become negligible and the solid response to shock compression becomes similar to that of an inviscid, compressible fluid. This is known as *''hydrodynamic approximation''* [4].



SHOCK CONDITIONS:

Integral mass, momentum and energy balance over a thin volume enclosing the shock front [4].

$$\begin{cases} [\rho]u_s = [\rho u] \\ [\rho u]u_s = [\rho u^2 + p] \\ \left[\rho\left(e + \frac{1}{2}u^2\right)\right]u_s = \left[\rho\left(e + \frac{1}{2}u^2\right)u + pu\right] \end{cases}$$

[□]=difference between upstream and downstream conditions

PART 1: MODELLING

The hydrodynamic model - The Hugoniot curve

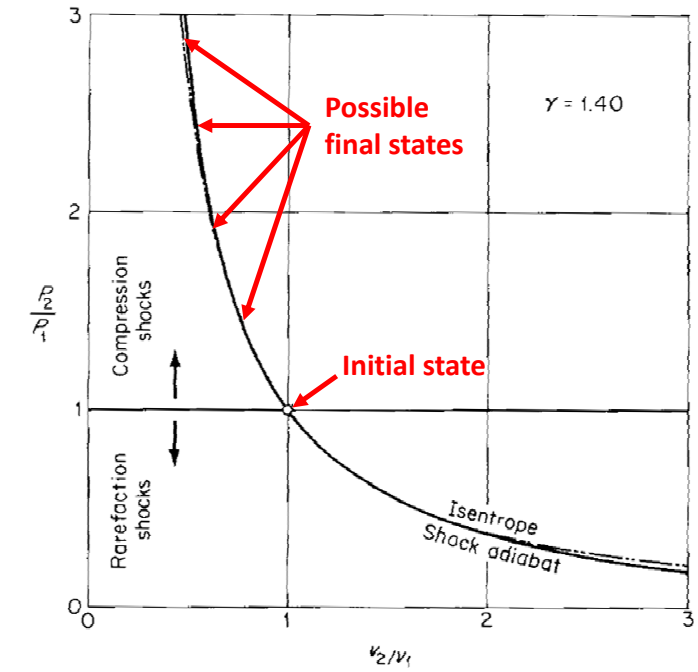
Combining the shock conditions, the **Hugoniot curve** (or shock adiabat) is obtained. It relates the initial and the possible final states of a material crossed by a shockwave [3,4].

The Hugoniot curve can be expressed in many equivalent ways. A commonly used form is the $U_S - u$ curve (Lagrangian shock velocity – solid particle velocity).

When the hydrodynamic approximation holds (p=5-10 GPa or higher), the $U_S - u$ curve assumes a linear form [4]:

$$U_S = C_B + S|\boldsymbol{u}|$$

where C_B and S are material constants.



Hugoniot curve for air, in the p-v plane [3]

PART 1: MODELLING

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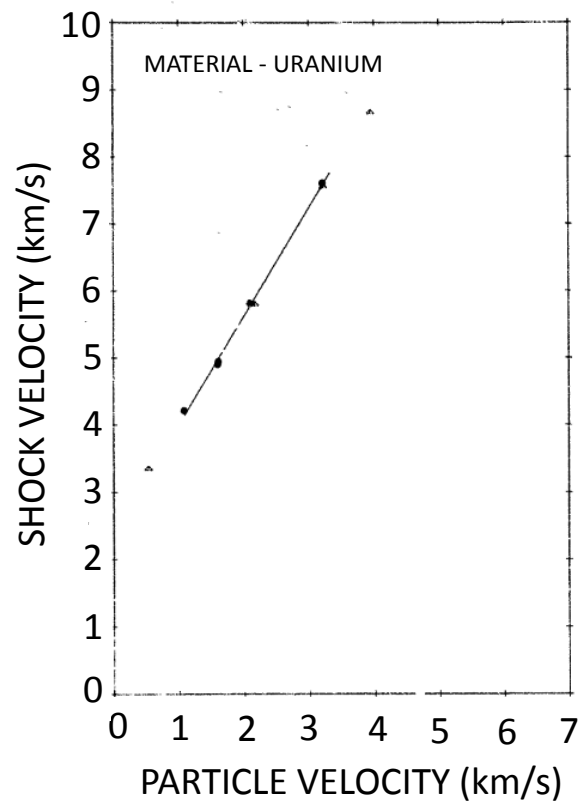

If the hydrodynamic approximation holds, the material behavior is described by the p-v-e Mie-Gruneisen equation of state [4]:

$$p - p_H = \frac{\gamma(v)}{v}(e - e_H)$$

where:

- p_H and e_H are the pressure and internal energy lying on a Hugoniot curve. If C_B and S are known, they can be obtained using the shock conditions.

- $\gamma(v)$ is the Gruneisen parameter. It can be calculated from S using the following relation [5]:

$$\gamma(v) = \left(\frac{v}{v_0} - 1\right)\left(S^2 - \frac{1}{3}S + \frac{5}{9}\right) + (2S - 1)$$

Thus, if C_B and S are known, the Mie-Gruneisen equation can be written, closing the thermo-mechanical problem.

