Foreseen capabilities, bootlenecks identification and potential limitations of Serpent MC transport code in large-scale Full 3-D Burnup Calculations

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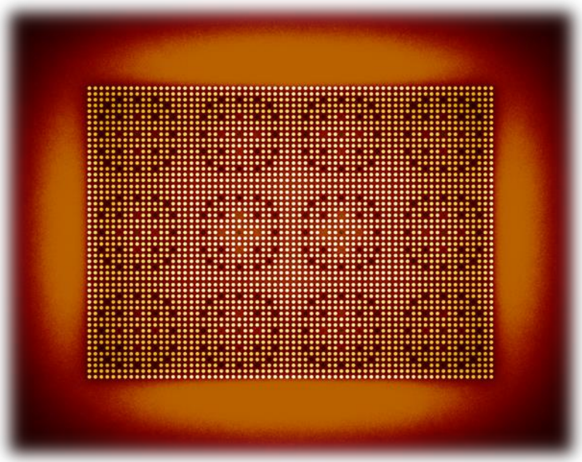

Presentation Overview

- Introduction & motivation
- Modelling goals for high fidelity calculations
- Screening of capabilities and bottlenecks in MC codes:
  - *Burnup instabilities for large problems*
  - *Memory consumption bottlenecks*
  - *Preliminary testing in HPC (parallelization & resources)*
- Discussions of main findings
- Conclusions (& further work)

1 – Introduction & motivation

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- ***Increasing effort*** to develop high accurate multi-physics approach for nuclear reactor analysis of complex phenomenology.
- ***Increasing demand*** from designers, operators, regulators and other stakeholders.
- Several projects around the world oriented to provide ***high-fidelity results*** → improvement of local phenomena calculation & provide reference solution).
- Under this framework, ***McSAFE*** project started in 2017 under Horizon 2020 (EU):

H2020 Mc SAFE High Performance Monte Carlo for Safety

McSAFE*: High –Performance* ***Monte******c****arlo Methods for* ***SAFE****ty Demonstration:*

- ✓ ***Cooperation*** between code developers, methods developers and industry stakeholders.
- ✓ **12 partners** from **9 countries** around EU and an extended community of users around world.

2 - McSAFE: goals for high fidelity calculations

- Move towards high fidelity multi-physics calculations using advanced codes and methodologies.
- High performance Montecarlo (MC) codes to become valuable tools for core design, safety analysis and industry like applications for LWRs of gen II and III.
- ***Final scope***: NPP core level calculations including depletion and TH-feedback in a full scope approach (i.e. pin level):

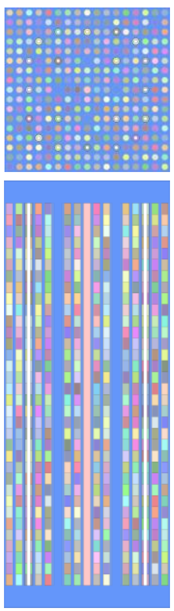
➡ ***Develop MC coupled TH calculations including burnup in an HPC environment for a full core LWR:***

→ Assessment of capabilities and bottlenecks

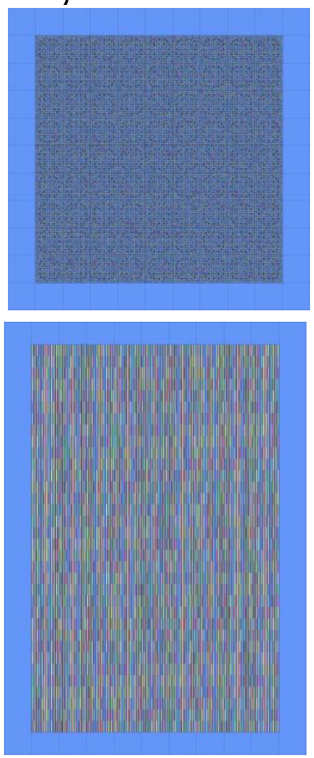
3 – Screening of capabilities

Problem analysis approach for this work

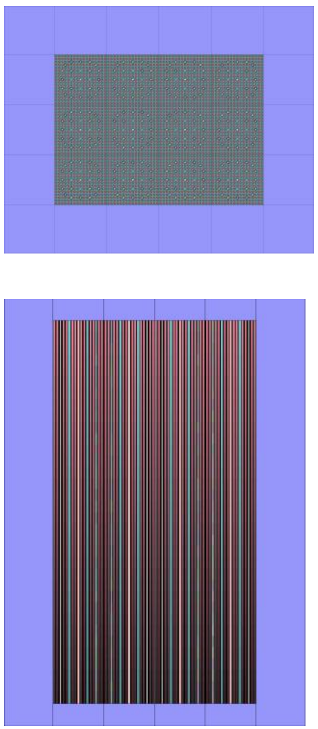
- Advanced MC code **Serpent 2** is considered (developed by VTT-Finland)
- High performance state-of-the-art MC code→ key part of McSAFE
- Increasing complexity approach→ basis BEAVRS 193 FA PWR benchmark
- Identification of issues, bottlenecks and resources requirements



