INSPYRE

Investigations Supporting MOX Fuel Licensing in ESNII Prototype Reactors

Using a basic research approach to improve fuel performance codes

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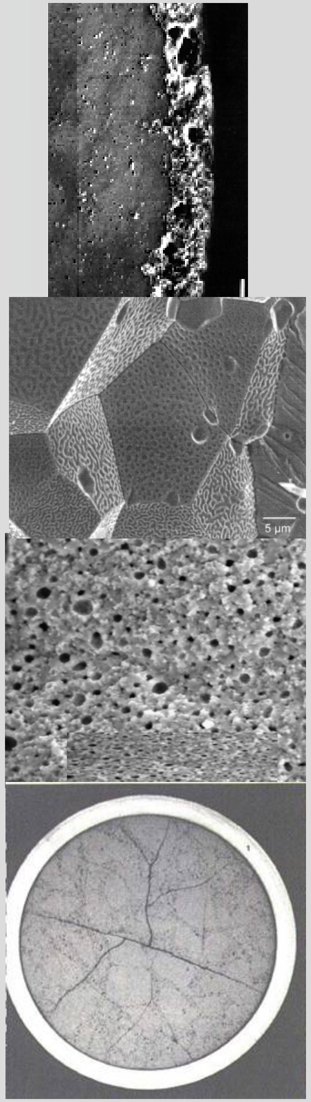
Objective and Approach

Nuclear fuels

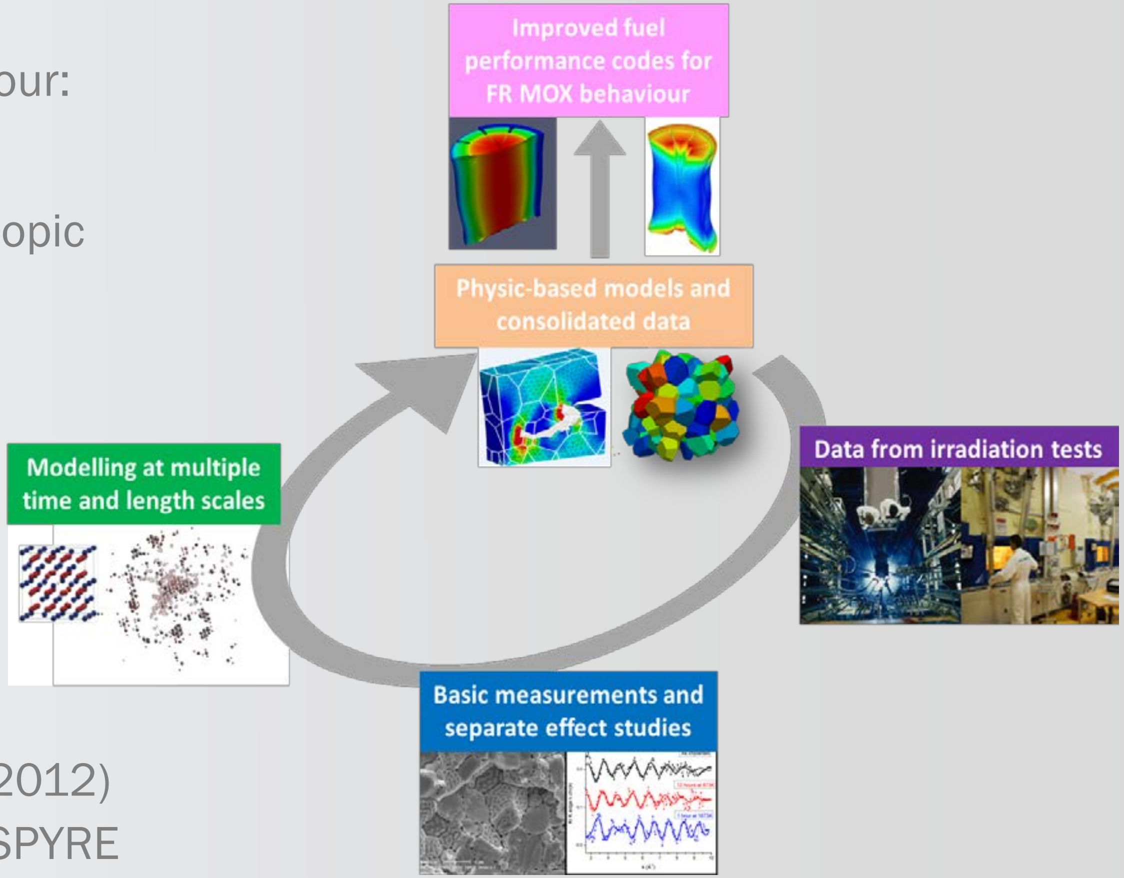
- Development of nuclear fuels: key for safety, efficiency, resources optimization and waste minimization
- Challenge for the current and next generations of nuclear reactors: improve the fuel performance and safety assessment, as well as the source term evaluation
- Behaviour of fuel and fission products is complex and combines coupled phenomena induced by irradiation, temperature, chemistry, mechanical effects
- Operational margins mainly determined by physico-mechanical behaviour of fuel elements
- Effects of accidents depend on physico-chemical behaviour of fuel as it contains the radioactive material that can eventually be released

