Nuclear Fuel Performance

NE-533

Spring 2025

Notes

- Wellness day on Tuesday 2/11
- No class
  - do something fun, take some time off, take care of yourself
- For events, activities, support:
  - https://wellness.ncsu.edu/wellness-day/

- Less fun news… paper project will be assigned next week
- Let me know if you prefer a specific topic area
- Reminder to make progress on your MOOSE project
- Exam on module 2 planned for Feb. 20

Last Time

- We developed analytical solutions for the stress in a pressurized cylinder with a thick wall
- Increases in temperature cause most materials to expand, which is a strain that doesn't inherently cause stress
- Thermal expansion can cause stress when
  - Deformation is constrained, there are gradients in the expansion coefficient, there is a temperature gradient
- We developed analytical equations for thermal stresses
  - in the cladding and in the fuel

NUMERICAL THERMO-MECHANICS

Now we can solve the temperature and the displacement vector for the full thermomechanical problem

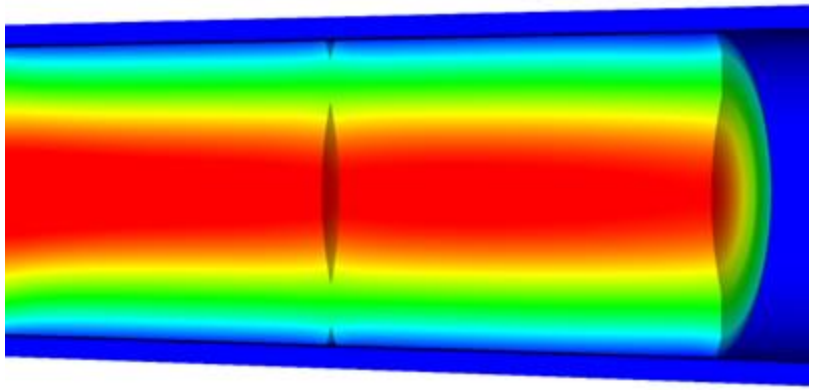
- T impacts the value of **u** through thermal expansion
- **u** impacts the value of T through changes in the thickness of the gap
- The value for T evolves with time
- The value for **u** also evolves with time, even though there is not time in its PDE

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

$$\boldsymbol{\sigma} = \boldsymbol{\mathcal{C}}(\boldsymbol{\epsilon} - \alpha(T - T_{fab})\mathbf{I})$$

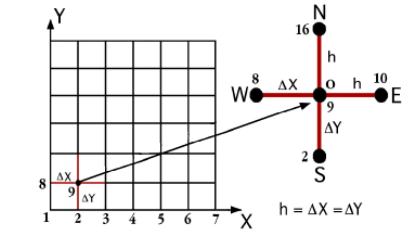
$$0 = \nabla \cdot \boldsymbol{\sigma}$$

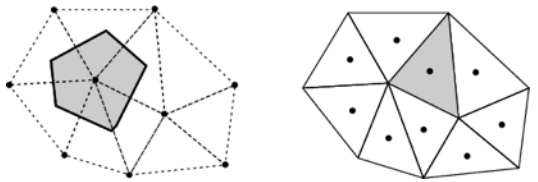
$$\boldsymbol{\epsilon} = \tfrac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)$$

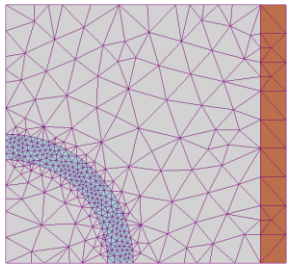


The primary tool for solving all thermomechanics problems is the finite element method

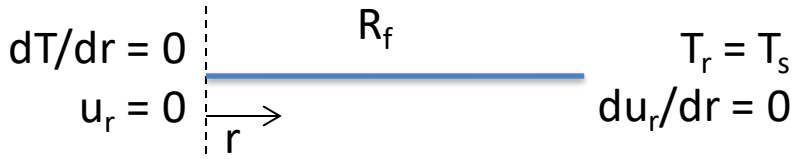
- **Finite difference**
  - Can solve the heat conduction equation
  - Can't easily solve the mechanics equations
- **Finite Volume**
  - Can solve the heat conduction equation
  - Can solve the mechanics equations
  - Eqns derived from fluid dynamics
- **Finite Element**
  - Can solve the heat conduction equation
  - Can solve the mechanics equations
  - Can handle any geometry
  - Can handle any boundary condition







The 1D thermomechanics problem definition

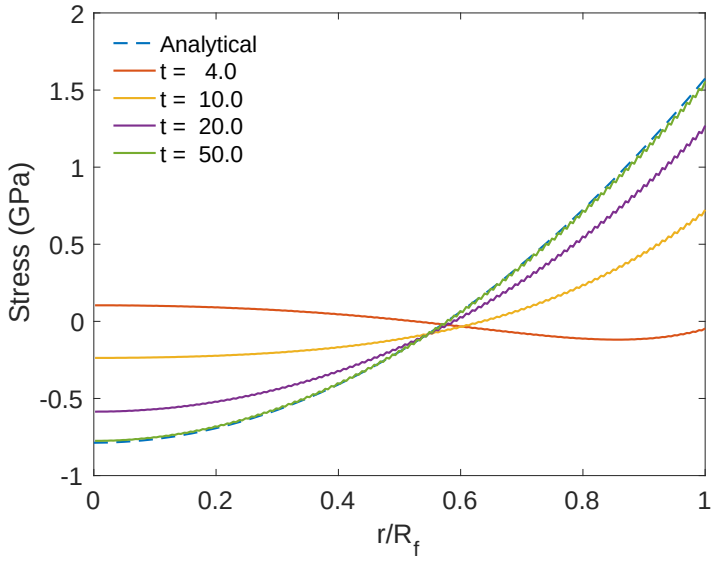


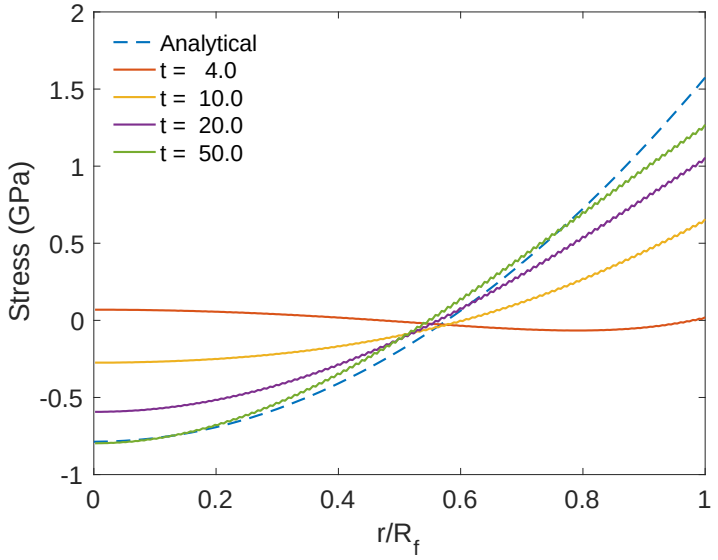
- The initial temperature is set to 273 K
- We will take 50 time steps of 0.5 s
- The full power of Q = 450 begins at time t = 0.
- UO_2 material properties are used for both the thermal and mechanics equations

Comparison to analytical theory

- If we use a constant thermal conductivity, analytical 1D model matches very well

- When k is a function of temperature, there is a difference between the FEM and analytical stress





There are various available tools for solving coupled thermomechanical problems with FEM

- Commercial tools
  - ABAQUS
  - ANSYS
  - COMSOL
- Open source
  - MOOSE
- NRC-based
  - FRAPCON/FRAPTRAN

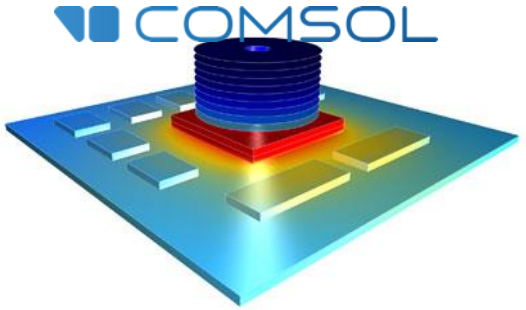
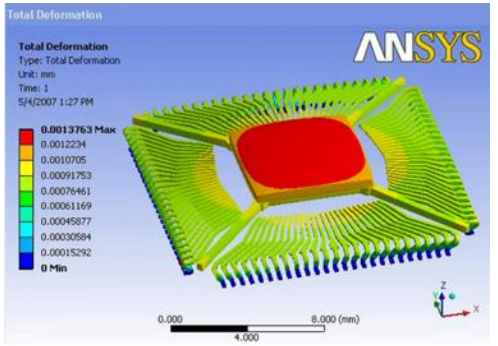


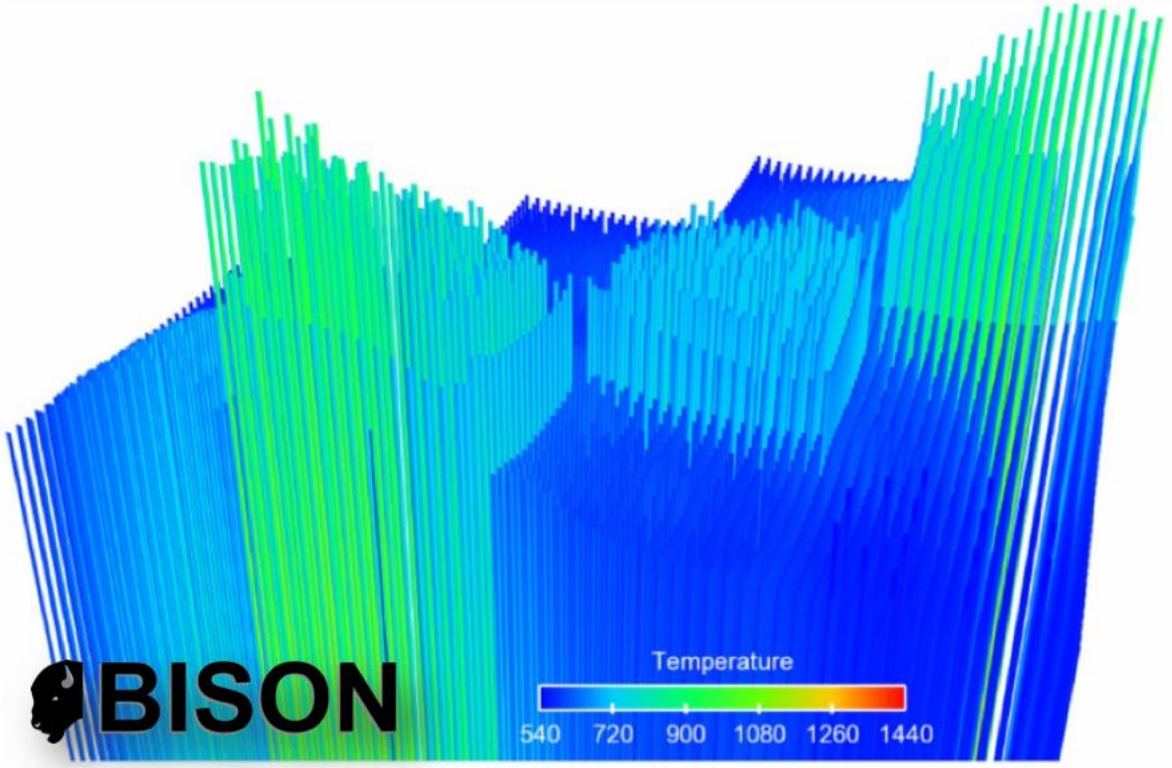
Figure 4. Temperature contour plot of exhaust manifold.