✓ ***FA level***: Burnup instabilities



✓ ***Array level***: memory bottlenecks



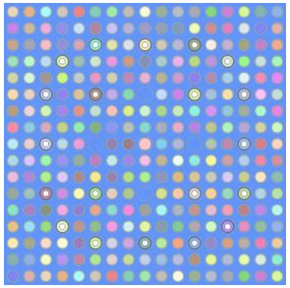
✓ ***Array level with TH capabilities***: HPC environment

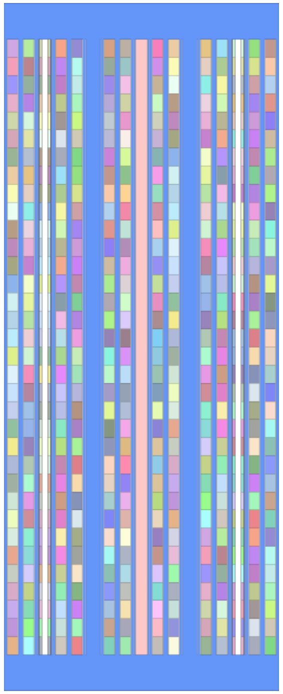
Define ***strategies***

3 – Screening of capabilities & limitations

1. Burnup instabilities in MC codes

- *Tests based on BEAVRS FA with 20BP were developed*:
  - ✓ Simplified 17x17 FA 3.1% wt with **20 BP.**
  - ✓ A 340 axial length - symmetrical w/o axial details (spacers or grids) – 34 axial divisions - Axially reflected (water).
  - ✓ Guide tubes and Instrumentation tubes modelled as empty tubes (i.e filled with coolant water and air respectively).
  - ✓ An overall total fission power of 17MW was considered to model approximate HFP case.
  - ✓ Burnup up to 12.5MWd/kgU → **9656 burnable zones.**





- What we are looking for → ***Potential instabilities*** in power profiles:
  - ✓ Due to burnup step bigger that traditional cell-core approach.
  - ✓ Due to MC statistical nature → induced Xe oscillations.

3 – Screening of capabilities & limitations

1. Burnup instabilities in MC codes

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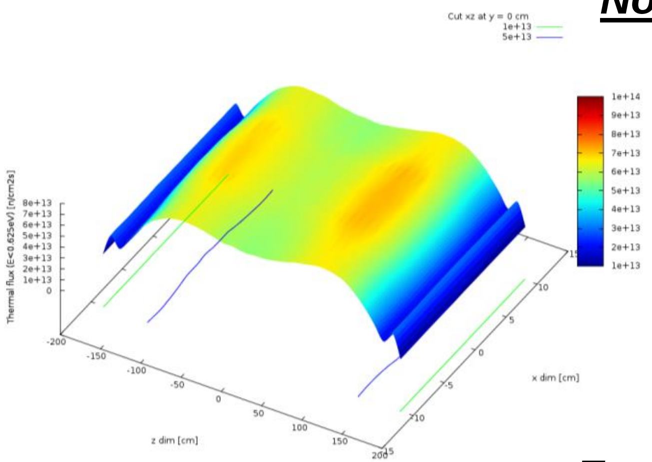
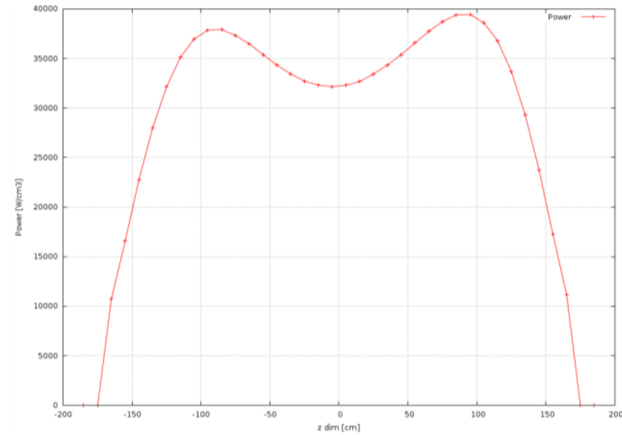
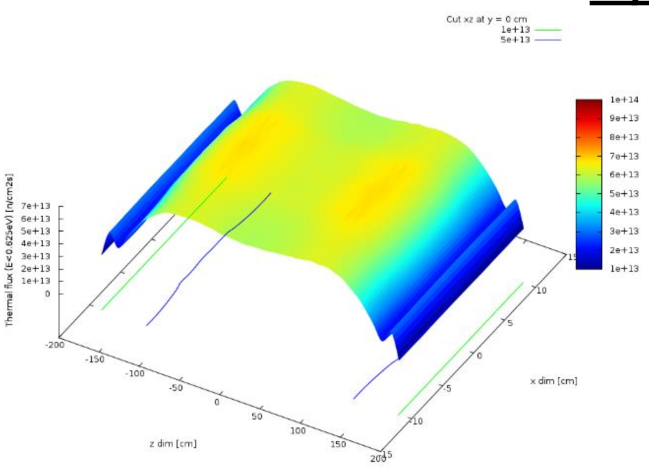
- Observed axial profiles w/ and w/o Xe in equilibrium (final step-qualitative):