⇨ Important to understand and be able to predict the behaviour of fuels under irradiation

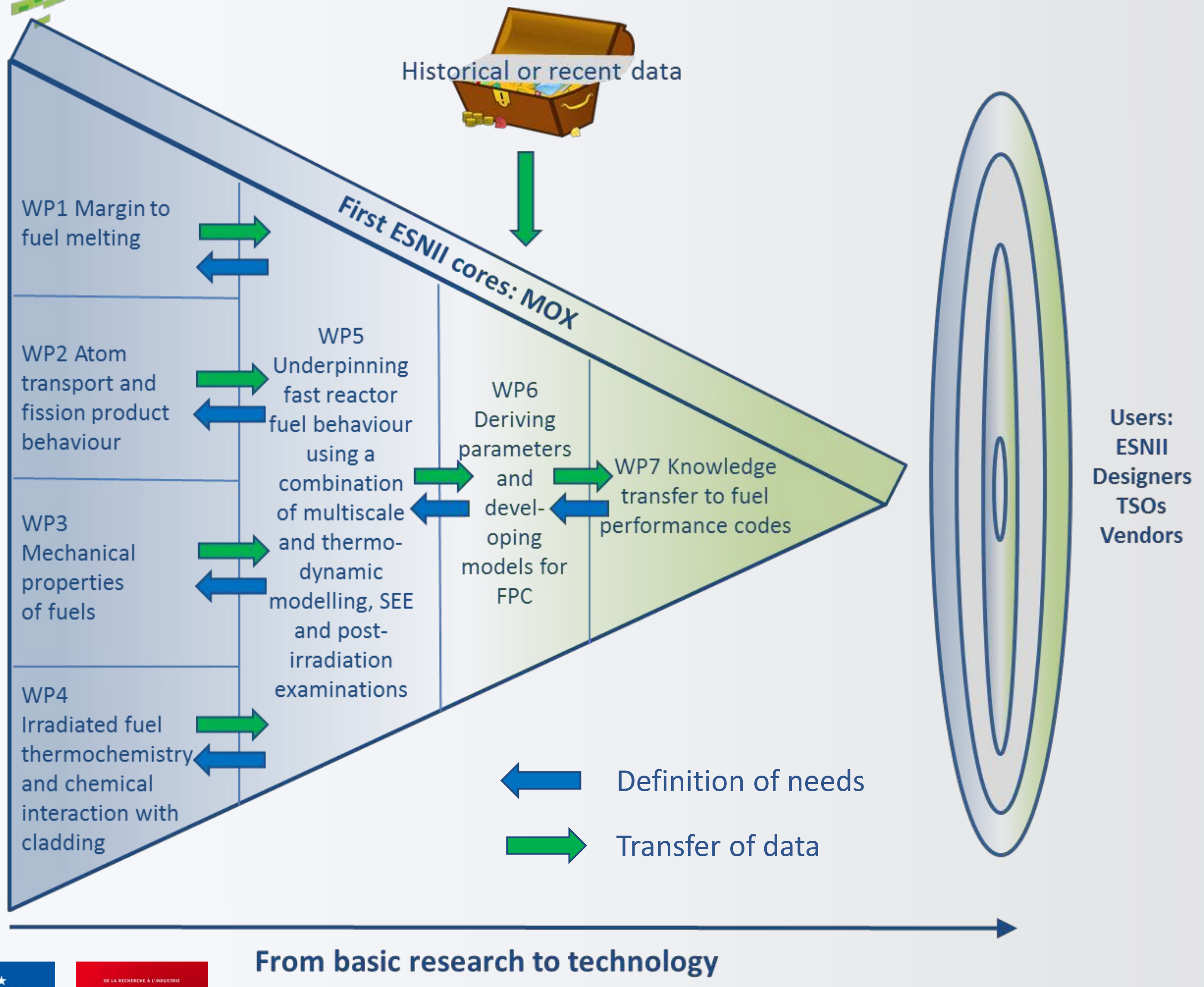


Approach: development of more mechanistic models and implementation in fuel performance and safety codes

- One effective way to bring further insight into fuel behaviour: decorrelate and identify phenomena at relevant scale
- Produce data necessary to develop and validate macroscopic models difficult and/or long to obtain experimentally
- Synergy between separate effect experiments and multiscale modelling (atomic, mesoscale, thermodynamic)
- Complement to irradiation experiments and examinations of irradiated materials
- Approach developed in the F-BRIDGE FP7 project (2008-2012) on UO_2 fuels and now applied on $(U,Pu)O_2$ fuels in the INSPYRE project (2017-2022)