MOOSE



The purpose of a fuel performance code is to simulate and evaluate fuel rod behavior

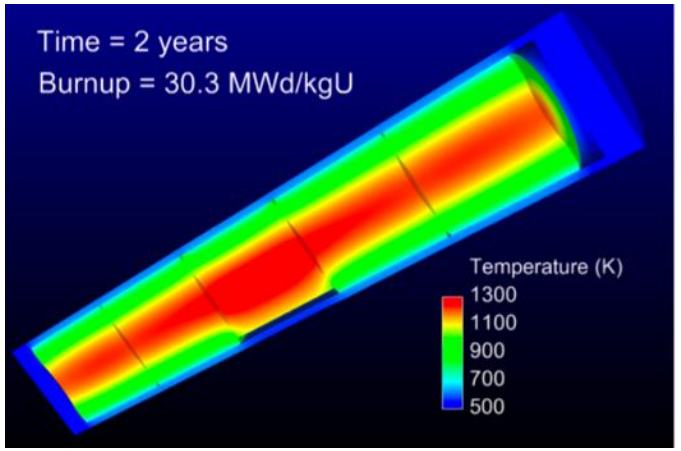
- The first fuel performance codes were developed in the mid seventies
- Advanced fuel performance codes are still under development today

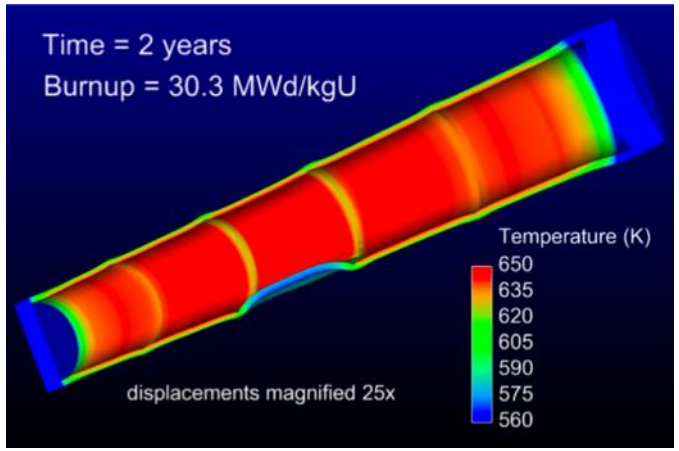


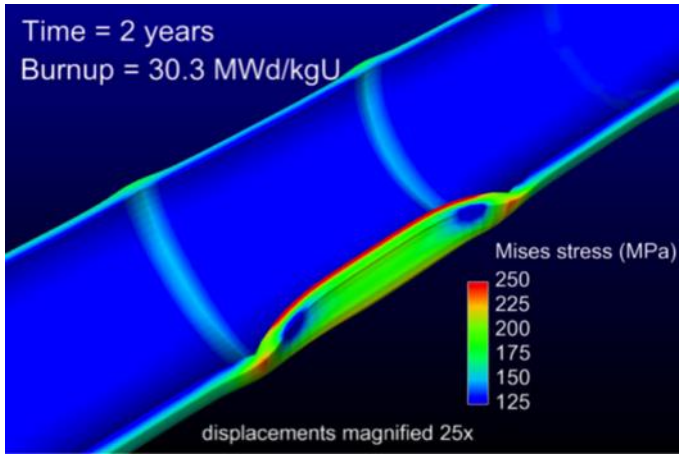
KAIST-3A benchmark results, showing displacement of 3432 rods, from Gaston et al. 2014

How are fuel performance codes used?

- The primary goals are to predict the fuel centerline temperature and the stress in the cladding
- Fuel performance codes aren't focused on predicting power production, but rather to predict safety margins, provide coupling to other codes



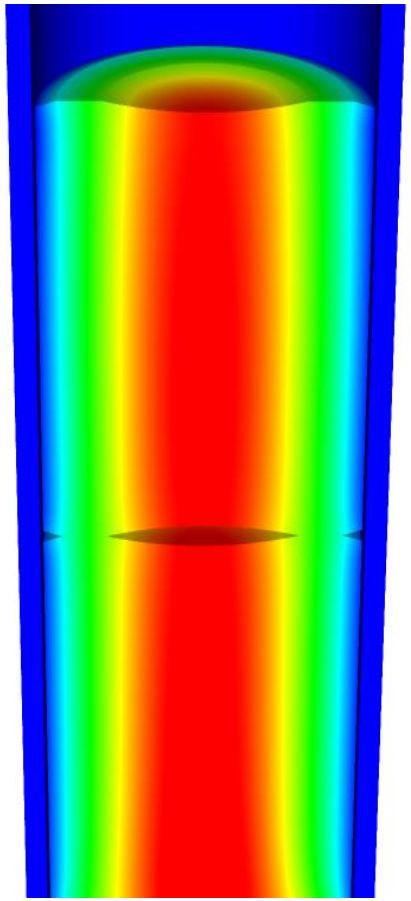




A fuel performance code must be able to predict:

Fuel
- Temperature profile
- Volumetric change

Cladding
- Temperature profile
- Stress



Gap
- Gap heat transport
- Mechanical interaction between fuel and cladding
- Gap pressure

The primary focus is solving the thermomechanical problem

Fuel

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved Numerically

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

Solved Numerically or analytically

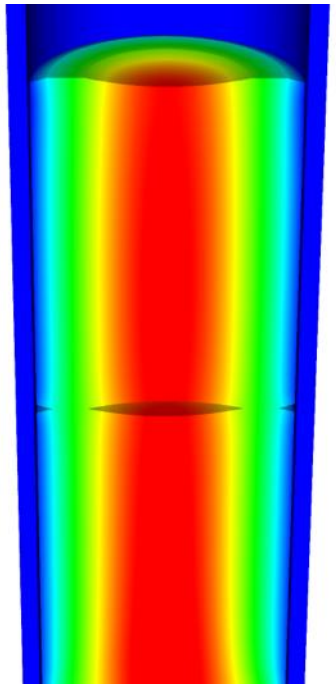
Cladding

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved Numerically or analytically

