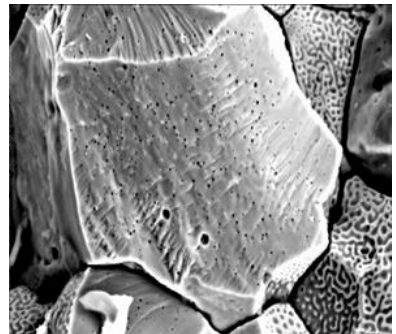
POLITECNICO
MILANO 1863



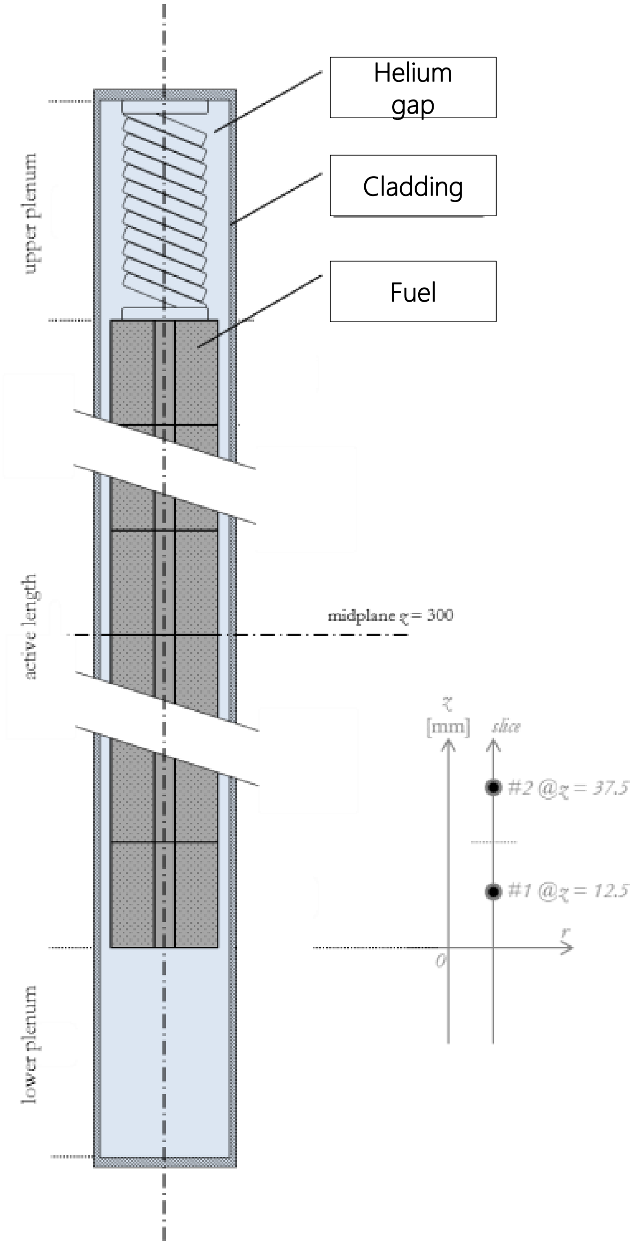
Sciantix

ONCORE, Technical Meeting on the Development and Application of Open-Source Modelling and Simulation Tools for Nuclear Reactors, Jun 20-24, 2022, POLIMI (Milano, IT)

SCIANTIX open-source code for fission gas behaviour: Objectives and foreseen developments

