Multiphysics and Multiscale Methodologies for Coupled Nuclear Reactor Simulations

Workshop on Computational Nuclear Science and Engineering

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Contents

Introduction

- One of the main subjects related with the use of nuclear energy is: **Nuclear Safety.**
- Originally, conservative methodologies for design and analysis of nuclear reactors were used.
- **Best-Estimate (BE) codes and approaches** have been developed to extend the safety analysis.
- The objective is: **to achieve the most realistic description of physical phenomena and avoid use of *fear* factors in the conservative calculations.**

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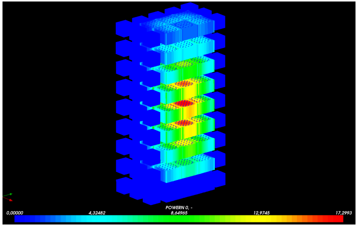
Introduction

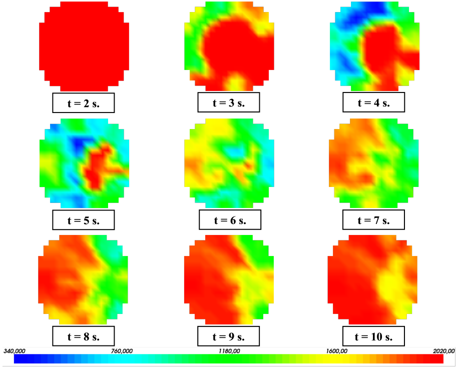
- State of the art codes are able to predict:
  - 3D thermalhydraulics parameters:
    - Coolant density
    - Fuel and moderator temperature
    - Void fractions, etc.
  - 3D-neutron flux distribution (power distribution).



3D-pin power distribution in a PWR minicore

Introduction

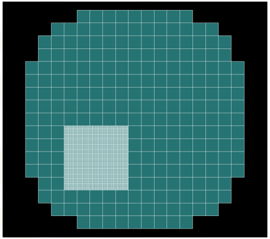
- State of the art codes can be used as standalone codes or coupled, to calculate:
  - Safety margins more accurately than the former developments.
  - Non-symmetrical core power perturbations, etc.

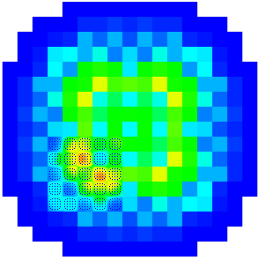


Boron slug at the inlet of a PWR core

Introduction

- State of the art codes can perform high fidelity calculations by means of multiscale approaches:
  - Move from fuel assembly based to pin based calculations.
  - Explore hot points at local refinements on mesh, etc.





Multiphysics methodologies

- The design and safety assessment of NPPs are complex problems requiring knowledge from different fields:
  - Fluid dynamics
  - Neutronics
  - Heat transfer
  - Structural mechanics
  - Chemistry, etc.
- Furthermore, these fields are in close interaction with each other:
  - Neutronics/Thermalhydraulics
  - Neutronics/Pin-mechanics
  - Thermalhydraulics/Pin-mechanics
  - Radiation/Structure
  - Fluid/Structure, etc.

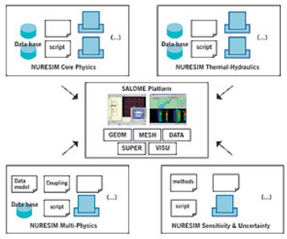
Multiphysics methodologies

- This multiphysic character of the nuclear technology was treated or described separately from the very beginning in different computer codes due to the limitations of the computer power.
- At present, computer power has been substantially increased so that the development of **coupled multiphysic solutions is the logical step to follow** by integrating the individual codes in the most appropriate way.
- The main goal of such developments is to **supply a more realistic description of key-phenomena for reactor design and safety reducing the degree of conservatism** of legacy codes.

