Working Party on Multiscale Modelling of Fuels and Structural Materials for Nuclear Systems **(WPMM)**

Expert Group on Multiscale Modeling of Fuels (M2F)

T. Besmann (Chair, University of South Carolina)
C. Valot (Vice-Chair, CEA)
M. Freyss (CEA)
S. Massara (NEA)

EGATFL-03 Task Force 1 Meeting

4th March 2015, Paris

NSC activities

Nuclear Science Committee (NSC)

Expert Group on Integral Experiments for Minor Actinide Management

Working Party on International Nuclear Data Evaluation Co-operation (WPEC)

- High Priority Request List for Nuclear Data
- Methods and Issues for the Combined Use of Integral Experiments and Covariance Data
- Co-ordinated Evaluation of ^{239}Pu in the Resonance Region
- Scattering Angular Distribution in the Fast Energy Range
- Evaluation of Experimental Data in the Resolved Resonance Region

Working Party on Scientific Issues of the Fuel Cycle (WPFC)

- Heavy Liquid Metal Technologies
- Fuel Recycling Chemistry
- Advanced Fuel Cycle Scenarios
- Innovative Structural Materials
- Innovative Fuels
- Task Force on Benchmarking of Thermal-hydraulic Loop Models for Lead-alloy-cooled Advanced Nuclear Energy Systems

Working Party on Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems (WPMM)

- Validation and Benchmarks of Methods
- Multi-scale Modelling Methods
- Structural Materials Modelling
- Multi-scale Modelling of Fuels
- Primary Radiation Damage

Working Party on Nuclear Criticality Safety (WPNCS)

- Advanced Monte Carlo Techniques
- Criticality Safety Benchmarks
- Burn-up Credit
- Criticality Excursions
- Assay Data of Spent Nuclear Fuel
- Uncertainty Analyses for Criticality Safety Assessment

Working Party on Scientific Issues of Reactor Systems (WPRS)

- Reactor Physics and Advanced Nuclear Systems
- Uncertainty Analysis in Modelling
- Reactor Fuel Performance
- Radiation Transport and Shielding

Executive Group of the NSC (Data Bank Management Committee)

Databases and Scientific Services

The Scientific Co-ordination Group of the Joint Evaluated Fission and Fusion (**JEFF**) Data Project

Thermodynamics of Advanced Fuels International Database (TAF-ID)

Expert Group on Accident Tolerant Fuels

Expert Group on MP Experimental Data, Benchmarking and Validation

NSC activities related to fuels

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NSC activities related to fuels and structural materials

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NSC material-related activities presented at EGATFL-03

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Outline

- **Working Party on Multiscale Modelling of Fuels and Structural Materials (WPMM)**
  - ❑ **Expert Group on Multiscale Modelling of Fuels (EGM2F)**
  - ❑ *Overview of Multiscale Modelling Methods EG (M3)*
  - ❑ *Overview of Structural Materials Modelling EG (SMM)*
  - ❑ *Overview of Primary Radiation Damage EG (PRD)*
  - ❑ *Overview of Task Force on Mechanisms of gaseous FP release*
- **Expert Group on Reactor Fuel Performance and IFPE Database (see next presentation)**