PART 1: MODELLING
The neutronics module

The neutron flux is estimated using the multi-group SP3 formulation of the transport equation:

$$\frac{1}{v_i}\frac{\partial \Phi_{0,i}}{\partial t} = \nabla \cdot D_{0,i}\nabla\Phi_{0,i} - \Sigma_{r,i}\left(\Phi_{0,i} - 2\varphi_{2,i}\right) + S_{n,i}(1-\beta)\chi_{p,i} + S_d\chi_{d,i} + S_{s,i} + \frac{2}{v_i}\frac{\partial \varphi_{2,i}}{\partial t}$$

$$\frac{9}{5}\frac{1}{v_i}\frac{\partial \varphi_{2,i}}{\partial t} = \nabla \cdot D_{2,i}\nabla\varphi_{2,i} - \Sigma_{t2,i}\varphi_{2,i} + \frac{2}{5}\Sigma_{r,i}\left(\Phi_{0,i} - 2\varphi_{2,i}\right) - \frac{2}{5}S_{n,i}(1-\beta)\chi_{p,i} - \frac{2}{5}S_d\chi_{d,i} - \frac{2}{5}S_{s,i} + \frac{2}{5}\frac{1}{v_i}\frac{\partial \Phi_{0,i}}{\partial t}$$

where S_n, S_s and S_d are the fission neutron, scattering neutron and delayed neutron source terms, respectively.

Delayed neutron precursor balance equation: $\frac{\partial c_k}{\partial t} + \nabla \cdot [c_k(\boldsymbol{u} - \boldsymbol{w})] = \beta_k \sum_i \bar{\nu}\Sigma_{f,i}\varphi_i - \lambda_k c_k$

Cross section for the *i*-th reaction in the *j*-th energy group: $\Sigma_{i,j} = \left[\Sigma_{i,j}^{o} + A_{i,j} log\frac{T}{T_{ref}}\right]\frac{\rho}{\rho_{ref}}$

In addition: a power iteration routine is implemented for the estimation of the multiplication factor k.

PART 2: VERIFICATION

Overview:

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Verification of the implemented models:

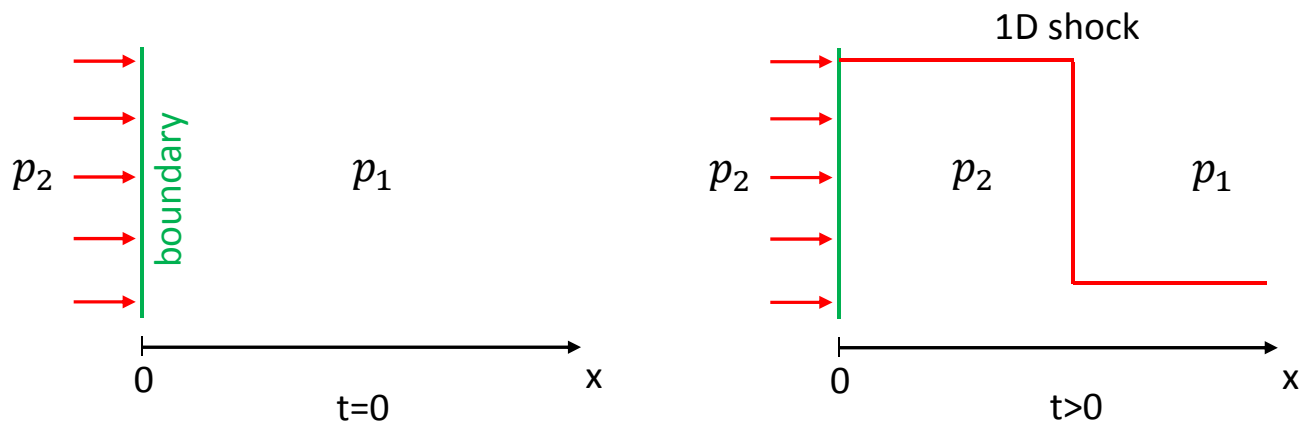
- **Thermal-mechanics:** correct prediction of the shock velocity and stability of the numerical solution;
- **Neutronics:** accuracy of the SP3 neutron transport model (especially in steep transients).

PART 2: VERIFICATION
Thermal-mechanics

In this part of the presentation, the correct implementation of the hydrodynamic model is verified.

To this aim, the propagation of 1D shocks in a semi-infinite medium is simulated, by applying different pressure steps at the domain boundary.

