

# Materials Modeling and Simulation of Nuclear Fuels (MMSNF) workshop series

Marius Stan

Senior Scientist, Argonne National Laboratory, Nuclear Engineering Division

Senior Fellow, University of Chicago, Computation Institute

# MMSNF in a nutshell

## Scope

- The workshop series aims at stimulating research and discussions on models and simulations of nuclear fuels and coupling the results into fuel performance codes [1].
- Although centered on multi-scale model development and computer simulations, close connections to theory, experiment and technology are encouraged

## Format

- Annual, itinerant (Americas, Europe, Asia)
- Every two years is part of the NuMat conference
- All talks are plenary (no parallel sessions) plus poster session
- All talks are contributed (no invited)
- The Chair of the Local Committee is also Program Chair and decides on the agenda, in consultation with the International Committee
- Each edition includes a new, “hot topic” session proposed by the Local Committee

## Other

- Small registration fee
- Some support for students

## The advent of “Modeling” and “Simulations”

### “Towards Building Modeling and Simulation for Nuclear Fuels Qualification

The goal of this project is to build a set of models and computer programs that are able to simulate the properties and behavior of the ceramic and metallic nuclear fuel materials during fabrication, operation, and storage. The programs will use information about the physico-chemical properties of materials and the dependence of these properties upon temperature, pressure, composition, irradiation, and other constraints imposed by the environment or by internal processes.

The computer programs and experimental setups will be grouped in modules able to simulate phenomena that occur during the various stages of processing the fuel: nuclear and chemical reactions, formation or decomposition of compounds, phase transformations, irradiation effects, swelling, creep, etc.

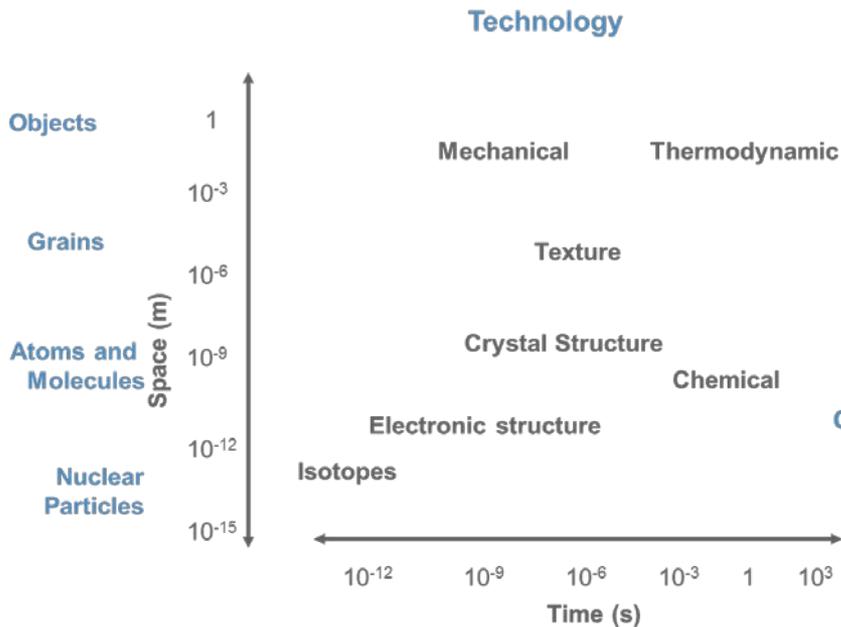
Given accurate data and reliable models for phenomena, the interconnected modules will guide the technological process of fabrication and assist the fuel operation. The information will be also useful for monitoring the fuel in storage.

