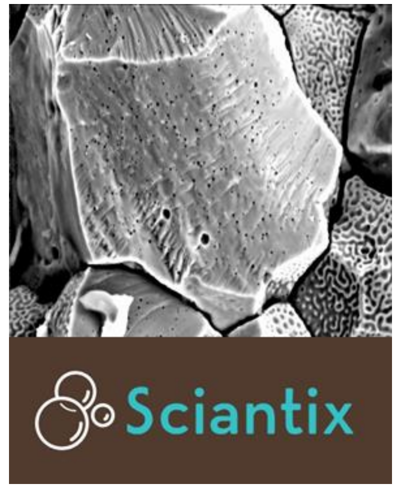
REDUCTION OF RADIOLOGICAL ACCIDENT CONSEQUENCES

POLITECNICO MILANO 1863

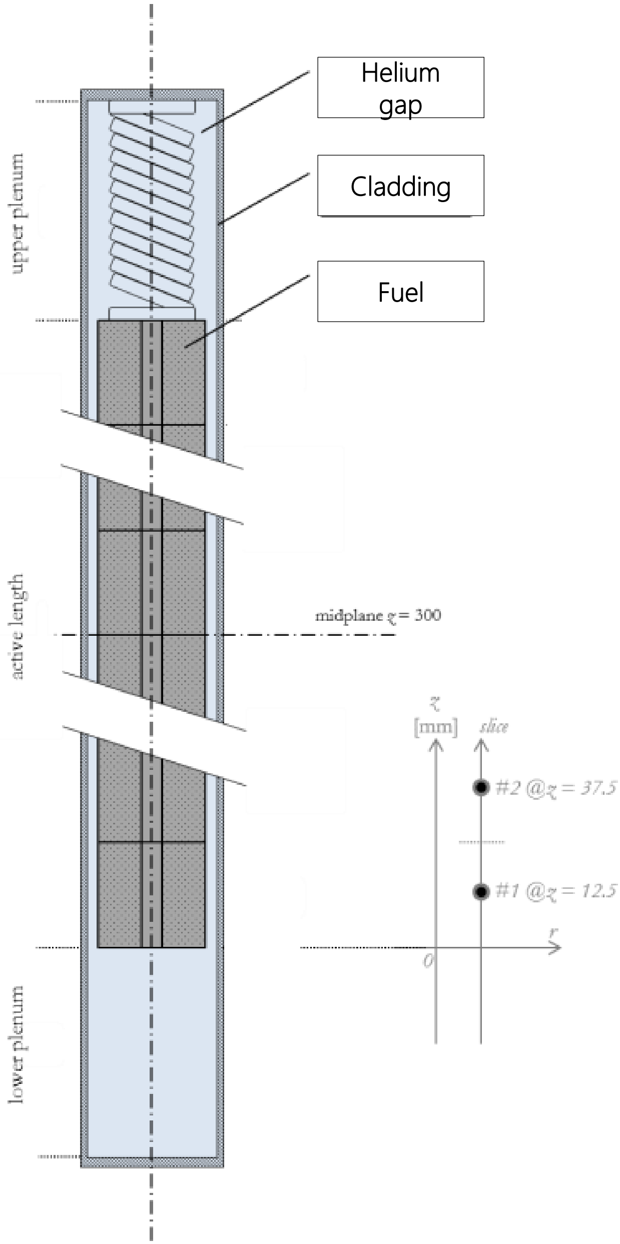


SCIANTIX Virtual Training - October 16, 2020

SCIANTIX: A new open source grain-scale code for fission gas behaviour modelling

D. Pizzocri, L. Luzzi, A. Magni

Object, nuclear fuel pin

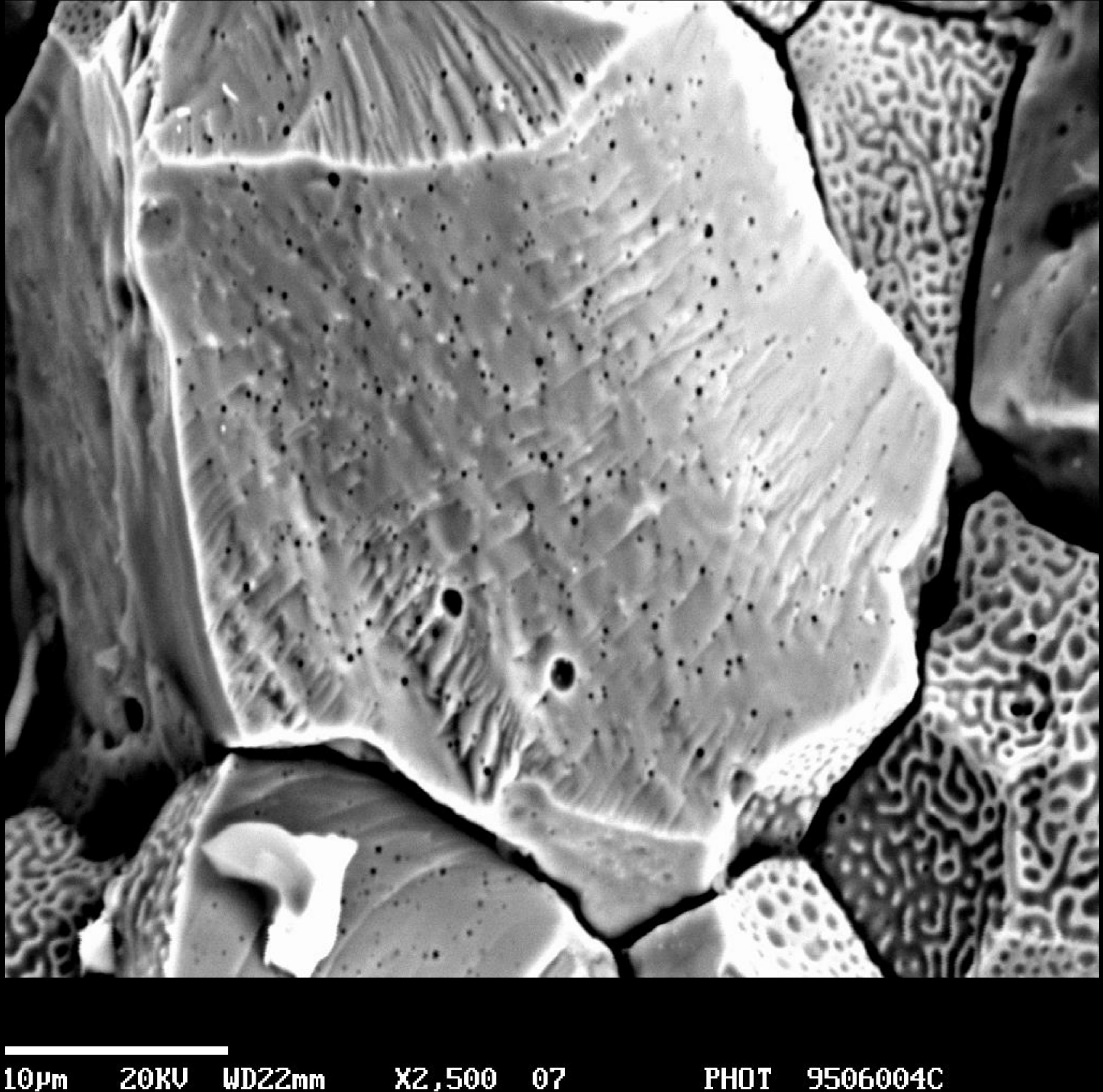


Nuclear fuel rod (ThR//FR) is made of a **stack of oxide (UO_2//MOX) fuel pellets** wrapped in **metallic (Zry//SS) cladding**