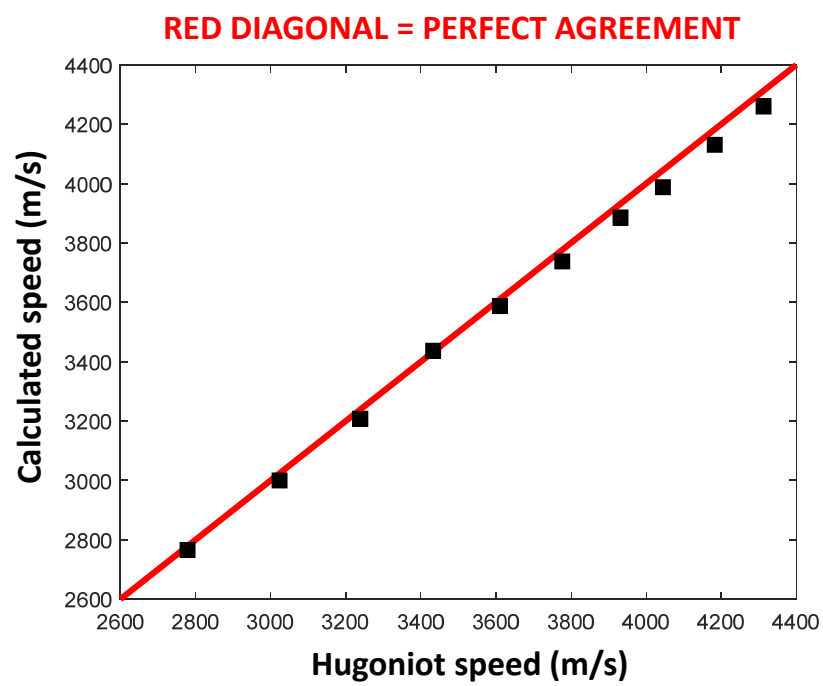
The velocity of the shock front is calculated by post-processing and is compared to the velocity predicted by the experimental $U_S - u$ Hugoniot curve: $U_S = C_B + S|\boldsymbol{u}|$



PART 2: VERIFICATION
Thermal-mechanics

Shock speed for different shock strengths in **metallic uranium**: $C_B = 2487\ m/s$ and $S = 1.539$ [6]

Pressure (GPa)	Calculated shock speed (m/s)	Shock speed from Hugoniot (m/s)	Relative error (%)
10	2766	2779	-0.47
20	3000	3024	-0.79
30	3208	3239	-0.96
40	3437	3433	0.12
50	3588	3611	-0.64
60	3738	3777	-1.03
70	3886	3932	-1.17
80	3988	4045	-1.41
90	4131	4183	-1.24
100	4260	4313	-1.23

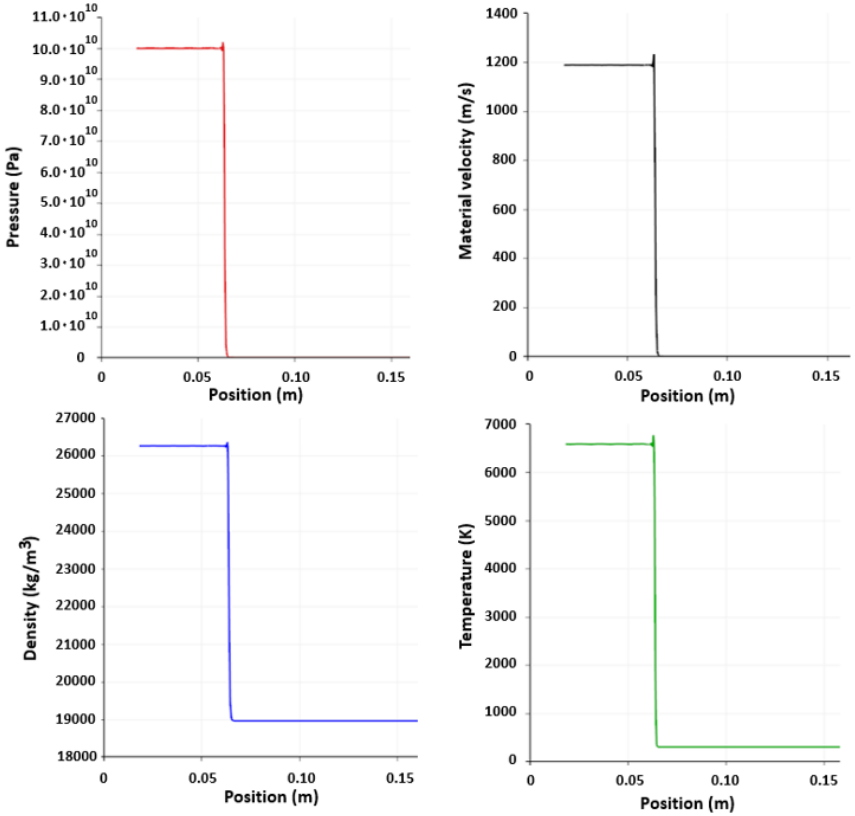


The error between the calculated velocity and the Hugoniot velocity is below 1.5%.

PART 2: VERIFICATION
Thermal-mechanics

- Shock conditions are satisfied for all the simulated shocks. Hence, there is coherence between the shock speed and the profiles of pressure, material velocity, density and temperature.