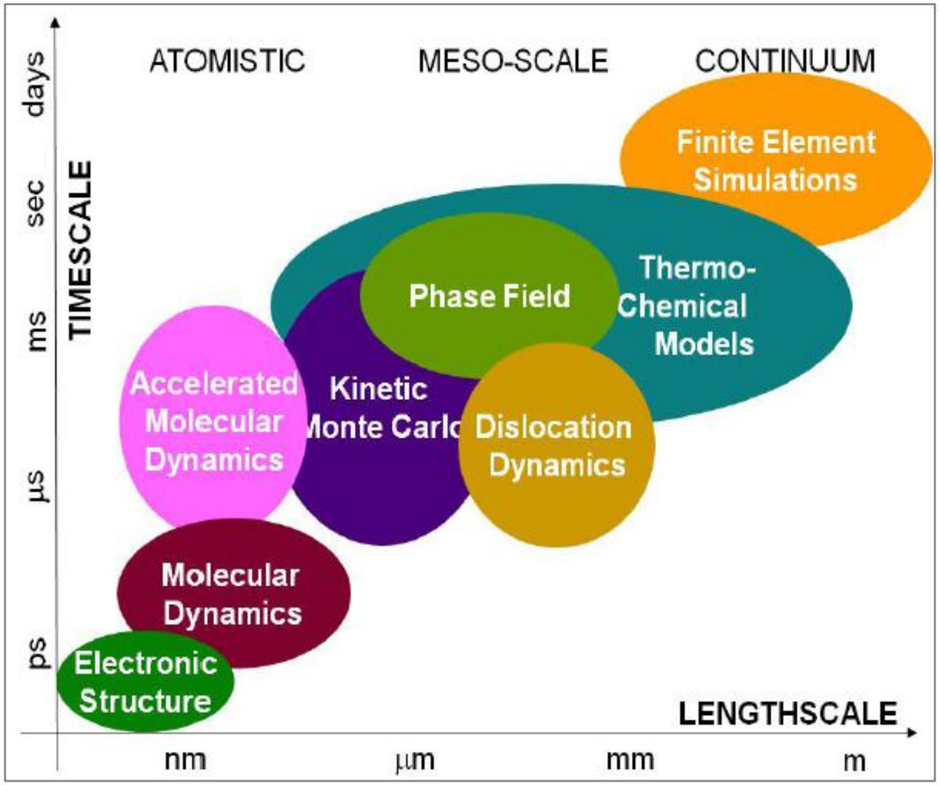
WPMM scope

Set up in 2008, renewed mandate 2014-2016

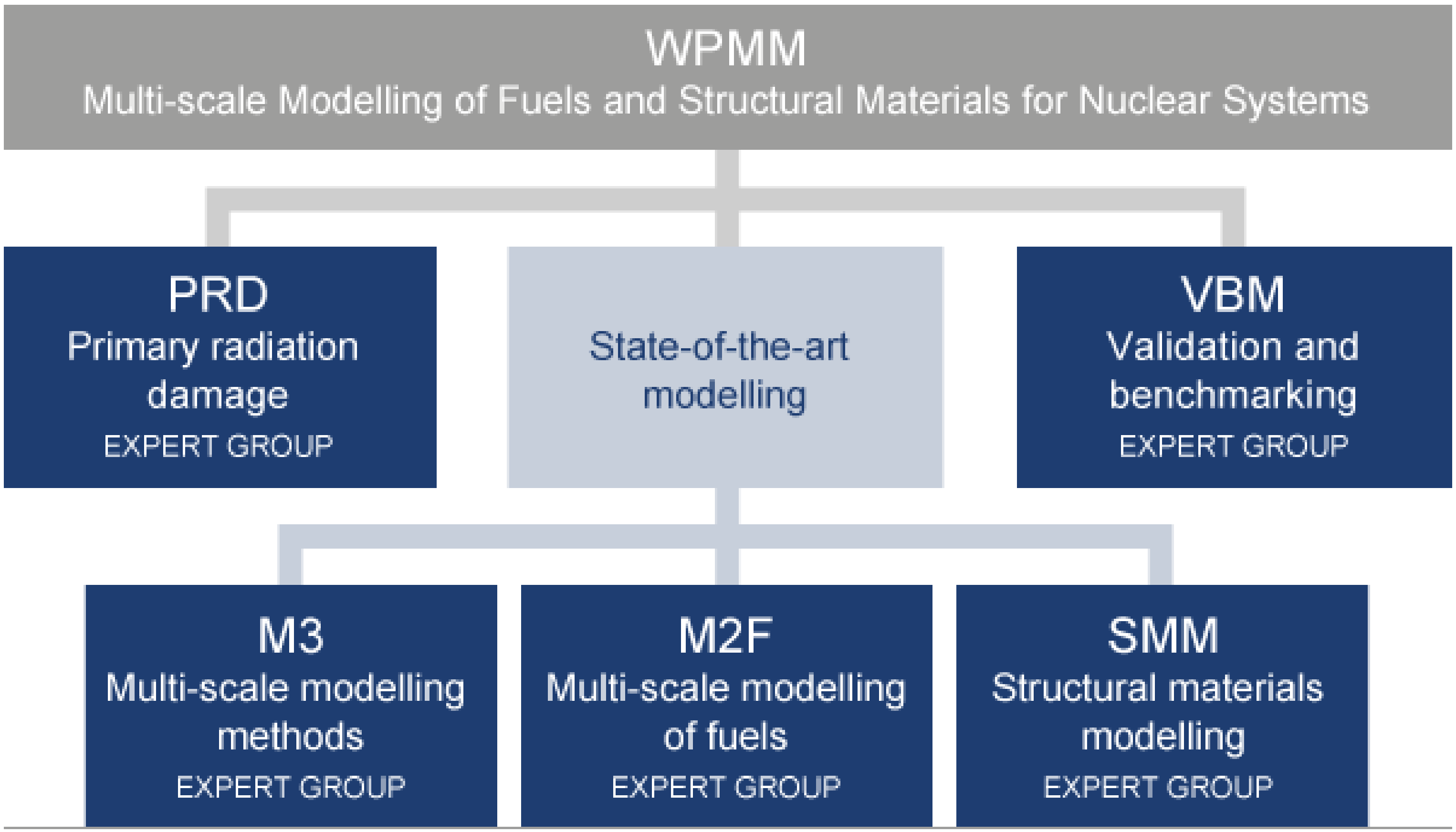
- Focused on materials science aspects of nuclear fuels and structural materials

- **Aims at promoting and developing multiscale models and simulations**

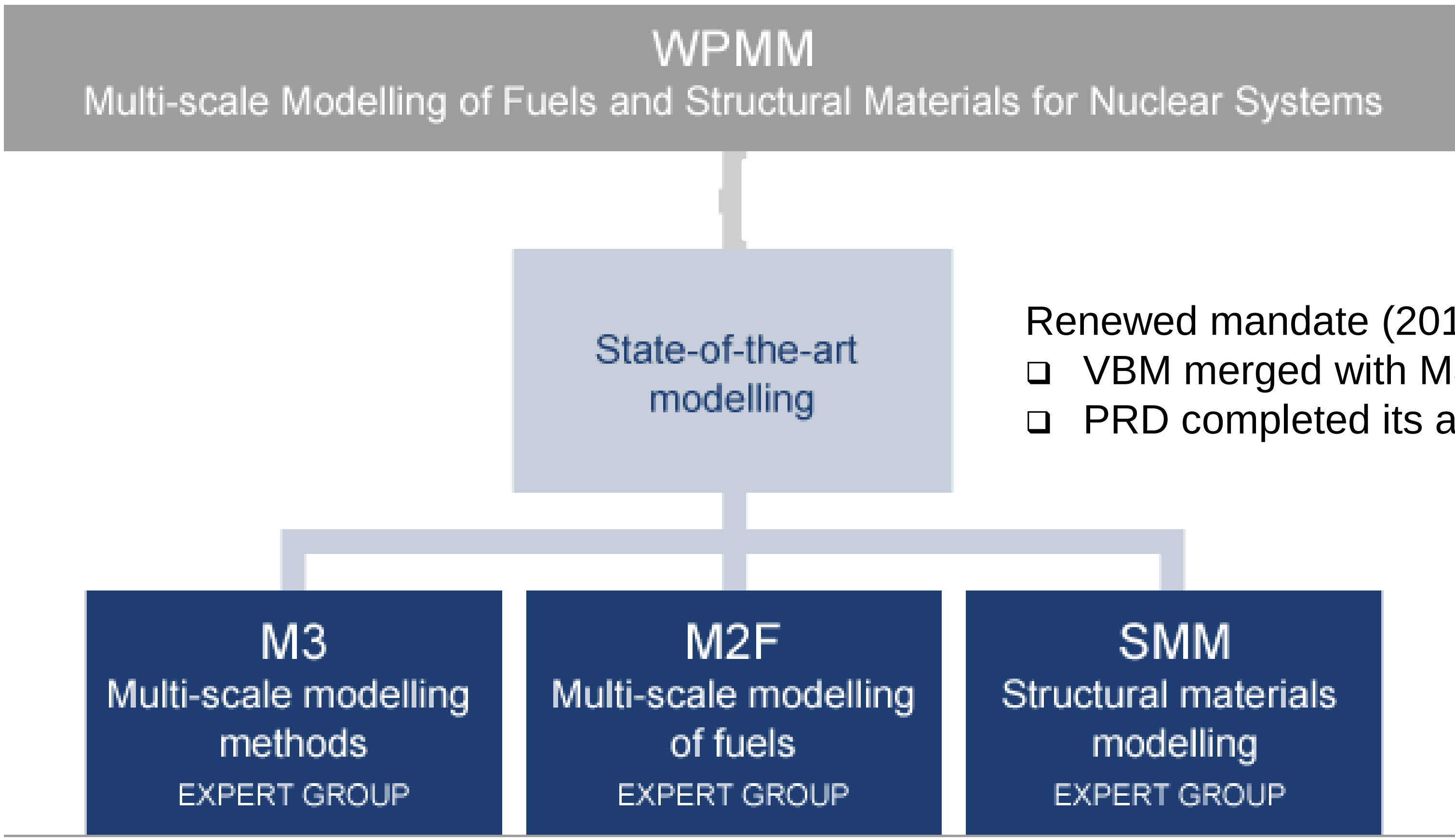
as **validated predictive** tools for nuclear fuel design, fabrication and performance