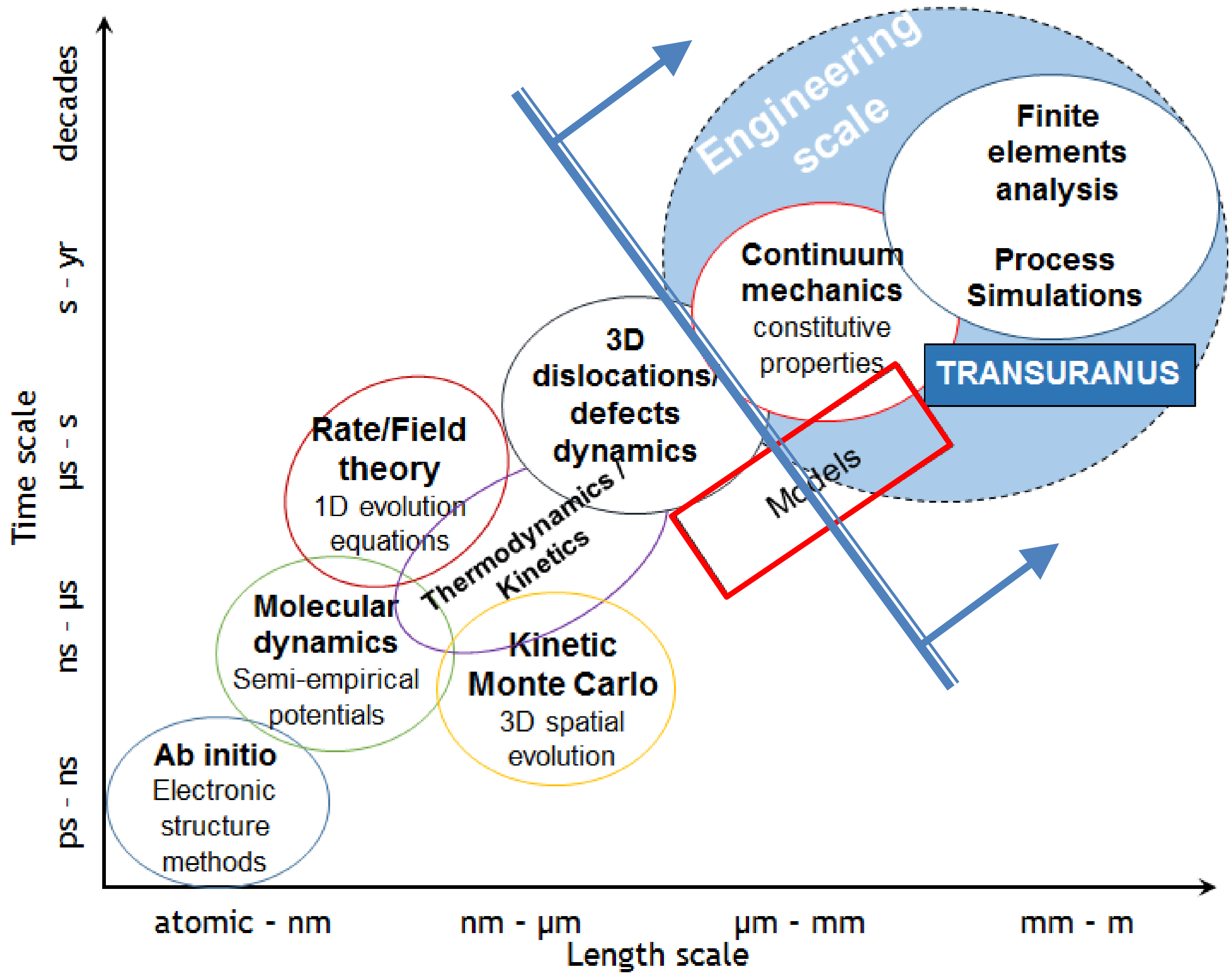
Its performance is fundamental for **safe operation** of the reactor (and **licensing** and **design**)

Need of **integral fuel performance codes (FPCs)** and integral irradiation experiments to assess the fuel rod **thermo-mechanical behaviour** (σ,ε, and T)

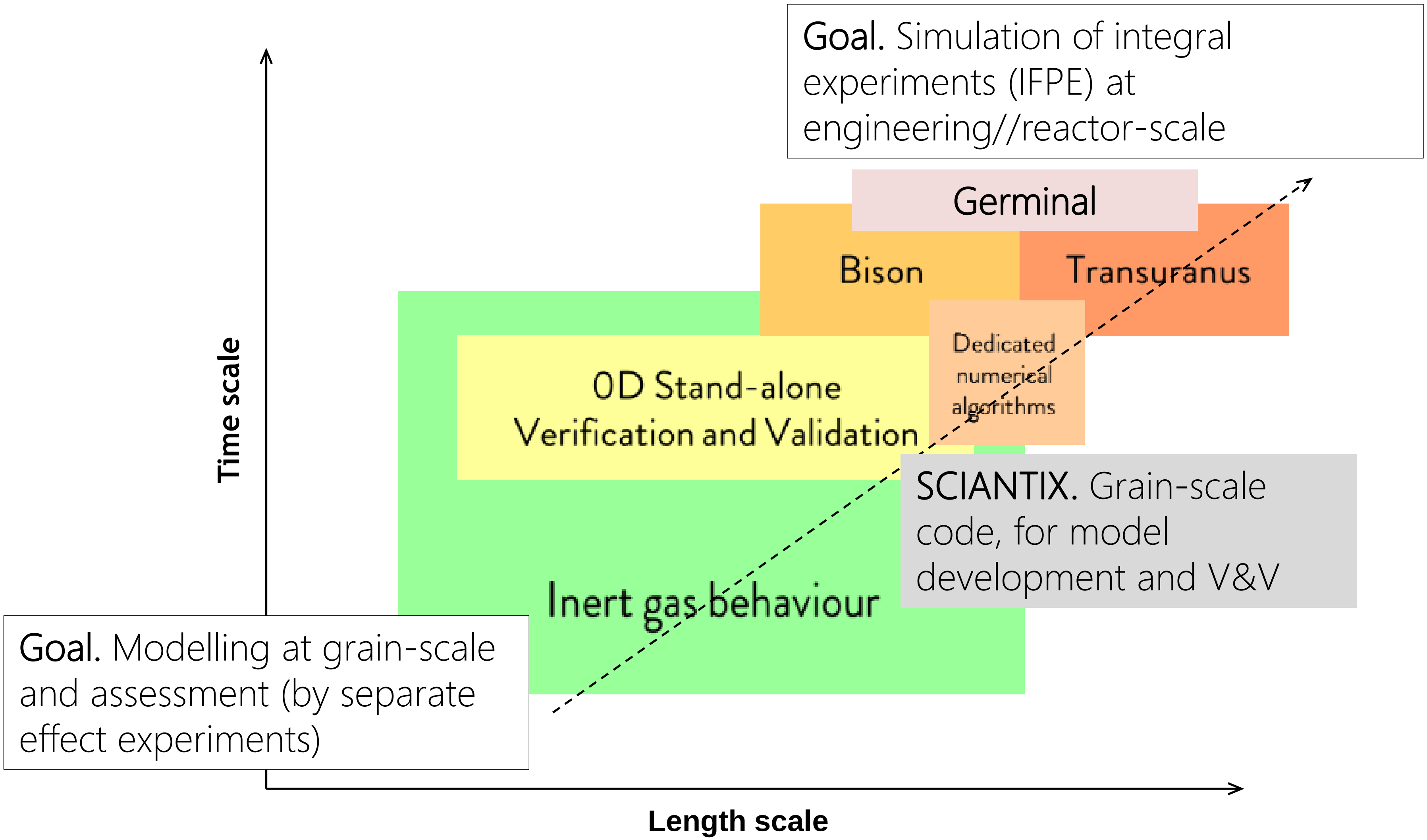
Focus on inert gas behavior, i.e., **gaseous swelling & fission gas release**