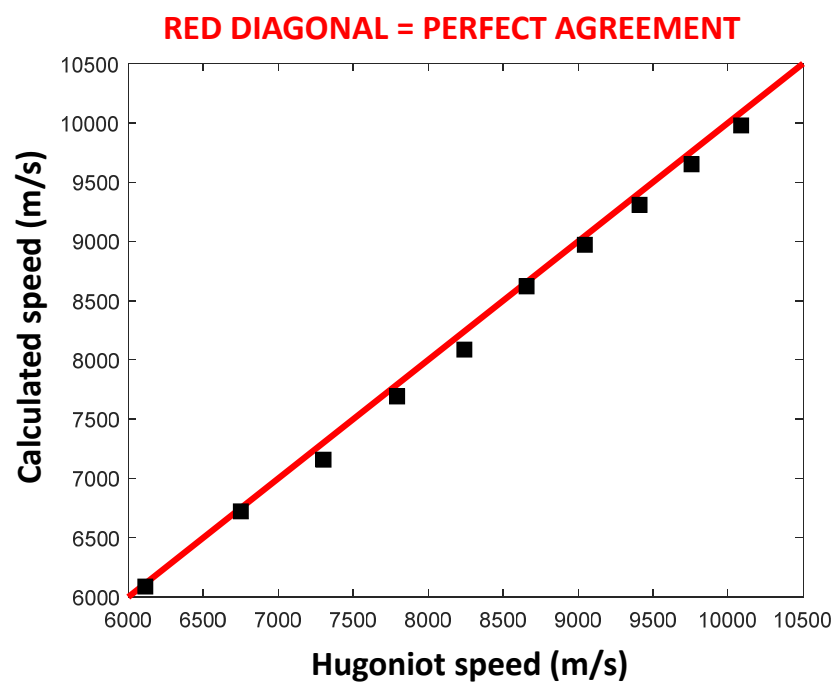
- On the right, the pressure, material velocity, density and temperature profiles are shown for a 100 GPa shockwave. Numerical oscillations at the shock front are very limited.



PART 2: VERIFICATION
Thermal-mechanics

Shock speed for different shock strengths in **aluminum**: $C_B = 5328\ m/s$ and $S = 1.338$ [4]

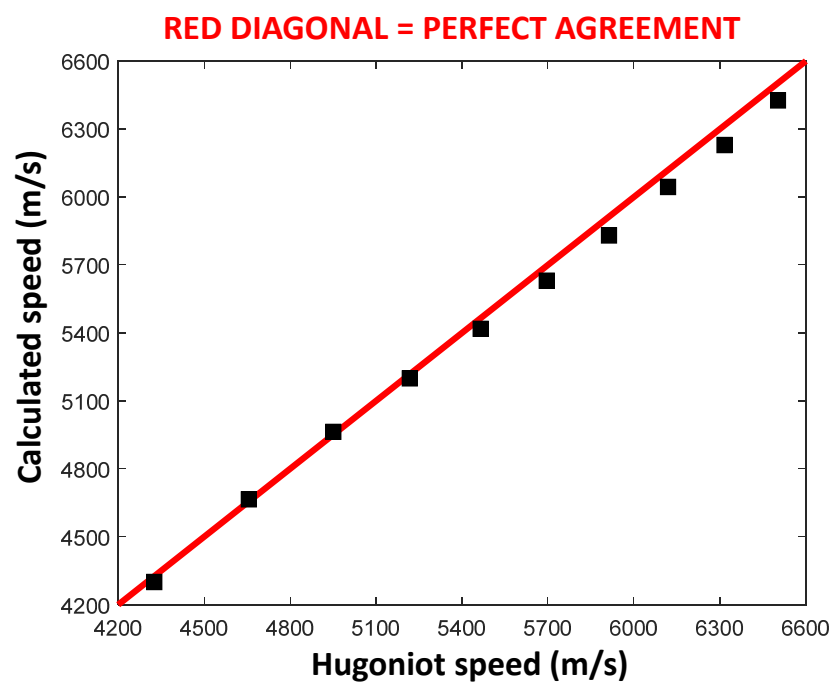
Pressure (GPa)	Calculated shock speed (m/s)	Shock speed from Hugoniot (m/s)	Relative error (%)
10	6088	6114	-0.43
20	6722	6751	-0.43
30	7158	7302	-1.97
40	7692	7793	-1.30
50	8087	8242	-1.88
60	8621	8657	-0.42
70	8971	9045	-0.82
80	9308	9410	-1.08
90	9651	9757	-1.09
100	9978	10088	-1.09



PART 2: VERIFICATION
Thermal-mechanics

Shock speed for different shock strengths in **copper**: $C_B = 3940\ m/s$ and $S = 1.489$ [4]

Pressure (GPa)	Calculated shock speed (m/s)	Shock speed from Hugoniot (m/s)	Relative error (%)
10	4300	4326	-0.60
20	4665	4656	0.19
30	4963	4951	0.24
40	5199	5218	-0.36
50	5418	5465	-0.86
60	5630	5696	-1.16
70	5830	5913	-1.40
80	6044	6119	-1.23
90	6229	6316	-1.38
100	6426	6503	-1.18



PART 2: VERIFICATION
Neutronics

In addition, a verification of the neutronics module is reported.

