INSPYRE
Investigations Supporting MOX Fuel Licensing
in ESNII Prototype Reactors

Fuel performance codes

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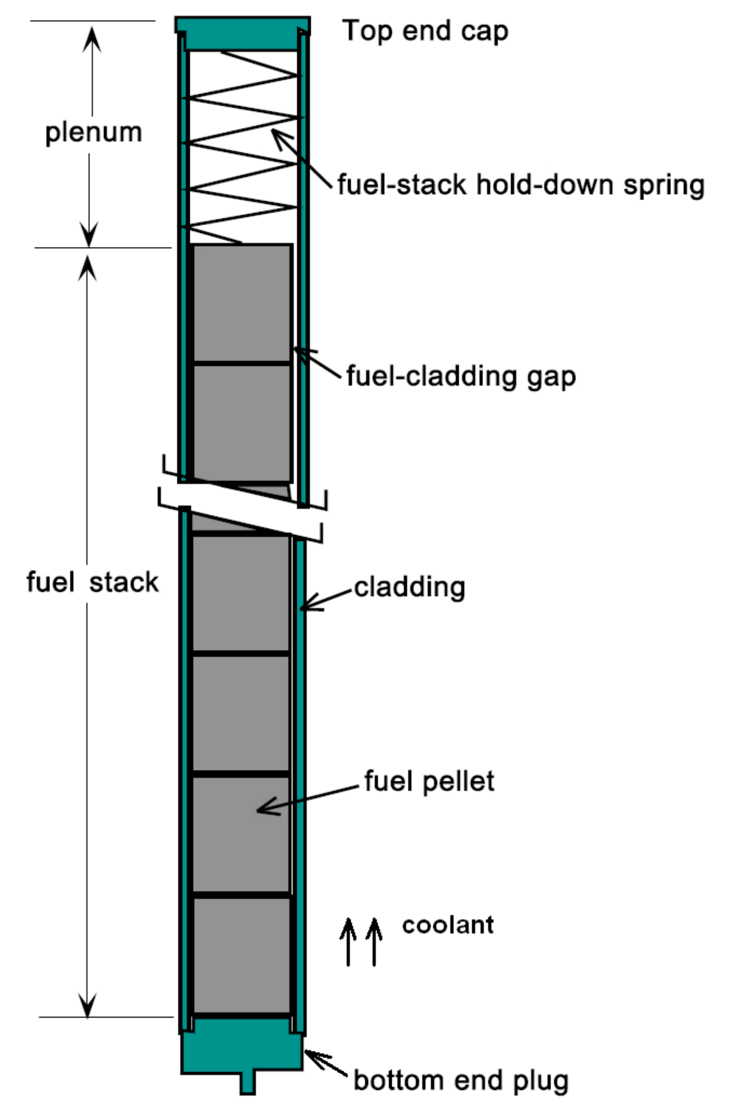
Introductory framework

Fuel pin "system" (i)



(Olander 2009)

Different **fuel types** (solid fuel pin, particle fuel, plate fuel, liquid fuel) for different nuclear **reactor types ...**

——> **the fuel pin/rod for solid-fuelled nuclear reactors**

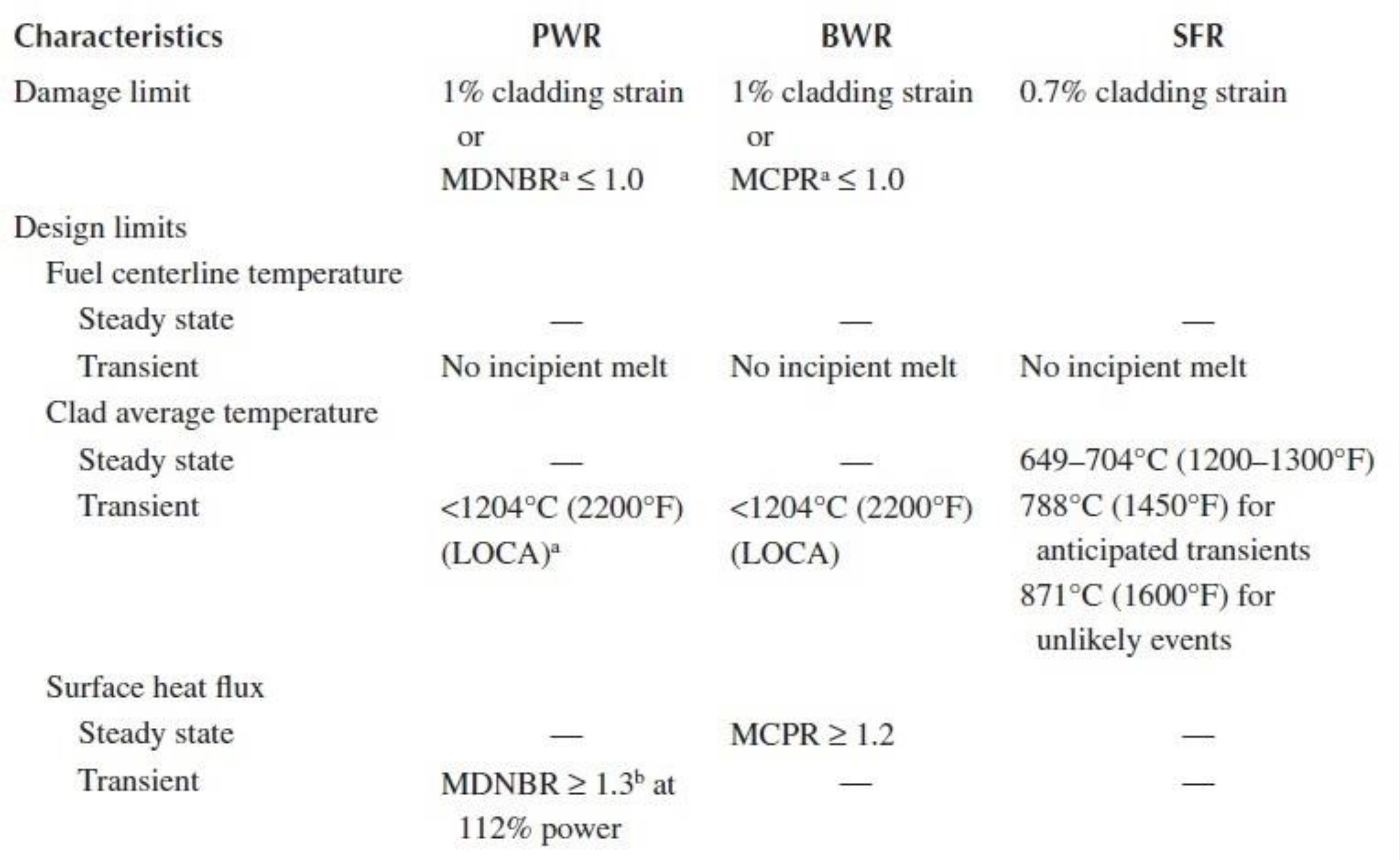
- made of a stack of fuel pellets wrapped in a cladding tube forming a **"coupled system"....**

.... fuel-cladding gap (open//closed) is a critical interaction zone that controls heat transfer from fuel pellets to cladding, and then to coolant, as well as mechanical forces and chemical environment during pellet-cladding-interaction (PCI failure potential)

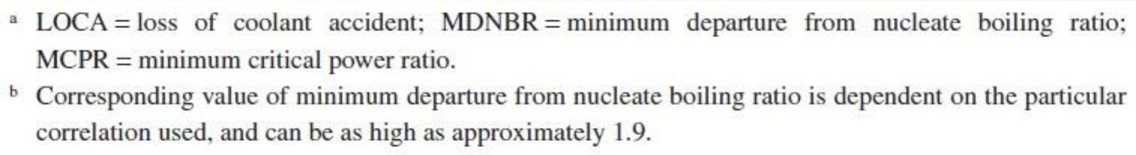
- its performance is fundamental for reactor **safe operation** (and for **design** & **licensing** as well)
- need of **Fuel Performance Codes (FPCs)**, and Separate-Effects & Integral Irradiation Experiments as well, to assess the **fuel pin thermal and mechanical behaviour + compliance with** functional requirements & design limits

Fuel pin "system" (ii)

- Typical fuel pin thermal design limits



Characteristics	PWR	BWR	SFR
Damage limit	1% cladding strain or MDNBR[a] ≤ 1.0	1% cladding strain or MCPR[a] ≤ 1.0	0.7% cladding strain
Design limits			
Fuel centerline temperature			
Steady state	—	—	—
Transient	No incipient melt	No incipient melt	No incipient melt
Clad average temperature			
Steady state	—	—	649–704°C (1200–1300°F)
Transient	<1204°C (2200°F) (LOCA)[a]	<1204°C (2200°F) (LOCA)	788°C (1450°F) for anticipated transients 871°C (1600°F) for unlikely events
Surface heat flux			
Steady state	—	MCPR ≥ 1.2	—
Transient	MDNBR ≥ 1.3[b] at 112% power	—	—



[a] LOCA = loss of coolant accident; MDNBR = minimum departure from nucleate boiling ratio; MCPR = minimum critical power ratio.

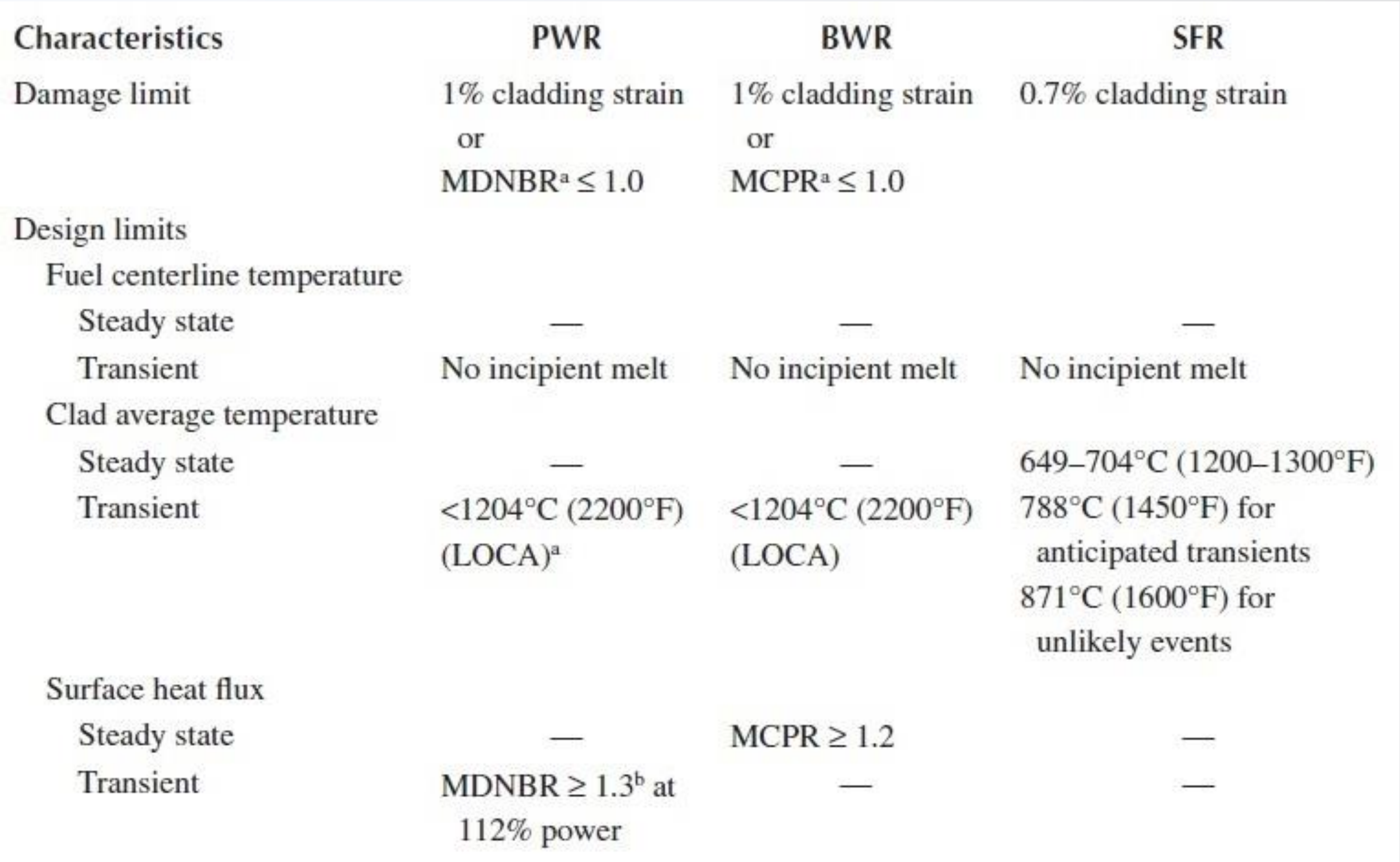
[b] Corresponding value of minimum departure from nucleate boiling ratio is dependent on the particular correlation used, and can be as high as approximately 1.9.

(Todreas - Kazimi 2011)

- **Design and licensing assessment** involves comparing calculated parameters ("performance indicators") with design limits, according to a number of design criteria, which ensure that the functional requirements of the fuel pins are met
- Different **functional requirements and design criteria** generally apply in normal operation, anticipated operational occurrences and accidents
- functional requirements and design criteria and vary from country to country due to the **differences in regulatory regimes**
- There are also variations due to **differences in reactor types** and, to some extent, **fuel types**

Fuel pin "system" (ii)

- Typical fuel pin thermal **design limits**



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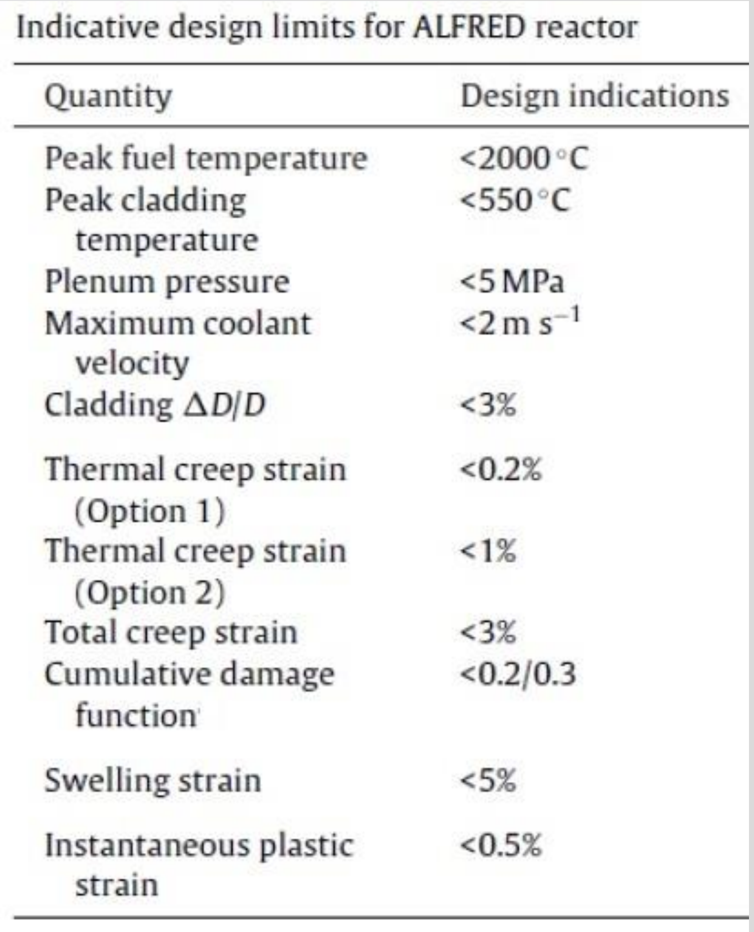


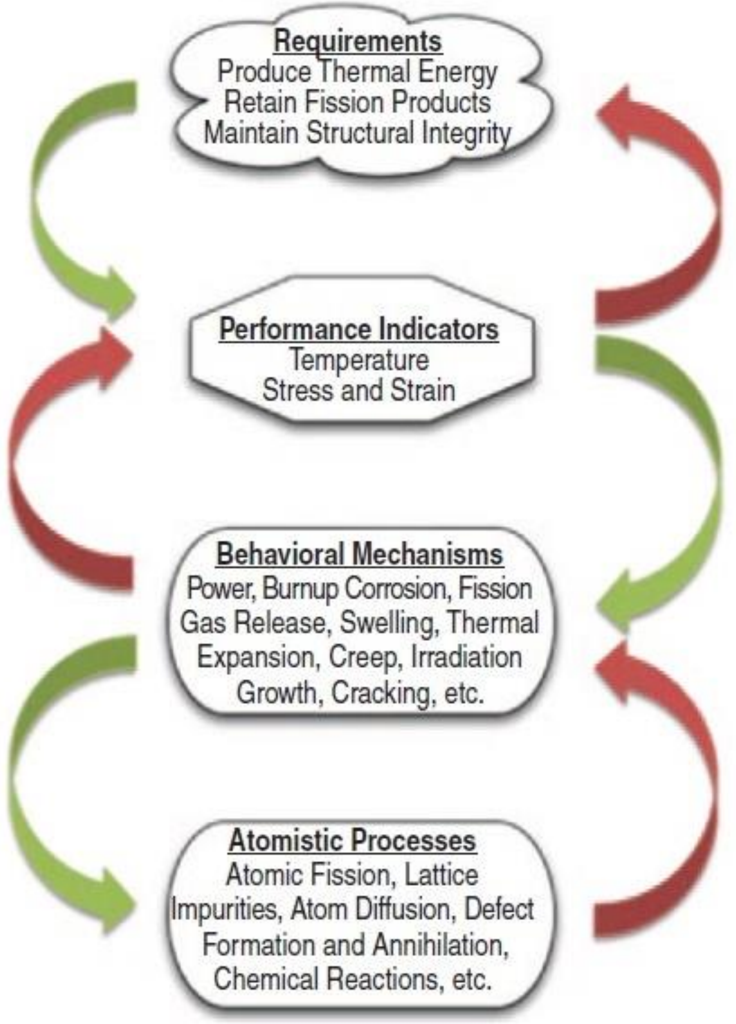
Indicative design limits for ALFRED reactor

Quantity	Design indications
Peak fuel temperature	<2000 °C
Peak cladding temperature	<550 °C
Plenum pressure	<5 MPa
Maximum coolant velocity	$<2\ \mathrm{m\ s^{-1}}$
Cladding $\Delta D/D$	<3%
Thermal creep strain (Option 1)	<0.2%
Thermal creep strain (Option 2)	<1%
Total creep strain	<3%
Cumulative damage function	<0.2/0.3
Swelling strain	<5%
Instantaneous plastic strain	<0.5%

(Luzzi et al. 2014)

Fuel pin "system" (iii)

- Sequential description: modelling & simulation of fuel pin behaviour



Requirements
Produce Thermal Energy
Retain Fission Products
Maintain Structural Integrity

Performance Indicators
Temperature
Stress and Strain

Behavioral Mechanisms
Power, Burnup Corrosion, Fission Gas Release, Swelling, Thermal Expansion, Creep, Irradiation Growth, Cracking, etc.

Atomistic Processes
Atomic Fission, Lattice Impurities, Atom Diffusion, Defect Formation and Annihilation, Chemical Reactions, etc.

(Rashid et al. 2011)

A **multi-component system** required to:

- produce thermal energy through fission
- efficiently transfer the thermal energy to the coolant system
- be carefully designed to retain fission products (FPs) by maintaining structural integrity under all operational conditions and accident events

The above **key requirements** lead to:

- various **performance indicators** (T, $\bar{\bar{\sigma}}$, $\bar{\bar{\epsilon}}$) describing the fuel system state
- **behavioural mechanisms** that dictate the evolution of the performance indicators
- **atomistic processes** that underlie all the thermal, mechanical, and chemical responses to the environment

These **steps** are highly interrelated as they also feed back up sequentially, and ultimately integrate hierarchically in time and space to determine the fuel pin performance

Fuel Performance Code (i)

- All this involves modelling & simulation of a large number of phenomena:

Given the coolant pressure, core inlet temperature and mass flow rate, and the irradiation history …

(i.e., the evolution of the axial distributions of pin power, bulk coolant temperature and fast neutron flux with time)

the Fuel Performance Code (FPC)

calculates the evolution of the **thermo-mechanical state of a fuel pin** ($\bar{\bar{\sigma}}$, $\bar{\bar{\epsilon}}$, $\bar{u}$, and T) during its lifetime in reactor

(Rossiter 2012)

- associated with **thermo-mechanical behaviour** of fuel and cladding materials (*standard* phenomena)

  (e.g., heat transfer by conduction, convection and radiation, thermal expansion, creep, elasticity, plasticity, fatigue, phase changes and melting)

- related to the **presence of a neutron flux**

  (e.g., cladding hardening, embrittlement, axial growth and void swelling)

- related to **fission, neutron capture and generation of fission products**

  (e.g., non-uniform heat generation, generation and release of fission gas, Xe, Kr, He, and fuel densification and swelling)

- related to **microstructural changes** in the fuel

  (e.g., formation of high burnup structure, grain growth and restructuring)

- related to **radial temperature gradients** in the fuel pellets

  (e.g., pellet cracking and fuel fragment relocation, pellet wheatsheafing/hour-glassing, axial extrusion, dish filling, oxygen migration and plutonium redistribution)

- **chemical** phenomena

  (e.g., fuel-clad bonding, stress-corrosion cracking and cladding oxidation, erosion and dissolution)

Fuel Performance Code (ii)

- The intriguing "complexity" and intricate "beauty" of fuel pin behaviour

Given the coolant pressure, core inlet temperature and mass flow rate, and the irradiation history …

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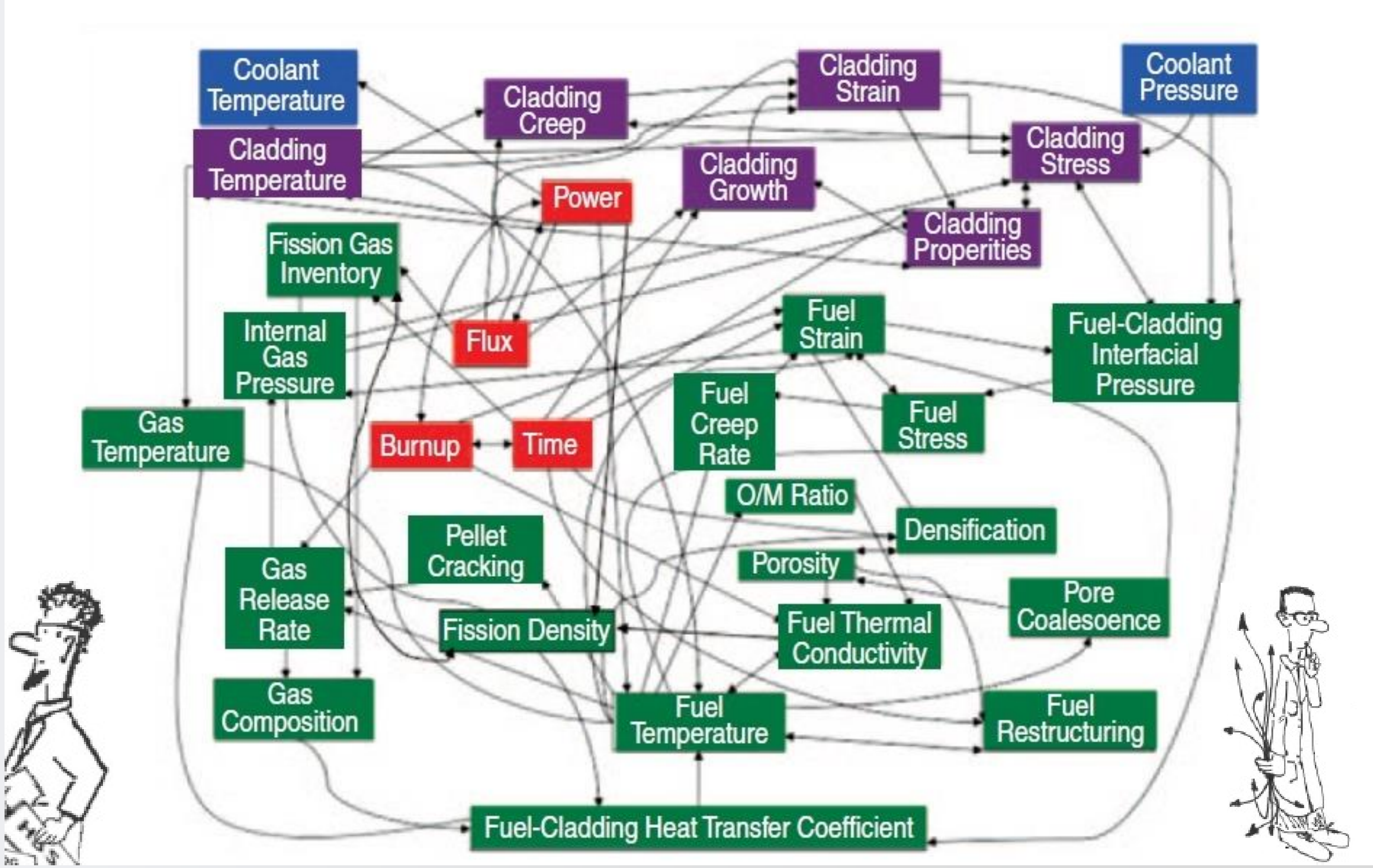
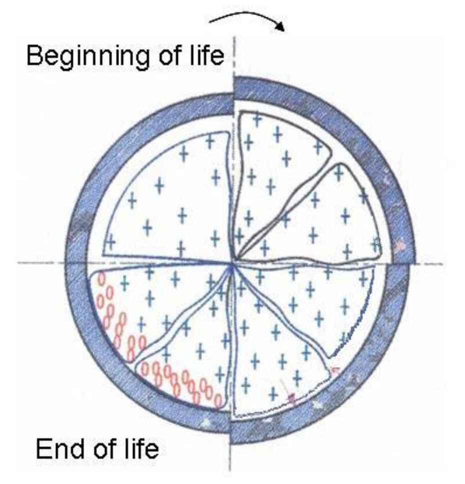


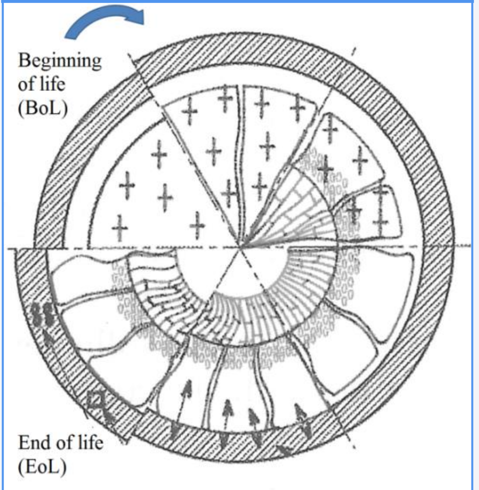
(Wirth 2017, Noirot 2016, Rashid et al. 2011, Lassmann 1980, Beyer et al. 1975, Horn 1973)

Complexity of fuel pin behaviour modelling (i)

LWR --> UO_2/Zy



FR --> $(U,Pu)O_2$/SS



- Complex **multi-physics phenomena** featured by *different time* (22 oom: ps-y) and *space scales* (10 oom: atomic/nm-m) concerning both fuel and cladding as a "coupled system":
  - very **different phenomenology and behaviour**, depending on reactor type/conditions and materials
  - **evolution with burnup** during irradiation and **synergy** → INTERRELATIONSHIP & FEEDBACK
- These conditions impose **challenging and unique modelling, simulation, and verification data requirements** in order to accurately determine the state of fuel pins during their lifetime in reactor
- **Numerous material and behavioural models** represent the engineering level multi-material/multi-domain complex interaction in the fuel pin:
  - they form the **internal capability of a FPC** and are generally characterized as "point models"

    (i.e., they describe material behaviour over a representative infinitesimal, or finite but small, volume, and are therefore independent of the FPC numerical or computational structure in which they reside)
  - Various **code styles**: geometrical representation (1½-D, 2-D, 3-D, "hybrid type") / numerical technique (finite difference, finite element) / type of analysis (steady-state, transient)

Complexity of fuel pin behaviour modelling (ii)

- Interacting phenomena and feedbacks in the fuel pin during irradiation

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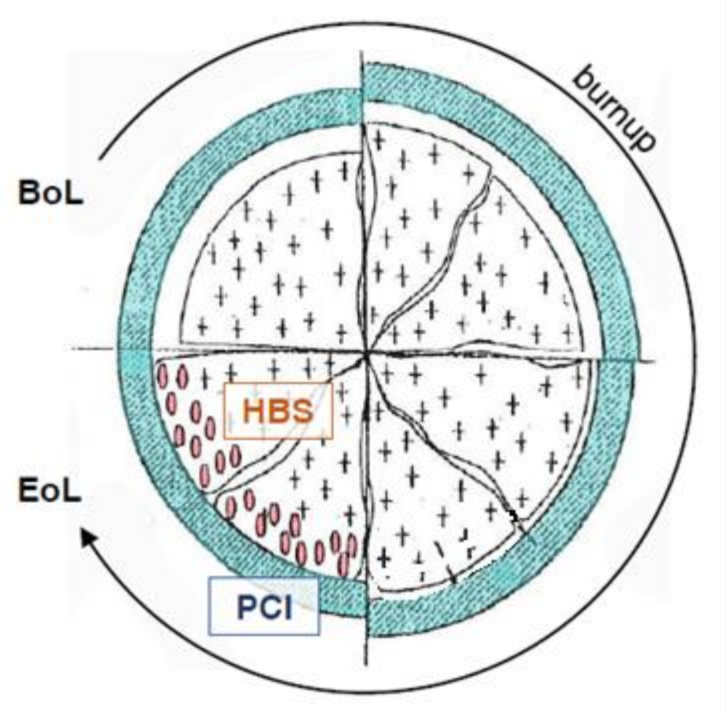

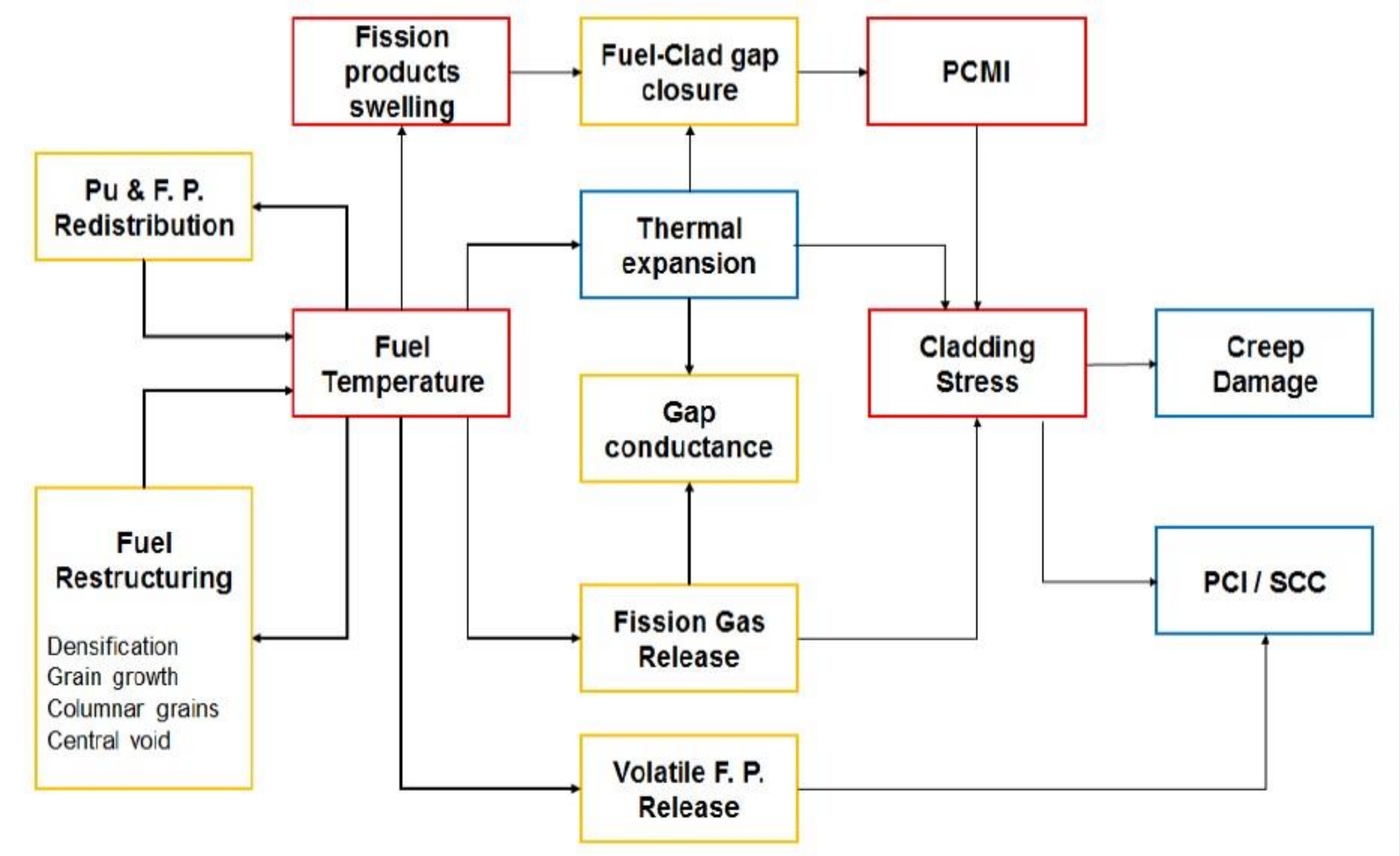

Fission products swelling

Fuel-Clad gap closure

PCMI

Pu & F. P. Redistribution

Thermal expansion

Fuel Temperature

Cladding Stress

Creep Damage

Gap conductance

Fuel Restructuring

Densification
Grain growth
Columnar grains
Central void

Fission Gas Release

PCI / SCC

Volatile F. P. Release

Complexity of fuel pin behaviour modelling (ii)

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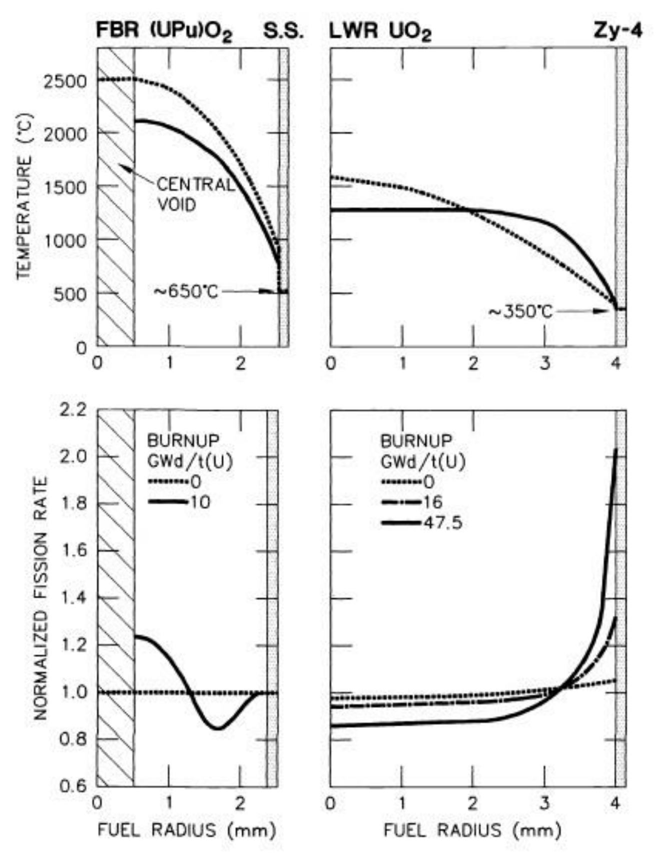
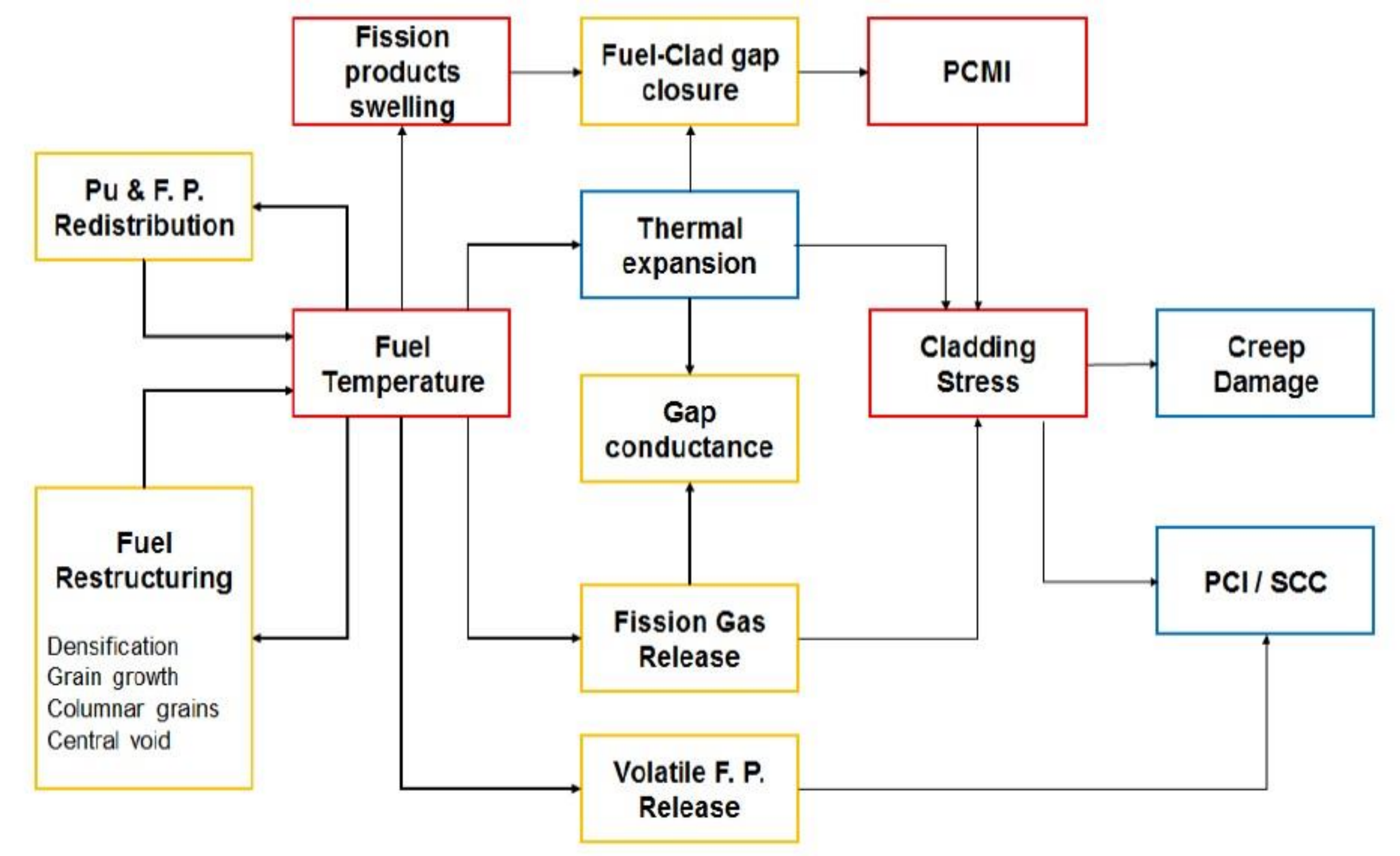
FR vs. LWR



(Lambert - Strain 1994)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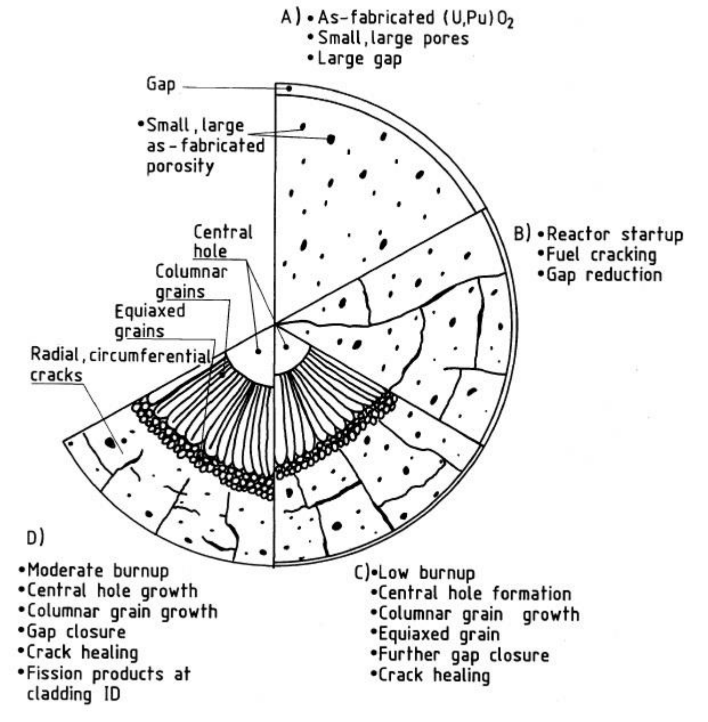
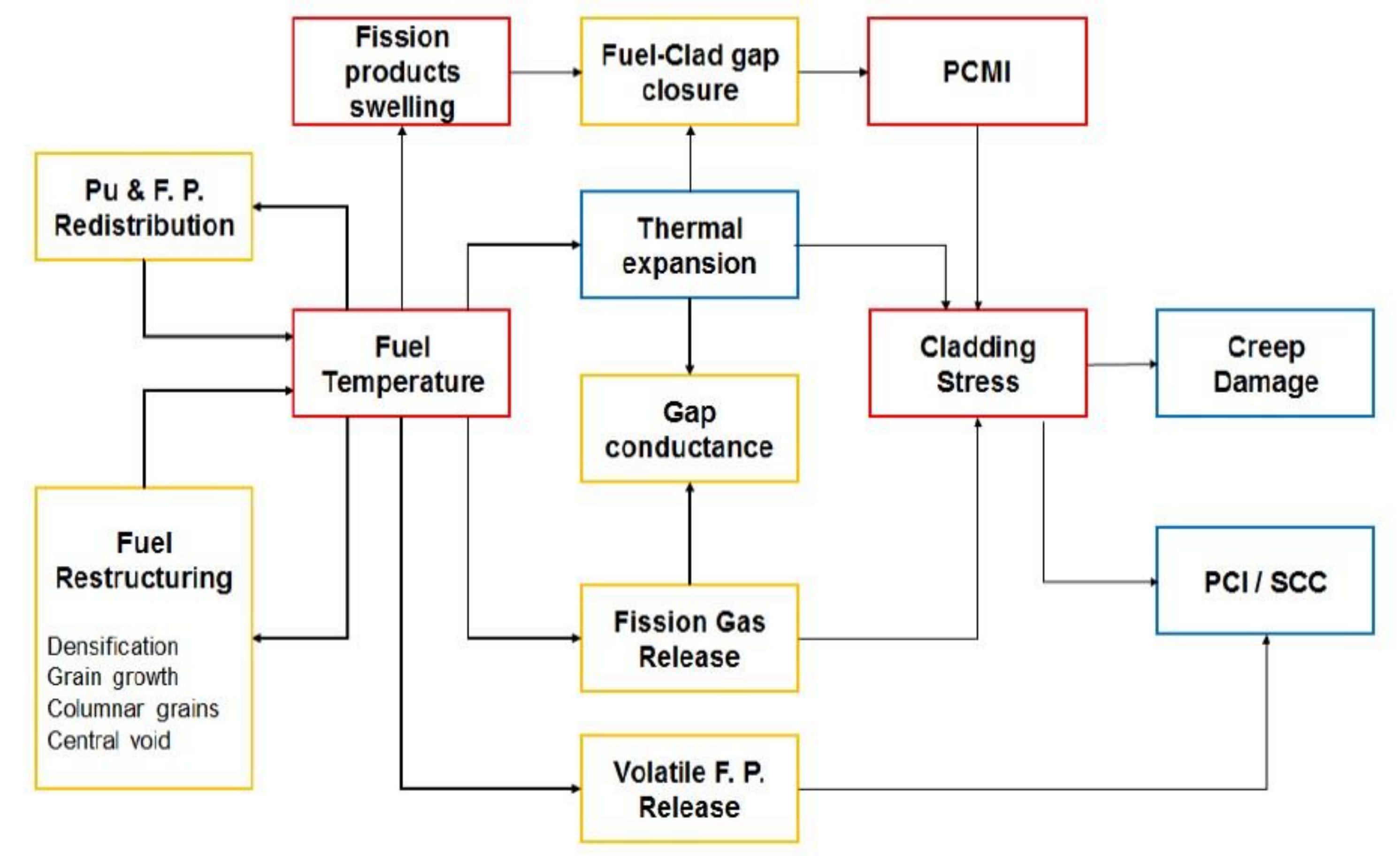


(Boltax 1994)



Complexity of fuel pin behaviour modelling (iii)

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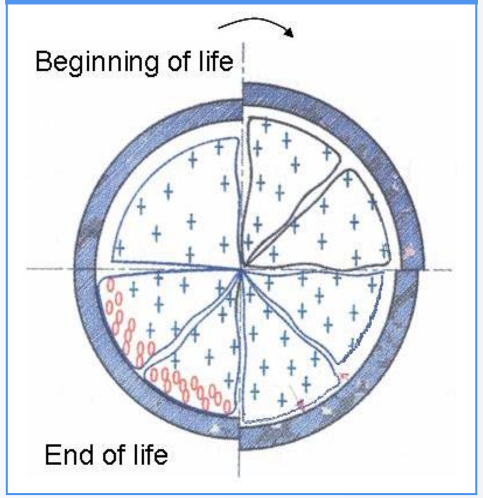