**The modules will assist the Nuclear Fuel Qualification”**

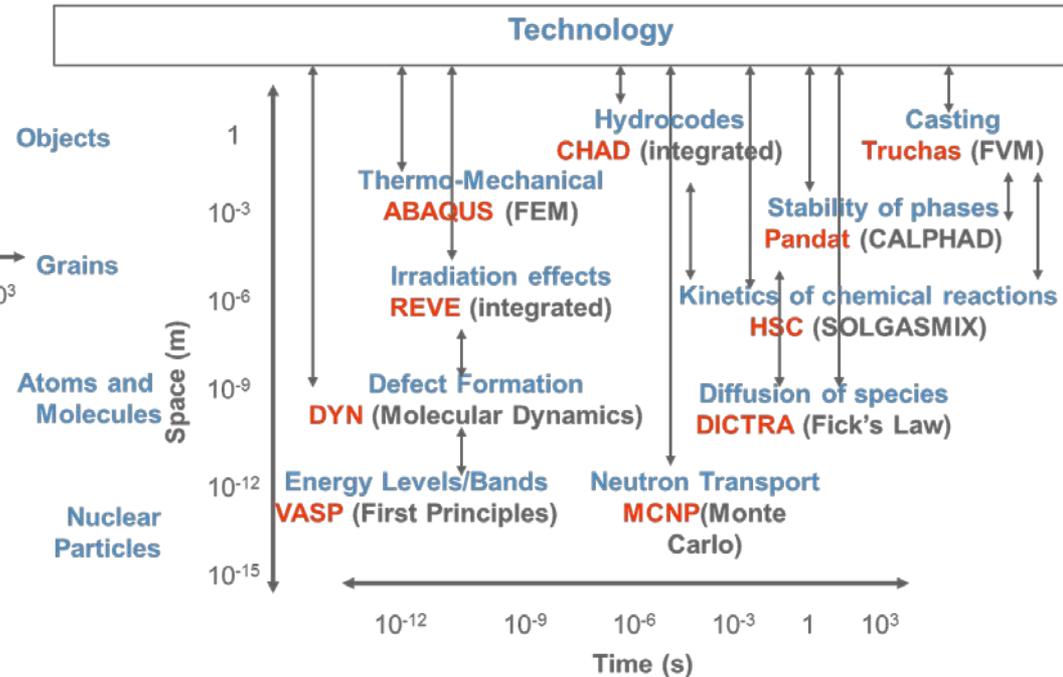


# All about multi-scale

## Modeling Scales



## Simulation Scales

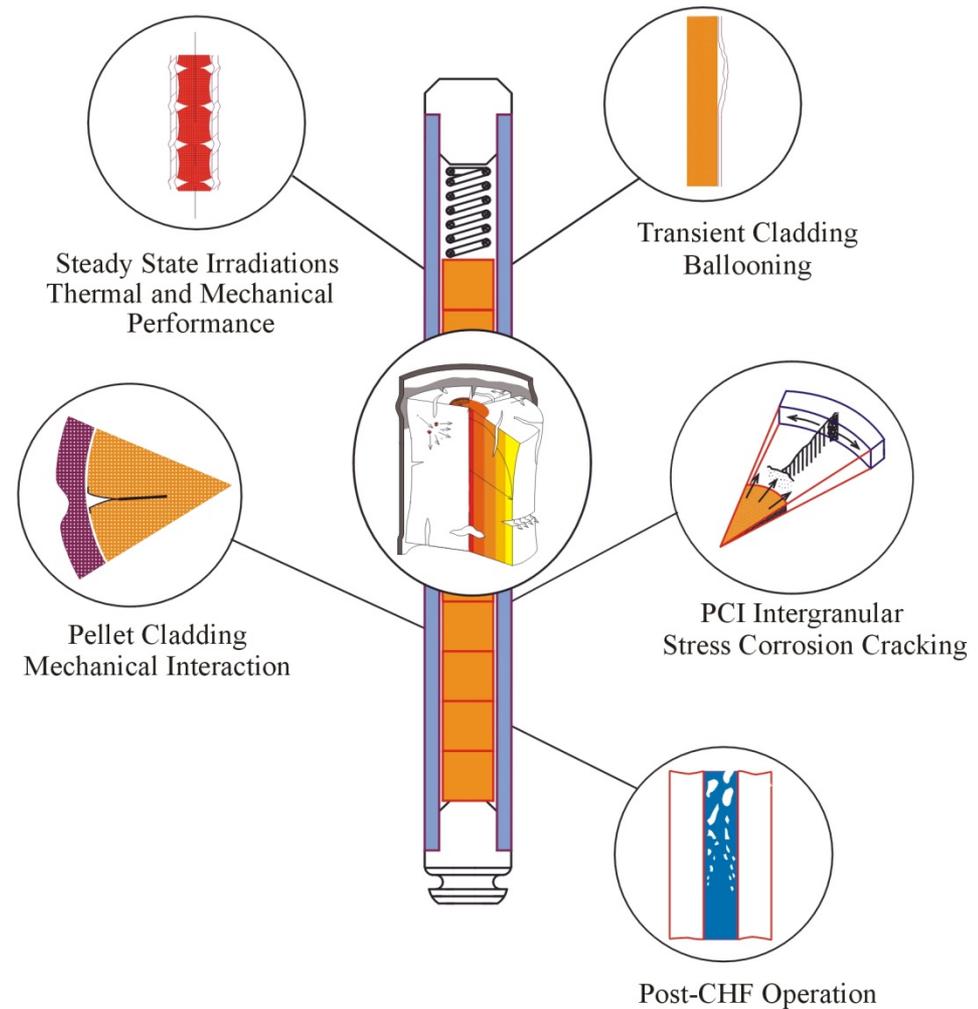


Scope: define mathematical models of fuel properties and run computer simulations of relevant phenomena