Study case: Lady Godiva super-prompt-critical burst, with initial 29.5 μs reactor period (about 21 pcm above prompt-critical).

Neutronics modelling: SP3 transport equation, using 1-group homogenized cross sections obtained by Monte Carlo simulation.

Thermal expansion: linear thermo-elastic model (*not shown for brevity*) with a spherical moving mesh.

The calculated results are in good agreement with both experimental data and analytical results [7]. In particular, the fission rate peak is well predicted by the proposed model.

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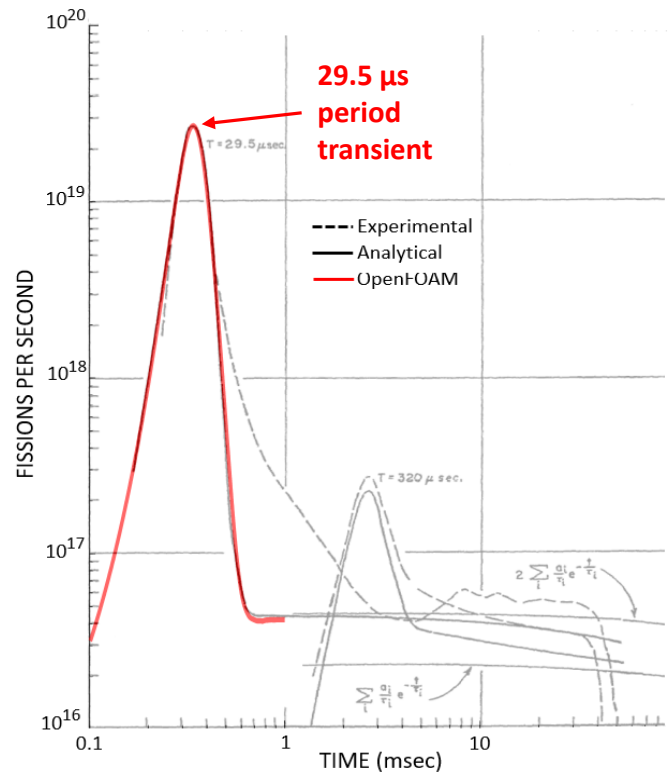

PART 3: COUPLED NEUTRONICS AND SHOCK PHYSICS

Overview:

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Content:

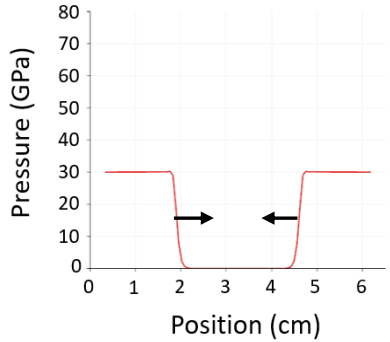
Two case studies are presented to demonstrate the coupling between neutronics and shock physics.

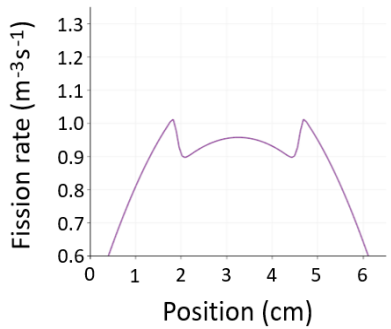
PART 3: COUPLED NEUTRONICS AND SHOCK PHYSICS

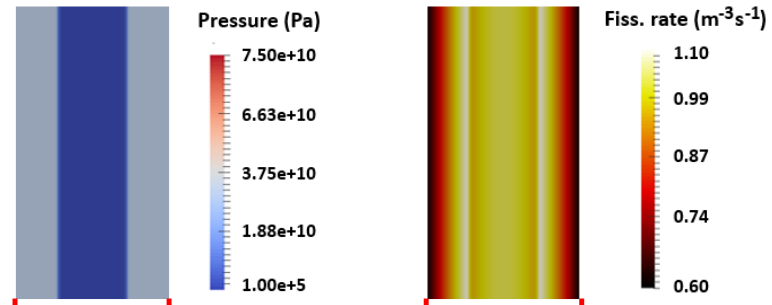
Case study: infinite slab

90% enriched uranium infinite slab: thickness = 6.5 cm, pressure applied at boundary= 30 GPa, initial multiplication factor $k = 0.98329$

