Integration of OpenCalphad thermo-chemical solver in PLEIADES/ALCYONE fuel performance code

C. Introini, J. Sercombe, J.-C. Dumas, P. Goldbronn, V. Marelle

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Work done in collaboration with the PLEIADES team and the support of B. Sundman OpenCalphad

Summary

- **Industrial context**
  - Iodine-Stress Corrosion Cracking during Pellet-Cladding Interaction
  - Numerical simulation of the Iodine-Stress Corrosion phenomenon
- **Overview of the PLEIADES/ALCYONE 2.0 fuel performance code**
- **On the use of thermochemistry in PLEIADES/ALCYONE 2.0**
  - The ANGE thermo-chemical solver
  - The OECD-NEA TAF-ID project
  - The OpenCalphad thermo-chemical solver & its integration in ALCYONE
- **Numerical simulations of in-reactor power transients (1D,2D,3D)**
  - Validation of the integration of OpenCalphad in PLEIADES/ALCYONE 2.0
  - Performance of the ALCYONE/OpenCalphad solver
  - Capacity of the ALCYONE/OpenCalphad with TAF-ID database
- **Conclusions & Future work**

Industrial context

Iodine-Stress Corrosion Cracking during Pellet-Cladding Interaction (PCI/I-SCC)

- One of the physical phenomena of major interest for cladding design and long term operation of Pressurized Water Reactors (PWRs)
- Chemistry of volatile fission products (iodine, cesium, tellurium) is of some importance with regards to PCI/I-SCC failures

  B. Baurens, et al., (2014). 3D thermo-chemical–mechanical simulation of power ramps with ALCYONE fuel code, J. Nucl. Mater. 452, 578-594.
- A "realistic" modelling of this phenomenon needs a precise description of FPs thermochemistry and their migration/release in the fuel under irradiation

Numerical simulation of Iodine-Stress Corrosion Cracking phenomenon

- Requires to have accurate, efficient and robust thermo-mechanical and thermochemical solvers

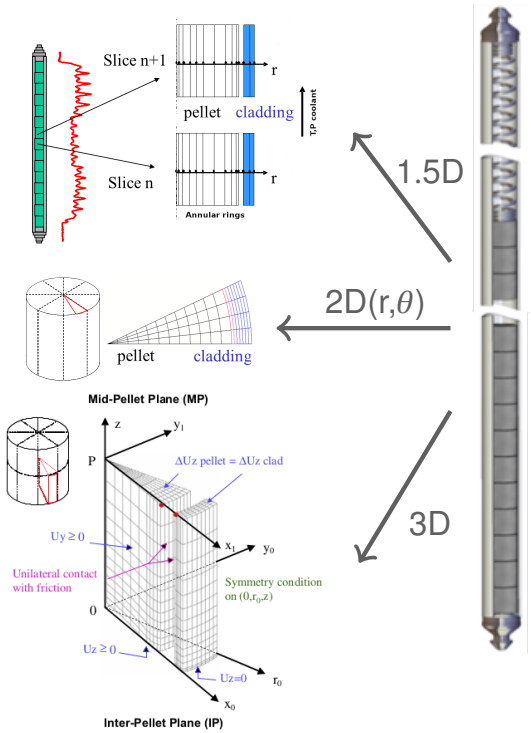
⇒ **Use of the validated PLEIADES/ALCYONE 2.0 fuel performance code**

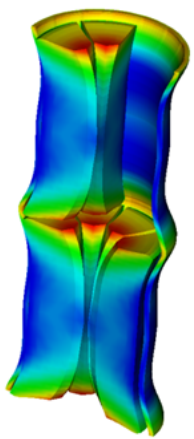
V. Marelle & al. , "New developments in ALCYONE 2.0 fuel performance code", Top Fuel, Boise ID. (2016)

Overview of PLEIADES/ALCYONE 2.0

A fuel performance code for Pressurized Water Reactors fuel rods

- Co-developed by CEA, EDF, Framatome
- Provides a multidimensional modeling for detailed analyses of PWR fuel elements behavior under irradiation
  - 1.5D scheme : rod discretized in axial segments
  - 2D(r,θ) scheme : mid-pellet plane of a pellet fragment
  - 3D scheme : one quarter of a pellet fragment
- Using the Finite Elements code CAST3M (CEA) to solve the thermo-mechanical problem
- Major phenomena considered in the 1D, 2D and 3D schemes





Fuel pellet

Power deposition, Heat conduction, Fission Gas Release, Diffusion of Fission Gas, Creep & cracking of the fuel pellet, Pellet densification, Pellet FG-induced swelling, Relocation of pellet fragments (1D), Properties depending on irradiation

Cladding material

Heat conduction, Irradiation creep, Thermal creep, Plasticity, Properties depending on irradiation

Pellet-Cladding interface

Heat convection, Contact with friction (3D), Pressure update (FG release, rodlet deformation)

From ANGE thermo-chemical solver to OpenCalphad thermo-chemical solver (1/3)