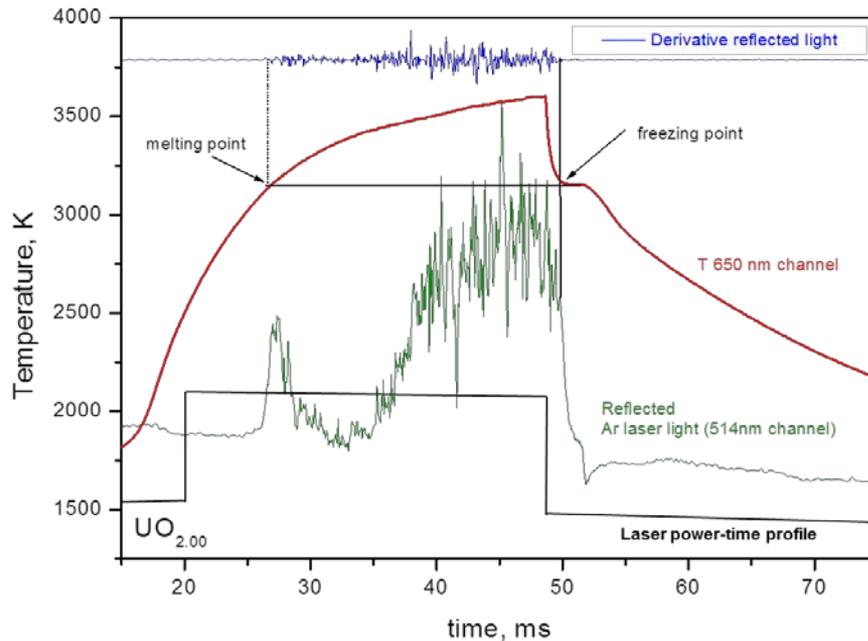
## The push for "fuel codes"

Agenda starts with presentations of FRAPCON, FRAPTRAN, TRANSURANUS, PLEIADES, PARFUME, BISMATH,... end ends with a discussion of FALCON

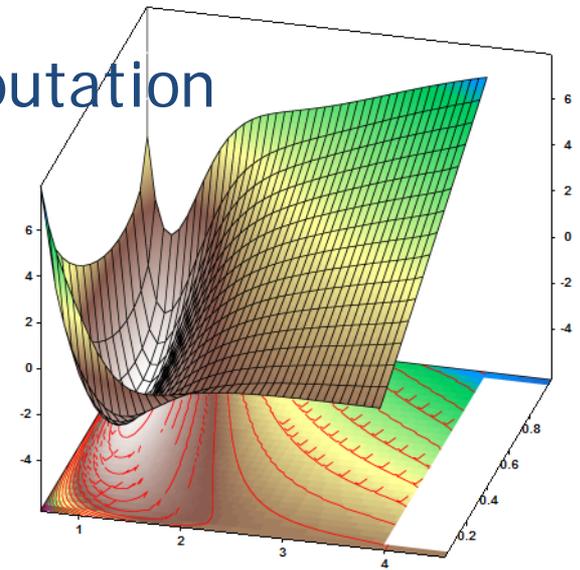


# The holy trinity: theory, experiment, computation

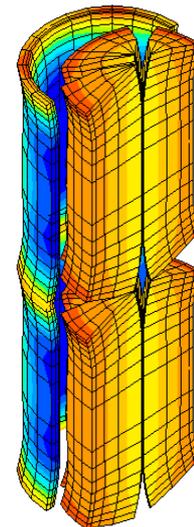
A more balance approach includes models, simulations and experimental results