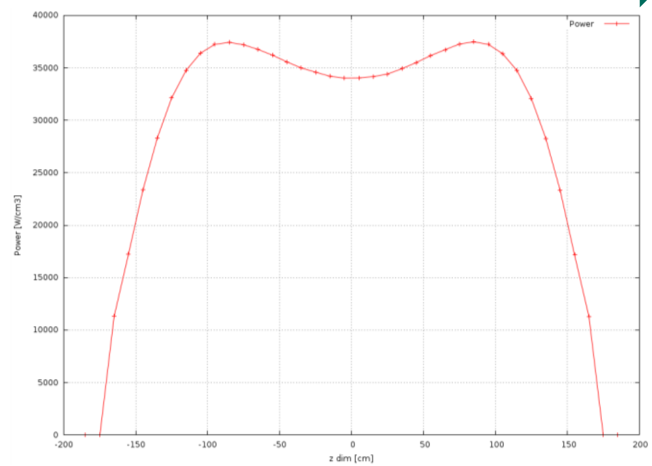
Non equilibrium Xe:





Equilibrium Xe:





Neutron Thermal flux z-x cut ***Integrated axial power***

- ✓ Power profile oscillations are clearly observable
- ✓ Foreseen for other isotopes of high XS
- ✓ High statistical convergence levels required
- ✓ Advanced methodologies under analysis

3 – Screening of capabilities & limitations

2. Memory consumption bottlenecks

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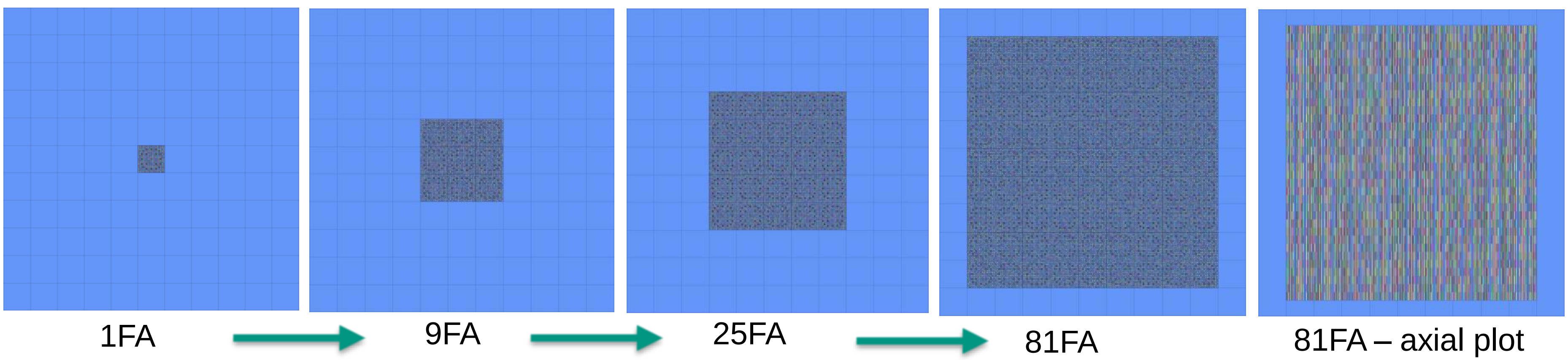
- High number of depletion zones → ***increasing RAM requirement***
- Usually HPC have high number of processors and low RAM → in KIT ***FH2 cluster is available*** → ~20000 cores but 64GB RAM
- How much RAM memory should we expect?
- To analyze this → parametric study w/FA fully divided, investigating total RAM