D. Pizzocri, A. Magni, G. Zullo, L. Luzzi

Object, nuclear fuel pin



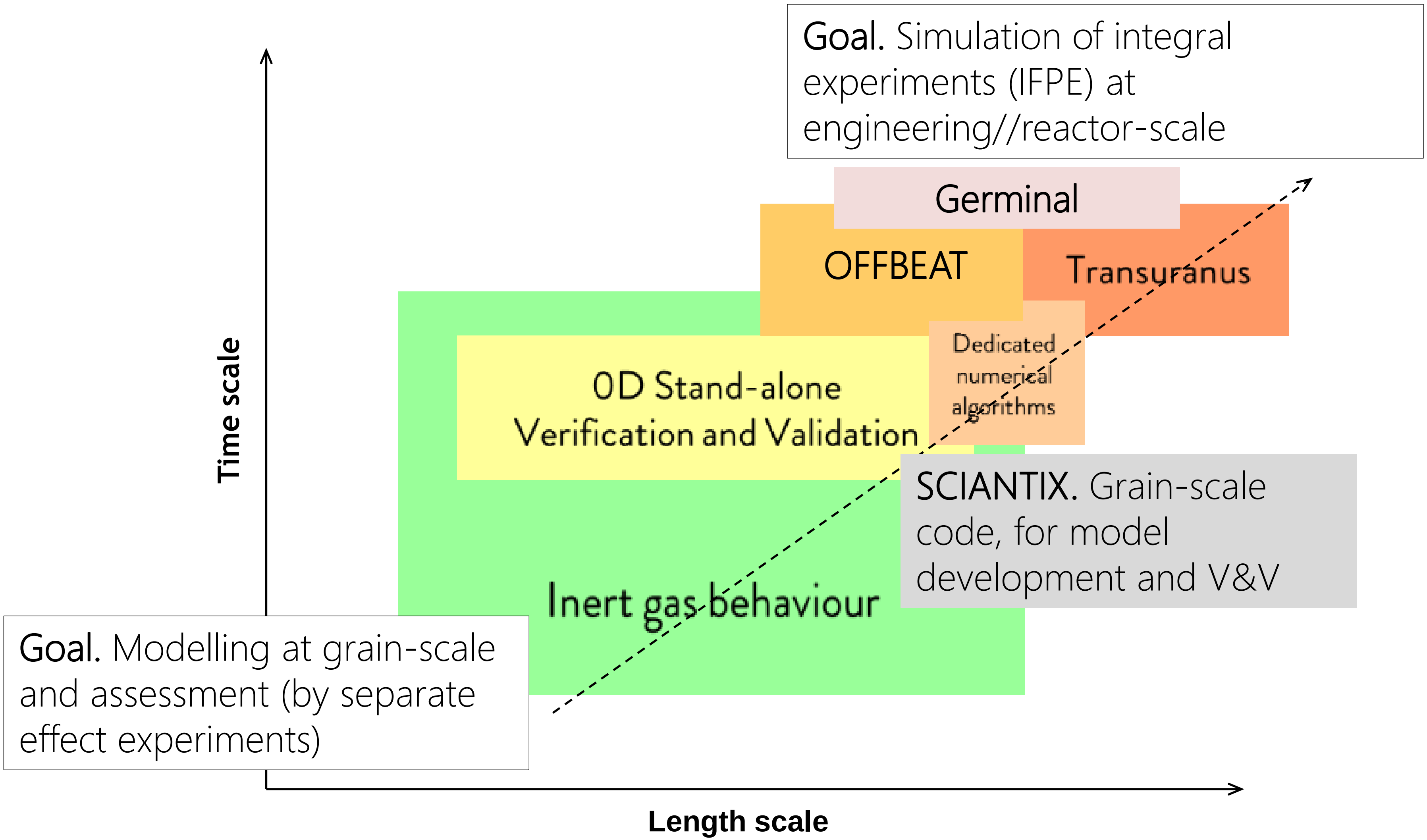
Nuclear fuel rod (ThR//FR) is made of a **stack of oxide (UO_2//MOX) fuel pellets** wrapped in **metallic (Zry//SS) cladding**

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

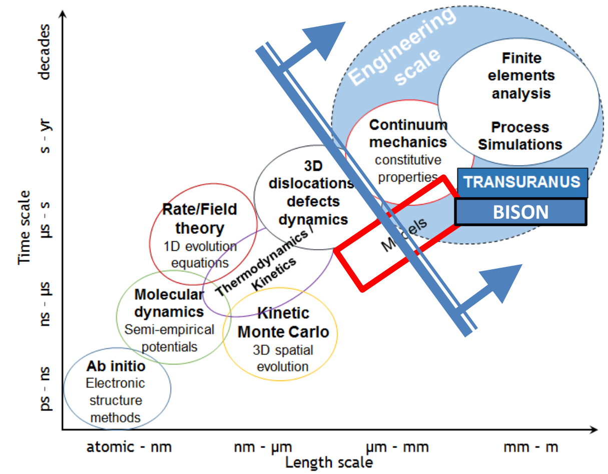
Multi-scale modelling approach, this work



Multi-scale modelling approach, requirements

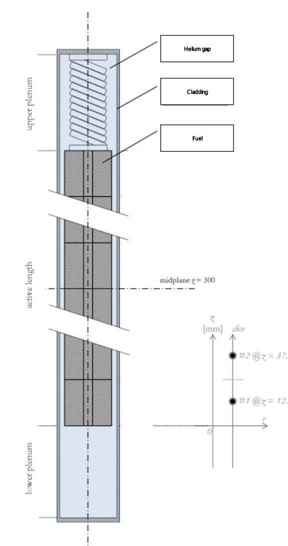
Physics-based modelling is fundamental in order to act as bridge between different scales