D. Manara, MMSNF-3.



B. Uberuaga, MMSNF-3.



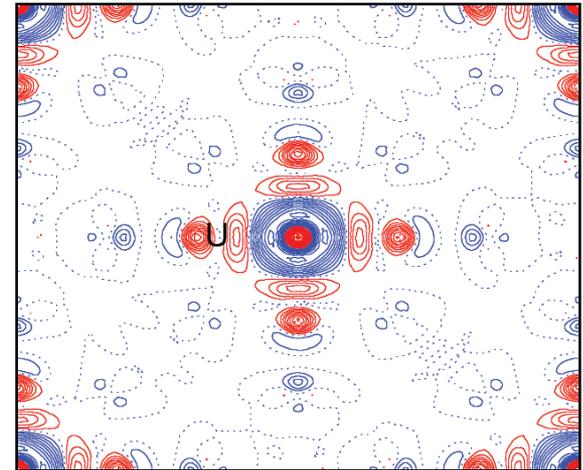
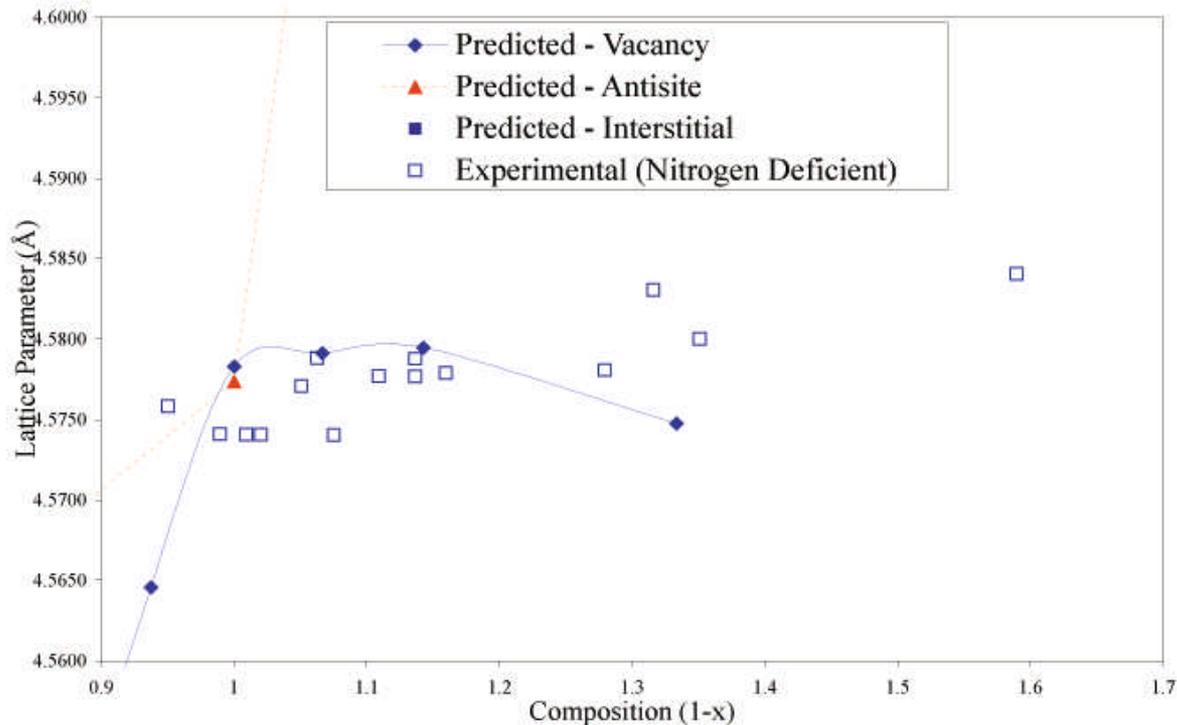
D. Plancq, MMSNF-3.



## What fuel?

Nitrides are promising and so are inert matrix and TRISO fuels. Can MMSNF help with the decision?

Lattice parameter as a function of nonstoichiometry for  $Zr(1-x)N$



E. Kotomin, MMSNF-4

C. Stanek, MMSNF-4



## Integration

Following extended discussions of theoretical, computational and experimental results, for the first time a session is dedicated to integration.