Structure of the WPMM Expert Groups (2009 – 2014)



Structure of the WPMM Expert Groups (2014 – 2015)



Renewed mandate (2014-17)

- VBM merged with M3
- PRD completed its activity

Structure of the WPMM Expert Groups (2015 – 2017)

WPMM
Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems

Task Force related to Structural Materials Modelling
(will be established in 2015)

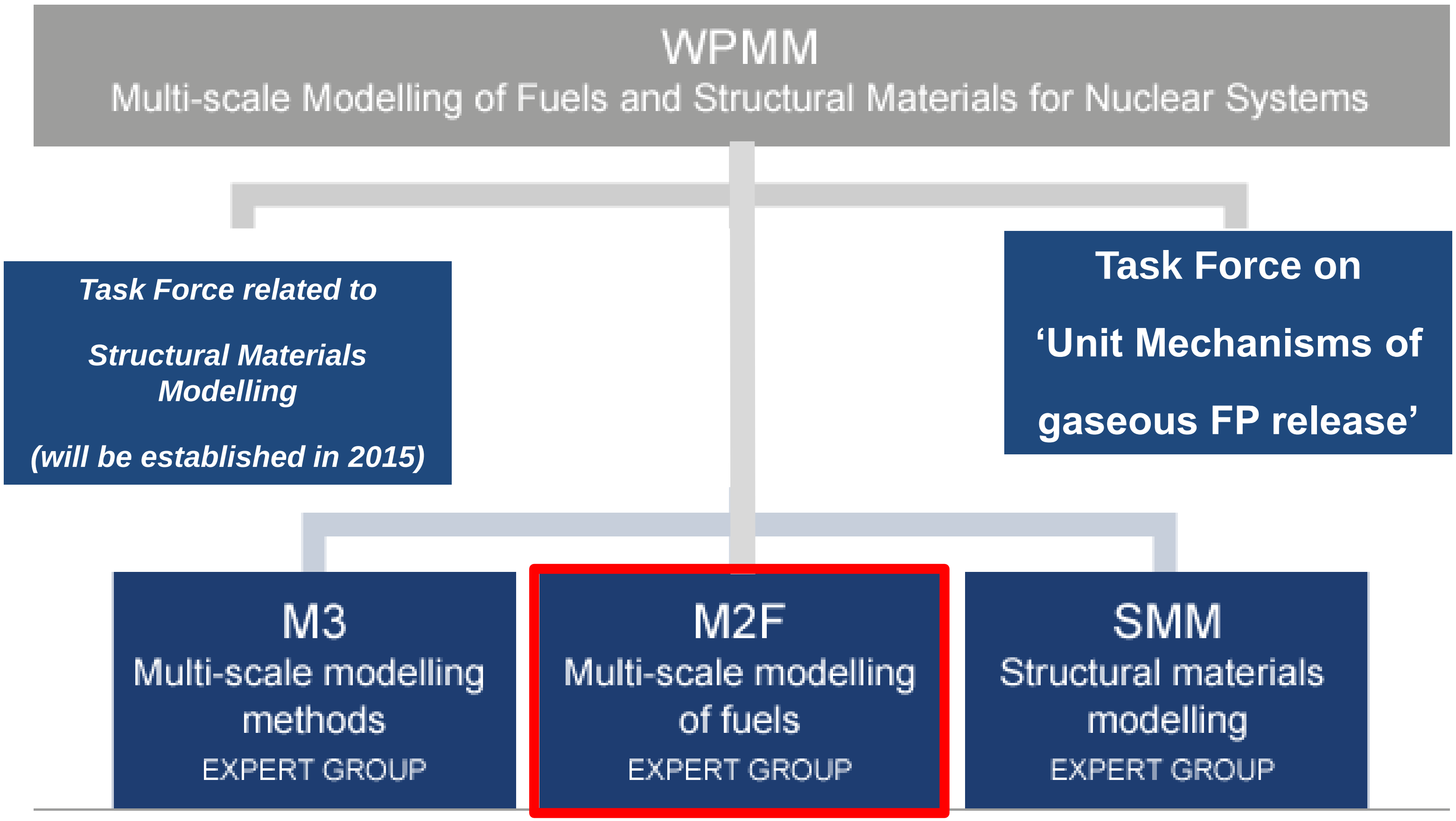
Task Force on 'Unit Mechanisms of gaseous FP release'

M3
Multi-scale modelling methods
EXPERT GROUP

M2F
Multi-scale modelling of fuels
EXPERT GROUP

SMM
Structural materials modelling
EXPERT GROUP

Structure of the WPMM Expert Groups (2015 – 2017)



EG M2F objectives

- Assess **multiscale modeling approaches** devoted to nuclear fuels from the atomic to the macroscopic scale in order to share and promote such approaches
- Address **all types of fuels**: current (mainly oxides) and advanced (oxide, carbide, nitride, metallic fuels, fuels with minor actinides)
- Foster **integration** of results from multi-scale modeling and simulation into performance codes
- Assess the quality of existing **links between the various scales** and list needs for strengthening multi-scale modeling approaches
- Promote exchange between multiscale modeling experts and **experimentalists**