→ **Number of depletion zones is # FA x 9656**

→ **~ Conservative approach for Full core 193 FA PWR (as BEAVRS) → BP positions replaced by guide tubes**

→ **An ad-hoc cluster node with ~400GB RAM was considered**

3 – Screening of capabilities & limitations

2. Memory consumption bottlenecks

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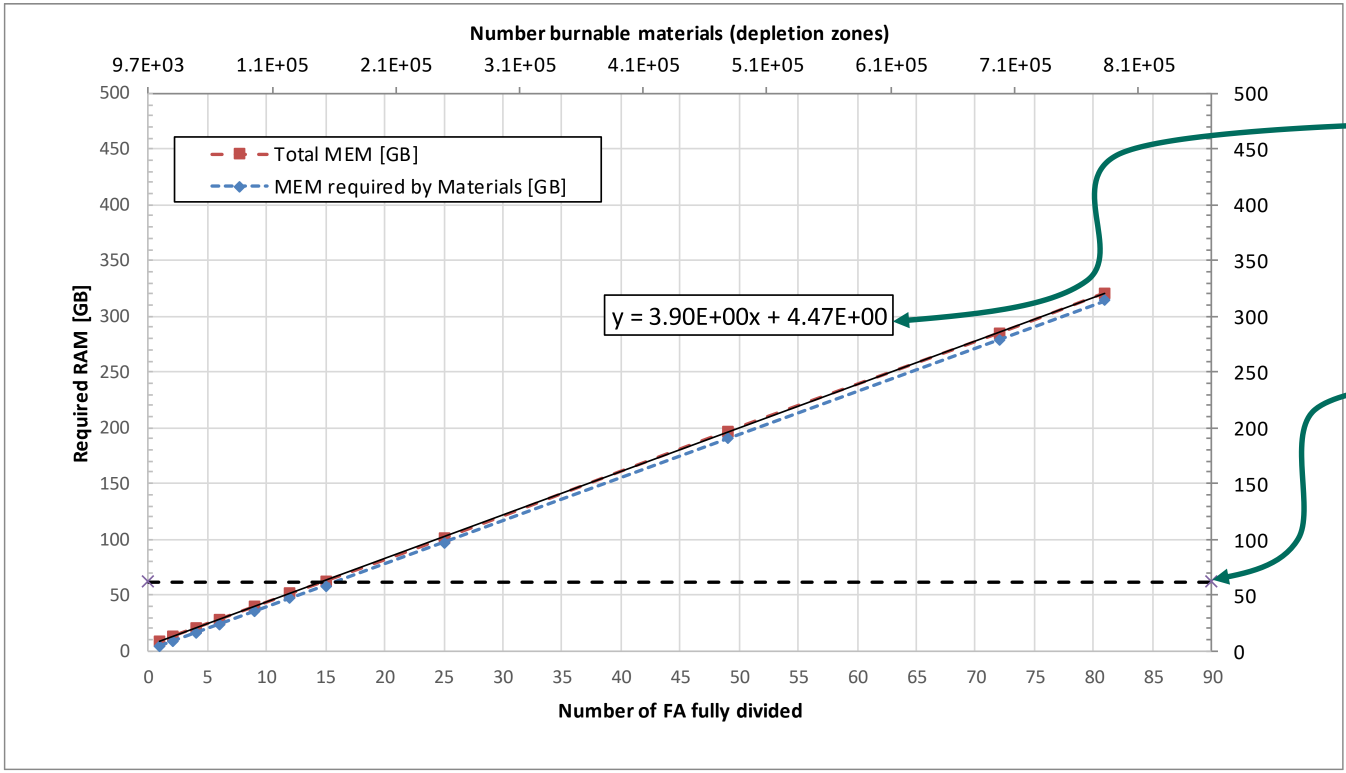
- RAM requirements for this increasing of fully divided FA



~4GB for XS data and miscellaneous

Available RAM per node in our FH2 HPC cluster ~64GB

→ RAM requirement increase linear with depletion zone → **~400kB per burn material**

→ **Maximum foreseen case in our available HPC → ~12FA**

→ **Biggest HPC worldwide have just ~10GB per node We need ~1TB for full PWR)**

Fit the problem in memory represents a bottleneck!