- 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



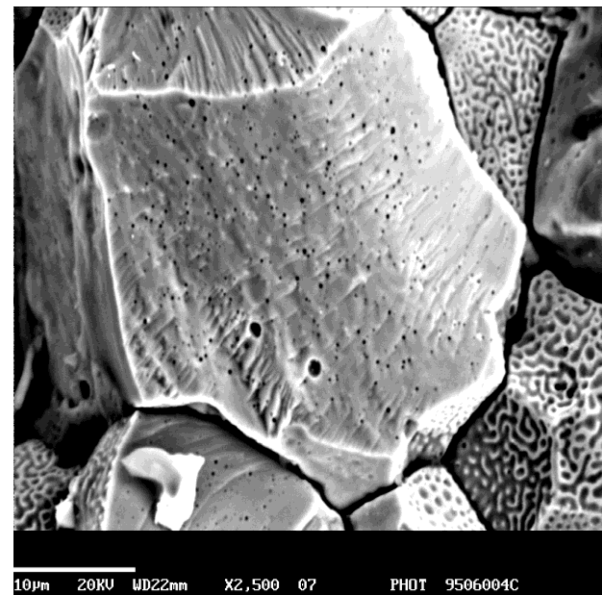
The SCIANTIX code, features

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**

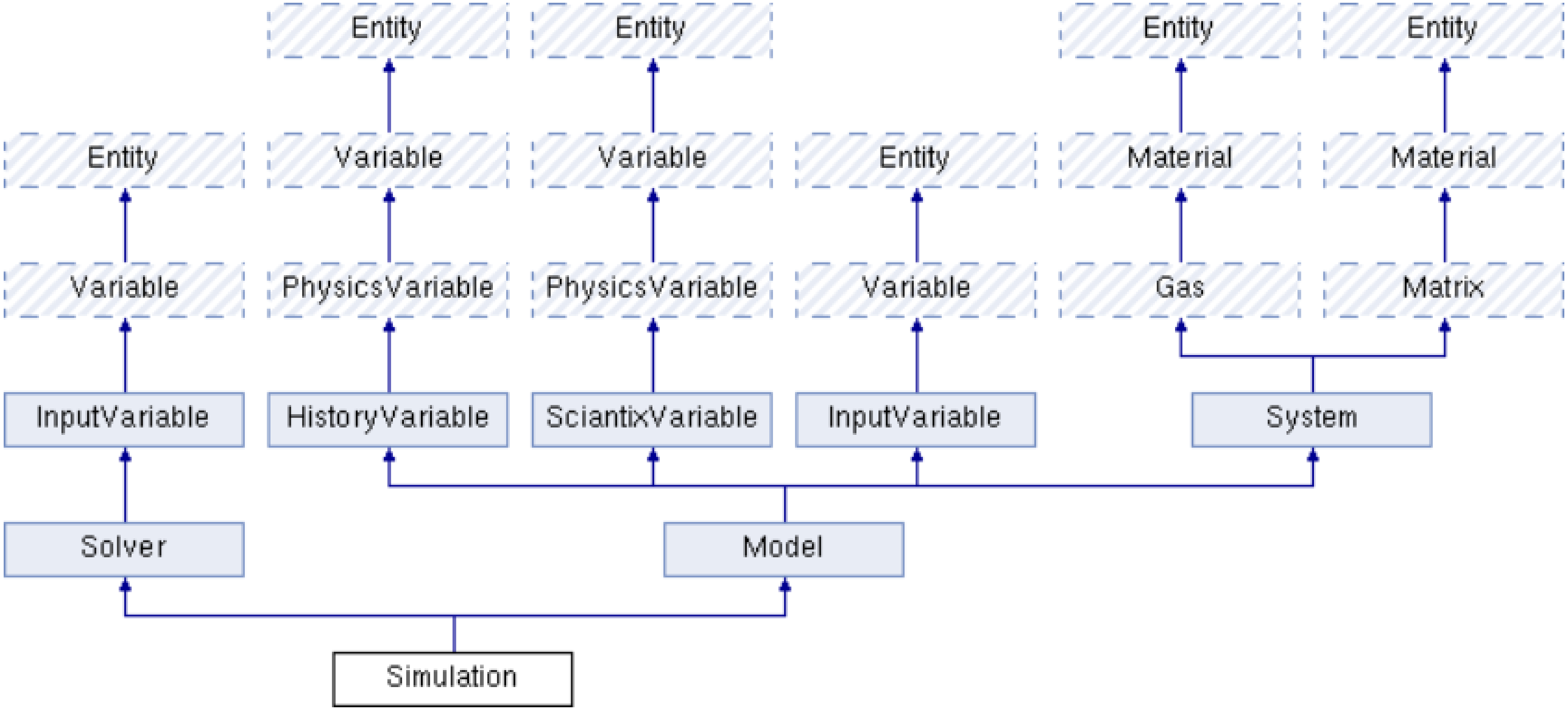
It can be **included in existing multiphysics platforms and fuel performance codes as a module (via simple interface)** to evaluate fission gas release and gaseous swelling or can be **used as stand-alone**