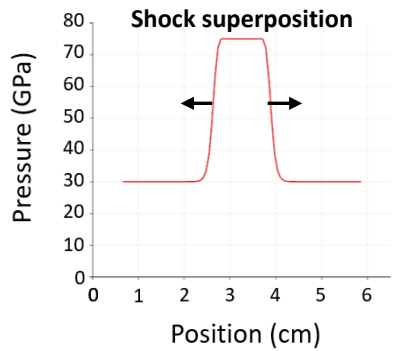
$t = 6\ \mu s$

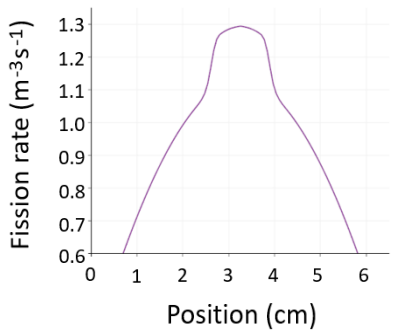


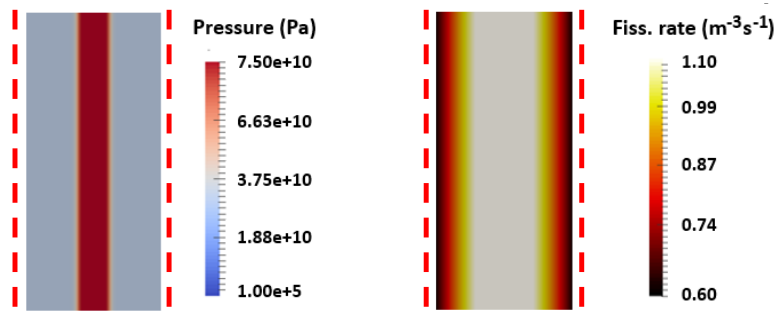




$t = 12\ \mu s$





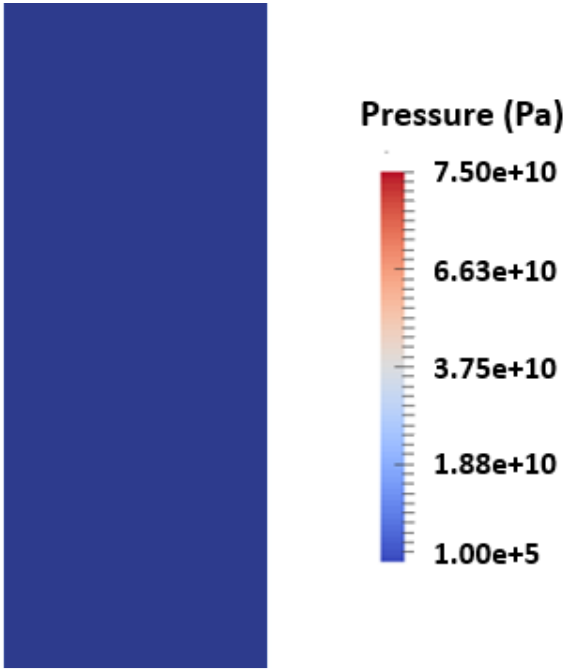


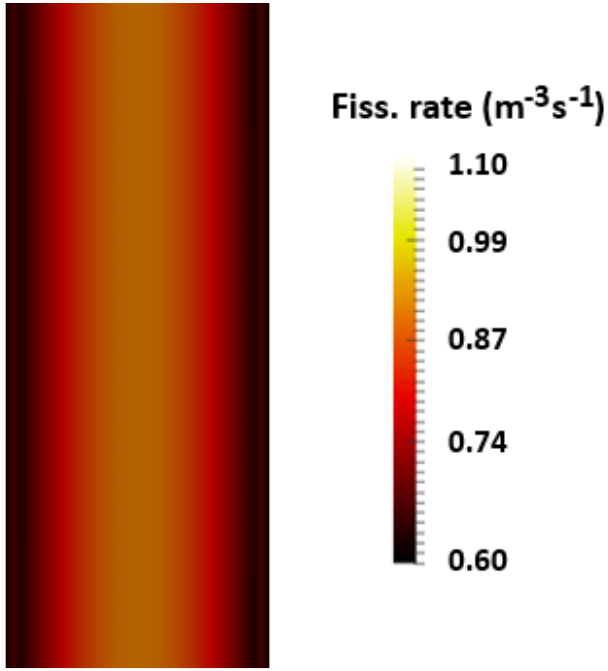
Due to the planar geometry, the surface area remains the same during compression → the system stays subcritical

(the multiplication factor does not change significantly during compression)