The INSPYRE project



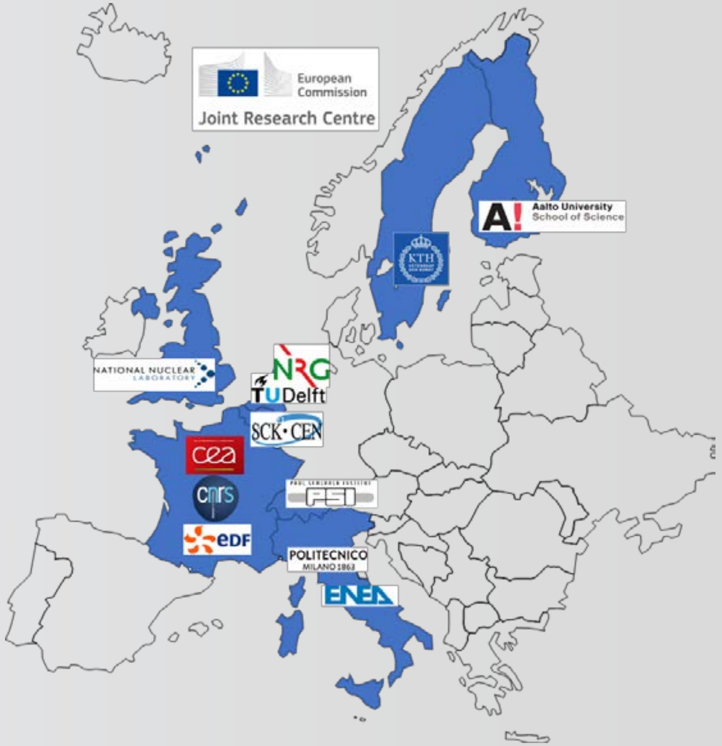
Fuels studied

Mainly Fast Reactor MOX fuel

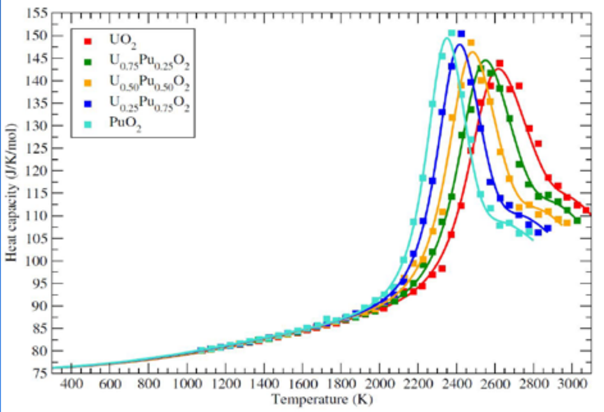
$(U,Pu)O_2$, pure or with a few % Am

A few studies on UO_2

Consortium



Development of a heat capacity law from atomic scale calculations



D. Bathellier *et al.*, J. Nucl. Mater. 2021 (to be published)

Heat capacity and margin to fuel melting

- Design rule: No melting of the fuel, so important to know the margin to fuel melting
- **Conductivity Integral Margin to melting** or power rating required to initiate centre melting

$$CIM = \int_{T_{op}}^{T_m} \lambda(T)dT$$

Melting temperature

Thermal conductivity

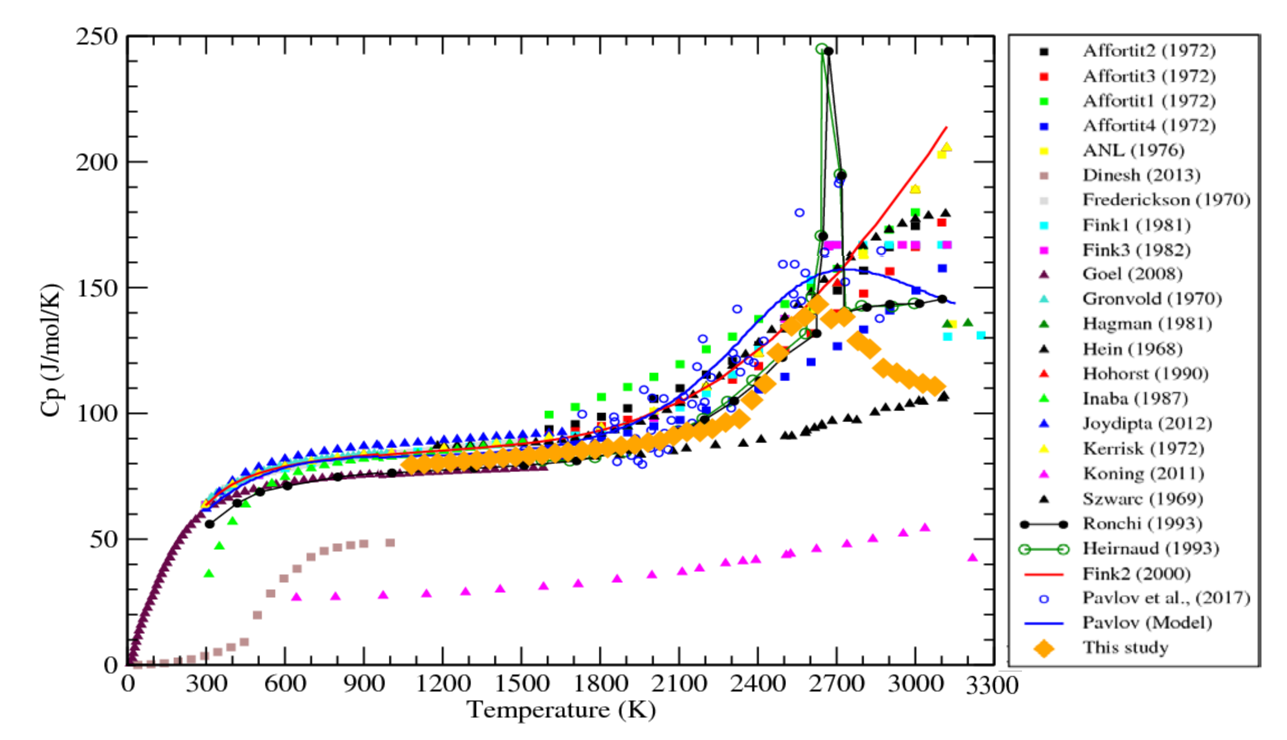
- Thermal conductivity $\lambda(T) = \alpha(T) \cdot c_p(T) \cdot \rho(T)$