- ANGE (*Advanced Numeric Gibbs Energy minimizer*)
  - A modified version of the equilibrium code SOLGASMIX
    Eriksson, G. et al., (1975). Thermodynamic studies of high temperature equilibria. XII. SOLGASMIX, A computer program for calculation of equilibrium compositions in multiphase systems, Chemica Scripta 8, 100-103.
  - ✓ Integrated in PLEIADES/ALCYONE 1.4 as a first step towards I-SCC simulations
    B. Baurens, et al., (2014). 3D thermo-chemical–mechanical simulation of power ramps with ALCYONE fuel code, J. Nucl. Mater. 452, 578-594.
  - ✓ Coupled with Lassmann's oxygen distribution model OXIRED
    K. Lassmann, (1987), The OXIRED model for redistribution of oxygen in nonstoechiometric Uranium-Plutonium-Oxides, J. Nucl. Mater. 150, 10-16

    ⇒ a numerical approach based on Finite Volumes (1D) and Finite Elements (2D,3D) methods is developed to solve the oxygen thermodiffusion problem coupled with equilibrium calculations
    P. Konarski & al. , 3D Simulation of power ramps with ALCYONE including fuel thermochemistry and oxygen thermodiffusion, Top Fuel (2018)
  - Minimization of the Gibbs free energy of the system under species balance constraint at fixed T,P,V with associate species description for (U,Pu,PF)$O_{2\pm x}$ solid solution *T.M. Besmannn, (2012), Computational Thermodynamics : Application to Nuclear Materials, Compr. Nucl. Mater. 1 455–470* and with thermodynamic functions from the TBASE database *E.H.P. Cordfuncke, R.J.M. Konings, (1993), J. Phase Equilibria 14 : 457*
  - ⚠ Cannot be used to solve chemical systems based on the Compound Energy Formalism as proposed in the TAF-ID database (`https://www.oecd-nea.org/science/taf-id/`)
    C. Guéneau et al., (2011). Thermodynamic modelling of advanced oxide and carbide nuclear fuels : Description of the U–Pu–O–C systems, J. Nucl. Mater., 419, 145-167

On the use of thermochemistry in PLEIADES/ALCYONE

From ANGE thermo-chemical solver to OpenCalphad thermo-chemical solver (2/3)

- OECD-NEA TAF-ID project (*Thermodynamics of Advanced Fuels - International Database*)
  (*cf.* C. Guéneau NuMat PS03 for more details about TAF-ID)
  - Aims at making a comprehensive, internationally recognised and quality-assured database of phase diagrams and thermodynamic properties for nuclear advanced fuels (Generation II-III reactors and Generation IV systems)
  - Development of the TAF-ID database consistent with the CALPHAD *CAlculation of PHAse Diagrams* method
    ⇝ calculation of phase diagrams and thermodynamic properties (heat capacity, enthalpy,...) as mathematical of the Gibbs free energy over a large composition, temperature and pressure range

- TAF-ID database *vs.* TBASE database

TBASE database
- 24 elements of the periodic table
- Associate species description for the oxide (*i.e.* sub-lattice description, cristalline structure)
- ~ 100 stoichiometric compounds
- No description of the liquid phases mixture

TAF-ID database
- 41 elements of the periodic table
- Compound Energy Formalism for the oxide (*i.e.* sub-lattice description, cristalline structure)
- ~ 150 stoichiometric phases
- Description of the liquid phases mixture (interesting for high temperatures)

✓ TAF-ID database provides a more complex description of the irradiated fuel (more complicated models, possible phases greater in number than in the TBASE database) and enables to describe the formation of liquid phases

⇒ **An upgrade of the thermo-chemical modeling in the PLEIADES 2.0 platform is necessary to use the TAF-ID database**

On the use of thermochemistry in PLEIADES/ALCYONE

OpenCalphad a free, efficient and robust thermo-chemical solver

- Developed under GNU GPL license by B. Sundman http://www.opencalphad.org/
  B. Sundman, et al, (2015), The implementation of an algorithm to calculate thermodynamic equilibria for multi-component systems with non-ideal phases in a free software, J. Nucl. Mater. 150, 10-16

✓ OpenCalphad 5.0 integrated in PLEIADES/ALCYONE 2.0 under CeCILL-C license
(*cf.* **J-C. Dumas NuMat O3.02 for details about the use of OpenCalphad in PLEIADES/GERMINAL (SFR))**

- A first minimizer : iterative algorithm similar to the one implemented in ANGE
  - Based on the Hillert's algorithm proposed in 1981
  - Strongly dependent on the initial set of phases and their constitutions
  - Does not ensure that the calculated equilibrium is a global minimum ⇝ "global minimisation"