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

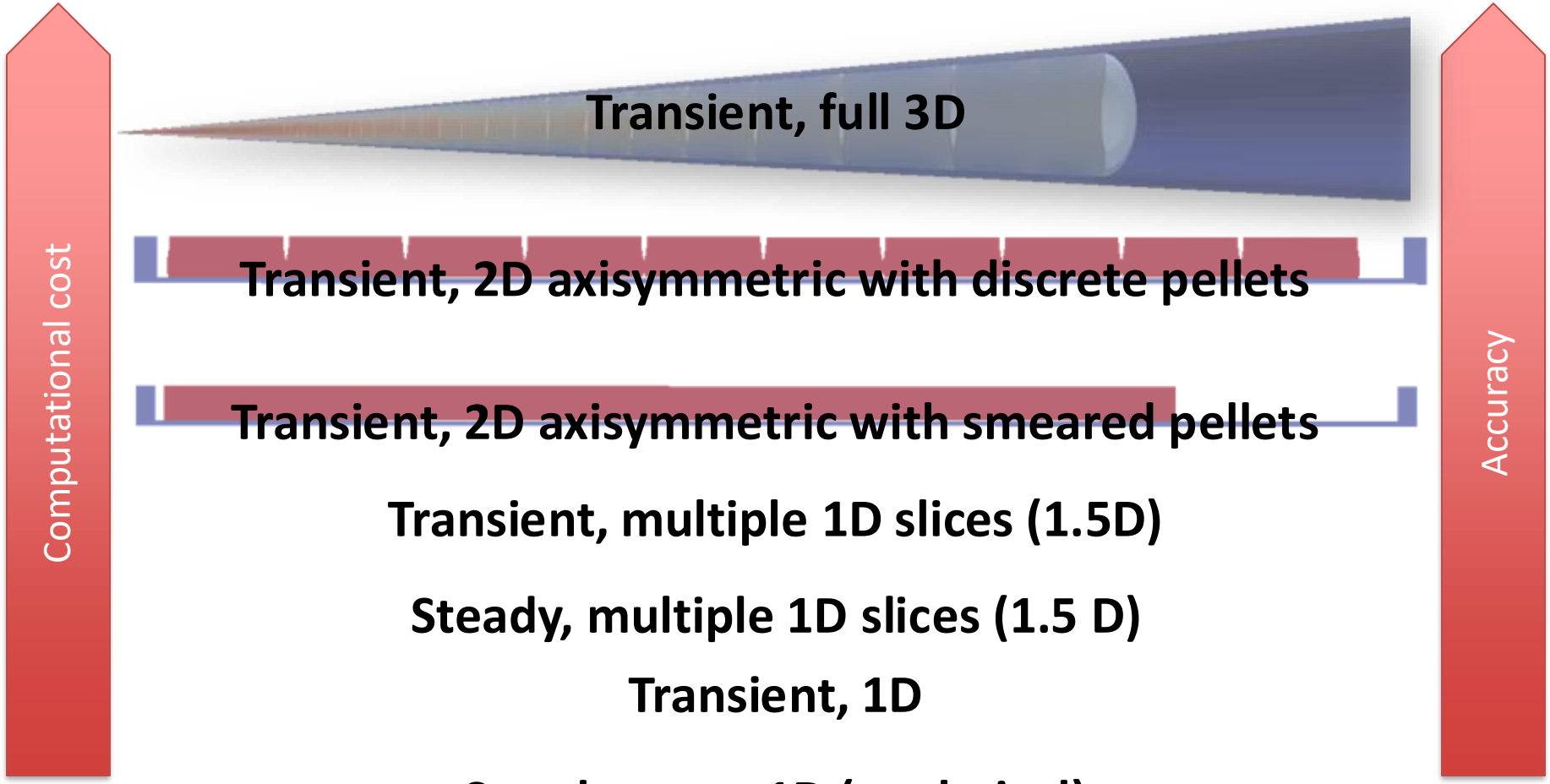
Solved Numerically



Gap

- The handling of the gap changes the most between different codes

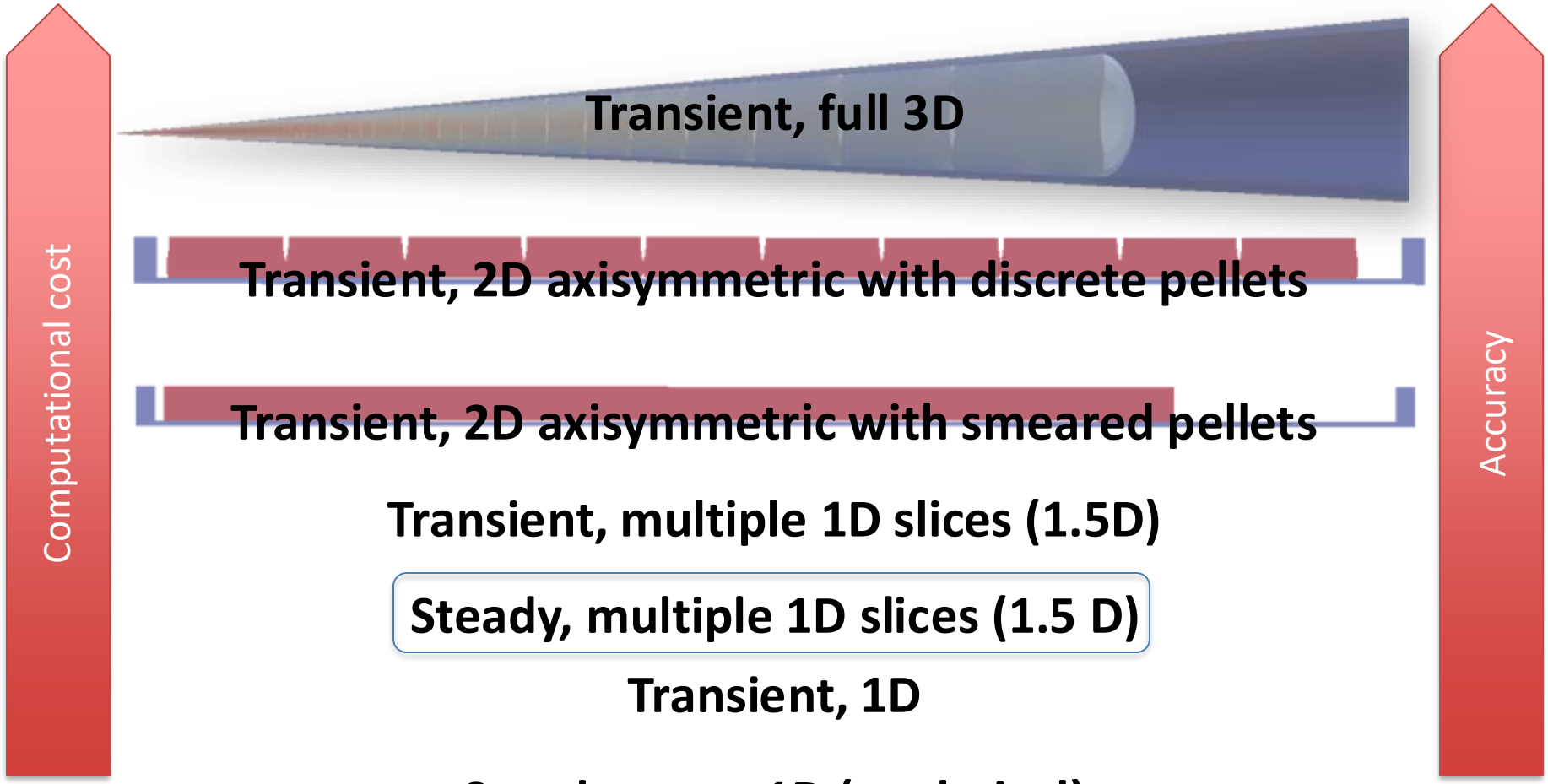
Various approaches to model the fuel rod



Early fuel performance codes were made for either steady state or transient operation

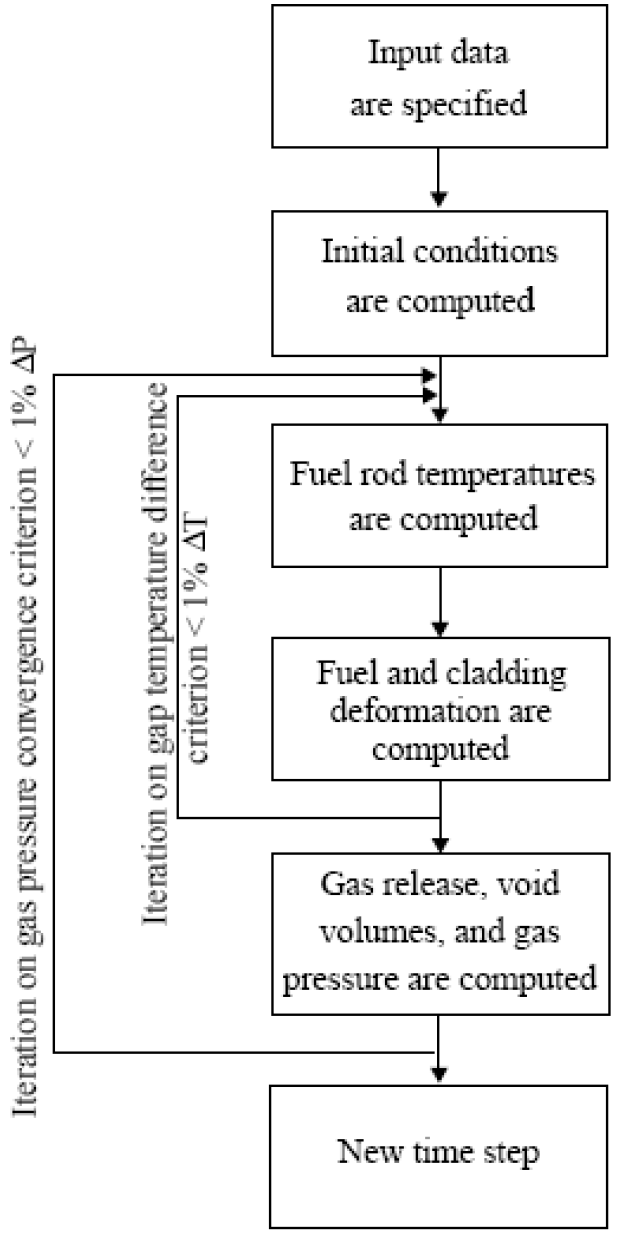
- Steady state codes
  - Leave off the time derivative part of the heat equation $\nabla \cdot (k \nabla T) + Q = 0$
  - The material properties still evolve with time as a function of burnup
  - The volumetric changes in the fuel are also a function of burnup
  - Creep of fuel and cladding change with time
- Transient codes
  - Include the time derivative $\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$
  - Have similar burnup dependent models like steady state codes, but don't include creep
  - Have additional models for rapid transients