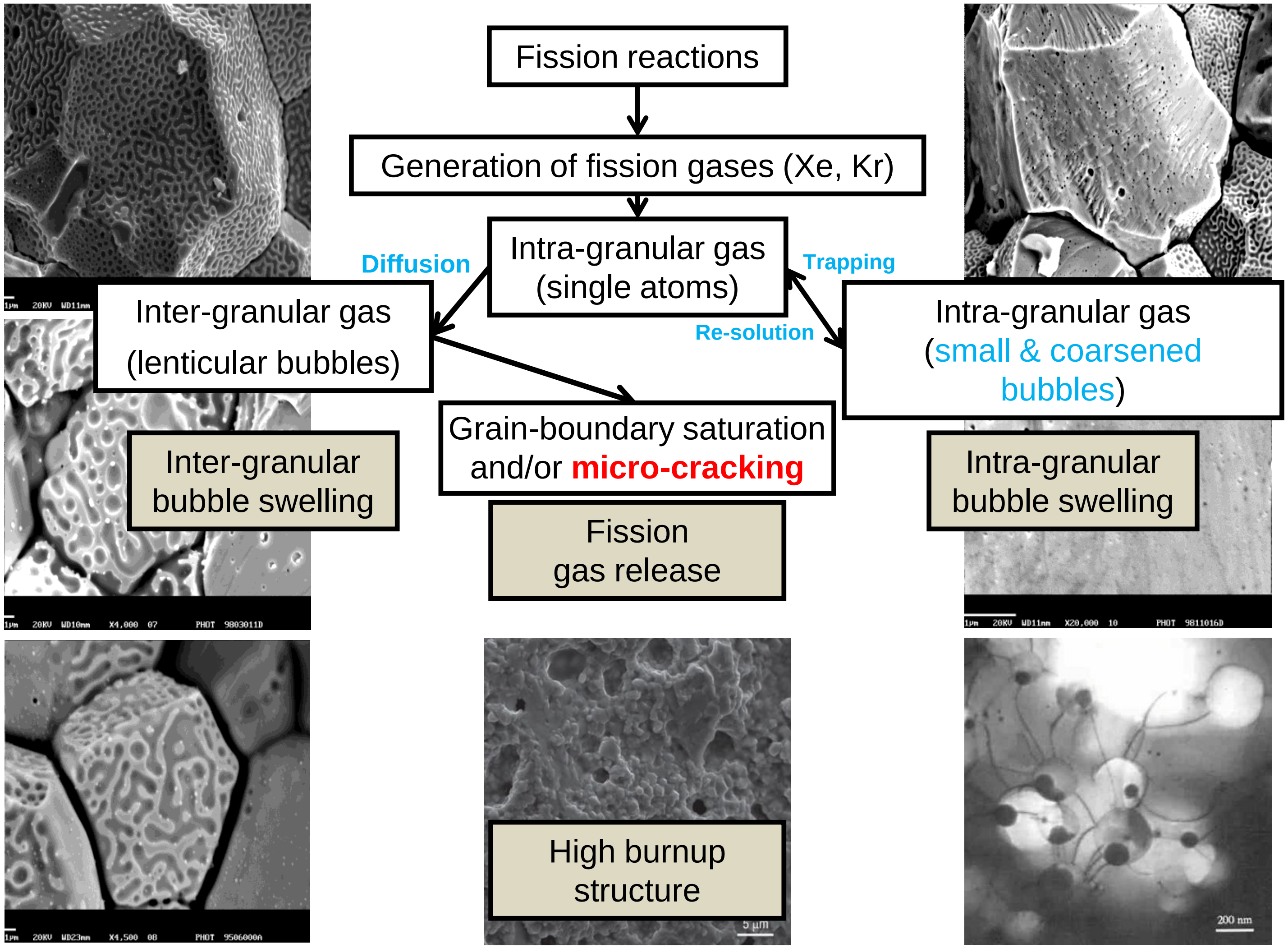
Available as open-source software (MIT license)

D. Pizzocri, T. Barani, L. Luzzi, 2020. SCIANTIX: A new open source multi-scale code for fission gas behaviour modelling designed for nuclear fuel performance codes, Journal of Nuclear Materials, 532, 152042