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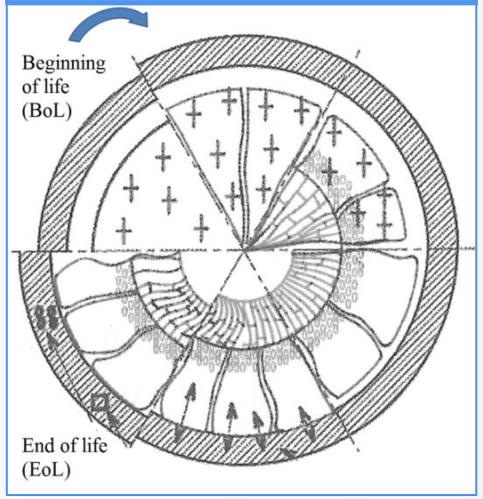

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Complexity of fuel pin behaviour modelling (iv)

- PCI-related effects are uniquely 3-D --> can be evaluated, in complete detail, only through 3-D modelling & simulation

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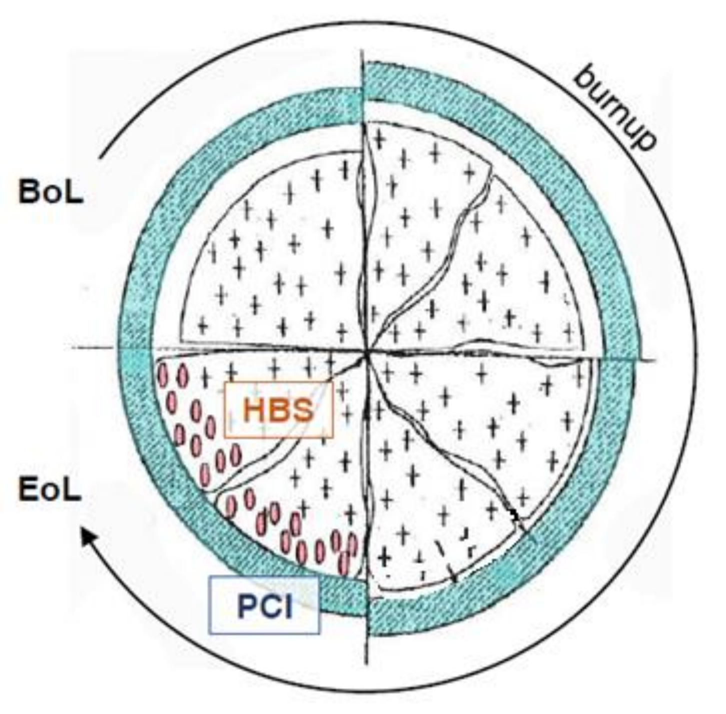
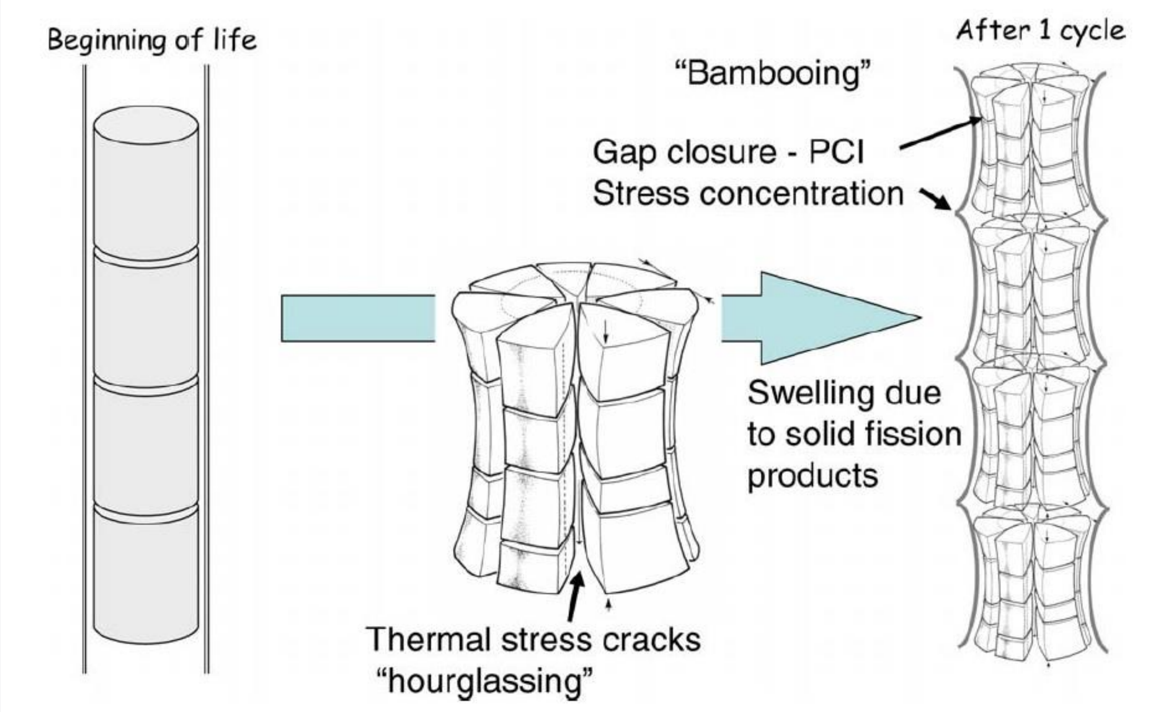
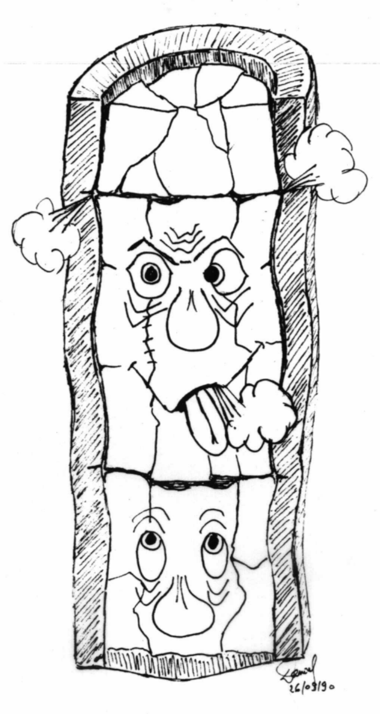




(Olander 2009)



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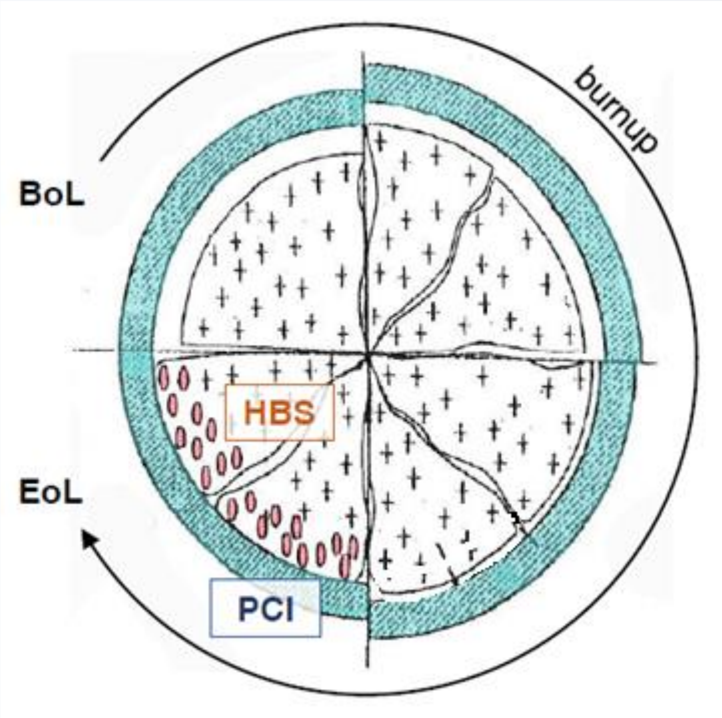

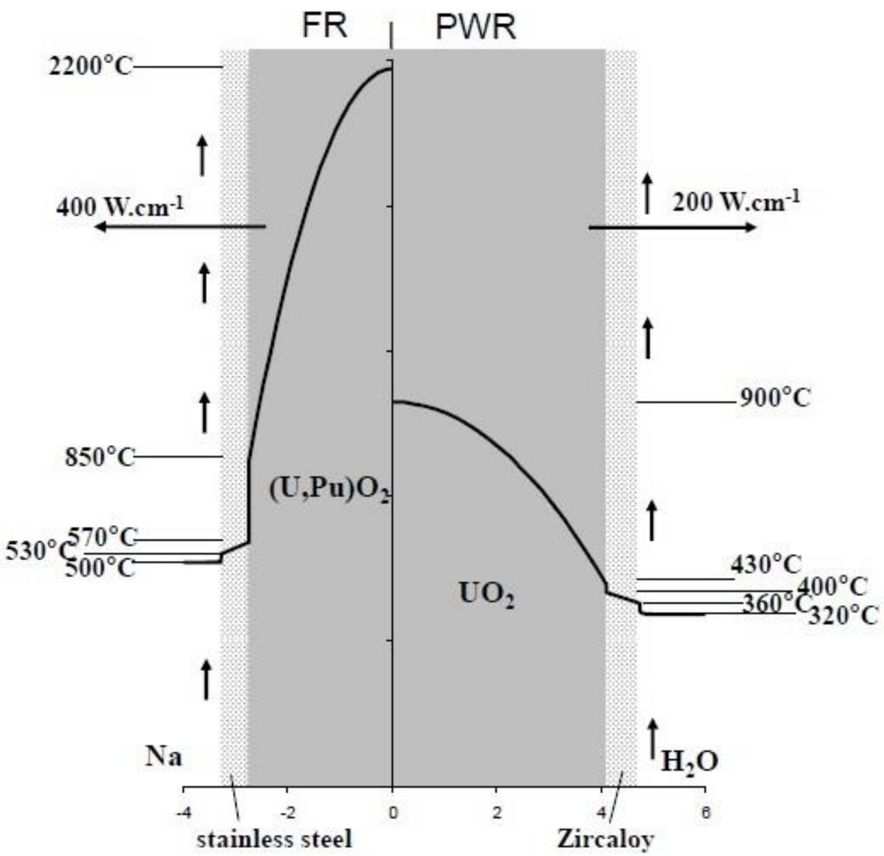

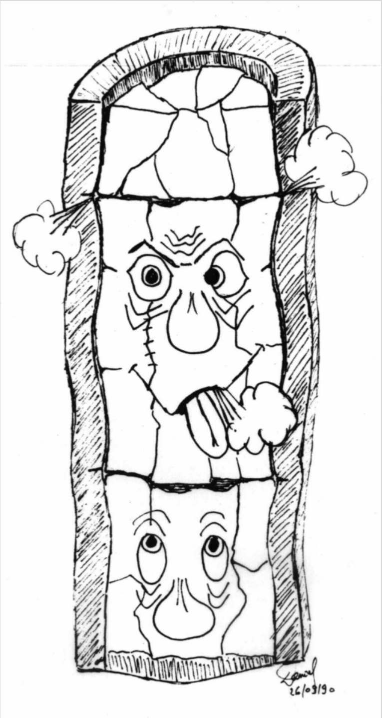

(Noirot 2016)

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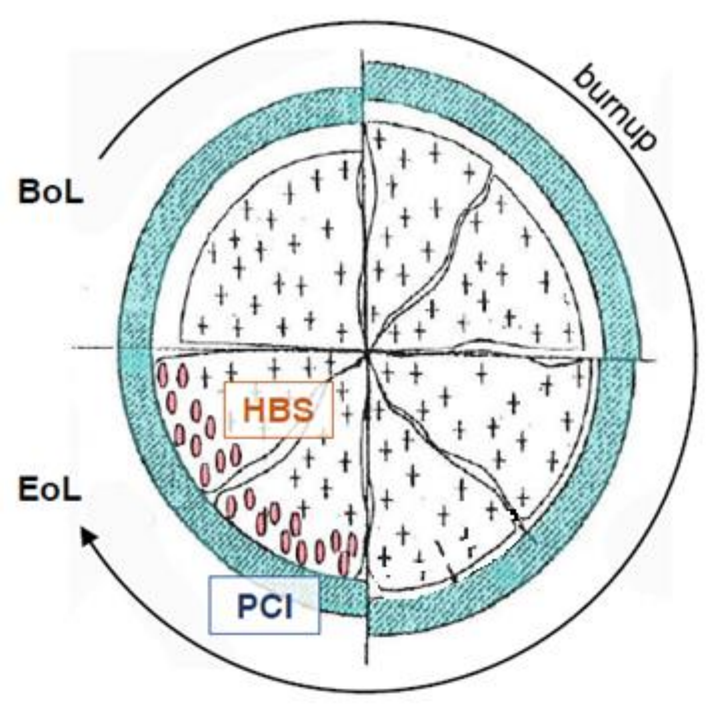
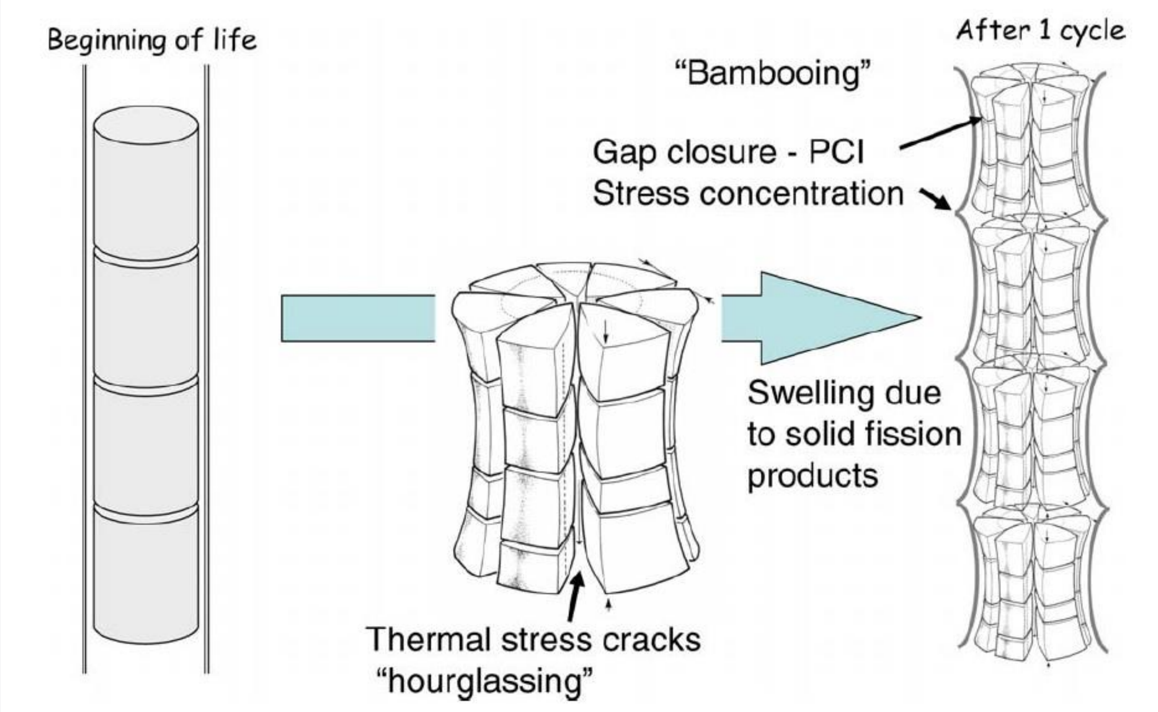
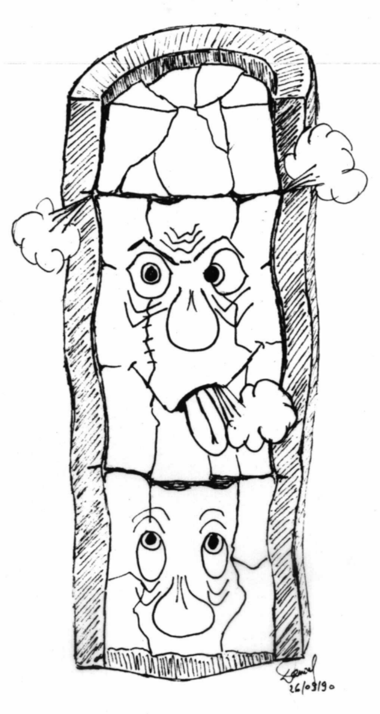




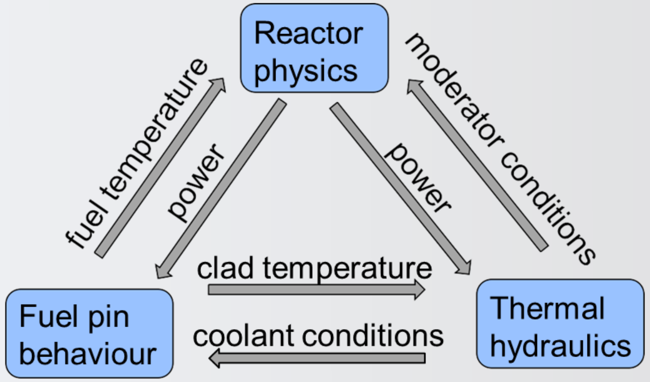


(Olander 2009)

Suite of computer codes for the modelling and simulation of in-pile fuel behaviour

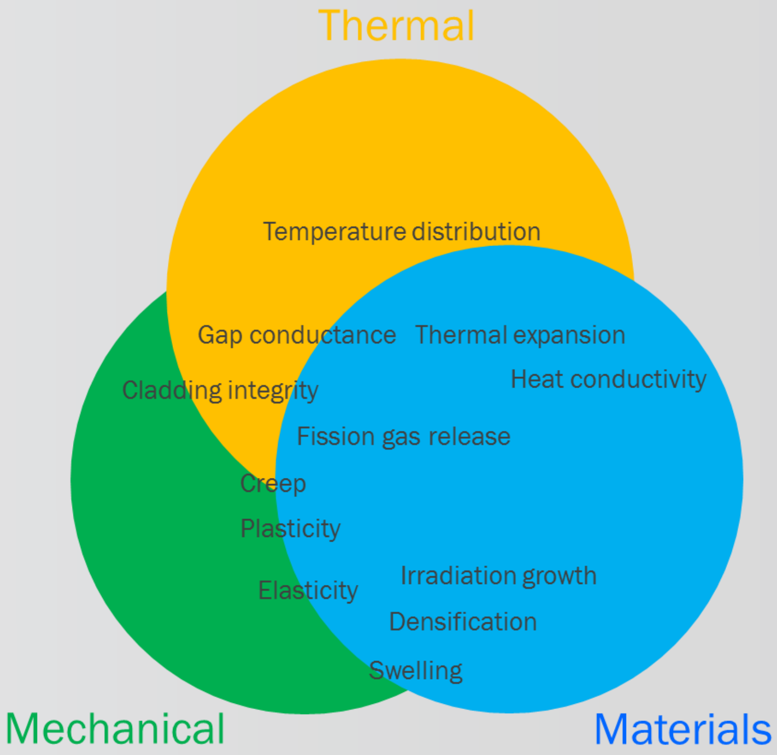
Involved disciplines and software tools

- Accurate description of fuel pin behaviour involves various disciplines
  - ➢ Reactor physics / neutronics
  - ➢ Thermal-hydraulics (system & core)
  - ➢ Chemistry
  - ➢ Nuclear and solid state physics
  - ➢ Metallurgy and ceramics
  - ➢ Applied mechanics
  - ➢ Software engineering / advanced computational methods



- To ensure safe and economic operation of fuel pins

→ predict their behaviour and life-time by means of a *convenient* suite/platform of computer codes



(Tulkki 2016)

Schematic of computer codes (i)

- **Design and licensing** of nuclear fuel require the behaviour under irradiation to be predicted. This includes:
  - the behaviour of *individual* fuel pins
  - the behaviour of fuel assemblies (also known as fuel bundles or elements), as well as of reactor *core as a whole*
- **The aim**:

  is to ensure that the fuel will operate safely and within design constraints, even under accident conditions

- The **behaviour of a <u>given fuel pin</u>** is governed by the evolution with time of:

  a) the pin power distribution <——

  b) the pin boundary conditions (primarily the axial distribution of coolant temperature and pressure), in turn dependent on <——

  c) the evolution with time of the thermal-hydraulic behaviour of the coolant in the primary circuit (‘system thermal-hydraulics’) <——

  d) the overall thermo-mechanical response of the fuel pin to the imposed powers and boundary conditions <——

- With respect to the <u>fuel assembly as a whole</u>, it is generally of interest only

  e) the mechanical behaviour, including stresses imposed by loads applied to the various assembly components (during normal operation, and accidents as well) <——

- Since the **fuel pin behaviour** *in its entirety* is **inherently complex**, and due to historical restrictions in computing power, **(a) to (e) are generally evaluated separately …**

This is achieved using a <u>suite of computer programs</u> with:

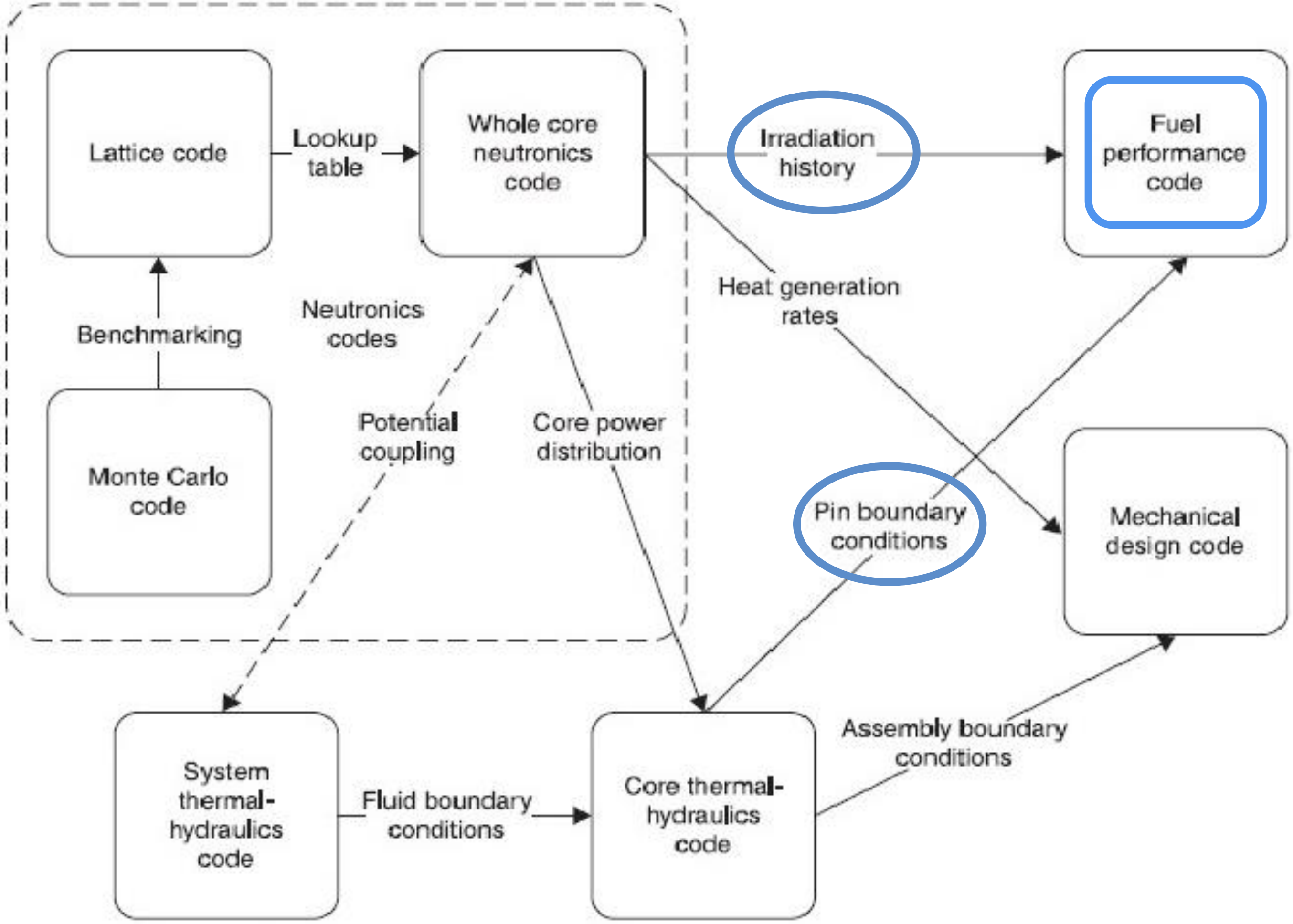
neutronics codes
core thermal-hydraulics codes
system thermal-hydraulics codes
Fuel Performance Codes (FPCs)
mechanical design codes

Other types of codes are used for *ad hoc* or specialized analysis (e.g., CFD, chemistry codes)

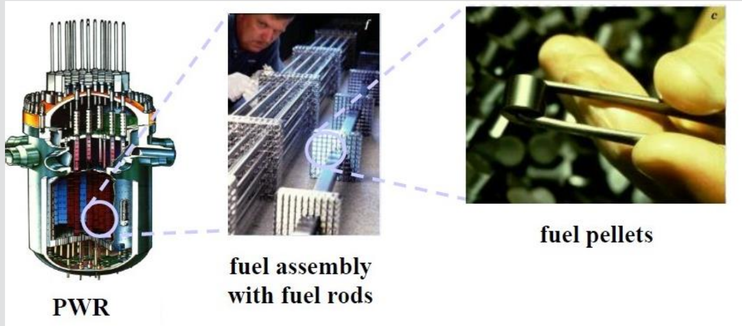
Schematic of computer codes (ii)

- Computer codes used for modelling fuel behaviour under irradiation and their interactions

computer program for analysing the fuel pin thermal and mechanical behaviour



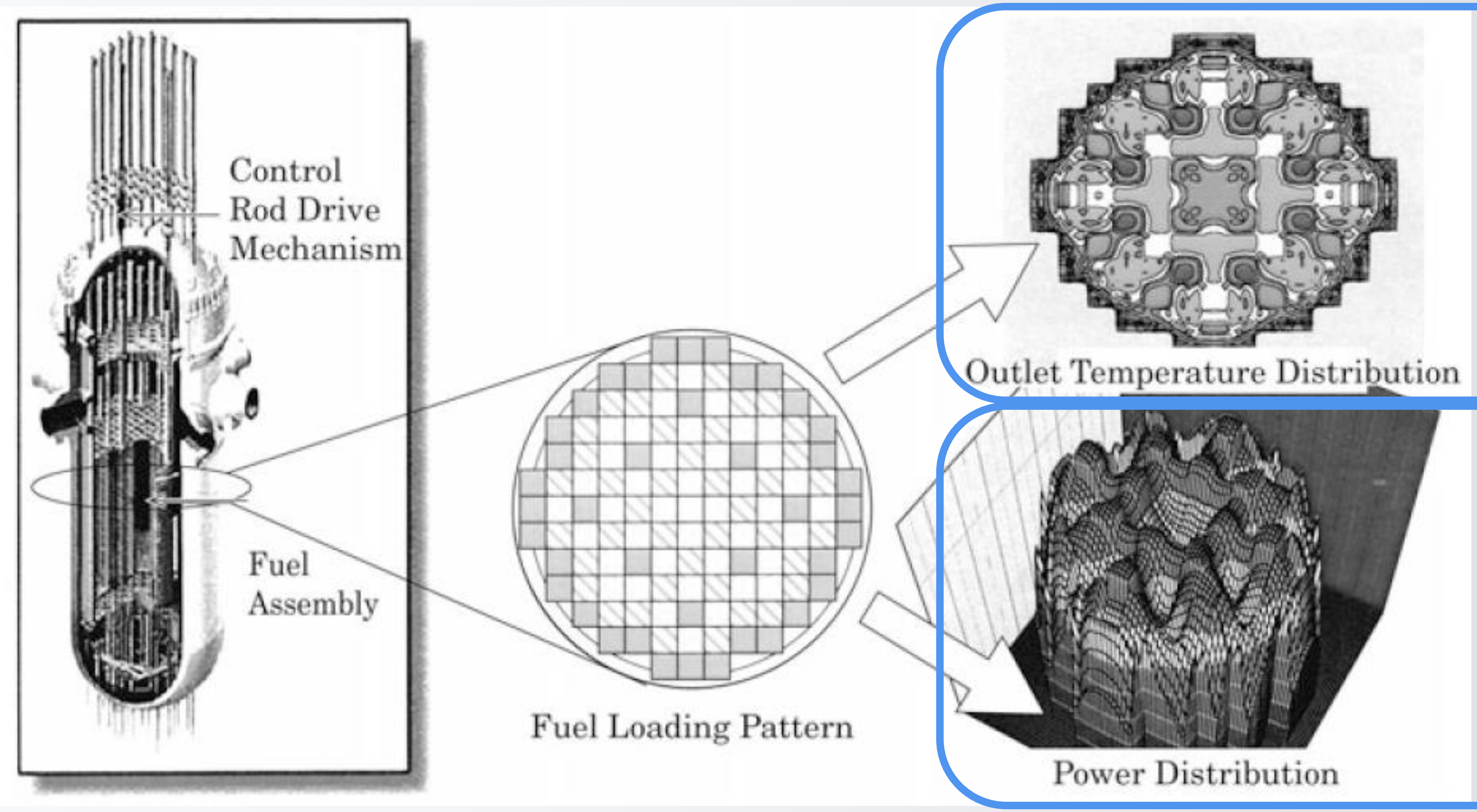
(Rossiter 2012)



- neutronics codes
- core thermal-hydraulics codes
- system thermal-hydraulics codes
- ✓ Fuel Performance Codes (FPCs)
  INDIVIDUAL FUEL PINS
- mechanical design codes

Schematic of computer codes (iii)

- Computer codes used for modelling fuel behaviour under irradiation and their interactions



SYSTEM THERMAL-HYDRAULICS CODE

CORE THERMAL-HYDRAULICS CODE

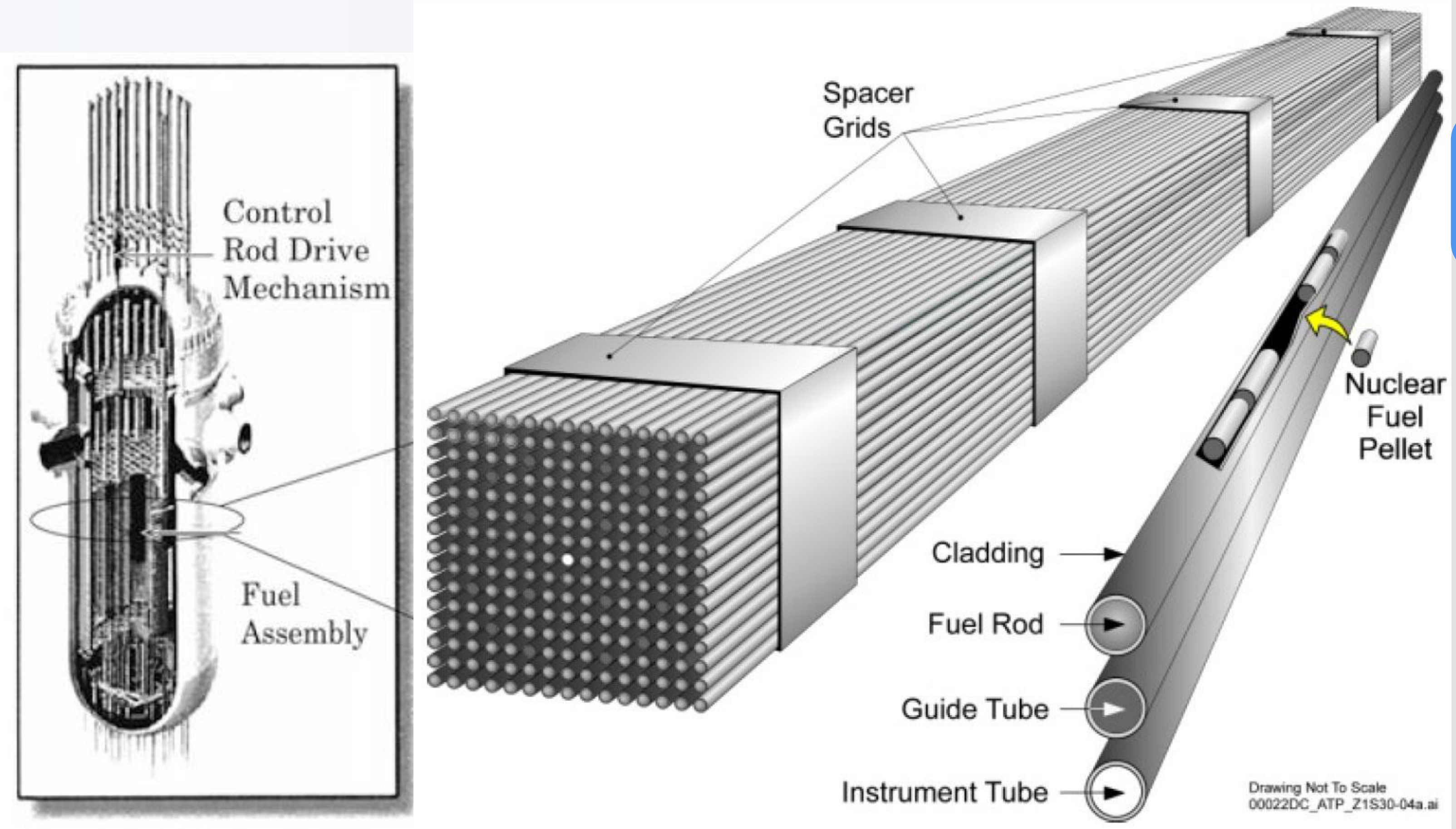
NEUTRONICS CODE

(Okumura et al. 2014)

POLITECNICO
MILANO 1863

Schematic of computer codes (iv)

- Computer codes used for modelling fuel behaviour under irradiation and their interactions



FUEL PERFORMANCE CODE

Average core conditions
Hot pin conditions...

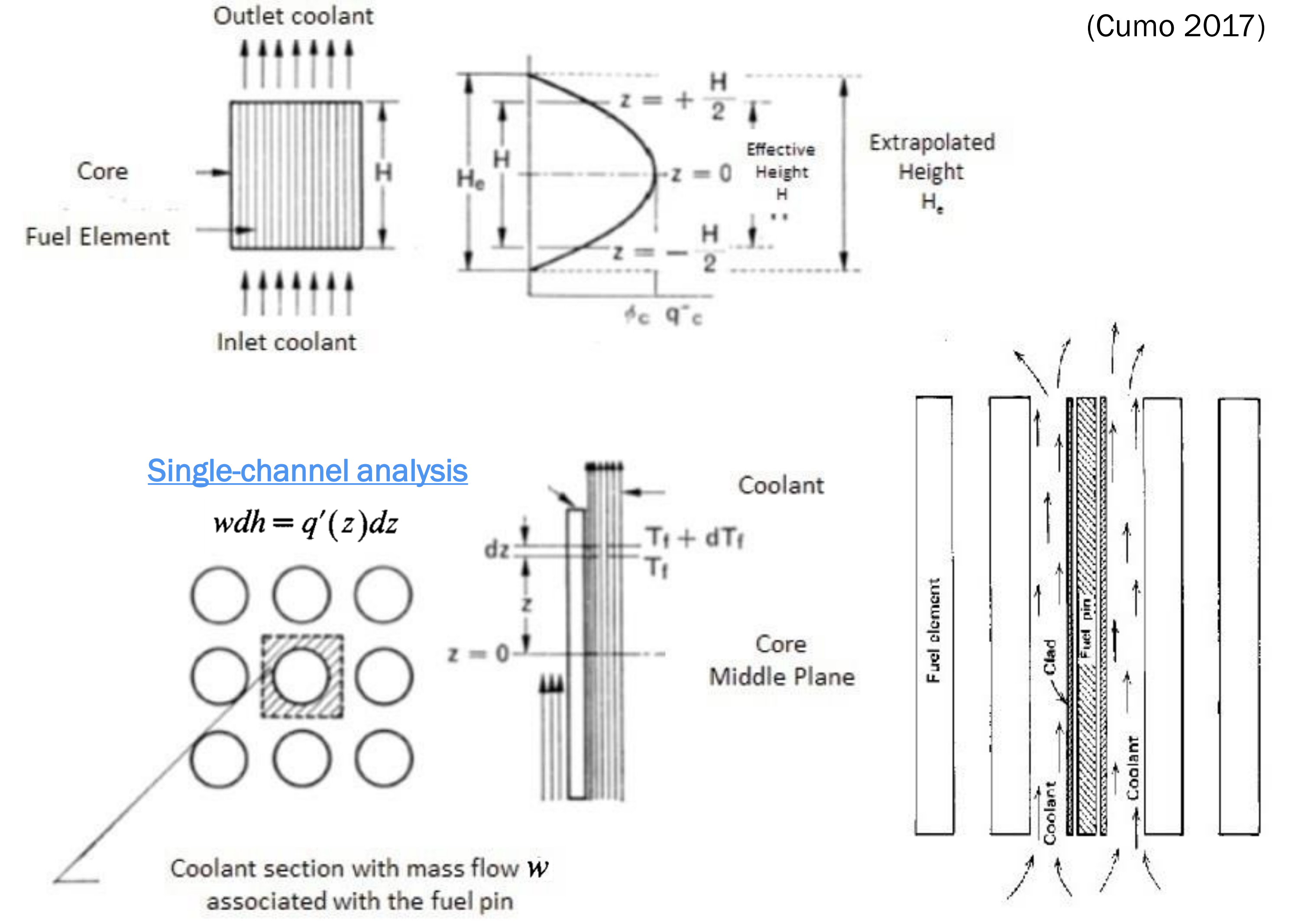
Approach of "the limiting pin“:

i.e., the pin featured by the minimum margin between the parameter of interest (performance indicator) and the corresponding design limit

- minimal computation time
- significant conservatism

Schematic of computer codes (v)

- Computer codes used for modelling fuel behaviour under irradiation and their interactions


(Cumo 2017)

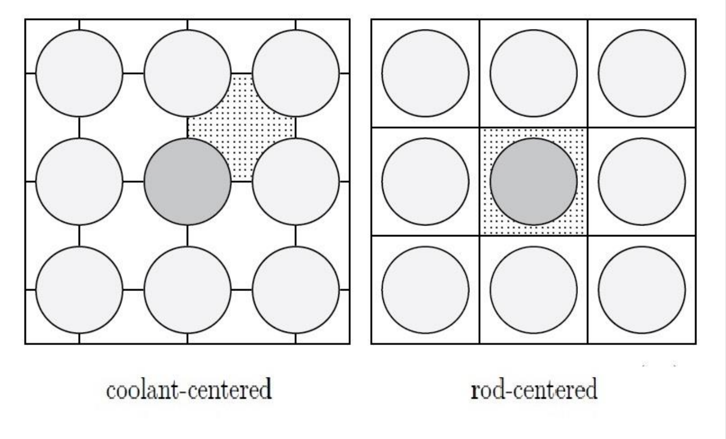
Single-channel analysis

$$wdh = q'(z)dz$$

FUEL PERFORMANCE CODE

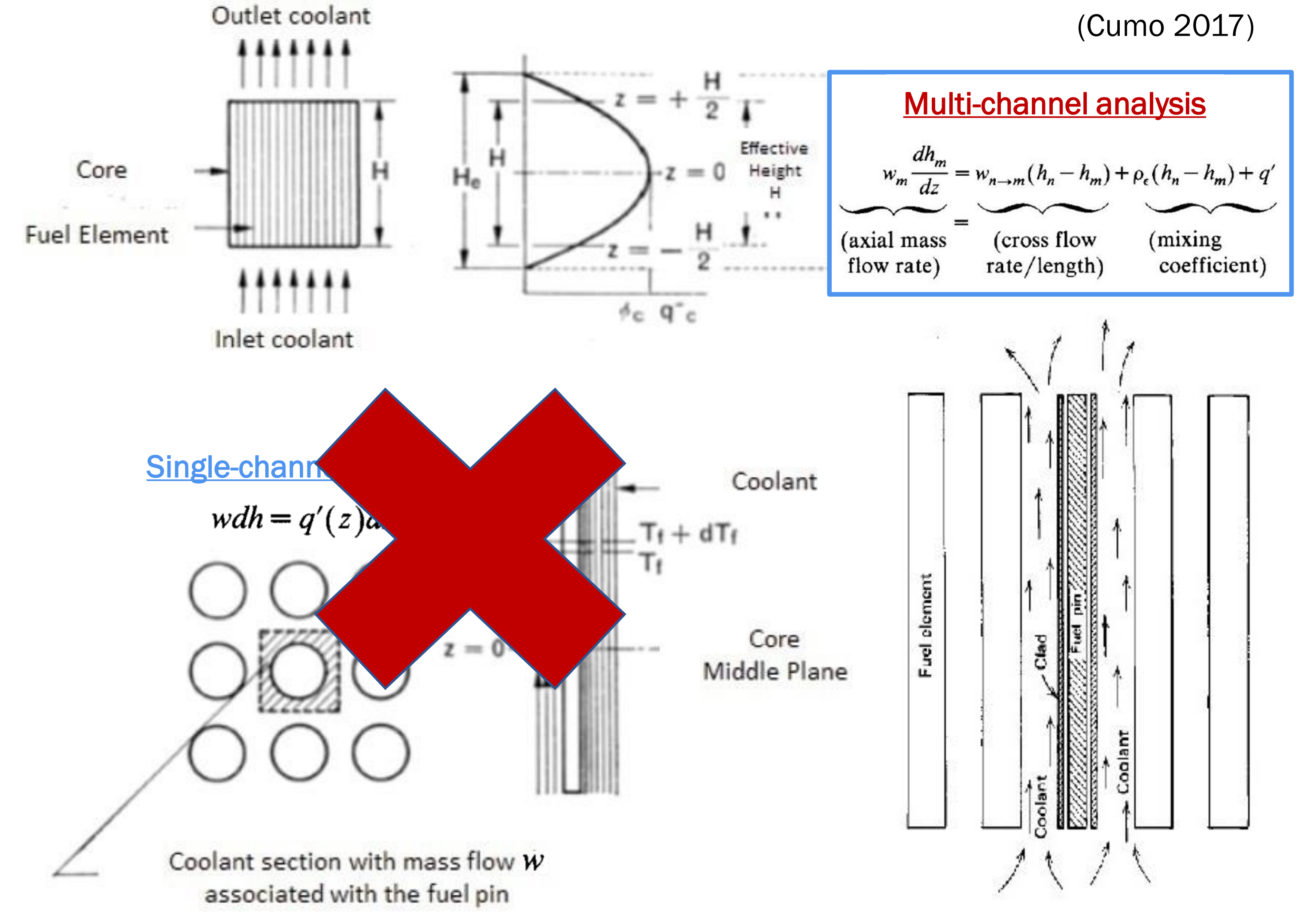
Average core conditions

Hot pin conditions...



Schematic of computer codes (vi)

- **Alternative** to "the limiting pin" approach ?