Start with FRAPCON

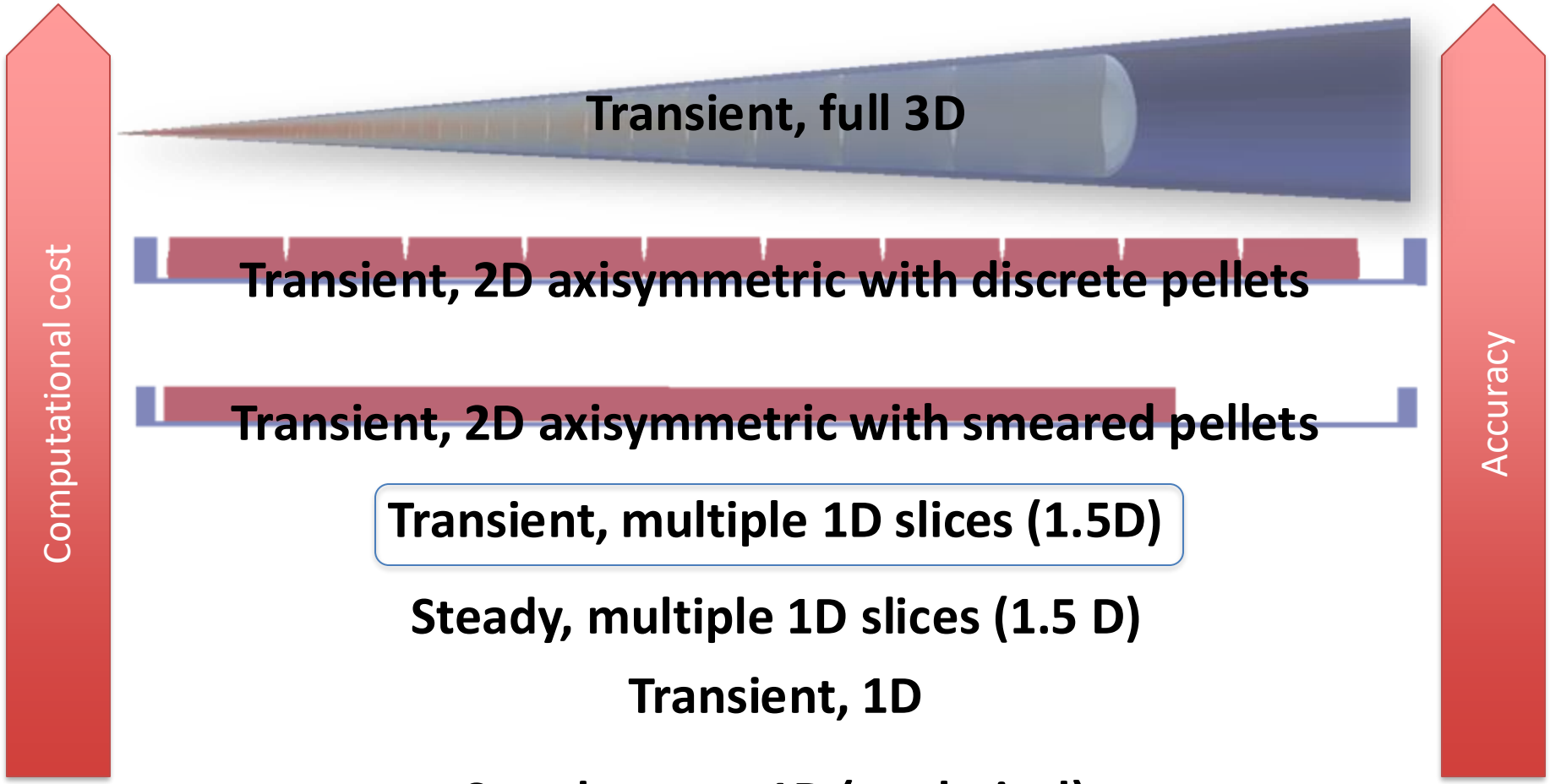


FRAPCON Flow Chart

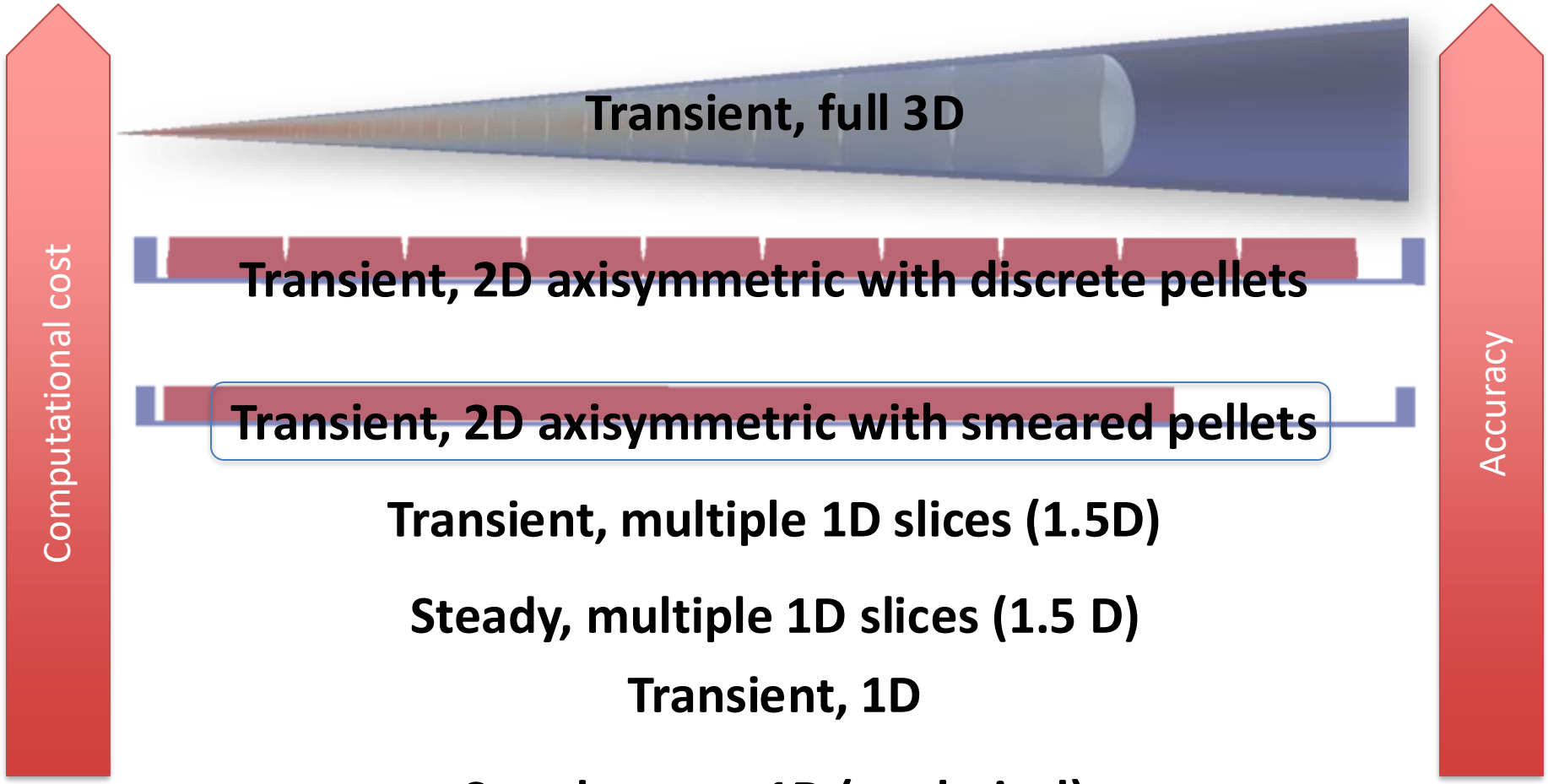
- FRAPCON is the NRC's steady-state fuel performance code
- FRAPCON has the ability to accurately calculate the high-burnup response of light-water reactor fuel rods
- FRAPCON iterates to determine fuel rod temperatures, fuel and cladding deformation
- This converged data is iterated to produce gas release, void volumes and plenum pressure
- Then marches forward in time



FRAPTRAN


Computational cost
Transient, full 3D
Transient, 2D axisymmetric with discrete pellets
Transient, 2D axisymmetric with smeared pellets
Transient, multiple 1D slices (1.5D)
Steady, multiple 1D slices (1.5 D)
Transient, 1D
Steady state, 1D (analytical)
Accuracy

FALCON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Transient, 2D axisymmetric with smeared pellets
Transient, multiple 1D slices (1.5D)
Steady, multiple 1D slices (1.5 D)
Transient, 1D
Steady state, 1D (analytical)
Accuracy

FALCON

- FALCON is a 2D fuel performance code developed by EPRI
- Development of FALCON started in 1996
- The beta version was released in 2003
- It was developed by ANATECH for EPRI
- FALCON is proprietary, owned by EPRI
- It is no longer under active development in the US

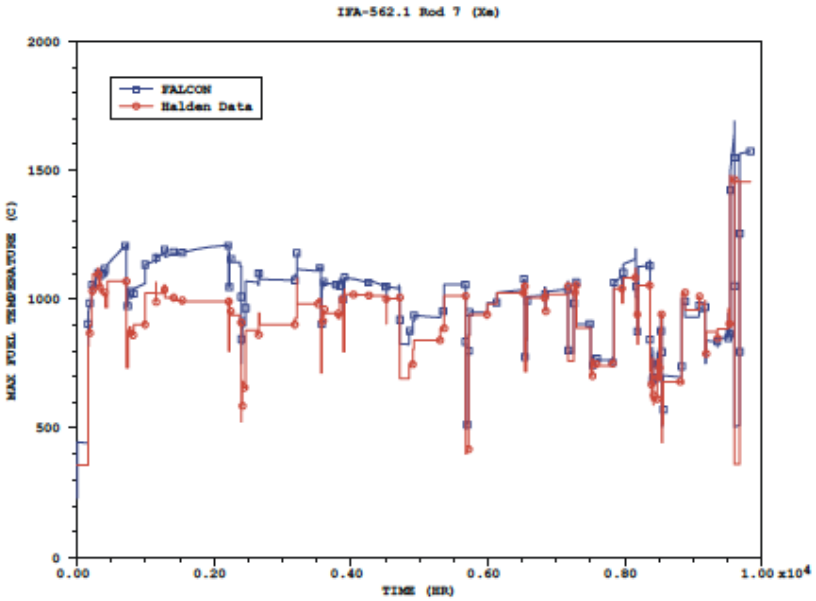


Figure 3-6
Calculated Fuel Temperatures Versus Measured Data for IFA-562.1 Rod 7 (Xe-filled)

FALCON is a 2D transient and steady state code

Fuel

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved with FEM

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

Solved with FEM

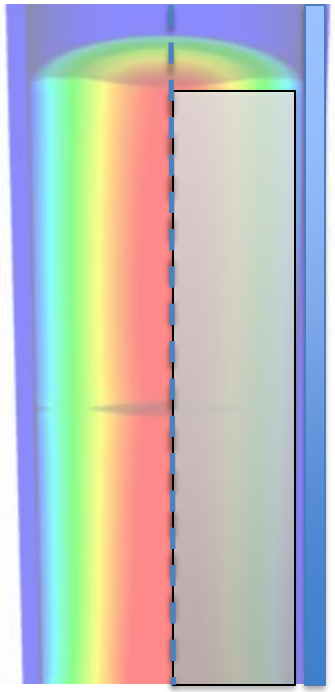
Cladding

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved with FEM

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

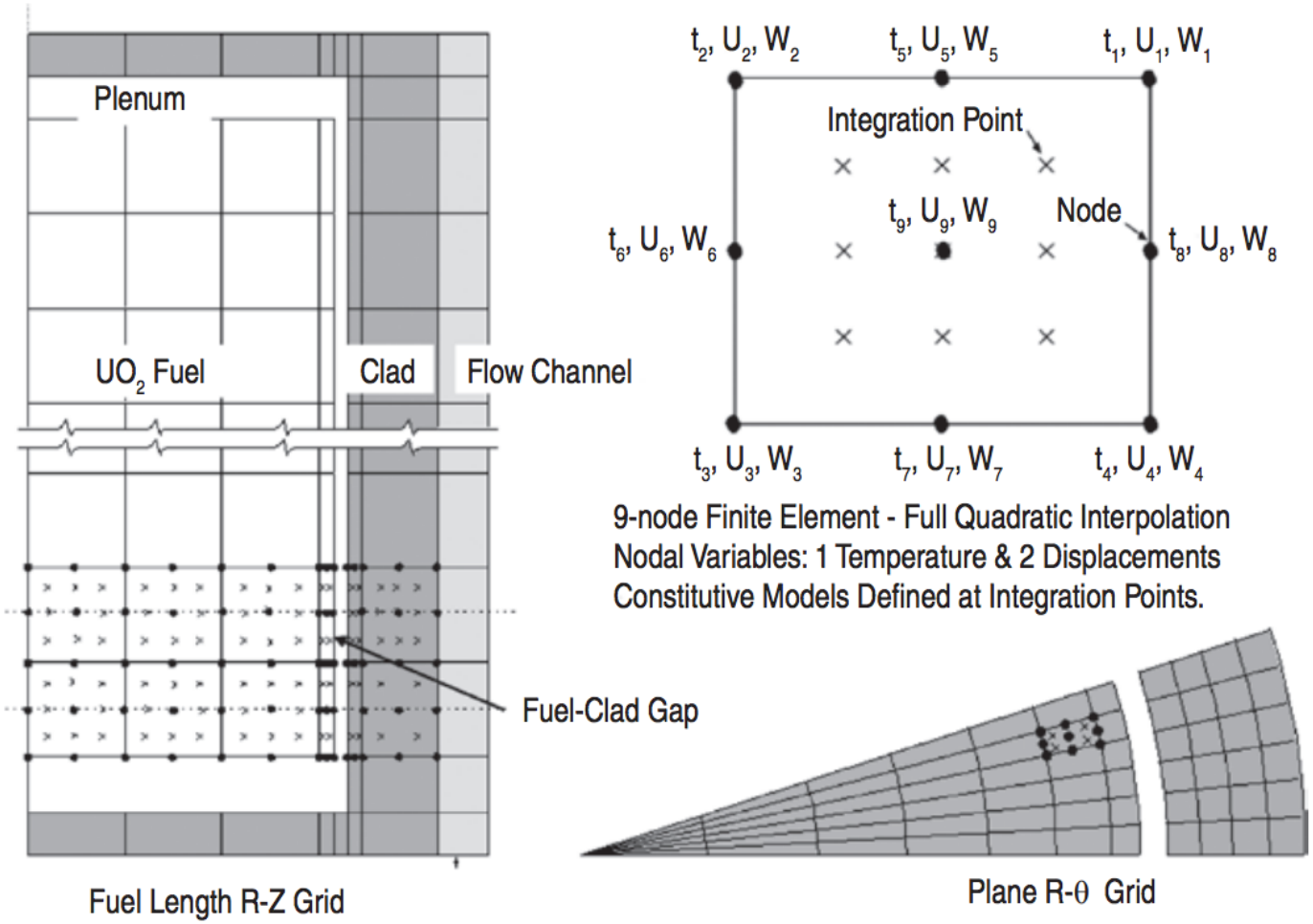
Solved with FEM



Gap

- Pressure is calculated using equation of state
- Simplified contact model is used for gap closure
- Gap heat transfer model is used

FALCON can predict the fuel performance in axisymmetric RZ space or in Rθ space



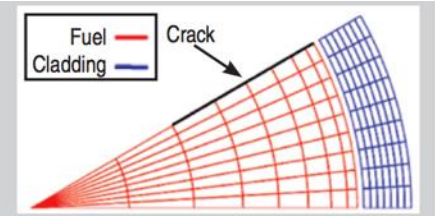


Figure 3. Standard PCI model.

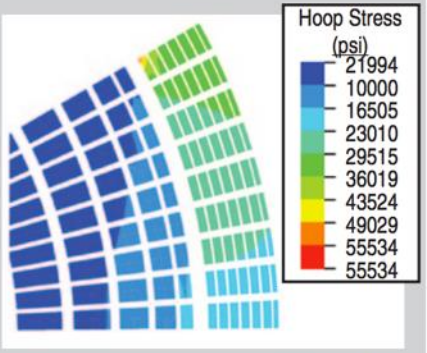


Figure 4. Calculated cladding hoop stress distribution (psi) using the standard PCI model.