Multiphysics methodologies

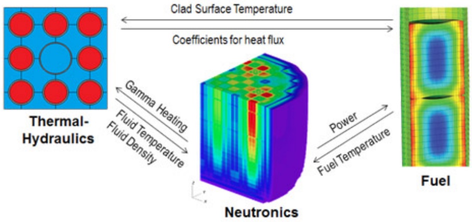
International developments

NURESIM: **NU**clear **RE**actors **SIM**ulation Platform



Source: www.ec.europa.eu

CASL: **C**onsortium for **A**dvanced **S**imulation of **L**ight Water Reactors



Source: www.casl.gov

Multiphysics methodologies

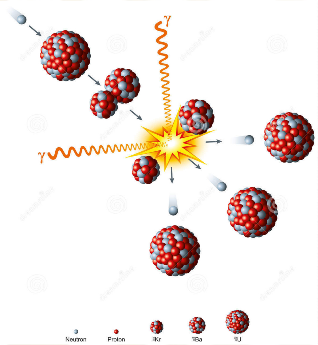
Neutronics

- The design and operation of a nuclear reactor is totally related with the capacity to predict the distribution of neutrons in space, energy and time.
- That can be done by solving the neutron transport equation or ***Boltzmann equation***.

$$\frac{1}{V(\vec{r},E)}\frac{\partial}{\partial t}\psi(\vec{r},E,\hat{\Omega},t) = -\hat{\Omega}\cdot\vec{\nabla}\psi(\vec{r},E,\hat{\Omega},t) - \Sigma_t(\vec{r},E,t)\psi(\vec{r},E,\hat{\Omega},t) +$$
$$\int_0^\infty dE' \int_{4\pi} \Sigma_s(\vec{r},E'\to E,\hat{\Omega}'\to\hat{\Omega},t)\psi(\vec{r},E',\hat{\Omega}',t)d\hat{\Omega}' +$$
$$(1-\beta(\vec{r}))\chi_p(\vec{r},E)\int_0^\infty dE' \int_{4\pi} \upsilon\Sigma_f(\vec{r},E',t)\psi(\vec{r},E',\hat{\Omega}',t)d\hat{\Omega}'$$
$$+\sum_{i=1}^{N_p}\chi_{d_i}(\vec{r},E)\lambda_i(\vec{r})C_i(\vec{r},t)$$

Multiphysics methodologies

Neutronics



- Neutron's density in multiplicative medium is proportional to the thermal power produced in a reactor core.
- Neutrons move in all directions and energies.
- Not all of them are produced at the same moment: prompt and delayed neutrons.
- Some neutrons leakage from system, some are captured and some more are absorbed causing further fissions.

Multiphysics methodologies

Neutronics

Two big branches are distinguished for dealing with the transport equation:

Deterministic codes

- Approximate solutions of the Boltzmann equation by means of a discretization of the domain under study.
- Discretizations in space, angular direction and energy are normally used as a function of time.

Monte Carlo codes

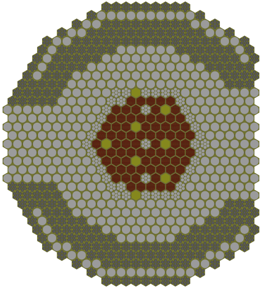
- Provide approximate solutions to a variety of mathematical problems by performing statistical sampling experiments.
- The macroscopic cross sections may be interpreted as a probability of interaction per unit distance travelled by a neutron.

Multiphysics methodologies

Neutronics

Monte Carlo codes:

- A set of neutron histories is generated by following individual neutrons through successive collisions.
- The locations of actual collisions and the results of such collisions, are determined from the range of possibilities by sets of random numbers.
- Exact geometry representation of the computational domain and continuous in energy of microscopic cross sections.