Multi-channel analysis

$$\underbrace{w_m \frac{dh_m}{dz}}_{\text{(axial mass flow rate)}} = \underbrace{w_{n\to m}(h_n - h_m)}_{\text{(cross flow rate/length)}} + \underbrace{\rho_\epsilon (h_n - h_m)}_{\text{(mixing coefficient)}} + q'$$

- **"whole core" fuel performance modelling** (thermo-mechanical behaviour of every fuel pin in the core is simulated)

- **Advantages:**

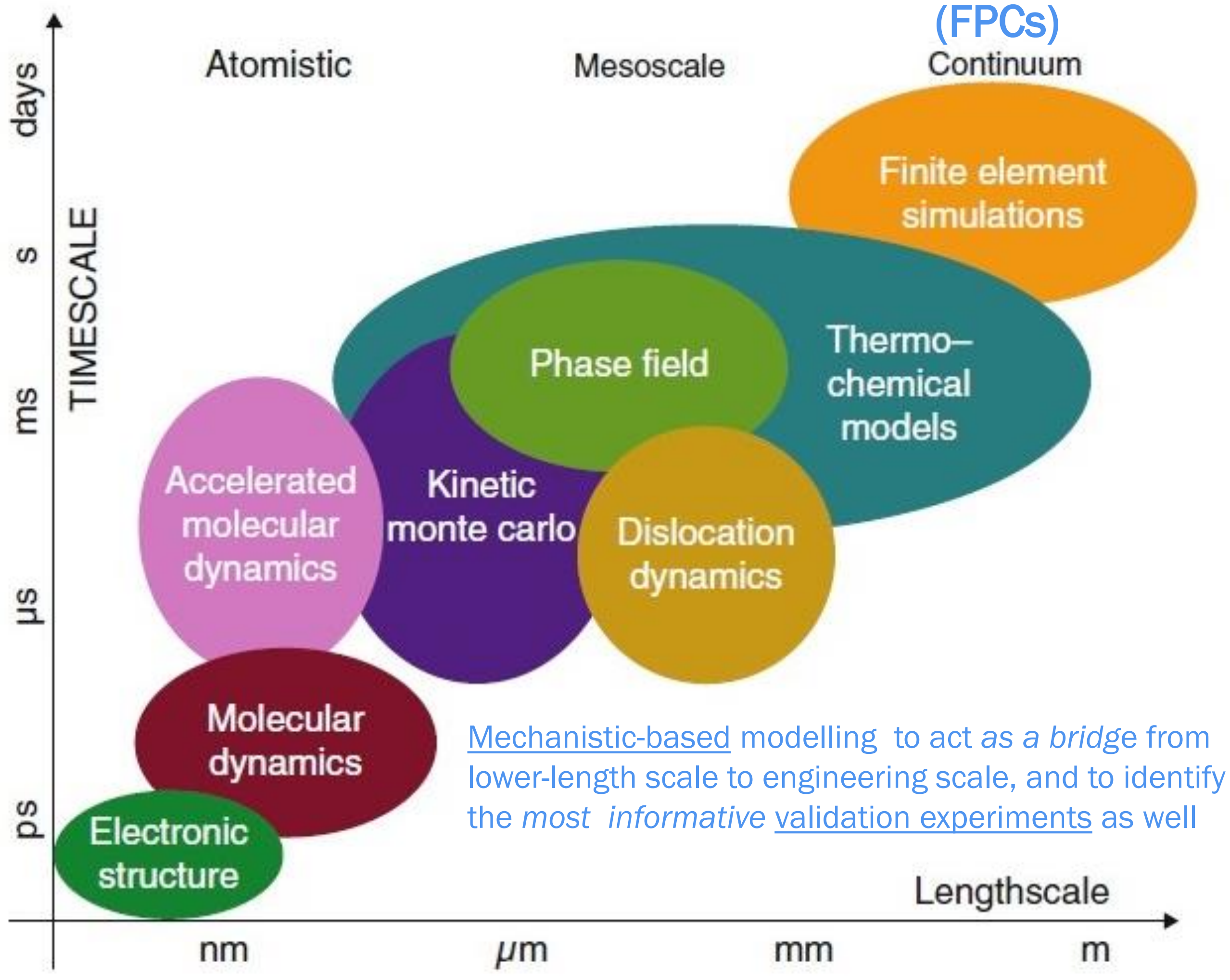
  reduced conservatism (and hence more margin to design limits), more easily quantifiable uncertainties, straightforward identification of the limiting pins, possibility to introduce more advanced methodologies…

- **Main disadvantage:**

  large amount of computing power

Notes on Advanced Fuel Modelling and Simulation (i)

- Multi-scale fuel performance modelling approach



Mechanistic-based modelling to act *as a bridge* from lower-length scale to engineering scale, and to identify the *most informative* validation experiments as well

(Stan et al. 2007)

- Current, near- and long-term **trends** in *high-fidelity* fuel pin behaviour modelling:

a) coupling of computer codes
b) implementation of more advanced modelling & simulation techniques

---> MOOSE, PLEIADES, SALOME, NURESIM **multi-physics platforms**

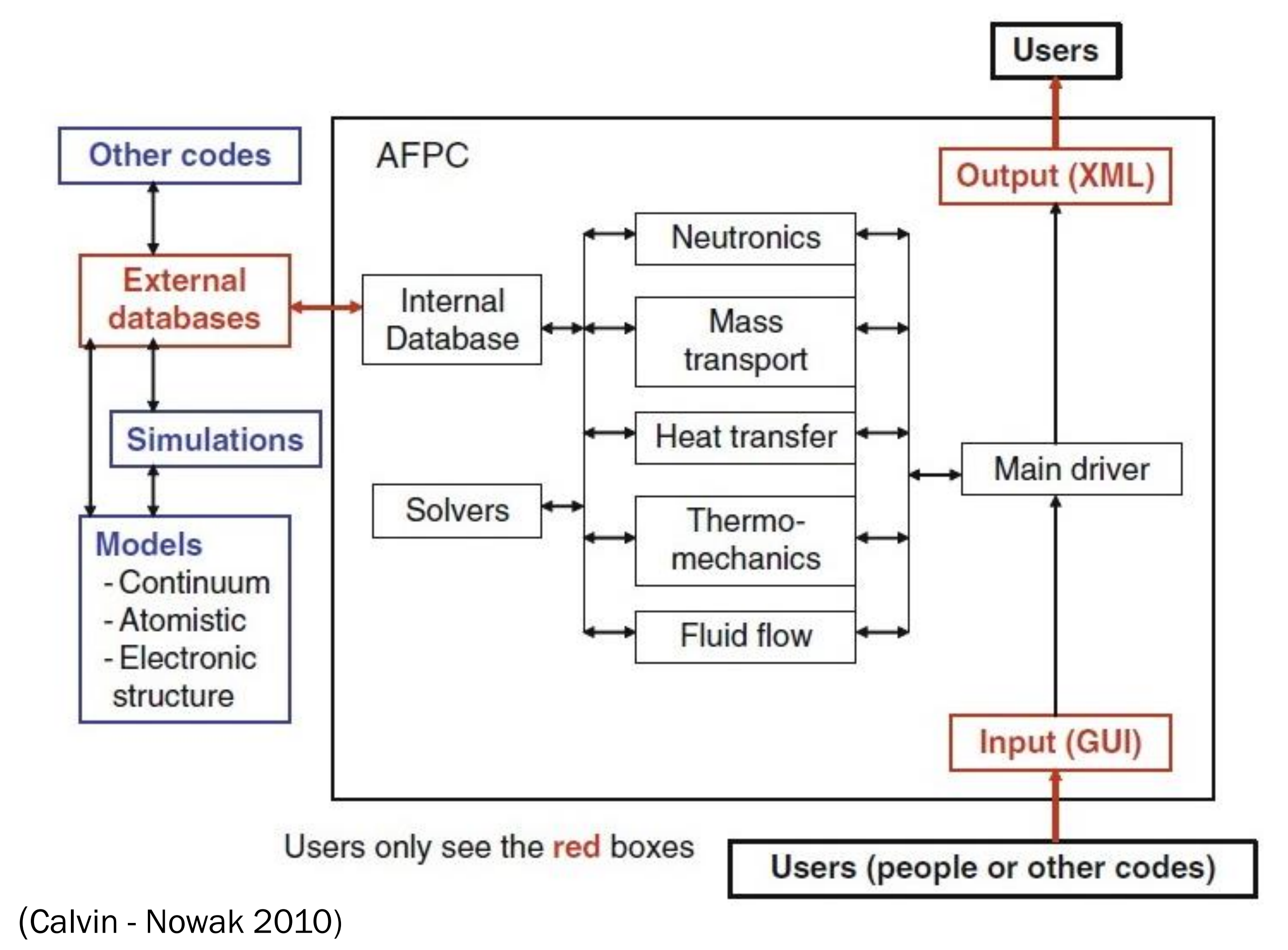
c) multi-scale fuel performance modelling

---> coupled with the need to move to **3-D fuel pin modelling**, the implementation in FPCs of **atomistically-informed engineering-scale models** should yield large advances in the simulation of fuel behaviour

d) "**whole core**" fuel performance modelling
e) advanced fuel performance capability (AFPC)

Notes on Advanced Fuel Modelling and Simulation (ii)

- Preliminary design of a new generation, advanced fuel performance capability (AFPC)



(Calvin - Nowak 2010)

To address material properties and phenomena, an AFPC must include, *at the minimum*:

- **Neutronics** (fission and neutrons diffusion)
- **Heat transfer** (conduction, convection, and radiation)
- **Mass transport** (species diffusion and gas accumulation)
- **Thermo-mechanics** (deformation, such as swelling, and stresses)
- **Fluid flow** (to model the coolant, *if necessary*)

This challenging endeavour involves:

- model development & software engineering

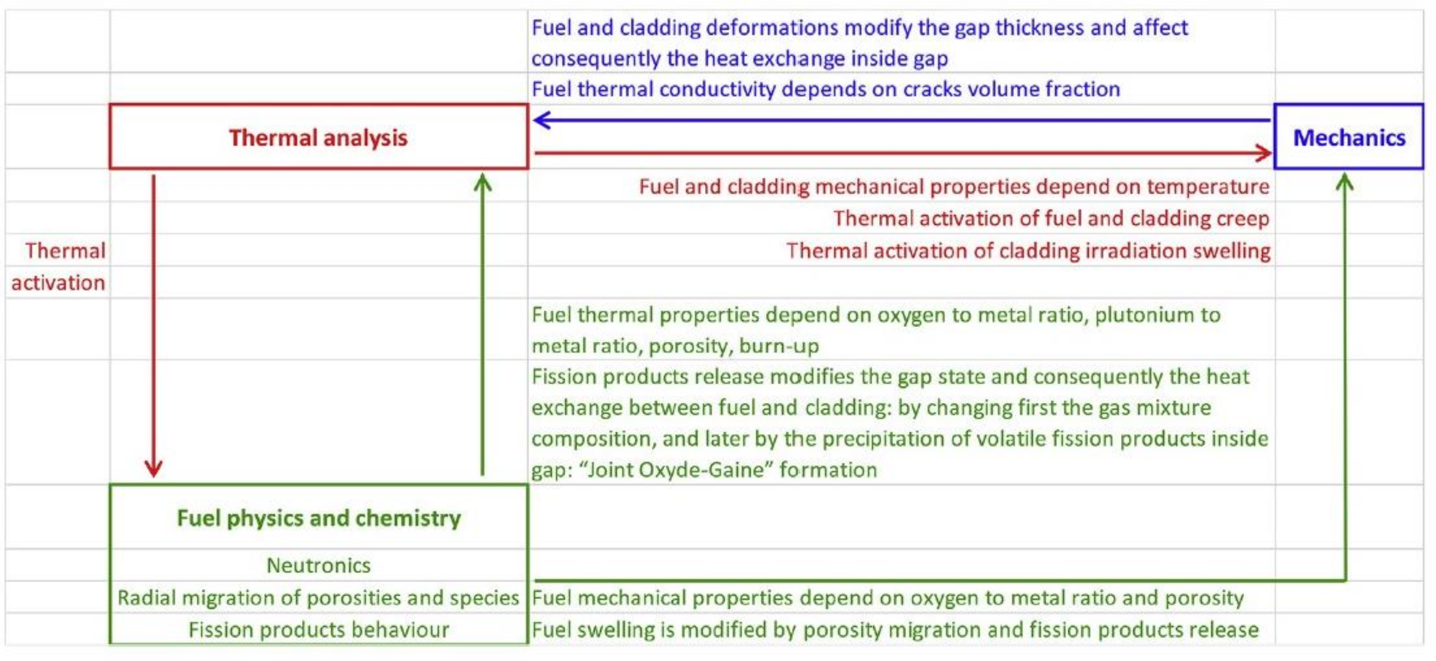
FUEL PERFORMANCE CODES

General outline

- Some topics *on the fly* …

- **Development/use of FPCs**
- **Geometric domains represented**
- **Mathematical/numerical frame**
- **Validation**
- Burnup analysis
- Thermal analysis
- Mechanical analysis
- Material and behavioural models (e.g., Fission Gas Behaviour)

…. but knowing that we have to *keep an eye* on the physical couplings and the calculation sequence



Thermal analysis

Mechanics

Fuel physics and chemistry

Fuel and cladding deformations modify the gap thickness and affect consequently the heat exchange inside gap

Fuel thermal conductivity depends on cracks volume fraction

Fuel and cladding mechanical properties depend on temperature

Thermal activation of fuel and cladding creep

Thermal activation of cladding irradiation swelling

Thermal activation

Fuel thermal properties depend on oxygen to metal ratio, plutonium to metal ratio, porosity, burn-up

Fission products release modifies the gap state and consequently the heat exchange between fuel and cladding: by changing first the gas mixture composition, and later by the precipitation of volatile fission products inside gap: "Joint Oxyde-Gaine" formation

Neutronics

Radial migration of porosities and species

Fission products behaviour

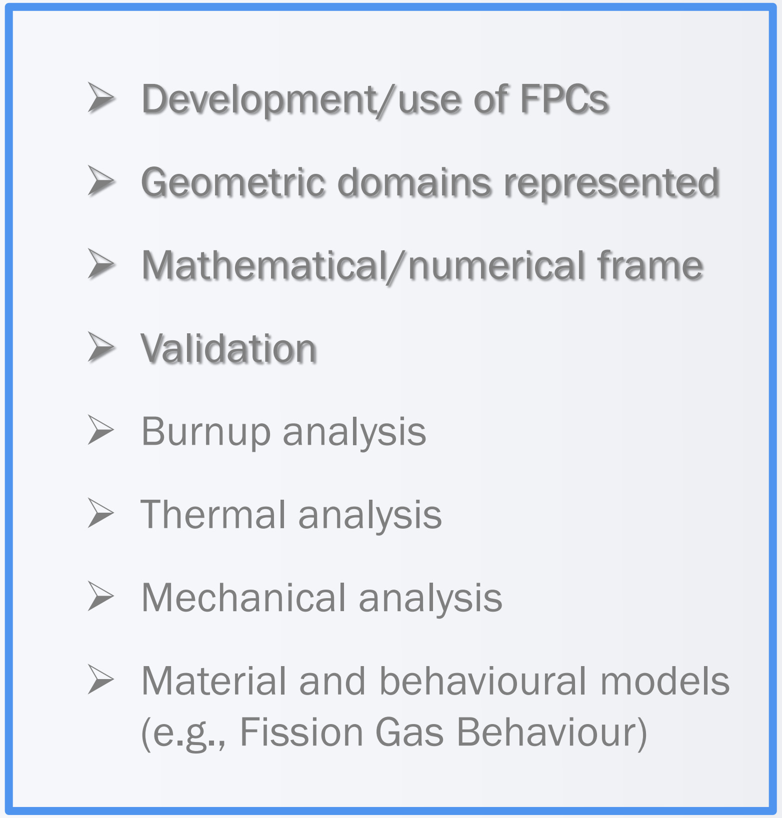
Fuel mechanical properties depend on oxygen to metal ratio and porosity

Fuel swelling is modified by porosity migration and fission products release

(Lainet et al. 2019)

General outline

- Some topics *on the fly* …



- ➢ **Development/use of FPCs**
- ➢ **Geometric domains represented**
- ➢ **Mathematical/numerical frame**
- ➢ **Validation**
- ➢ Burnup analysis
- ➢ Thermal analysis
- ➢ Mechanical analysis
- ➢ Material and behavioural models (e.g., Fission Gas Behaviour)

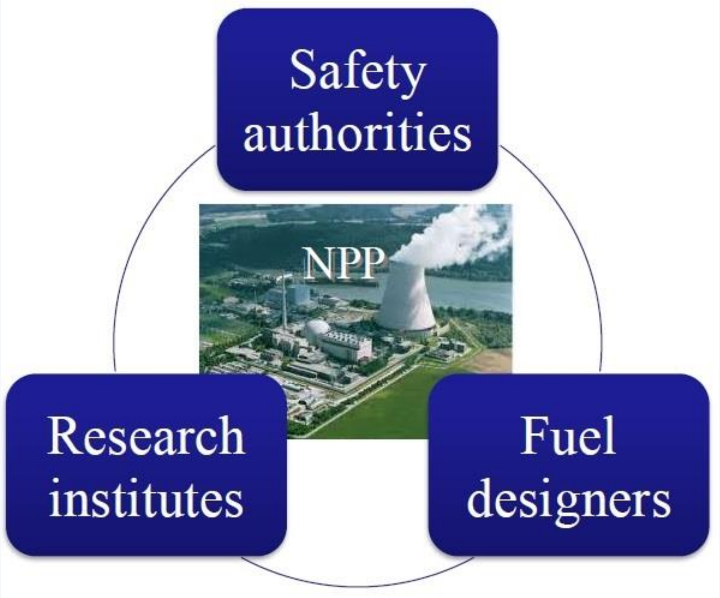
TUTORIAL
&
CASE STUDY
(FPCs in FRs)

- Development/use of FPCs
- Geometric domains represented
- Mathematical/numerical frame
- Validation
- Burnup analysis
- Thermal analysis
- Mechanical analysis
- Material and behavioural models (e.g., Fission Gas Behaviour)

Development/use of FPCs

Development / use of FPCs (i)

- Who // which ?
  - Fuel designers and vendors // Copernic, …
  - Research institutes // Alcyone, Bison, Cosmos, Enigma, Falcon, Femaxi, Frapcon, Fraptran, Germinal, MFPR, Scanair, SFPR, START, Transuranus, …
  - Safety authorities // Frapcon, Fraptran, …
  - Utilities & industry // Cyrano, Galileo, Pad, Rodex, …

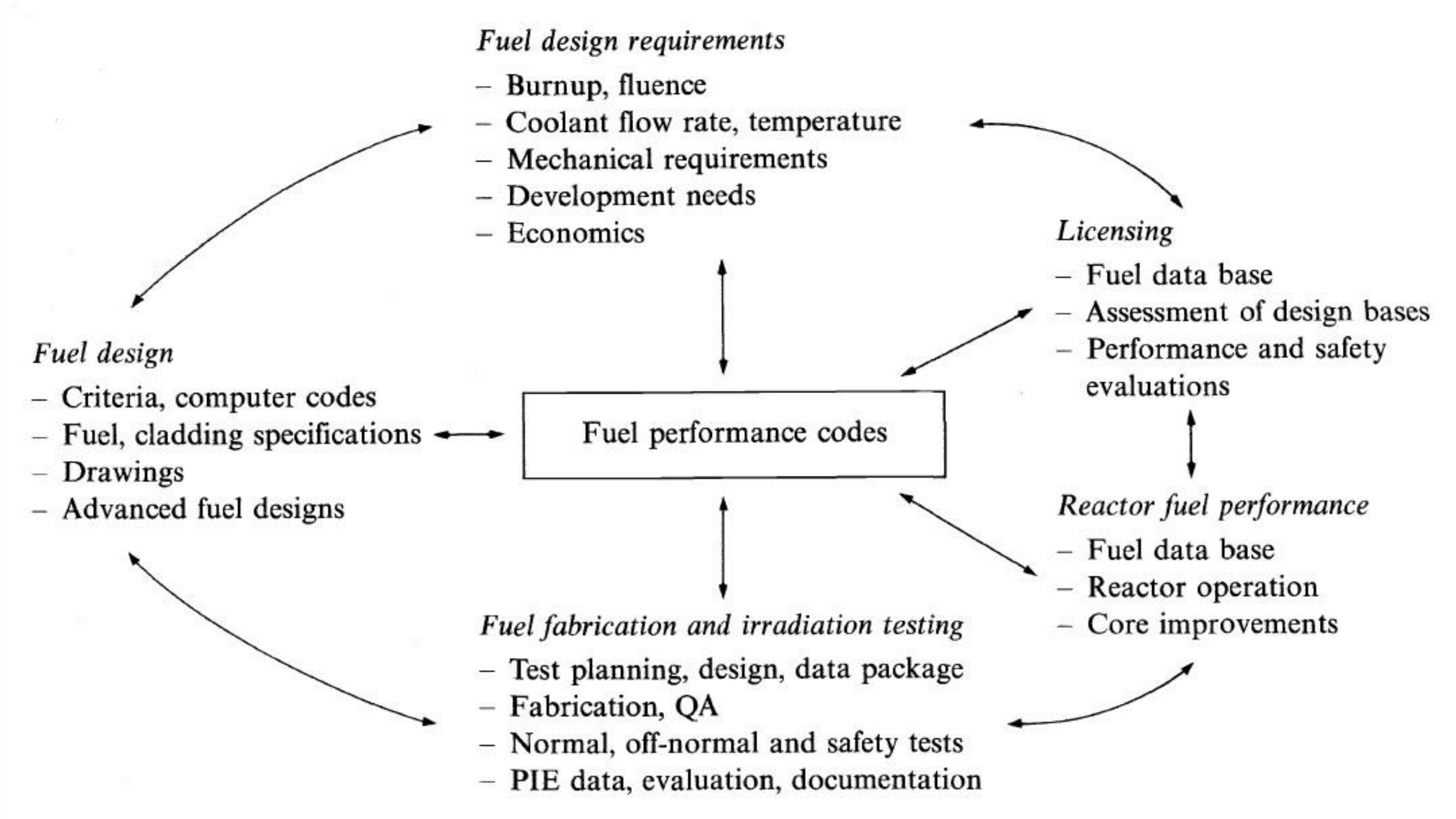


Country	Organization	Code name (precursor codes)
Argentina	CNEA	BACO, DIONISIO
Belgium	Belgonucleaire	COMETHE
	SCK-CEN	MACROS (ASFAD)
China	Xi'an Xiaotong Univeristy	FROBA
	CIAE	FTPAC
	NPIC	FUPAC
	CGNPC	JASMINE
Czech Republic	UJV	PIN-MICRO (GAPCON-THERMAL2)
France	CEA	ALCYONE (METEOR-TRANSURANUS)
	Framatome	COPERNIC (TRANSURANUS), GALILEO (COPERNIC/RODEX/CARO)
	EdF	CYRANO
	IRSN	SCANAIR
Germany	Siemens	CARO
	Framatome	GALILEO (COPERNIC/RODEX/CARO)
	GRS	TESPA-ROD (TESPA)
	JRC	TRANSURANUS (URANUS)
Hungary	MTA EK	FUROM (PIN-MICRO)
India	BARC	FAIR, PROFESS
	PNC	FUDA
Japan	CRIEPI	EIMUS (FEMAXI-III)
	JAEA	FEMAXI, RANNS
	SEPC	IRON (FEMAXI-III)
	NFD	TRUST
Korea	KAERI	COSMOS, INFRA
Russian Federation	VNIINM	START, RAPTA
	TRINITI	RTOP
	IBRAE	SFPR (MFPR)
Sweden	Westinghouse Sweden Electric	STAV
United Kingdom	NNL, EDF Energy	ENIGMA (MINIPAT, SLEUTH, HOTROD)
USA	USNRC	FRAPCON, FRAPTRAN (FRAP), FAST
	Siemens	RODEX
	EPRI	FALCON (FREY, ESCORE)
	INL	BISON
	Framatome	GALILEO (COPERNIC/RODEX/CARO)
	Westinghouse	PAD

(Van Uffelen et al. 2019)

Development /use of FPCs (ii)

- FPCs —> central role in the overall fuel design & development process



Fuel design requirements
- Burnup, fluence
- Coolant flow rate, temperature
- Mechanical requirements
- Development needs
- Economics

Fuel design
- Criteria, computer codes
- Fuel, cladding specifications
- Drawings
- Advanced fuel designs

Fuel performance codes

Licensing
- Fuel data base
- Assessment of design bases
- Performance and safety evaluations

Reactor fuel performance
- Fuel data base
- Reactor operation
- Core improvements

Fuel fabrication and irradiation testing
- Test planning, design, data package
- Fabrication, QA
- Normal, off-normal and safety tests
- PIE data, evaluation, documentation

(Boltax 1994)

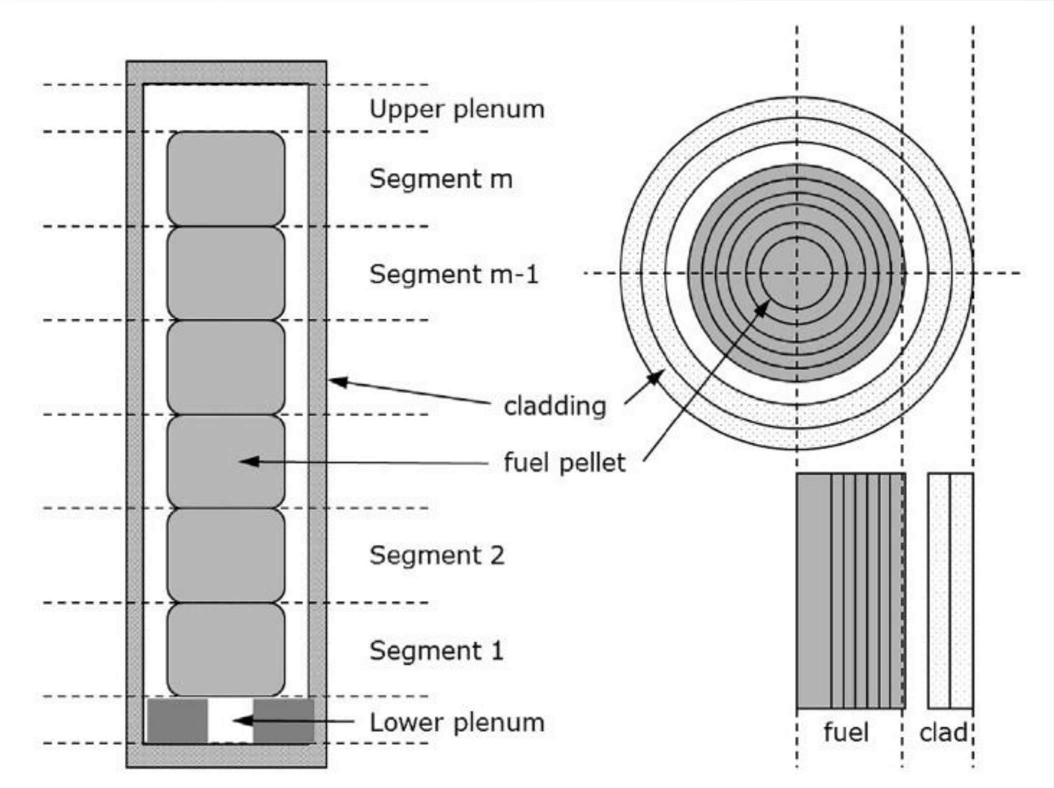
- The design process *starts with* fuel design requirements ...
- ... however, there is no clear end point because the process *continues indefinitely* as long as replacement fuel is required, and there is an incentive to improve the fuel (e.g., cost reduction, safer operation, extended burnup)

- Development/use of FPCs
- **Geometric domains represented**
- Mathematical/numerical frame
- Validation
- Burnup analysis
- Thermal analysis
- Mechanical analysis
- Material and behavioural models (e.g., Fission Gas Behaviour)

Geometric domains represented

Geometric representation (i)

- Simple representation of the fuel pin in a FPC

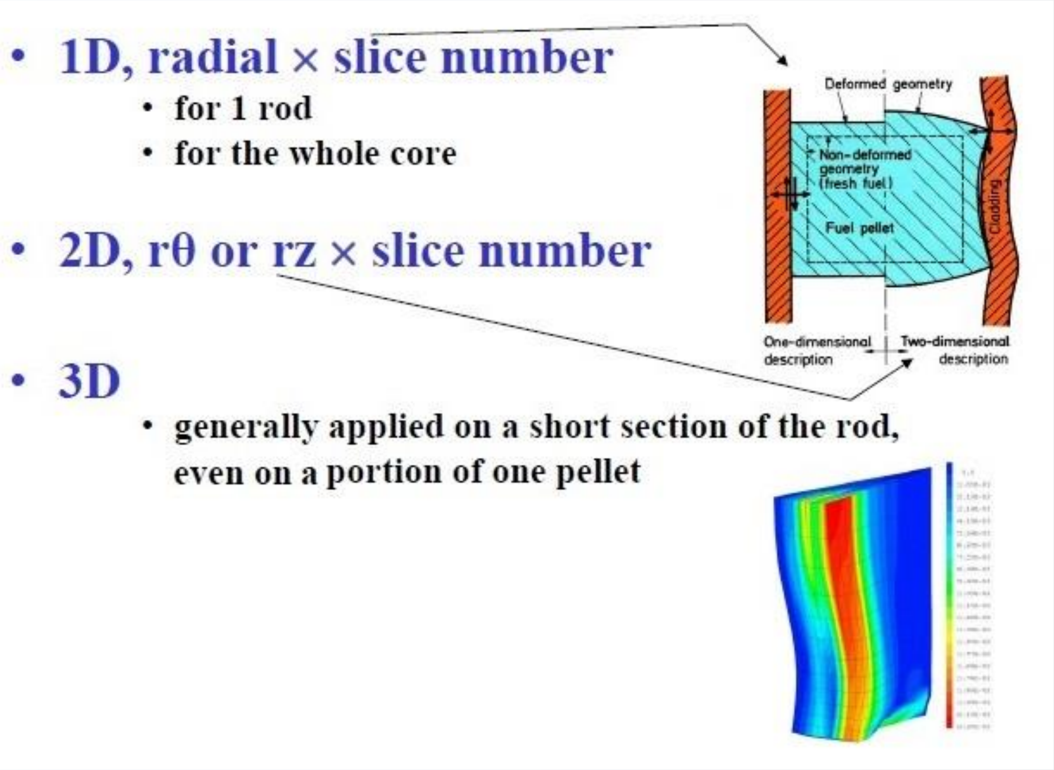


(Van Uffelen et al. 2019)

- **Active length** of the fuel pin (i.e., the part containing the fuel pellets or bar) is usually represented by a series of axial zones (or segments/slices). In each axial zone, the fuel is divided into radial annuli (or rings), usually of equal volume, but sometimes of equal thickness
- **Cladding** may also be divided into several rings (especially, if liner or corrosion layer is being simulated)
- **Free volumes** associated with fuel-cladding gap, pellet dishes and chamfers, pellet cracks, pellet/bar hole (*if any*), any upper and lower plena are also generally modelled

Geometric representation (i)

- Simple representation of the fuel pin in a FPC



- **1D, radial × slice number**
  - for 1 rod
  - for the whole core
- **2D, rθ or rz × slice number**
- **3D**
  - generally applied on a short section of the rod, even on a portion of one pellet

(Noirot 2016)

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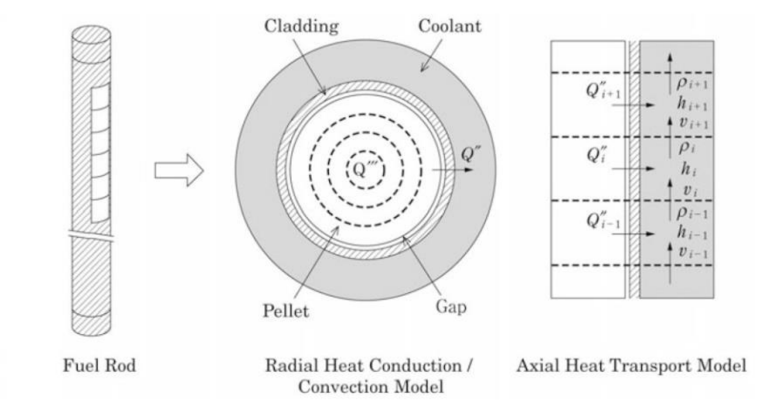
- Cladding may also be divided into several rings (especially, if liner or corrosion layer is being simulated)
- Free volumes associated with fuel-cladding gap, pellet dishes and chamfers, pellet cracks, pellet/bar hole (*if any*), any upper and lower plena are also generally modelled
- Further details depend on the **sophistication of the simulation**, which can be – under some necessary simplifications – 1½-D, 2-D or 3-D (steady-state and/or transient)

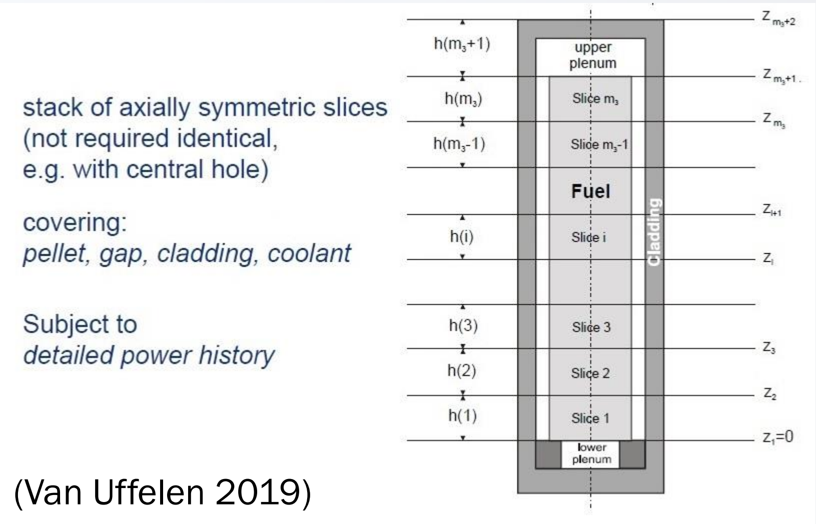
Geometric representation (ii)

- **Axisymmetric, axially-stacked, one-dimensional radial representation** (referred to as 1½-D /1.5D)

"Single-channel" heat transfer calculation model



(Okumura et al. 2014)


stack of axially symmetric slices (not required identical, e.g. with central hole)

covering: *pellet, gap, cladding, coolant*

Subject to *detailed power history*

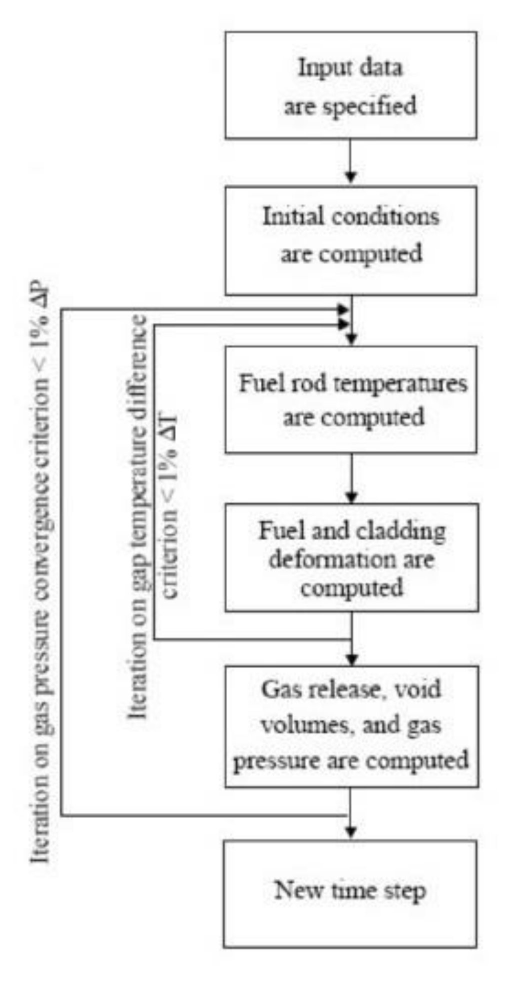
(Van Uffelen 2019)

- Cladding-coolant interface is represented by an annular flow channel: **only radial** (i.e., no axial or hoop) **heat flow** is assumed, and the fuel pin rings are all considered to be subject to the same axial strain
- **"Generalized plane strain"**, in conjunction with **axial-symmetry**, allows shear stresses to be ignored –> stresses along radial, hoop and axial directions are principal stresses $(\sigma_r, \sigma_\theta, \sigma_z \rightarrow s_I, s_{II}, s_{III})$
- **Thermal** (energy conservation) **and mechanical equations** (force bal., stress-strain + strain-displacement relationships) are typically solved by a **finite difference scheme**
- **Coupling between axial zones** (–> "half dimension" in the 1½-D) is restricted... to the coolant enthalpy, pin internal pressure and gas transport. Usually, **small-strain/small-displacement** theory for the kinematic representation
- A **1½-D code** cannot simulate phenomena caused by shear stresses, (e.g., pellet hourglassing, clad ridging, axial extrusion, pellet cracking, *although the fact that the pellets are cracked is taken into account*)

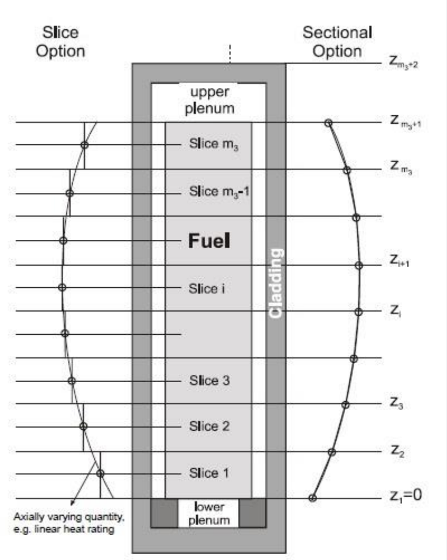
Geometric representation (ii)

- **Axisymmetric, axially-stacked, one-dimensional radial representation** (referred to as 1½-D /1.5D)

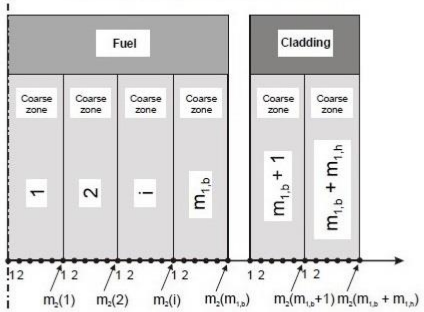
FRAPCON flowchart (simpl.)



TRANSURANUS nodes



(Van Uffelen 2019)



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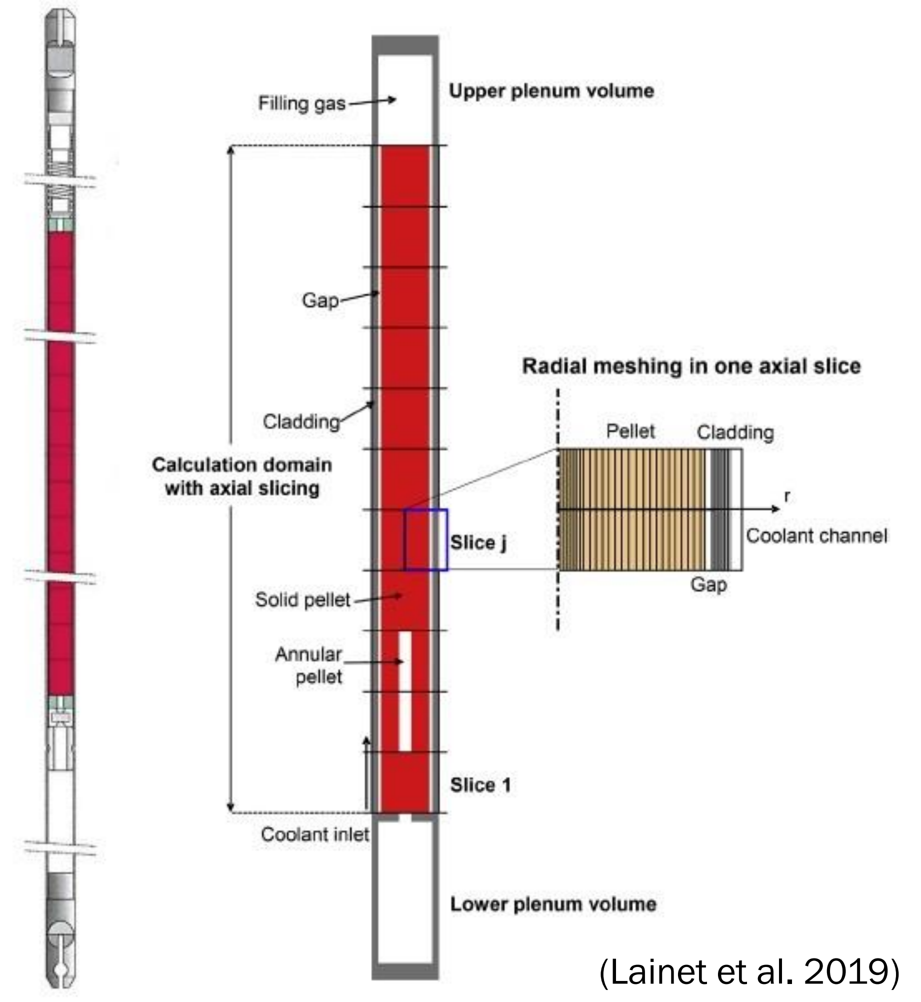
Geometric representation (ii)

- **Axisymmetric, axially-stacked, one-dimensional radial representation** (referred to as 1½-D /1.5D)

1.5D fuel pin representation used by GERMINAL V2



(Lainet et al. 2019)

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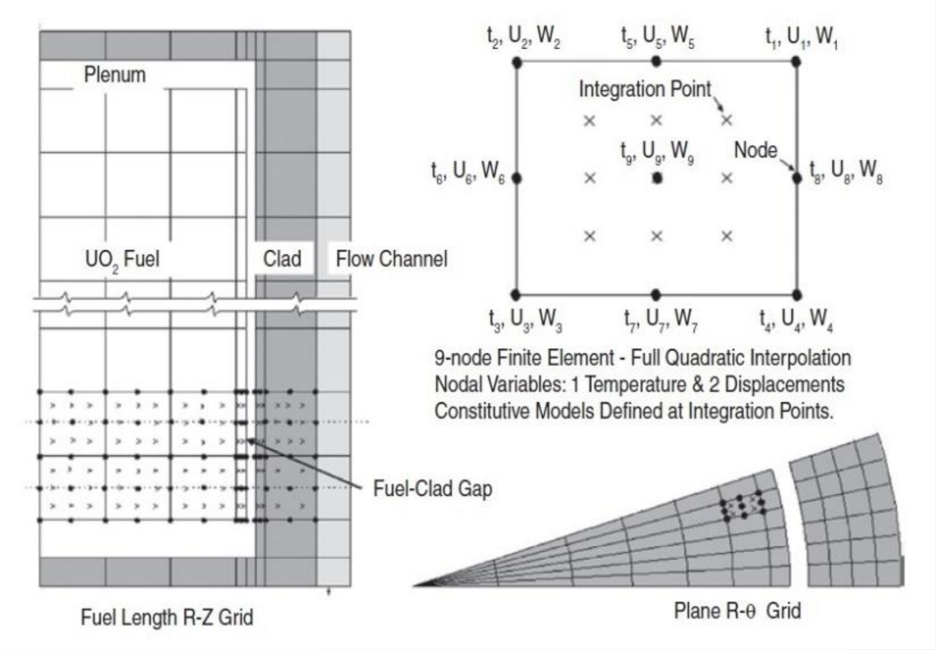
- A **1½-D code** cannot simulate phenomena caused by shear stresses, (e.g., pellet hourglassing, clad ridging, axial extrusion, pellet cracking)
- Examples of 1.5D codes are GERMINAL, TRANSURANUS

Geometric representation (iii)

- 2-D (r-z and r-θ), fully thermal-mechanically coupled, (FEM) finite-element-based

FALCON spatial models and FEM structure



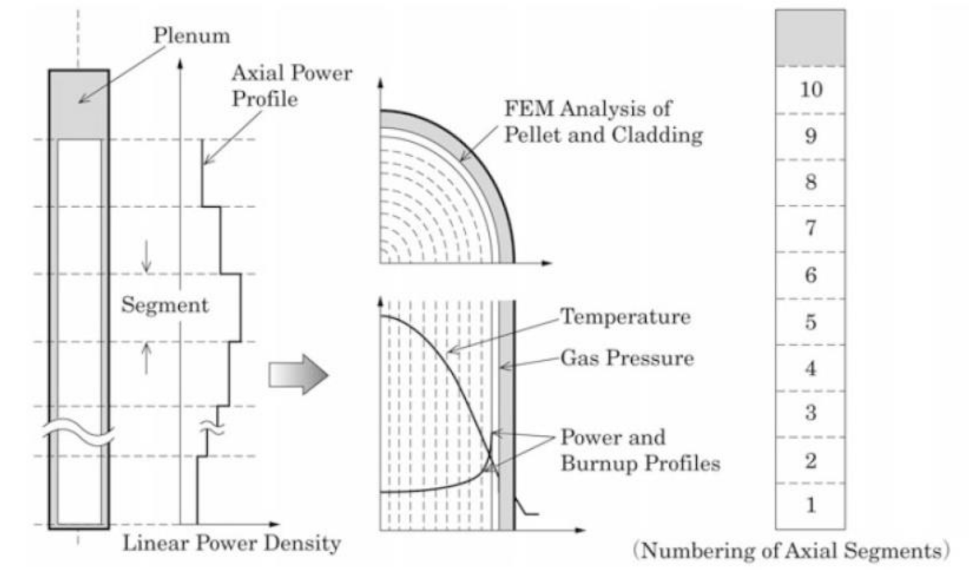
(Rashid et al. 2011)

- Fuel pin geometry representation (effectively only applicable to pelleted fuel) by means of either **axisymmetric (r-z) or plane (r-θ) grids** treated as 2-D continua
- There is radial and axial modelling of a fuel pellet in each axial zone --> **axial-symmetry** is still assumed, but not **"generalized plane axial strain"**
- **Thermal and mechanical equations** are typically solved by a **finite element technique** (FEM)
- **Examples of 2-D codes** are FALCON, FEMAXI

Geometric representation (iii)

- 2-D (r-z and r-θ), fully thermal-mechanically coupled, (FEM) finite-element-based

FEMAXI-6 calculation model



(Okumura et al. 2014)

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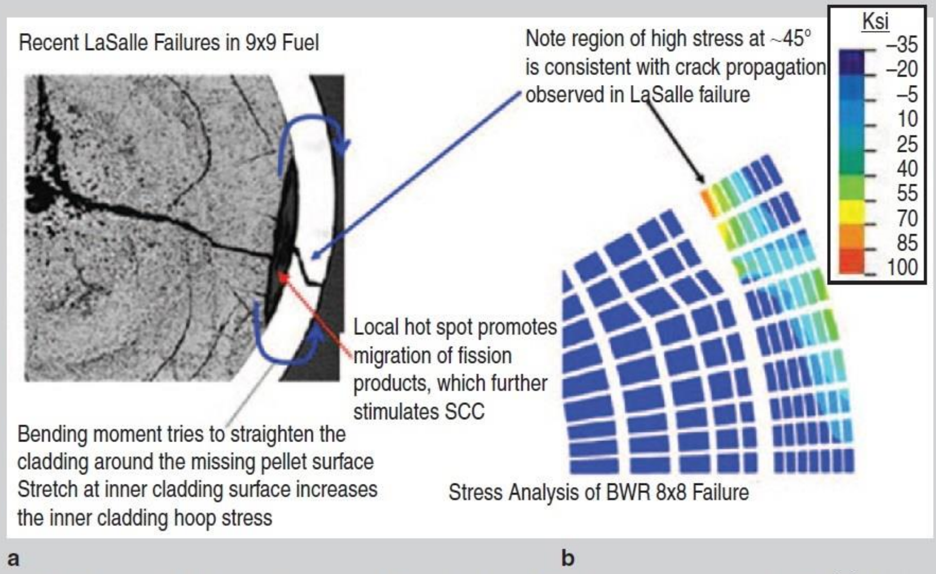
Geometric representation (iii)

- 2-D (r-z and r-θ), fully thermal-mechanically coupled, (FEM) finite-element-based

Modelling and simulation of manufacturing-induced Missing Pellet Surface (MPS) conditions with FALCON



(a) MPS induced failure pattern, and (b) calculated cladding hoop stress (psi) distribution.