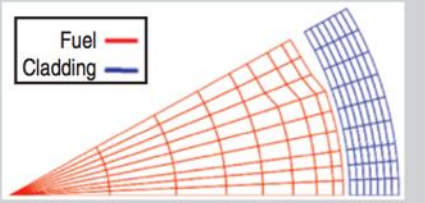
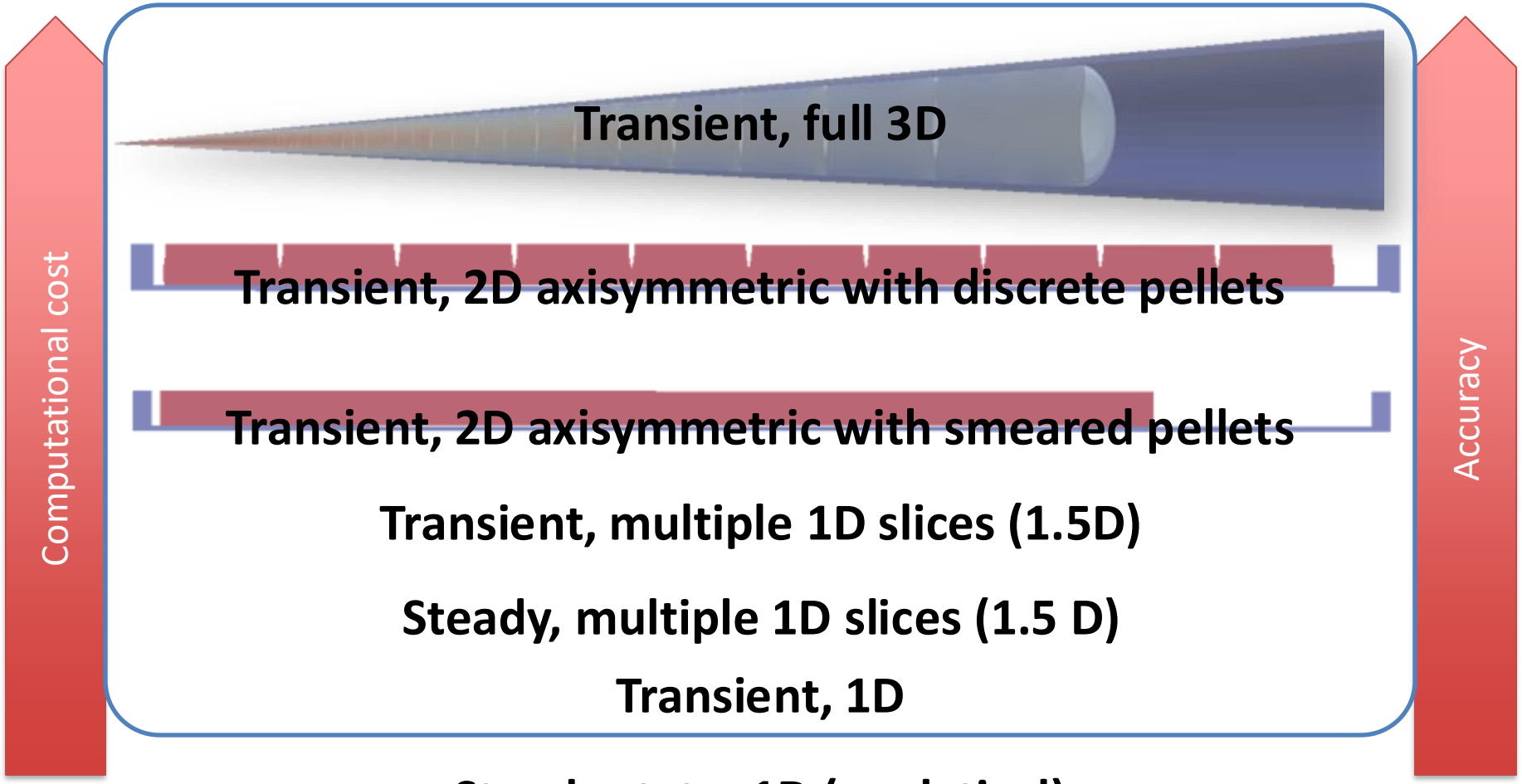


Figure 5. Missing pellet surface (MPS) PCI model.

BISON


Computational cost
Transient, full 3D
Transient, 2D axisymmetric with discrete pellets
Transient, 2D axisymmetric with smeared pellets
Transient, multiple 1D slices (1.5D)
Steady, multiple 1D slices (1.5 D)
Transient, 1D
Steady state, 1D (analytical)
Accuracy

BISON

- The next generation fuel performance code under development in the US
- It uses the MOOSE framework
- Development was begun in 2008
- The first paper using BISON was published in 2009 and the paper summarizing its full capabilities was published in 2012
- It was developed at Idaho National Laboratory, with some support by ANATECH
- BISON is available for free, but it is export controlled and requires a license agreement be signed

BISON models the fuel behavior ranging from 1D to full 3D and uses FEM

Fuel

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved with FEM

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

Solved with FEM

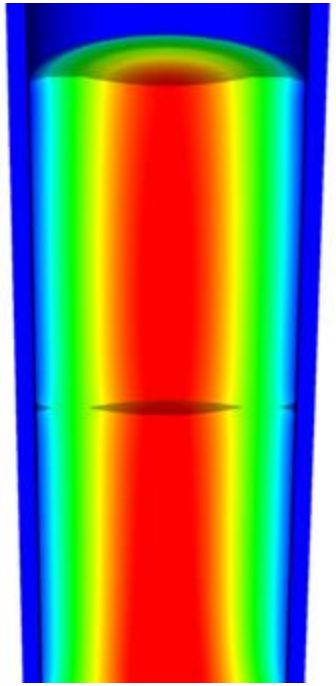
Cladding

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

Solved with FEM

$$0 = \nabla \cdot \boldsymbol{\sigma}$$

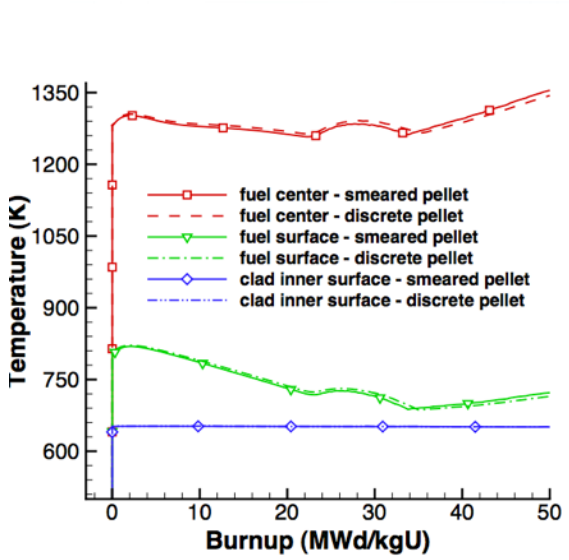
Solved with FEM

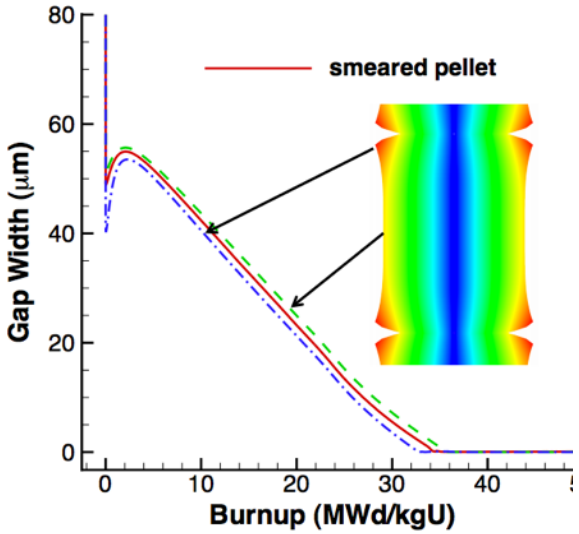


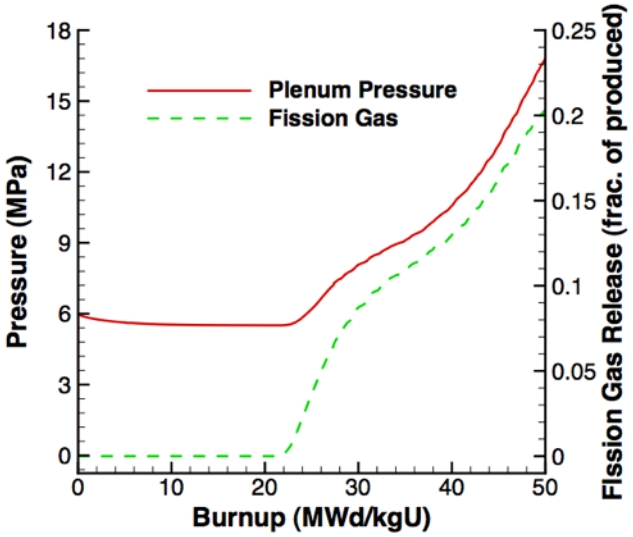
Gap

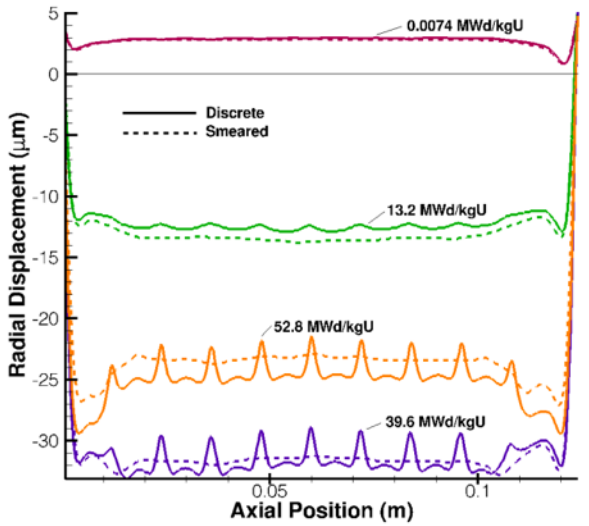
- Pressure is calculated using equation of state
- Fully implemented implicit contact algorithm
- Gap heat transfer model is used

Can handle smeared or discrete pellets, asymmetric pellet geometry and deformation