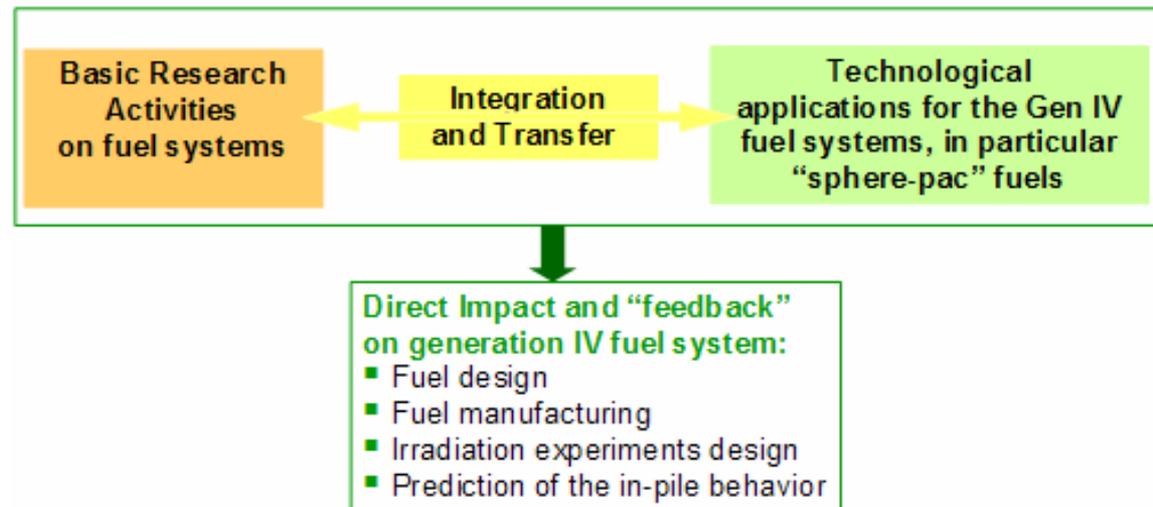
## Thermodynamics

Thermodynamic stability of fuels and reactor materials is examined using electronic structure, molecular dynamics and CALPHAD methods.



## In the spot light

MMSNF gets the attention of national and international programs such as F-BRIDGE (EC) and GNEP (USA). Models and simulations are now “cool”.

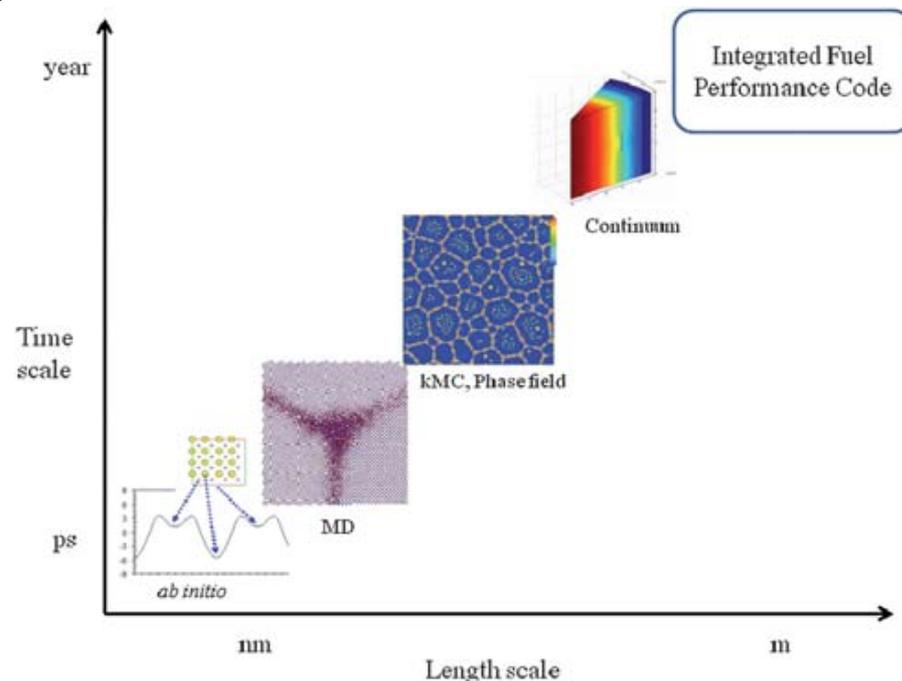
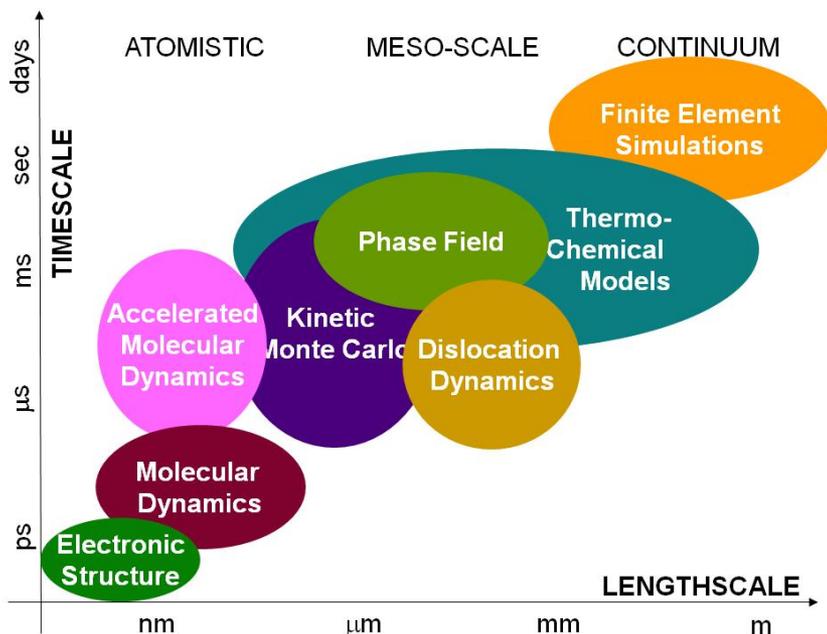