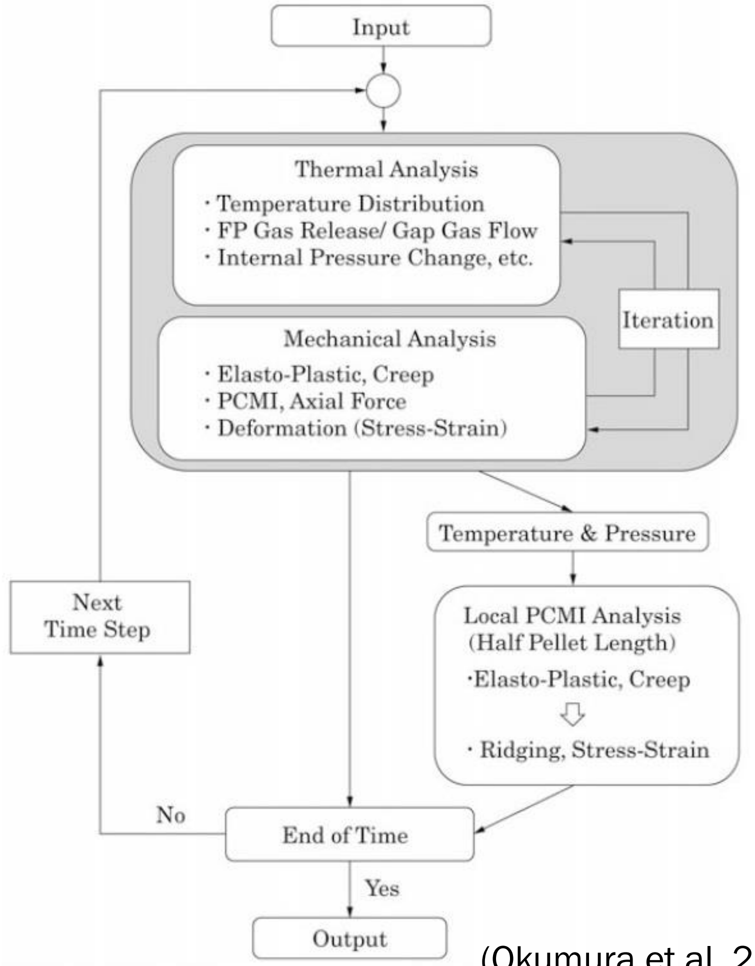
(Rashid et al. 2011)

- **Advantage** --> 2-D phenomena such as pellet hour-glassing, clad ridging. large-strain ballooning-type displacements (LOCA), axial extrusion, **MPS (missing pellet surface) induced failure pattern** can be modelled explicitly, *in some way…*
- **Disadvantage** --> increased complexity, and therefore also slower running time
- **"Hybrid" codes** of 1½-D and 2-D representations, e.g., ENIGMA nominally with a 1½-D scheme --> effects of shear stresses approximated by means of models for axial extrusion and for pellet hour-glassing; hoop cladding stress concentration over radial fuel cracks calculated using a model *ad hoc*.

Geometric representation (iv)

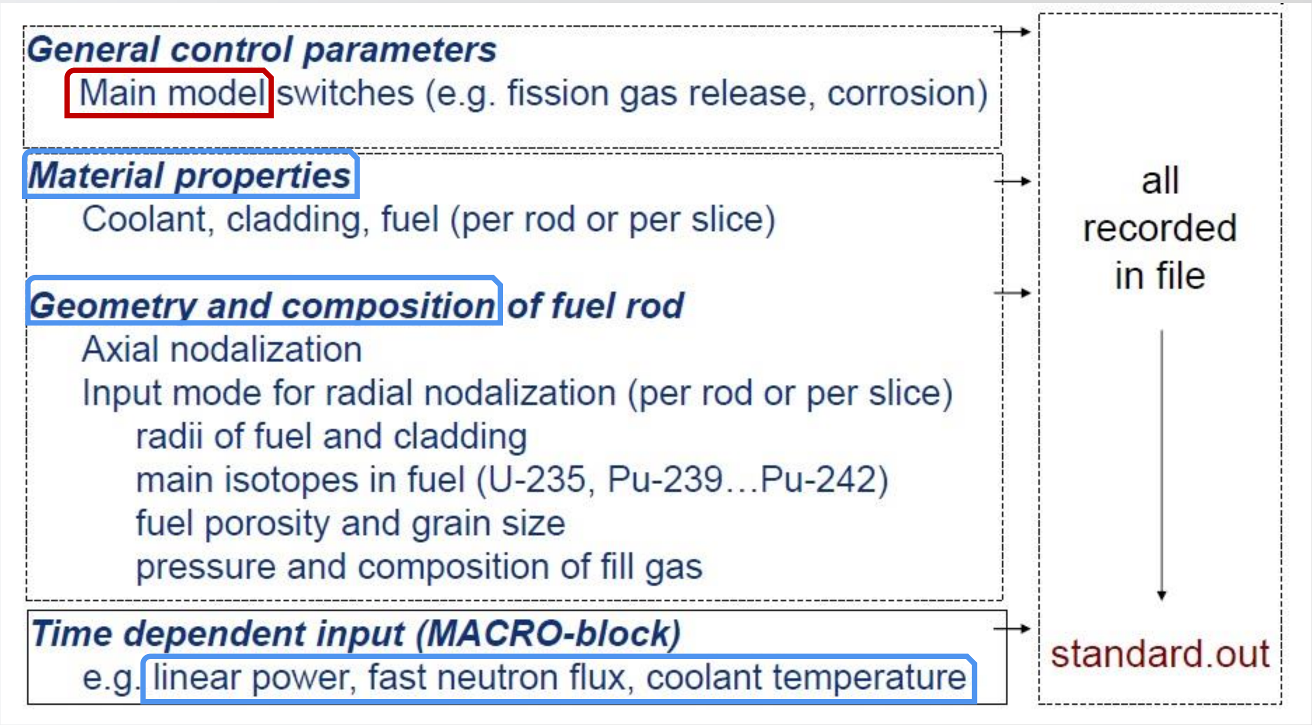
- What is needed for thermo-mechanical solutions in all classes of codes (1½-D, 2-D, 3-D, hybrid type)

FEMAXI-6 structure



(Okumura et al. 2014)

- INPUT for thermo-mechanical analysis (e.g., TRANSURANUS)



General control parameters
Main model switches (e.g. fission gas release, corrosion)

Material properties
Coolant, cladding, fuel (per rod or per slice)

Geometry and composition of fuel rod
Axial nodalization
Input mode for radial nodalization (per rod or per slice)
radii of fuel and cladding
main isotopes in fuel (U-235, Pu-239…Pu-242)
fuel porosity and grain size
pressure and composition of fill gas

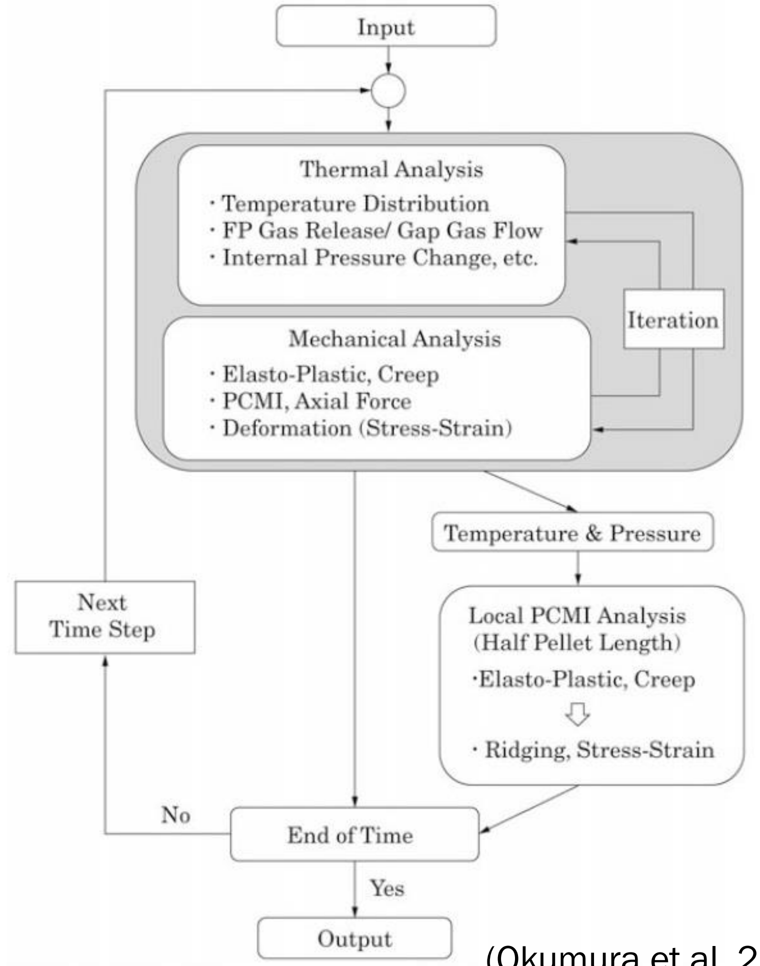
Time dependent input (MACRO-block)
e.g. linear power, fast neutron flux, coolant temperature

(Van Uffelen 2019)

Geometric representation (iv)

- What is needed for thermo-mechanical solutions in all classes of codes (1½-D, 2-D, 3-D, hybrid type)

FEMAXI-6 structure



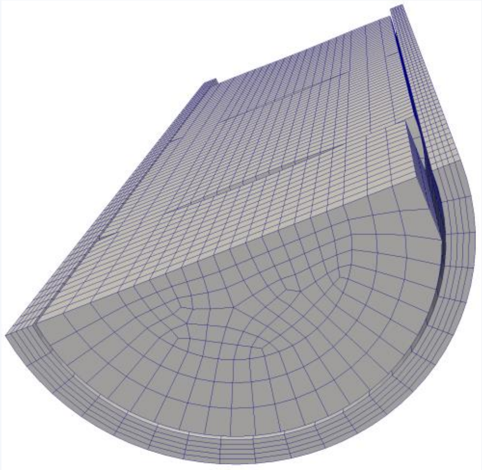
(Okumura et al. 2014)

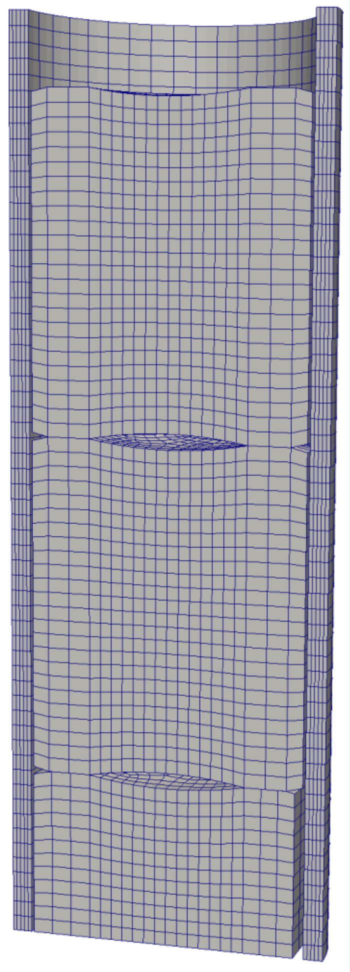
- Thermo-mechanical solutions
  - … *traditionally* proceed in a series of **step-by-step calculations** in which the **temperatures** are calculated in the fuel pellets and the cladding, using fission power input derived from separate neutronics code calculations
  - …. followed by the calculations of pellet and cladding **displacements**, **strains** and **stresses**, with both sets of calculations performed within an iteration loop
  - **Convergence** is usually judged by the status of the gap, which can oscillate between open and closed conditions, or between soft and hard pellet-cladding contact
  - *Currently*… thermal and mechanical equation **solvers**, **fully-coupled**, and with state-of-the-art finite element modelling techniques, are tending to be implemented
  - Drivers for these developments are the increased accuracy and the possibility of more generic application

Geometric representation (v)

- 3-D, fully thermal-mechanically coupled, (FEM) finite-element-based

3-D FEM mesh





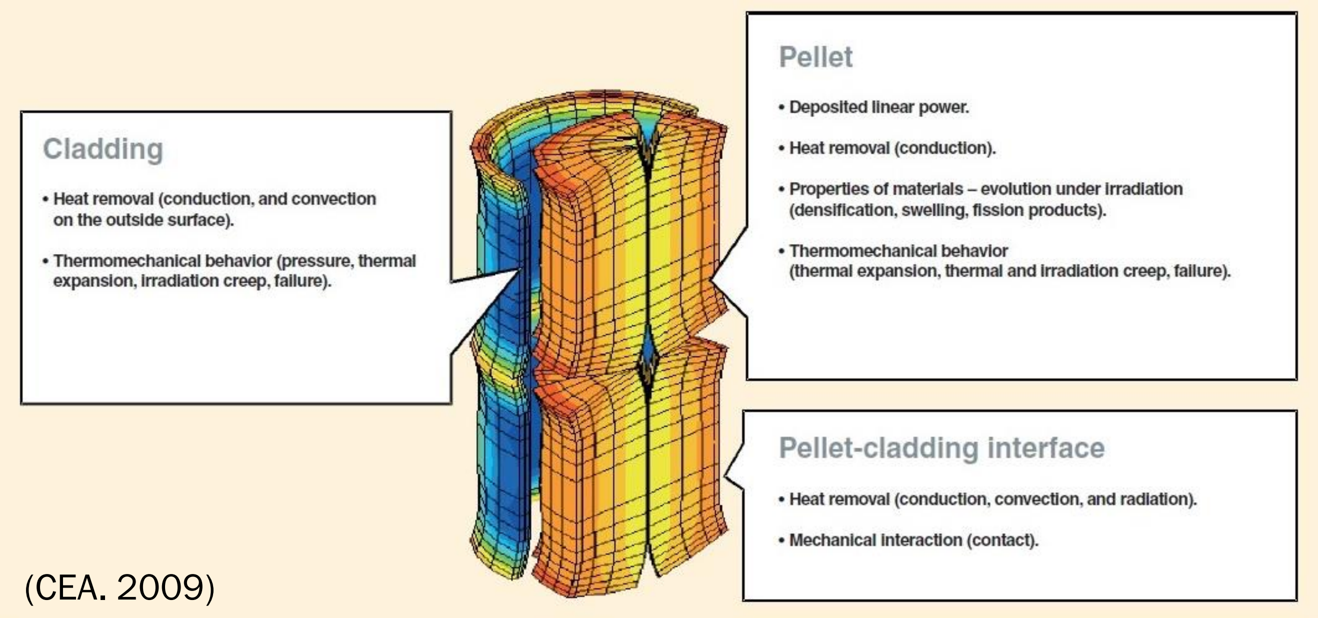
- **Three-dimensional modelling** of the fuel pellets/bar and cladding. As in the 2-D representation, thermal and mechanical equations are typically solved by **a finite element technique** (FEM)
- but applied for the **analysis of limited regions only** (short section of the rod, a portion of one pellet)
- **Advantage over 2-D codes** --> PCI-related effects or pellet-cladding eccentricity (which cannot be modelled when axial-symmetry is assumed) can be simulated
- **Disadvantage** --> increased complexity, and therefore also slower running time
- Due to intricacies of 3-D representation, **advanced numerical techniques** generally required in the solution scheme
- **Examples of 3-D codes** are ALCYONE, BISON

Geometric representation (v)

- 3-D, fully thermal-mechanically coupled, (FEM) finite-element-based

3-D thermo-mechanical, finite-element model of PWR fuel pellet stack

(short section) with ALCYONE makes it possible now ....



Cladding

- Heat removal (conduction, and convection on the outside surface).
- Thermomechanical behavior (pressure, thermal expansion, irradiation creep, failure).

Pellet

- Deposited linear power.
- Heat removal (conduction).
- Properties of materials – evolution under irradiation (densification, swelling, fission products).
- Thermomechanical behavior (thermal expansion, thermal and irradiation creep, failure).

Pellet-cladding interface

- Heat removal (conduction, convection, and radiation).
- Mechanical interaction (contact).

(CEA. 2009)

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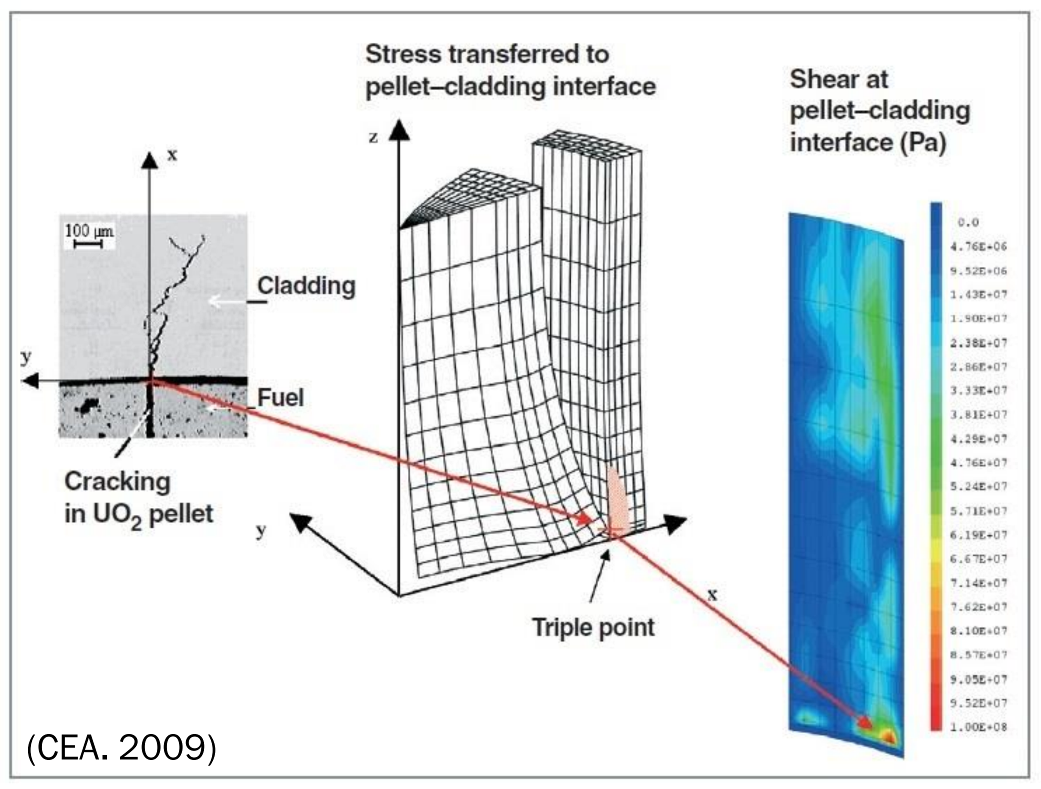
Geometric representation (v)

- 3-D, fully thermal-mechanically coupled, (FEM) finite-element-based

... to account for the localization typical of PCI failures



(CEA. 2009)

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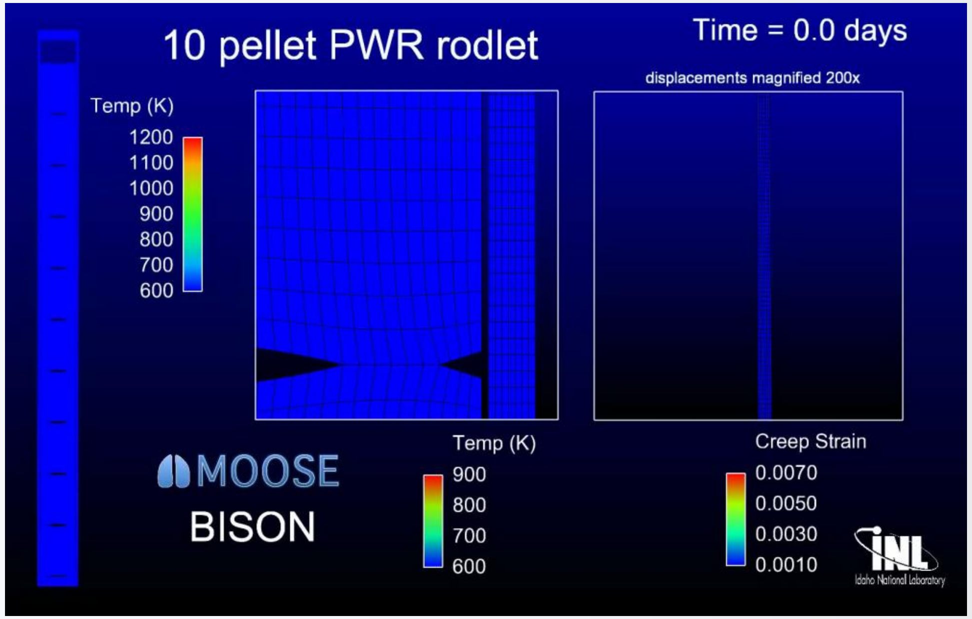
POLITECNICO MILANO 1863

Geometric representation (v)

- 3-D, fully thermal-mechanically coupled, (FEM) finite-element-based

3-D thermo-mechanical, finite-element model of a 10 pellet PWR fuel rodlet with BISON makes it possible to consider local effects such as ridging and stress concentration due to "bambooing"



(bison.inl.gov)

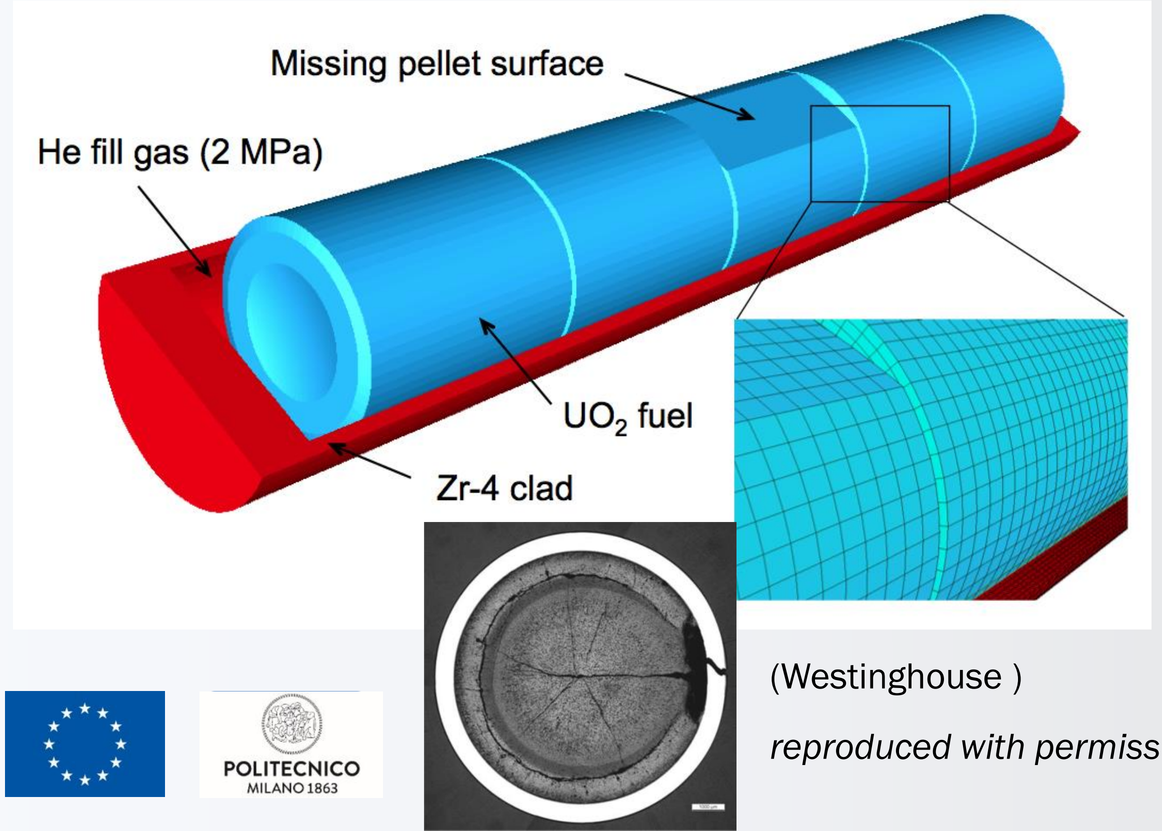
BISON animation showing the predicted thermo-mechanical behaviour of a 10 pellet PWR fuel rodlet during 2.4 years of fuel life. The **central panel** shows the evolution of thermal and mechanical contact, at the intersection of two pellets and the cladding. The **rightmost panel** shows cladding deformation with the development of a "bamboo" appearance, due to hard contact, with "hourglass-shaped" fuel pellets

https://www.youtube.com/watch?v=Vm8QYjLm9m0&list=PLX2nBoWRisnW7DGDdHr--IWPnPM3_G1f1&index=1

Geometric representation (vi)

- 3-D, fully thermal-mechanically coupled, (FEM) finite-element-based

3-D thermo-mechanical, finite-element model of a defective rod with BISON makes it possible to consider detrimental effects of a Missing Pellet Surface (MPS) imperfection



(Westinghouse)

reproduced with permission

- ➢ **Three-dimensional modelling** of the fuel pellets/bar and cladding. As in the 2-D representation, thermal and mechanical equations are typically solved by **a finite element technique** (FEM)
- ➢ but applied for the **analysis of *limited* regions only** (short section of the rod, a portion of one pellet)
- ➢ **Advantage over 2-D codes** --> PCI-related effects or pellet-cladding eccentricity, MPS (which cannot be modelled when axial-symmetry is assumed) can be simulated
- ➢ **Disadvantage** --> increased complexity, and therefore also slower running time
- ➢ Due to intricacies of 3-D representation, **advanced numerical techniques** generally required in the solution scheme
- ➢ **Examples of 3-D codes** are ALCYONE, BISON

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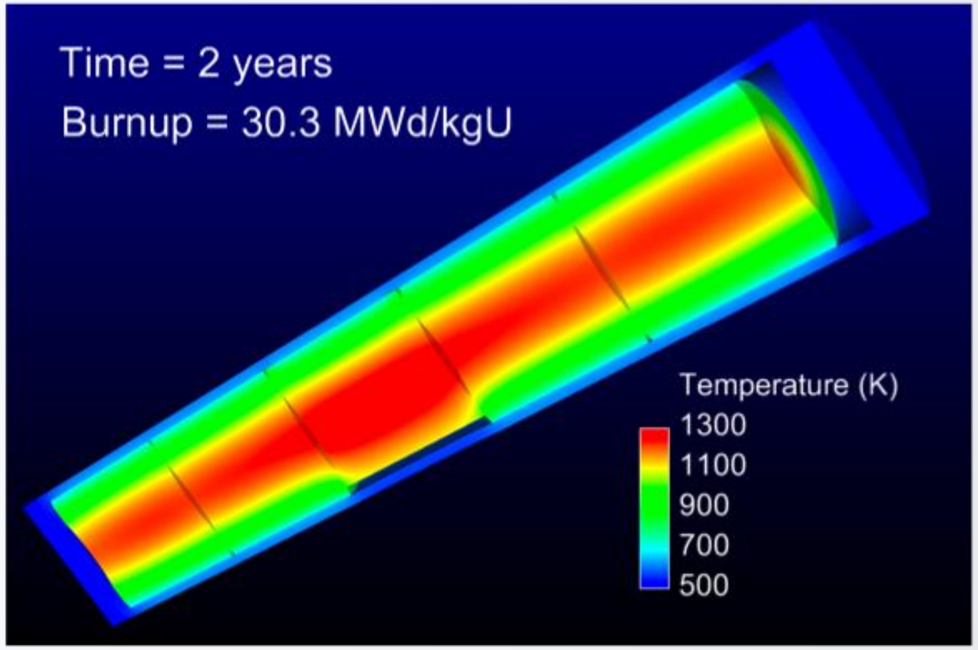

Fuel temperature (Pastore 2015)

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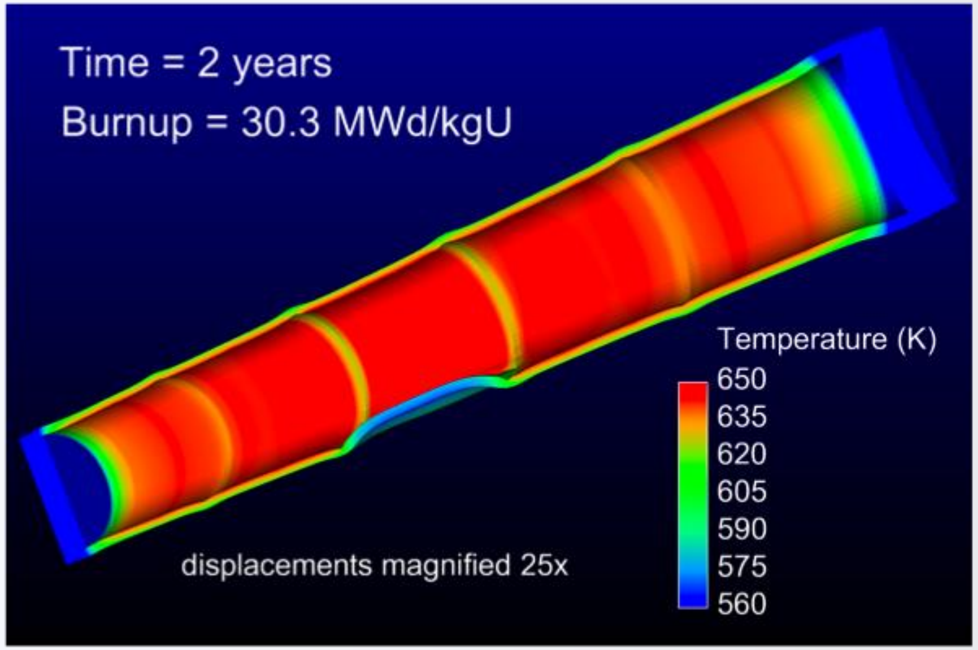

Cladding temperature (Pastore 2015)

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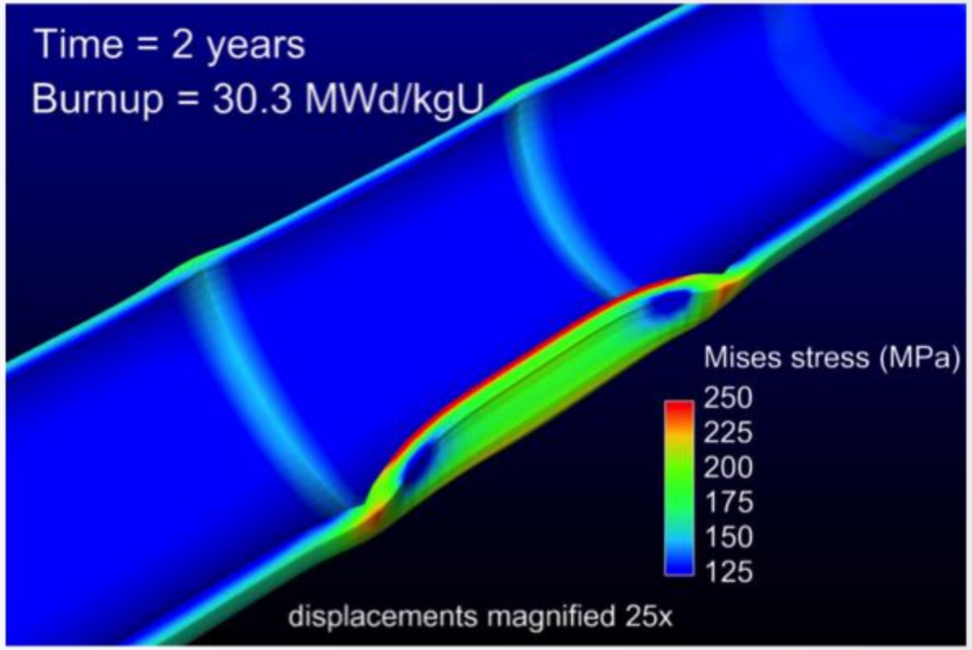

Cladding stress (Pastore 2015)

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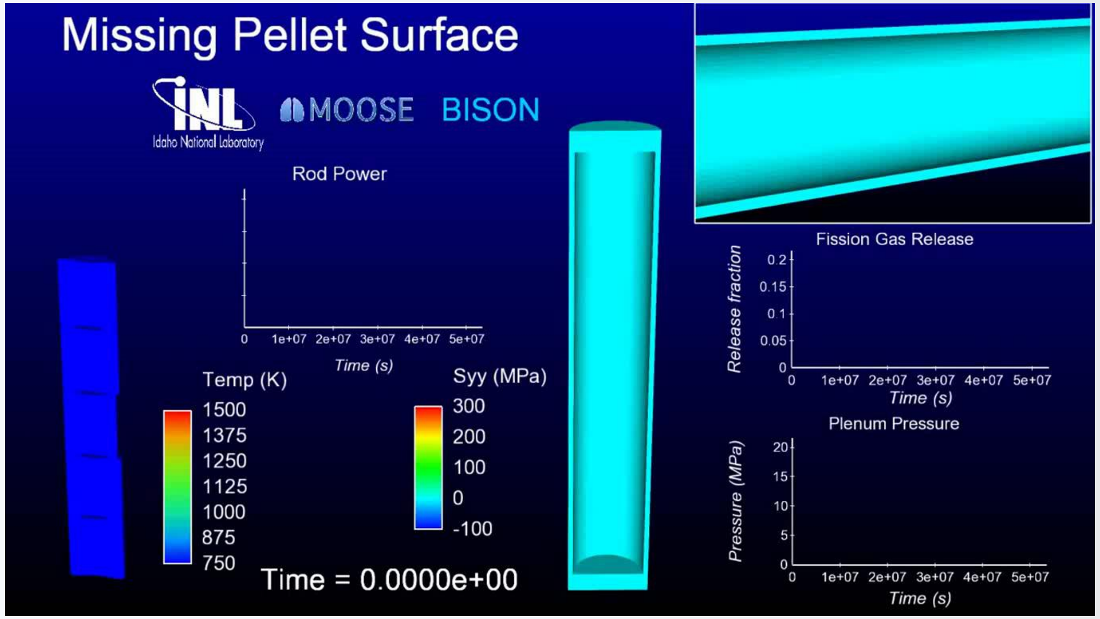


(bison.inl.gov)

https://www.youtube.com/watch?v=EfZtf7FLI-M&list=PLX2nBoWRisnW7DGDdHr--IWPnPM3_G1f1&index=2

BISON animation showing the detrimental effects of a fuel pellet imperfection known as a Missing Pellet Surface (MPS). The **leftmost plot** shows high local fuel temperatures, due to an increased gap width at the MPS. The clad hoop stress is also significantly increased, as shown in the **centre** and **top right plots**. **Line plots** document the rod power, FGR (fission gas release) fraction, and plenum pressure

- Development/use of FPCs
- Geometric domains represented
- Mathematical/numerical frame
- Validation
- Burnup analysis
- Thermal analysis
- Mechanical analysis
- Material and behavioural models (e.g., Fission Gas Behaviour)

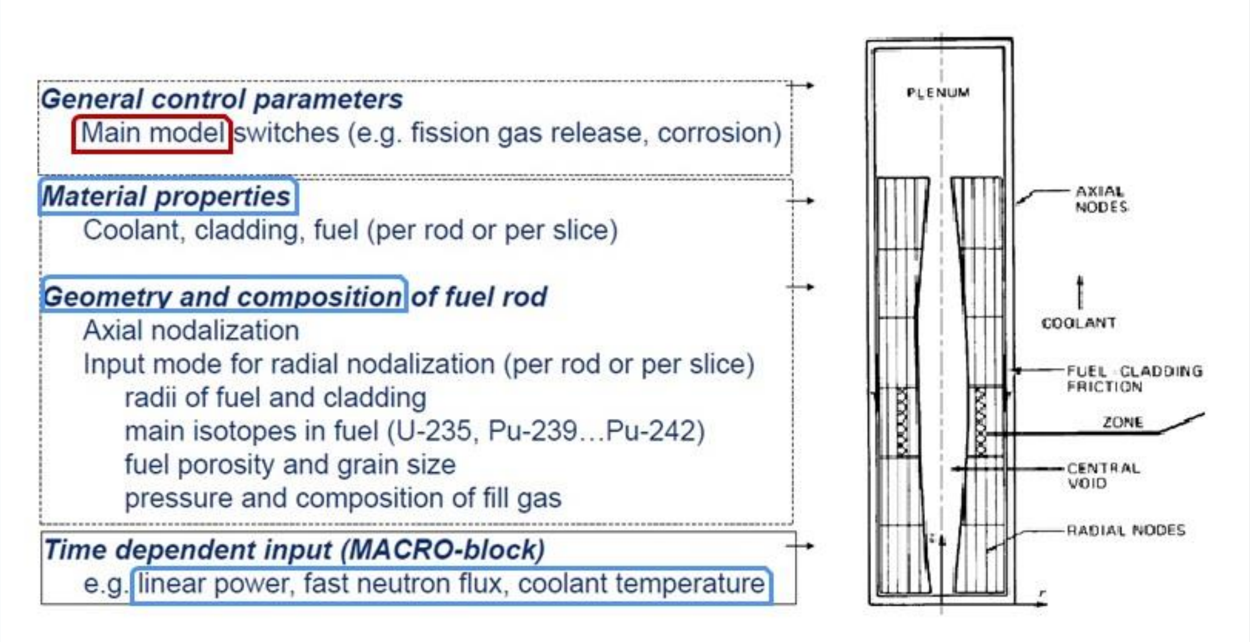
Mathematical/numerical frame

Mathematical/numerical frame (i)

- FPCs feature a frame into which time-dependent input, geometry and composition, material properties and behavioural models are /can be incorporated ....

LIFE - 4 code models

TRANSURANUS code input



General control parameters
Main model switches (e.g. fission gas release, corrosion)

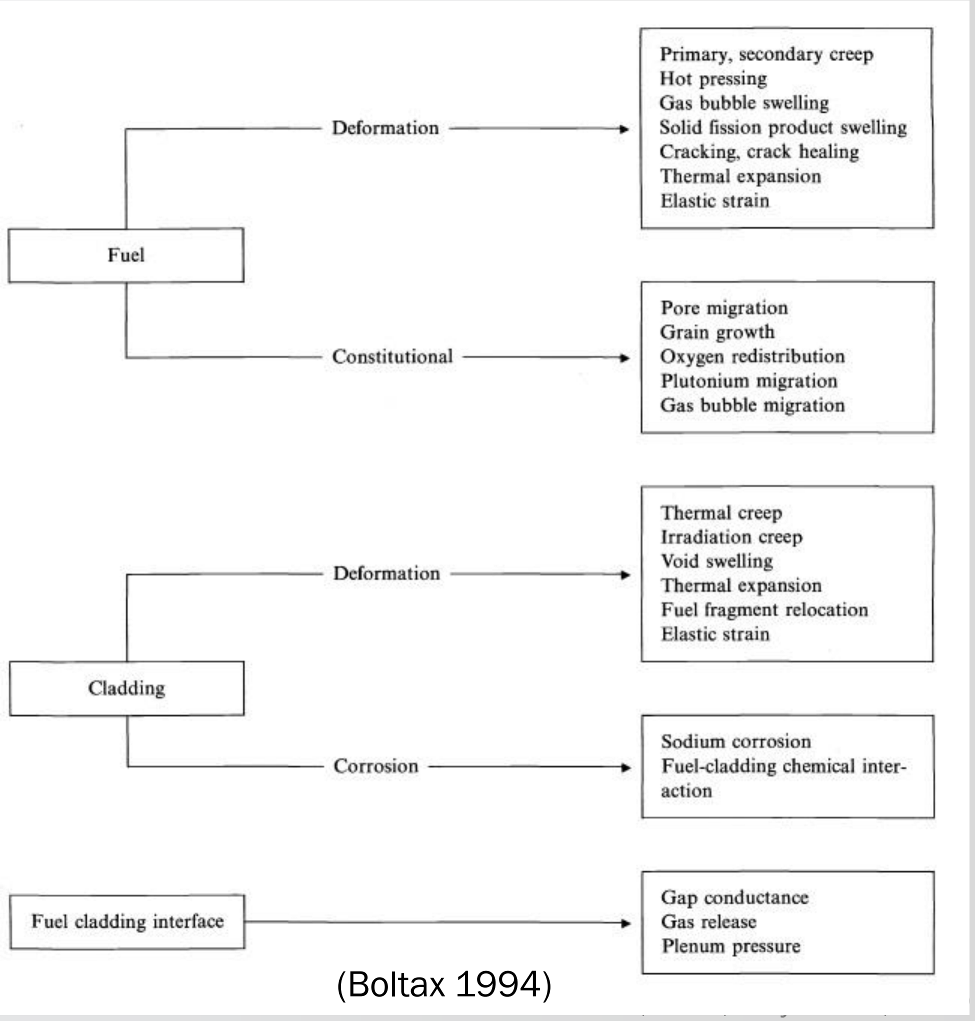
Material properties
Coolant, cladding, fuel (per rod or per slice)

Geometry and composition of fuel rod
Axial nodalization
Input mode for radial nodalization (per rod or per slice)
radii of fuel and cladding
main isotopes in fuel (U-235, Pu-239…Pu-242)
fuel porosity and grain size
pressure and composition of fill gas

Time dependent input (MACRO-block)
e.g. linear power, fast neutron flux, coolant temperature

(Van Uffelen 2019)

Olander 1976



(Boltax 1994)

Mathematical/numerical frame (i)

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Input and uncertainties

(Noirot 2016)

Fuel design and fabrication

- geometries
- compositions, enrichments, impurities
- porosities (from density / theoretical density)
- grain size

specifications with known limits

Irradiation data

- reactor data such as neutron spectrum, coolant chemistry and flux
- irradiation history ← *locally, high uncertainties*

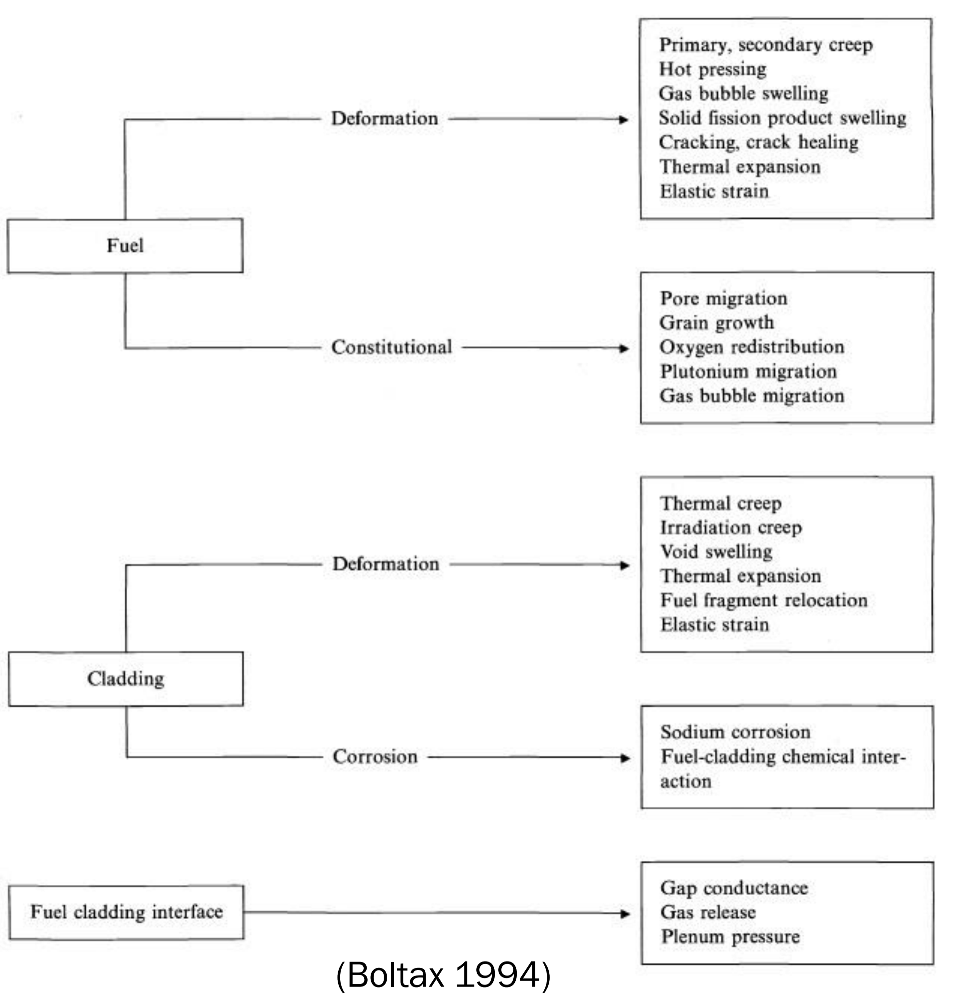
Material properties

- thermal properties
- mechanical properties

high uncertainties

Models uncertainties + necessary simplifications

LIFE - 4 code models



(Boltax 1994)

Mathematical/numerical frame (ii)

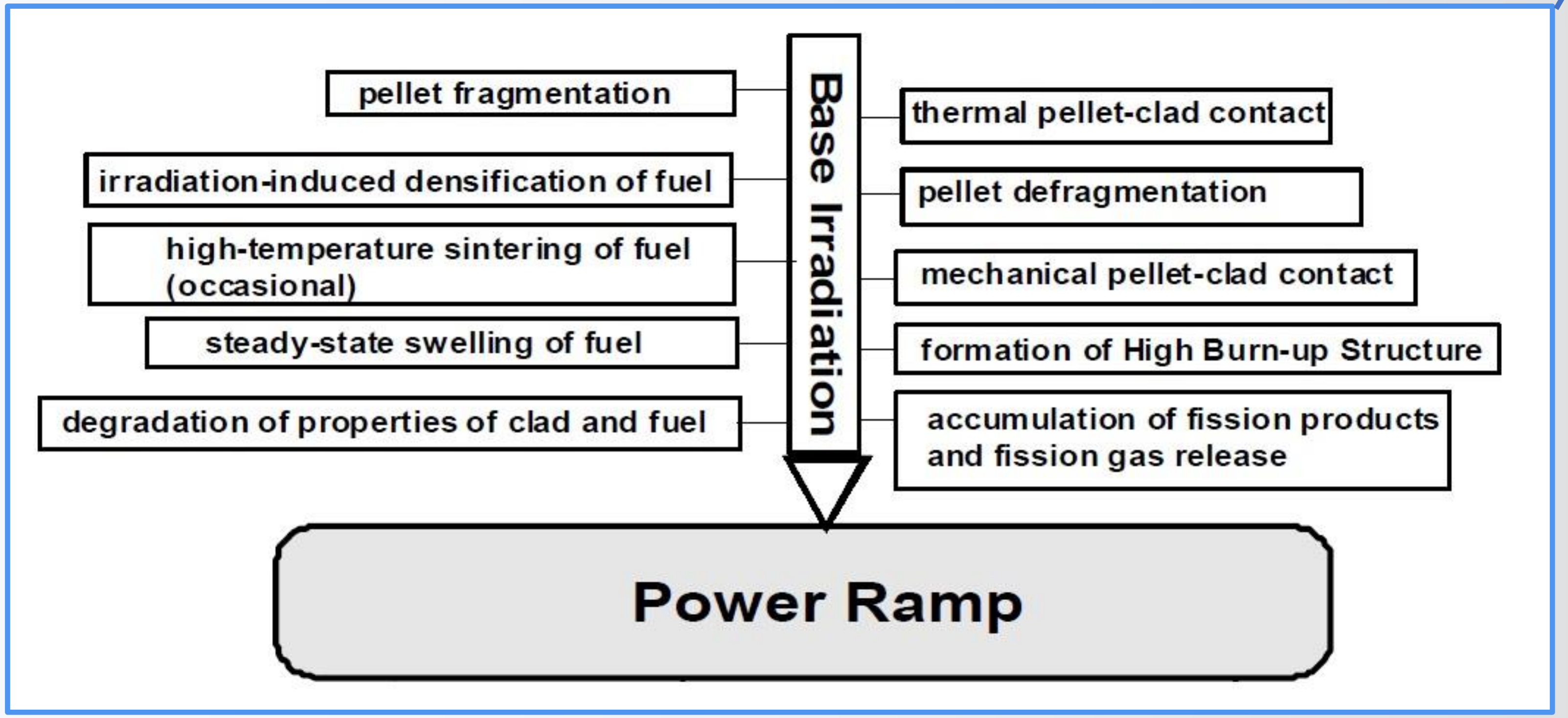
- FPCs feature a frame into which time-dependent input, geometry and composition, material properties and behavioural models are /can be incorporated ….