EG M2F objectives

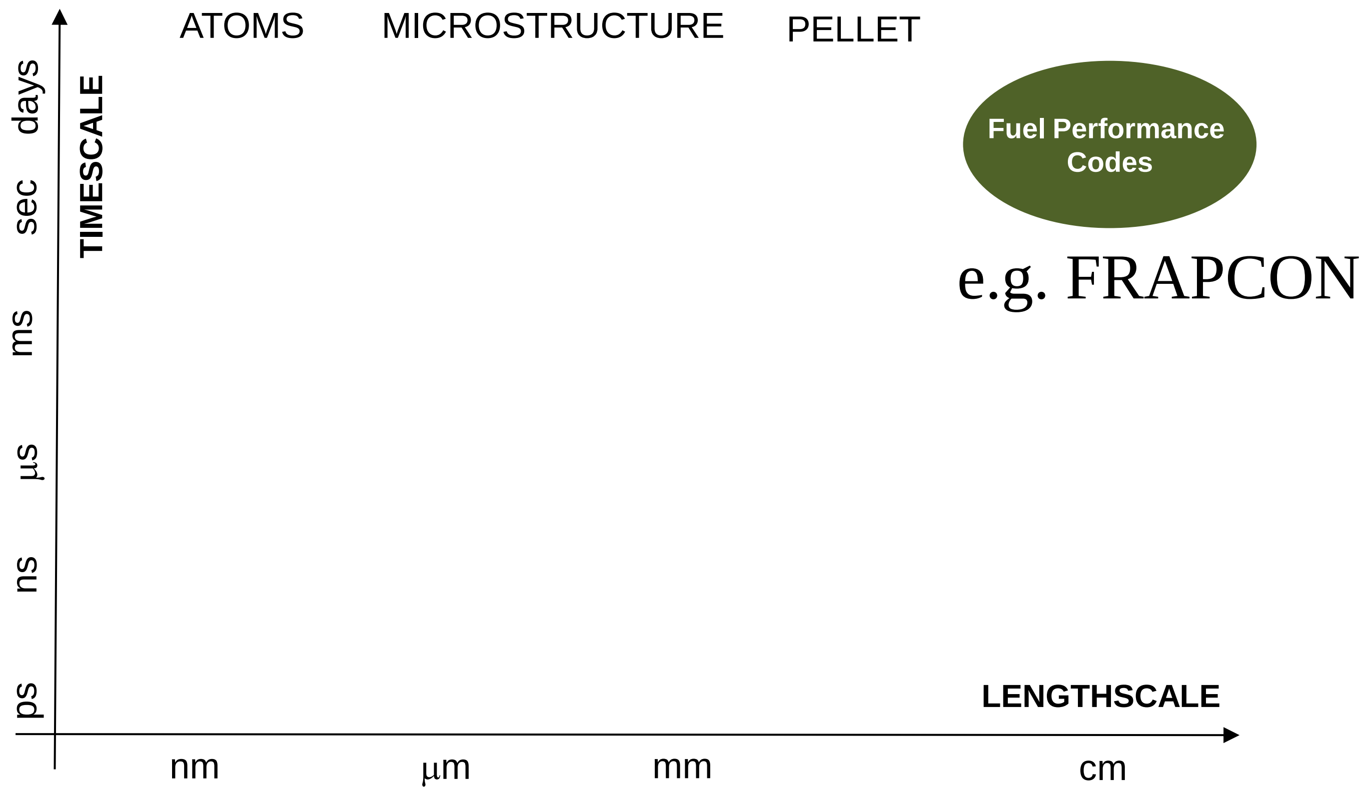
- Identify the most relevant experimental data or experimental characterization techniques that are missing for **validation of fuel multiscale modeling**

- Address **key engineering issues** associated with each type of fuels, for which combining modeling and experiment could contribute to reducing the time and resources needed to develop/improve fuels

  ➔ **Set up of Task Forces**

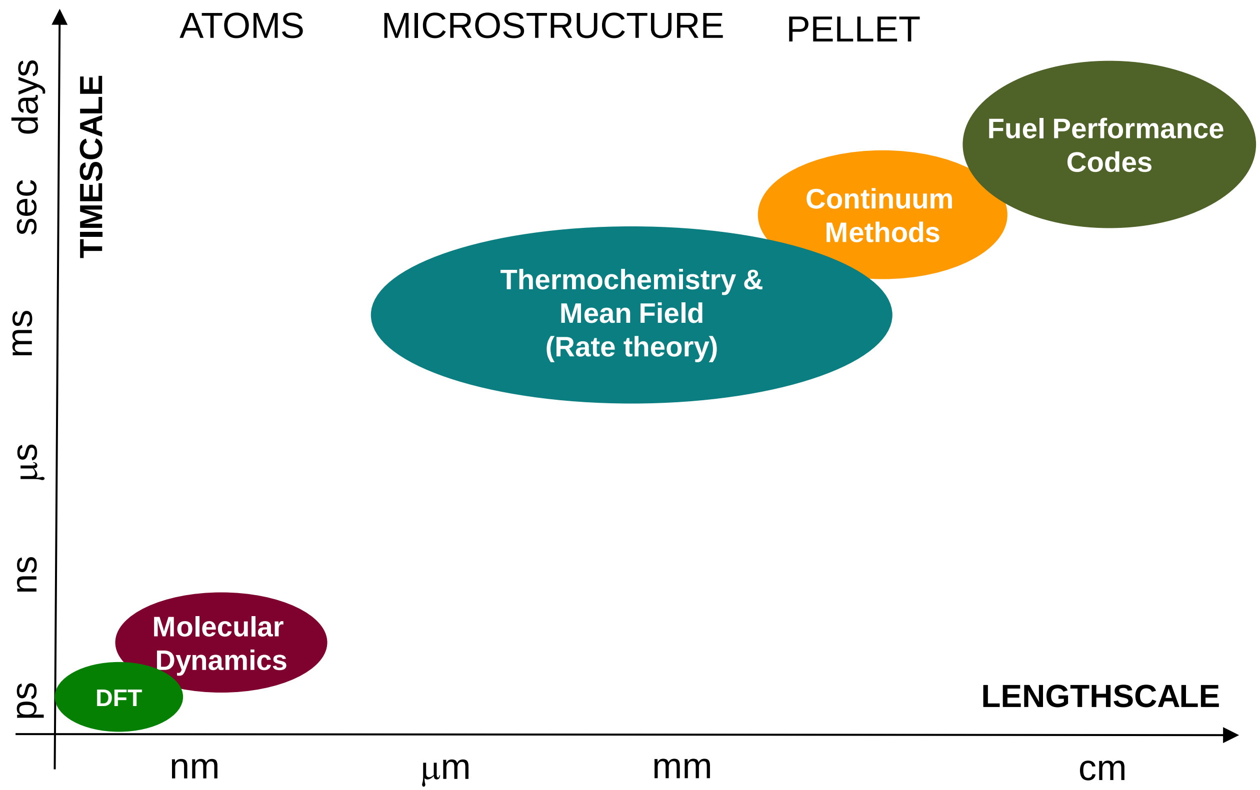
- Foster international **cooperation on multiscale modeling** of nuclear fuels by sharing **state-of-the-art models, expertise, progress and key issues in multiscale modeling**