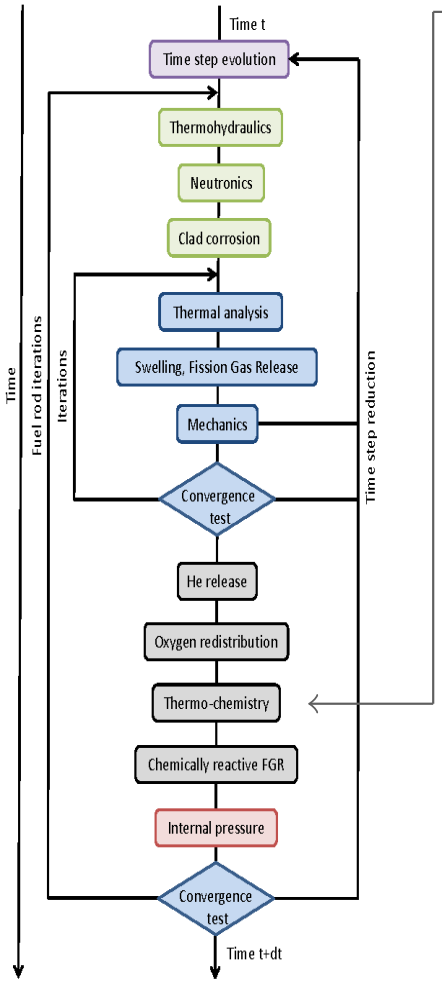
- The "global minimisation" (not available in ANGE)
  - An initial calculation of the Gibbs energy of all phases (assumed stoichiometric) is done over a grid of compositions to find initial values for the iterative algorithm ⇝ ensures that the calculated equilibrium is a global minimum
  - Minimizer that automatically detects miscibility gaps
  - ⚠ **More accurate but more expensive in terms of CPU time**

✓ Can use the TBASE and OECD-NEA TAF-ID databases

✓ Many functionalities provided by the stand-alone version of OpenCalphad (*e.g.* iterative calculations, phase diagrams, calculation of thermodynamic properties) with most of them available when OC is interfaced with a fuel performance code

Integration of OpenCalphad in PLEIADES/ALCYONE 2.0

Integration of the OpenCalphad solver in the ALCYONE coupling scheme



- OpenCalphad solver called after multiphysics convergence loop
- At each time-step, OpenCalphad calculations are done at each node

Temperature [K]
Pressure [Pa]
Composition [mol/mol]

→ OpenCalphad solver →

Gas, Condensed Species
Solid Solution [mol/mol]
O/M ratio, chemical potentials

✓ OpenCalphad solver isofunctional with ANGE solver (non-regression goal)

✓ OpenCalphad solver coupled with Lassmann's oxygen distribution model OXIRED

\+ Specific management of residual species to avoid convergence difficulties

\+ Dynamic post-processing based on SQLite3 databases ⇝ useful to deal with different multi-component systems with different databases (TBASE,TAF-ID)

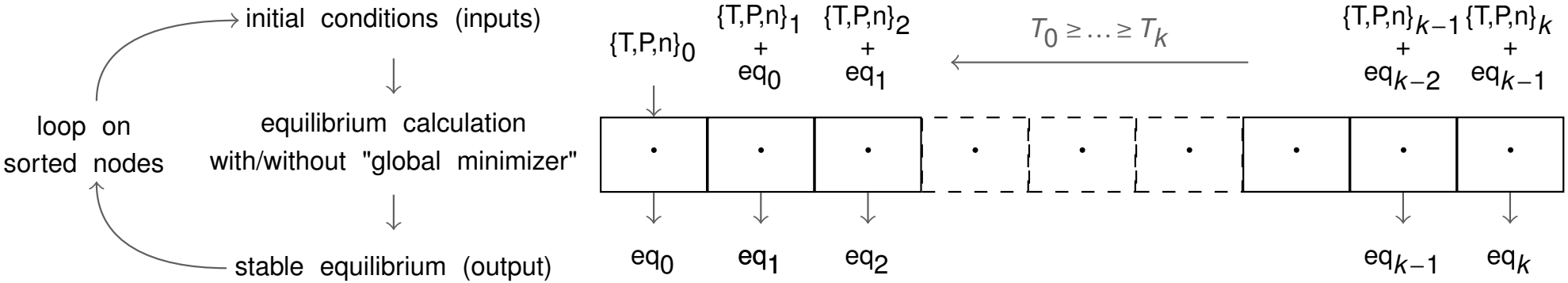
\+ **Parallelization of equilibrium calculations** : first implementation based on a multi-processing approach⇝optimization & assessment of performances in progress

\+ **Implementation of numerical strategies to reduce the CPU time**

Numerical strategies implemented to reduce the CPU time

Spatial strategy

- At each time-step, the mesh nodes are sorted in function of temperature (predominant variable of interest)
  - The mesh nodes can be sorted in descending (default, natural order in 1D) or ascending order of temperature
- Each calculated equilibrium at a node is used as the start value for the calculation done on the thermally closest neighboring node