… also supported by uncertainty analysis (UA) & sensitivity analysis (SA)

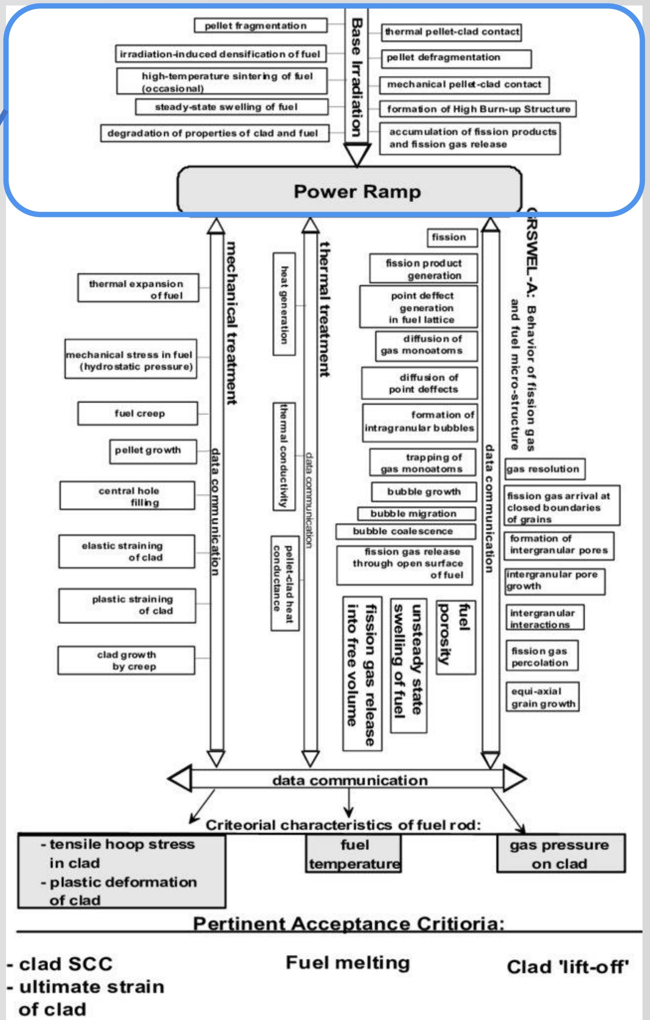
→ Models (at every single-scale level) have to be **computationally efficient !**

(Novikov et al. 2004)

for Base Irradiation



START-3 code models

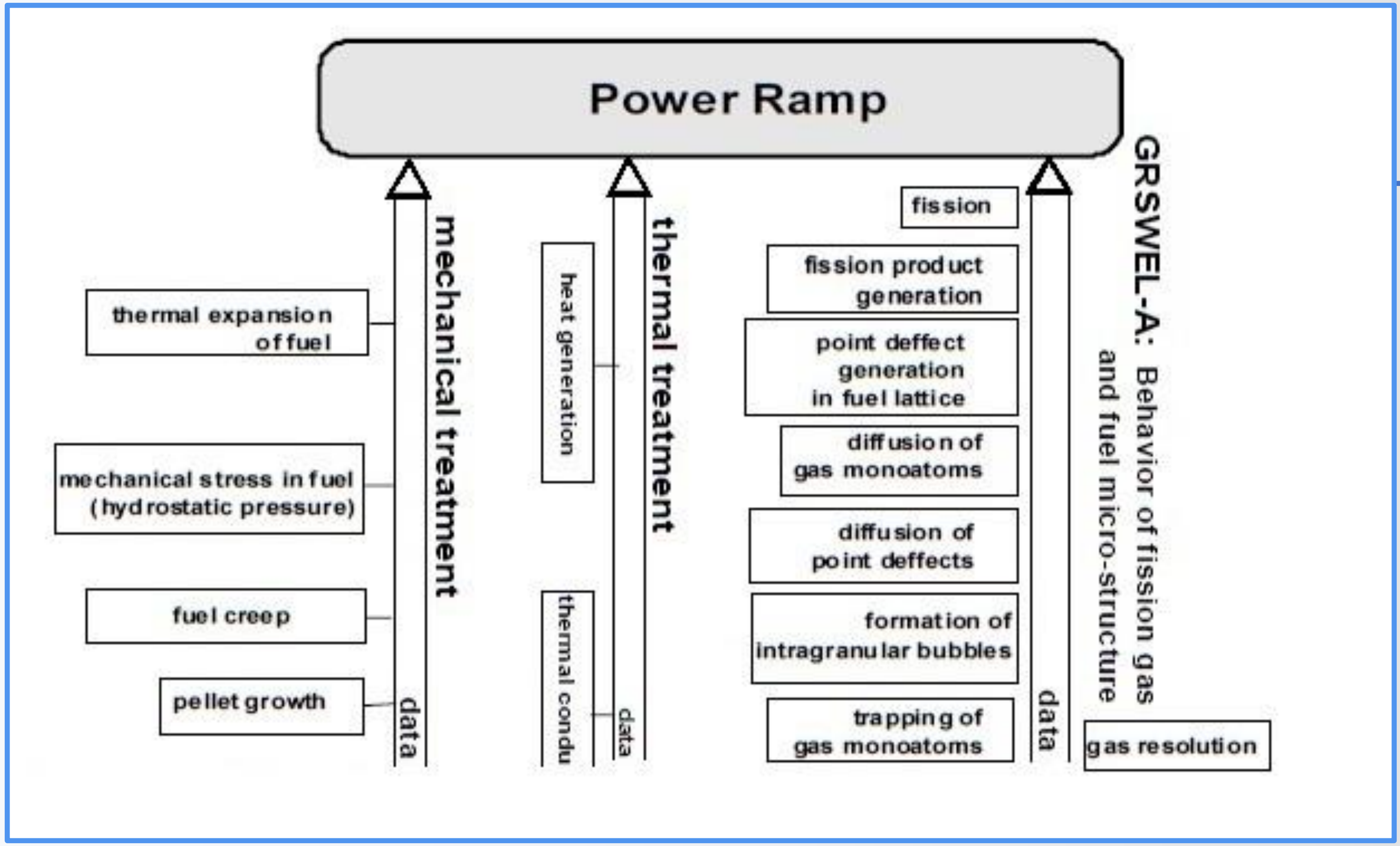


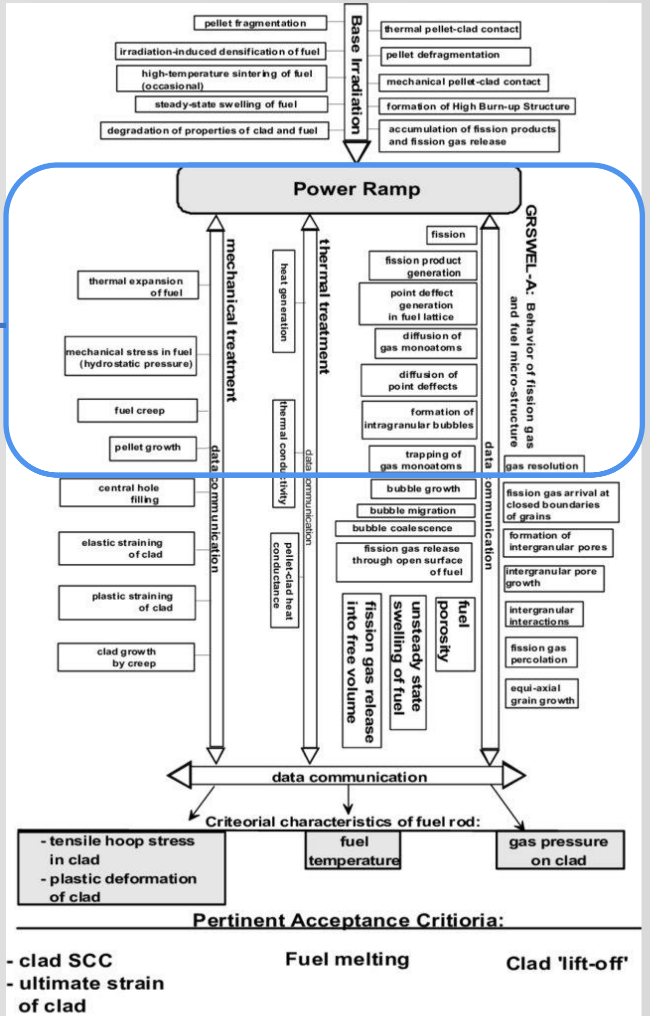
Mathematical/numerical frame (ii)

- FPCs feature a frame into which time-dependent input, geometry and composition, material properties and behavioural models are /can be incorporated ….

START-3 code models

for Power Ramp





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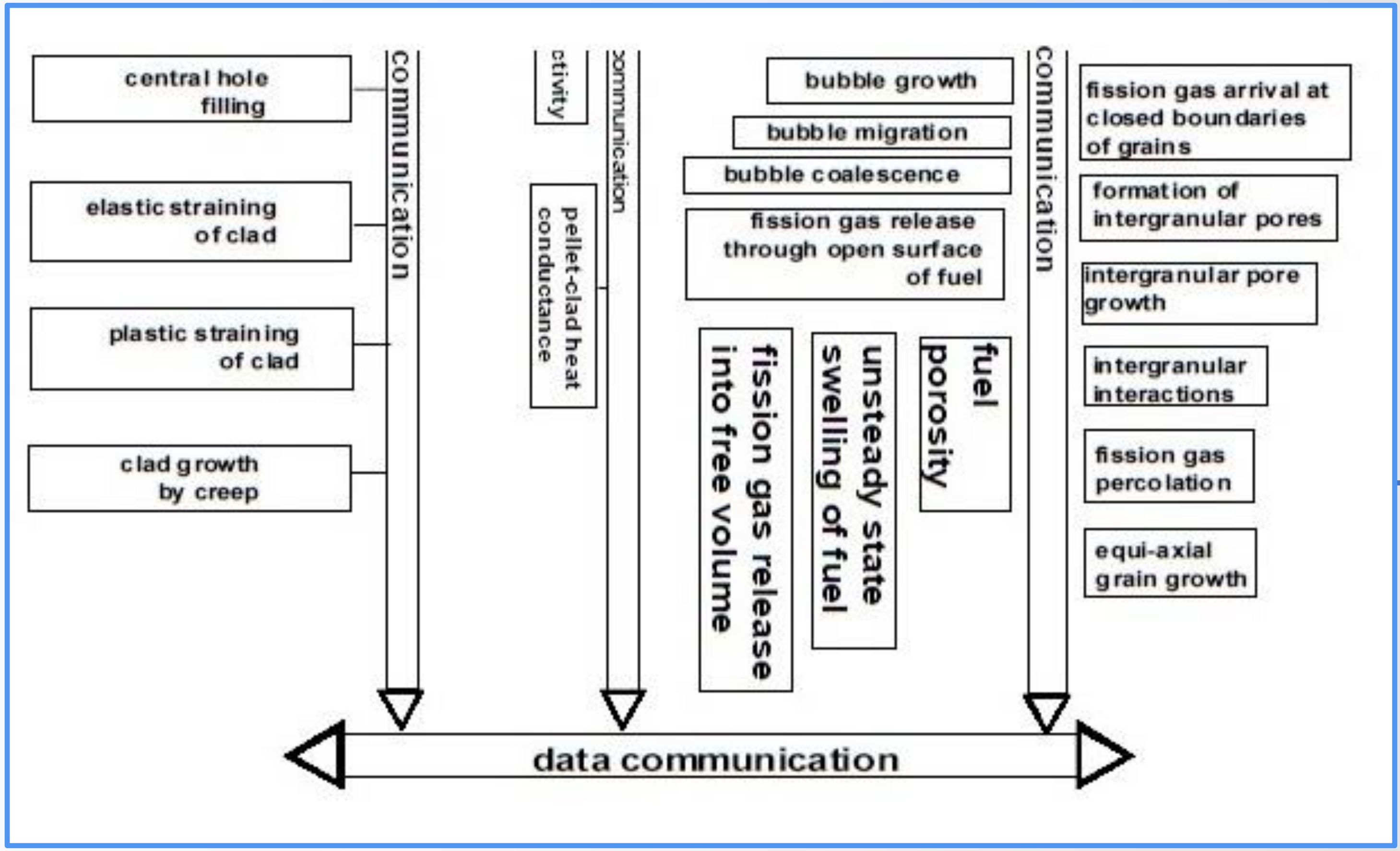

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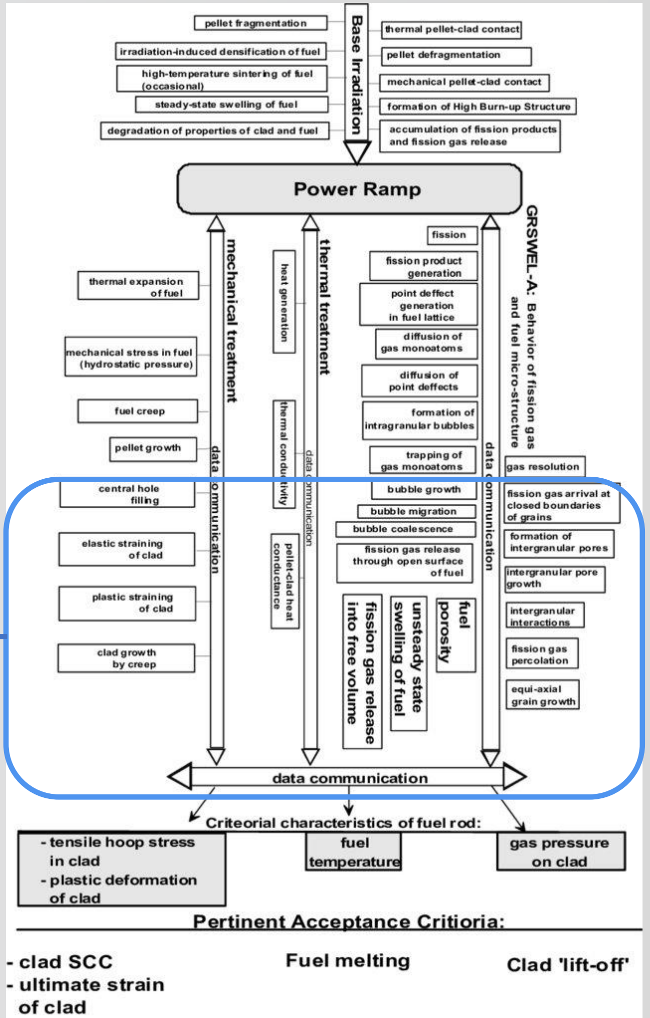
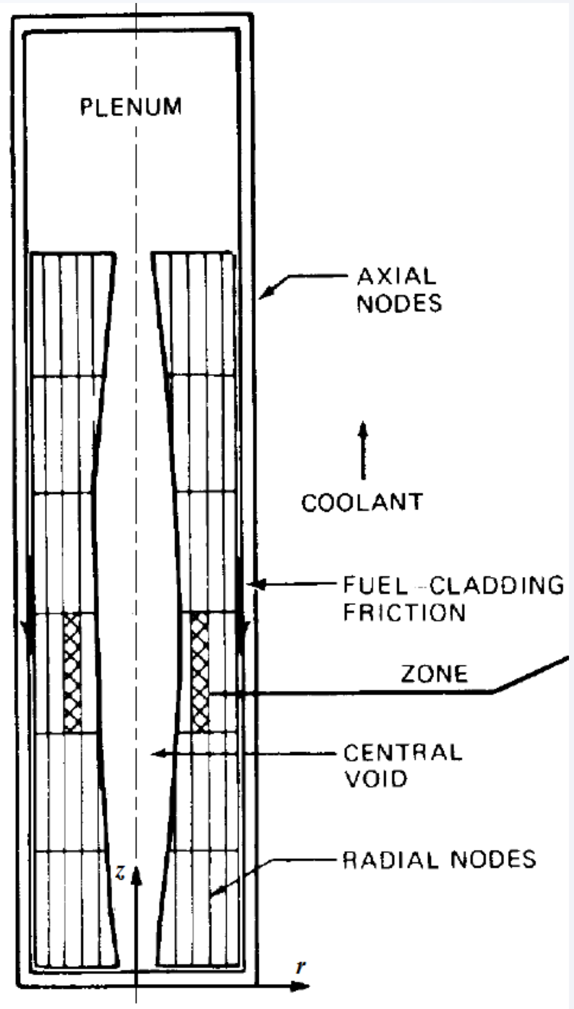
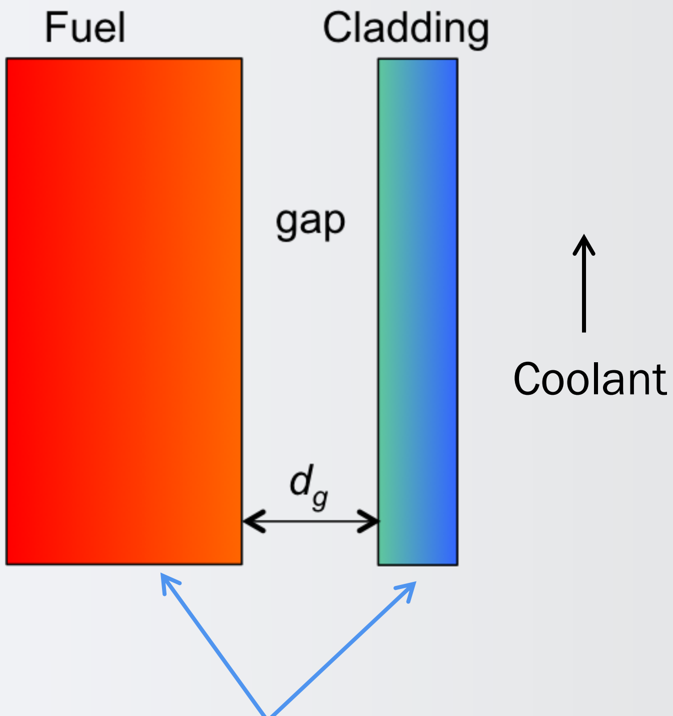


Mathematical/numerical frame (iii)

- Thermal Analysis



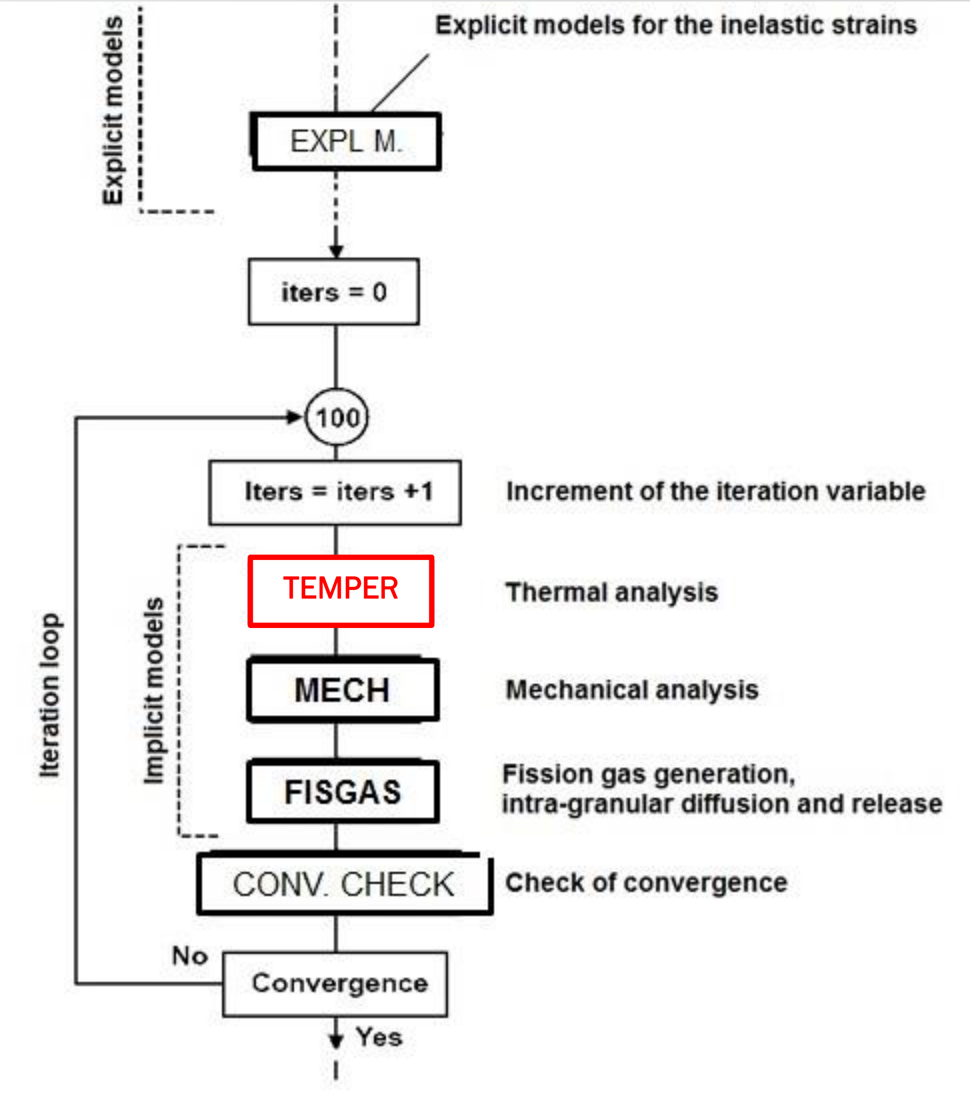


$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot k \nabla T + q'''$$

BCs:

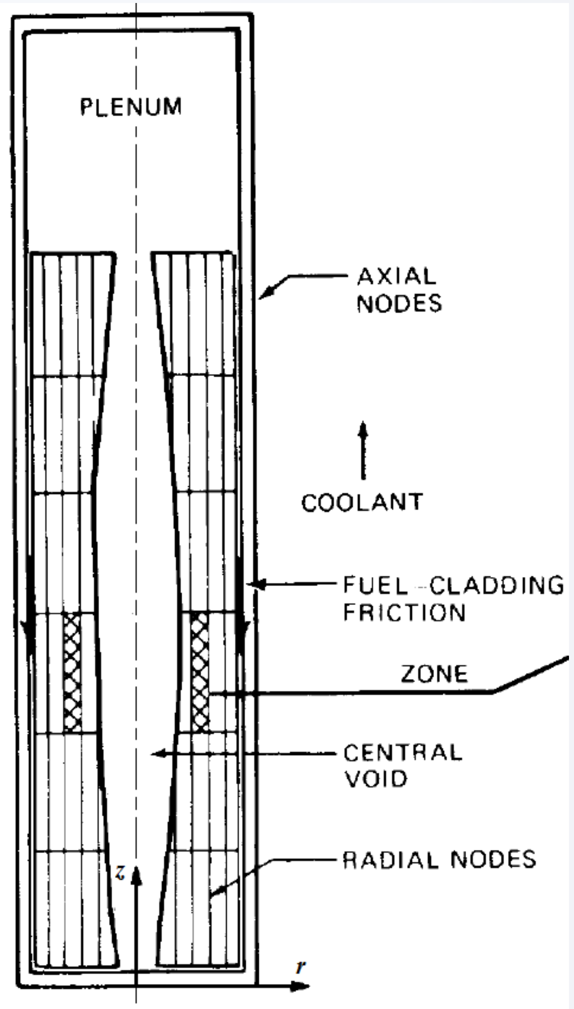
Symmetry at fuel centreline

Convective at clad outer wall



Mathematical/numerical frame (iv)

- Mechanical Analysis



In 1D (radial), *for simplicity*

- **Constitutive equations:**

$$\boxed{\varepsilon_i = \varepsilon_i^E + \varepsilon_i^T + \varepsilon_i^S + \varepsilon_i^{VP} \quad \text{for } r, \theta, z}$$

- **Compatibility equations:**

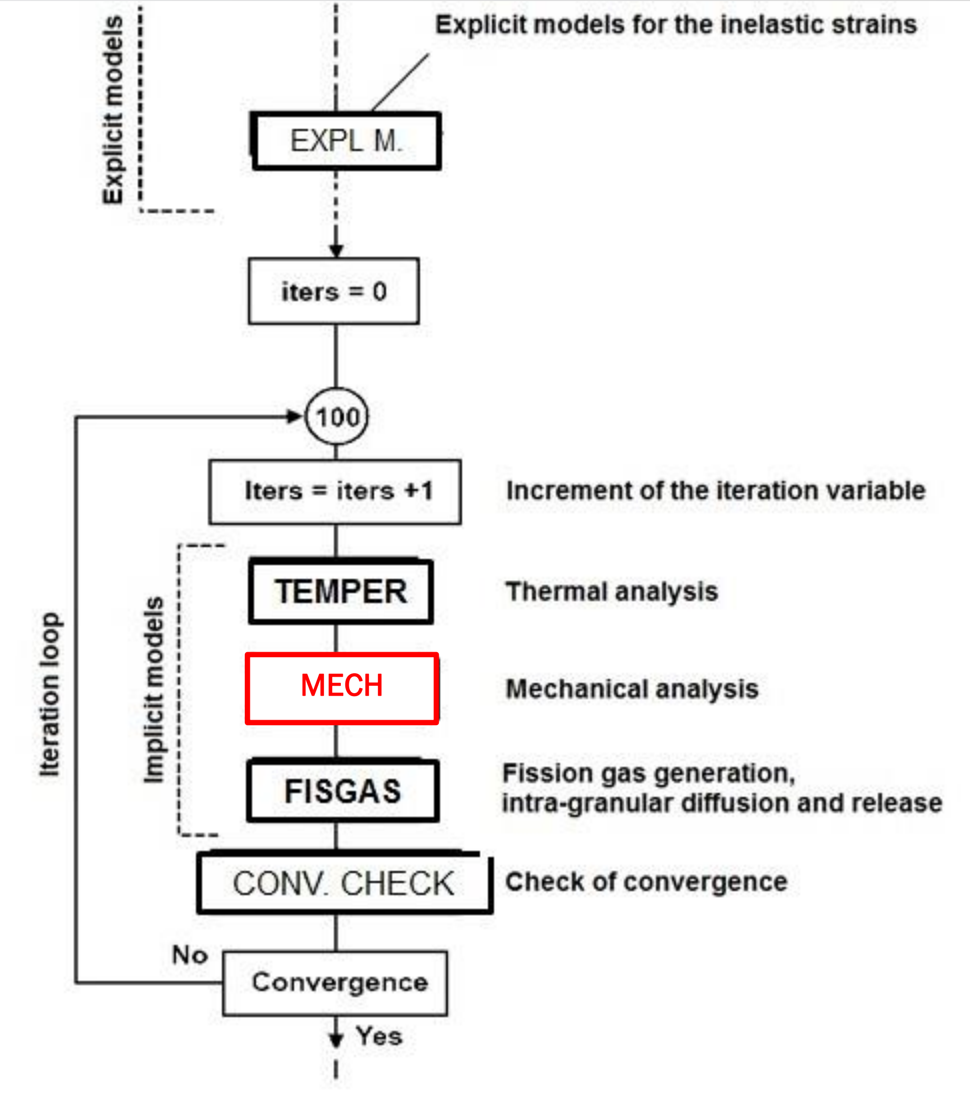
$$\boxed{\begin{cases} \varepsilon_r = \dfrac{du_r}{dr} \\ \varepsilon_\theta = \dfrac{u_r}{r} \\ \varepsilon_z = \dfrac{du_z}{dz} = const \end{cases}}$$

- **Equilibrium:**

$$\boxed{\sigma_\theta = \sigma_r + r\frac{d\sigma_r}{dr}}$$

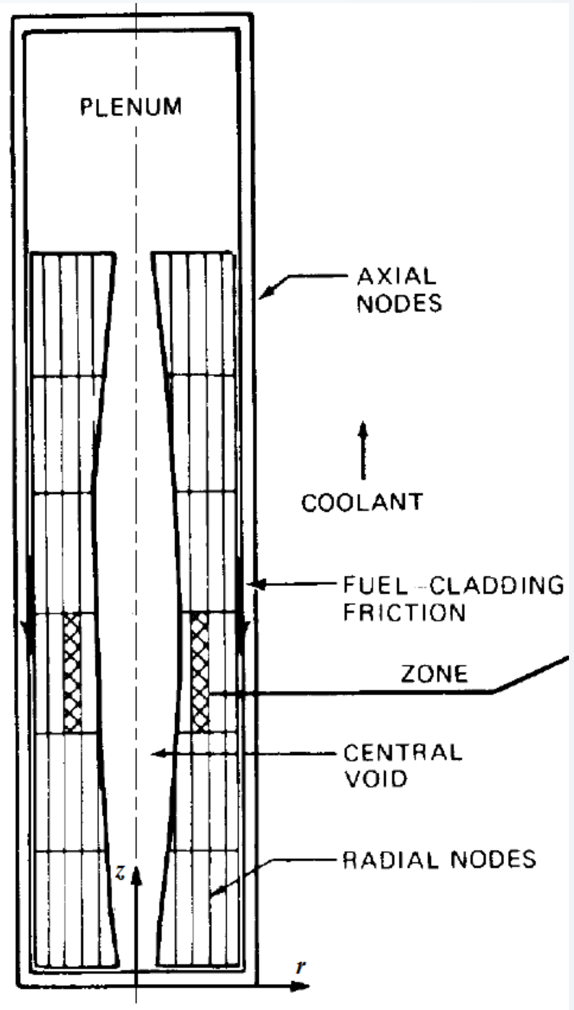
From this set of eqs, we can get one ordinary differential equation for radial displacement u_r as a function of elastic & inelastic strains

We need to implement physical models for the material behaviour (e.g., for inelastic strains like swelling, creep)

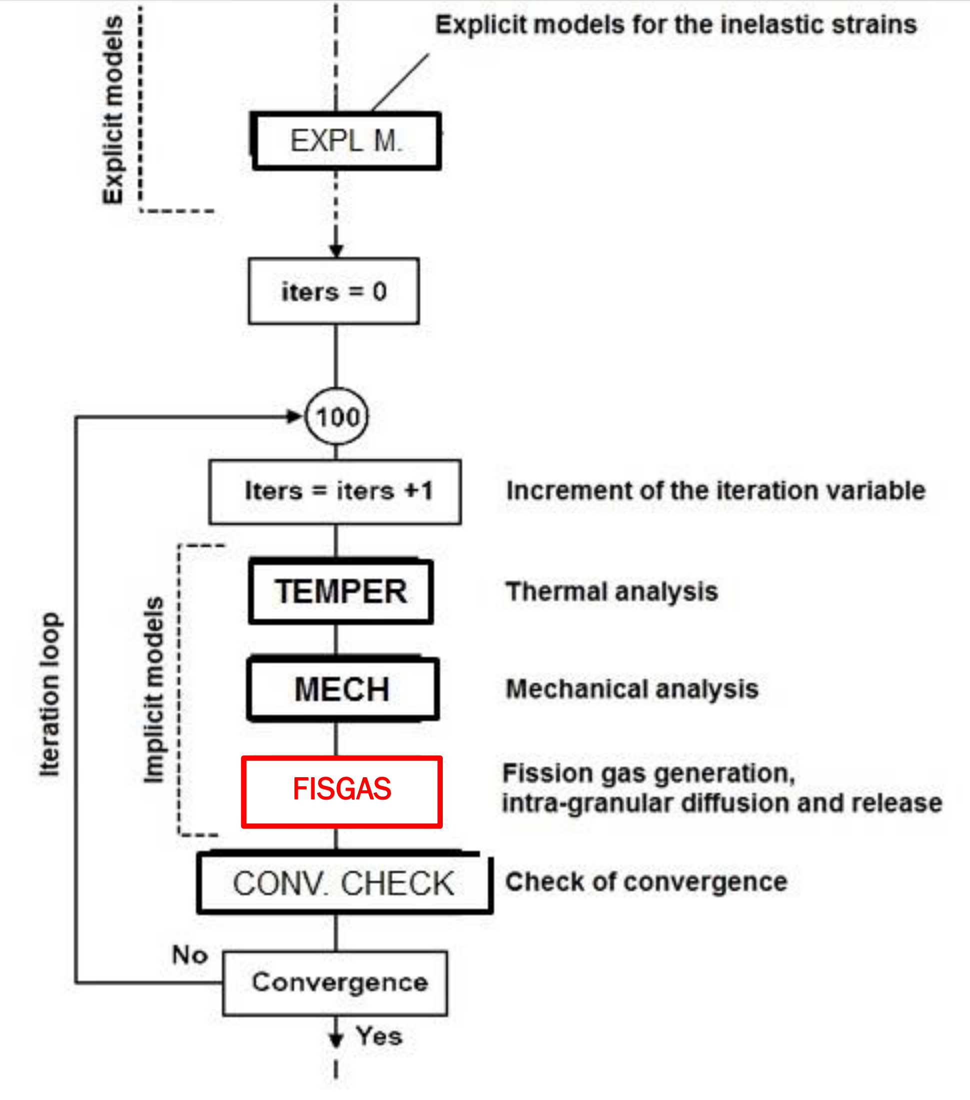


Mathematical/numerical frame (v)

- Fission Gas Behaviour (FGB)



- One of these inelastic strains is the **gaseous swelling** strain induced by fission gas accumulation in the fuel
- Also, fission gas is released in the fuel-cladding gap, and in the other free volumes as well (**FGR - fission gas release**)
- FGR modifies the properties of the gap (thermal conductance, pressure)



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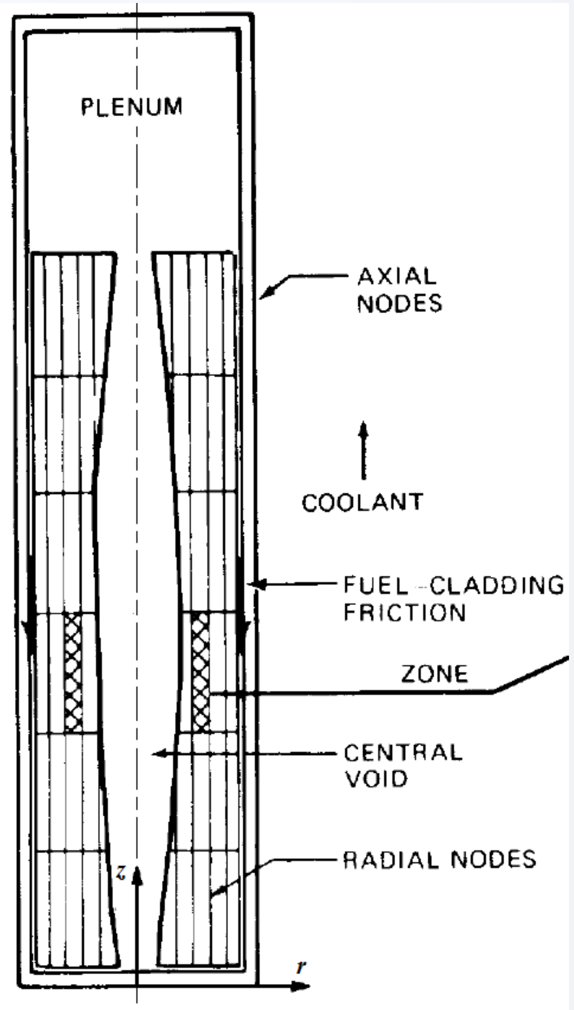

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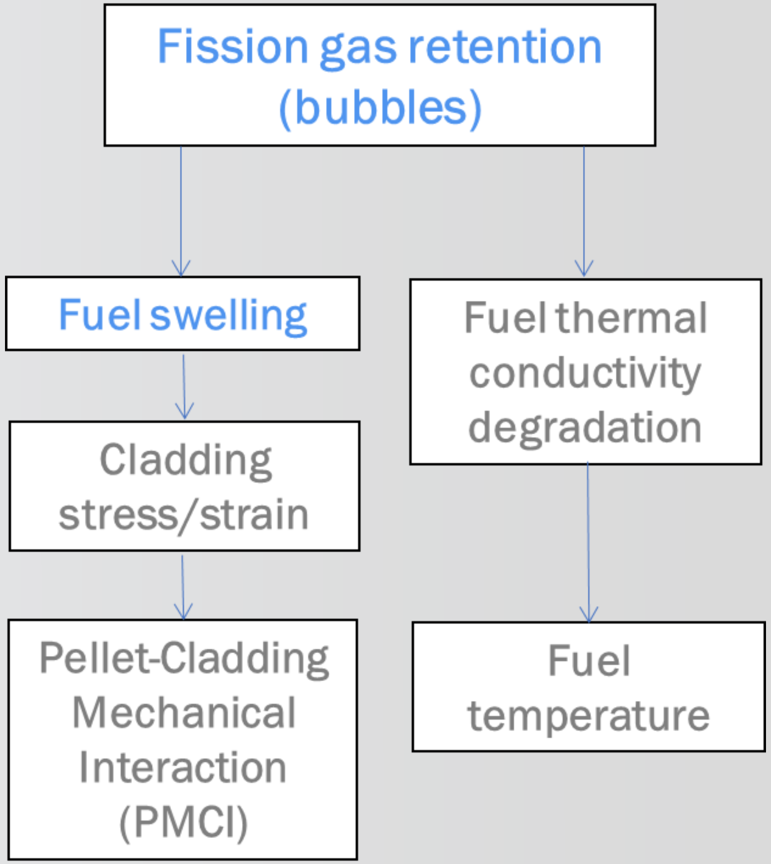

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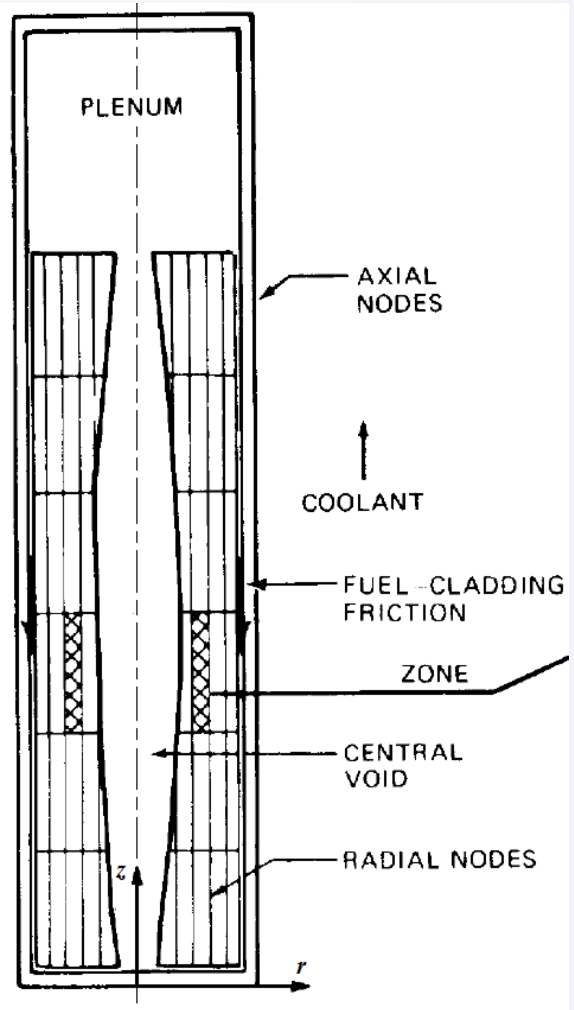

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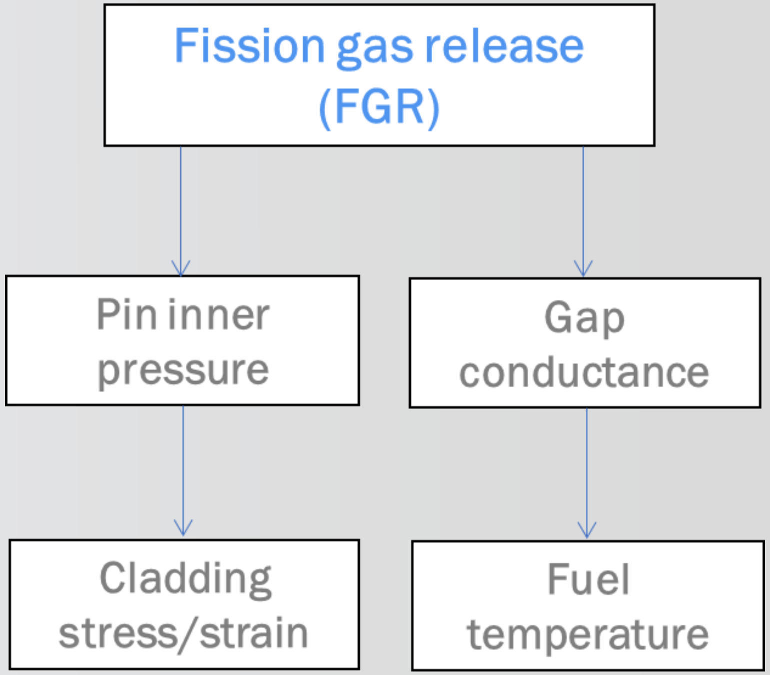

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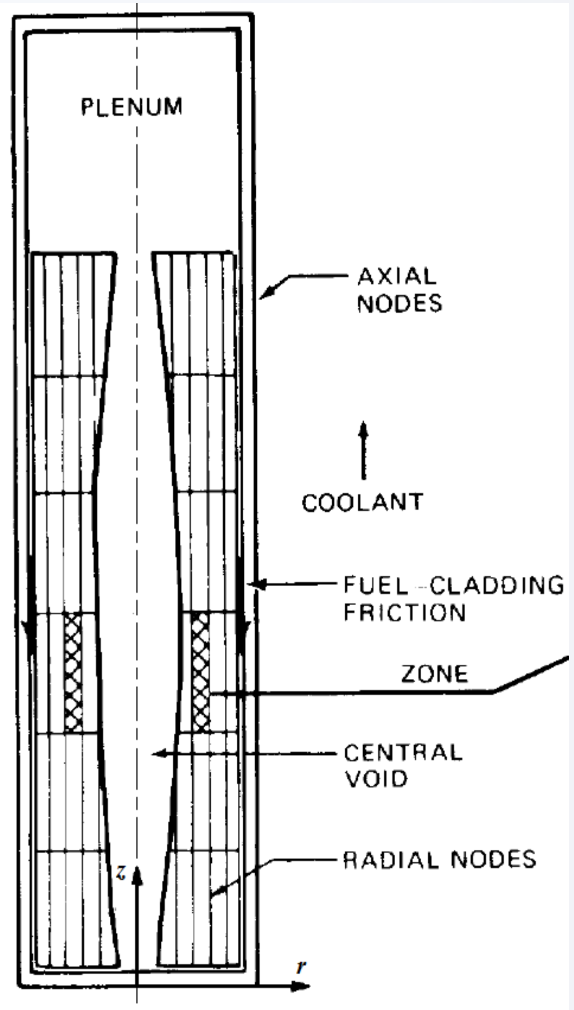

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- Calculation of gaseous swelling and FGR requires modelling the **complex fission gas behaviour…** and is coupled to the thermal-mechanical analysis as well!