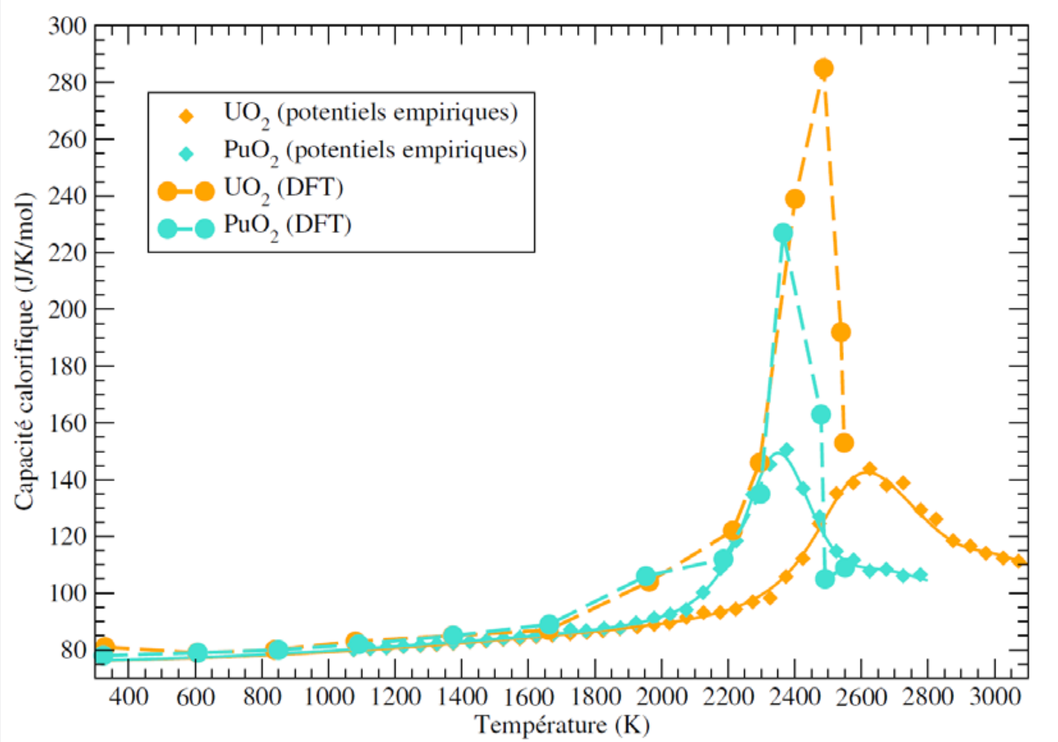
Thermal diffusivity   Heat capacity   Volumic density

- c_p necessary to get thermal conductivity from thermal diffusivity measurements
- c_p also an important parameter in fast transients, e.g. reactivity insertion accident
- Very little information on heat capacity of MOX, especially at high temperature, and on impact of composition

Calculation of heat capacity at the atomic scale

- Molecular dynamics simulation combined to CRG interatomic potential
- Validation through comparison with latest experimental data on UO_2 and with electronic structural calculations on UO_2 and PuO_2