C. Valot, F-BRIDGE program



## Connecting the scales

The multi-scale concept is refined and applied to fuels design. The first MMSNF-based journal article is published.



R. Devanathan, *et al.*, Energy Env. Sc., **3** (2010) 1406-1426.



## Yes, we can.

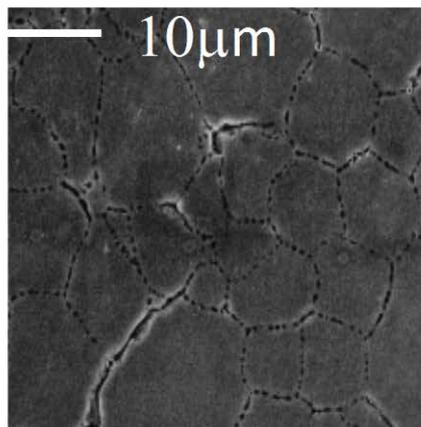
MMSNF is part of the first NuMat conference. Multi-scale predictions of fuel properties are presented:

- “Ab-initio molecular dynamics simulations of actinide materials”
- “Atomistic Modeling of Fuel-Cladding Interaction”
- “Intragranular bubbles impact on nuclear fuel properties”
- “Integrating Mesoscale Models of Microstructural Evolution of Uranium Dioxide Fuel within Continuum-scale Models of Thermo-mechanical Behaviour of Nuclear Fuel Elements”

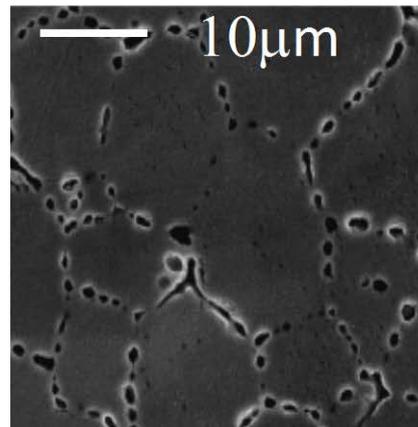
We made significant progress. What's next?



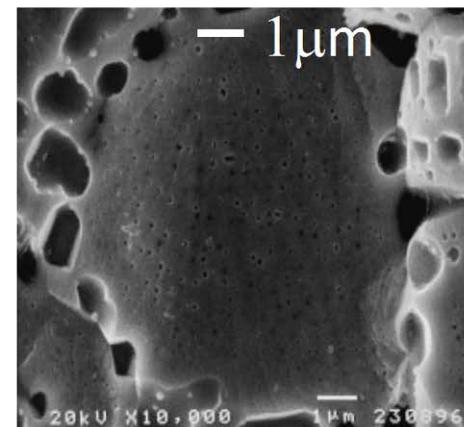
## Meso-scale



5mins/1715°C



300mins/1715°C



5hours/1715°C

Fission gas bubble evolution in UO<sub>2</sub> during heat treatment

Challenge: Develop models of fuel micro(nano) structures and simulate the behavior in reactor conditions. Then optimize.

## Heterogeneity

MMSNF is part of the second NuMat conference.

Heterogeneity is discussed at atomistic and meso-scale levels, with impact on materials design.



## Extreme conditions

Irradiation effects and high temperature thermo-chemistry take center stage.