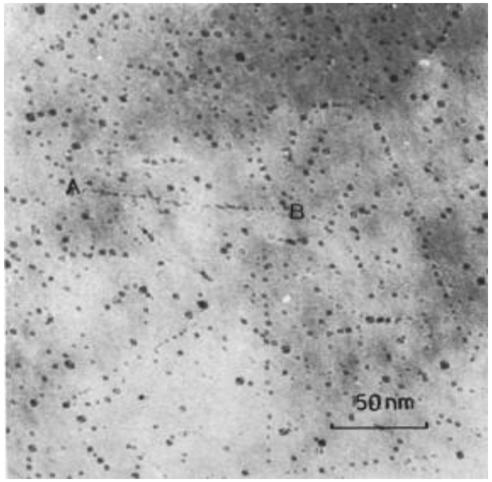
Object-oriented structure



The SCIANTIX code, physical aspects

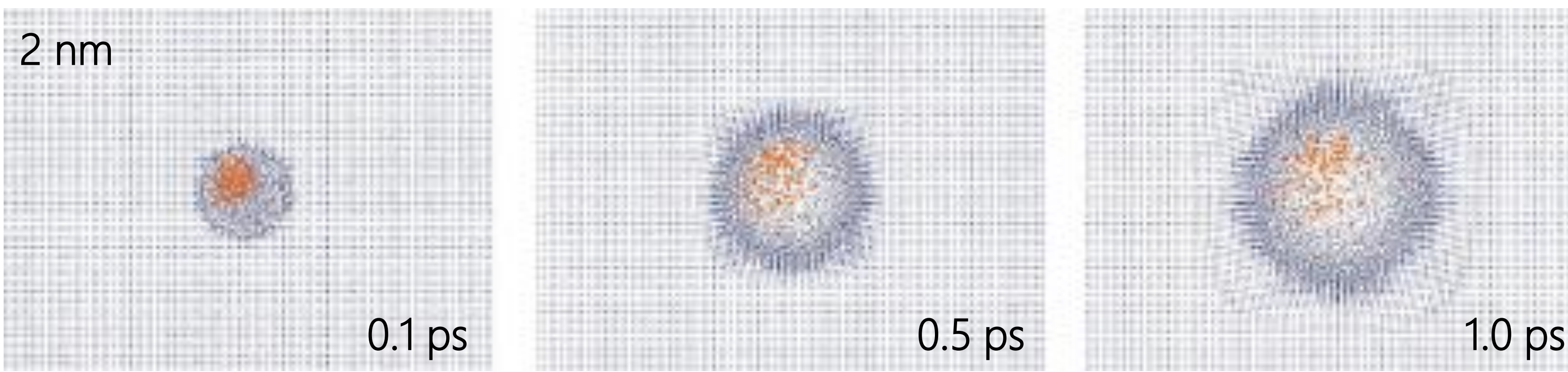


Applicative modelling example
Intra-granular model



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

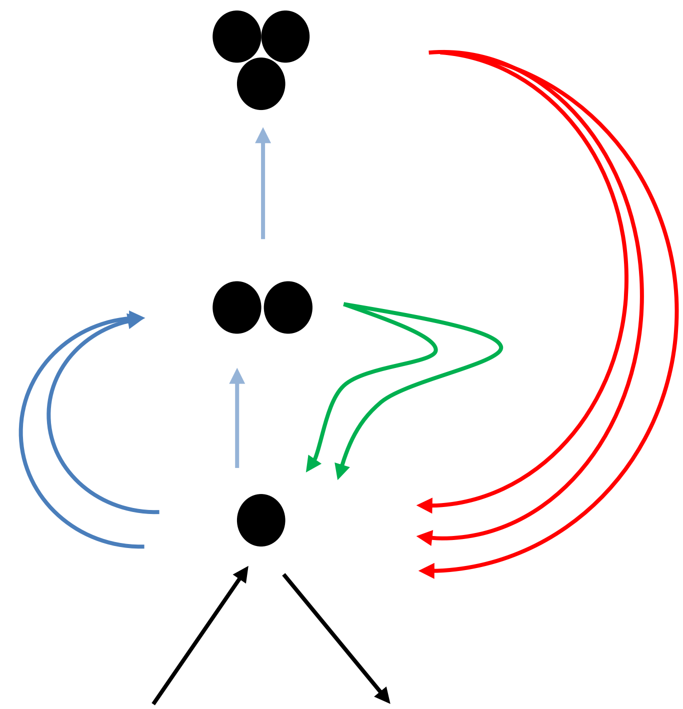


Govers et al., J. Nucl. Mater., 2012

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



$$\frac{dN}{dt} = \nu - b_{\bar{n}} N$$

$$\frac{d\bar{n}}{dt} = g_{\bar{n}} c_1 - b_{\bar{n}} \bar{n}$$

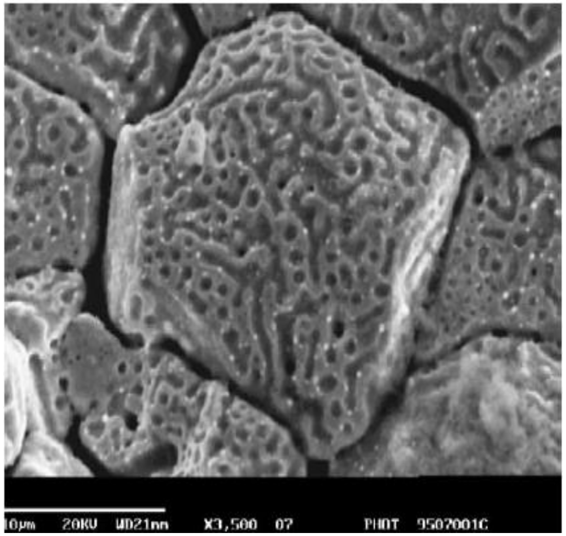
$$\frac{d\mathrm{Var}[n]}{dt} = \cdots$$

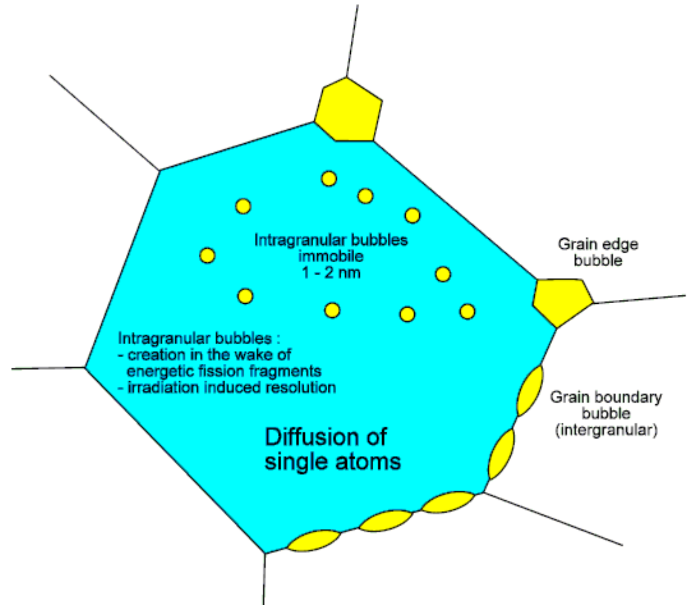
```
case 1 :
{
  std::string reference = "Pizzocri et al., JNM, 502 (2018) 323-330";
  std::vector<double> parameter;
  parameter.push_back(model[sm["Resolution rate"]].getParameter().front());
  parameter.push_back(model[sm["Nucleation rate"]].getParameter().front());

  model[model_index].setParameter(parameter);
  model[model_index].setRef(reference);

  break;
}
```