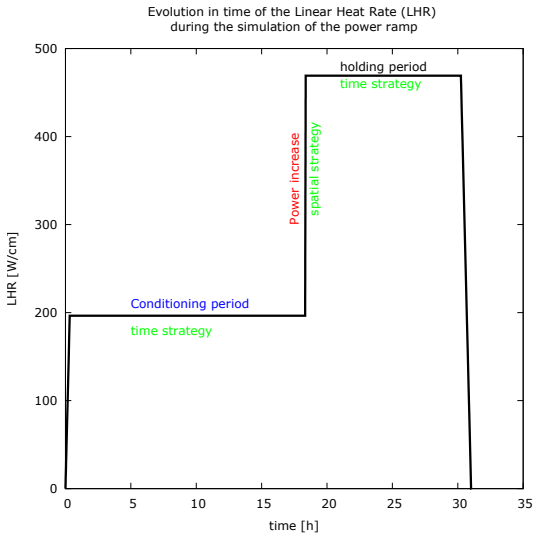
- Contrary to the other nodes, the hottest (*resp.* the coldest) is always calculated with the "global minimization" and an automatic recalculation with the other minimizer is done in case of non convergence of the calculations
- A periodic use of the global minimizer remains possible depending on the complexity of the multi-component systems considered

⇒**Fast convergence and, consequently, reduction in CPU time are expected**

Numerical strategies implemented to reduce the CPU time

Time strategy

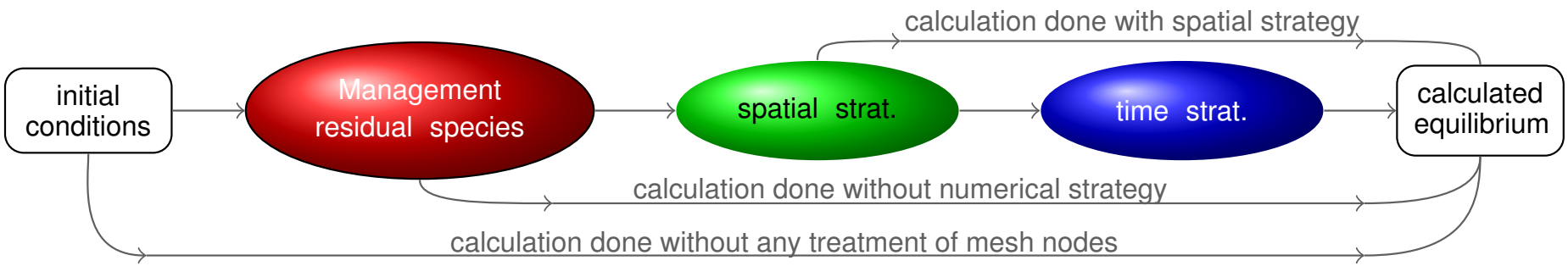
- For each mesh node, the equilibrium calculated at the previous time-step is used as start value at the current time-step
  - Strategy automatically activated during the conditioning and the holding periods based on a linear power criterion
  - Spatial strategy is always used during the power increase period
  - Strategy using the backup/recovery functionalities proposed by the OpenCalphad code (~ file read/write function).



⇒**What is the impact of "read/write file" function on CPU time ?**

Management of the negligible species (not detailed)

- At each time-step, a table of correspondence between a set of nodes and a given set of elements is made by eliminating elements in negligible quantities ($\epsilon \leq 10^{-9}$ mol/mol)



Numerical simulations

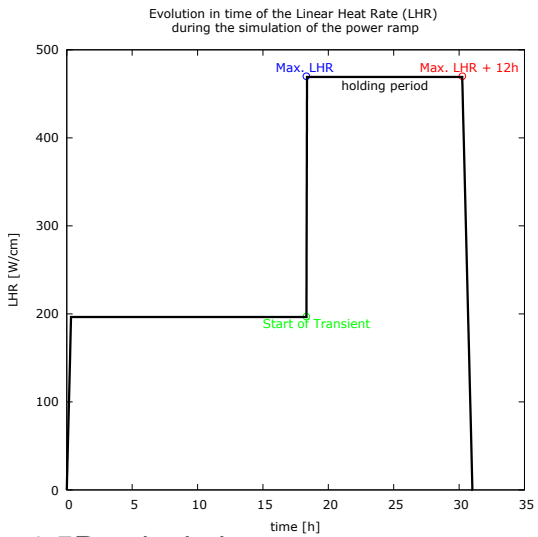
Multi-dimensional simulations performed with the TBASE & TAF-ID databases

- ALCYONE/OpenCalphad *vs.* ALCYONE/ANGE with an equivalent TBASE database
  - A set of 1.5D, 2D(r,θ) and 3D calculations are done by considering different combinations of numerical strategies
  - $\Rightarrow$ to verify the implementation of the OC thermo-chemical solver against ANGE solver
  - $\Rightarrow$ to assess the performances of ALCYONE/OpenCalphad versus those of ALCYONE/ANGE
- ALCYONE/OpenCalphad with TBASE *vs.* ALCYONE/OpenCalphad with TAF-ID
  - A set of 1.5D, 2D(r,θ) and 3D calculations are done with nodes treated in descending order of temperature
  - $\Rightarrow$ to assess and compare the performances of ALCYONE/OpenCalphad with TAF-ID to those obtained with TBASE
  - $\Rightarrow$ to assess the capacity of ALCYONE/OpenCalphad to simulate multi-component systems with TAF-ID
- ALCYONE/OpenCalphad with TAF-ID
  - 2D(r,θ) and 3D calculations are performed in parallel with default spatial strategy
  - $\Rightarrow$ to illustrate the gain in terms of CPU time when equilibrium calculations are parallelized
  - A 3.5D calculation is performed with nodes treated in descending order of temperature
  - $\Rightarrow$ to show the capacity of PLEIADES/ALCYONE 2.0 to simulate in-reactor power transients involving complex multi-component systems with TAF-ID database