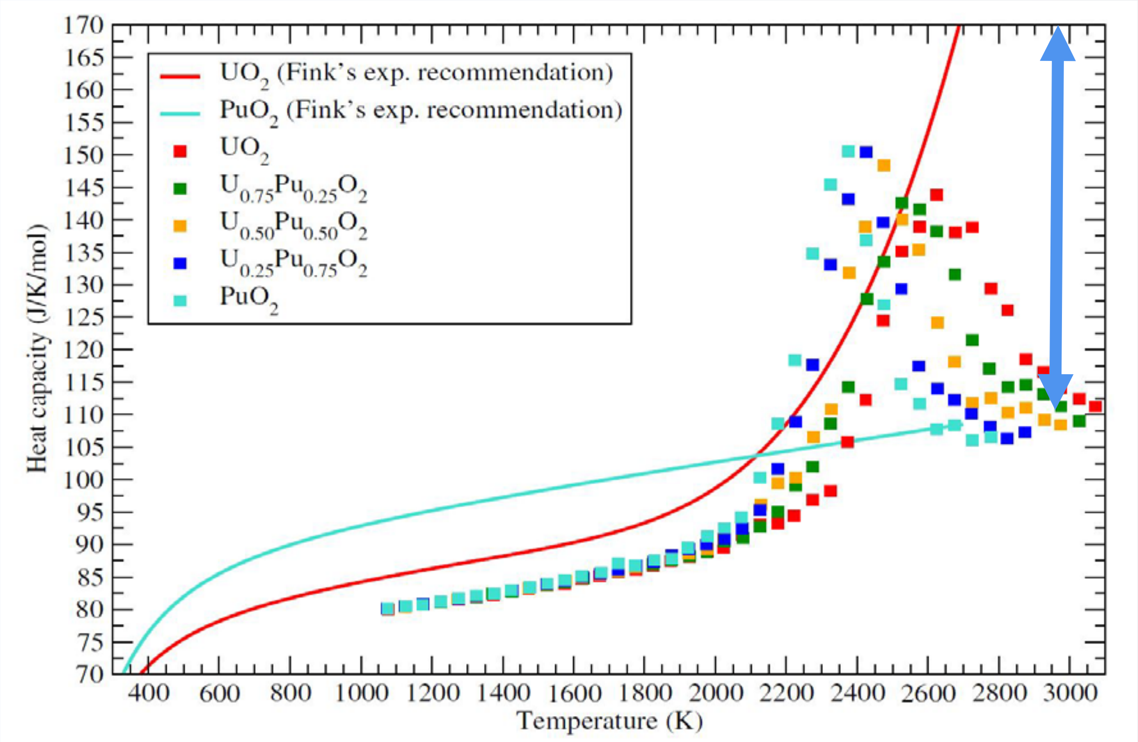


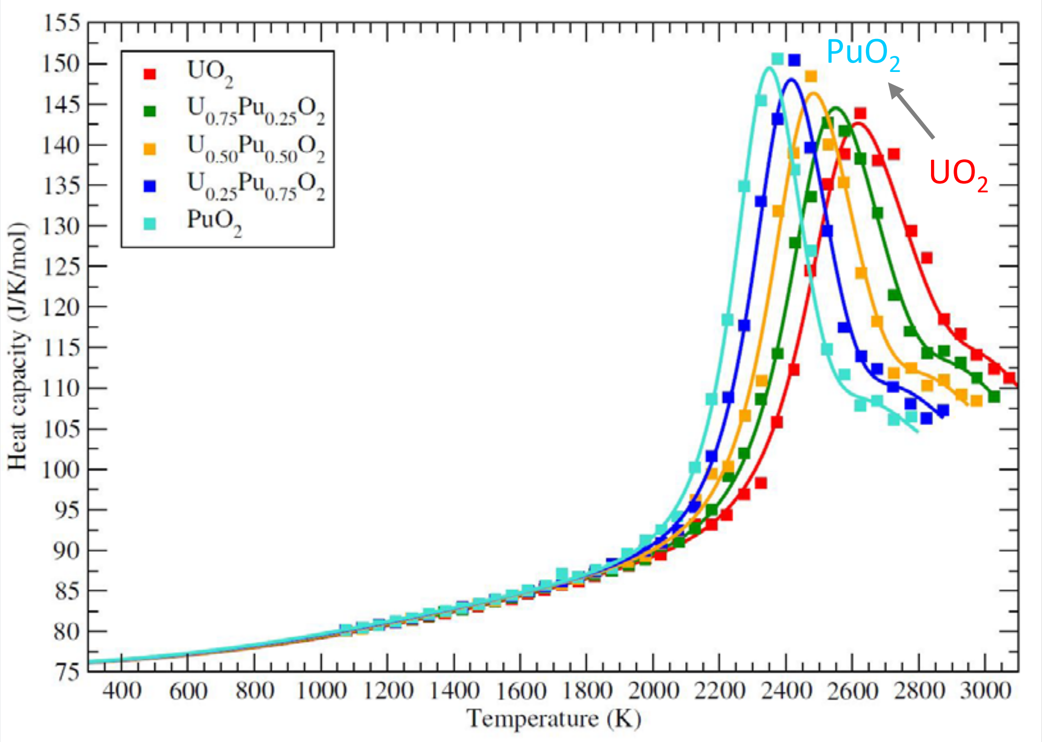


Peak in Cp observed just below melting temperature: Bredig Transition

M.W.D Cooper *et al.*, J. Phys. Condens. Matter, 26, 105401 (2014)