Sciantix

Pizzocri et al., 2018. JNM

Inter-granular model

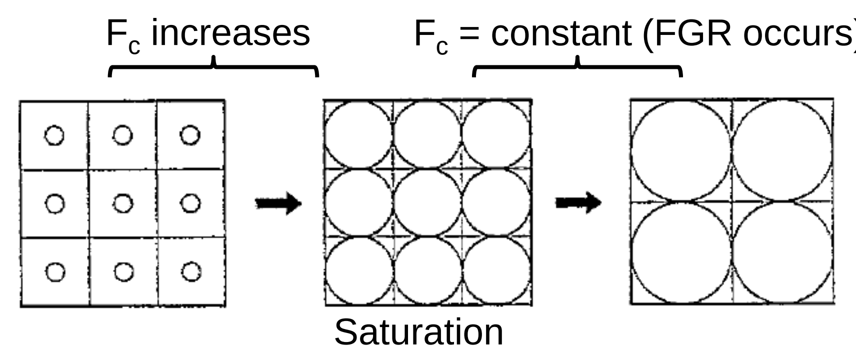




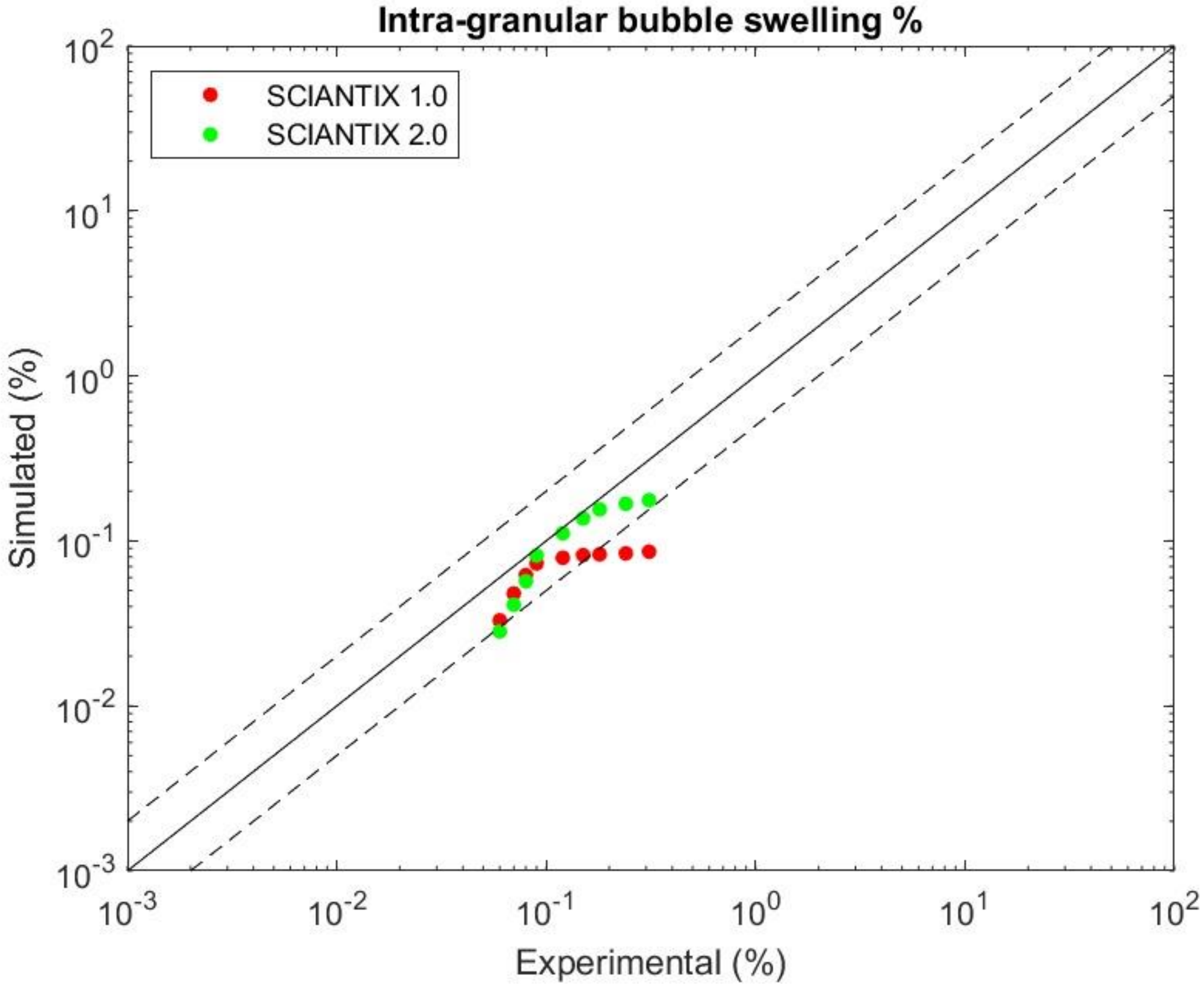
- Grain-boundary bubbles **growth** by vacancy absorption and **coalescence**
- A **saturation value of the fractional coverage** of the grain-faces is considered
- At saturation, further bubble growth is compensated by **gas release**

