RELAP5-3D/PHISICS Coupling Advancements

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Outline

- Part I
  - Code structure
  - PHISICS modules (steady state)
  - Coupling schemes (steady state)
  - NGNP example
- Part II
  - PHISICS modules (time dependent)
  - Coupling schemes (time dependent)
  - Validation activity
  - Future development
  - Release

Outline Part I

- What is PHISICS
- Modules
  - INSTANT (Spherical harmonics nodal transport)
  - MIXER
  - MRTAU (depletion)
  - Criticality Search
  - Time Driver (in part II)
  - RELAP5-3D Coupler
- Calculation Patterns with RELAP5-3D (part I)
- Examples

- *RELAP5-3D/PHISICS coupling adds the following features*
  - *Spatial/angular mesh refinement*
  - *Unlimited number of energy group*
  - *Cross section tabulation*
  - *In the future: depletion, time dependent, decay heat, adjoint sensitivity analysis*
- *We can match computational time with higher accuracy*
- *We preserve compatibility with past input decks*

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What is PHISICS?

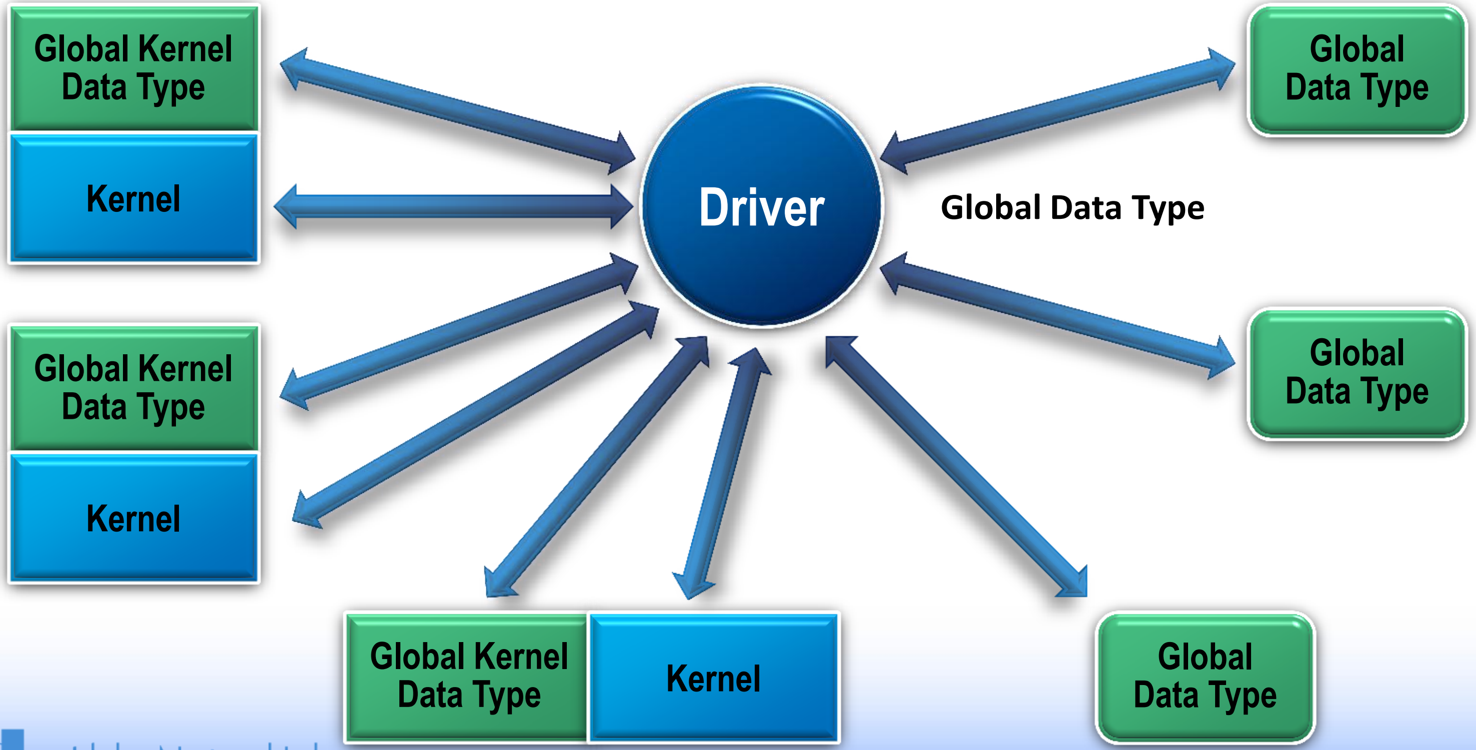
PHISICS

Parallel and Highly Innovative Simulation INL Code System

- **Collection of kernels/modules. Their combined capabilities make PHISICS an attractive code for reactor physics analysis**
- **Its latter coupling with RELAP5-3D creates a unique bundle where state of the art reactor physics is directly coupled with one of the most used system codes, leading to new attractive features**

Software Infrastructure

- Each kernel solves one specific equation set connected to a reactor physics problem
- Each Kernel could be called through its interface leading to different calculation patterns



INSTANT

- **INSTANT is the transport/diffusion nodal solver**
- **Solution is based on the second order formulation of the transport equation projected on the angular spherical harmonics**

Capability Summary	
Energy	Unlimited
Spatial Order	33
Angular Order	33 (it is also the order of the angular scattering supported)
MESHES	Cartesian 2/3D, Hex 2/3D, Triangular, Wedges
Adjoint	Fundamental, Source (no generalized source)

Using PHISICS Within RELAP5-3D

- **Accessible through new keyword "instant"**

```
$-----------------------------------------------------------
$            REACTOR KINETICS INPUT
$-----------------------------------------------------------
30000000  instant  gen
30000001  no-gamma  3600.0e+6   0.0076  6  1.0 0.48
…
```

- **Coupling it is not through PVM !!!**

- **There is compatibility with past input decks**

- **More accurate simulation might require additional inputs → for this you might need to provide additional files**

Cross Section Management (MIXER)

- **Cross section manipulation is agnostic with respect to the usage of micro, macro, or mixed**
- **Cross sections are tabulated with respect to an arbitrary number of parameters: fuel temperature, coolant temperature, coolant density, control rod (CR) position, boron concentration, etc.**

$$\sigma(P) = \sigma_i + \sum_{j=1}^{dimension} \frac{\sigma_j - \sigma_i}{P_j - P_i}(P - P_i)$$

- **Unlimited number of energy groups**
- **Unlimited number of tabulation points (with cross terms)**
- **Flexibility to follow a specific isotope separately**

MIXER within RELAP5-3D

The new cross section handling capabilities are accessible through…

phis_ma

```
$---------------------------------------------------------
$          REACTOR KINETICS INPUT
$---------------------------------------------------------
30000000  instant  phis_ma
30000001  no-gamma  3000.0e+6   0.0076  6  1.0 0.48
...
```

Tabulated macros only

No densities input

Depletion module not active

phis_mi

```
$---------------------------------------------------------
$          REACTOR KINETICS INPUT
$---------------------------------------------------------
30000000  instant  phis_mi
30000001  no-gamma  3000.0e+6   0.0076  6  1.0 0.48
...
```

Tabulated macros / micros mixed

Isotopic densities input

Depletion module active

- **Compatible with RELAP5-3D CR model**
- **Kinetic nodes to TH mapping: as in “Gen”**

FB Zones and Regions for:

- **Structure temperature**
- **Fluid temperature**
- **Fluid density**
- **Poison concentration**

Depletion (MRTAU)