PART 3: COUPLED NEUTRONICS AND SHOCK PHYSICS

Case study: infinite slab





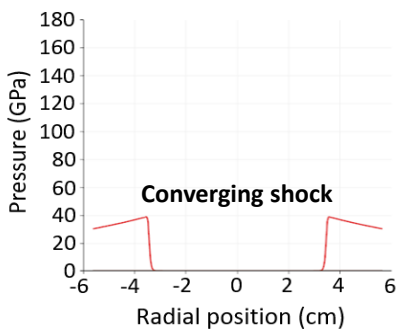
$t = 0 \div 19\ \mu s$

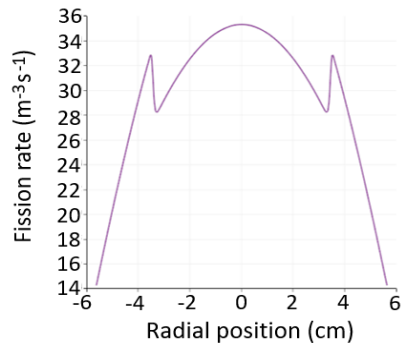
PART 3: COUPLED NEUTRONICS AND SHOCK PHYSICS

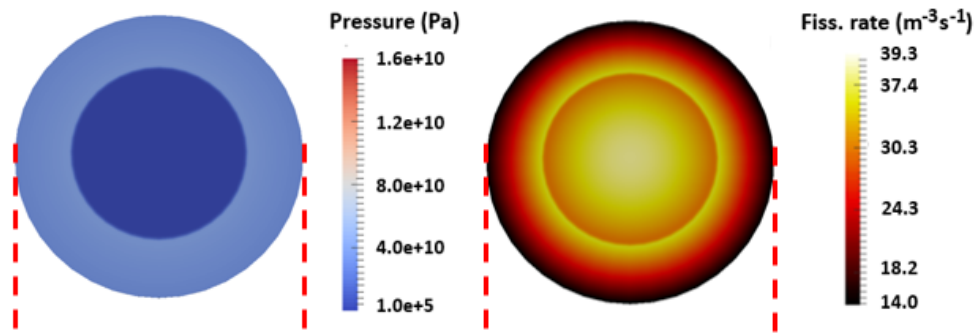
Case study: infinite cylinder

90% enriched uranium infinite cylinder: radius = 6 cm, pressure applied at boundary = 30 GPa, initial multiplication factor $k = 0.97911$