FISSION GAS BEHAVIOR IN NUCLEAR FUEL

A MODELLING AND EXPERIMENTAL CHALLENGE

> *< Among the myriad phenomena that occur simultaneously in a nuclear fuel element under irradiation, none has so frustrated the designer, so challenged the experimentalist, or so intrigued the theorist as the behavior of the fission products >*
>
> (Olander 1976)

> *< Although written in 1976 this statement is still valid, and even after more than 30 years of research, fission gas release and swelling is still a subject of controversial discussions >*
>
> (Lassmann - Benk 2000)

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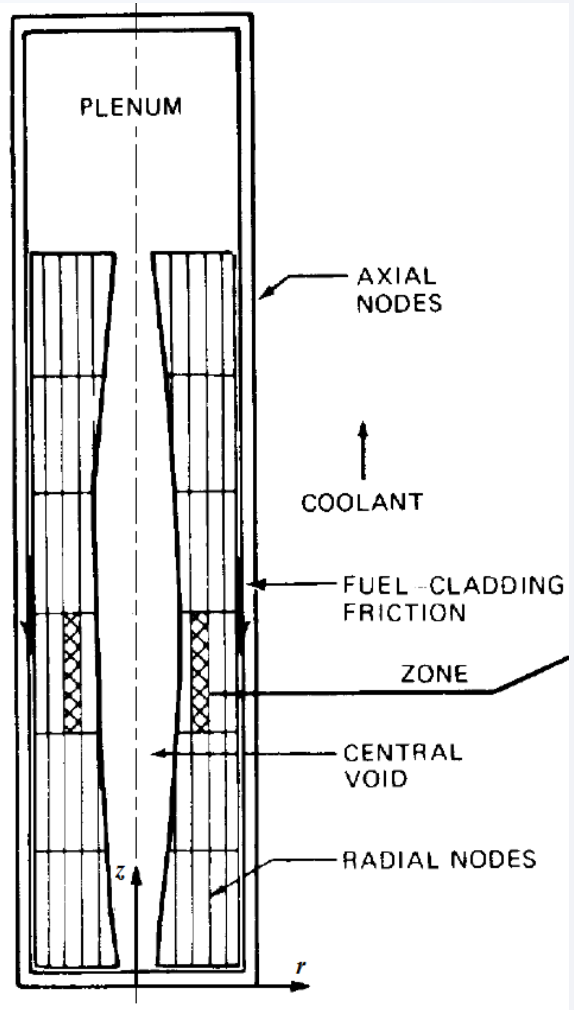

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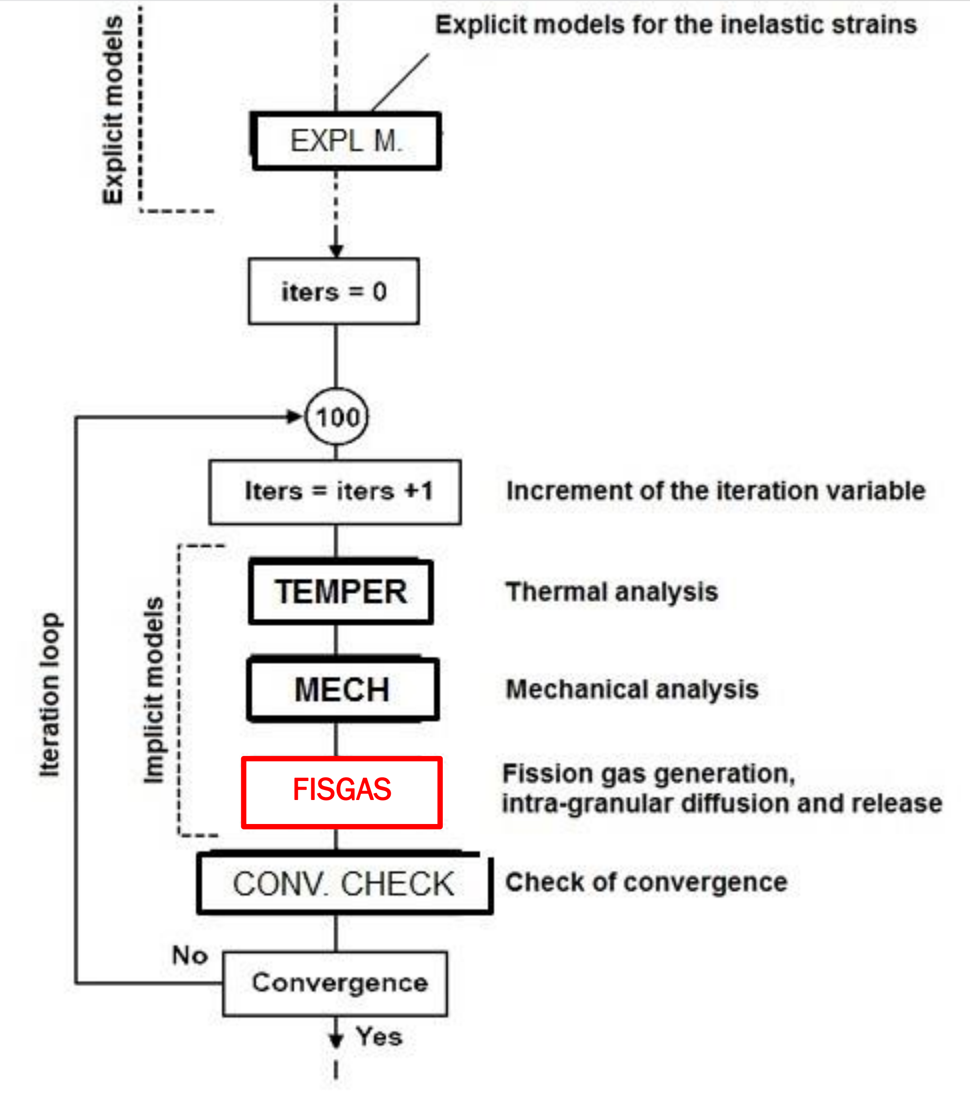
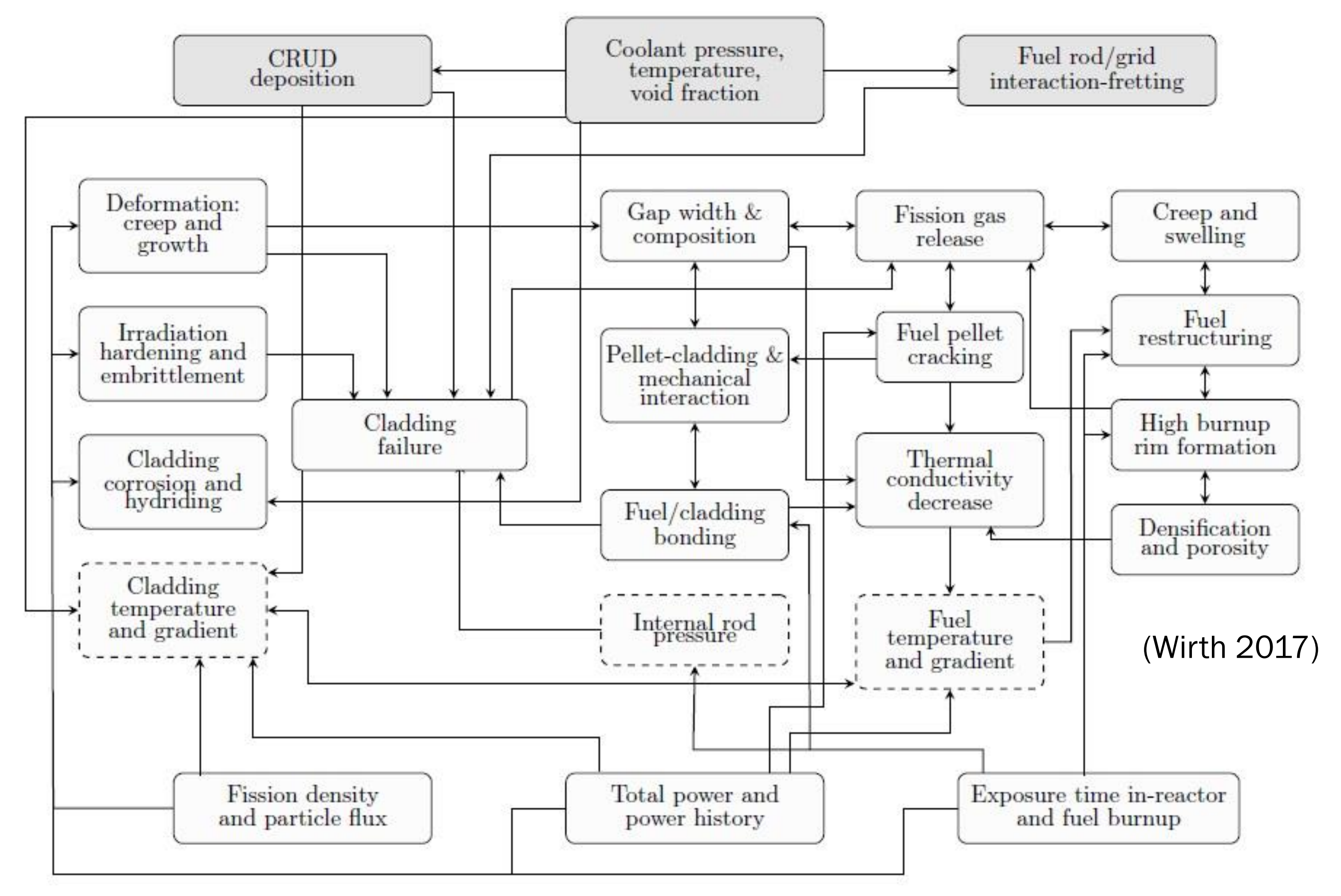


Material and behavioural models

- Complex phenomena, behavioural evolution and interactions to be incorporated in FPCs



(Wirth 2017)

- **Traditionally, FPC modelling** employs continuum mechanics techniques at the macroscopic scale, where the molecular nature of the materials is usually ignored
- **From a correlation-based to a physics-based approach** (*possibly* according to a hierarchical **multi-scale modelling** for a better simulation of fuel pin behaviour under irradiation), *also* **supported by** uncertainty analysis (**UA**) **&** sensitivity analysis (**SA**)
- The models (at every single-scale level) have to be computationally efficient to allow for error propagation and quantification-margin-uncertainty analysis
- This will provide a more theoretical or *in silico*, and so less empirical, basis for fuel pin performance modelling, hence enabling more generic application to novel fuel designs, in particular of Gen-IV reactors

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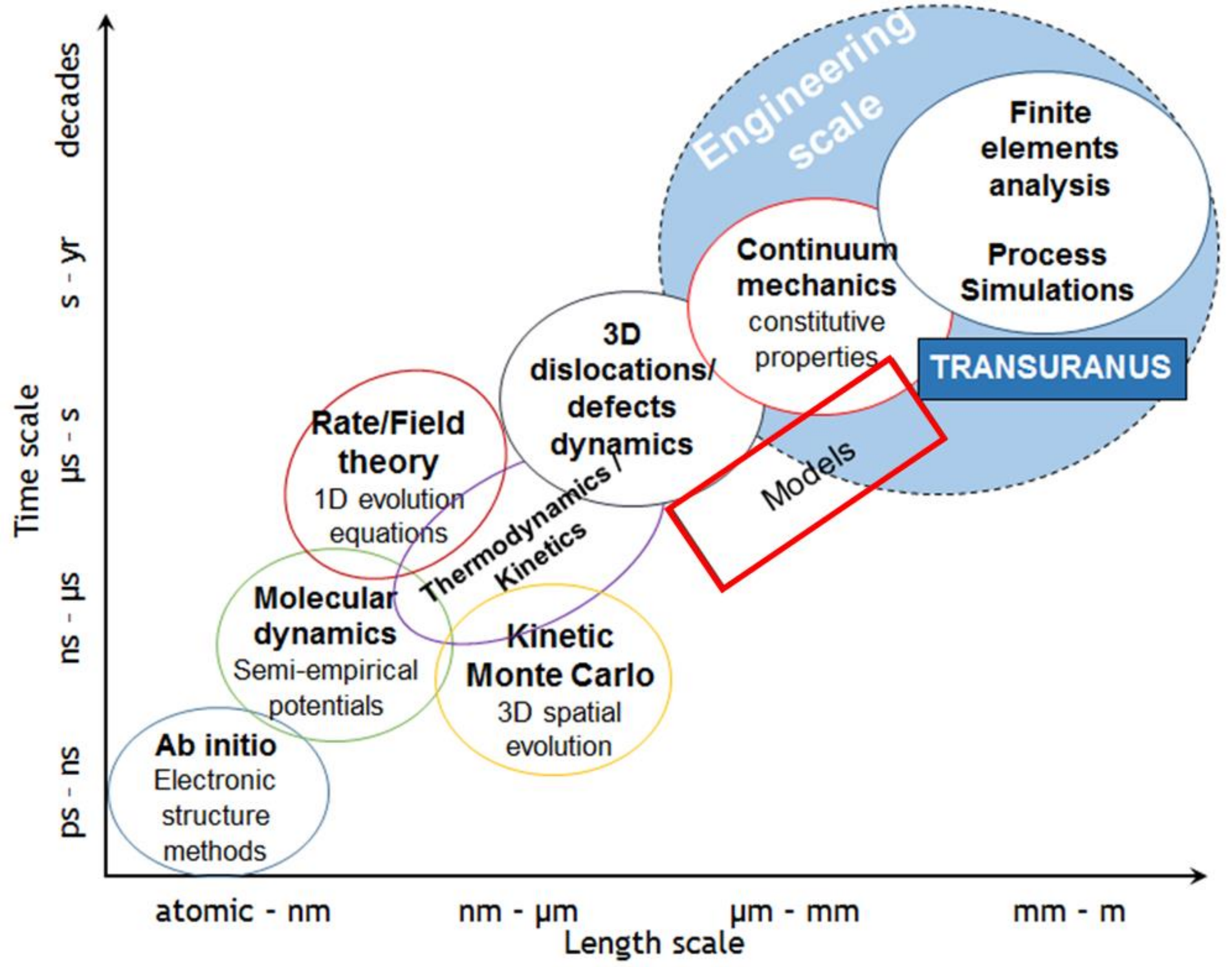

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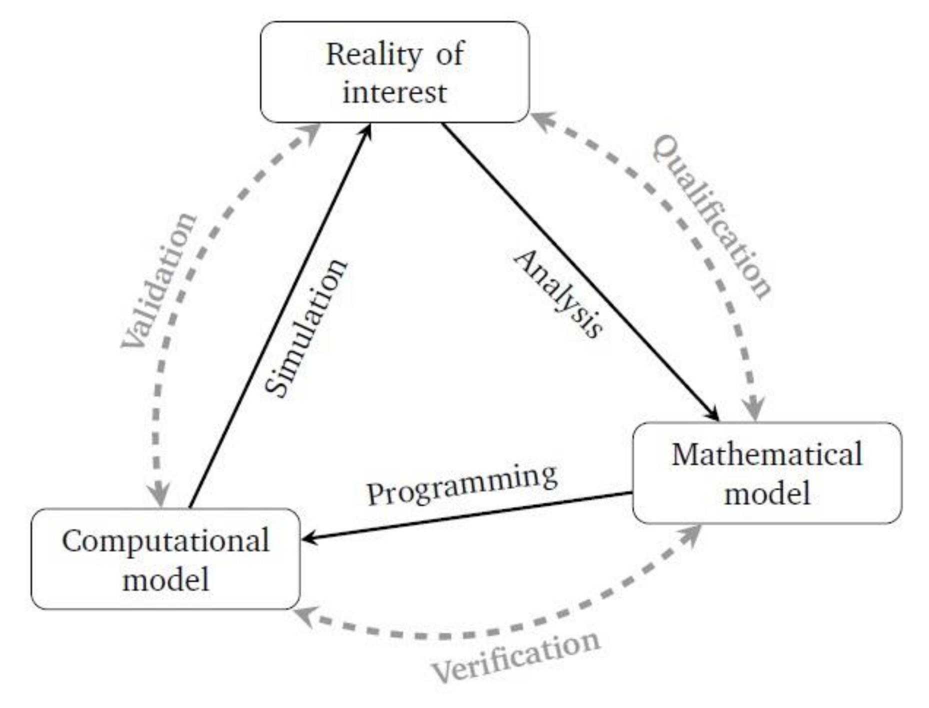

Validation

Validation (i)

- Fuel pin behaviour modelling inevitably requires:
  - material properties data + dedicated experiments
  - quantification of behavioural model parameters
  - overall validation of the global "fuel pin" behaviour
  - code-to-code comparison and benchmarking

(Noirot 2016)

In-pile dedicated tests

- temperature measurements
- pressure measurements
- diameter measurements
- sweeping gas analysis of the in-pile release
- post-test examinations

Out-of-pile annealing tests

- for gas models, without irradiation

Post-Irradiation Examinations (PIE)

- diameter measurements, 1D at mid-pellet, 3D including ridges
- axial gamma scanning
- rod length measurement
- fission gas release
- free volume

} *pin pressure*

- density measurements
- porosity measurements
- EPMA and SIMS Xe measurements
- EPMA and SIMS FP creation measurements
- Zirconia thickness (non-destructive and ceramography)
- gap (ceramography measurement)
- intergranular gas measurements
- fuel thermal conductivity

Validation (ii)

- Fuel pin behaviour modelling inevitably requires:
  - material properties data + dedicated experiments
  - quantification of behavioural model parameters
  - overall validation of the *global* "fuel pin" behaviour
  - code-to-code comparison & benchmarking

❖ Experimental data on **material properties** can be fitted (in an equation form) to a set of logical independent variables or experimental parameters

(e.g., thermal conductivity of the fuel is typically fitted to temperature, burnup, plutonium content, stoichiometry, and porosity; pellet cracking and fragment relocation effects can be taken into account, as well)

(Rashid et al. 2011)

❖ **Behavioural models**, such as irradiation creep in cladding, can be based on certain fundamental hypothesis

(e.g., dislocation glide or vacancy loop collapse)

➢ Such a hypothesis needs to be tested with dedicated Separate-Effects Experiments. If the experiments confirm the hypothesis, a correlation can be developed

(which in this case will depend at least on stress, temperature, material cold work condition, and neutron flux)

❖ Finally, we need an overall validation of the **global behaviour,** as confirmed by Integral Irradiation Experiments & by actual in-reactor experience, Last, but not least, we also need **code-to-code** comparison & **benchmarking**

Validation (iii)

- Predictions from modelling could be used as a guidance to understand the materials (fuel + cladding) behaviour ---> it is necessary to keep data sets used for *calibrating* a FPC separate from the data sets used for *checking* the FPC predictions …

(Rashid et al 2011, Rossiter 2012)

- ➢ Determination of material properties, and their evolution with irradiation, using sub-macroscopic scale models

  (e.g., molecular dynamics models for a novel material, meso-scale modelling for a heterogeneous composite of two standard materials or for a porous material)

- ➢ **Resulting properties** can then be used in traditional FPCs for macroscopic modelling to see whether their predictions are enhanced toward greater fidelity to the experiments on which validation of FPCs is based

- ➢ **Alternatively,** the microscopic and macroscopic models can be coupled each other to allow a seamless interface

  (however, atomistic simulations cannot be independently verified even with the best available microscopy, since they are made at sub-lattice scale by definition)

Some limitations of FPCs

----> Any code is only as good as its validation … (i.e., as the measured data used to confirm the accuracy of its predictions)

- ➢ A **first limitation** is connected to the validation range (i.e., the range of fuel designs, material compositions, burnups, etc. for which FPC predictions have been compared to measurements). If the FPC is used outside its range of applicability, the predictions are then subject to significant, and non-quantifiable, uncertainties

- ➢ A **second limitation** of codes used for fuel behaviour modelling (in particular, FPCs) is that several phenomena of interest are stochastic (e.g., pellet cracking and fuel fragment relocation)

TOO GOOD TO LEAVE ON THE SHELF...

Useful reading

- D.R. Olander, Fundamental Aspects of Nuclear Reactor Fuel Elements, ERDA Technical Information Center, Oak Ridge, 1976.
- H. Bailly, D. Ménessier, C. Prunier, The Nuclear Fuel of Pressurized Water Reactors and Fast Neutron Reactors - Design and Behaviour, Lavoisier Publishing Inc., Paris, 1999.
- B.R.T. Frost, Nuclear Materials. In: Materials Science and Technology - A Comprehensive Treatment, Vol. 10, VCH, Weinheim, 1994.
- D.G. Cacuci, Handbook of Nuclear Engineering. Springer-Verlag, New York, 2010.
- N.E. Todreas, M.S. Kazimi, Nuclear Systems, Vol. 1: Thermal Hydraulic Fundamentals, Taylor & Francis, London, 2011.
- A.E. Waltar, D.R. Todd, P.V. Tsvetkov, Fast Spectrum Reactors, Springer, 2012.
- R.J.M. Konings, Comprehensive Nuclear Materials. Elsevier, Amsterdam, 2012.
- D.R. Olander, A. Motta, Light Water Reactor Materials, Vol. I: Fundamentals, American Nuclear Society, 2017.

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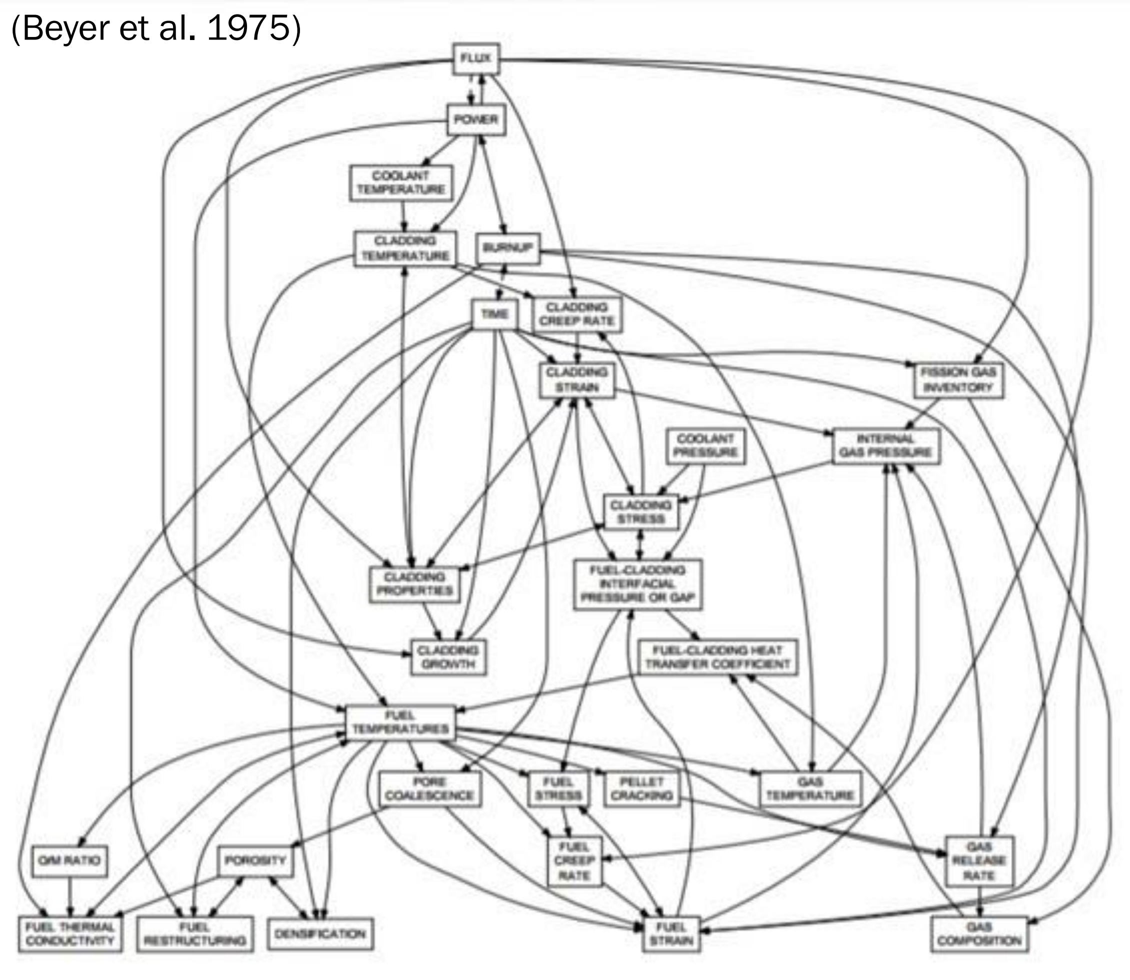
Reference sources (i)

- **Beyer et al. 1975** - GAPCON-THERMAL-2: A Computer Program for Calculating the Thermal Behavior of an Oxide Fuel Rod, BNWL-1898, Battelle Pacific Northwest Laboratories.
- **Boltax 1994** - Mixed Oxide Fuel Pin Performance. In: B.R.T. Frost (Ed.), Materials Science and Technology - A Comprehensive Treatment, vol. 10, VCH.
- **Calvin - Nowak 2010** - High Performance Computing in Nuclear Engineering. In: D.G. Cacuci (Ed.), Handbook of Nuclear Engineering. vol. II, Springer-Verlag.
- **CEA. 2009** - J-L. Guillet, Y. Guérin (Eds.), Nuclear fuels, DEN Monographs, CEA Saclay and Groupe Moniteur.
- **Cumo 2017** - Nuclear plants, Sapienza Università Editrice.
- **Horn 1973** - Babcock and Wilcox Company.
- **Lainet et al. 2019** - GERMINAL, a fuel performance code of the PLEIADES platform to simulate the in-pile behaviour of mixed oxide fuel pins for sodium-cooled fast reactors, Journal of Nuclear Materials, vol. 516.
- **Lambert - Strain 1994** - Oxide Fuels. In: B.R.T. Frost (Ed.), Materials Science and Technology - A Comprehensive Treatment, vol. 10, VCH.
- **Lassmann 1980** - The structure of fuel element codes, Nuclear Engineering and Design, vol. 57.
- **Lassmann - Benk 2000** - Numerical algorithms for intragranular fission gas release, Journal of Nuclear Materials, vol. 280.
- **Luzzi et al. 2014** - Application of the TRANSURANUS code for the fuel pin design process of the ALFRED reactor, Nuclear Engineering and Design, vol. 277.
- **Noirot 2016** - Modeling of fuel behavior, International School in Nuclear Engineering - Nuclear fuels for light water reactors and fast reactors, CEA.

Reference sources (ii)

- **Novikov et al. 2004** - Modelling of Thermal Mechanical Behaviour of High Burn-up VVER Fuel at Power Transients with Especial Emphasis on Impact of Fission Gas Induced Swelling of Fuel Pellets, International Seminar on Pellet-Clad Interaction in Light Water Reactor Fuels.
- **Okumura et al. 2014** - Nuclear Reactor Calculations. In: Y. Oka (Ed.): Nuclear Reactor Design, Springer.
- **Olander 1976** - Fundamental Aspects of Nuclear Reactor Fuel Elements, ERDA Technical Information Center.
- **Olander 2009** - Nuclear fuels – Present and future, Journal of Nuclear Materials, vol. 389.
- **Rashid et al. 2011** - Light Water Reactor Fuel Performance Modeling and Multi-Dimensional Simulation, JOM: the journal of the Minerals, Metals & Materials Society, vol. 63.
- **Rossiter 2012** - Understanding and modelling fuel behaviour under irradiation. In: I. Crossland (Ed.), Nuclear fuel cycle science and engineering, Woodhead Publishing Limited.
- **Stan et al. 2007** - Models and simulations of nuclear fuel materials properties, Journal of Alloys and Compound, vol. 444-445.
- **Todreas - Kazimi 2011** - Nuclear Systems, vol. 1: Thermal Hydraulic Fundamentals, Taylor & Francis.
- **Tulkki 2016** - Nuclear fuel behaviour, PHYS-E0562, VTT.
- **Van Uffelen 2019** - Fuel performance modelling by means of TRANSURANUS, TRANSURANUS training course, JRC.
- **Van Uffelen et al. 2019** - A review of fuel performance modelling, Journal of Nuclear Materials, vol. 516.
- **Wirth 2017** - Computational Modeling of Nuclear Fuels. In: D.R. Olander, A. Motta (Eds.), Light Water Reactor Materials, vol. I: Fundamentals, American Nuclear Society.


(Beyer et al. 1975)

Thank you for your attention

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This project is part of the research activities portfolio of the Joint Programme on Nuclear Materials.

SUPPLEMENTARY MATERIAL

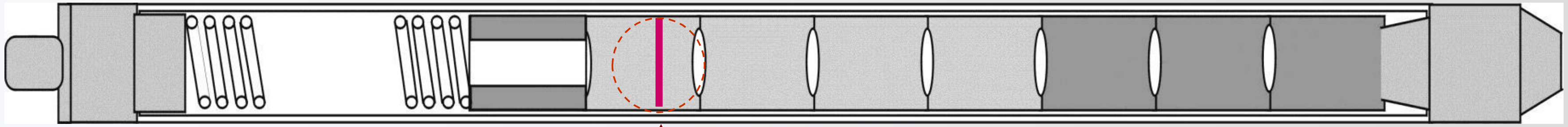
—> TUTORIAL ON FUEL PERFORMANCE CODES

- Development/use of FPCs
- Geometric domains represented
- Mathematical/numerical frame
- Validation
- **Burnup analysis**
- Thermal analysis
- Mechanical analysis
- Material and behavioural models (e.g., Fission Gas Behaviour)

Burnup analysis

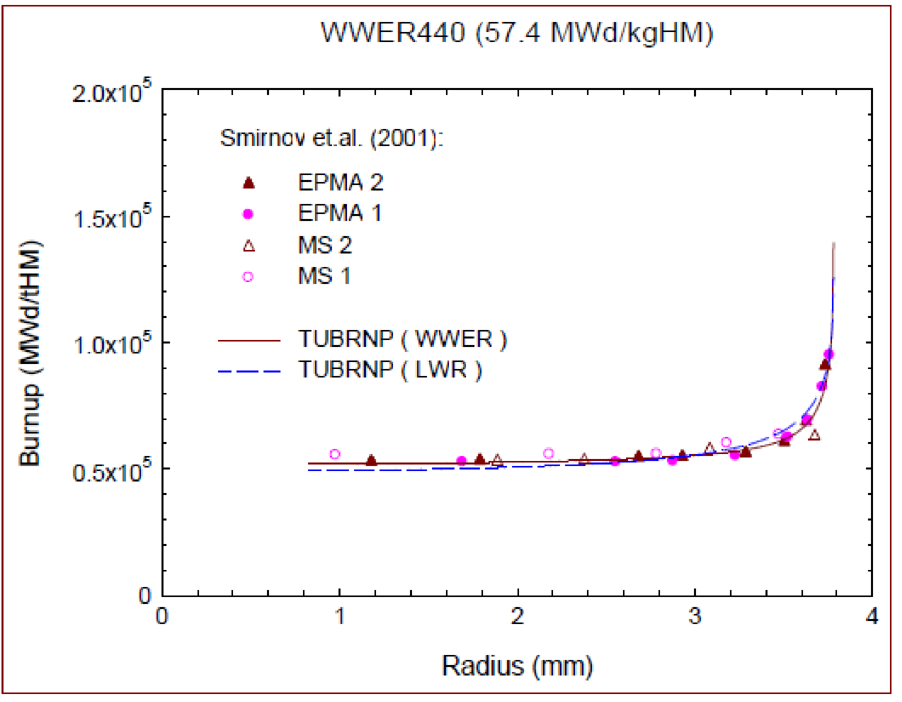
Burnup analysis (i)

- Why do we need a burn-up model in fuel performance calculations ?



Burn-up - to be distinguished:

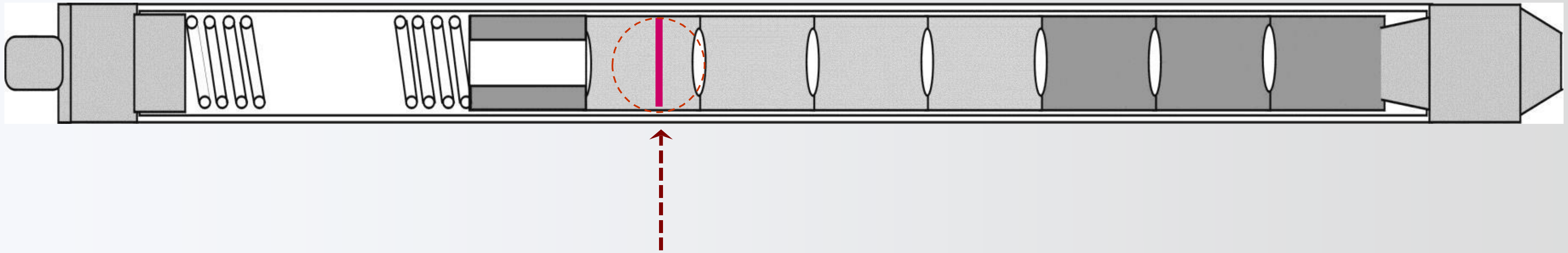
- local burnup
- section average burnup
- fuel rod average burnup



(Van Uffelen 2019)

Burnup analysis (i)

- Why do we need a burn-up model in fuel performance calculations ?



To calculate at each *radial position* in the fuel:

- the fraction of fissile material burnt (local burn-up)
- the build-up and fission of the Pu, Am and Cm isotopes and
- the build-up of fission products

→

radial power density distribution → source term for temperature calculations

radial burn-up distribution → local material properties

→ local concentrations of fission products

Burnup analysis (ii)

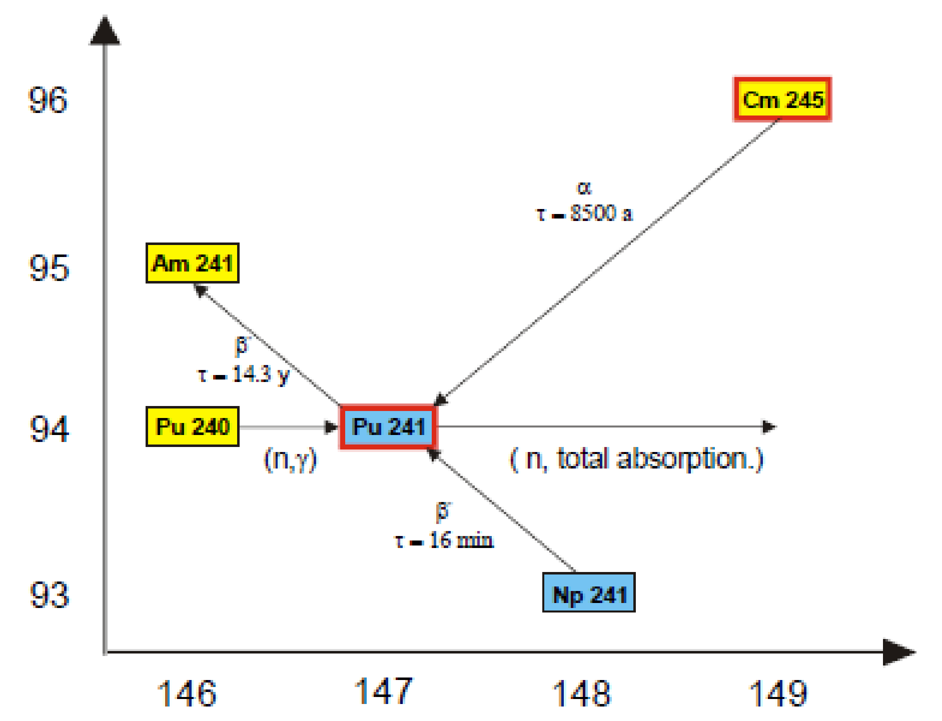
- ---> complete solution (?)

Complete system of isotope evolution equations

- total neutron absorption on ${}^{m}_{z}X$
+ neutron capture on ${}^{m-1}_{z}X$
+ ... add. nuclear reactions, e.g. (n,2n)

- total decay of ${}^{m}_{z}X$
+ build-up from α-decay of ${}^{m+4}_{z+2}A$
+ build-up from β-decay of ${}^{m}_{z-1}B$
+ build-up from add. decay modes (e.g. electron conversion)

Example: ${}^{m}_{z}X = {}^{241}_{94}Pu$
but to be solved for all isotopes
in all radial zones !



Burnup analysis (ii)

- ---> complete solution (?)

Complete system of isotope evolution equations

$$
\begin{aligned}
dN_m(r,t) = & \left[-\int N_m(r,t)\,\sigma_{a,m}(E)\Phi(r,E,t)dE + \int N_{m-1}(r,t)\sigma_{c,m-1}(E)\,\Phi(r,E,t)dE \right] dt + \dots \\
& - \left[\lambda_m N_m(r,t)\right] dt + \left[\lambda_{\alpha,m+4} N_{m+4}(r)\right] dt + \left[\lambda_{\beta m'} N_{m'}(r)\right] dt + \dots
\end{aligned}
$$

For all isotopes, in all radial zones (!)

→ feasible today, but coupling with fuel performance code is still challenging:

- time-step control required for short-lived isotopes
- fuel geometry changing during irradiation

→ But **full set is not required …**

- only the fissioning nuclides are relevant for the radial power profile
- only the relative radial power profile is required

Burnup analysis (iii)

- —> alternative …

Common approach: one-group effective cross sections

- total neutron absorption on ${}^{m}_{z}X$

\+ neutron capture on ${}^{m-1}_{z}X$

\+ … add. nuclear reactions, e.g. (n,2n)

$$
\begin{aligned}
dN_m(r,t) = &-\left[\int N_m(r,t)\,\sigma_{a,m}(E)\Phi(r,E,t)dE\right]dt \\
&+\left[\int N_{m-1}(r,t)\sigma_{c,m-1}(E)\,\Phi(r,E,t)dE\right]dt \\
&+\ldots
\end{aligned}
$$

Neutron transport (e.g., MCNP) for calculation of flux and effective cross sections combined with depletion calculations (e.g., ORIGEN) for time increment defining one-group effective cross sections, depending on location and time

$$\sigma_x(r,t) = \frac{\int \sigma_x(E)\Phi(r,E,t)dE}{\int \Phi(r,E,t)dE} \qquad \Phi(r,t) = \int \Phi(r,E,t)dE$$

$$\rightarrow dN_m(r,t) = \left[-\sigma_{a,m}(r,t)N_m(r,t)\,\Phi(r,t) + \sigma_{c,m-1}(r,t)N_{m-1}(r,t)\Phi(r,t)\right]dt$$

(Van Uffelen 2019)

Burnup analysis (iii)

- –-> alternative ...

Common approach: one-group effective cross sections

Priority: modeling relative radial power profiles
= source term for fuel performance calculations
(radially averaged or "linear" power is given on input)

↓

Diffusion of thermal neutrons

$$q'''(r) \propto \sum_k \sigma_{f,k} N_k(r) \Phi(r) \qquad \Phi(r) = c \cdot I_0(\kappa r) \quad \text{with} \quad \kappa = \sqrt{\frac{\Sigma_{a,tot}}{3\Sigma_s}} \approx \sqrt{\frac{\sum_k \sigma_{a,th,k} N_k}{3\sigma_s N_{tot}}}$$

+

$$dN_m(r) = \left[-\sigma_{a,m} N_m(r)\, f_m(r) + \sigma_{c,m-1} N_{m-1}(r) f_{m-1}(r) \right] \Phi(r) dt$$

(only) for U-235 ... U-238, Np-237, Pu-238 ... Pu-242,
Am-241..Am-244, Cm-242..Cm-245, He-4
+ most relevant decay terms

Limited equations

- one-group eff. cross sections
- resonance form factors (only for U-238, Pu-240)

Example

TUBRNP module

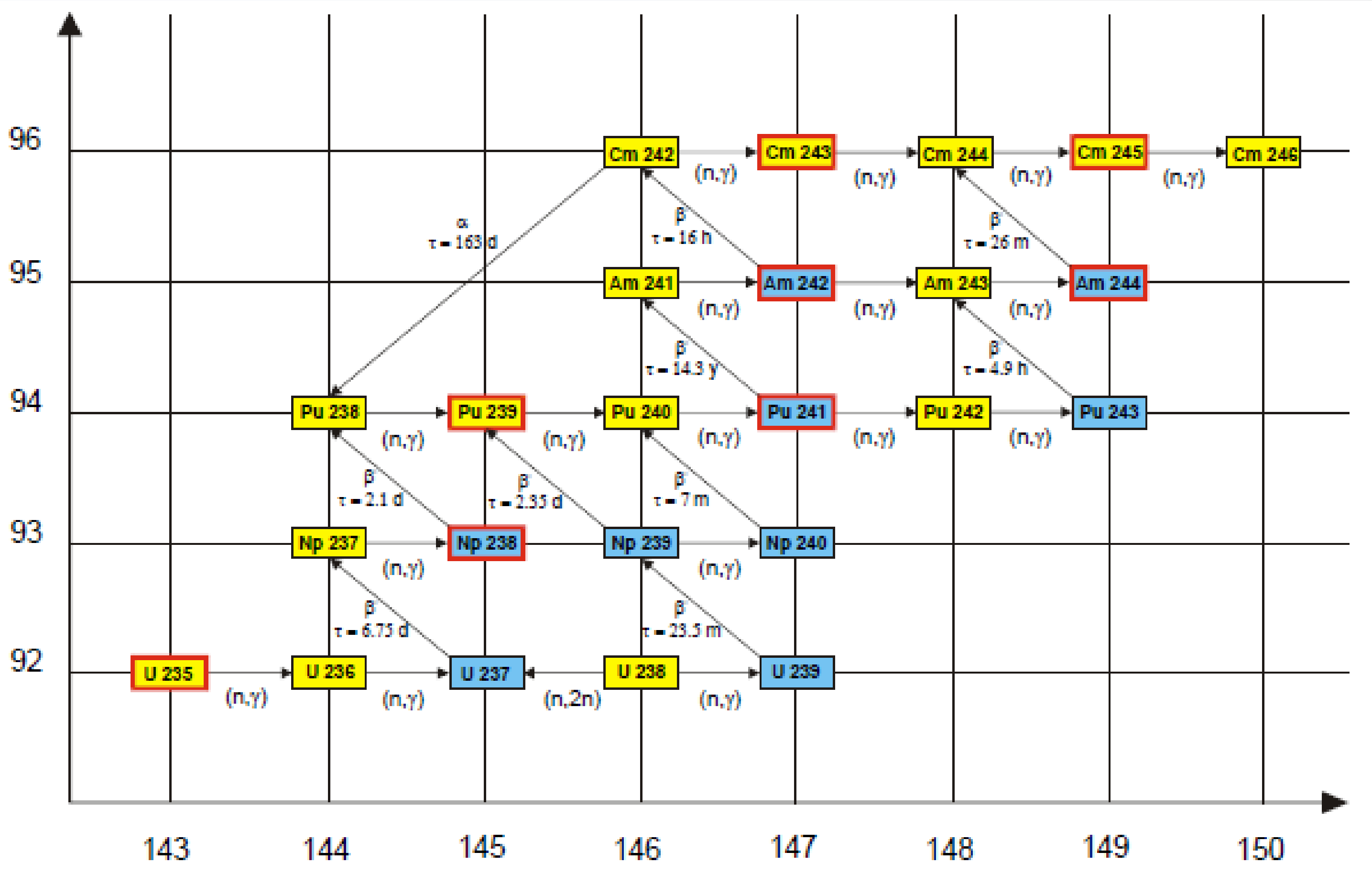
in TRANSURANUS

(Van Uffelen 2019)

Burnup analysis (iii)

- ---> alternative …

Common approach: one-group effective cross sections



Example

TUBRNP module

in TRANSURANUS

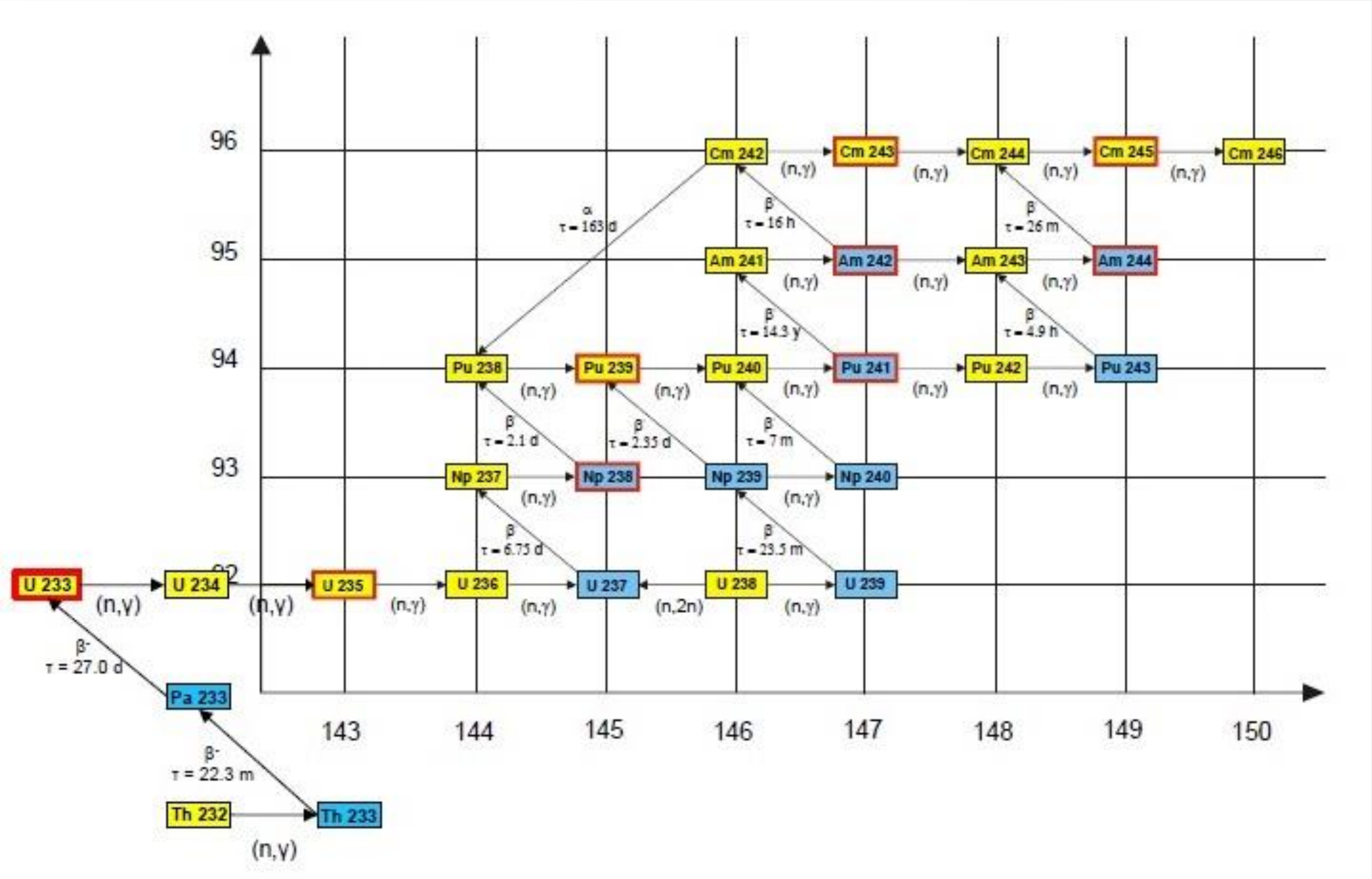
(Van Uffelen 2019)

---> major actinides & fission products (including α-decays, branching ratios for ^{242}Am, β-decays, helium issues…)

Burnup analysis (iii)

- ---> alternative …

Common approach: one-group effective cross sections



Example

TUBRNP module

in TRANSURANUS

(Van Uffelen 2019)

---> major actinides & fission products (including α-decays, branching ratios for ^{242}Am, β-decays, helium issues)

---> extended to Th-fuels

Burnup analysis (iv)

- ---> validation ...