Computational Approaches: Practicing Engineer



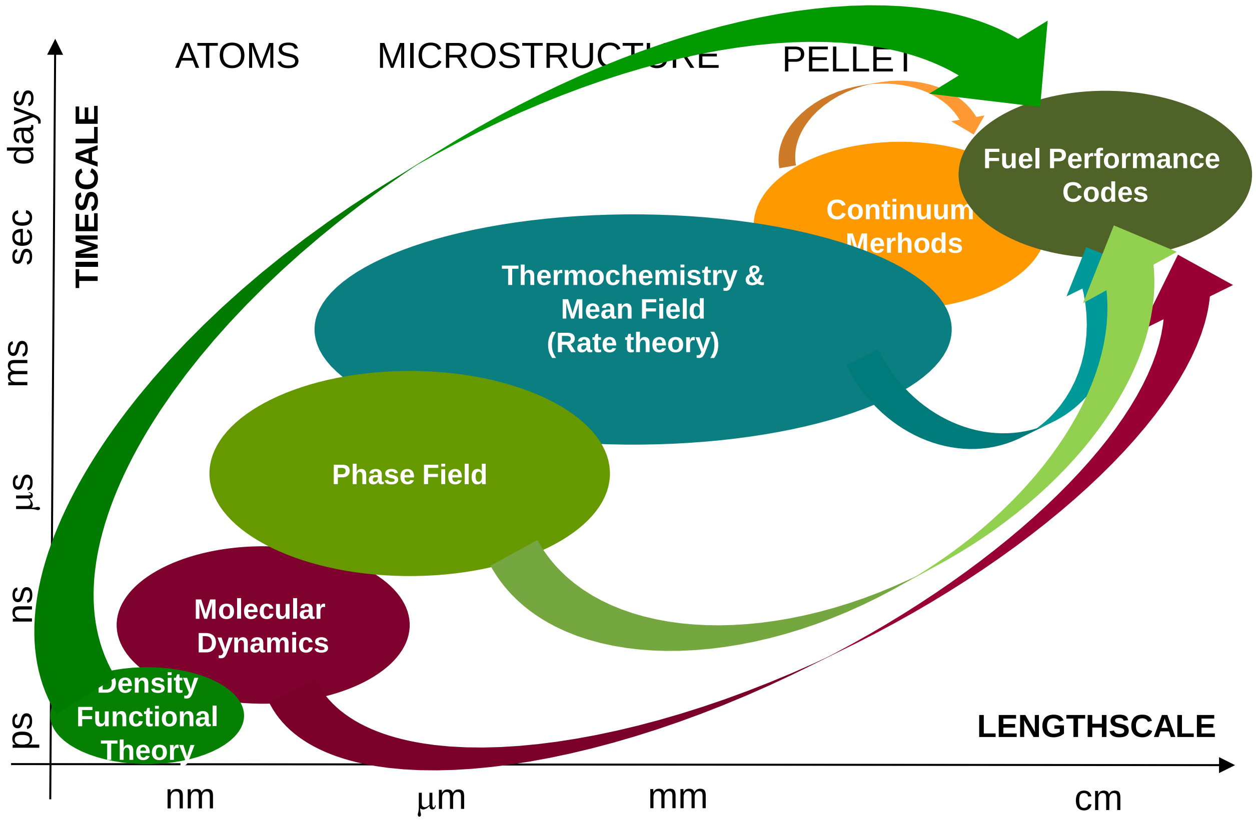
From S. Phillpot (Univ. Florida), OECD-NEA NSC Meeting, 13/06/14 (figure adapted from Marius Stan, DOE)

Computational Approaches: ~1985



From S. Phillpot (Univ. Florida), OECD-NEA NSC Meeting, 13/06/14 (figure adapted from Marius Stan, DOE)