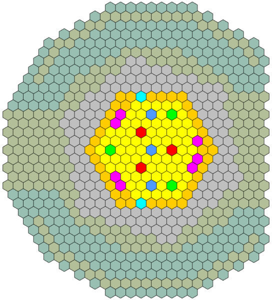


Multiphysics methodologies

Neutronics

Deterministic codes:

- Due to the complexity of Boltzmann equation in realistic problems, it is virtually impossible to obtain analytical solutions.
- Depending on the numerical method for solving the Boltzmann equation, several approximations and methods have been studied.
- Approximations in geometry and energy are usually done.
- Execution times could be smaller than in MC.

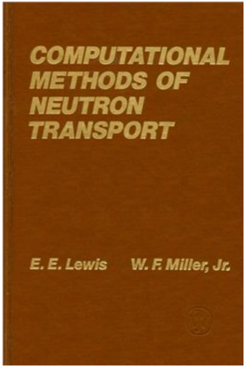


Multiphysics methodologies

Neutronics

Some common methods used in deterministic codes:

- Transport cell lattice calculations:
  - Collision probability methods
  - Method of Characteristics
- Transport core calculations:
  - Method of Spherical Harmonics
  - Discrete Ordinates Method
- Neutron diffusion calculations:
  - Finite Difference methods
  - Modern Nodal Methods



Multiphysics methodologies

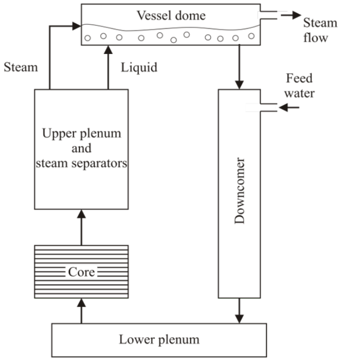
Thermalhydraulics

- The evaluation of the safety of NPPs is closely related to the ability to determine the temporal and spatial distributions of the fluid thermalhydraulic conditions.
- Associated effects from heat sources and heat sinks throughout the reactor coolant system, and especially in the core region must be also determined.
- The established method to evaluate those complex conditions is by deployment of advanced numerical thermalhydraulic simulation tools based on well validated physical and numerical solution models.

Multiphysics methodologies

Thermalhydraulics

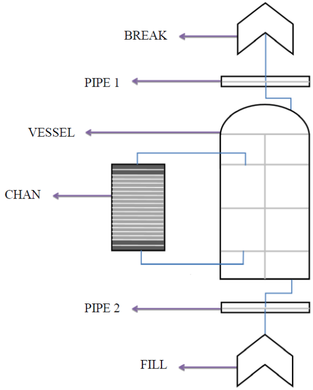
- The physical phenomena to be simulated are very numerous and, some times, problem dependent:
  - Heat conduction
  - Fluid dynamics
  - Heat transfer for single and two phase flow
  - Boron transport in liquid
  - Non-condensable gases
  - Special models: reflood, stratification, condensation, critical flow, counter current flow, etc.



Multiphysics methodologies

Thermalhydraulics

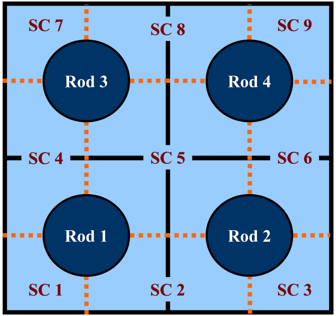
- **System codes:**
  - The reactor hydraulic system is modelled with 1D fluid computational elements, interconnected by means of flow junctions.
  - Special models to simulate the behaviour of coolant pumps, pressurizers, steam generators.
  - Conservation of mass, momentum and energy are solved in such a 1D network by means of numerical methods that provide the time evolution of the variables of the system.
  - Some of these codes make use of a more sophisticated modelling for the reactor vessel and core, even in 3D.