- **MRTAU Kernel is a Bateman solver**

Isotopic Density Vector

$$\dot{N} = \bar{\bar{\Lambda}}\bar{N}$$

$$\bar{N} = \bar{N}_0 e^{-\bar{\bar{\Lambda}}t}$$

Micro Reaction Rate, Capture, Natural Decay

- **Two algorithms are available for the exponential evaluation: CRAM and Taylor**
- **MRTAU is controlled by a separate input file and can be used with the "phis_mi" option**
- **Decay heat can be calculated by MRTAU and requested with keyword "MRTAU" on W1 card 30000001**

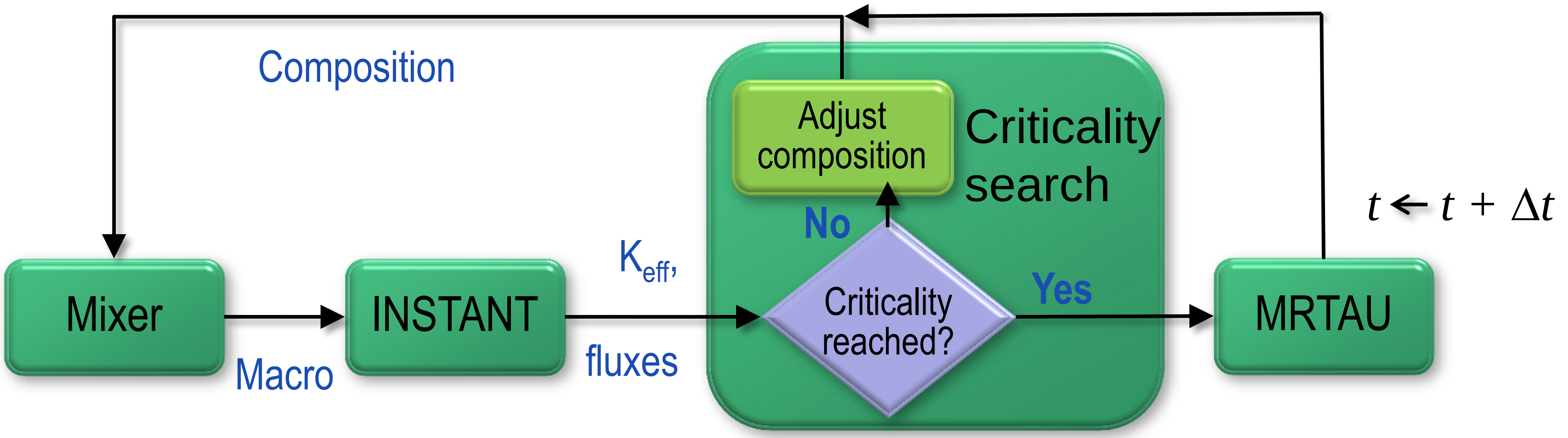
Criticality Search

Given

- **Target k_{eff}**
- **Region**
- **Isotope**

Seeks the density matching the target

- **If Macro-isotope → Material movement**
- **If Micro-Isotope → Number density**



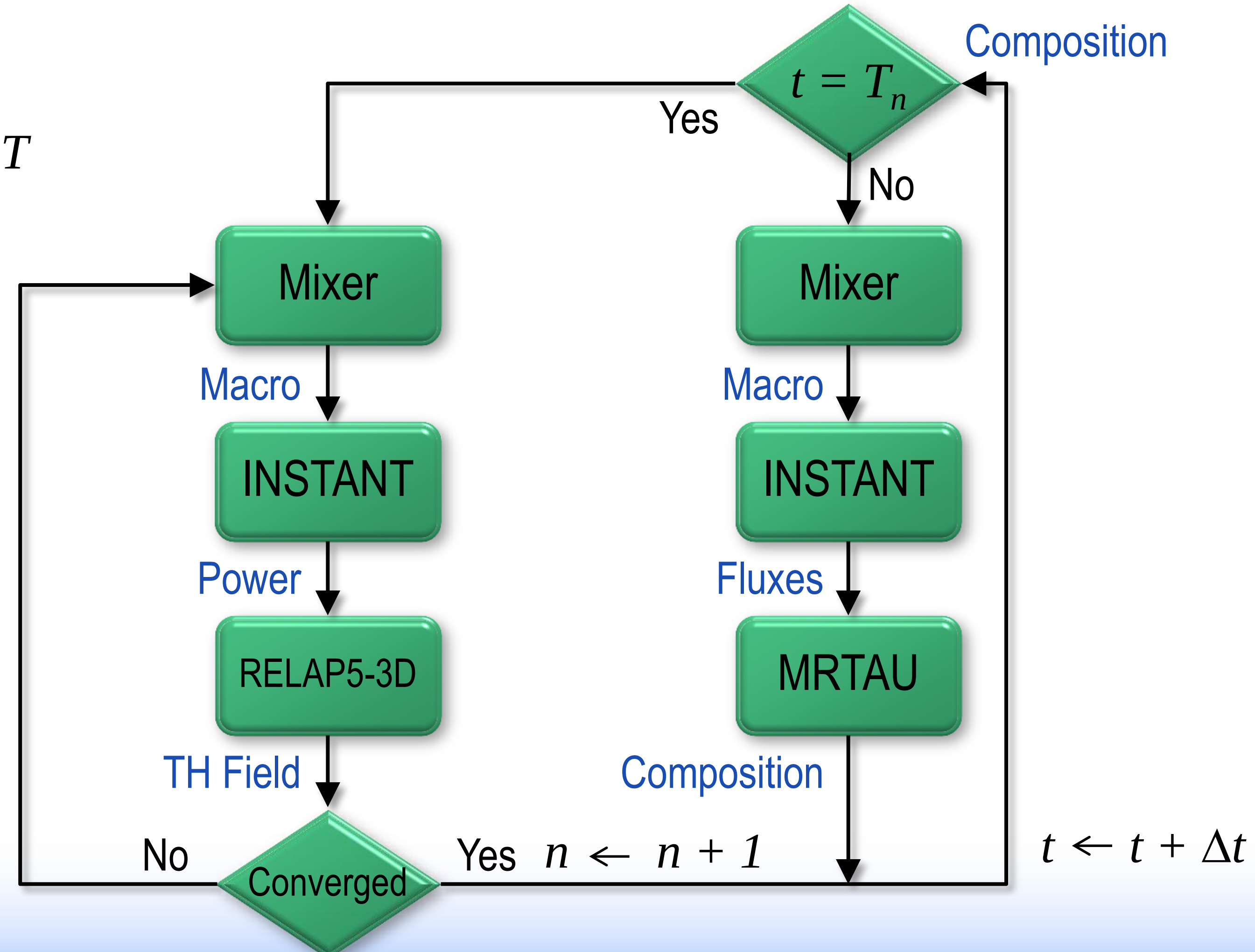
RELAP5-3D Coupling

Several coupling schemes are available with RELAP5-3D and they fall in two main classes

- **Depletion time evolution**
  - **TH**
  - **Neutronics steady state**
  - **Depletion**
  - **Mixing**
- **Time dependent**
  - **TH**
  - **Neutronics time dependent**
  - **Depletion**
  - **Mixing**