10μm 20KV WD22mm X2,500 07 PHOT 9506004C

Multi-scale modelling approach



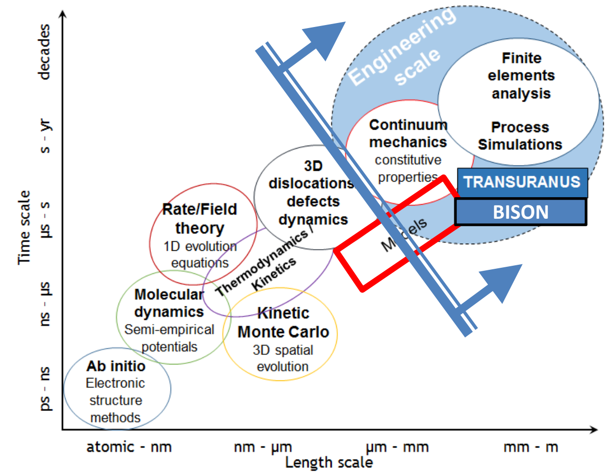
Multi-scale modelling approach, this work



Multi-scale modelling approach, requirements

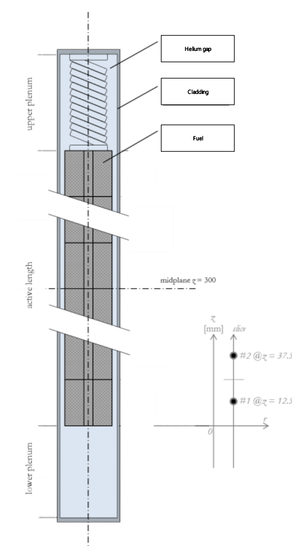
Physics-based modelling is fundamental in order to act as bridge between different scales

- Can be **informed by lower-length scale calculations and experiments**, in terms of physical phenomena and model parameters
- Need to **overcome correlation-based approaches** currently used **in FPCs**



Low computational time is needed for effective use *within* fuel performance codes

- IGB model called at each thermo-mechanical iteration, in each time-step of the FPC simulation, in each mesh point
- The huge number of calls implies that **numerical robustness** is a requirement



The SCIANTIX code, features

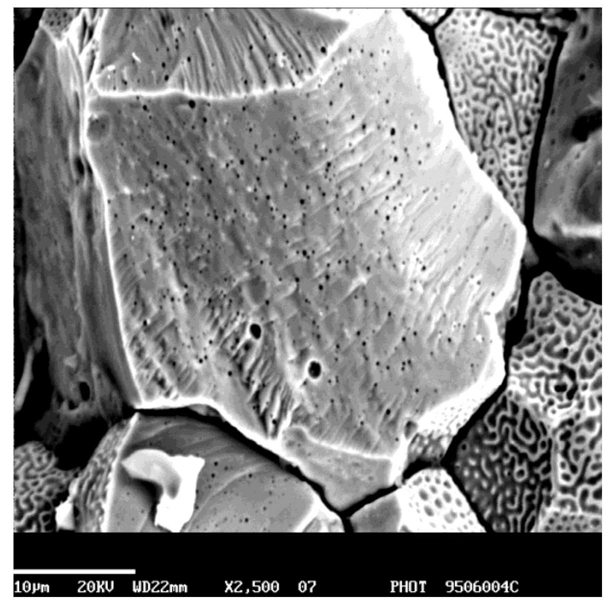
Developed at Politecnico di Milano

It is a **0D stand-alone code, designed to be included as a mechanistic fission gas behaviour module in existing fuel performance codes**

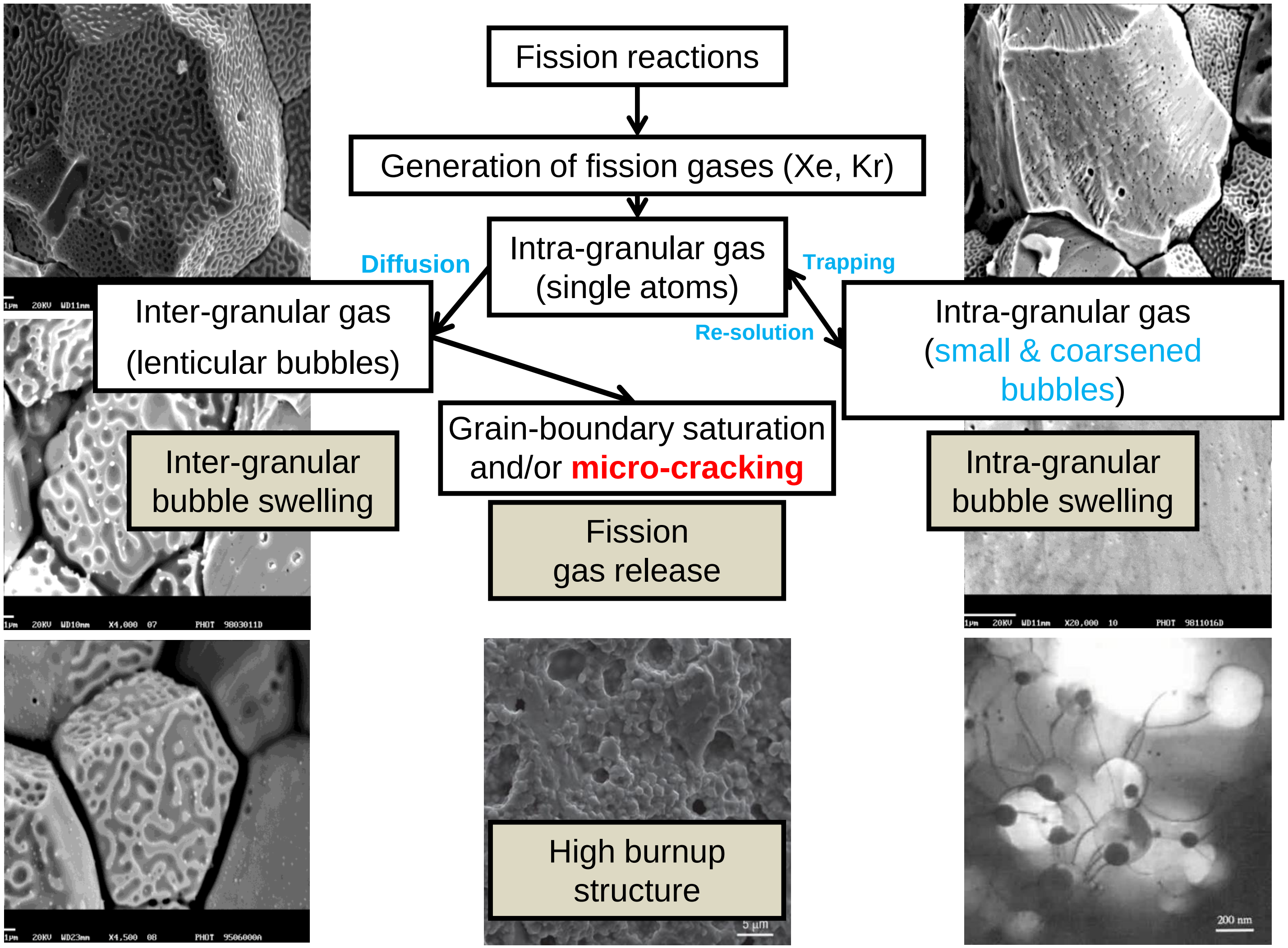
Constitutes the natural environment for the development, verification, and validation of fission gas behaviour models, and for the **simulation of separate-effect test experiments**