Numerical simulations

Characteristics of the simulated long hold time power ramp (release of FPs greater than 10%)

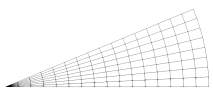
Fuel		Cladding	
Cr Doped UO_2		M5®	
Conditioning period		**Holding period**	
P(W/cm)	Time (h)	P (W/cm)	Time (h)
196	18.68	468	12



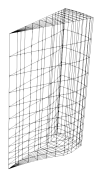
1.5D calculations
41 nodes per slice
10 slices computed on 10 CPUs
(MPI functionalities of PLEIADES 2.0)

Representative Elements	Creation [mol/molUO_2/at%]	Family
Xe+Kr	3.058e-3	Inert fission gas
Cs(+Rb)	1.699e-3	
I(+Br)	1.308e-4	Volatile FPs
Te(+Se)	3.022e-4	
Ba(+Sr)	1.381e-3	stable oxides
Zr(+Nb)	2.622e-3	
Mo	2.334e-3	
Ru+Tc+Rh	2.440e-3	Metallic FPs
Pd(+*Ag+In+Sn+...*)	1.020e-3	
Ce	1.239e-3	FPs in solid
Eu(+Sm)	3.808e-4	
La(+Y)	9.310e-4	
Gd(+Nd+Pm)	1.918e-3	solution in UO_2
Cr	5.062e-3	dopant
O	2.007	

2D(r,θ) calculations
1 pellet fragment (MP plane)
145 nodes



3D calculations
1/32 fuel pellet
1417 nodes



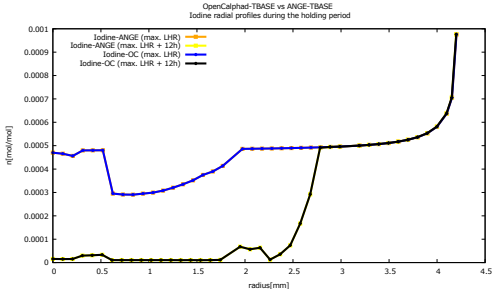
3.5D calculation
26 slices over 26 CPUs
1/32 fuel pellet per slice
1417 nodes per slice

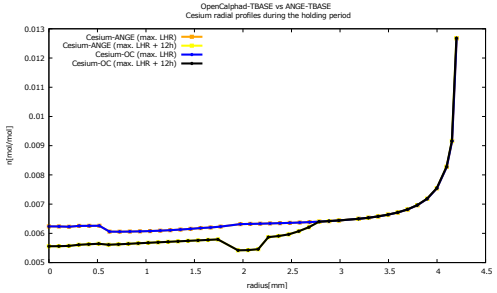
All calculations have been performed on the computing server : 44 cores, 352Go, Intel Xeon E5 2699Av42.40GHz

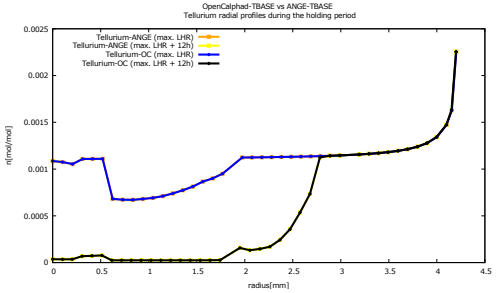
ALCYONE/OpenCalphad *vs.* ALCYONE/ANGE (TBASE)

ALCYONE/OpenCalphad *vs.* ALCYONE/ANGE : non-regression of the integration (1/2)

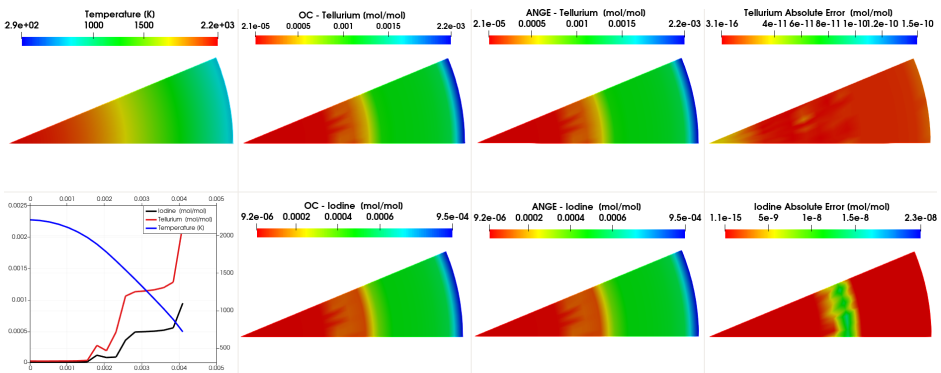
Radial profiles of Iodine (left), Cesium (center) and Tellurium (right) at the end of the holding period (1.5D)