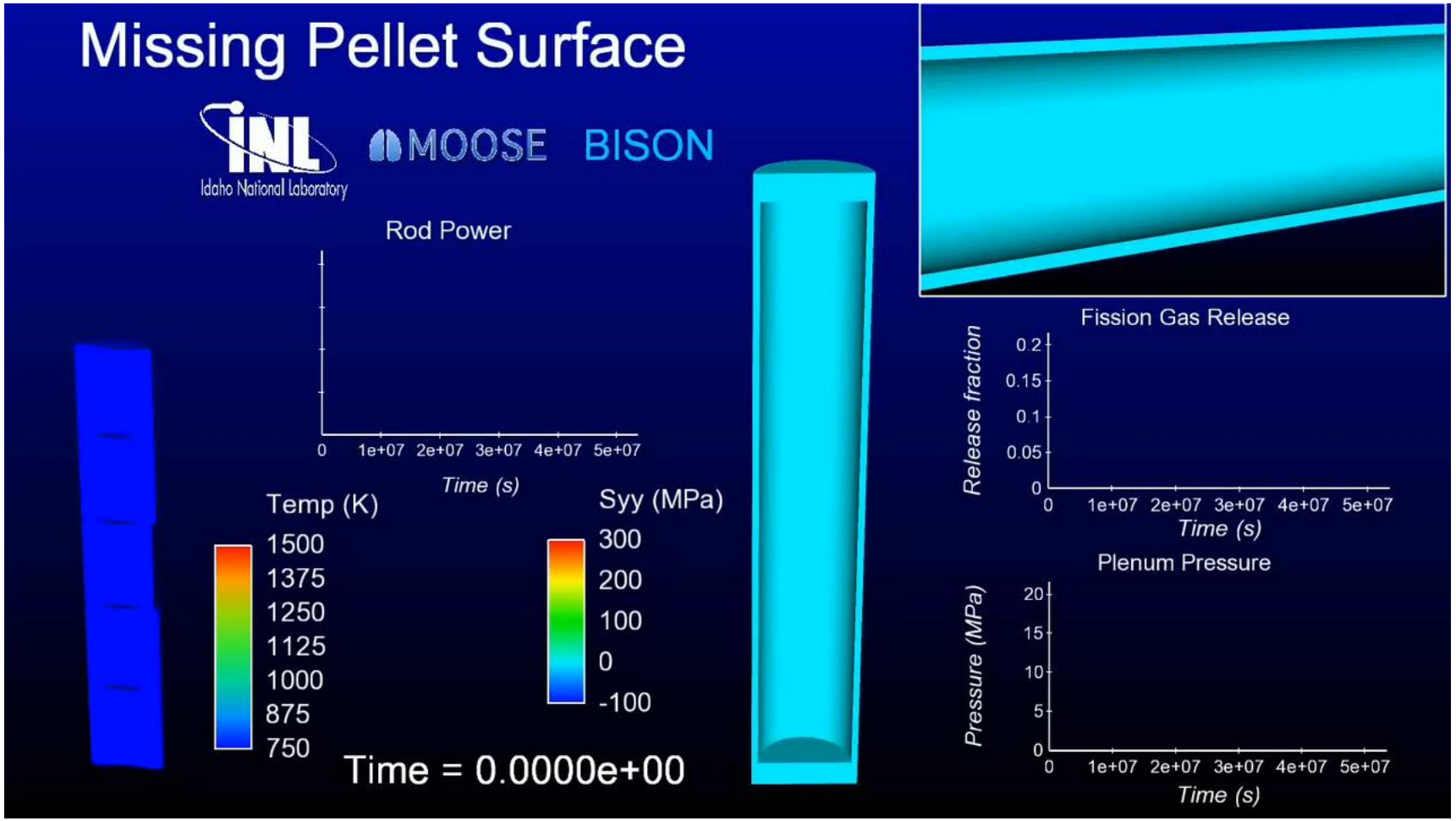








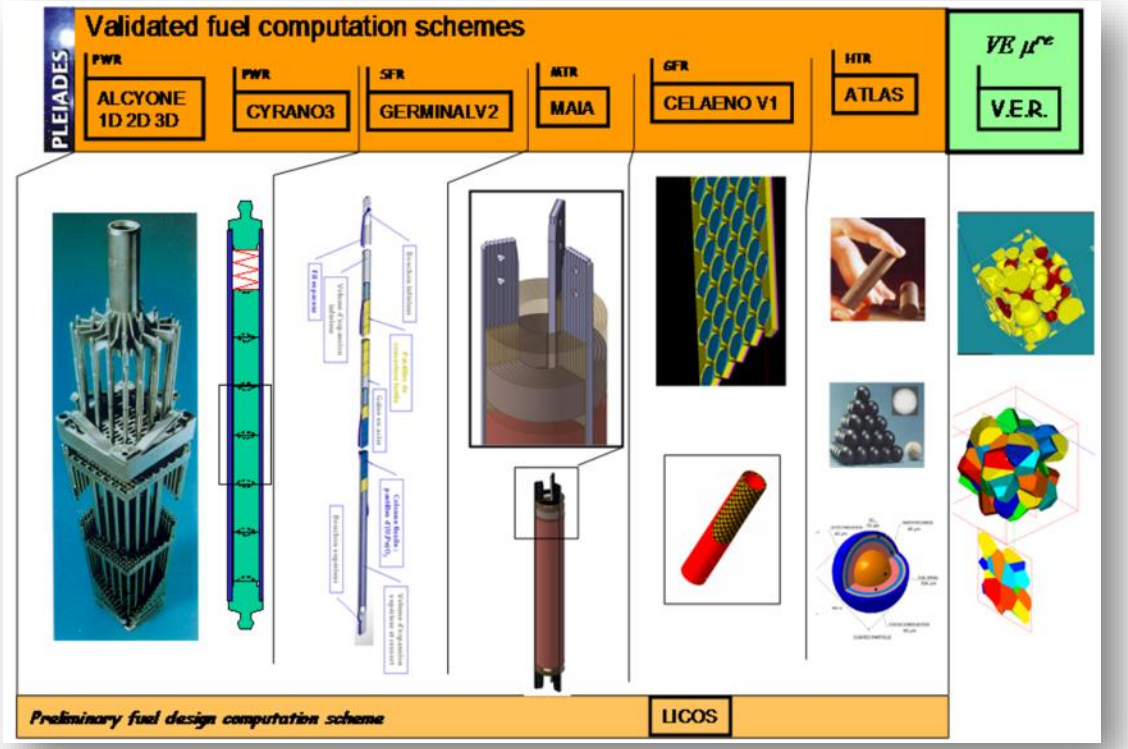
Because of its unique 3D capability, BISON can model truly 3D fuel performance problems



Other countries have other fuel performance codes

Table 1
List of fuel rod performance codes developed in different parts of the world for light water reactor fuel. More information is provided in Appendix: Overview of main fuel rod performance code developments across the globe.

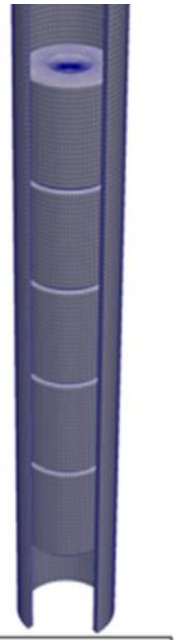
Country	Organization	Code name (precursor codes)
Argentina	CNEA	BACO, DIONISIO
Belgium	Belgonucleaire	COMETHE
	SCK-CEN	MACROS (ASFAD)
China	Xi'an Xiaotong Univeristy	FROBA
	CIAE	FTPAC
	NPIC	FUPAC
	CGNPC	JASMINE
Czech Republic	UJV	PIN-MICRO (GAPCON-THERMAL2)
France	CEA	ALCYONE (METEOR-TRANSURANUS)
	Framatome	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



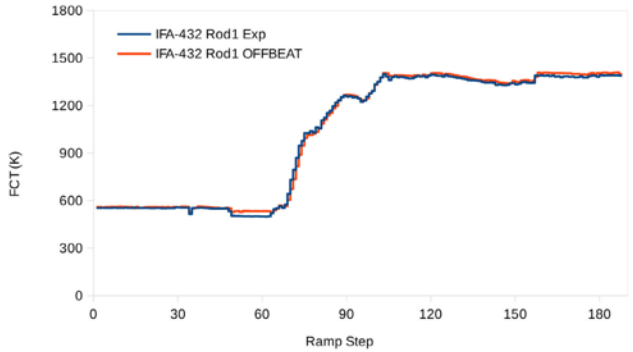
http://www.materials.cea.fr/en/PDF/PLEIADES-Platform.pdf

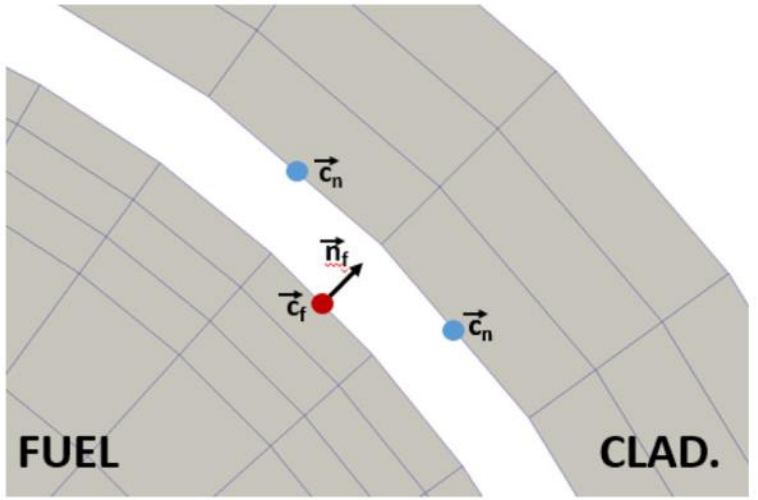
OFFBEAT – new(ish) tool

- The OpenFOAM Fuel BEhavior Analysis Tool (OFFBEAT) is a multi-dimensional fuel performance code developed in Switzerland
- The code can be used both for studying complex 2D or 3D local effects and for more traditional 1.5D base irradiation analyses
- OFFBEAT is based on the open-source C++ library OpenFOAM, thus the governing equations are discretized with modern finite volume techniques