It can be **included in existing multiphysics platforms and fuel performance codes as a module (via simple interface)** to evaluate fission gas release and gaseous swelling or can be **used as stand-alone**

Available as open-source software (MIT license)



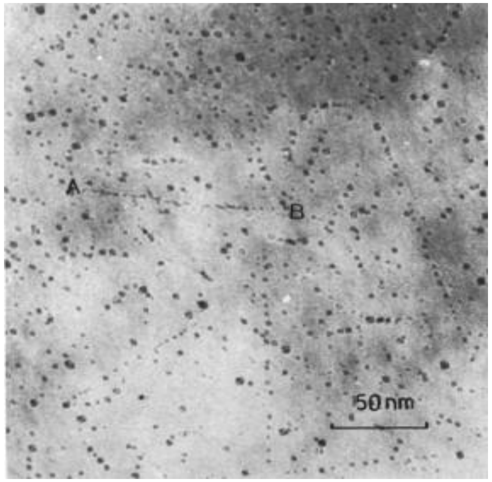
The SCIANTIX code, physical aspects



Applicative modelling example

Intra-granular bubble evolution

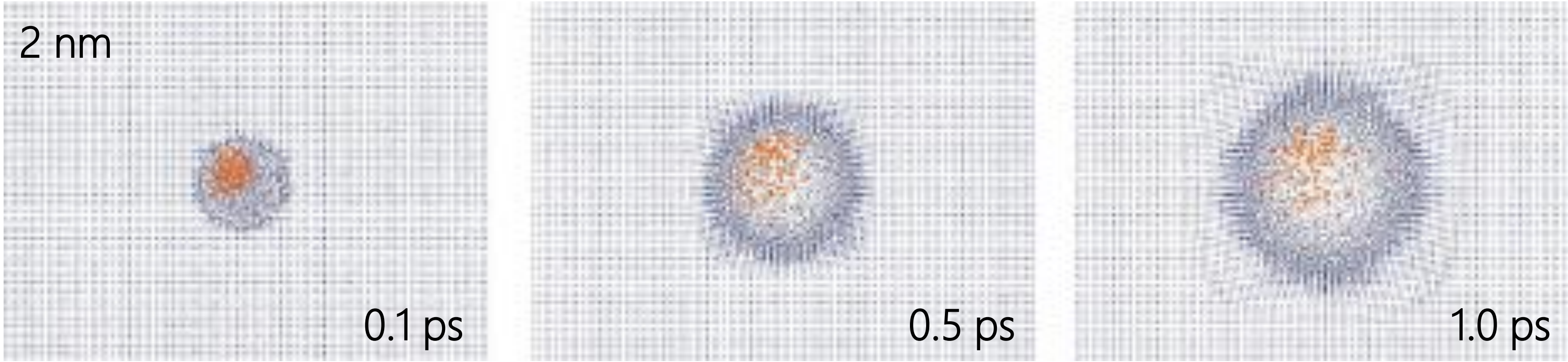
State of the Art. Correlations for bubble radius and bubble concentration, f(T)



Baker, J. Nucl. Mater., 1977

Lower length-scale information available

- **Bubble nucleation** appears to be driven by fission fragments
- **Bubble re-solution** appears to be (mainly) *heterogeneous* and again driven by fission fragments



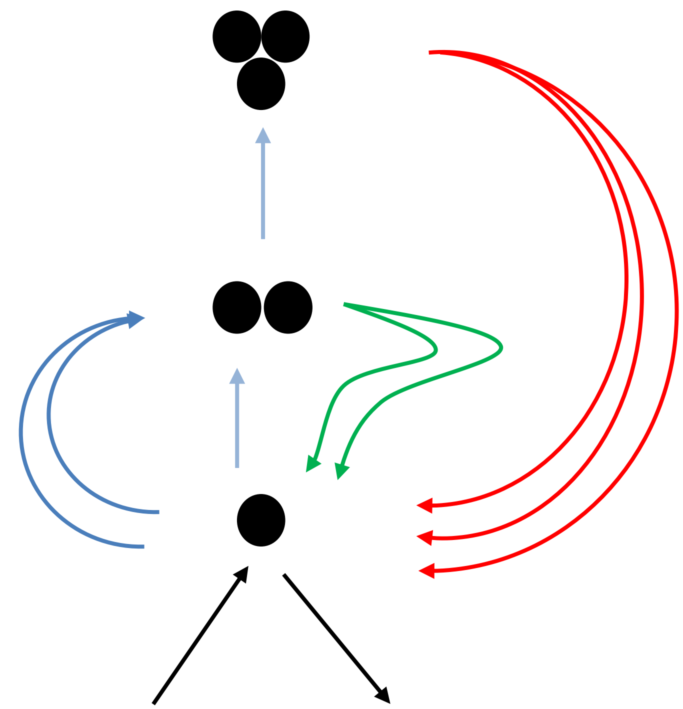
Govers et al., J. Nucl. Mater., 2012

D. Pizzocri, G. Pastore, L. Luzzi, T. Barani, A. Magni, P. Van Uffelen, S.A. Pitts, J.D. Hales, *A model describing intra-granular inert gas behavior in oxide fuel for advanced engineering tools*. 2018, Journal of Nuclear Materials, 502, 323-330.

Physically-based single-size model derived **from cluster dynamics Fokker-Planck expansion in the phase space,** at order zero

Assumption of first moment expansion implies single-size model and is valid for peaked distributions (confirmed from LLS)

All clusters with size *n* > 2 are considered immobile and counted as bubbles



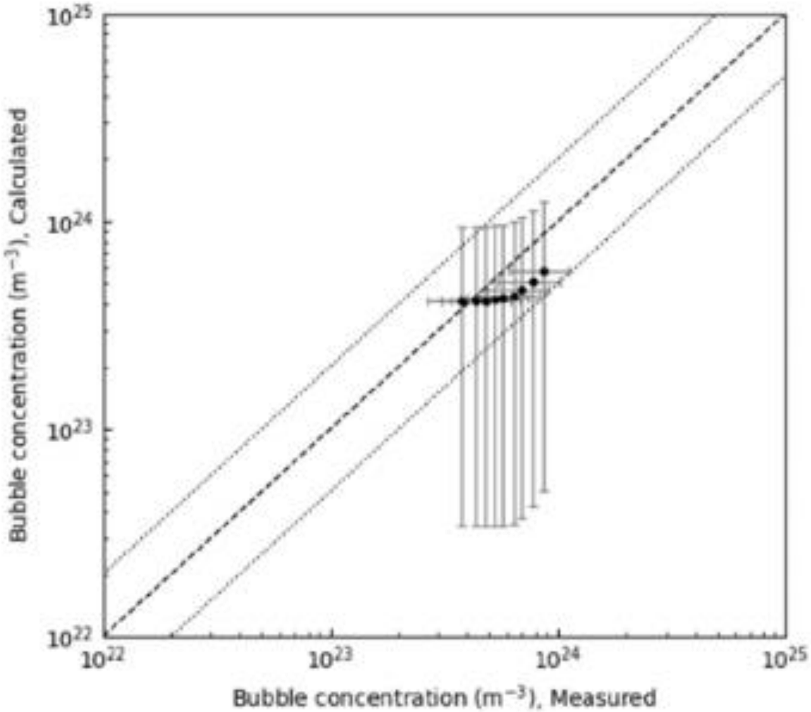
$$\frac{\mathrm{d}N}{\mathrm{d}t} = \nu - \mathrm{b}_{\bar{n}} N$$