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

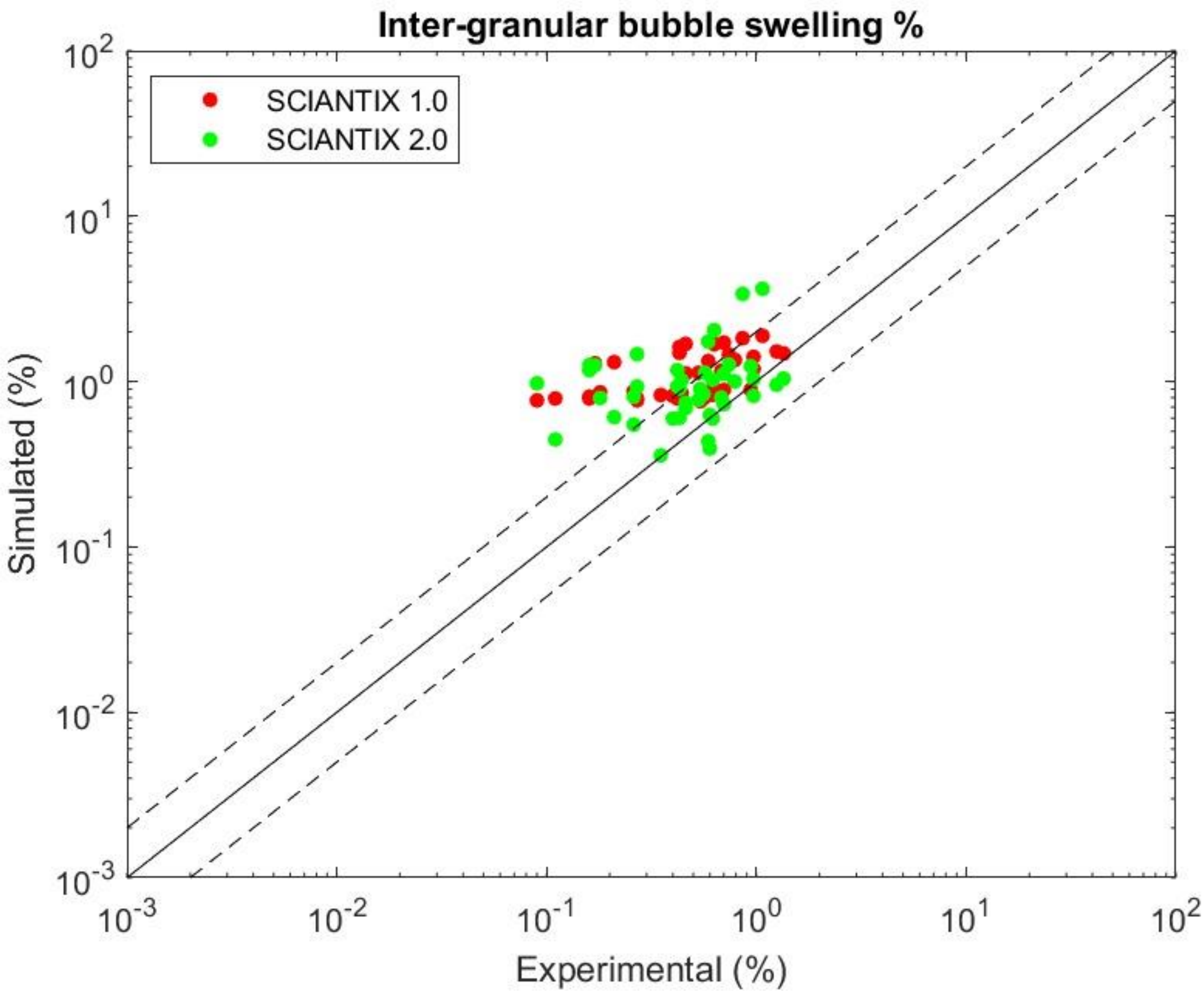
$$\frac{dF_c}{dt} = \frac{d\left(N_{gf} A_{gf}\right)}{dt} = 0 \quad if \;\; F_c = F_{c,sat}$$