Multiphysics methodologies

Thermalhydraulics

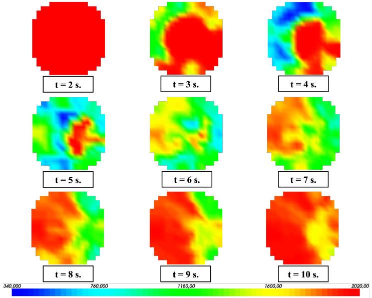
- **Subchannel codes:**
  - Better modelling of the thermalhydraulic conditions inside fuel assemblies in the vicinity of fuel rods.
  - The distribution of pressure drop and void fraction inside a reactor fuel assembly.
  - Local thermalhydraulic conditions, such as mass fluxes in fuel channels, pressure gradients between flow channels, arrangement of the rods, etc.
  - Conservation of mass, momentum and energy are solved in the predominant direction (axial) and the transversal to the axial one (cross flow).



Multiphysics methodologies

Thermalhydraulics

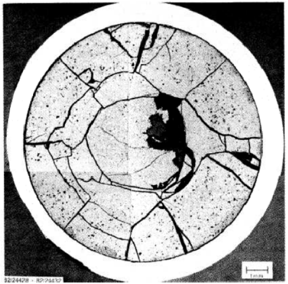
- **Computational Fluid Dynamic (CFD) codes:**
  - The fundamental bases are the Navier–Stokes equations (conservation equations), which define any single-phase fluid flow.
  - The fundamental concept of numerical schemes is based on the approximation of partial derivatives by algebraic expressions that can be solved numerically using computers.
  - Almost exact geometry can be simulated and equations can be solved in a fine mesh, the finer the mesh the more accurate result.
  - Require huge amount of computational resources.



Multiphysics methodologies

Fuel rod mechanics

- In nuclear reactors, the fuel is exposed to very strong thermal, mechanical and radiation loads during its operational life, which cause significant changes to its microstructure altering its mechanical and thermal properties.
- The material composition of the fuel also changes during burn-up resulting in several consequences for the fuel rod:
  - Internal rod pressure increases
  - Cracking of the fuel pellets
  - Pellet-clad contact
  - Increase the mechanical stresses in the clad

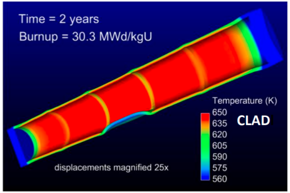


Multiphysics methodologies

Fuel rod mechanics

- There are two types of codes for the analysis of nuclear fuel behaviour:
  - **The simplified:** solve the heat transfer equations and is able to calculate the deformations based in the properties of the materials given by input.
  - **The mechanistic:** are able to calculate directly those properties as a function of the operational conditions and the history of the fuel.

[BISON, bison.inl.gov]



Source of image:

`https://snetp.eu/wp-content/uploads/2021/02/Presentation_Lelio-Luzzi.pdf`

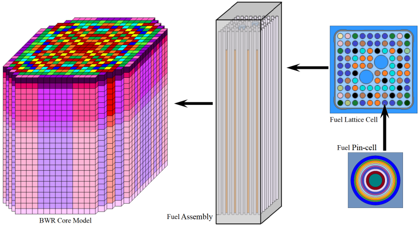
Multiscale methodologies

- A multiscale approach tries to describe all phenomena occurring in a physical system at different spatial scales and how they are connected.
- The reactor vessel's radius can be several meters long, an assembly is usually 20 cm, the fuel rod diameter is approximately 1 cm and the size of the bubbles in the coolant is of the order of millimetres.
- The fluid passing through all these elements is governed by the same physical laws, however, the hypotheses used in every scale are chosen in agreement with the effects that must be reproduced at a given scale.

Multiscale methodologies

Multiscale approach in the neutronic branch

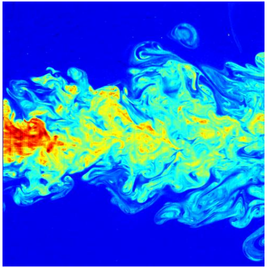
- The neutronic core behaviour can be described in a macro scale by means of point kinetics.
- In a more detailed representation (still at macro scale), the neutron diffusion equation can be solved in 3D for spatially homogenized fuel assemblies.
- The development of more heterogeneous fuel designs (MOX fuels, burnable poisons, water holes, etc) fosters the transition from FA-based analysis to pin-based neutronic simulations (macro to meso scale).