Computational Approaches: 2015



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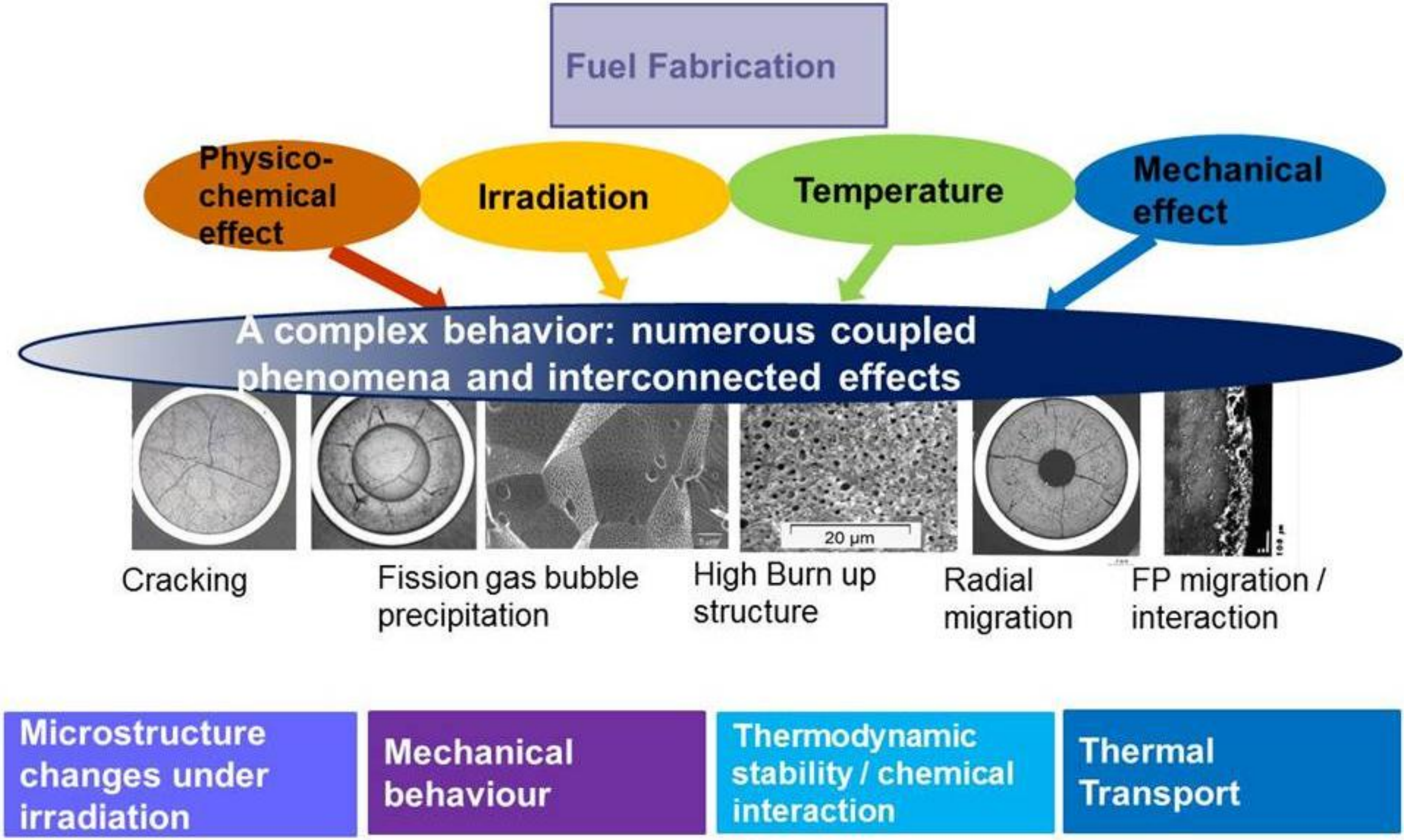
EG M2F deliverable

State-of-the-art report on fuel multi-scale modeling approaches, including :

- **Key engineering issues** that are relevant for the various fuels
- A worldwide **state-of-the-art review** of modeling approaches, from the atomic scale (first-principles and empirical potentials methods) to the macroscopic scale (fuel performance codes)
- A focus on **mid-term and long-term challenges** for the future (approximations, methods, scales, key experimental data, characterization techniques missing or to be strengthened)

Draft version available since October 2013, reviewed in 2014, final version currently being edited, the report will be published in April 2015

Part I : Underlying phenomena of nuclear fuel behavior



Part I : Underlying phenomena of nuclear fuel behavior

- **I.01 Microstructural changes of fuel under irradiation**

Radiation damage, fission gas bubble formation, high burn-up effects, …

P. Garcia, G. Carlot, B. Dorado, S. Maillard, G. Martin, J. Y. Oh, C. Sabathier, M.J. Welland

- **I.02 Nuclear fuel deformation**

Creep, swelling, cracking, pellet-clad interaction *L. Van Brutzel, R. Dingreville,T. Bartel*

- **I.03 Chemical interactions**

Fuel/cladding, fuel/coolant, cladding/coolant chemical interactions

C. Guéneau, J. Piron, J-C. Dumas, V. Bouineau, B.J. Lewis, F.C. Iglesias, C. Desgranges, C. Toffolon

- **I.04 Property / process relationships in fuel fabrication**

Microstructure, porosity, density optimisation,… *V. Tikare*

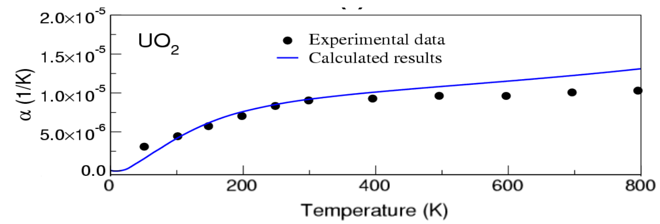
- **I.05 Phenomena in thermal transport in fuels**

Phonons / radiation damage interactions, conductivity models…

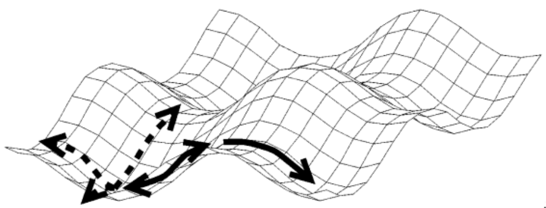
A. Chernatynskiu, A. El-Azab, J. Tulenko, S. Phillpot

Part II: Methodologies for determining nuclear fuel properties

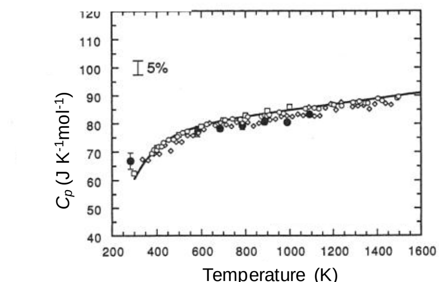
- **II.01 Theoretical estimation of thermal expansion of nuclear fuels**
  - *Y. Yun*



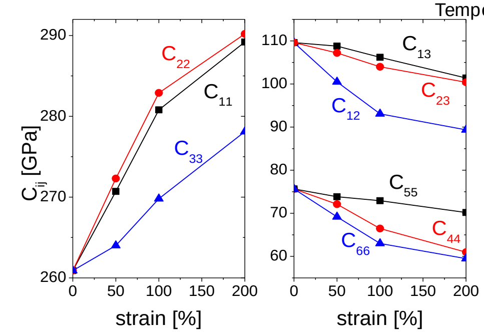
- **II.02 Atomic transport properties**
  - *M. Freyss*