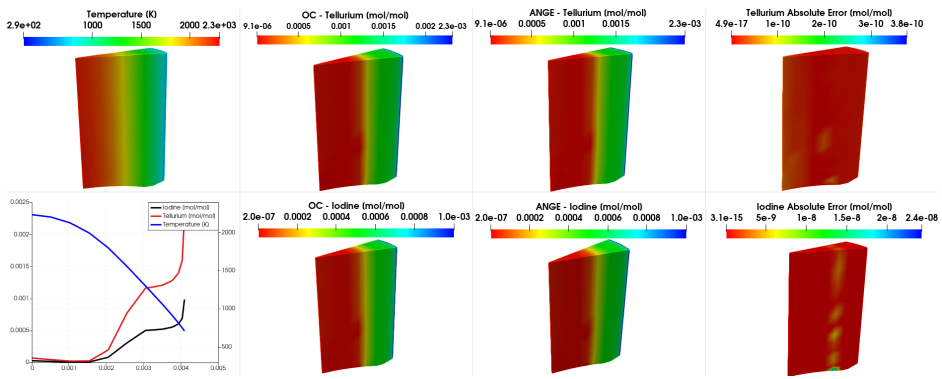






Temperature & Volatile FPs (Tellurium (top), Iodine (bottom)) at the end of the holding period [2D(r,θ) (left), 3D (right)]



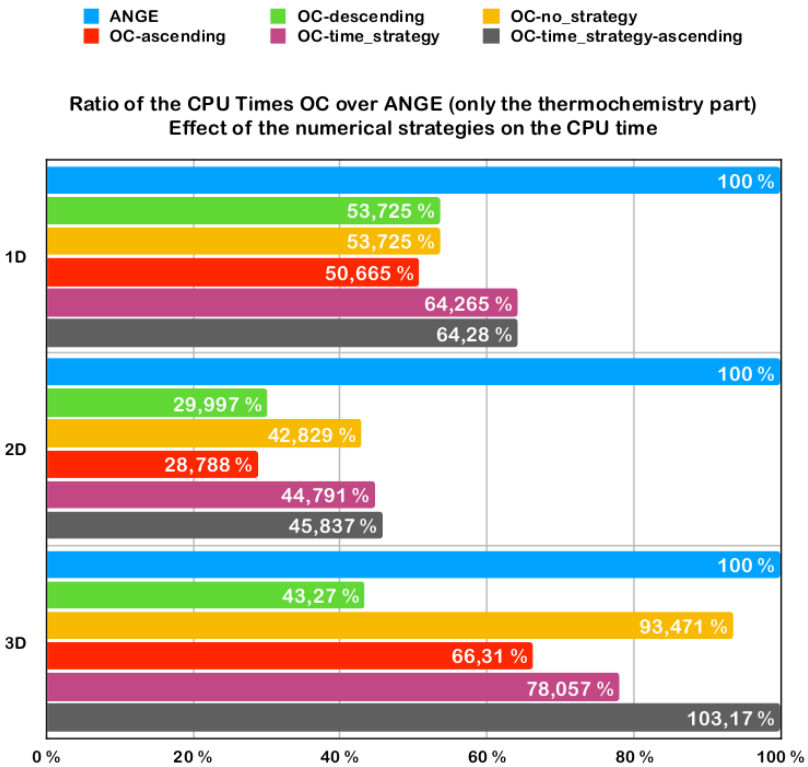


- **High release of volatile FPs at the pellet center during the holding period** ($T \geq 2000\,K$)
- **Similar quantities of volatile FPs given by OpenCalphad & ANGE (1.5D,2D(r,θ),3D)**

⇒**Validation of ALCYONE/OpenCalphad implementation *vs.* ALCYONE/ANGE**

ALCYONE/OpenCalphad *vs.* ALCYONE/ANGE (TBASE)

ALCYONE/OpenCalphad *vs.* ALCYONE/ANGE : performance (2/2)



ALCYONE/OpenCalphad faster than ALCYONE/ANGE

- Time strategy less efficient than spatial strategy

⇒ **"backup/recovery" functionalities too expensive**

- Spatial strategies more efficient than time strategy

⇒ **The most efficient strategy in 1.5D & 2D(r,θ) consists in treating mesh nodes in ascending order of temperature**

⇒ **The most efficient strategy in 3D consists in treating mesh nodes in descending order of temperature**

⇒ **The more nodes there are, the more efficient the strategy is**

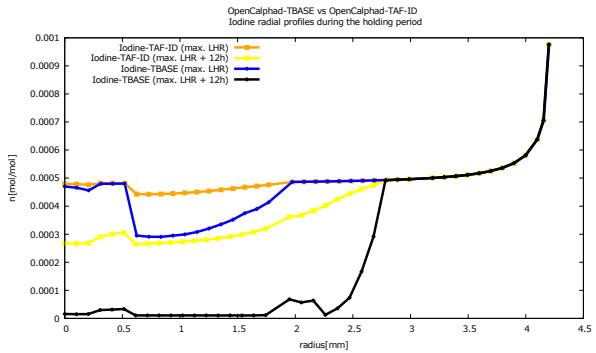
In these tests, ALCYONE/OC is 2-3.5 times faster than ALCYONE/ANGE