Multiscale methodologies

Multiscale approach in the thermal branch

- **Macro-scale with System codes:** reproduce the behaviour of the different components without paying much attention to physical processes at smaller scales.
- **Meso-scale with Subchannel and some coarse mesh CFD codes:** physical phenomena important for evaluation of local safety parameters like the heat removal of a single pin inside a fuel assembly.
- **Micro-scale with fine mesh CFD codes:** physical phenomena taking place at a very small spatial scale, e.g. boundary layer effects, turbulences, velocity gradients, etc.



Source of image: C. Fukushima and J. Westerweel, `https://commons.wikimedia.org/w/index.php?curid=3082535`

Multiscale methodologies

Different codes

Type of codes	Physics	Scale	Examples
System	Thermal-hydraulics	Macro	ATHLET [Lerchl1998], RELAP5 [RELAP2000], TRACE [TRACE2008], CATHARE [Barre1990]
Cell Lattice	Neutronics Deterministic	Meso	HELIOS [Pralong2005], CASMO [Rhodes2006], APOLLO2 [SanchezR2003], SCALE [Bowman2007], DRAGON [Marleau2008]
Monte Carlo	Neutronics Stochastic	Meso	MCNP [MCNP2006] , TRIPOLI [Brun2009], SER-PENT [Leppanen2009], KENO [Hollenbach2005]
Reactor Dynamic	Neutronics	Meso	DYN3D* [Grundmann2005], NEM [Beam1999], NESTLE [Turinsky1994], PARCS* [Downar2006], QUABOX/CUBBOX [Langenbuch1984], CRONOS [Lautard1999], TORT-TD [Seubert2011], DeCART [Han2004], COBAYA [Jimenez2010]
Subchannel	Thermal-hydraulics	Meso	COBRA[Wheeler1976], MATRA [MATRA1998], FLICA4[Toumi2000],SUBCHANFLOW [GomezR2010]
CFD/DNS	Thermal-hydraulics	Macro Meso Micro	ANSYS-CFX [ANSYS2009], TRIO-U [Barthel2009],TURBIT [Grötzbach1977], NEPTUNE-CFD [Guelfi2005], OpenFOAM [OPENFOAM2010]
Fuel Mechanics	Fuel behaviour	Meso	DRACCAR [Papin2006], FRAPCON [Berna1997] TRANSURANUS [Lassmann1992], SCANAIR [Federici], FRAPTRAN [Cunningham]

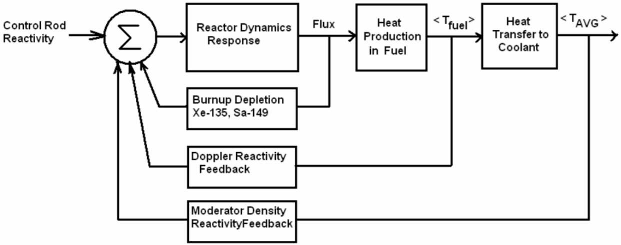
* A simplified thermal-hydraulics and fuel rod mechanics model are included in such codes for taking into account the effect of thermal-hydraulic feedback, as it will be discussed in the next sections.

Coupling methodologies

- The coupling between multiphysics and multiscale methodologies is a very complex subject with many possible combinations.
- In the past, the thermalhydraulic analyses of plant transients and of reactor core behaviour were performed separately, even though they may address the same reactor conditions.
  1. The thermalhydraulic analysis used simplified neutronic models (PK) and focused on the entire reactor system.
  2. The result provided the necessary boundary conditions for the core: mass flow and temperature distribution of coolant and fuel, together with time-functions for pressure.
  3. A more detailed 3D neutronics calculation can be done with BC from step 2.
- In reality these BC are functions of the power generation i.e. the neutronics.

Coupling methodologies

- The coupled code calculation approach constitutes the normal evolution of these methods.
- Especially in cases with strong feedback between the NK and the TH is present, as well as when neutron flux distortions are important to analize.