Depletion Time Evolution

$\Delta t \leq \Delta T$

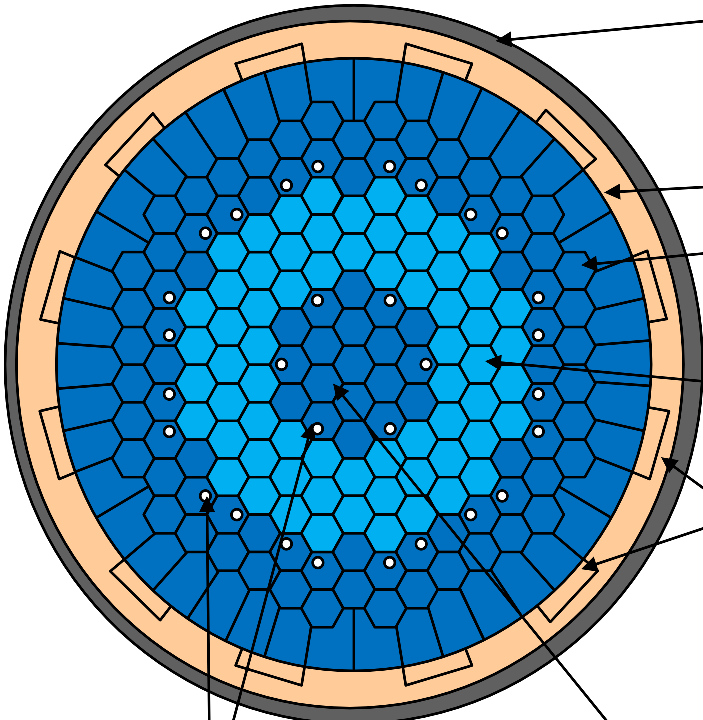


MHTGR

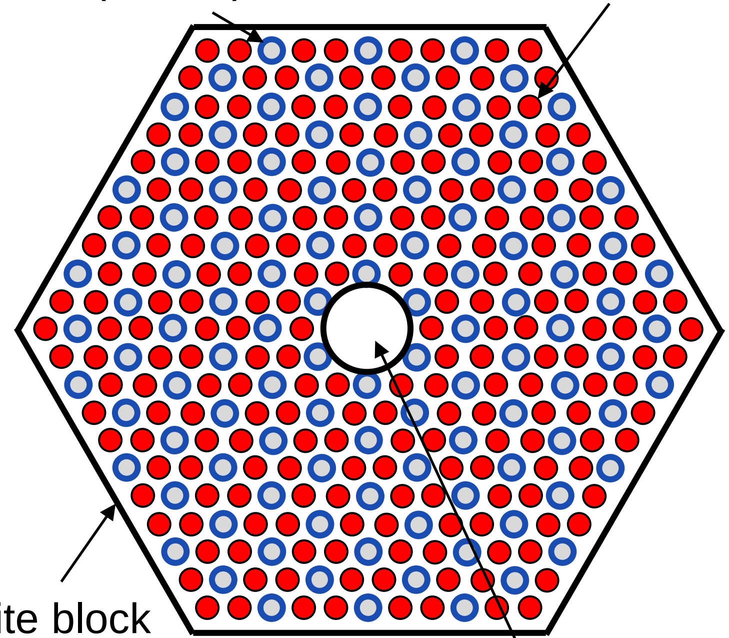
- ***NGNP supports the PHISICS/RELAP5-3D coupling for the MHTGR benchmark***
- **Features needed by the benchmark not supported by NESTLE/RELAP5-3D**
  - **High order cross section behavior (two point linear dependency of cross-section not sufficient to capture feedback)**
  - **Twenty-six energy groups needed**
  - **Triangular mesh for CR location**
- **Benchmark characteristics (neutronics)**
  - **4000 neutronic nodes**
  - **Twenty-six energy groups, ~170 tabulation points, anisotropic scattering, 230 material definitions**
  - **Fuel and reflector macroscopic cross sections, *Xe* and *I* microscopic absorption**

MHTGR RELAP5-3D models

Core



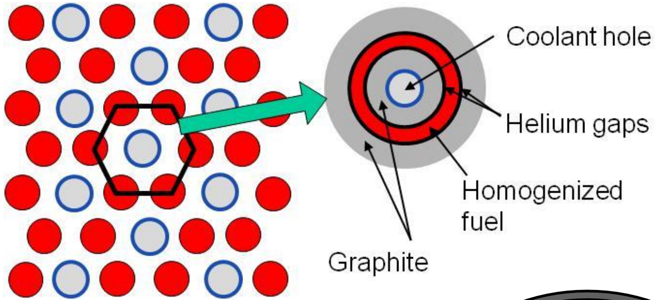
Fuel element



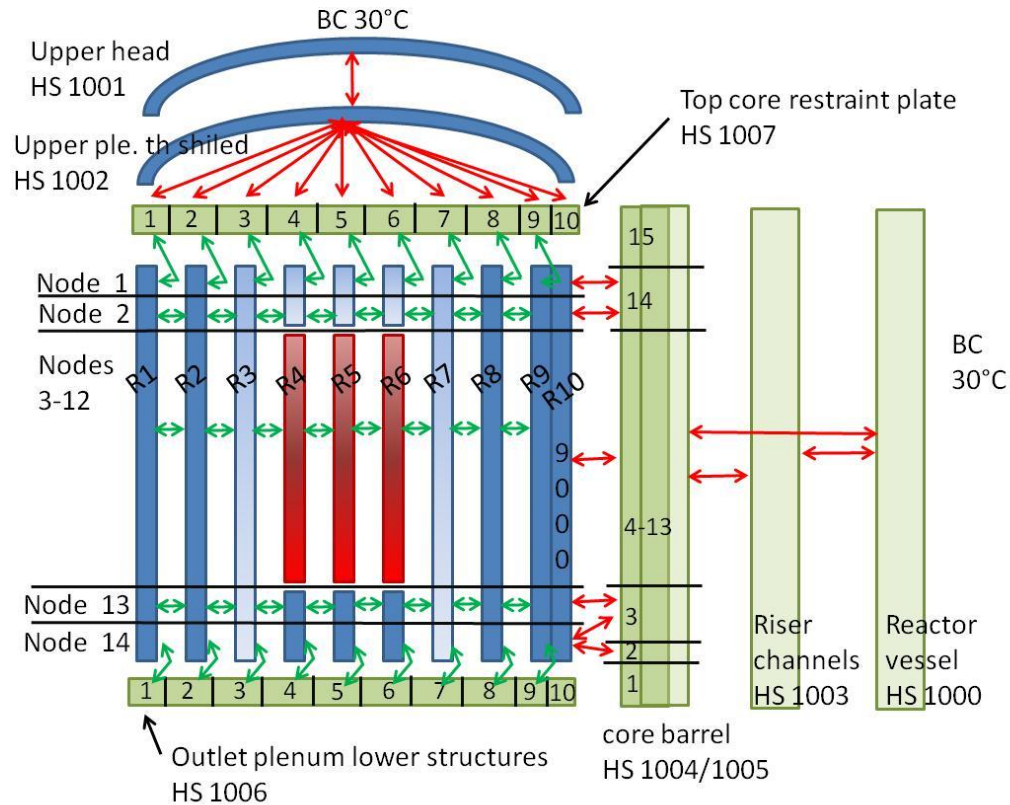
Fuel pins: graphite matrix filled with TRISO particles

MHTGR RELAP5-3D models (ring-wise)

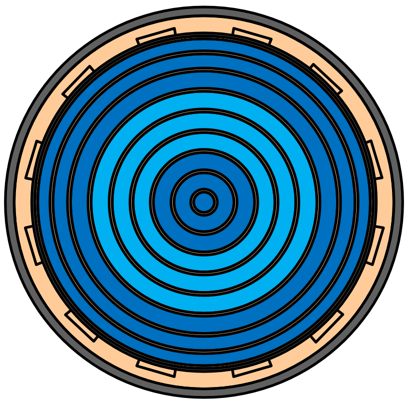
Unit cell



Conduction/radiation



Feed-back zones



- One unit cell (heat-structure) per ring
- One bypass pipe per ring
- Rings connected by conduction/radiation enclosures
- "Ring-wise" feedbacks for PHISICS