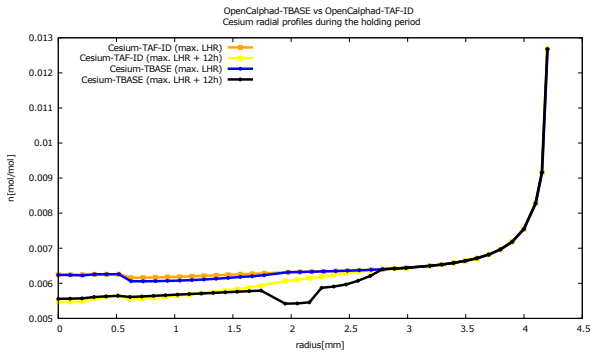
- ✓ Higher performance are obtained during simulations with moderate FPs release
- ✓ ALCYONE/OpenCalphad remains faster than ALCYONE/ANGE with the oxygen distribution model OXIRED (not presented here)

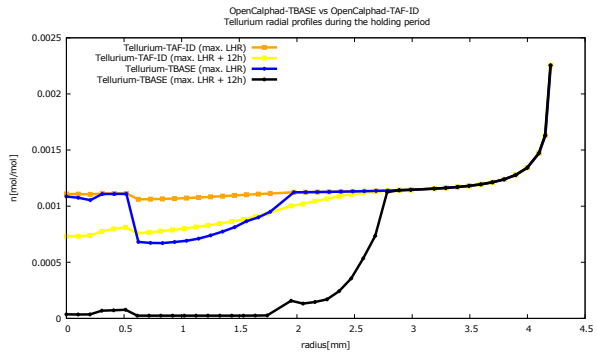
ALCYONE/OpenCalphad : TBASE *vs.* TAF-ID

ALCYONE/OpenCalphad (TBASE) *vs.* ALCYONE/OpenCalphad (TAF-ID) : qualitative comparisons

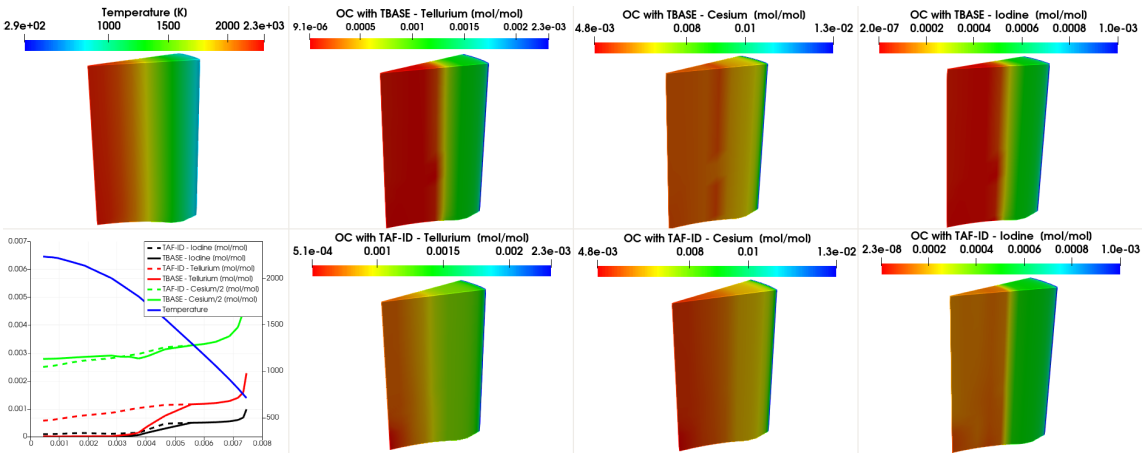
Radial profiles of Iodine (left), Cesium (center) and Tellurium (right) at the end of the holding period (1.5D)





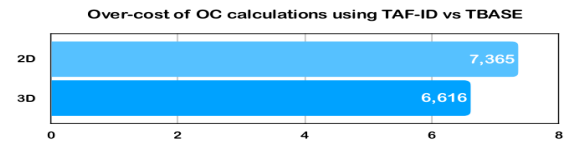


Temperature, Tellurium, Cesium, Iodine at the end of the holding period

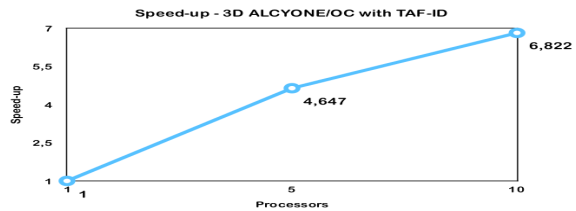


Volatile FPs release consistent with temperature profile
Lower release of FPs (I,Cs,Te) with TAF-ID (results analysis in progress)