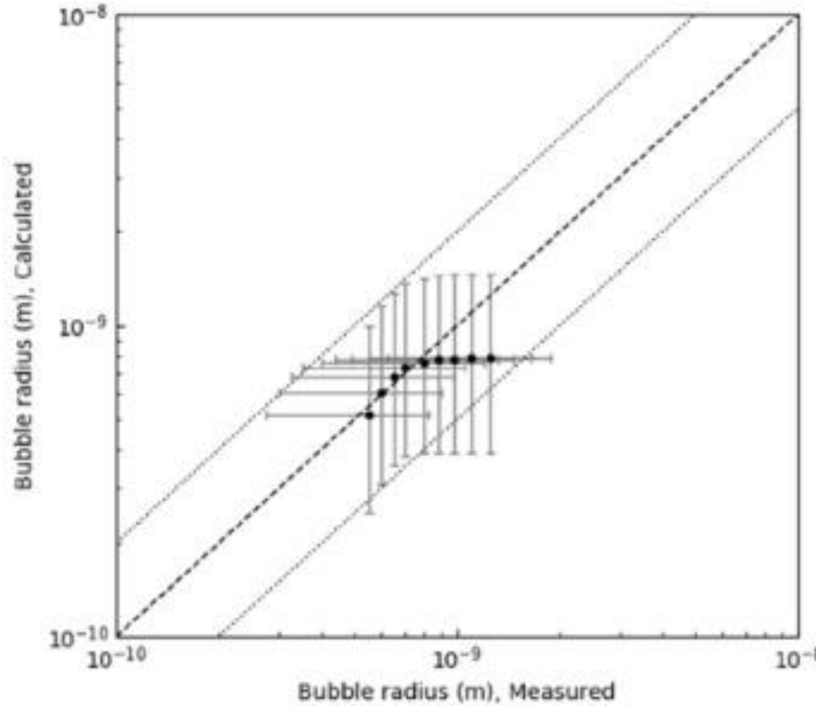
$$\frac{\mathrm{d}\bar{n}}{\mathrm{d}t} = \mathrm{g}_{\bar{n}} c_1 - \mathrm{b}_{\bar{n}} \bar{n}$$

$$\frac{\mathrm{dVar}[n]}{\mathrm{d}t} = \cdots$$

```
Intragranular_bubble_concentration[1] =
Solver::Decay(Intragranular_bubble_concentration[0],
              resolution_rate,
              nucleation_rate,
              dTime_s);
```

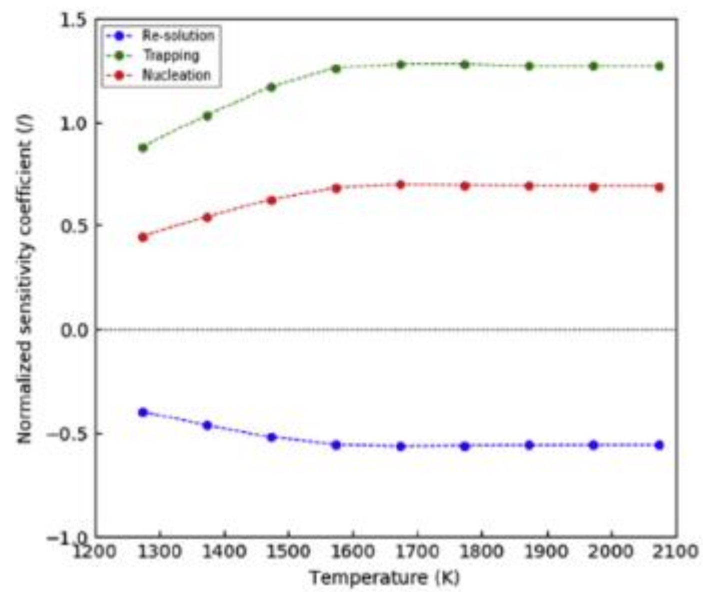
Sciantix





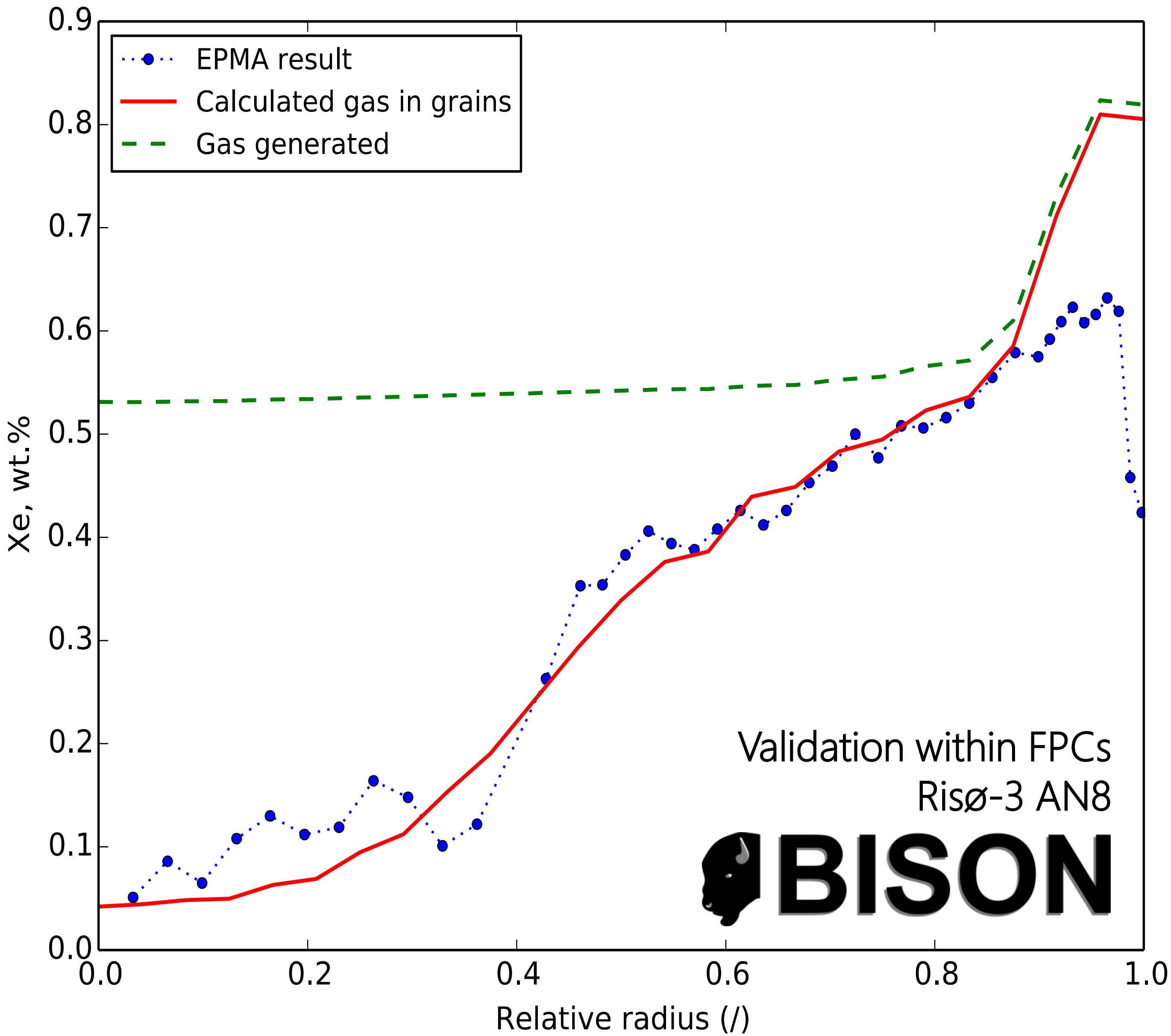
Separate effect **validation performed in SCIANTIX**: good agreement with experimental data