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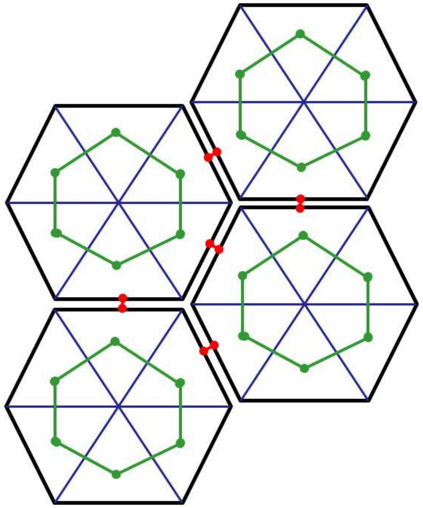
MHTGR RELAP5-3D models (1/6 block, 1/3 core)

Pushing RELAP5-3D to its limits

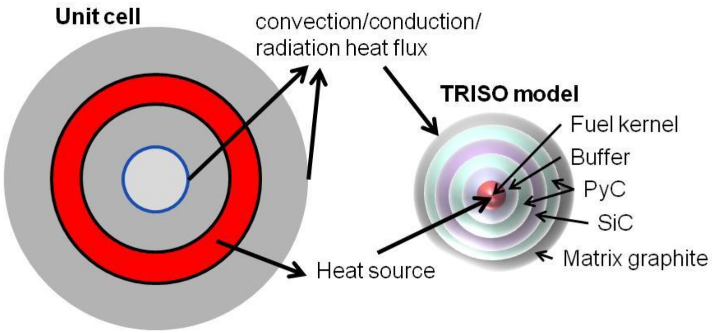
- One unit cell (heat-structure) per 1/6 block
- One bypass pipe per block face
- “Intrablock” conduction between 1/6 blocks
- Radiation between block faces
- Refined feedback for PHISICS
  - Particle model for Doppler feedback

    One particle per 1/6 block and axial level

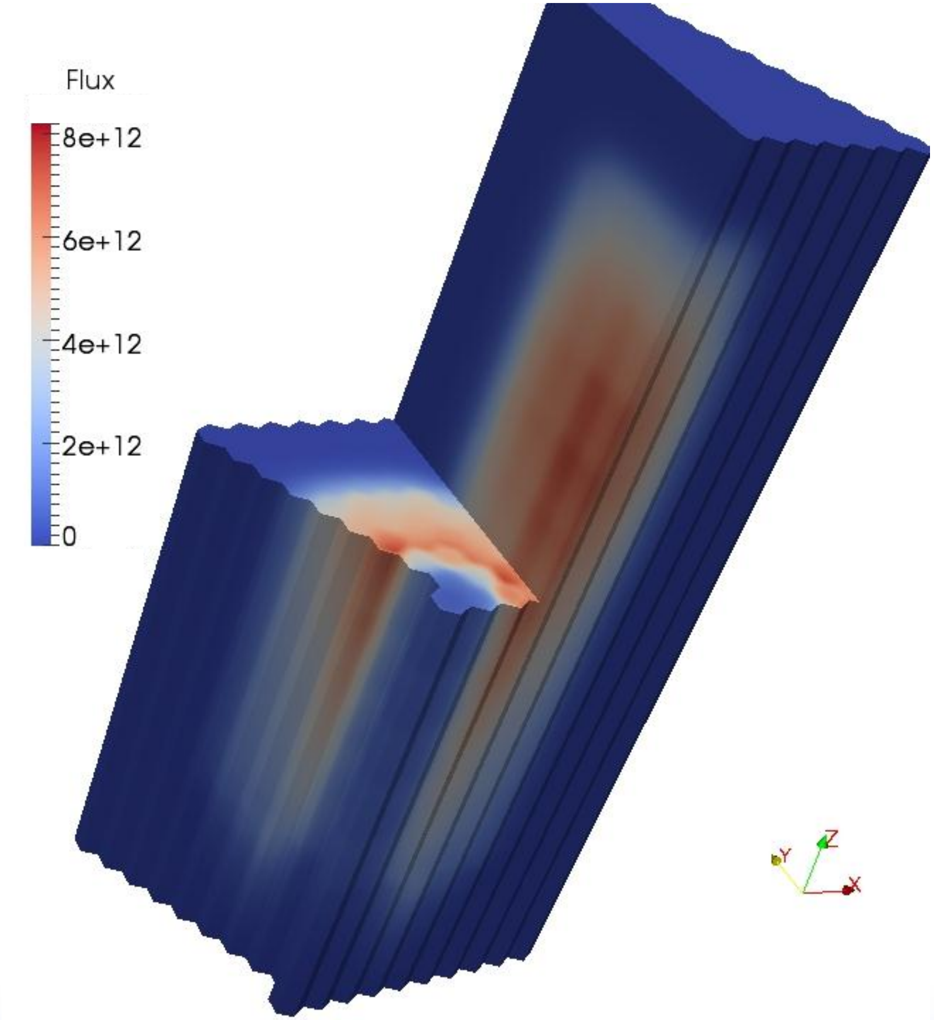


- 800+ material definitions to accommodate fluency and burn-up dependence
- 120+ bypass pipes, 130+ cooling pipes (14 axial nodes)
- 3400+ HS, 1220 particle HS
- 7000+ surfaces in radiation/conduction enclosures
- 1200+ neutronic feedback zones
- 220 decay heat tables

… it’s a huge bookkeeping exercise



NGNP MHTGR results



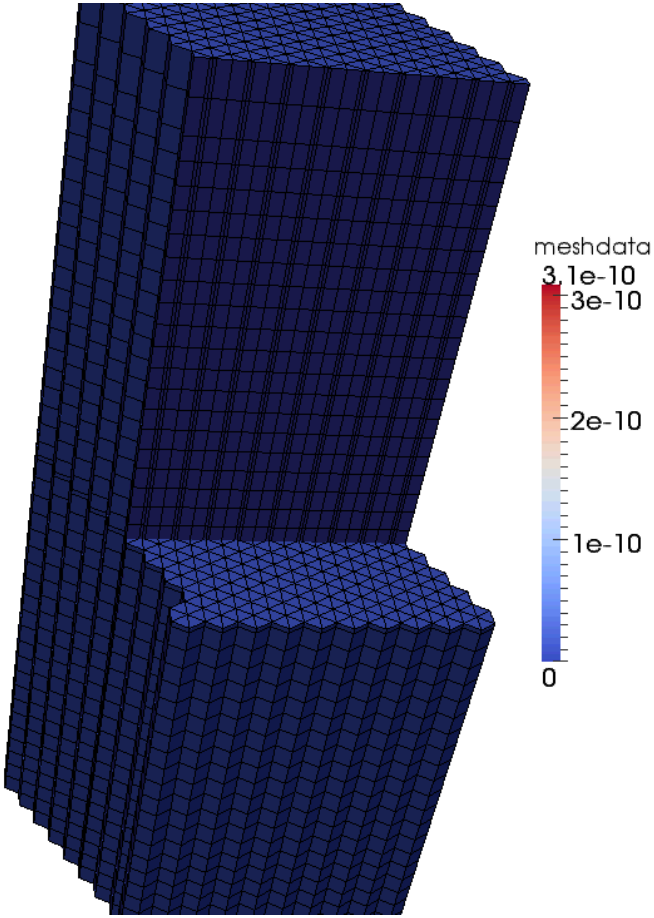
- full XS library, 26 groups
- block-wise kinetics
- detailed 1/6 block TH