Heat capacity results for $U_{1-y}Pu_yO_2$



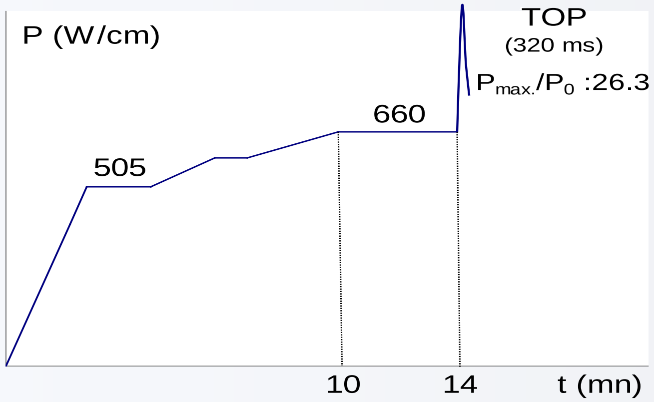


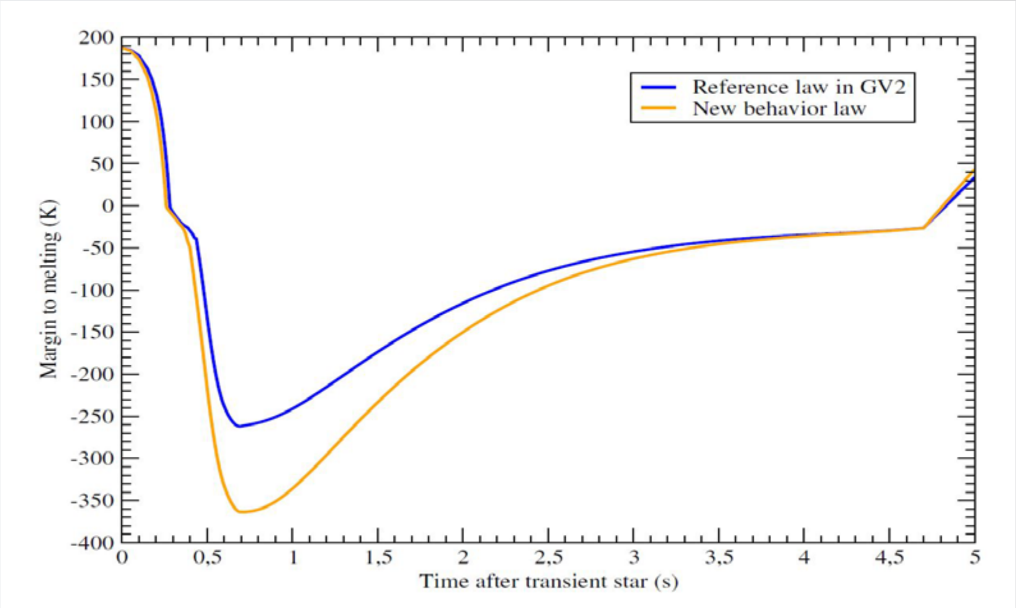
- Heat capacity of (U,Pu)O_2 also shows a Bredig transition ⇨ significant difference at high T
- Pu content impacts temperature and intensity of peak at high T
- Linear variation from UO_2 to PuO_2
- New law $c_p(T, x, y)$ with y Pu content and x deviation from stoichiometry was developed and introduced in Germinal code

Application of new law to transient power test simulation

Re-irradiation in CABRI of a fuel pin of the OPHELIE6 assembly (annular pellets) previously irradiated in normal operating conditions in the French nuclear Phénix reactor (BU 5 at %)