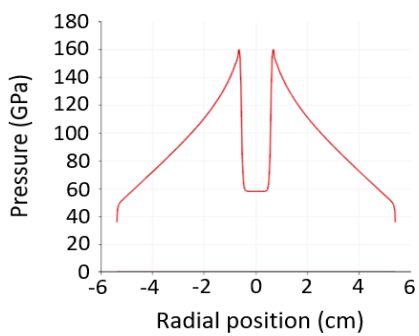
$t = 8\ \mu s$

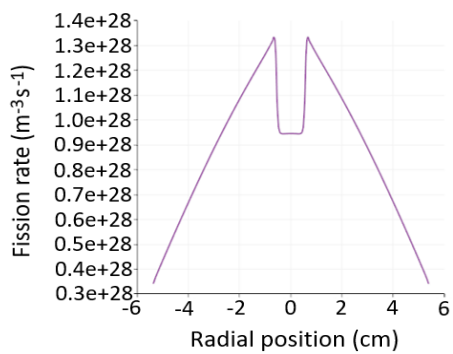


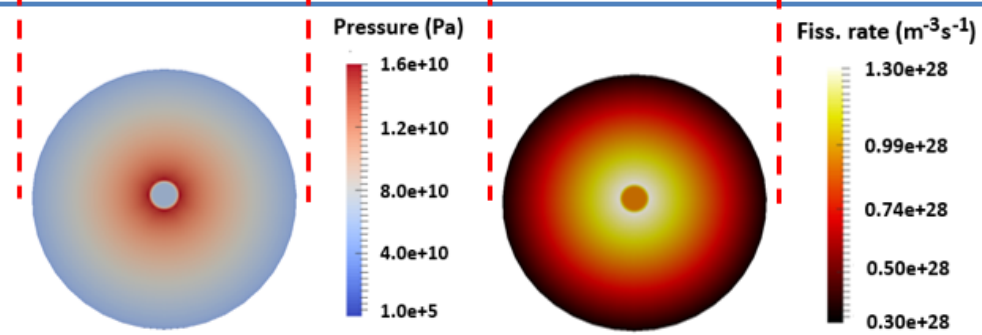




$t = 16\ \mu s$





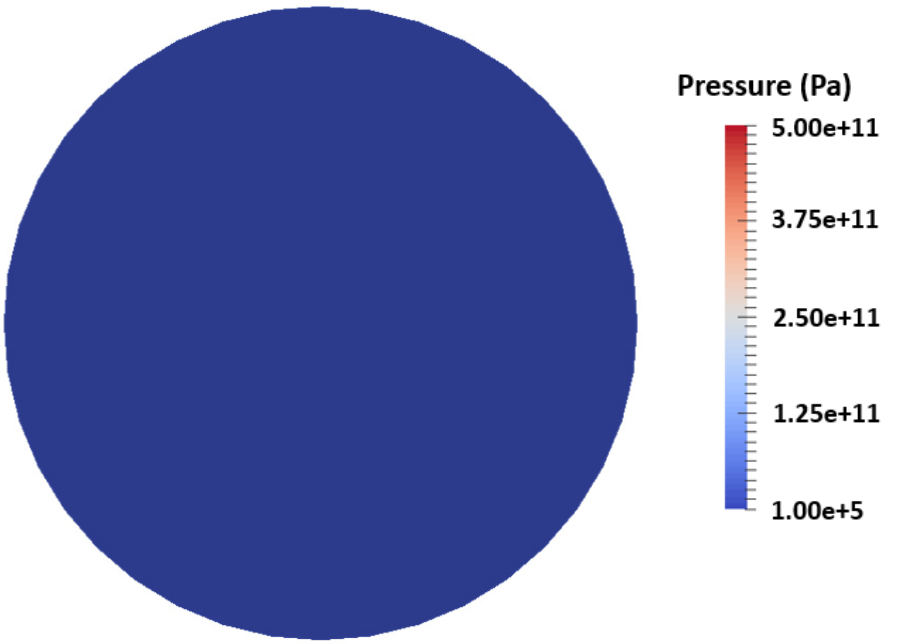


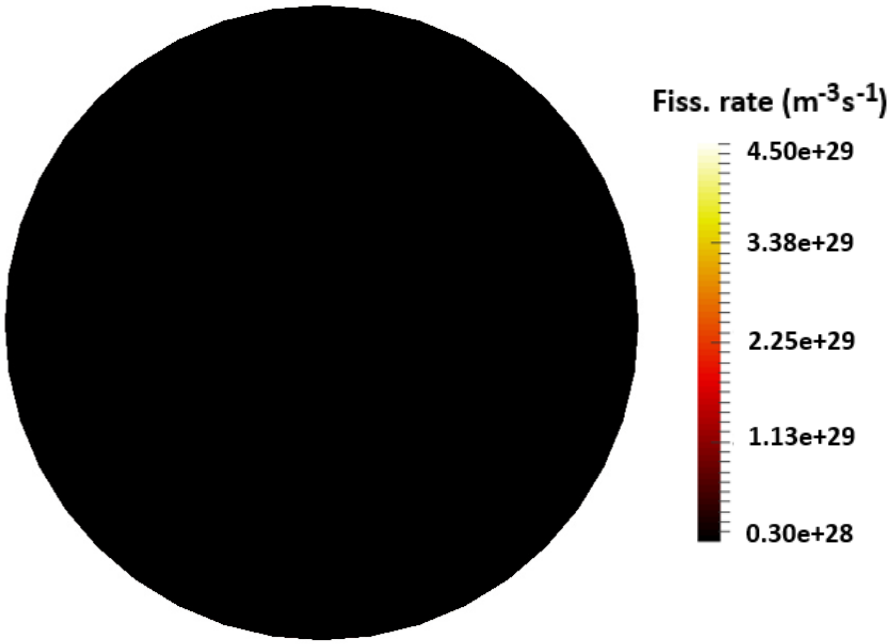
Due to the cylindrical geometry, the surface area decreases during compression→ the system becomes supercritical

(at $t = 16\ \mu s$ the multiplication factor is $k = 1.06520$)

PART 3: COUPLED NEUTRONICS AND SHOCK PHYSICS

Case study: infinite cylinder





$t = 0 \div 17\ \mu s$

CONCLUSIONS

In this work, a multiphysics model for nuclear criticality safety applications is implemented in OpenFOAM.

- Specific models were developed for neutronics and shock physics, as well as a coupling strategy between them;
- All the developed models have been validated/verified against experimental and analytical data;
- The coupling between neutronics and shock physics is presented for two simple case studies, highlighting the impact of geometry on reactivity.

Future efforts will be devoted to couple this model with other available modules, e.g.:

- Thermal-hydraulics models for liquid fuels and/or liquid moderators [8];
- Combustion models, chemical models, etc., to study other types of accidents [1,2].

BIBLIOGRAPHY

[1] DOE Technical Standard, Preparing critical safety evaluations at department of energy nonreactor facilities (2017).

[2] OpenFOAM documentation available at http://www.openfoam.org/docs/.

[3] Thompson, P.A., Compressible-fluid dynamics, McGraw Hill New York, 1972.

[4] Davison, L., Fundamentals of Shock Wave Propagation in Solids, Springer-Verlag Berlin Heidelberg, 2008.

[5] Grodzka, P.G., Gruneisen parameter study, Lockheed Missiles and Space Company (1967).

[6] Isbell, W.M., Shipman, F.H., Jones, A.H., Hugoniot equation of state measurements for eleven materials to five Megabars, Material & Structures Laboratory Manufactory Development, General Motor Company, 1971.

[7] Wimett, T.F., Time behavior of Godiva through prompt critical, Report LA-2029, Los Alamos National Laboratory, 1960.

[8] Cervi, E., Lorenzi, S., Cammi, A., Luzzi, L., Development of a multiphysics model for the study of fuel compressibility effects in the Molten Salt Fast Reactors.

THANK YOU FOR THE ATTENTION

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