- steady state with *Xe* equilibrium

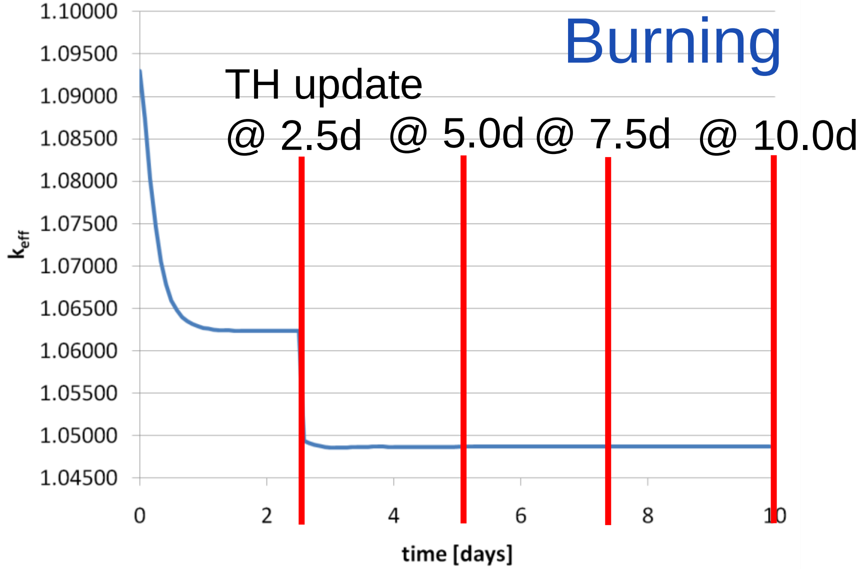
←Converged flux for group 18

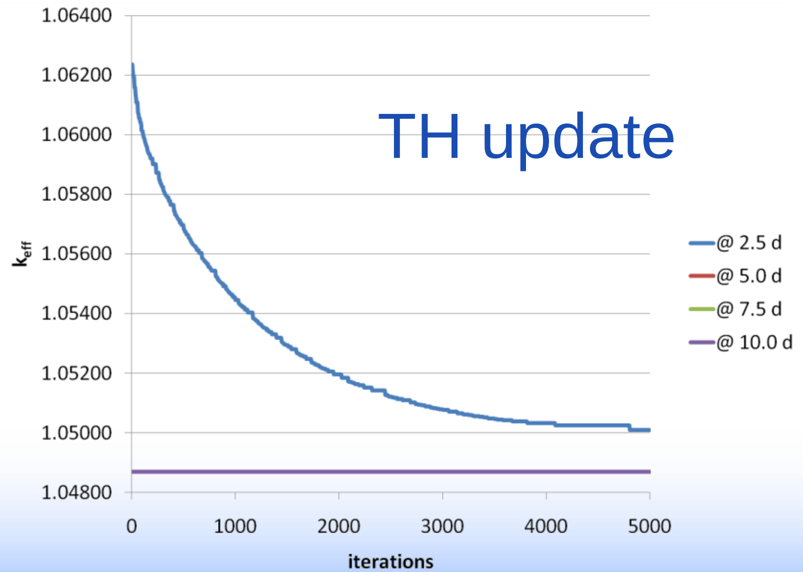
	PHISICS/RELAP5-3D
Keff converged	1.04859

NGNP MHTGR results



Xenon build-up





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RELAP5-3D/PHISICS coupling advancements II

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Outline

- Time driver module
- Calculation Patterns with RELAP5-3D (part II)
  - Time dependent
- Ongoing work
  - PWR TH/neutronics/burn-up benchmark
  - Assembly shuffling
  - Perturbation Analysis
- Code licensing
- Conclusions

Time Dependent Theory

- **A second order backward Euler scheme is re-casted as a steady state source problem (always stable)**

$$\begin{cases} \vec{\Omega}\cdot\vec{\nabla}\psi^{-,i+1} + \tilde{\Sigma}_T\psi^{+,i+1} = H^{+}\psi^{+,i+1} + \tilde{S}^{+,i+1} + \frac{1}{k}F\psi^{+,i+1} \\ \vec{\Omega}\cdot\vec{\nabla}\psi^{+,i+1} + \tilde{\Sigma}_T\psi^{-,i+1} = H^{-}\psi^{-,i+1} + \tilde{S}^{-,i+1} \end{cases}$$

$$\begin{cases} \tilde{S}^{\pm,i+1} = S^{\pm,i+1} + \frac{1}{s\Delta t}\psi^{\pm,i} \\ \tilde{\Sigma}_T = \frac{1}{s\Delta t} + \Sigma_T \end{cases}$$

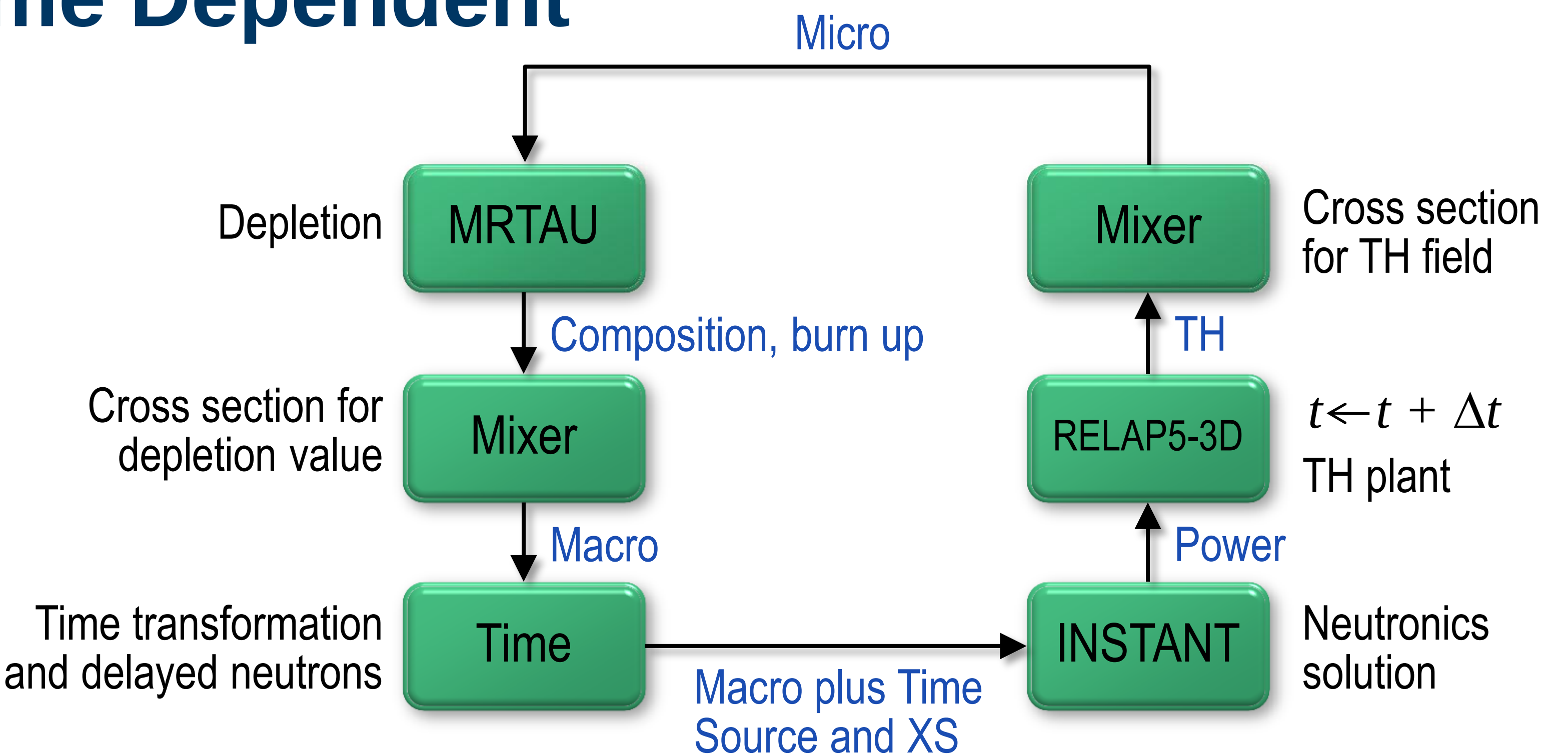
- **Computation of the delayed neutron source is obtained by operator split and then direct integration**