Fast transient power test



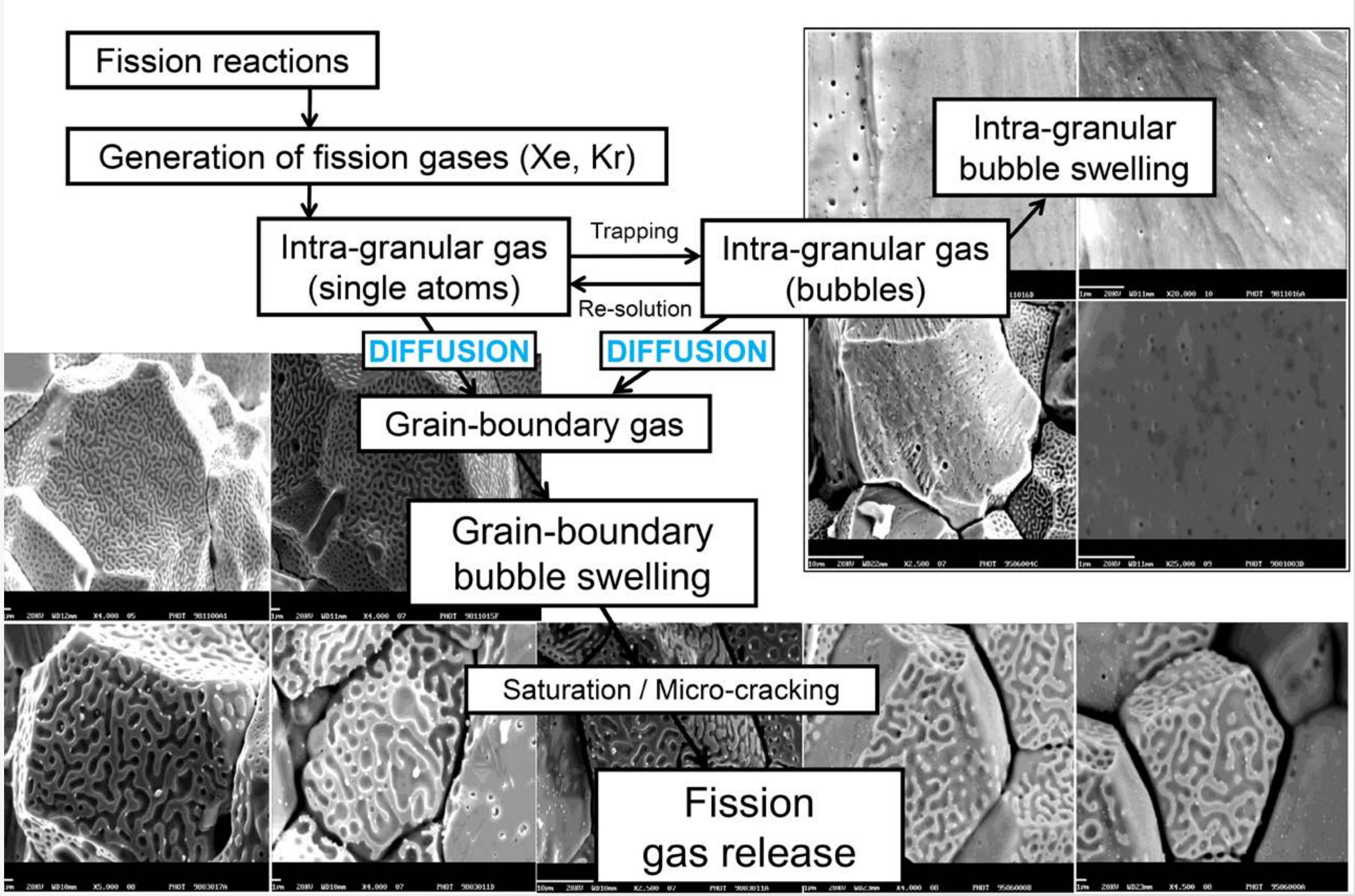


- Significant impact of the new law ⇨ melting appears slightly faster and lasts longer. When heat capacity of solid phase decreases with all other quantities remaining equal, more material will melt to store the same injected energy.
- Simulation results farther from experimental results
- Other properties need to be updated consistently

Description of inert gas behaviour: the SCIANTIX module

D. Pizzocri *et al.*, J. Nucl. Mater. 502, 323 (2018)
D. Pizzocri *et al.*, J. Nucl. Mater. 532, 152042 (2020)

Inert gas behaviour in fuel under irradiation



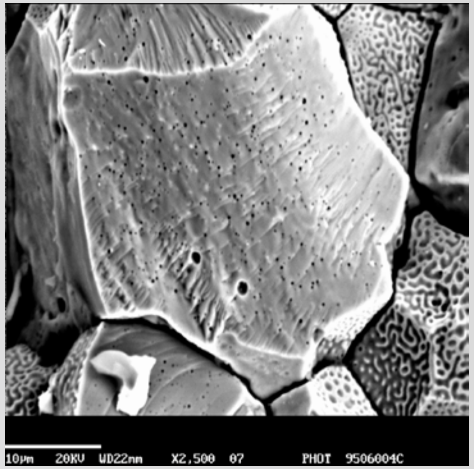
SCIANTIX

- 0D stand-alone code developed at Politecnico di Milano designed to be included as a module in existing fuel performance codes
- Single-size model derived from cluster dynamics
- Fokker-Planck expansion in the phase space at order zero
- Assumption of first moment expansion valid for peaked distributions of bubble size (observed experimentally by White)
- All clusters with size n > 2 are considered immobile and counted as bubbles
- Number of bubbles N and average size $\bar{n}$ can be obtained by solving the coupled equations

$$\boxed{\begin{cases} \dfrac{\mathrm{d}N}{\mathrm{d}t} = \nu - \mathrm{b}_N N \\ \dfrac{\mathrm{d}\bar{n}}{\mathrm{d}t} = \mathrm{g}_{\bar{n}} c_1 - \mathrm{b}_{\bar{n}} \bar{n} \end{cases}}$$

With ν nucleation rate
b_N,$\mathrm{b}_{\bar{n}}$ resolution rates
$\mathrm{g}_{\bar{n}}$ trapping rate
c_1 concentration of single gas atoms

- Physical parameters taken from lower scale modelling or experiments
- Model can be improved when new results are obtained