3D Model



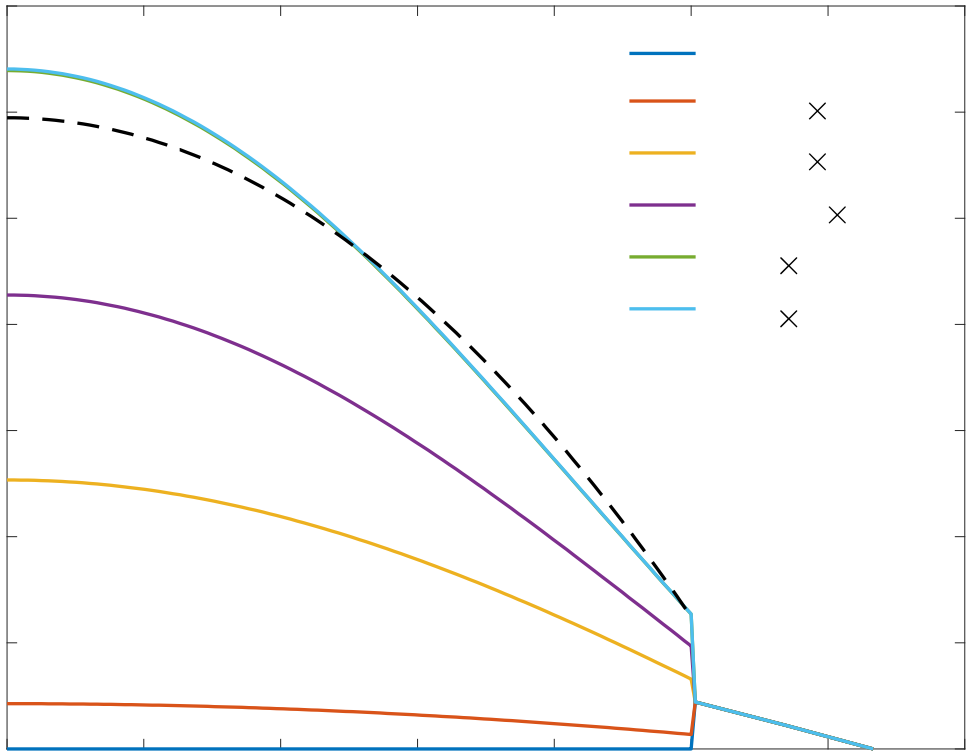


Summary

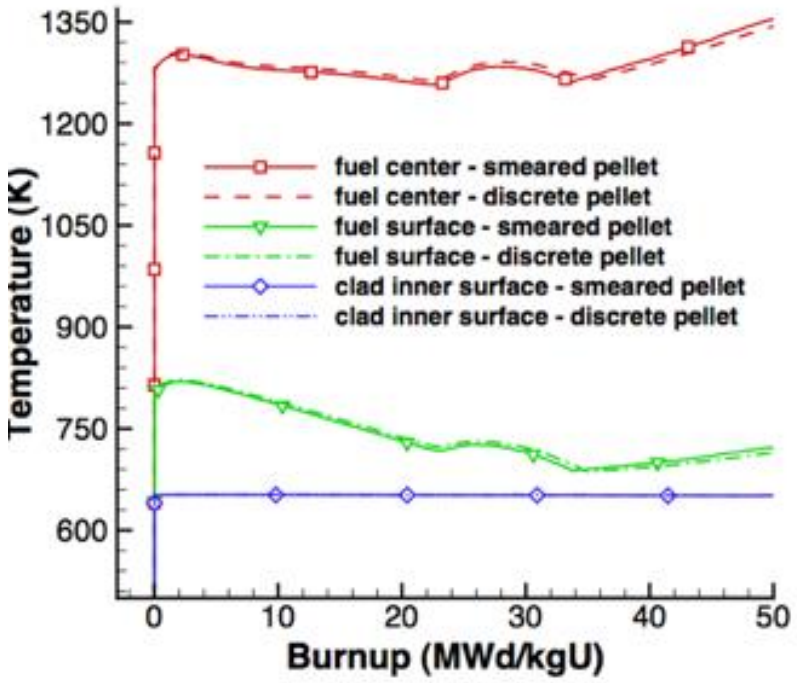
- Fuel performance codes are focused on predicting the center temperature of the pellet and the stress in the cladding
- All fuel performance codes
  - Numerically model the temperature in the fuel
  - Numerically model the stress in the cladding
  - Consider gap pressure, closure, and heat transfer
- The primary US codes are
  - FRAPCON – Steady state 1.5D, uses finite difference
  - FRAPTRAN – Transient 1.5D, uses finite difference
  - BISON – Steady or transient, 1D – 3D, uses finite element

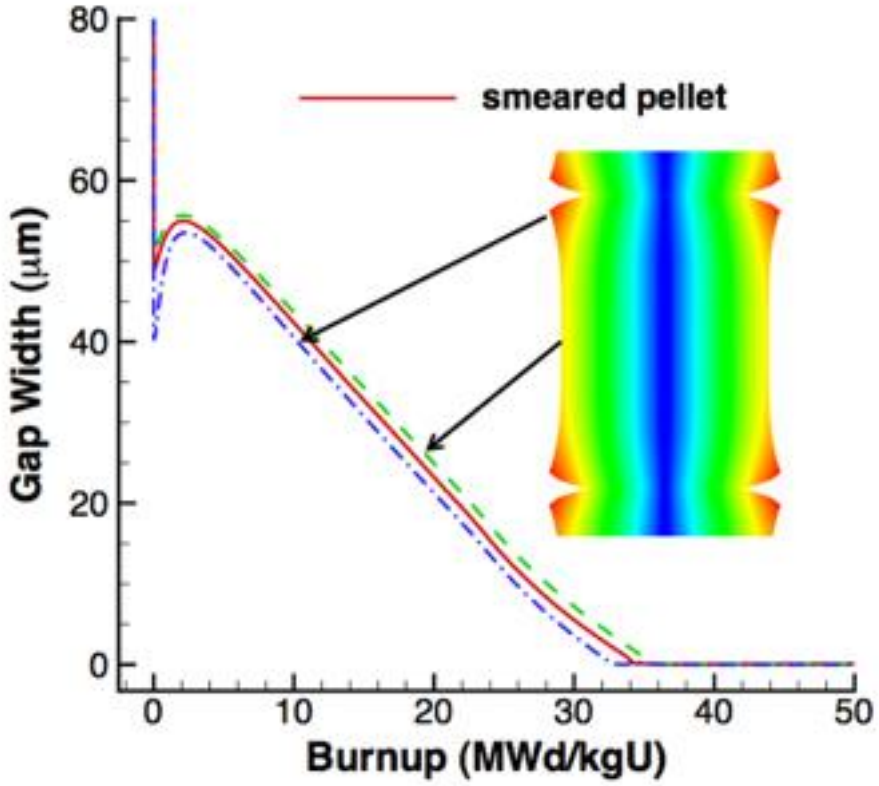
MATERIAL PROPERTY EVOLUTION

Pretty much everything we have learned so far, nothing changes once the fuel and cladding reach steady state



Fuel is dynamic!





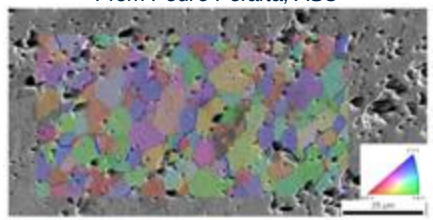
Property changes due to microstructure evolution during reactor operation must be considered

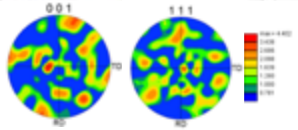
Insertion in reactor → Removal from reactor

Fuel Fabrication
- Sintered UO^2
- Height 2 cm
- Diameter 1 cm
- ~10 µm grain size
- Density > 95%

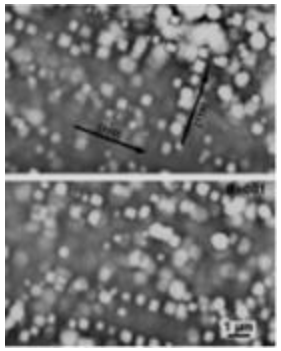
From Pedro Peralta, ASU

Early life
- Thermal expansion
- Fracture
- Point defect and fission gas generation
- Fuel Densification

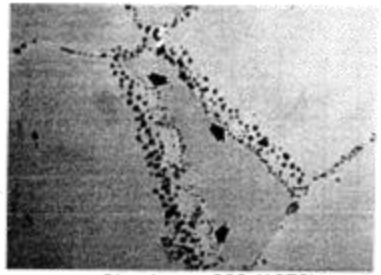




Mid Life
- Point defect diffusion
- Point defect clustering
- Fission gas segregation to GB and voids
- Bubble nucleation



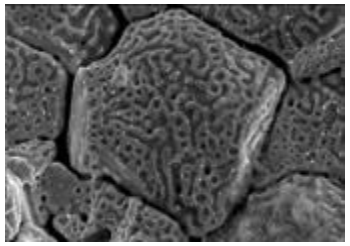
Zinkle and Singh 2000

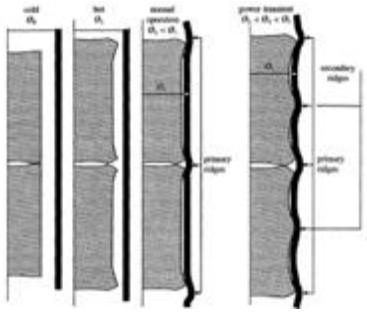


Olander, p. 323 (1978)

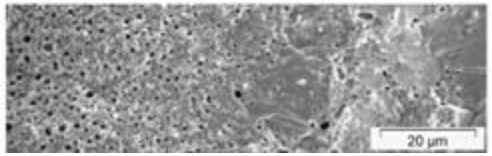
Late life
- Fission product swelling
- Bubble percolation and fission gas release
- Cladding creep
- Fuel creep

Brohan 2000

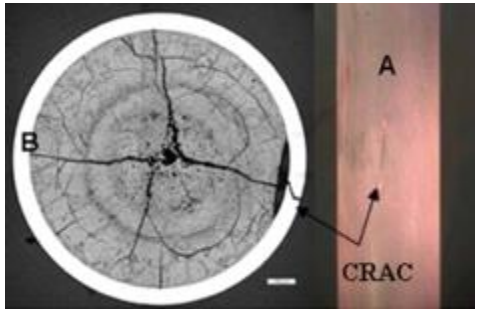




Fuel failure
- Pellet/cladding interaction
- Cladding corrosion
- Cladding fracture

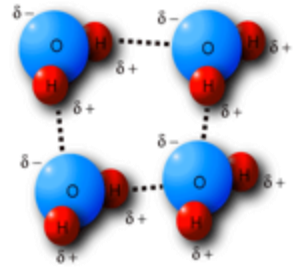


Santana et al. 2011

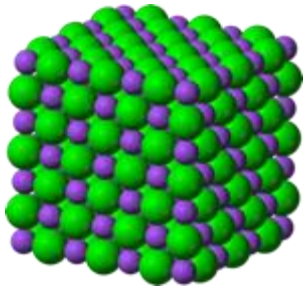


The properties and performance of a material are a result of factors across various length scales