Pastore et al., 2013, NED

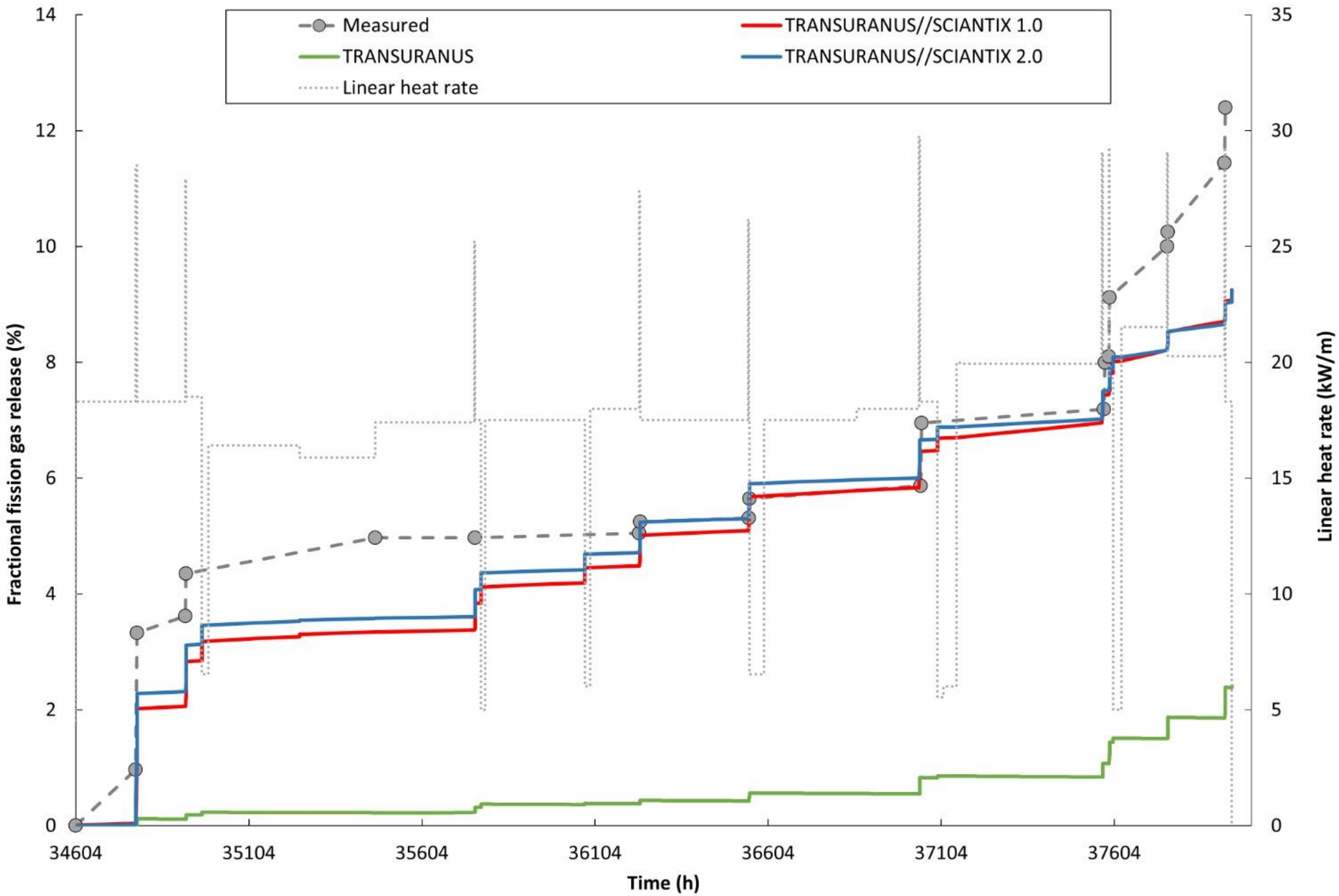


Data from Baker, 1977. JNM



Data from White et al., 2006

Coupling with fuel performance codes



HATAC C2

SCIANTIX capabilities, summary

- Intra- and inter-granular fission gas behaviour
- Consistent representation of fission gas release and swelling
- Up to date state-of-the-art models available
- Validated on separate effect experiments
- Succesfully coupled with several fuel performance codes
- Available open source under MIT license
  https://gitlab.com/poliminrg/sciantix

E&T

- Used and developed in 10+ MSc theses since 2018
- Used and developed in 5 PhD theses
- Training sessions organized in the frame of H2020 Projects
  (30+ participants)

SCIANTIX2.0 achievements and future developments

- The development of an **object-oriented version** has been performed, to ease the incorporation/coupling in/with other opensource tools and ensure the maintainability of the code

- The **documentation** of the code is progressively going to be integrated with a video-manual and doxygen

- The **verification** of solvers via MMS is soon to be included in the repository

- The inclusion of a set of regression tests has been realized

Acknowledgements
Involvement in on-going international projects

INSPYRE — Investigations Supporting MOX Fuel Licensing in ESNII Prototype Reactors

PATRICIA

Extend modelling of FGB in MOX fuels FRs

- Helium behaviour
- Grain-boundary venting
- Columnar grains

R2CA — REDUCTION OF RADIOLOGICAL ACCIDENT CONSEQUENCES

Include description of fission products in LWRs

- Production and transport of key FPs
- Coupling with FRAPCON/FRAPTRAN

OperaHPC — Coupling and extension for HPC tools

EGRFP/NEA — Code-to-code benchmark on transients