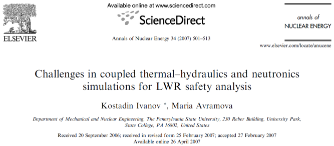


Source of image: Dr. John H. Bickel, `https://www.nrc.gov/docs/ML1214/ML12142A130.pdf`

Coupling methodologies

- In the literature, six basic components of the coupling methodologies have been identified in order to be able to couple two codes:

1. The way of coupling (internal or external)
2. The coupling approaches (serial integration or parallel processing coupling)
3. Spatial mesh overlays (fixed or flexible)
4. Coupled time steps algorithms (synchronization of the time steps)
5. Coupling numerics (explicit, semi-implicit and implicit)
6. Coupled convergence schemes must be considered and implemented.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Challenges in coupled thermal–hydraulics and neutronics simulations for LWR safety analysis

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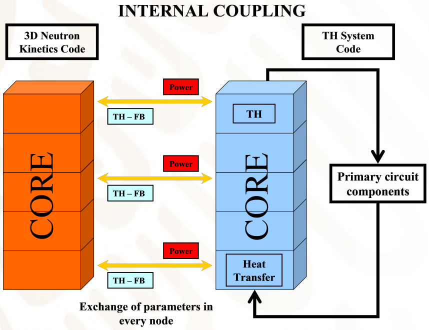
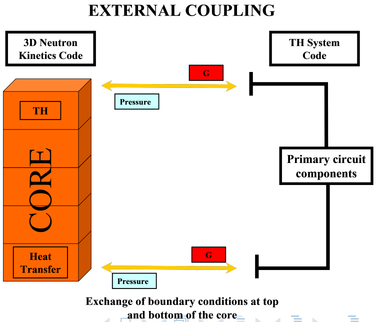
Coupling methodologies

Reactor dynamics code with System code

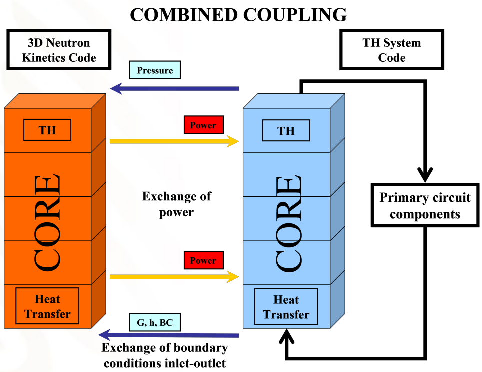
- Three different ways of coupling can be implemented: internal, external and combined.





Coupling methodologies

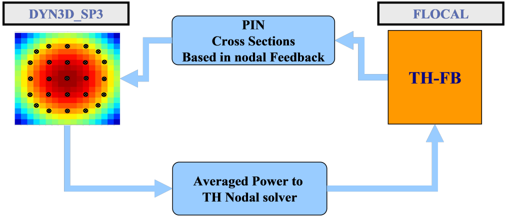
Reactor dynamics code with System code



Coupling methodologies

Reactor dynamics code coupled with simplified thermal-hydraulics code

- The external and combined coupling described before requires that the reactor dynamics code is internally coupled with a two phase flow thermalhydraulics model capable of calculating assembly averaged feedback parameters.
- Feedback parameters are used to actualize the cross sections for a later calculation of the reactor power.

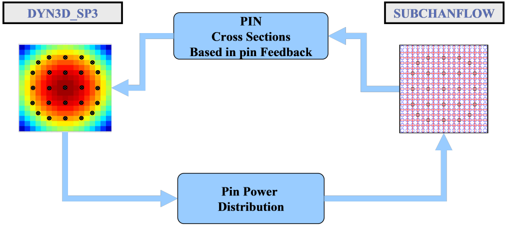


One and a half way coupling

Coupling methodologies

Reactor dynamics code coupled with subchannel code

- To increase the degree of detail in the thermalhydraulic solution, a subchannel codes is needed.
- In this case, pin based cross sections with pin based thermalhydraulic feedback parameters are obtained, avoiding the averaging process.