1) Priority ---> Experimental Data

Electron Probe Micro Analysis (EPMA)

- Provides local concentrations of elements (e.g., Pu, U, Nd, Xe)

Secondary Ionization Mass Spectrometry (SIMS)

- provides relative local concentrations of isotopes (e.g., Pu-239, Pu-240)

Radiochemical analyses

- provide radially-averaged concentrations of elements and isotopes

2) Complementary ---> Detailed neutron-physical simulations

Monte-Carlo Burn-up codes (e.g., Monteburns, ALEPH, VESTA, SERPENT)

Lattice codes (e.g., HELIOS)

Example

TUBRNP module

in TRANSURANUS

(Van Uffelen 2019)

---> major actinides & fission products (including α-decays, branching ratios for ^{242}Am, β-decays, helium issues)

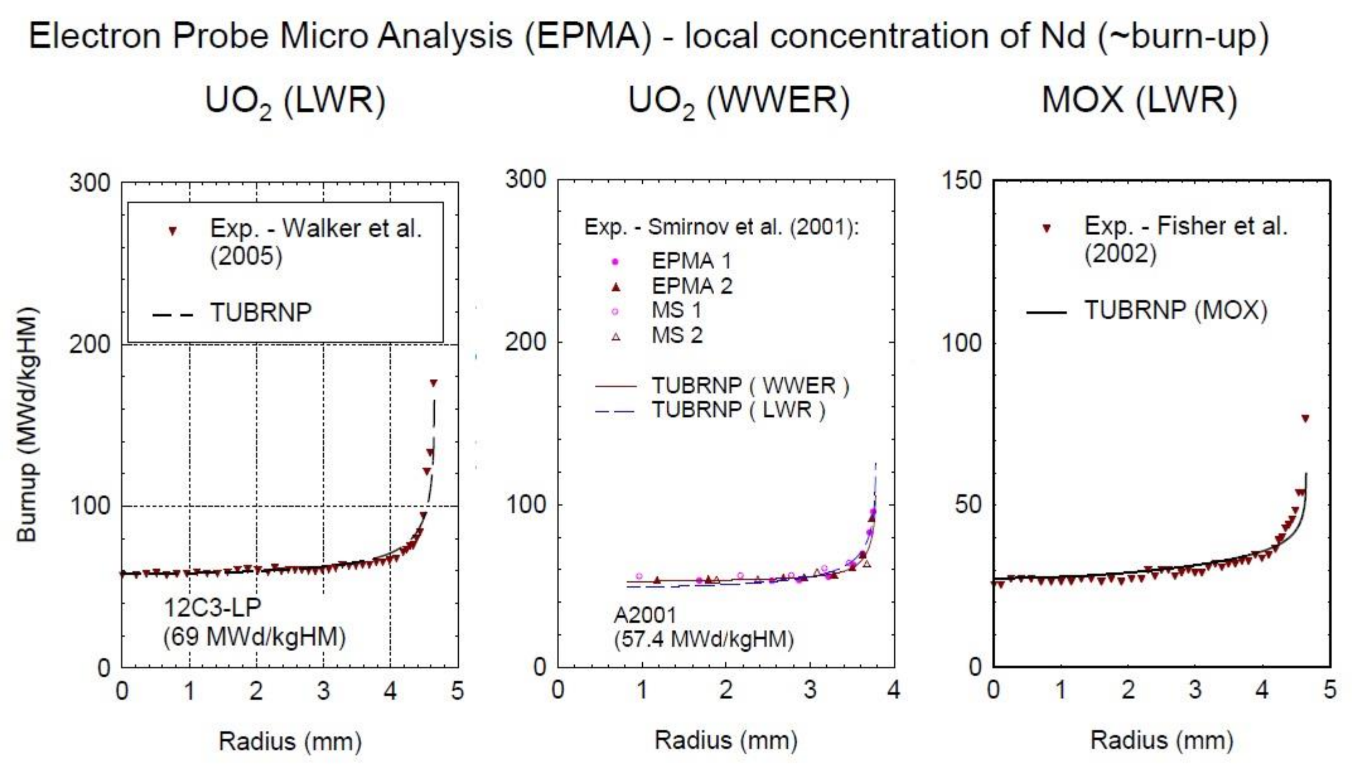
---> extended to Th-fuels

---> **extensively validated**

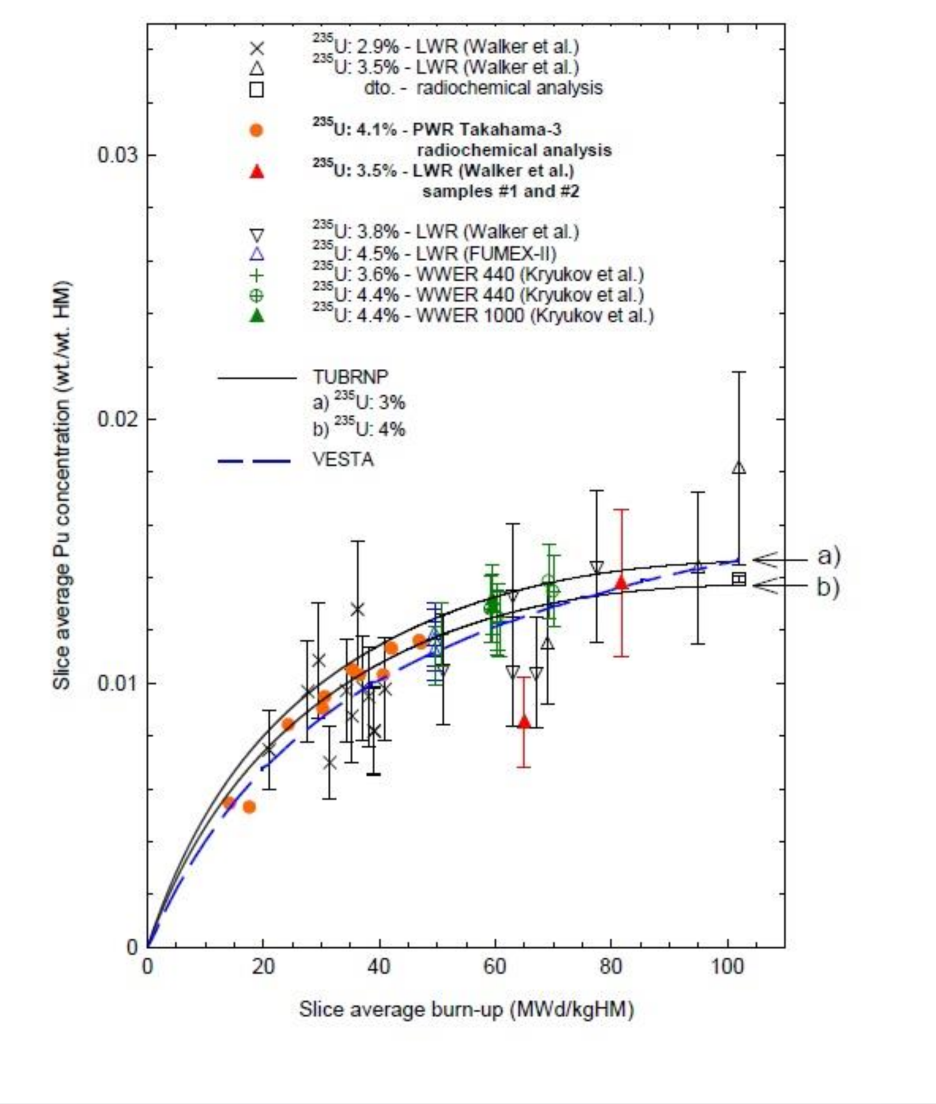
Burnup analysis (iv)

- ---> example: TUBRNP validation …

1) Priority ---> Experimental Data



Electron Probe Micro Analysis (EPMA) - local concentration of Nd (~burn-up)



(Van Uffelen 2019)

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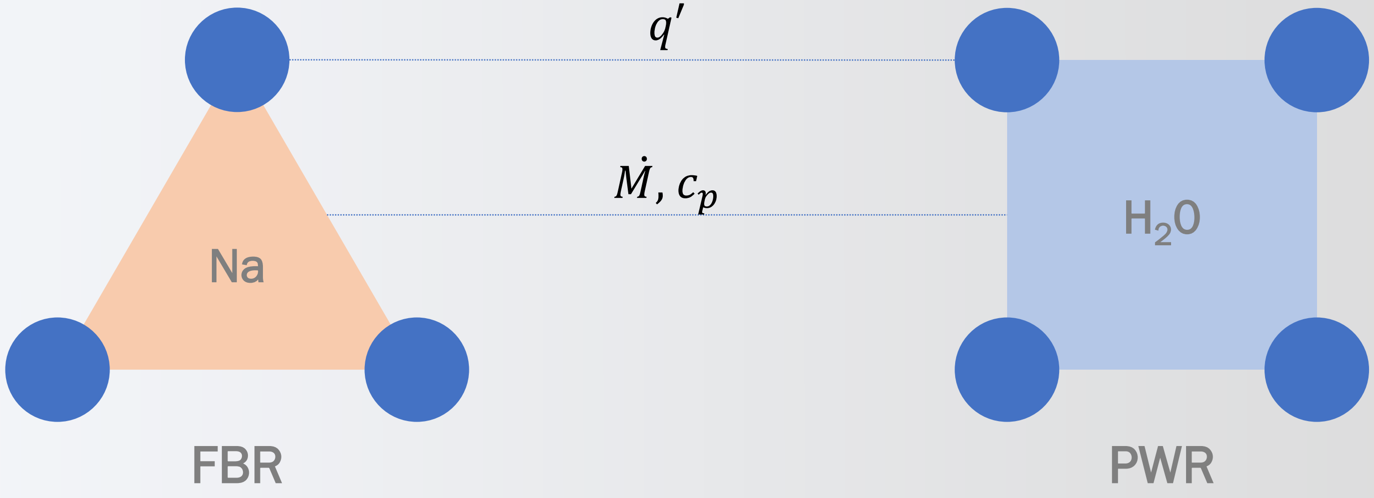
- Mechanical analysis
- Material and behavioural models (e.g., Fission Gas Behaviour)

Thermal analysis

Thermal analysis of fuel pins (i)

- **"Single-channel" analysis** *(coolant-centred)*
- Hp. Single-phase flow, steady-state conditions
- Hp. No azimuthal dependency in heat generation & cooling
- Hp. Radially uniform power generation, dq'''/d*r* = 0
- Hp. L/D >> 10

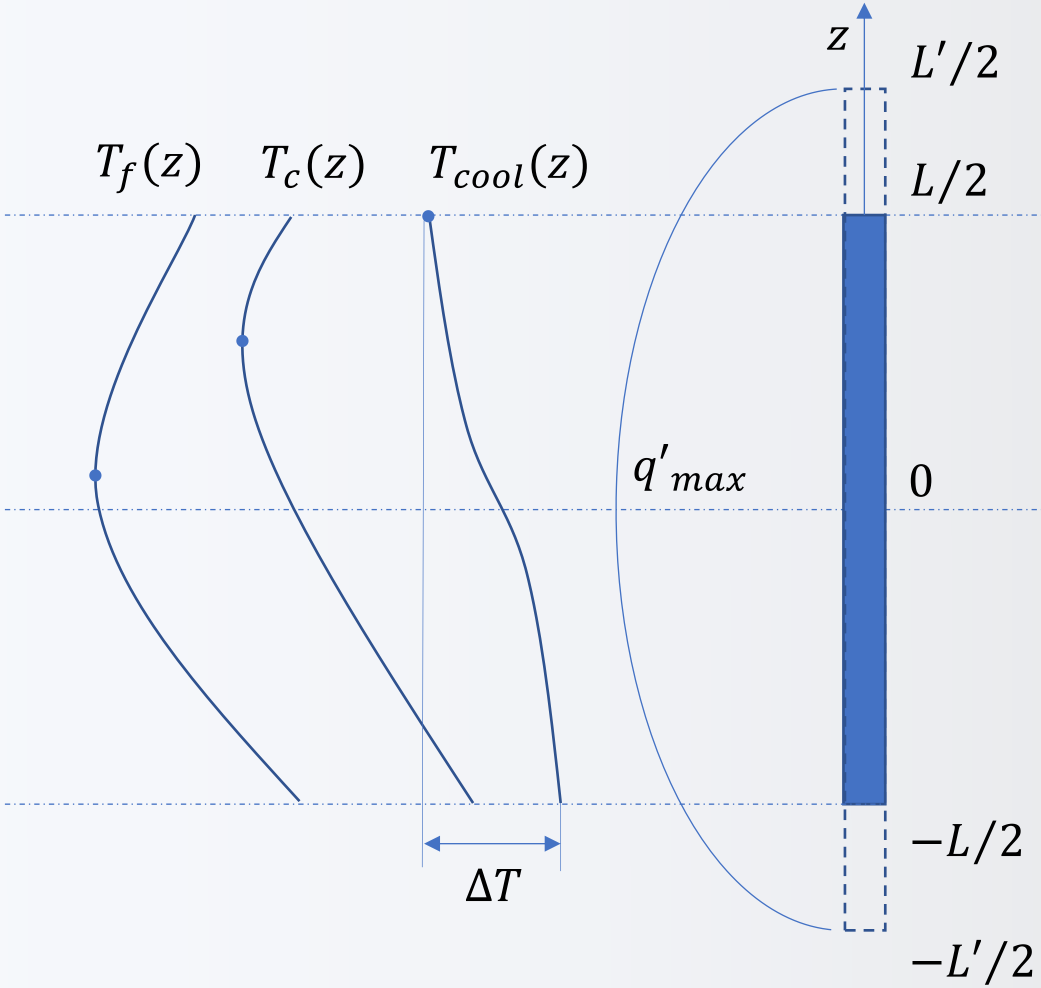
- not true if the pin is in special locations, in the periphery, close to control rods
- not true at beginning of life (eccentricity, fragment relocation)
- often not true in FRs

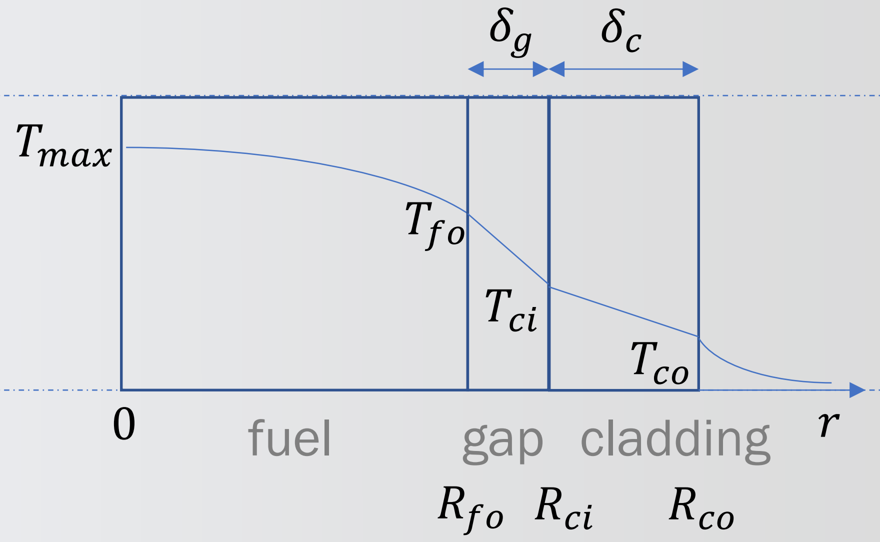


$$f = \frac{1}{6} \cdot 3 = \frac{1}{2}$$

$$f = \frac{1}{4} \cdot 4 = 1$$

Thermal analysis of fuel pins (ii)





$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot k \nabla T + q'''$$

Hp.

$$\frac{1}{r}\frac{\mathrm{d}T}{\mathrm{d}r}\left(kr\frac{\mathrm{d}T}{\mathrm{d}r}\right) + q''' = 0$$

Thermal analysis of fuel pins (iii)

- Axial problem

$$q'(z) \longrightarrow q'(z) = q'_{max}\cos\left(\frac{\pi z}{L'}\right)$$

$$f\,q'(z)\mathrm{d}z = \dot{M}c_p\mathrm{d}T_{cool}$$

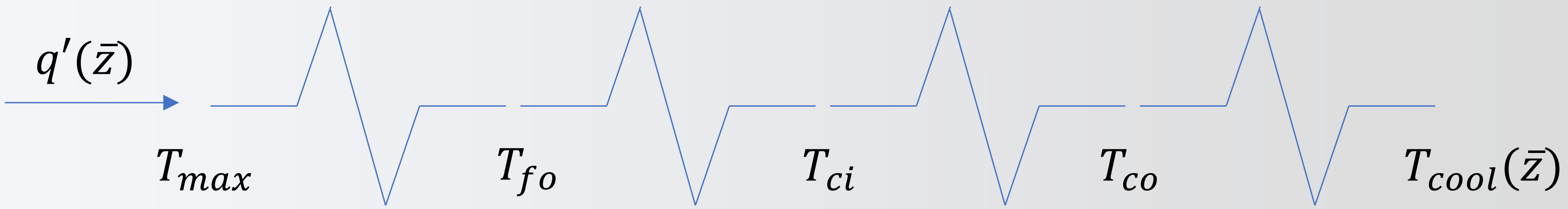
$$\boxed{T_{cool}(z) = T_{cool,in} + \frac{f}{\dot{M}c_p}\int_{-L/2}^{z} q'(z)\mathrm{d}z = T_{cool,in} + \frac{\Delta T}{2}\left[1 + \frac{\sin(\pi z/L)}{\sin(\pi L/2L')}\right]}$$

$$\Delta T = \frac{2L' f q'_{max}}{\pi \dot{M} c_p}\sin\left(\frac{\pi L}{2L'}\right) \approx \frac{2L' f q'_{max}}{\pi \dot{M} c_p}$$

$$\boxed{T_{co}(z) = T_{cool}(z) + \frac{q'(z)}{2\pi R_{co} h}}$$

Thermal analysis of fuel pins (iv)

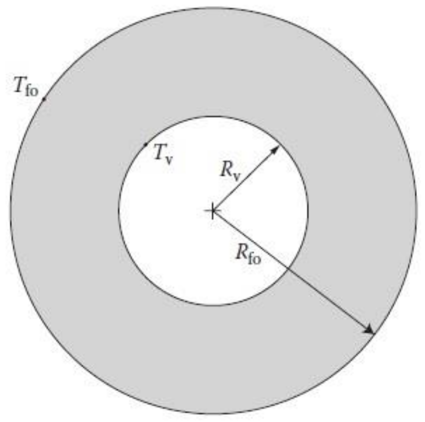
- Radial problem



FUEL	GAP	CLAD	COOLANT
solid pellet $\frac{1}{4\pi\bar{k}_f}$	$\frac{1}{2\pi R_g h_g}$	$\frac{\ln(R_{co}/R_{ci})}{2\pi k_c}$	$\frac{1}{2\pi R_{co} h}$
$\downarrow$	$\downarrow$ gap open	$\downarrow$ $\ln\left(1+\frac{\delta_c}{R_{ci}}\right) \sim \frac{\delta_c}{R_{ci}} \ll 1$	
$\int_{T_{fo}}^{T_{max}} k_f \mathrm{d}T = \frac{q'}{4\pi}$	$\frac{\delta_g}{2\pi R_{fo} k_g}$	$\frac{\delta_c}{2\pi R_{ci} k_c}$	

Thermal analysis of fuel pins (v)

- Radial problem

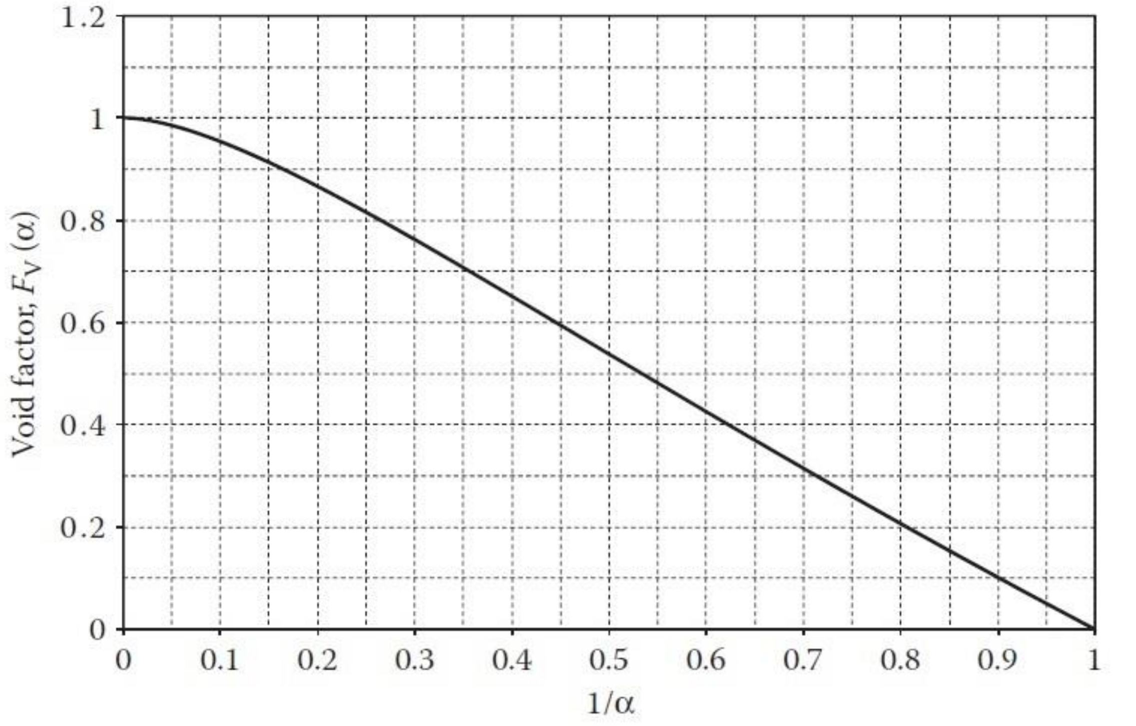


Cross section of an annular pellet.

FUEL

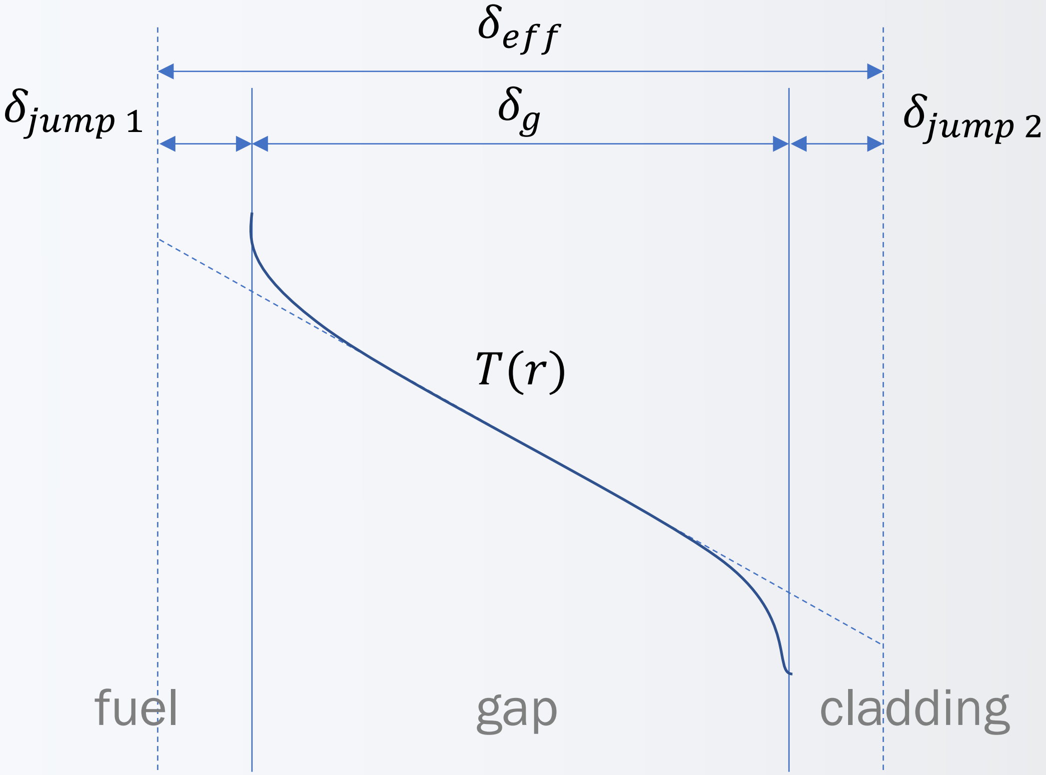
annular pellet $\dfrac{F_V}{4\pi\bar{k}_f}$

$$\int_{T_{fo}}^{T_{max}} k_f \mathrm{d}T = \frac{q'}{4\pi} F_V$$



Void factor function. For an annular region, α is the ratio of the outer to the inner radius.

Thermal analysis of fuel pins (vi)



OPEN GAP

$$h_g \approx \frac{k_{gas}}{\delta_{eff}} + \frac{4\sigma T_{fo}^3}{\frac{1}{\varepsilon_f} + \frac{1}{\varepsilon_c} - 1}$$

$$\delta_{eff} = \delta_g + \delta_{jump\ 1} + \delta_{jump\ 2}$$

10 μm He

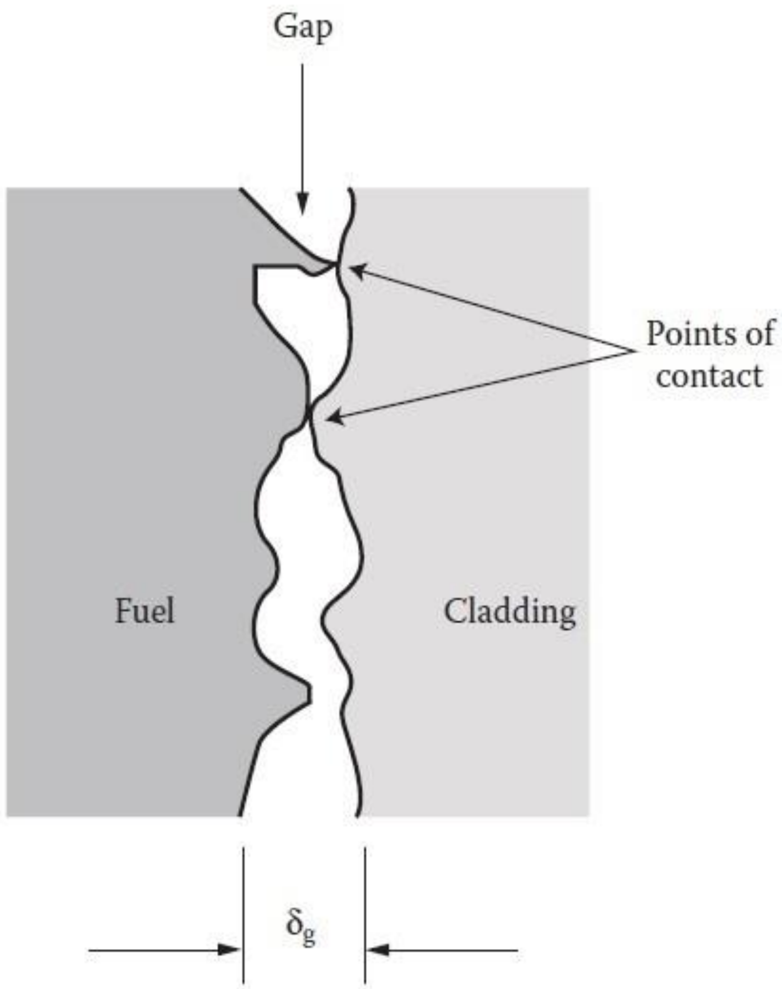
1 μm Xe

$$k_{gas} = (k_1)^{x_1}(k_2)^{x_2}$$

$$k_{gas} = A\ 10^{-6} T(\mathrm{K})^{0.79}\ \frac{\mathrm{W}}{\mathrm{cm\ K}}$$

$A =$ 15.8 He
1.97 Ar
1.15 Kr
0.72 Xe

Thermal analysis of fuel pins (vii)



Close-up view of fuel-cladding contact

OPEN GAP

$$h_g \approx \frac{k_{gas}}{\delta_{eff}} + \frac{4\sigma T_{fo}^3}{\frac{1}{\varepsilon_f} + \frac{1}{\varepsilon_c} - 1}$$

$$\delta_{eff} = \delta_g + \delta_{jump\,1} + \delta_{jump\,2}$$

10 µm He

1 µm Xe

$$k_{gas} = (k_1)^{x_1}(k_2)^{x_2}$$

$$k_{gas} = A\,10^{-6}T(\mathrm{K})^{0.79}\,\frac{\mathrm{W}}{\mathrm{cm\,K}}$$

$A =$ 15.8 He
1.97 Ar
1.15 Kr
0.72 Xe

CLOSED GAP

$$h_{contact} = C\,\frac{2k_f k_c}{k_f + k_c}\,\frac{p_c}{H\sqrt{\delta_g}}$$

$$h_{g,closed} = h_{g,open} + h_{contact}$$

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- **Mechanical analysis**
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Mechanical analysis

Mechanical analysis (i)

- Hp. Continuum mechanics
- Hp. Deformable body without lacerations

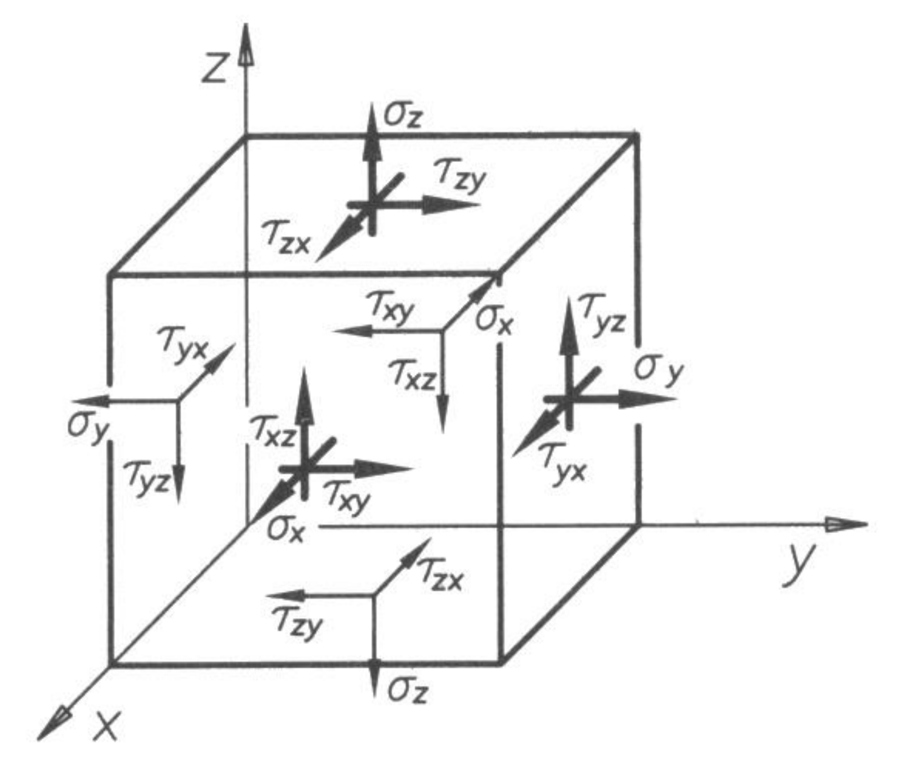
- *Engineering notation*
  - Orthogonal reference system
  - Rectangular coordinates (*x, y, z*)

$$\begin{cases} \boldsymbol{\bar{u}} & 3\boldsymbol{u_j} & \text{displacement} \\ \boldsymbol{\bar{\varepsilon}} & 6\boldsymbol{\varepsilon_{ij}} & \text{strain} \\ \boldsymbol{\bar{\sigma}} & 9\boldsymbol{\sigma_{ij}} & \text{stress} \end{cases}$$

Unknowns

$$\bar{\bar{\sigma}} = \begin{vmatrix} \sigma_x & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_y & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_z \end{vmatrix}$$

$$\bar{\sigma}_n = \sum_{i=1}^{3} \bar{\sigma}_i n_i$$



Visual representation

Mechanical analysis (ii)

- Governing equations
- Hp. Cauchy continuum (non-polar materials)
- / denotes partial derivatives

$$\varepsilon_{ij} = \frac{1}{2}\left(u_{j/i} + u_{i/j}\right)$$

6 Eqs. Strain compatibility (imposing simply-connected body)

$$\begin{cases} \sigma_{ij} = \sigma_{ji} \\ \sum_{i=1}^{3} \sigma_{ij/i} + F_j = 0 \end{cases}$$

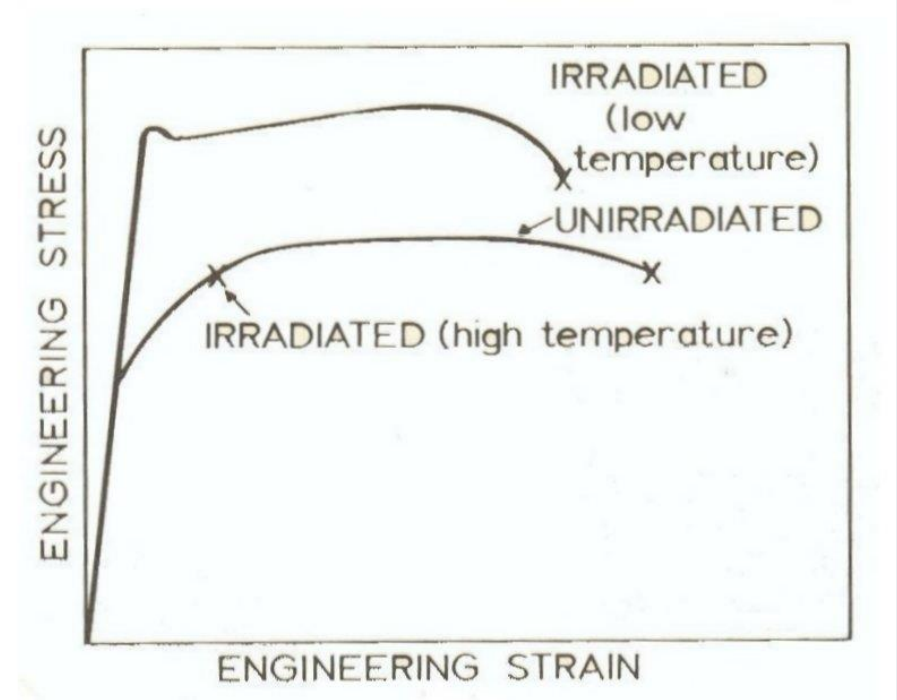
6 Eqs. Static equilibrium in the undeformed configuration
(Hp. of infinitesimal or "small" strains)

MATERIAL BEHAVIOUR

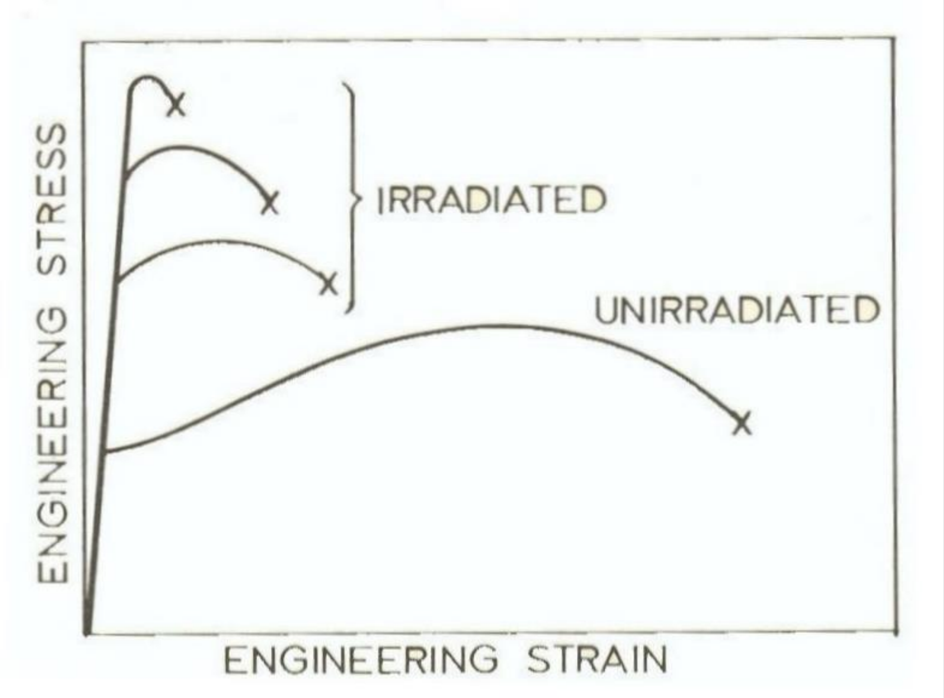
6 Eqs. Constitutive laws (depend on the material, $\bar{\bar{\sigma}} \sim \bar{\bar{\varepsilon}}$)

Mechanical analysis (iii)

- Material behaviour, Constitutive Equations
- Elastic & Plastic
- Effect of irradiation…



fcc, austenitic steel



bcc, ferritic steel

Mechanical analysis (iv)

- Elasticity
  - Bi-univocal relation between stresses and strains
  - Law of this dependency has to be found **experimentally**
- **Linear elasticity**
  - No yielding in the material
  - Compatibility imposed on infinitesimal relative displacements
  - The superposition principle holds…

HOOKE'S LAW

$$\varepsilon_{ij} = \sum\nolimits_{1}^{3} rs\, C_{ijrs}\sigma_{rs}$$

$$\sigma_{ij} = \sum\nolimits_{1}^{3} rs D_{ijrs}\varepsilon_{rs}$$

3^4 = 81 components → <u>2 independent components</u>

- Symmetry of $\bar{\bar{\varepsilon}}$ and $\bar{\bar{\sigma}}$
- Reversibility: strain energy density independent of loading history
- Macroscopically homogeneous & perfectly isotropic material

Mechanical analysis (v)

- With $\delta = \sum_1^3 \varepsilon_{ii} = tr\left(\overline{\overline{\varepsilon}}\right) = \frac{\Delta V}{V}$

Lamé's relations

$$\sigma_{ij} = \sum_1^3 rsD_{ijrs}\varepsilon_{rs} \longrightarrow \begin{cases}\sigma_{ii} = 2\mu\varepsilon_{ii} + \lambda\delta \\ \sigma_{ij} = 2\mu\varepsilon_{ij}\end{cases}$$

In terms of engineering elastic moduli

$$\begin{cases} E = \dfrac{\mu(3\lambda + 2\mu)}{\lambda + \mu} \\ \nu = \dfrac{\lambda}{2(\lambda + \mu)} \\ G = \dfrac{E}{2(1 + \nu)} = \mu \end{cases} \longrightarrow \begin{cases} \varepsilon_{ii} = \dfrac{1}{E}\left[\sigma_{ii} - \nu \sum_{jj} \sigma_{jj}\right] \\ \varepsilon_{ij} = \dfrac{1}{2G}\sigma_{ij} \end{cases}$$

Mechanical analysis (vi)

- Thermo-elasticity

$$\begin{cases} \bar{u} & [u_x, u_y, u_z] \\ \bar{\varepsilon} & \begin{bmatrix} \varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\ \varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\ \varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz} \end{bmatrix} \\ \bar{\sigma} & \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} \\ \bar{F} & [F_x, F_y, F_z] \end{cases} \longrightarrow \left\{ \begin{array}{l} \varepsilon_{xx} = \frac{1}{E}\left[\sigma_{xx} - \nu\left(\sigma_{yy} + \sigma_{zz}\right)\right] \\ \varepsilon_{yy} = \frac{1}{E}\left[\sigma_{yy} - \nu\left(\sigma_{xx} + \sigma_{zz}\right)\right] \\ \varepsilon_{zz} = \frac{1}{E}\left[\sigma_{zz} - \nu\left(\sigma_{xx} + \sigma_{yy}\right)\right] \end{array} \right. \boxed{\begin{array}{l} + \alpha(T - T_0) \\ + \alpha(T - T_0) \\ + \alpha(T - T_0) \end{array}}$$

$$\varepsilon_{xy} = \frac{1}{2G}\sigma_{xy}$$
$$\varepsilon_{xz} = \frac{1}{2G}\sigma_{xz}$$
$$\varepsilon_{yz} = \frac{1}{2G}\sigma_{yz}$$

$$\{\ T \qquad T(x, y, z) \longrightarrow \bar{\nabla} \cdot k \bar{\nabla} T + q'''(x, y, z) = 0$$

+ Strain compatibility
+ Static equilibrium

α is the linear thermal expansion coefficient ($\alpha \equiv \Delta L / L \Delta T \approx \frac{\beta}{3} \equiv \Delta V / V \Delta T$)

β being the volumetric thermal expansion coefficient

Mechanical analysis (vii)

- Thermal stresses

  - Homogeneous and isotropic material
  - Uniformly heated//cooled
  - Free to expand//contract thermally

→ **NO THERMAL STRESSES !**

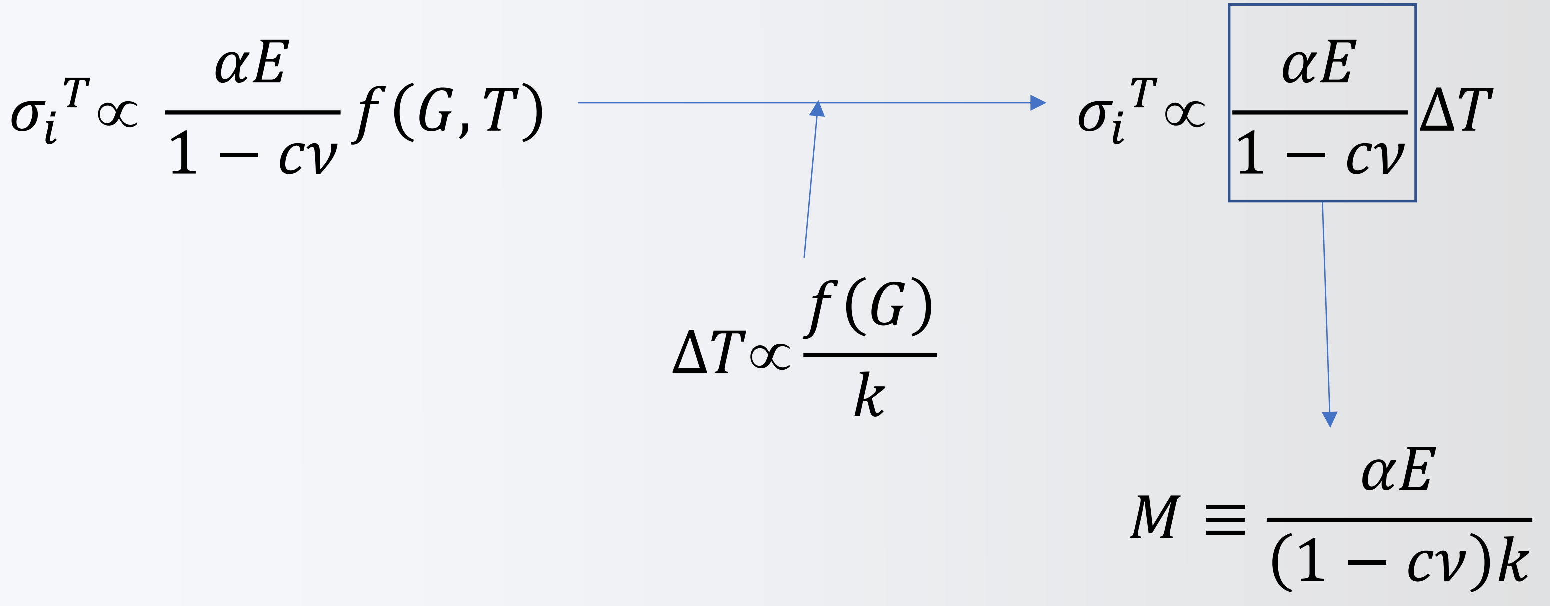
  - Thermal expansion//contraction <u>completely</u> prevented in uniform heating//cooling
  - Non-uniform temperature (thermal gradient) but free to expand//contract
  - Mixed effect: non-uniform temperature + <u>partial</u> restraints in one or more directions

$$\sigma_i{}^T \propto \frac{\alpha E}{1 - c\nu} f(G, T)$$

G : geometry of the component
T : temperature distribution

Mechanical analysis (viii)

- Thermal stresses



$$\sigma_i^{\,T} \propto \frac{\alpha E}{1-c\nu} f(G,T)$$

$$\Delta T \propto \frac{f(G)}{k}$$

$$\sigma_i^{\,T} \propto \boxed{\frac{\alpha E}{1-c\nu}} \Delta T$$

$$M \equiv \frac{\alpha E}{(1-c\nu)k} \qquad [M] = \frac{\text{MPa m}}{\text{W}}$$