UA & SA with respect to model parameters via **Total Monte Carlo** (low computational time)

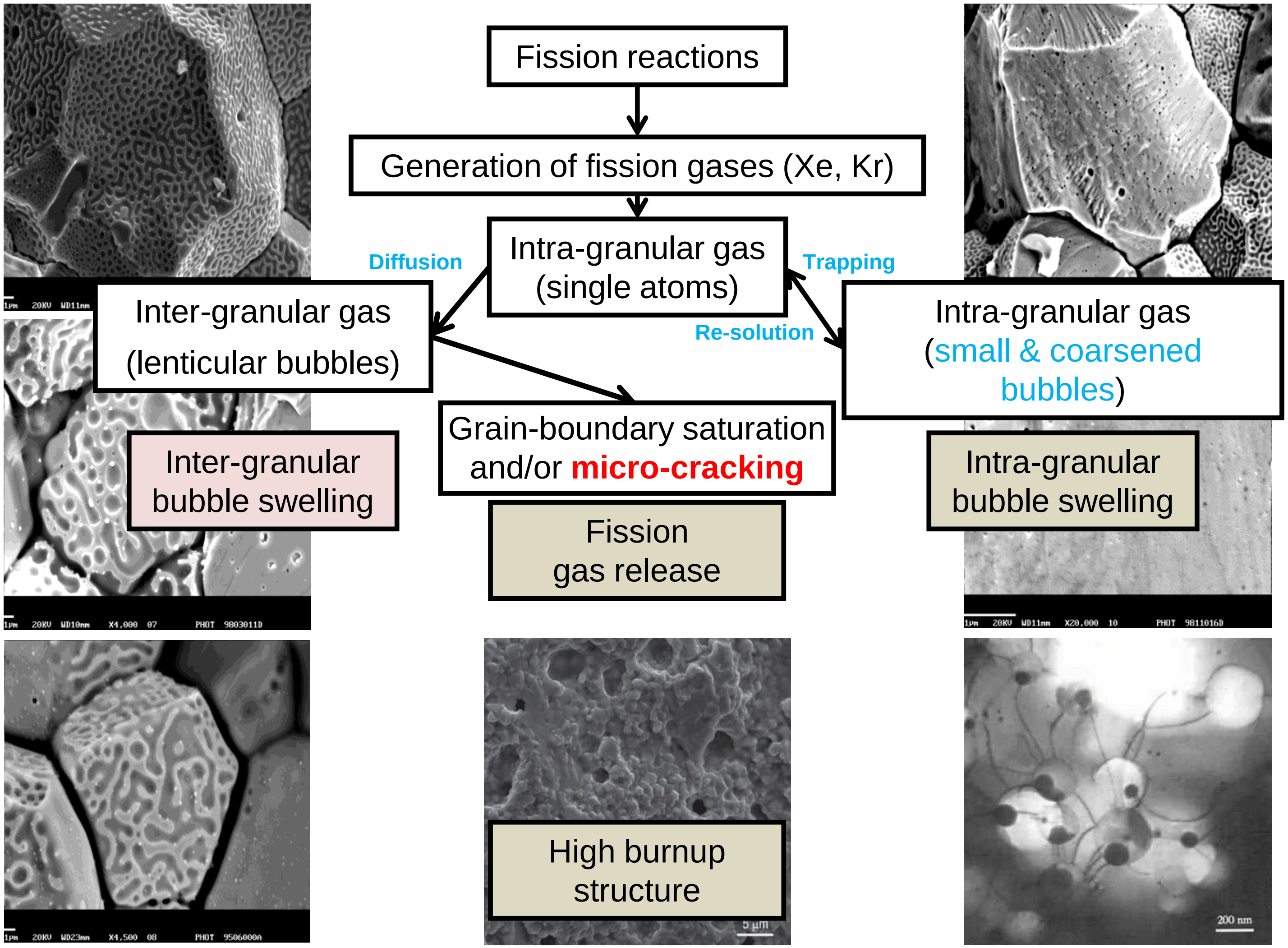


Data from Baker, 1977. JNM

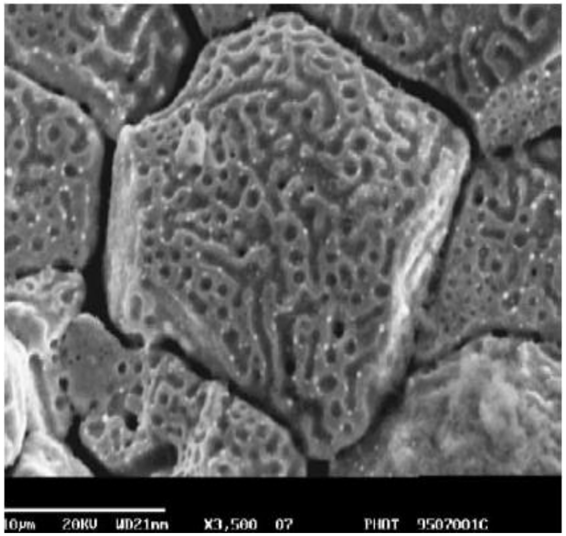
This case is going to be detailed and simulated in the training !

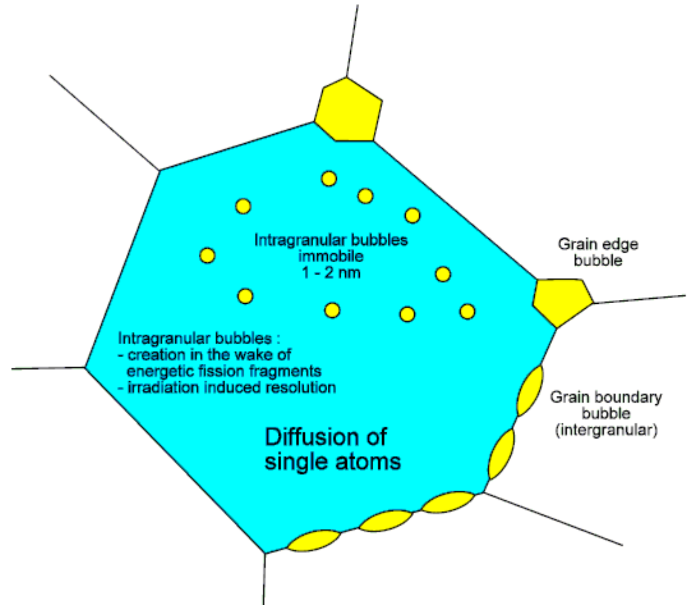

EPMA result
Calculated gas in grains
Gas generated
Xe, wt.%
Relative radius (/)
Validation within FPCs
Risø-3 AN8
BISON
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0.0
0.2
0.4
0.6
0.8
1.0