$$N_f^i = N_f^{i-1}e^{-\lambda_f \Delta t_i} + \frac{1-e^{-\lambda_f \Delta t_i}}{\lambda_f}\sum_{g=1}^{G}\beta_{f,g}\upsilon\Sigma_{\mathrm{F,g}}\Phi_{\mathrm{g}}^{\mathrm{i-1}}$$

$$S_{d,g}^{i+1} = \sum_{f=1}^{nf}\chi_{f,g}\lambda_f N_f^i$$

$$S_{Tot}^{i+1} = \tilde{S}^{\pm,i+1} + S_d^{i+1}$$

Time Dependent

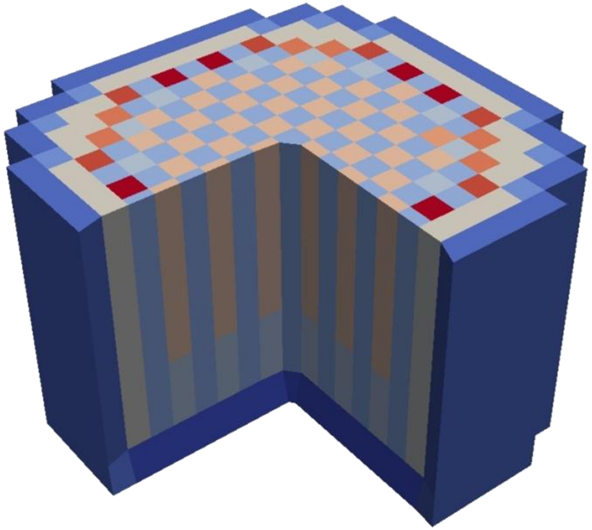


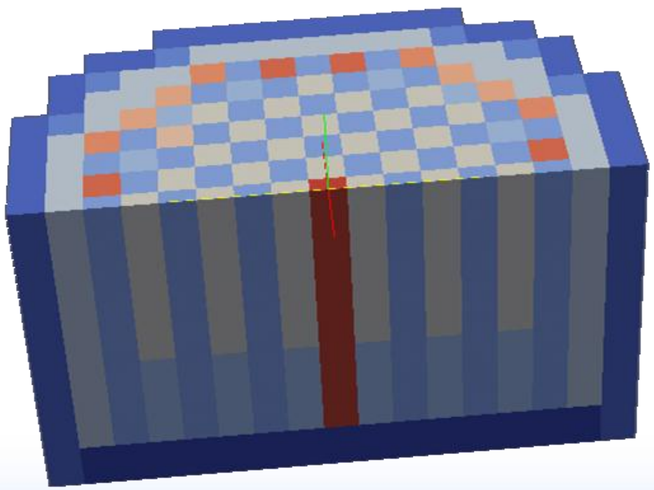
- “Pre-burnig” possible in one stop calculation, i.e. before the time dependent loop starts, MRTAU can pre-burn the core with the initial temperature distribution to a desired burn-up level
- Full restart capabilities for PHISICS/RELAP5-3D are implemented, i.e. a “Depletion Time Evolution” calculation can be performed before a transient is restarted

PWR Description

- **Full core model**
- **17x17 radial nodes**
- **13 axial levels**
- **11 Materials**
- **36 TH feedback zones**
- **2 Energy groups**
- **6 families delayed neutrons**

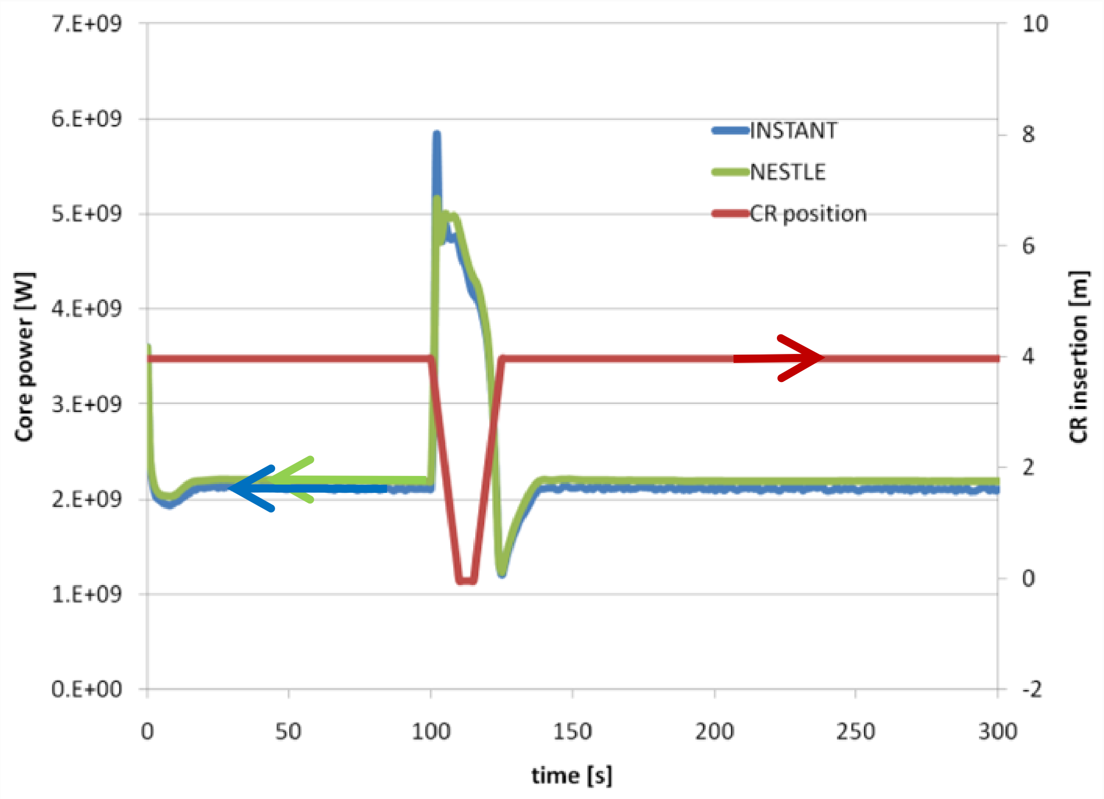
CR out





CR in

Time Dependent: CR movement



- Stability satisfied in the initial phase of the simulation
- Peak in reasonable agreement with REALP5-3D NESTLE
- Convergence studies might improve agreement
- After CR reinsertion power is re-stabilized at initial value