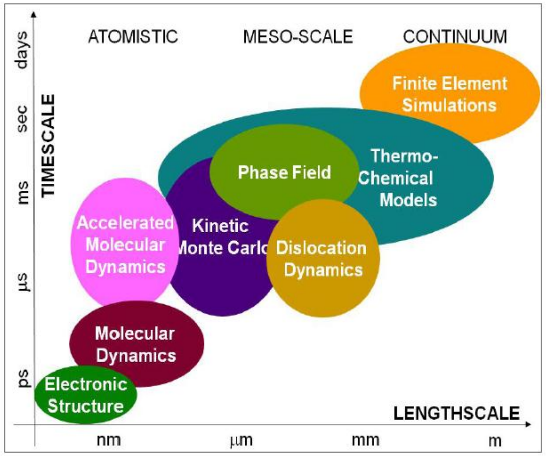
- **II.03 Free energy and heat capacity**
  - *M. Kurata, R. Devanathan*



- **II.04 Elastic and viscoplastic properties**
  - *R. Lebensohn*



Part III: Principles of modeling techniques for fuels



- III.01 **Density Functional Theory** - *M. Freyss*
- III.02 **Classical Molecular Dynamics** - *R. Devanathan, M. Krack, M. Bertolus*
- III.03 **Dislocation Dynamics** - *L. Van Brutzel*
- III.04 **Assessment of atomic scale modeling methods for UO_2** - *M. Bertolus, M. Freyss, M. Krack, R. Devanathan*
- III.05 **Phase Field** - *B. Radhakrishnan, S.B. Gorti, K. Clarno, M. Tonks*
- III.06 **Peridynamics** – *D. Littlewood*
- III.07 **Kinetic Monte Carlo** - *V. Tikare*
- III.08 **Rate Theory** - *S. Maillard, R. Skorek, P. Maugis, M. Dumont*
- III.09 **Thermochemical Modeling** - *B. Sundman, C. Guéneau*
- III.10 **Viscoplastic Models** - *R. Masson, V. Blanc, J.M. Gatt, J. Julien, R. Largenton, B. Michel*
- III.11 **Finite Element Modeling** - *M. Tonks, R. Williamson, R. Masson*
- III.12 **Integration/Multiscale** – *C. Valot, L. Malerba*
- III.13 **Fuel Performance Codes** - *P. Van Uffelen*

Structure of the WPMM Expert Groups (2015 – 2017)

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Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems

Task Force related to

Structural Materials Modelling

(will be established in 2015)

Task Force on

'Unit Mechanisms of

gaseous FP release'

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Multi-scale modelling methods
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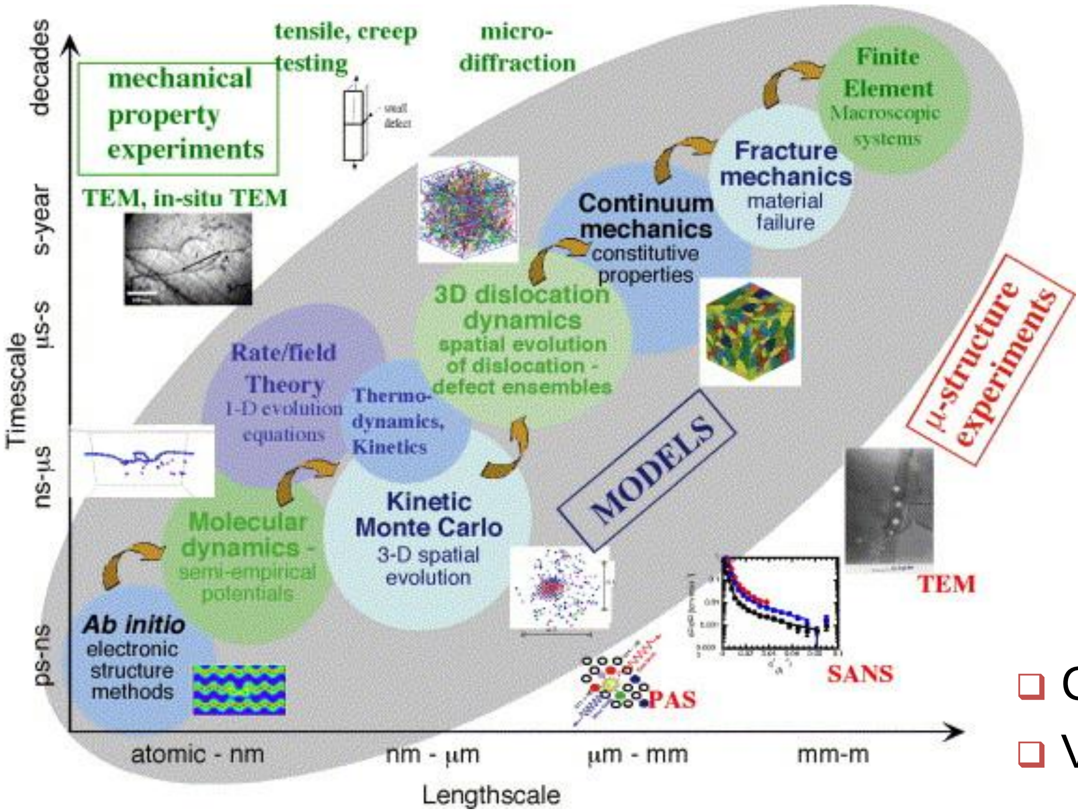
EG on Multiscale Modelling Methods (M3)