The SCIANTIX code, physical aspects



Inter-granular, LWR approach





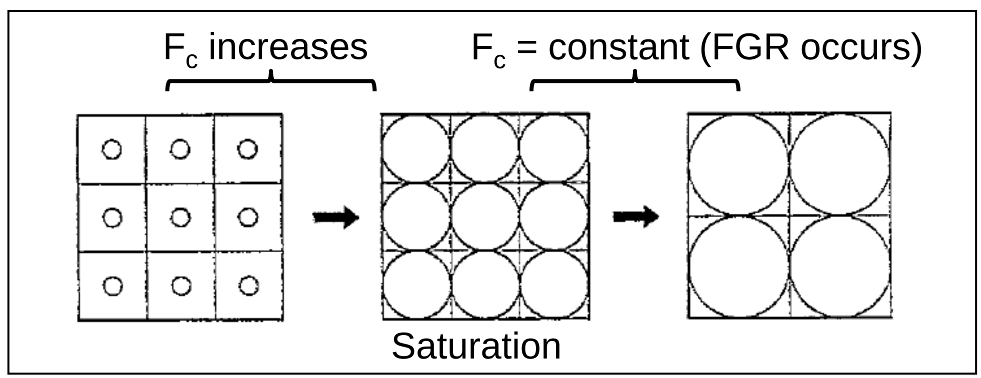
Grain-boundary bubbles **growth** by vacancy absorption and **coalescence**

A **saturation value of the fractional coverage** of the grain-faces is considered

At saturation, further bubble growth is compensated by **gas release**

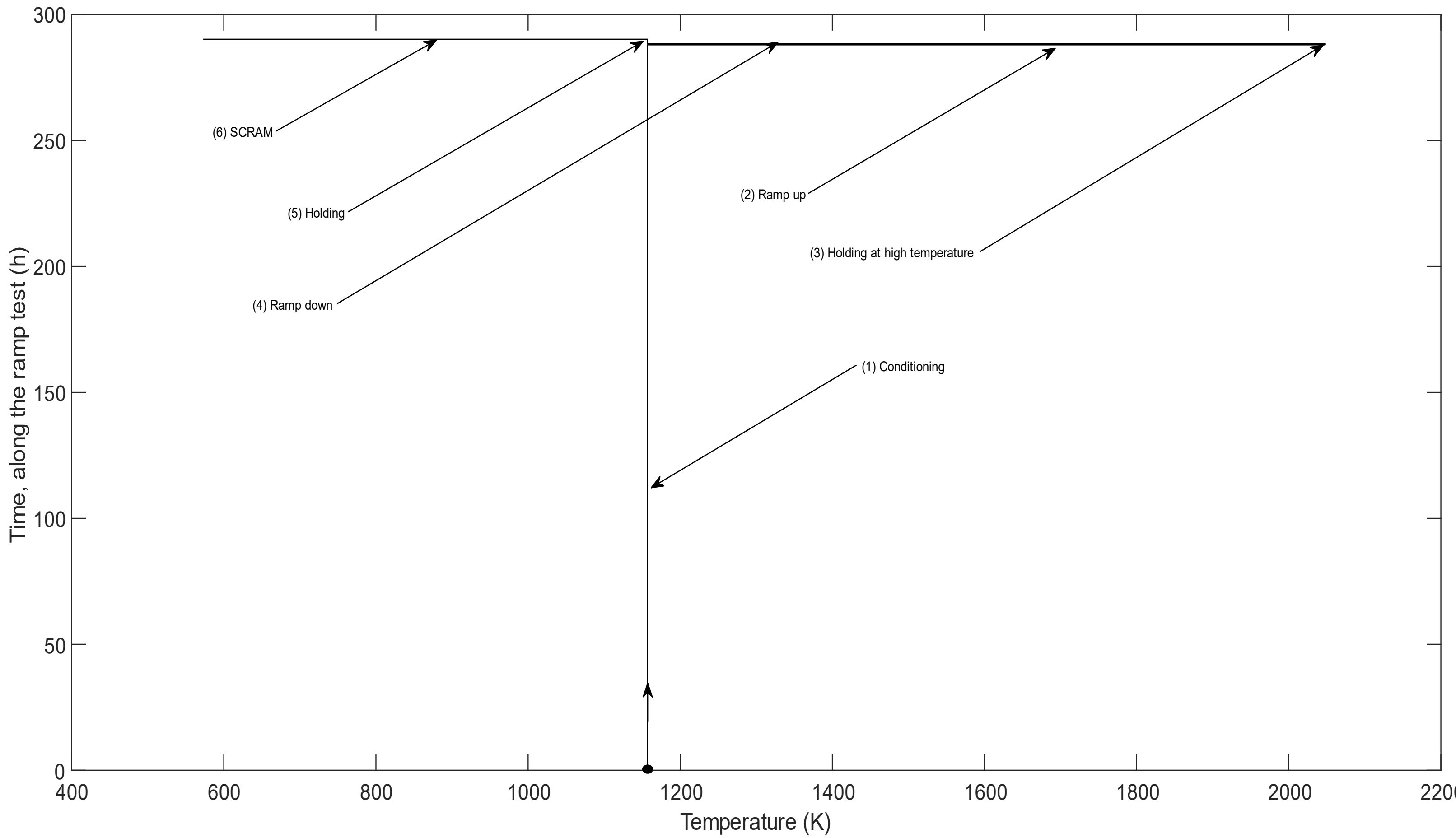
\+ Grain-boundary <u>micro-cracking</u>

$$\frac{dF_c}{dt} = \frac{d\left(N_{gf} A_{gf}\right)}{dt} = 0 \quad if \;\; F_c = F_{c,sat}$$