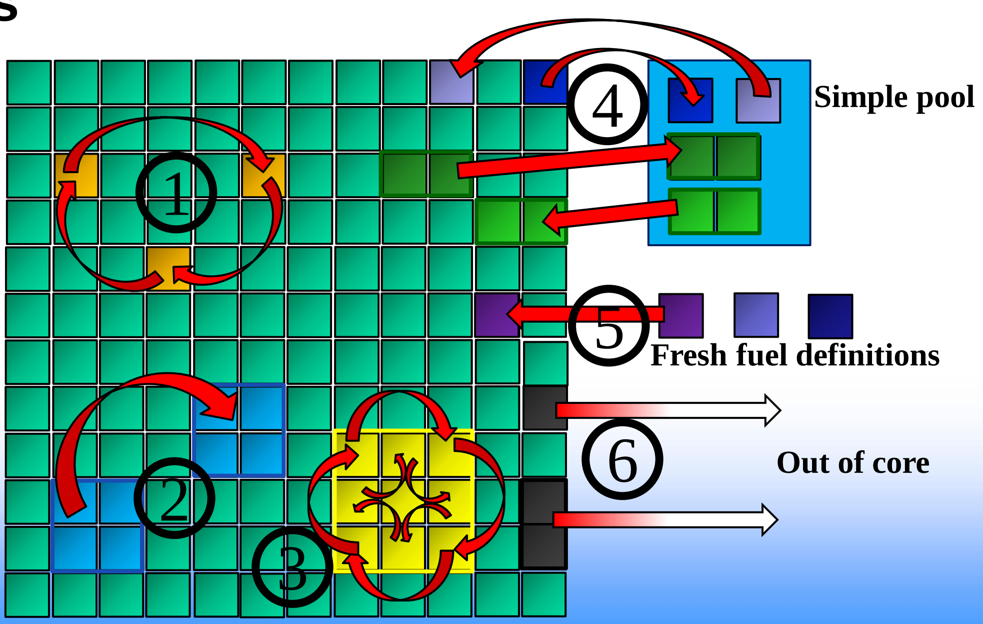
- 300s total transient time
- CR movement: withdrawn from 100s to 110s, reinserted from 115s to 125s

Shuffling scheme

(Allan Mabe Master Thesis)

The composition shuffling module is able to do

1) **arbitrary in-core movements**
2) **grouped in-core movement (for assemblies)**
3) **group rotation (for assemblies)**
4) **grouped/individual core to pool movements**
5) **fresh fuel to core movements**
6) **Grouped/individual movements out of the core (trash)**



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The Pool Approach

Moving toward an integrate reactor analysis tool it is important…

- **Being capable to trace fuel inside and outside the core since things happens also outside**

- **We have the capability to perform isotopic changes for stand alone depletions but it is not yet integrated with RELAP5-3D**

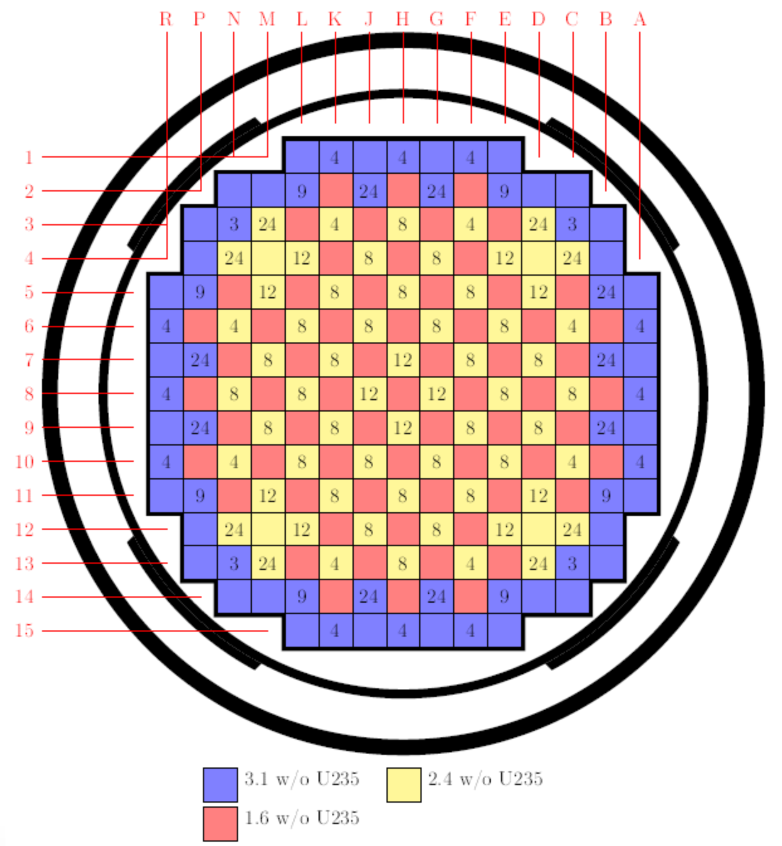
- **A more detailed isotopic heat production would allow for dealing with pool heating problems**

Ongoing: PWR depletion/TH benchmark

(Francesco Lodi Master Thesis)

- **Full core coupled thermal-hydraulics/depletion benchmark**
- **Real plant data available**
- **15x15 assemblies, 32 axial levels**
- **17 different assembly types**
    - **3 different enrichments**
    - **burnable absorber**
    - **control rods**

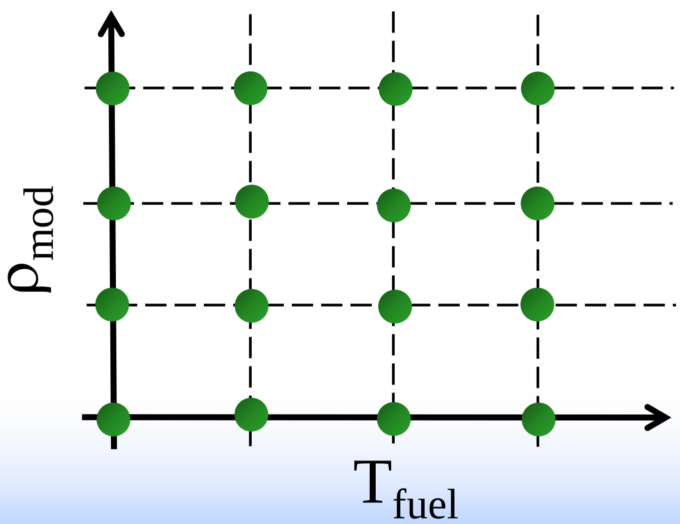
- **Benchmark goals:**
    - **First two cycles in normal operation**
    - **Assembly shuffling between cycles**



PWR depletion/TH benchmark

Cross section library generated with HELIOS

- **~180 isotopes**
- **69 different materials**
  - Assembly types, reflector, spacers, etc..
- **4 tabulation dimensions (4 points each)**
  - Burn-up
  - Fuel temperature
  - Moderator density
  - Boron concentration
- **All cross points considered**
  - 256 tabulation points



PWR depletion/TH benchmark

Zero power figure of merits

- **Critical boron concentration at different temperatures**
- **Reactivity variations for temperature changes**
- **Boron and control rod worth**
- **U235 fission rate**

PWR depletion/TH benchmark

- **3x3 computational nodes per assembly**
  ~60’000 nodes

- **Node-wise depletion**

- **Two cycle goal (24 GWd/HMton)**
  - **compare fission chamber response**
  - **other hot full power figures to be defined**

Perturbation Analysis

(Christopher Kennedy PhD)

- **Reactor Design has been relaying on sensitivity coefficient to**
  - **Short the design process**
  - **Perform safety evaluation**
  - **Evaluate uncertainty**