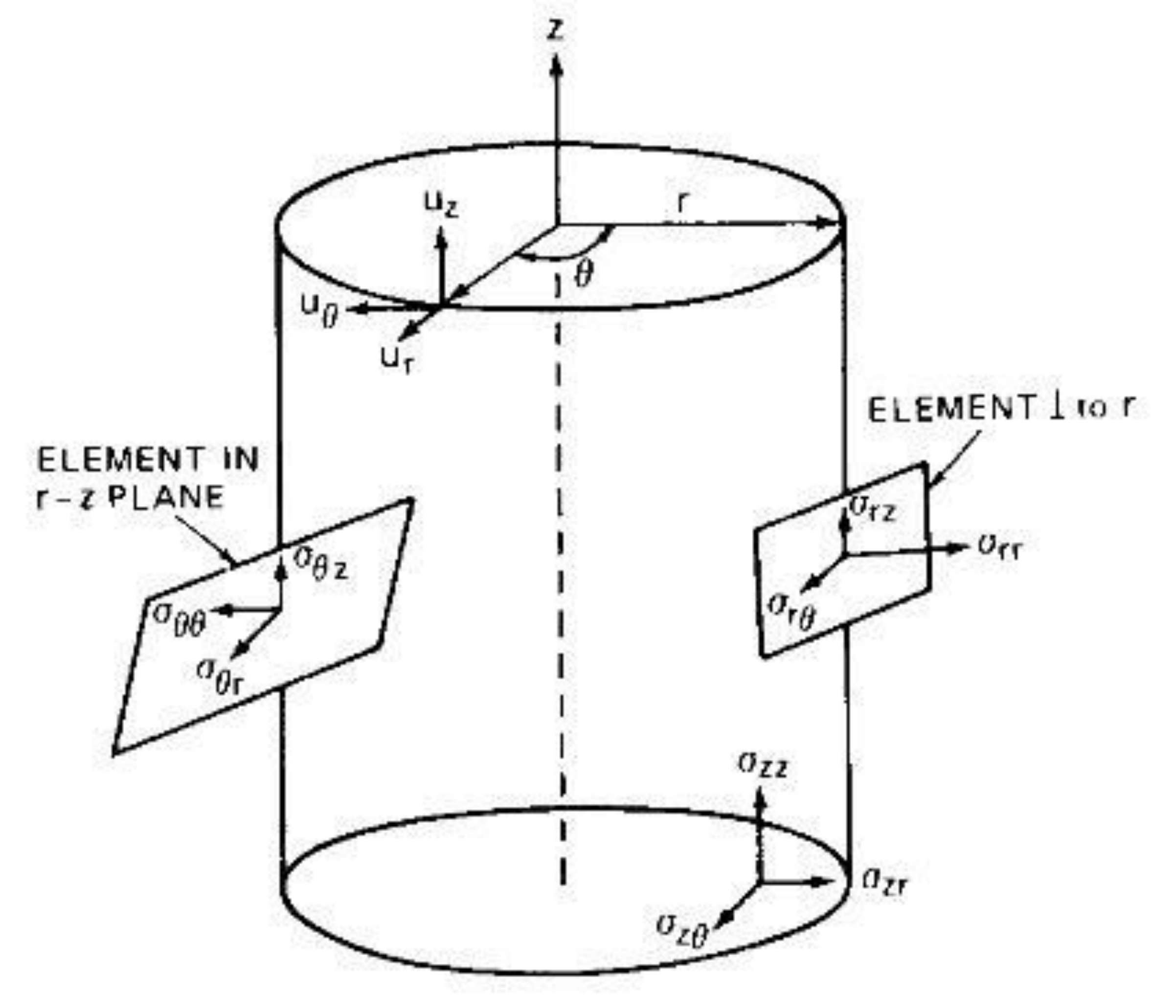
Ferritic steel, bcc : *M* = 0.12
Austenitic steel, fcc : *M* = 0.36

Mechanical analysis of fuel pins (i)

$$\boxed{x_j = r, \vartheta, z}$$

$$\left.\begin{array}{ll}
\bar{u} & [u_r, u_\vartheta, u_z] \\
\overline{\varepsilon} & \begin{bmatrix} \varepsilon_{rr} & \varepsilon_{r\vartheta} & \varepsilon_{rz} \\ \varepsilon_{\vartheta r} & \varepsilon_{\vartheta\vartheta} & \varepsilon_{\vartheta z} \\ \varepsilon_{zr} & \varepsilon_{z\vartheta} & \varepsilon_{zz} \end{bmatrix} \\
\overline{\sigma} & \begin{bmatrix} \sigma_{rr} & \sigma_{r\vartheta} & \sigma_{rz} \\ \sigma_{\vartheta r} & \sigma_{\vartheta\vartheta} & \sigma_{\vartheta z} \\ \sigma_{zr} & \sigma_{z\vartheta} & \sigma_{zz} \end{bmatrix} \\
\bar{F} & [F_r, F_\vartheta, F_z]
\end{array}\right\}$$

$$T \qquad T(r, \vartheta, z)\}$$



Mechanical analysis of fuel pins (ii)

- **Axial-symmetry** of geometry and applied load

$$\begin{cases} \sigma_{\vartheta z} \equiv \tau_{\vartheta z} = 0 \\ \sigma_{\vartheta r} \equiv \tau_{\vartheta r} = 0 \end{cases}$$

- Equilibrium (symmetry of the Cauchy tensor)

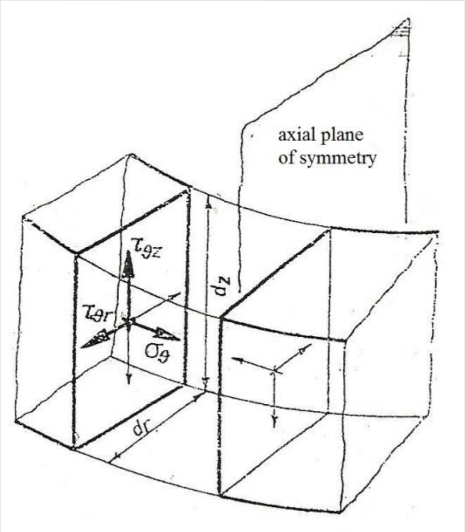
$$\begin{cases} \tau_{z\vartheta} = \tau_{\vartheta z} = 0 \\ \tau_{r\vartheta} = \tau_{\vartheta r} = 0 \\ \tau_{rz} = \tau_{zr} \end{cases}$$

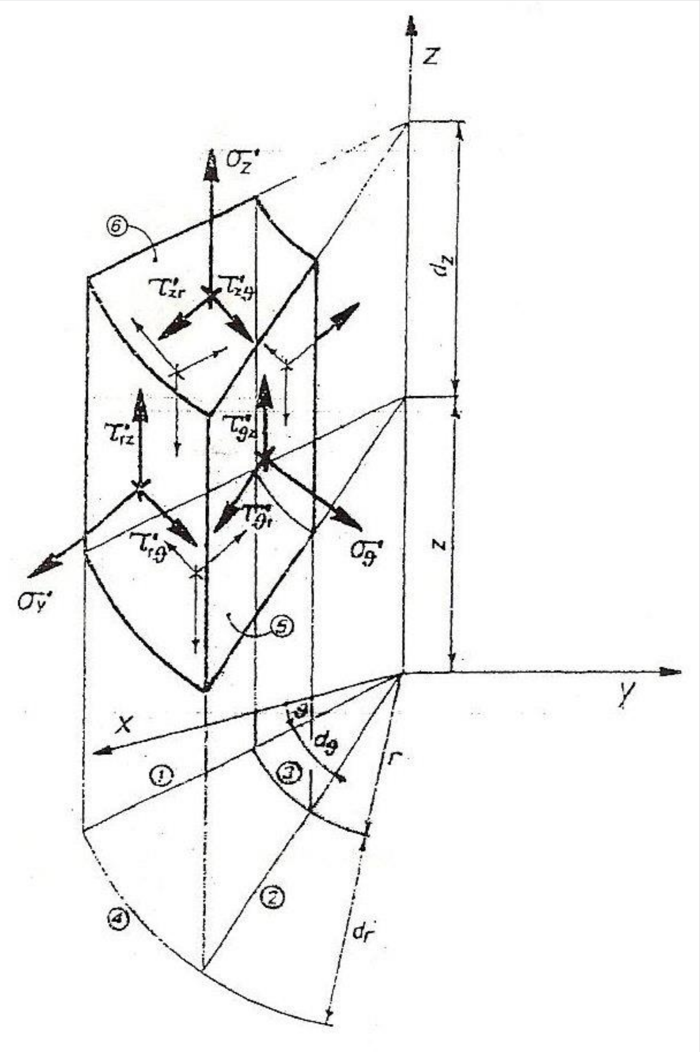
- **Ortho-cylindricity**
  - u_r independent of *z*
  - u_z independent of *r*
  - $\varepsilon_z = u_{z/z}$ independent of *r*

$$\varepsilon_{rz} = \varepsilon_{zr} \equiv \frac{1}{2}\left(u_{r/z} + u_{z/r}\right) = 0$$

$$\tau_{zr} = 2G\varepsilon_{zr} = 0$$

- Neglect volume forces *F*





Mechanical analysis of fuel pins (iii)

- Constitutive Eqs. of Cladding and Fuel

$$\varepsilon_i = \varepsilon_i^E + \varepsilon_i^T + \varepsilon_i^S + \varepsilon_i^{VP} + \left[\varepsilon_i^C\right]$$

  - *E* : elastic strain
  - *T* : thermal strain
  - *S* : swelling + [fuel densification]
  - *VP* : visco-plastic strain
  - *C* : [fuel cracking]

Component	Isotropic ?	Permanent ?
Elastic	NO	NO
Thermal	YES	NO
Swelling	YES	YES
Creep/plastic	NO	YES
Axial growth (e.g., Zy)	NO	YES

Thermo-elastic component

$$\begin{cases} \varepsilon_r^E = \dfrac{1}{E}\left[\sigma_r - \nu(\sigma_\vartheta + \sigma_z)\right] \\ \varepsilon_\vartheta^E = \dfrac{1}{E}\left[\sigma_\vartheta - \nu(\sigma_r + \sigma_z)\right] \\ \varepsilon_z^E = \dfrac{1}{E}\left[\sigma_z - \nu(\sigma_r + \sigma_\vartheta)\right] \end{cases}$$

(cladding ≠ fuel)

$$\left\{\varepsilon_r^T = \varepsilon_\vartheta^T = \varepsilon_z^T = \alpha(T - T_0)\right.$$

(cladding ≠ fuel)

Mechanical analysis of fuel pins (iv)

- Constitutive Eqs. of Cladding and Fuel

$$\varepsilon_i = \varepsilon_i^E + \varepsilon_i^T + \varepsilon_i^S + \varepsilon_i^{VP} + \left[\varepsilon_i^C\right]$$

  - *E* : elastic strain
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  - *VP* : visco-plastic strain
  - *C* : [fuel cracking]

Component	Isotropic ?	Permanent ?
Elastic	NO	NO
Thermal	YES	NO
Swelling	YES	YES
Creep/plastic	NO	YES
Axial growth (e.g., Zy)	NO	YES

Swelling + [fuel densification]

$$\begin{cases} \varepsilon_r^S = \varepsilon_\vartheta^S = \varepsilon_z^S = \varepsilon^S = \dfrac{1}{3}\left[\left(\dfrac{\Delta V}{V}\right)_{\text{voids}}\right] \div \sigma_h \text{ (hydrostatic stress)}, T, dpa \text{ (dose)} & \text{(cladding)} \\ \varepsilon_r^S = \varepsilon_\vartheta^S = \varepsilon_z^S = \varepsilon^S = \dfrac{1}{3}\left[\left(\dfrac{\Delta V}{V}\right)_{\text{solid FPs}} + \left(\dfrac{\Delta V}{V}\right)_{\text{gaseous FPs}} - \left(\dfrac{\Delta V}{V}\right)_{\text{densification}}\right] & \text{(fuel)} \end{cases}$$

$(\Delta V/V)_{\text{solid FPs}}$ $\div$ burn-up

$(\Delta V/V)_{\text{gaseous FPs}}$ $\div\ \sigma_h$, size and concentration of fission-gas bubbles vs. T

$(\Delta V/V)_{\text{densification}}$ $\div\ \sigma_h$, reduction in volume of the pores

Mechanical analysis of fuel pins (v)

- Constitutive Eqs. of Cladding and Fuel

$$\varepsilon_i = \varepsilon_i^E + \varepsilon_i^T + \varepsilon_i^S + \varepsilon_i^{VP} + \left[\varepsilon_i^C\right]$$

- *E* : elastic strain
- *T* : thermal strain
- *S* : swelling + [fuel densification]
- *VP* : visco-plastic strain
- *C* : [fuel cracking]

Component	Isotropic ?	Permanent ?
Elastic	NO	NO
Thermal	YES	NO
Swelling	YES	YES
Creep/plastic	NO	YES
Axial growth (e.g., Zy)	NO	YES

Visco-plastic strain (cladding ≠ fuel)

$$\begin{cases} \varepsilon_r^{VP} = \dfrac{\varepsilon_{eq}}{\sigma_{eq}}\left[\sigma_r - \dfrac{1}{2}(\sigma_\vartheta + \sigma_z)\right] = \dfrac{3}{2}\dfrac{\varepsilon_{eq}}{\sigma_{eq}} S_r \\ \varepsilon_\vartheta^{VP} = \dfrac{\varepsilon_{eq}}{\sigma_{eq}}\left[\sigma_\vartheta - \dfrac{1}{2}(\sigma_r + \sigma_z)\right] = \dfrac{3}{2}\dfrac{\varepsilon_{eq}}{\sigma_{eq}} S_\vartheta \\ \varepsilon_z^{VP} = \dfrac{\varepsilon_{eq}}{\sigma_{eq}}\left[\sigma_z - \dfrac{1}{2}(\sigma_r + \sigma_\vartheta)\right] = \dfrac{3}{2}\dfrac{\varepsilon_{eq}}{\sigma_{eq}} S_z \end{cases}$$

$$\left(\frac{dV}{V}\right)^{VP} = \sum_i \varepsilon_i^{VP} = 0$$

$$\varepsilon_i^V = \varepsilon_i^V(t)$$

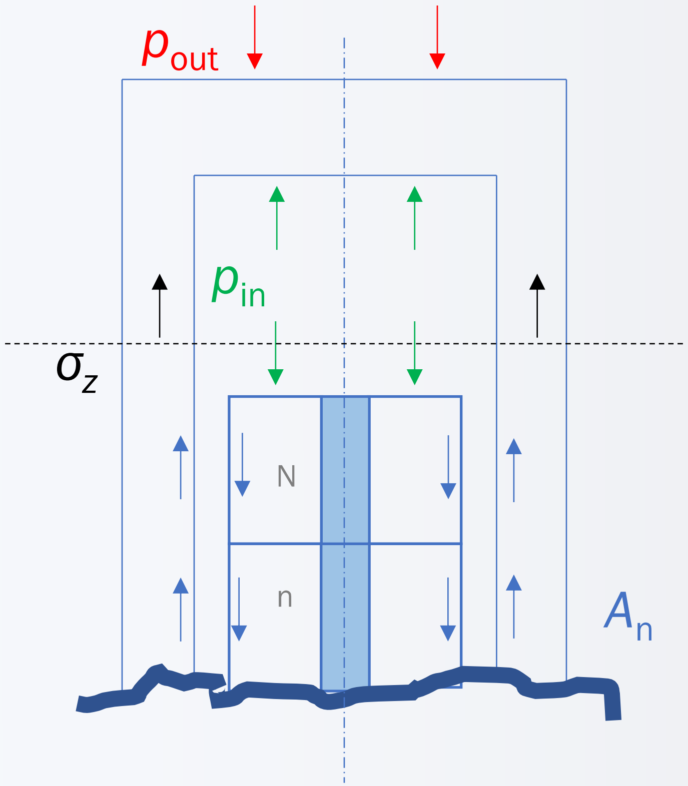
For instantaneous plastic strain ----> (more complex for creep strain)

$$\varepsilon_i^P(t + \Delta t) = \varepsilon_i^P(t) + \Delta\varepsilon_i^P = \varepsilon_i^P(t) + \frac{3}{2}\frac{\varepsilon_{eq}^P}{\sigma_{eq}} S_i \qquad S_i \equiv \sigma_i - \sigma_h \text{ (stress deviator)}$$

$$\varepsilon_{eq}^P = A(T)\sigma_{eq}^{n(T)}$$

Mechanical analysis of fuel pins (vi)

- Axial balance



Fuel

$$2\pi \int_0^R \sigma_z(r) r dr = \pi(R^2 - r_0{}^2) p_{in} + A_n + \sum_{k=n+1}^{N} A_k$$

Cladding

$$2\pi \int_R^{R+t} \sigma_z(r) r dr = \pi(R+t)^2 p_{out} - \pi R^2 p_{in} - A_n - \sum_{k=n+1}^{N} A_k$$

- Different conditions can be applied for A_n (e.g., stick, slip,…)

Thermo-elastic analysis of fuel pins

$$\sigma_\theta = \sigma_r + r\frac{d\sigma_r}{dr}$$

$$\begin{cases} \varepsilon_r = \dfrac{du_r}{dr} \\ \varepsilon_\theta = \dfrac{u_r}{r} \Rightarrow \varepsilon_r = \varepsilon_\theta + r\dfrac{d\varepsilon_\theta}{dr} \\ \varepsilon_z = \dfrac{du_z}{dz} \end{cases}$$

$$\boldsymbol{\varepsilon_i = \varepsilon_i^E + \varepsilon_i^T} + \varepsilon_i^S + \varepsilon_i^{VP} + \left[\varepsilon_i^C\right]$$

NB: considering also these strains, we get instead an ordinary differential equation for radial displacement u_r (more complex to solve …)

Generalized Plain Strain

$$\frac{d\varepsilon_z}{dr} = 0$$

$$\frac{d}{dr}\left(r^3\frac{d\sigma_r}{dr}\right) + \frac{E\alpha r^2}{(1-\nu)}\frac{dT}{dr} = 0$$

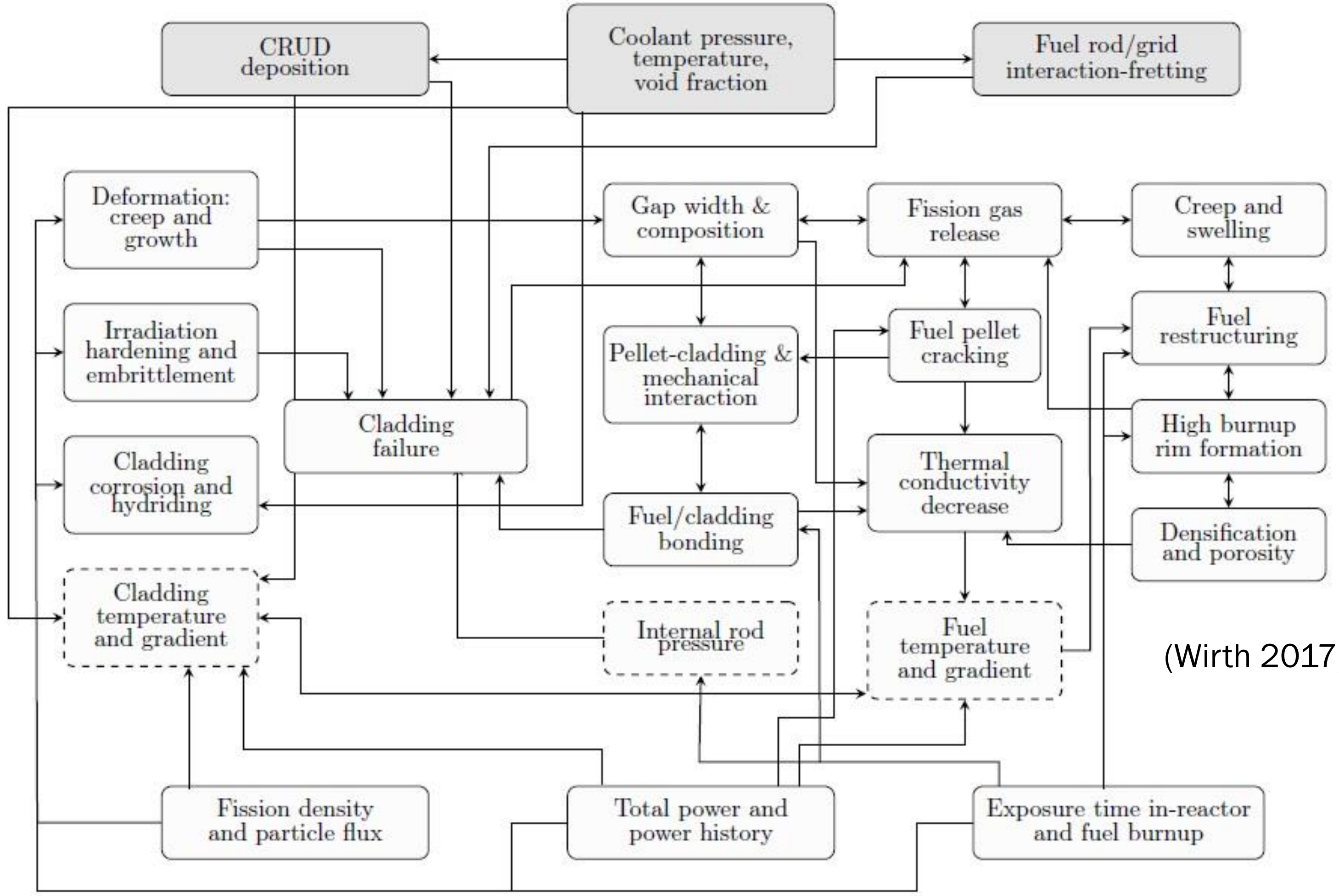
ε_z is constant, but not necessarily zero

- Development/use of FPCs
- Geometric domains represented
- Mathematical/numerical frame
- Validation
- Burnup analysis
- Thermal analysis
- Mechanical analysis
- **Material and behavioural models (e.g., Fission Gas Behaviour)**

Material and behavioural models

Material and behavioural models

- Complex phenomena, behavioural evolution and interactions to be incorporated in FPCs

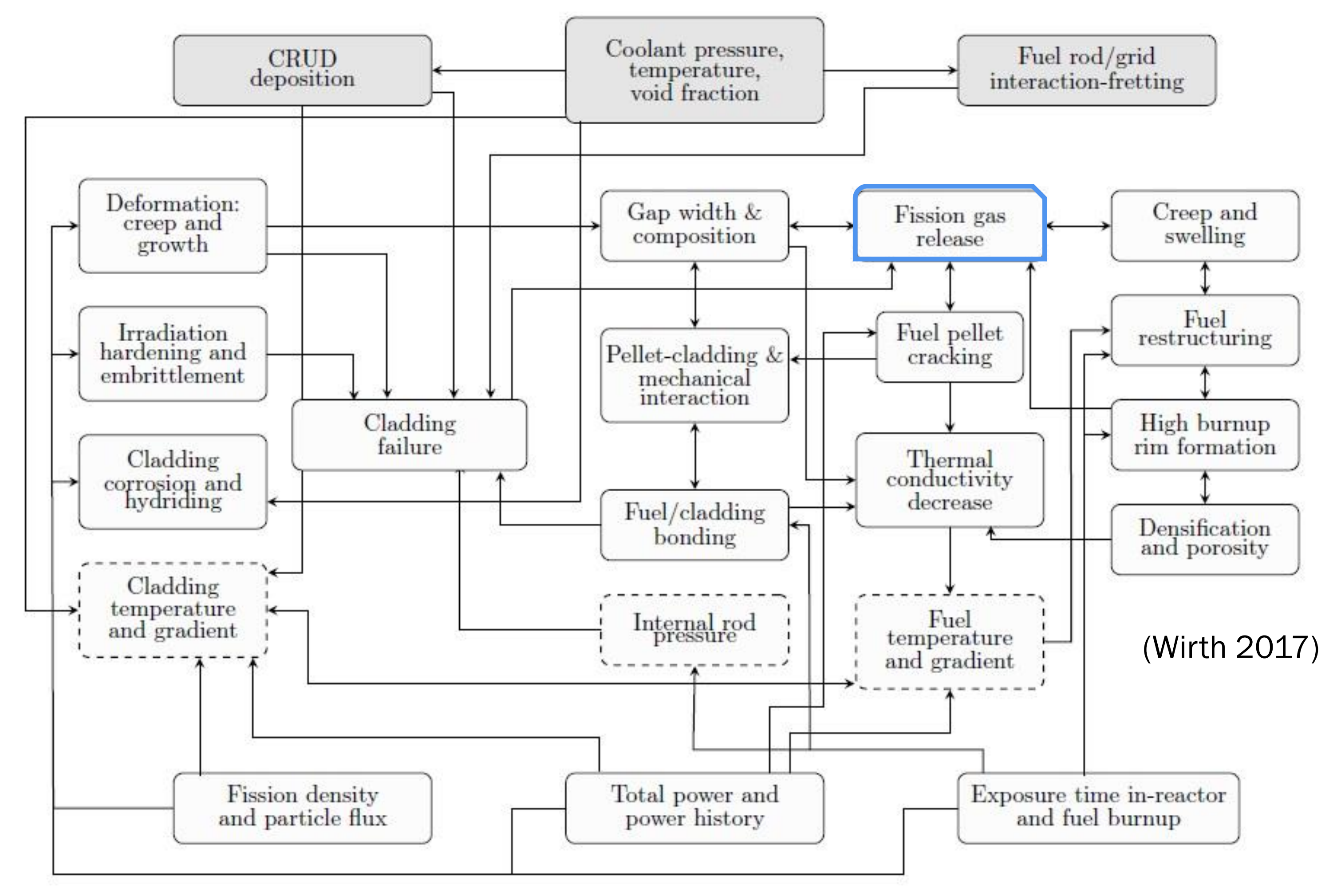


(Wirth 2017)

- **Traditionally, FPC modelling** employs continuum mechanics techniques at the macroscopic scale, where the molecular nature of the materials is usually ignored
- **From a correlation-based to a physics-based approach** (*possibly* according to a hierarchical **multi-scale modelling** for a better simulation of fuel pin behaviour under irradiation), *also* **supported by** uncertainty analysis (**UA**) **&** sensitivity analysis (**SA**)
- The models (at every single-scale level) have to be **computationally efficient** to allow for error propagation and quantification-margin-uncertainty analysis
- This will provide a more theoretical or *in silico*, and so less empirical, basis for fuel pin performance modelling, hence enabling **more generic application** to novel fuel designs, in particular in Gen-IV reactors

Fission Gas Behaviour (i)

- Just few notes on Fission Gas Behaviour (FGB) —> effects



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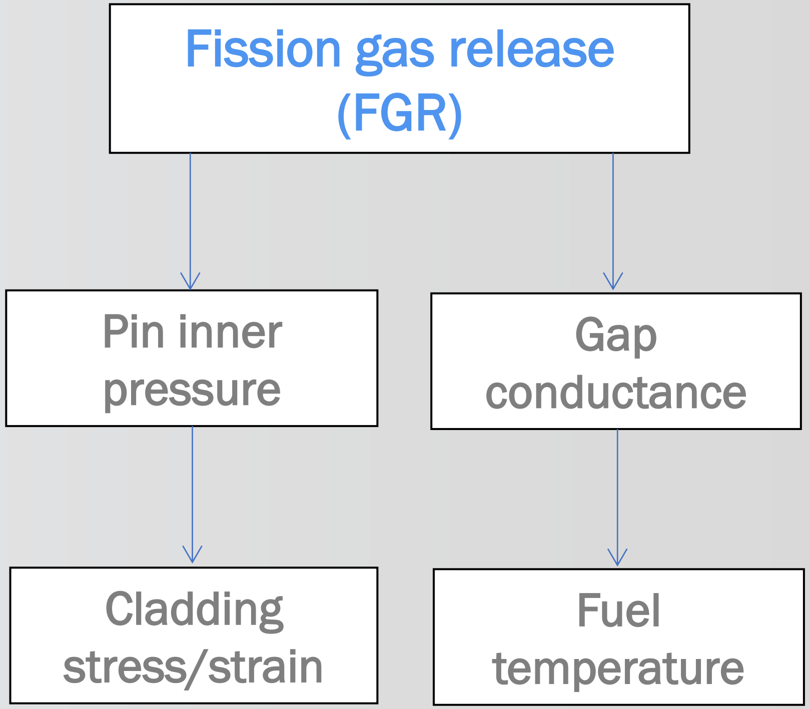


Fission gas release (FGR)

Pin inner pressure

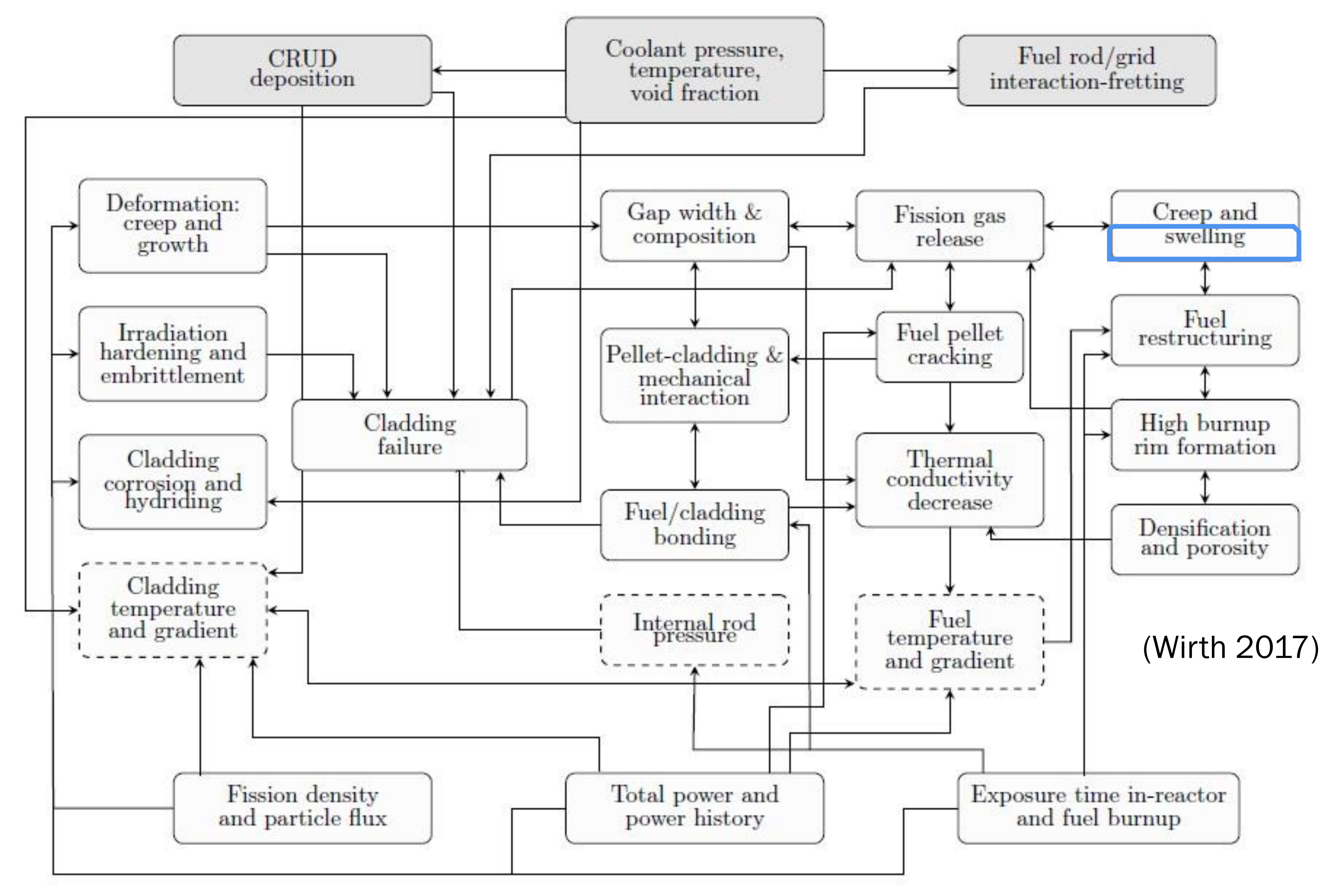
Gap conductance

Cladding stress/strain

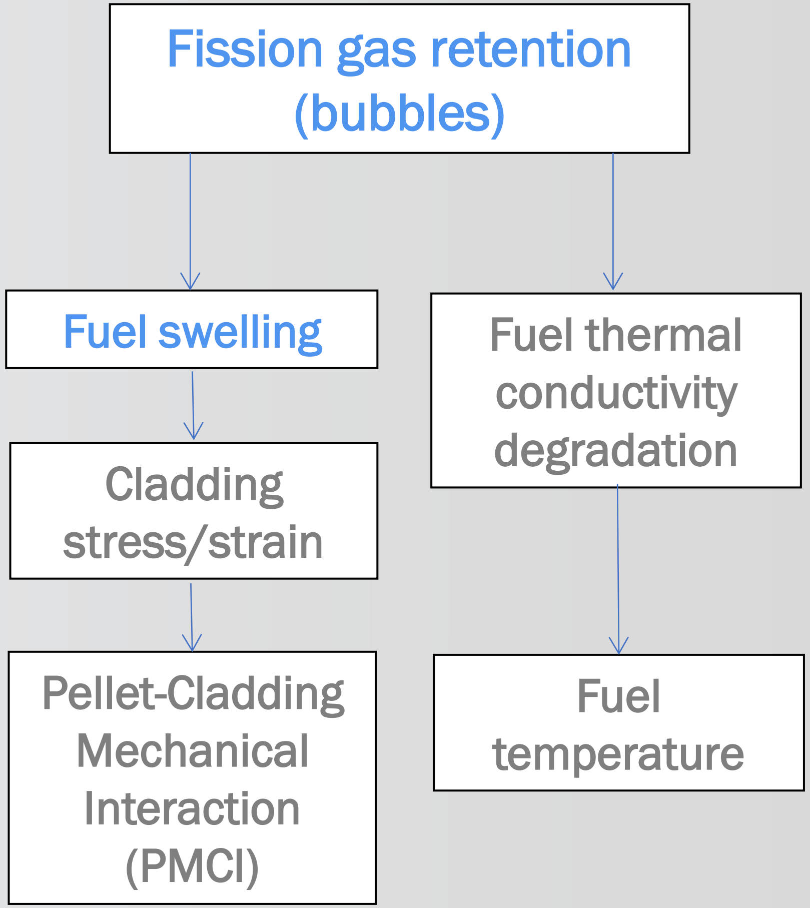
Fuel temperature

Fission Gas Behaviour (ii)

- Just few notes on Fission Gas Behaviour (FGB) —> effects



(Wirth 2017)



Fission gas retention (bubbles)

Fuel swelling

Fuel thermal conductivity degradation

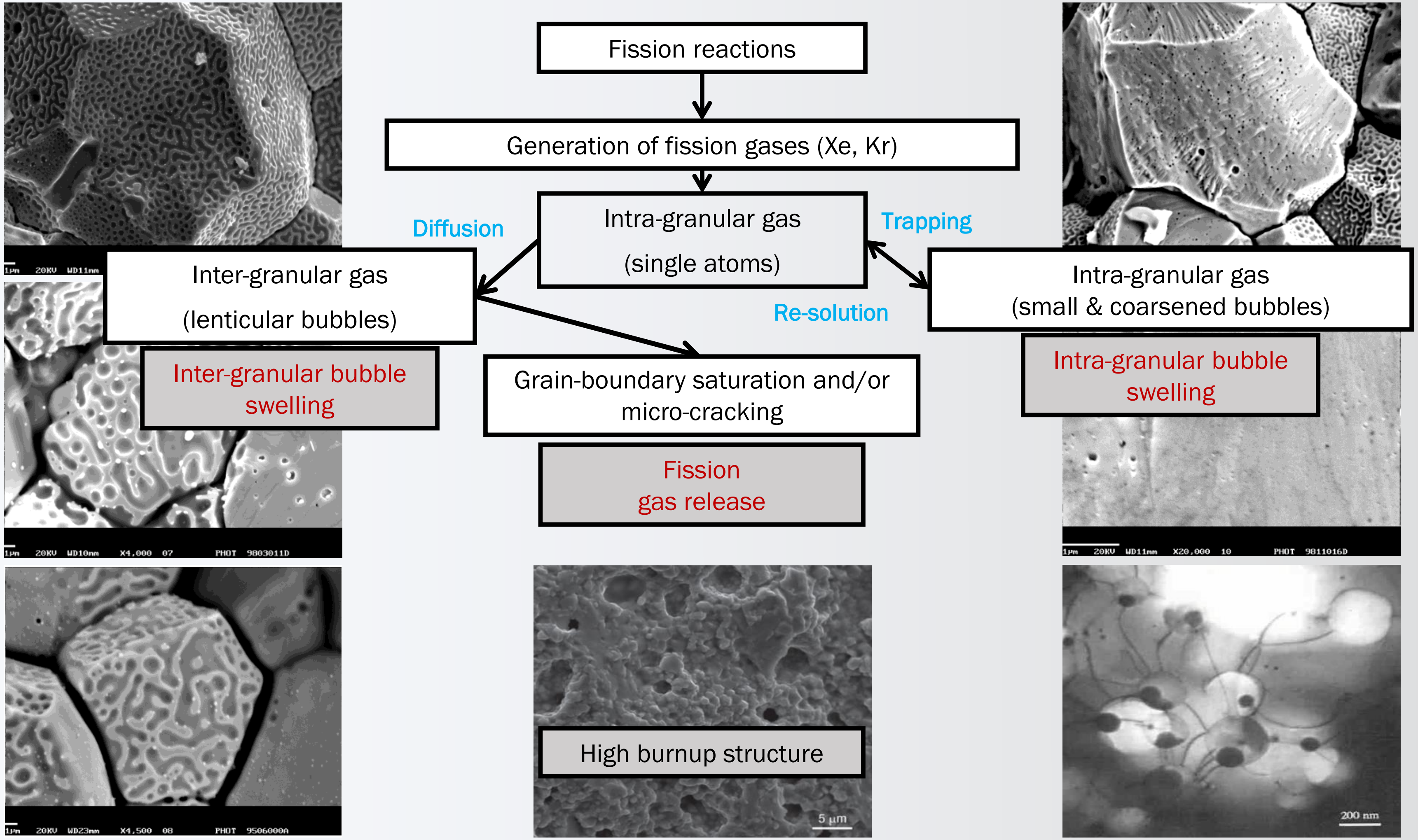
Cladding stress/strain

Pellet-Cladding Mechanical Interaction (PMCI)

Fuel temperature

Fission Gas Behaviour (iii)

- Given the impact on thermo-mechanical behavior, FGB needs to be considered …



Fission reactions

Generation of fission gases (Xe, Kr)

Intra-granular gas

(single atoms)

Diffusion

Trapping

Re-solution

Inter-granular gas

(lenticular bubbles)

Inter-granular bubble swelling

Intra-granular gas

(small & coarsened bubbles)

Intra-granular bubble swelling

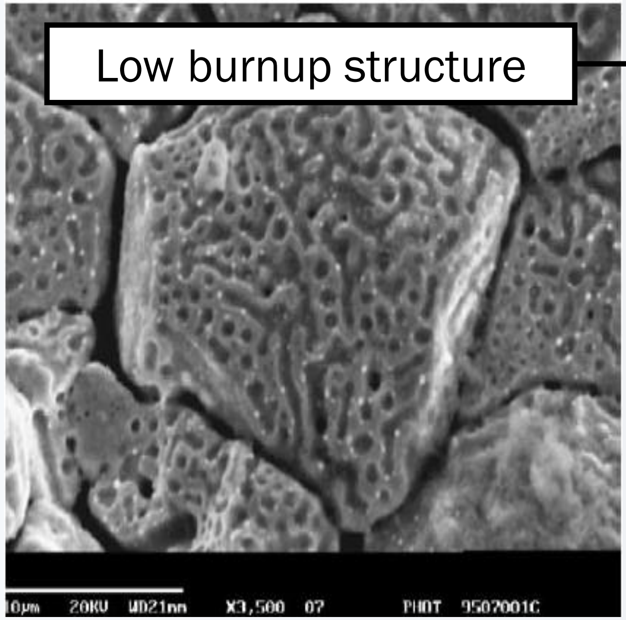
Grain-boundary saturation and/or micro-cracking

Fission gas release

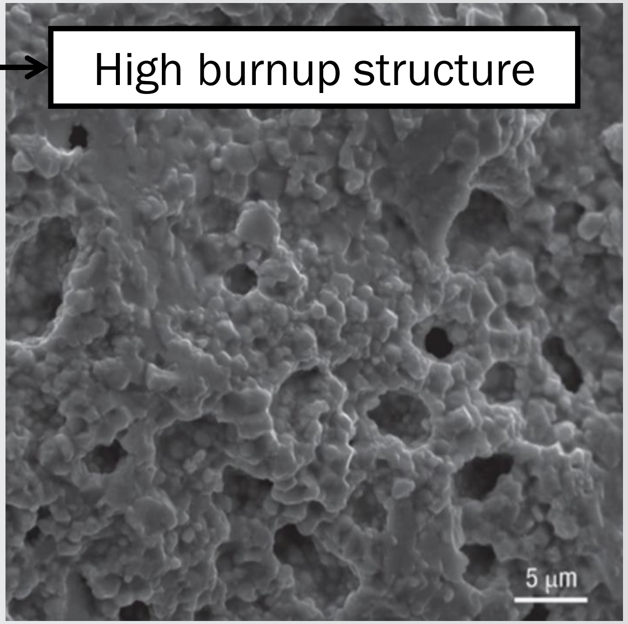
High burnup structure

Fission Gas Behaviour (iv)

- Given the impact on thermo-mechanical behavior, FGB needs to be considered …


Low burnup structure

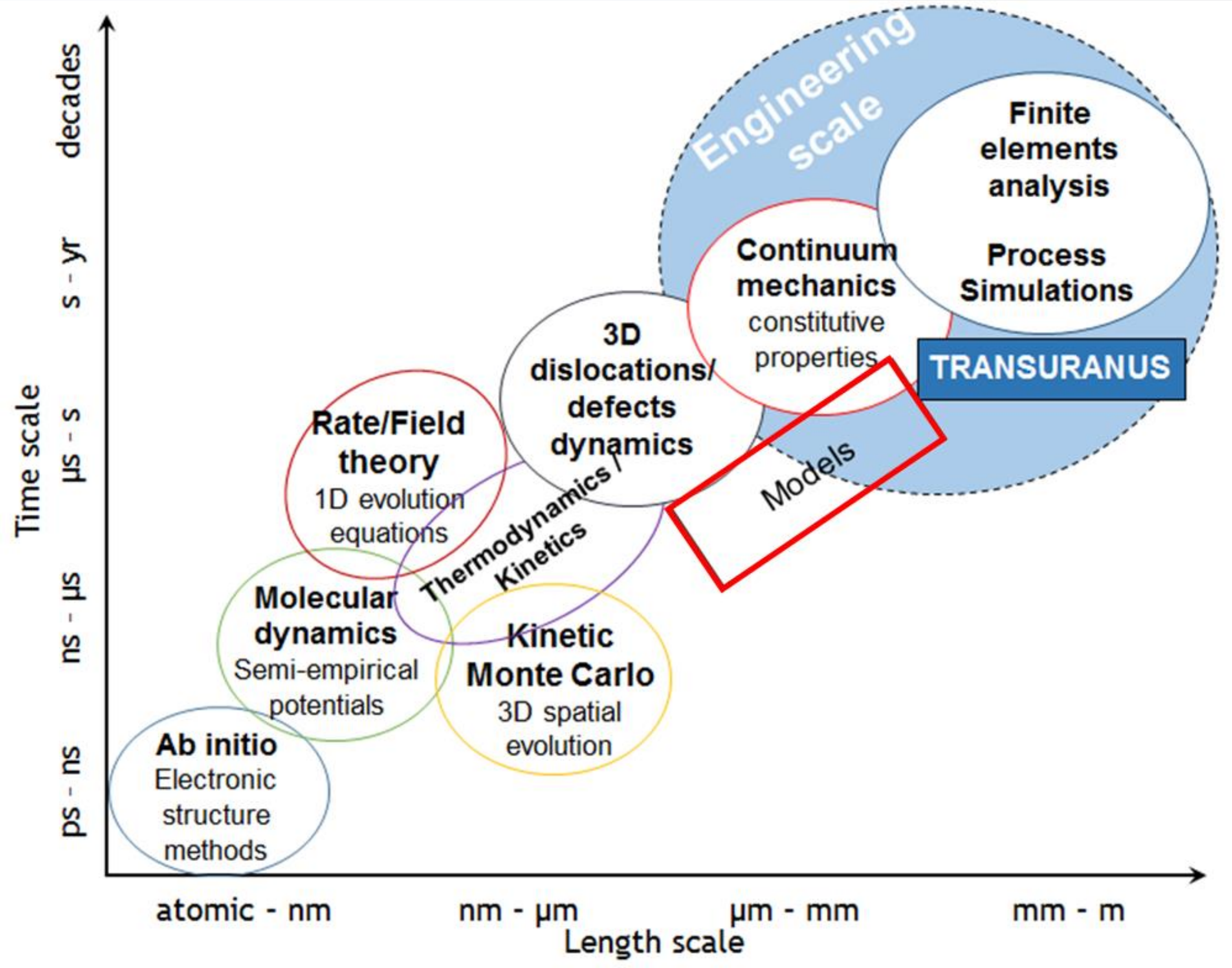
- Dislocation pile-up
- Grain recrystallization/ polygonisation
- Depletion of intra-granular fission gas
- Development of novel porosity


High burnup structure

- **High Burnup Structure (HBS)** formation leads to localized contribution to fission gas swelling, which may be significant during (accidental) transients
- Novel porosity affecting the thermo-mechanical properties of the fuel
- In fast reactor (U,Pu)O_2 fuel, many other phenomena (higher *T* and *gradT*)

Fission Gas Behaviour (v)

- Given the impact on thermo-mechanical behavior, FGB needs to be considered …



… according to a *suitable* multi-scale fuel performance modelling approach !