Pastore et al., 2013, NED

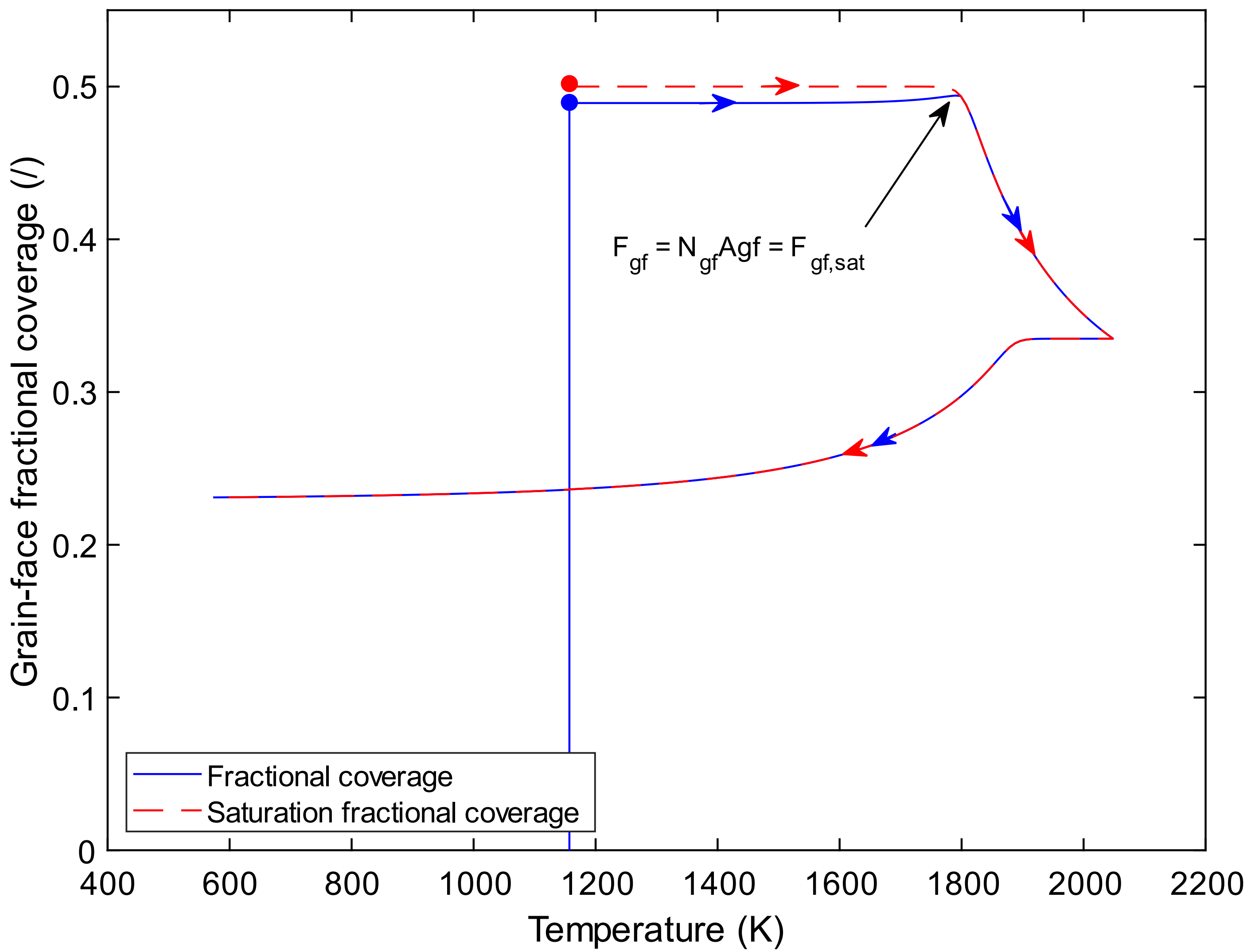
Inter-granular gas behaviour, LWR approach
Showcase of a high temperature transient



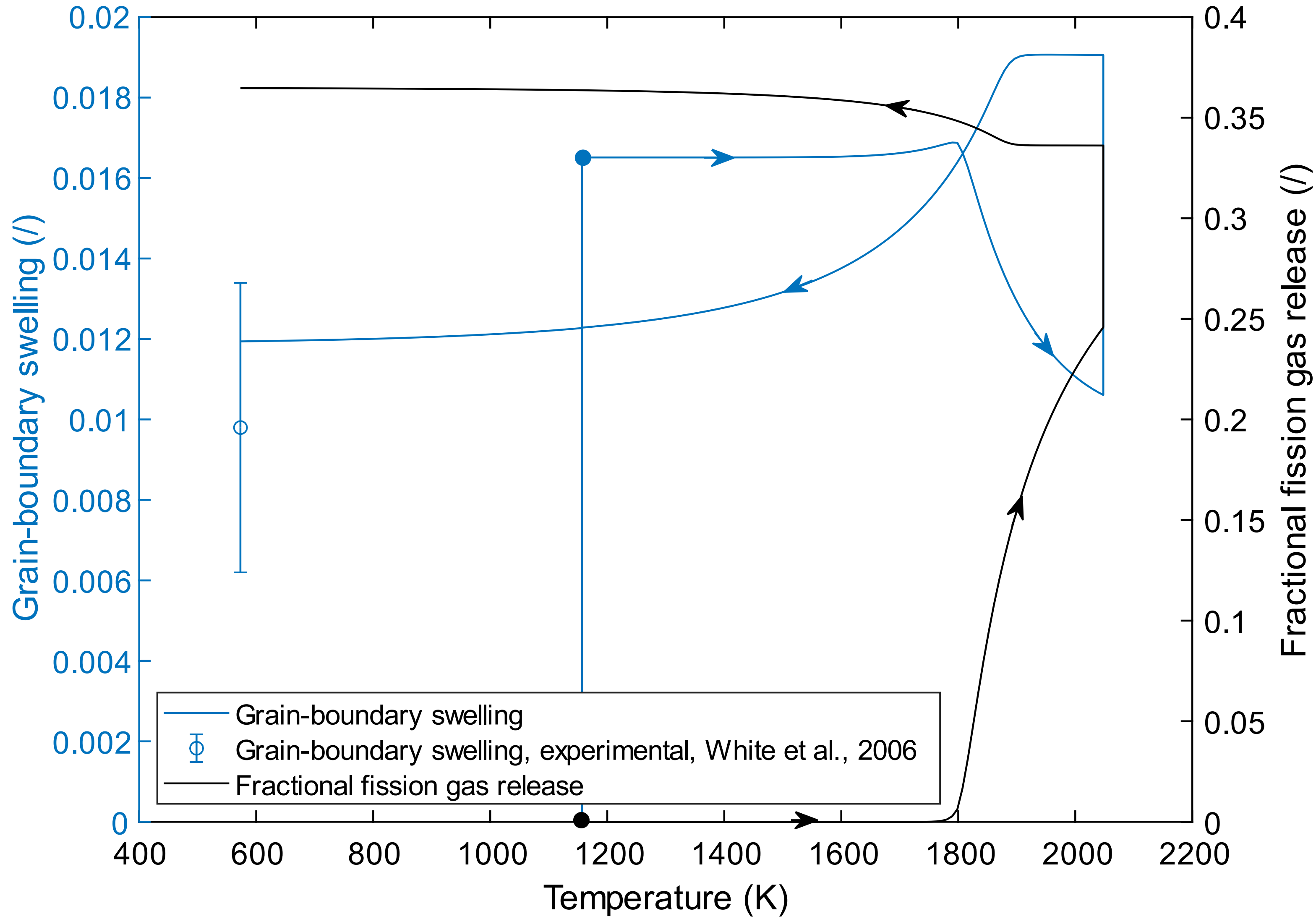
White et al., 2006

This case is going to be detailed and simulated in the training !

Inter-granular gas behaviour, LWR approach



Inter-granular gas behaviour, LWR approach



SCIANTIX future developments

Extend modelling of FGB in MOX fuels FRs

- Helium behaviour (solubility & production)
- Columnar grains → ROM for fission gas diffusion
- Continue the work with GERMINAL (& TRANSURANUS)

Include description of fission products

- Production and transport of key FPs (new-ANS5.4)
- Thermochemistry treatment (as MFPR-F)
- Medium/long-term targeting JOG in FPCs (INSPYRE follow up)

Improve modelling of high burnup structure

- Important for LWRs and FRs
- Extend Fokker-Planck approach to rate theory
- Average value & Variance for different variables

Acknowledgements

The development of SCIANTIX has received funding from the Euratom research and training programme 2014-2018 through the INSPYRE project under grant agreement No 754329

INSPYRE
Investigations Supporting MOX Fuel Licensing in ESNII Prototype Reactors

The development of SCIANTIX has received funding from the Euratom research and training programme 2018-2020 through the R2CA project under Grant Agreement n° 847656

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& Thank you for your kind attention !