Some performance results (2D(r,θ), 3D)



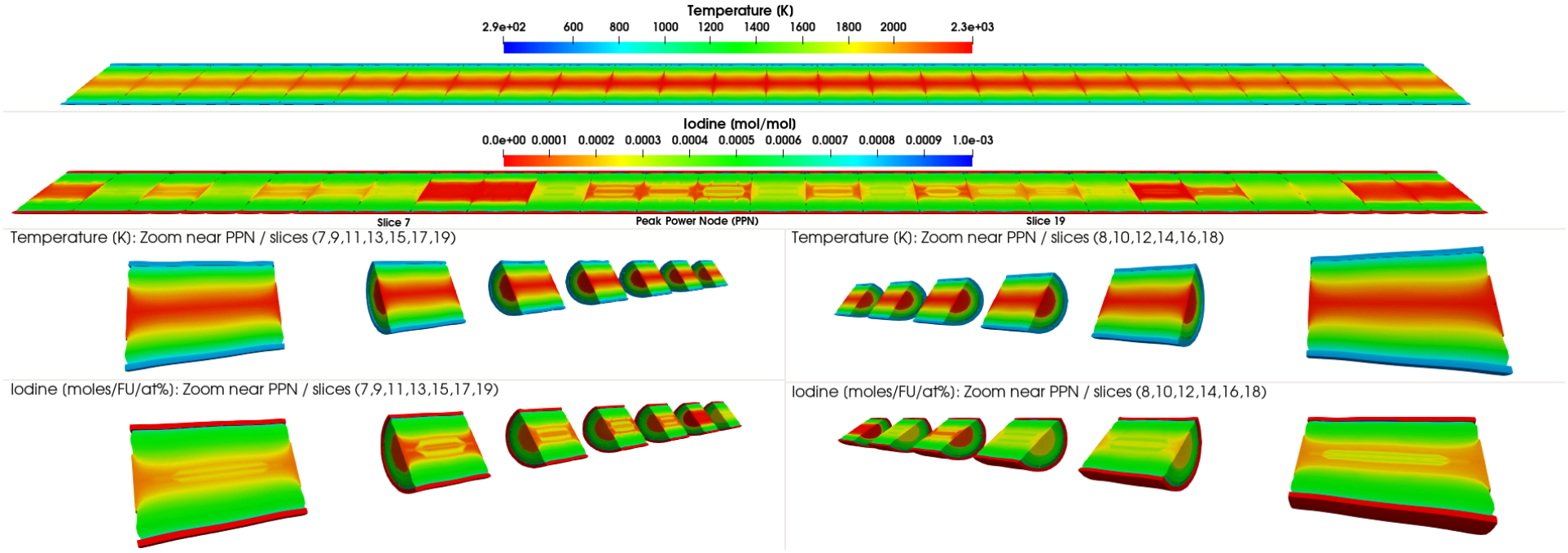
Expected increase of the CPU time
because of more complicated models



First promising performance results
Optimization work is in progress

ALCYONE/OpenCalphad with the TAF-ID database

First promising results obtained on a 3.5D simulation of a long power ramp with TAF-ID



The results illustrate the capacity and robustness of ALCYONE/OpenCalphad to simulate complex in-reactor power ramp using thermodynamics data coming from TAF-ID database

- 26 fuel pellets/26 CPUs : 1 slice per pellet, 1 slice per CPU, 1417 nodes per pellet
  - ⇒ **CPU time of the 3.5D simulation ~ CPU time of 3D pellet fragment**
  - ⇒ **total CPU time ~20h : thermomechanics (~ 8h) + thermochemistry (~12h)**

Conclusions & Future work

Integration of OpenCalphad thermo-chemical solver in PLEIADES/ALCYONE 2.0

- **ALCYONE/OpenCalphad is much faster than ALCYONE/ANGE with TBASE database**
  - ✓ 2-3.5 times faster on a simulated power ramp
  - ✓ Performance clearly enhanced when the mesh nodes are treated in order of descending temperature
  - ✓ Higher performances are seen on simulations with moderate fission gas release
- **Capacity and robustness of ALCYONE/OpenCalphad to simulate multi-dimensional power transients with TAF-ID database**
  - ✓ OpenCalphad/TAF-ID : an advanced thermo-chemical model in PLEIADES/ALCYONE 2.0
  - ✓ Expected increase of the CPU time because of more complicated models
  - ✓ Parallelization of equilibrium calculations reduces the increase of CPU time (optimization in progress)

Towards a more important use of TAF-ID with new physical couplings

- **First promising results with TAF-ID but the validation of this database is needed for in-reactor power transients calculations**
- **Future developments will be dedicated to the coupling of thermal diffusion, oxygen redistribution and local equilibrium calculations with fuel melting based on phase-field approach**

M.J. Welland, et al., (2011), Review of high temperature thermochemical properties and application in phase-field modelling of incipient melting in defective fuel, J. Nucl. Mater. 412, 342-349

Commissariat à l'énergie atomique et aux énergies alternatives
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