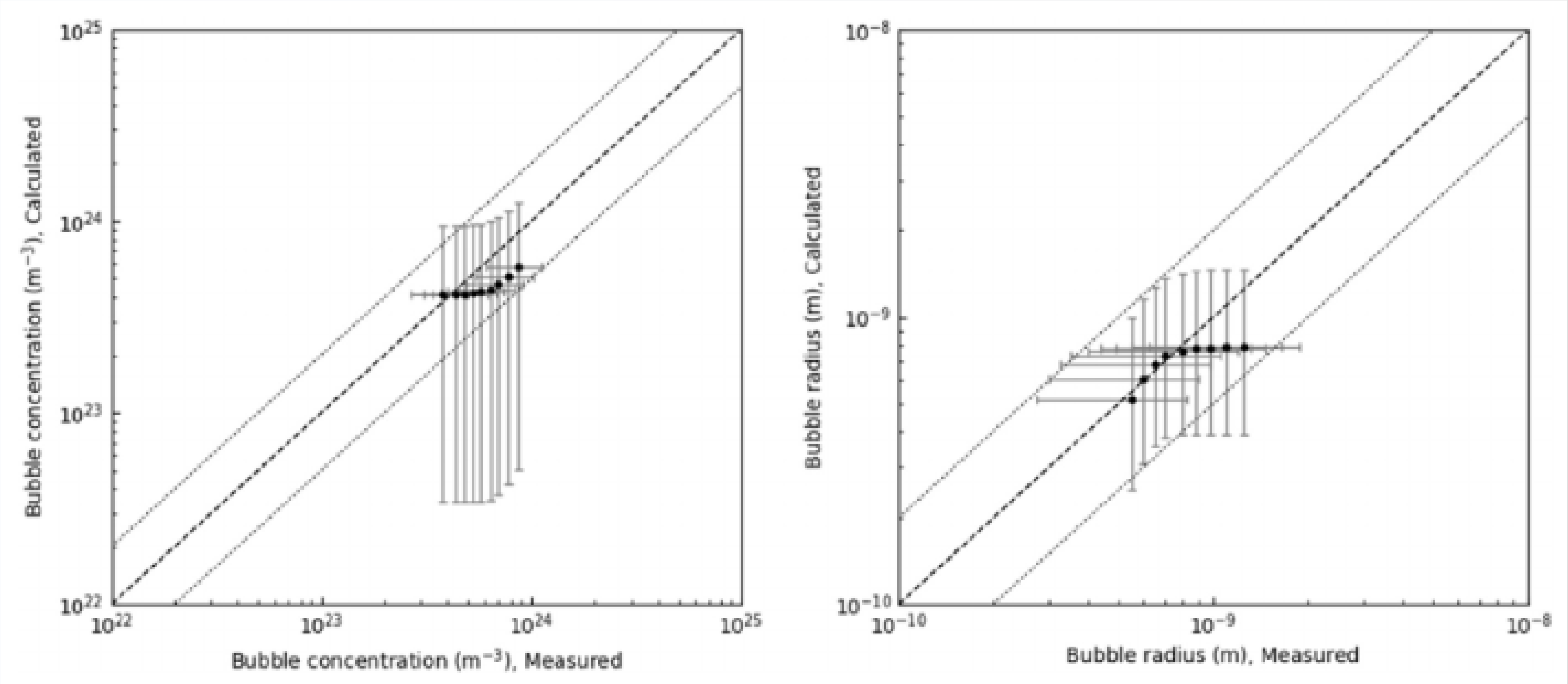


R.J. White, J. Nucl. Mater. 325, 61 (2004)

Available as open-source software (MIT license) at https://gitlab.com/poliminrg/sciantix

Validation on experimental data

Validation performed on data on irradiated fuel (20 Gwd/t)
from Baker, J. Nucl. Mater. 66, 283 & 71, 117 (1977)



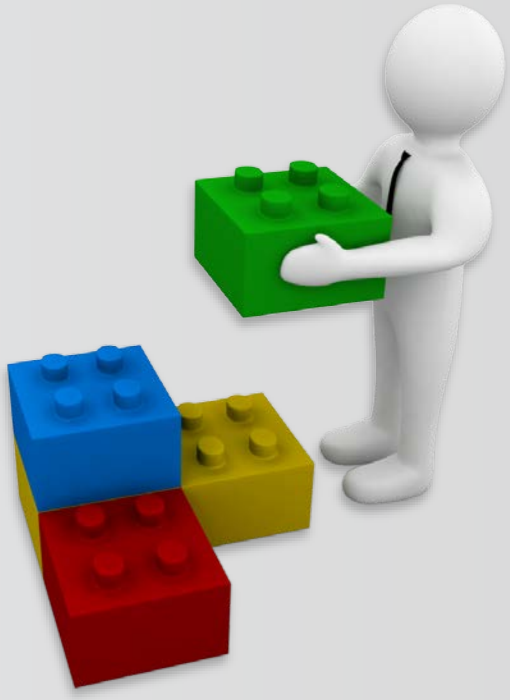
UA & SA with respect to model parameters performed via total Monte Carlo

First step towards description of more complex systems, with larger bubbles

Conclusions

Results and perspectives

- INSPYRE basic research studies brought important results on the behaviour of fuels under irradiation which were or are being implemented in fuel performance codes and thermodynamic databases
- Significant progress made for thermal properties, inert gas behaviour, fission product compounds
- Studies starting on Am-bearing fuels
- Work started for mechanical properties. Linear regime well described. More investigation needed for non-linear behaviour: creep and fracture, description of heterogeneous materials



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