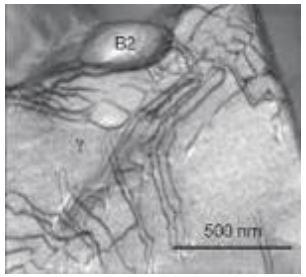
Chemical bonds



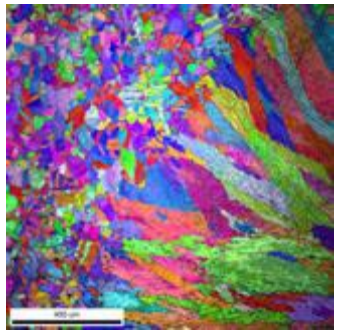
Crystal structure



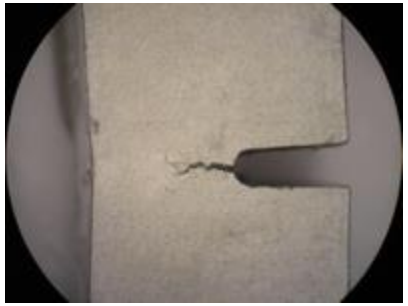
Defect interactions



Microstructure

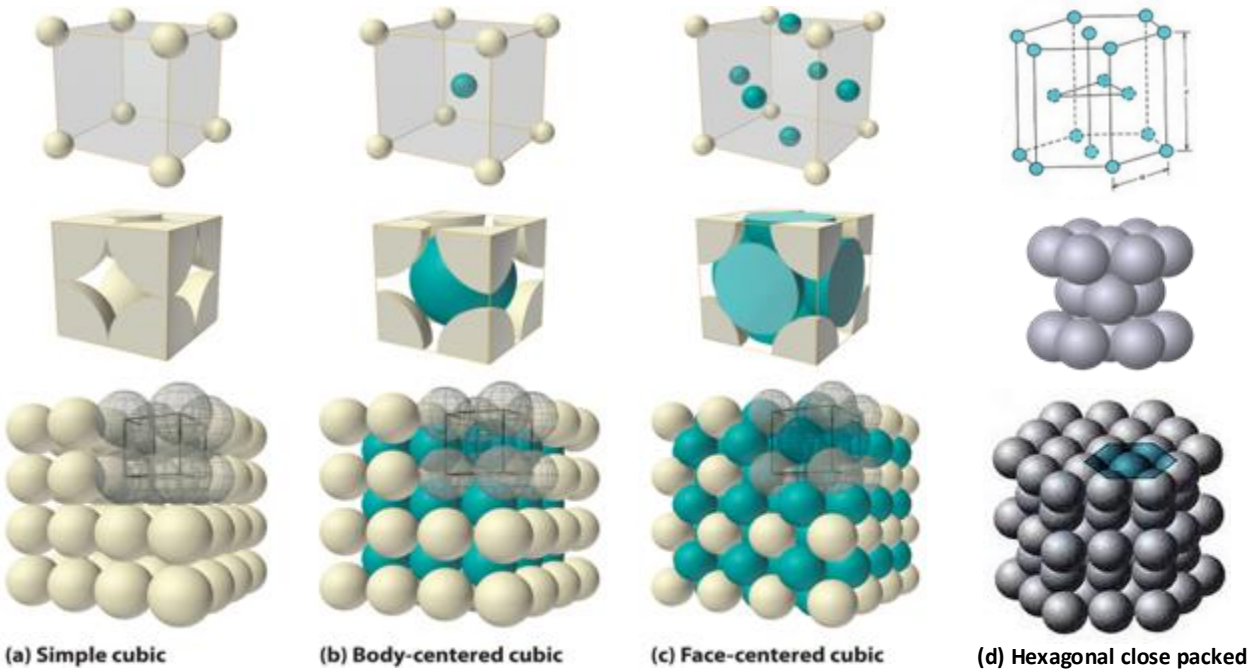


Material properties and performance



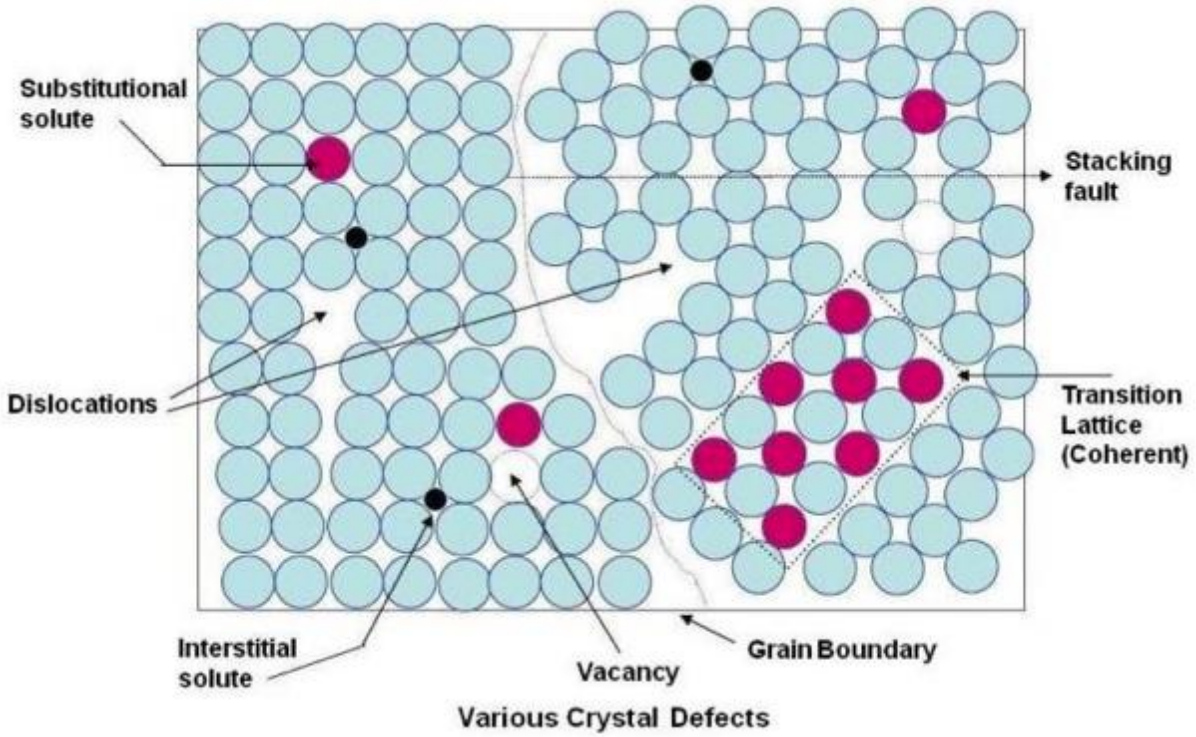
The crystal structure of a material is the shape of the ordered structure of the atoms

- The atoms of many materials form an organized lattice, these are called **crystalline materials.** All reactor materials are crystalline.
- The configuration of the atoms in the lattice impacts the properties of the material (density, thermal expansion coefficient, elastic modulus, etc.)
- All major light water nuclear materials are either cubic or hexagonal



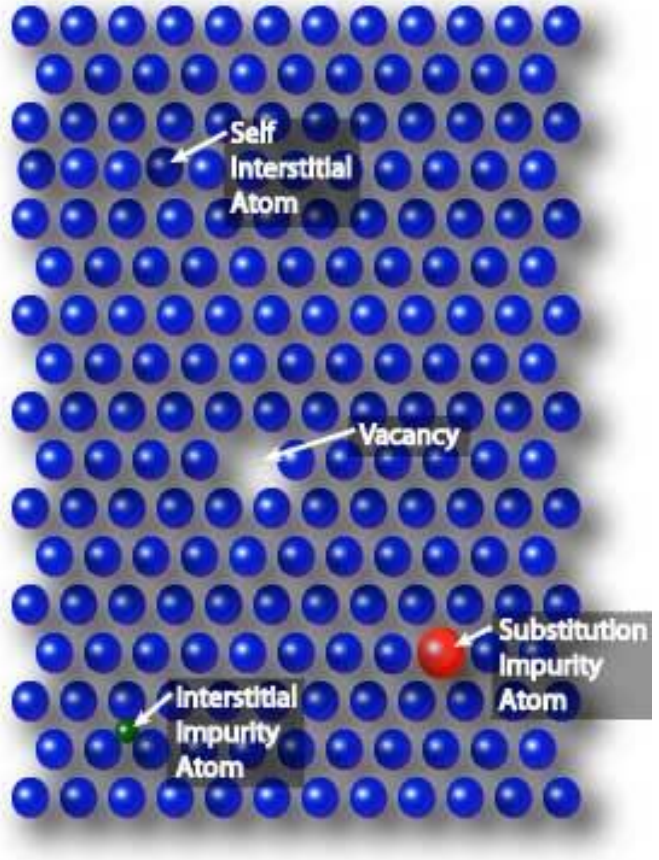
Crystalline materials

- In crystalline materials, the lattices are not perfect, they have defects
- Defects can be 0D, 1D, 2D, 3D
- The interactions between defects seriously impact material properties and how they perform



Point defects

- Point defects (zero-dimensional defects) are lattice imperfections related to one or two lattice sites
- There are several types of point defects
  - **Vacancies**
  - **Self interstitial atoms (SIA)**
  - **Interstitial impurity atoms**
  - **Substitutional impurity atoms**
- Point defects control the mobility of atoms and, therefore influence all processes that depend on diffusion



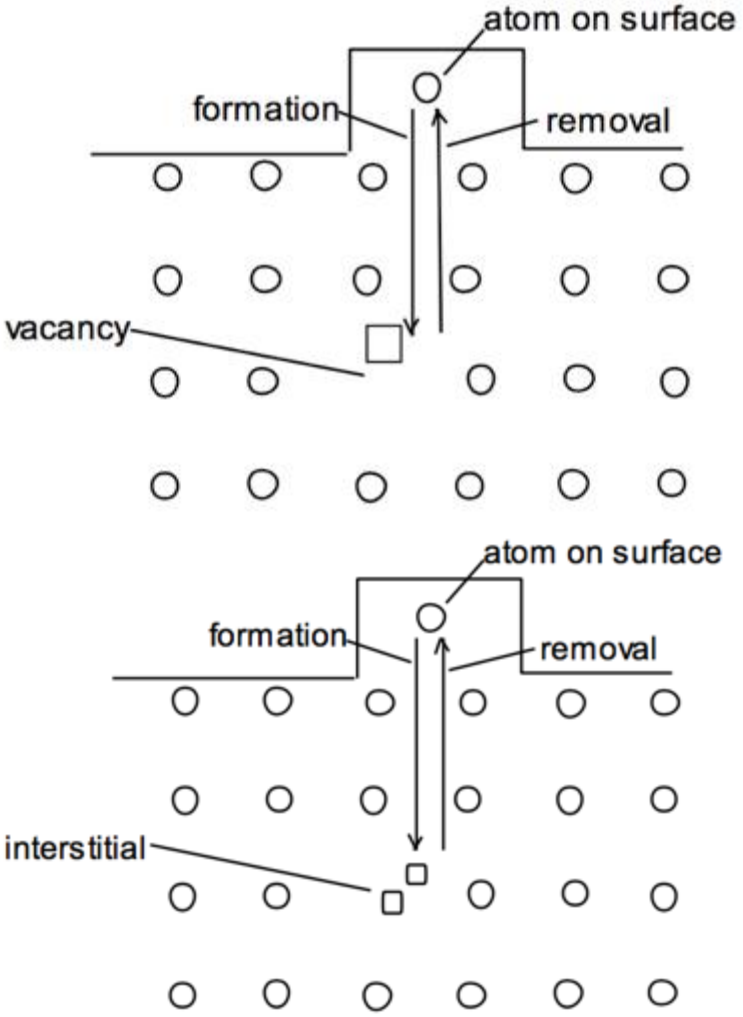
Point defects

- Vacancies and interstitials form naturally in materials
- Extra atoms can sit on a surface, creating a vacancy, or a surface can have a missing atom, creating a self interstitial atom (SIA)
- We define the number of vacancies or interstitials in terms of a concentration

$$C_V = \frac{N_V}{N_S} = \frac{number\ of\ \ empty\ sites}{total\ number\ of\ \ sites}$$

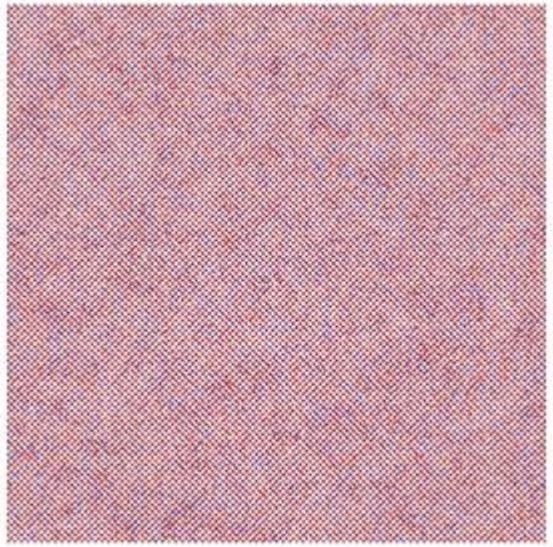
- There exists an equilibrium concentration of point defects

$$C_v = \exp\left(\frac{S_f^v}{k}\right)\exp\left(\frac{-E_f^v}{kT}\right)$$



Radiation damage

- Ionizing radiation can introduce defects into the crystal lattice, called radiation damage
- PKA collisions create a collision cascade, which results in the generation of defects (point and clusters)



Duration (ps)	Event	Result	Parameters
10^{-6}	Transfer of energy from energetic particle	Creation of PKA	$\Sigma_n(E_p, E)$

10^{-6} to 0.2	Slowing down of PKA, generation of displacement cascade	Recoil atoms
		Vacancies
		Subcascades
			E_d = energy
			ν_{NRT} = # atoms
			T = energy transferred

0.2 – 0.3	Thermal spike cool down	Stable interstitials, clusters, atomic mixing	V(T) = # stable defects
			F = clustering fraction

3 – 10	Cascade cooling to bulk solid temperature	SIA depleted zone in cascade core	Loop collapse probability
> 10	Diffusion of defects and interaction with sinks	Microstructure evolution	Many