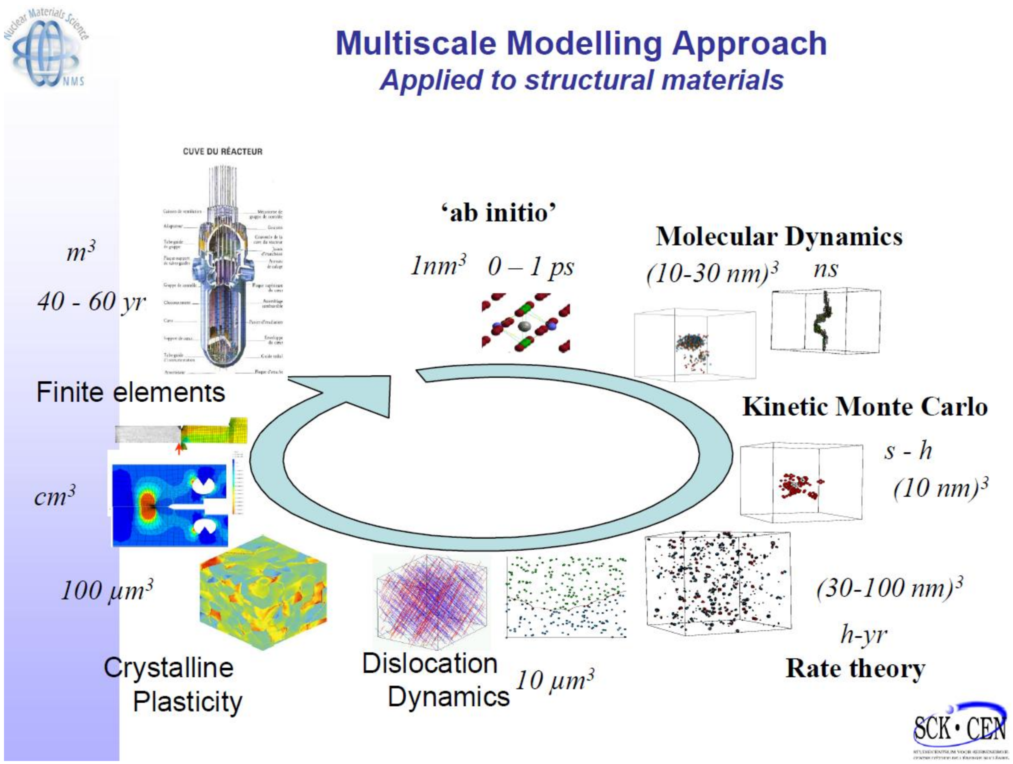
Objective: assess the possibilities and limits of both numerical methods applied to multi-scale modelling of materials for nuclear energy and means to link them



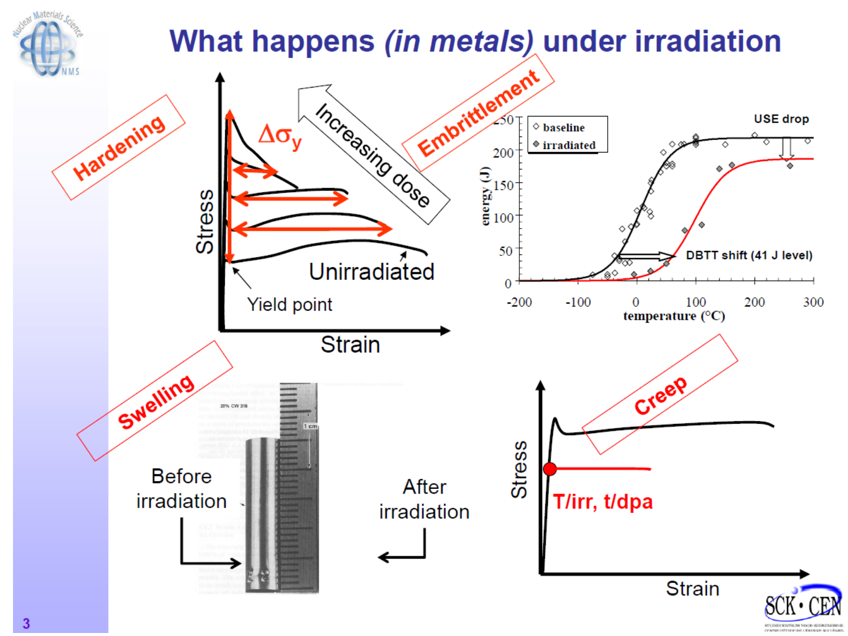
- Outline of the methods as applied to nuclear materials
- Advantages & disadvantages
- Limits, needs & recommendations
- Foster exchange of experience and dissemination of knowledge

- Chair: V. Tikare (SNL, USA)
- Vice-Ch.: M. Crack (PSI, Switzerland)

EG on Structural Materials Modelling (SMM)



- ❑ **New Chair: P. Olsson, (KTH, Sweden)**
- ❑ Vice-Ch.: L. Malerba (SCK-CEN, Belgium)



- ➢ Invented to allow the investigation of phenomena that cannot be studied experimentally - ideally *ab initio*
- ➢ Should be able to reproduce / predict how the nanostructure and the microchemistry changes under irradiation
- ➢ Should be able to reproduce / predict changes of mech. ppties under irradiation

EG on Primary Radiation Damage (PRD)

Objectives:

- to assess the limitations of the NRT-dpa standard
- to revisit the NRT-dpa standard and examine the possibility of proposing a new improved standard of primary damage characteristics.

Association Euratom-Tekes

Physics overview

Dpa in metals does not correspond to anything!

- The final damage is ~ 2 - 10 times smaller than the dpa number
- The real number of displaced atoms that have moved from their lattice sites can be ~ 10-100 times higher
  - Ion beam mixing experiments show this!
- Example: Self-recoils in Cu:

Recoil energy (keV)	# Frenkel pairs*	# dpa from NRT (E_d = 25 eV)	# Displaced atoms*
0.4	1.8	6	28
2	6.4	26	370
10	15	126	3000

*[MD data from: Nordlund et al, PRB 57 (1998) 7556]

Kai Nordlund, Department of Physics, University of Helsinki 16

Association Euratom-Tekes

Athermal-recombination corrected dpa

Sketch of final form

- The final result **for arc-dpa** is:

$$N_d(E) = \begin{bmatrix} 0 & E < E_d \\ 1 & E_d < E < 2E_d/0.8 \\ \dfrac{0.8E}{2E_d}\xi(E) & 2E_d/0.8 < E < \infty \end{bmatrix}$$

where $\xi(E)$ is given by

$$\xi(E) = \frac{1-c}{(2E_d/0.8)^b} E^b + c$$

- Chair: Kai Nordlund (Univ. Helsinki, Finland)
- Liaison: F. Willaime (CEA, France)

The final report will be published in March 2015 on the NEA website

Task Force on "Unit mechanisms of gaseous FP release"

- Established in 2014 between 12 experts, coordinated by M. Tonks (INL, USA)

- Scope: ***summarizing existing research*** *on the basic mechanisms behind the various stages of fission gas release during normal reactor operation and* ***identify critical areas*** *where experimental and simulation work is needed*
  - Identify fission gas behaviour mechanisms
  - Determine critical modelling parameters
  - Relate model parameters to physics-based phenomena
  - Critically assess existing data
  - Recommend new, key experiments/simulations

- Deliverable: OECD-NEA Technical Report & Journal article
  - First draft scheduled for mid-2015
  - Final report scheduled mid-2016