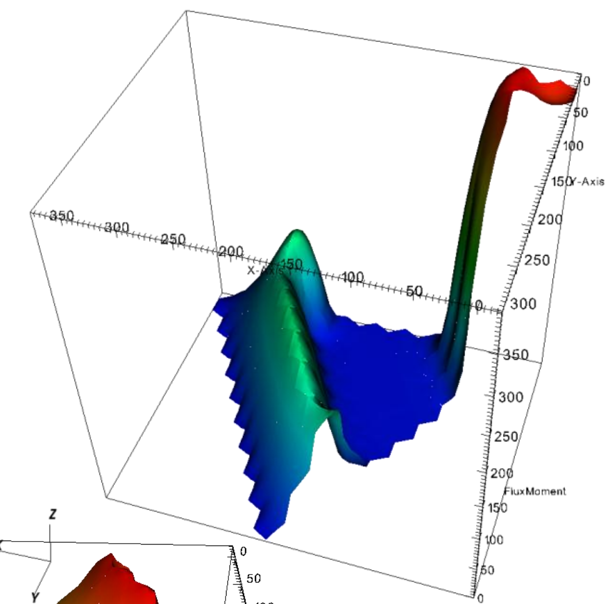
$$\frac{\partial FoM}{\partial p}$$

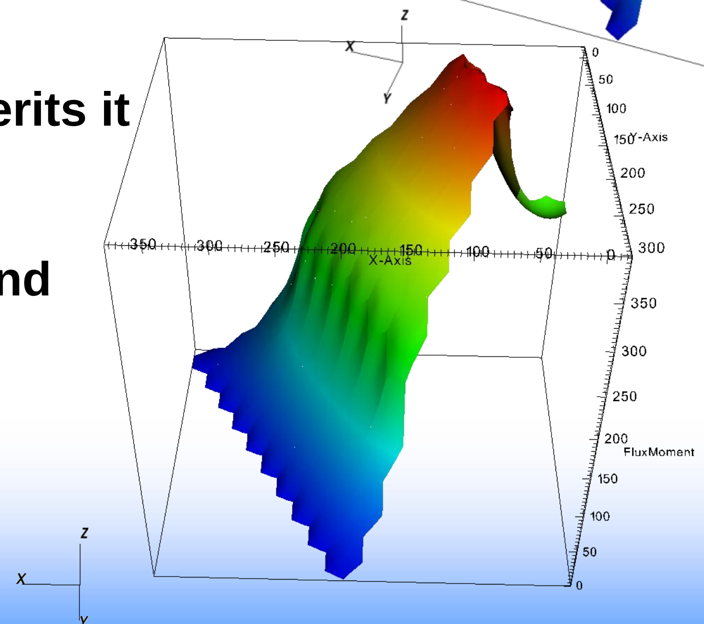
- **Neutronics is a easy problem (linear) therefore adjoint analysis was possible**

Perturbation Analysis in PHISICS

- Since incipit INSTANT had the capability to perform critical adjoint calculation
- Critical adjoint could be used only for sensitivity for K_{eff}
  - Temperature coefficients
  - Void coefficient

- For more complex figure of merits it is needed the generalized perturbation theory (GPT)
  - All type of reaction rates and their linear combination

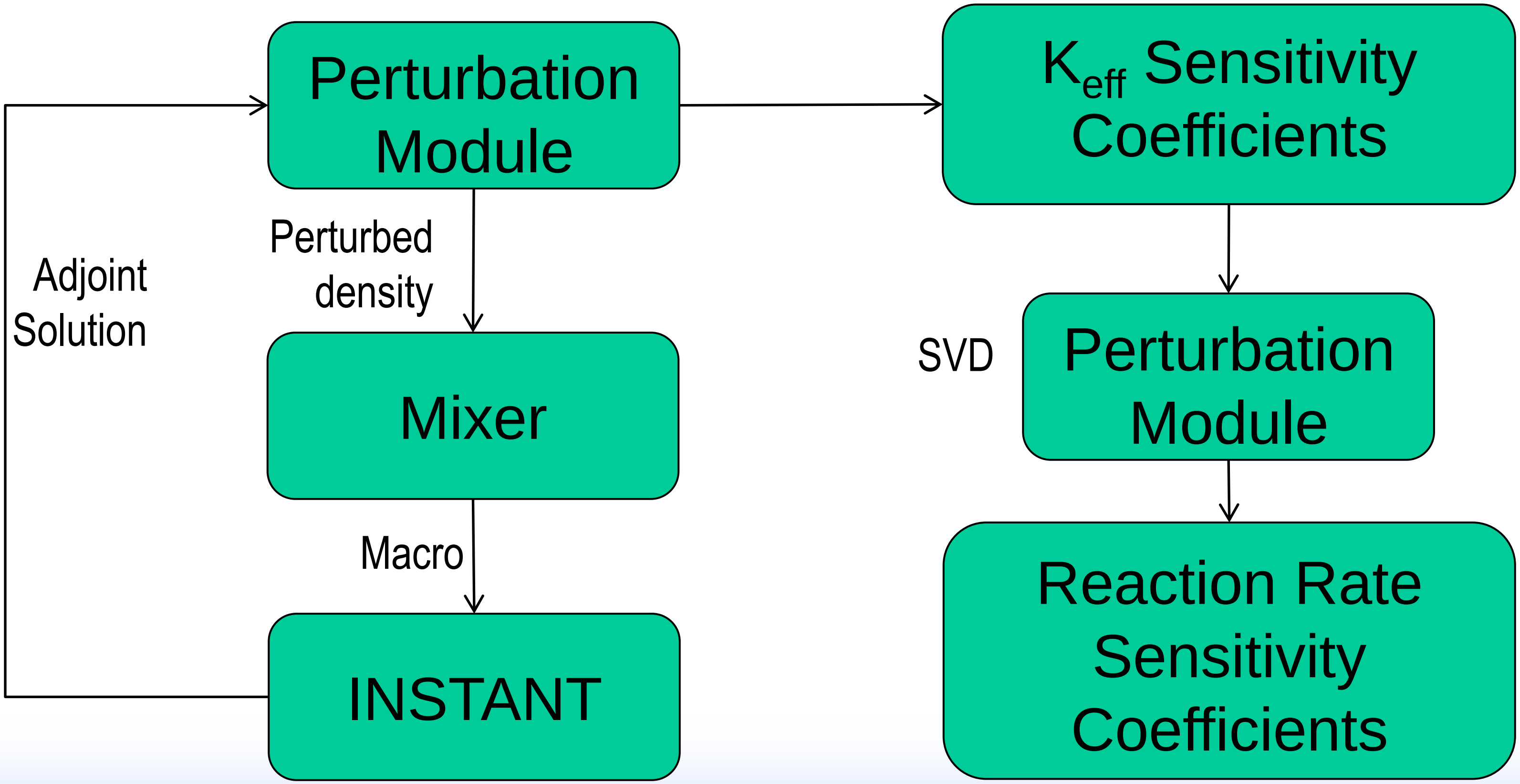




GPT Free Implementation

- In cooperation with NCSU INL has developed a GPT free approach
- In short the K_{eff} sensitivity is seen as a linear combination of the sensitivity of interest
- Sensitivity of interest are extracted from several sampling of the sensitivity of the K_{eff}
- Advantages:
  - No need to implement GPT
  - Number of sampling could be less than the number of sensitivity parameters

GPT Free Schema



RELAP5-3D + PHISICS + GPT free

- **The GPT free module is coming along as we speak so not yet integrated…**

- **The reason why we are looking forward for this implementation:**
  - **Sensitivity coefficient at every possible stage of the reactor simulation in terms of**
    - **Depletion**
    - **TH field**

More Ongoing Developments

- What has not been mentioned so far:
  - Inline cross section homogenization with HELIOS
  - Monte Carlo coupling of the depletion module

How to get RELAP5-3D with PHISICS

- **Coupling available in RELAP5-3D v4.0.3**
- **University**
  - **Executable for free but unsupported (only Linux version) after a regular RELAP5-3D license**
  - **Source code available (RELAP5-3D as a precompiled library)**
    - **Access to INL repository and capability to run locally**
    - **RELAP5-3D executable license required**
    - **INL will retain copyrights of the developments**
    - **Development proposal required**
- **Commercial use TBD but available**

Conclusions

- More additions have been performed toward the generation of a reactor analysis tool with TH and neutronics at the state of the art
- MHTGR benchmark is going smoothly assessing a good level of maturity of the code
- PWR coupled depletion is a challenging benchmark that we expect to accomplish without major road stoppers
- Code capabilities are growing and more is in the pipeline