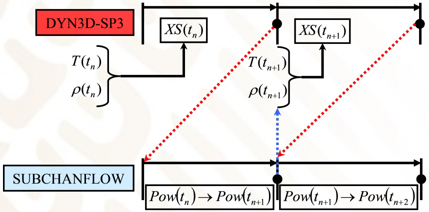


Two way coupling

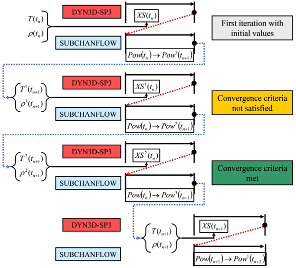
Coupling methodologies

Coupling numerics

- Beyond the time step size, the point at which data is exchanged between the two codes is important, most common types of coupling are explicit, and semi-implicit also known as fixed point iteration (FPI) or nested loop.



Explicit



Semi-implicit (Fixed Point Iteration)

Coupling methodologies

Convergence criteria

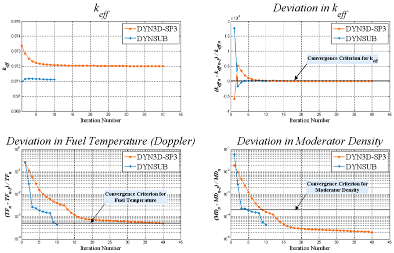
- The convergence criteria for ending the NK-TH iteration process are based in the change in k_{eff} which is determined in the NK calculation, and the maximal deviations for the fuel Doppler temperatures and coolant densities in the TH calculation.

$$Dev\_k_{eff} = \frac{k_{eff}^{n} - k_{eff}^{n-1}}{k_{eff}^{n}} \le \varepsilon_k$$

$$Dev\_TF_{DOPPLER} = \max_i \left(\frac{TF_{DOPPLER,i}^{n} - TF_{DOPPLER,i}^{n-1}}{TF_{DOPPLER,i}^{n}} \right) \le \varepsilon_{TF}$$

$$Dev\_TF_{DOPPLER} = \max_i \left(\frac{TF_{DOPPLER,i}^{n} - TF_{DOPPLER,i}^{n-1}}{TF_{DOPPLER,i}^{n}} \right) \le \varepsilon_{TF}$$

Different convergence criteria

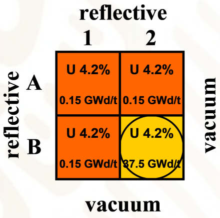


Convergence process

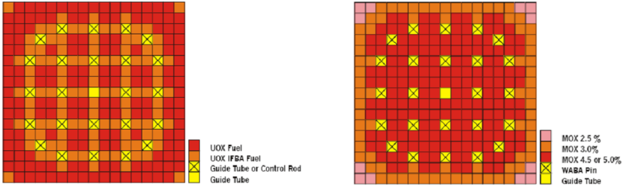
Coupling methodologies

Coupling example

- A fast running test case (2x2 minicore) based in the *OECD/NEA and U.S. NRC PWR MOX/UO2 core transient Benchmark*.



Minicore configuration

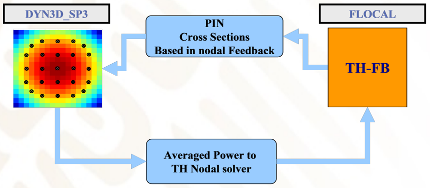


Fuel assembly configuration

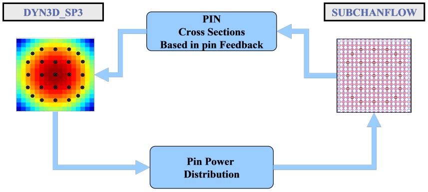
Coupling methodologies

Coupling example

- One and a half way coupling vs. Two way coupling:



One and a half way coupling



Two way coupling

Coupling methodologies

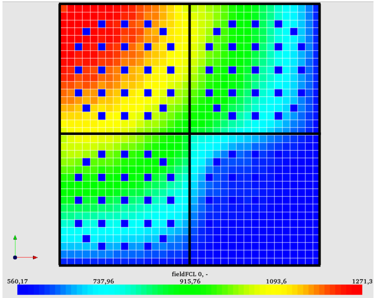
Coupling example

- Results with one and a half way coupling and two way coupling:

Assembly ID Fuel centreline temperature Moderator temperature

A1 **1145.60 K** **570.14 K**	**A2** **821.70 K** **564.53 K**
B1 **821.70 K** **564.53 K**	**B2** **607.20 K** **560.81 K**

Results with one and a half way coupling

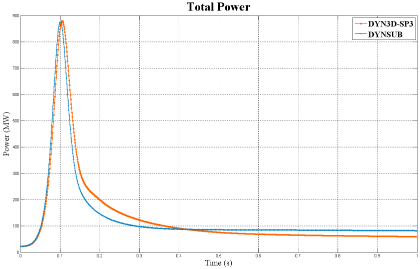


Results with two way coupling

Coupling methodologies

Coupling example

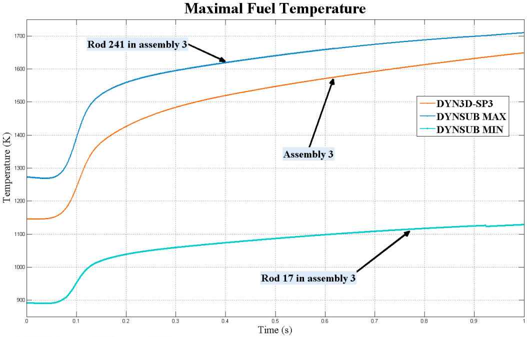
- A transient can be studied: very fast rod ejection.
- The rapid increase in reactivity brings the system to a prompt critical state and a significant power rise is expected in the initial milliseconds.
- The strong negative fuel temperature (Doppler) feedback reactivity is the only inherent reactivity feedback responsible to avoid a bigger power excursion and to mitigate the power peak.



Coupling methodologies

Coupling example

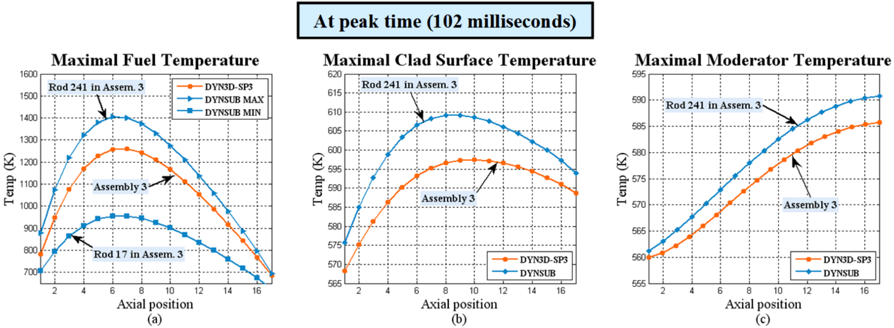
- Maximal fuel temperature for every single rod in the two way coupling using a subchannel code.



Coupling methodologies

Coupling example

- Much more information can be obtained when the two way coupling methodology is used.



Remarks

- There is a bunch of physical phenomena interacting inside a nuclear reactor (multiphysics).
- They interact at different scales (multiscale).
- The Best Estimate codes (multiphysics and multiscale codes) supply a more realistic description of key-phenomena for reactor design and safety, reducing the degree of conservatism of legacy codes.
- With the current computer power it is possible to analyze more and more phenomena in a coupled way.
- The more physical phenomena working together, the more reliable result.
- **And all this is very good :-) for Nuclear Safety analyses.**

END

Thanks a lot for your attention