3 – Screening of capabilities & limitations

3. Testing in a HPC environment

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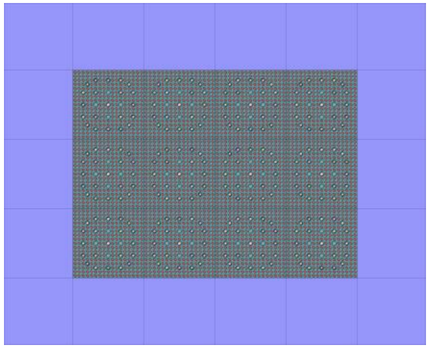
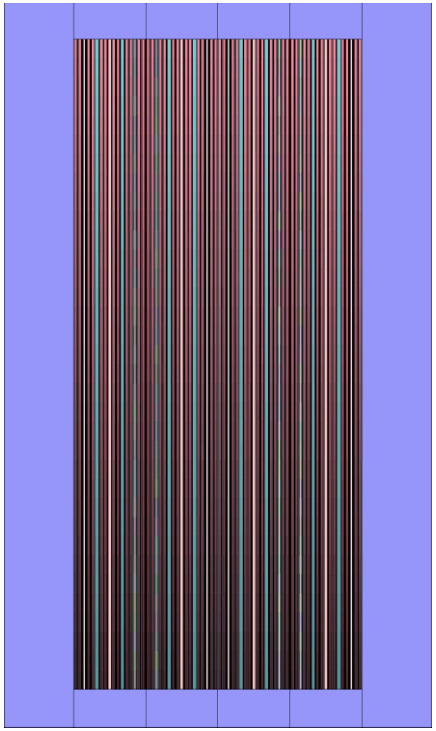
- The most demanding problem that can be nowadays fitted in FH2 HPC was considered:
  - ✓ *A 12 FA array, fully divided (~1e5 burnable zones) was modeled*
  - ✓ *Burn calculations (~1e5 burnable zones)*
  - ✓ *2e9 active histories (2000 active cycles, 1e6 histories each)*
  - ✓ *Up to 100 MPI nodes, 20 CPUs each (up to 2000 cores in total)*
  - ✓ *A PIN by PIN dummy multi-physics feedback was included for fuel and coolant to estimate overhead*
  - ✓ *Power and thermal flux detectors by pin*
- ***Requirements and convergence analyzed***
- ***Multi-physics overhead was analyzed***
- ***Scalability in HPC analyzed***



Top view



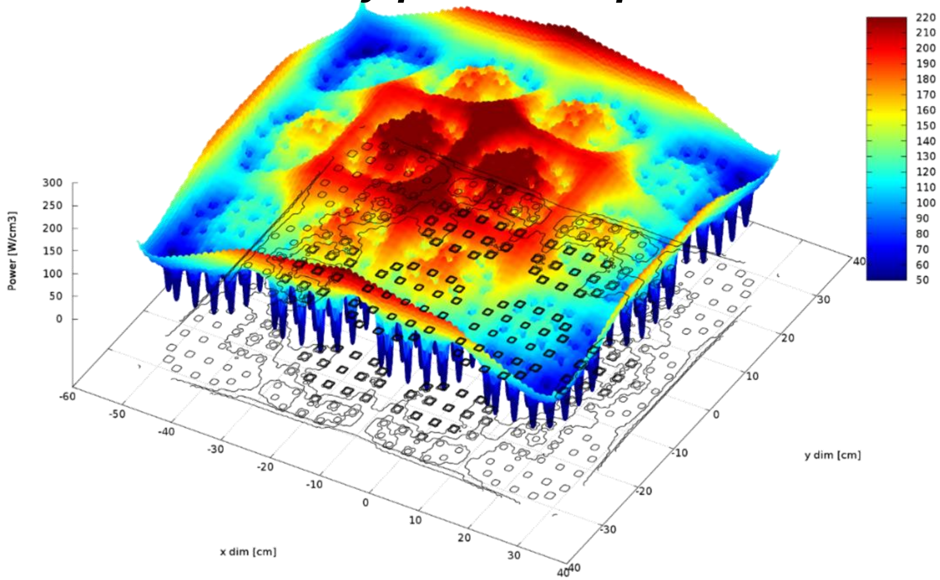
Axial view

3 – Screening of capabilities & limitations

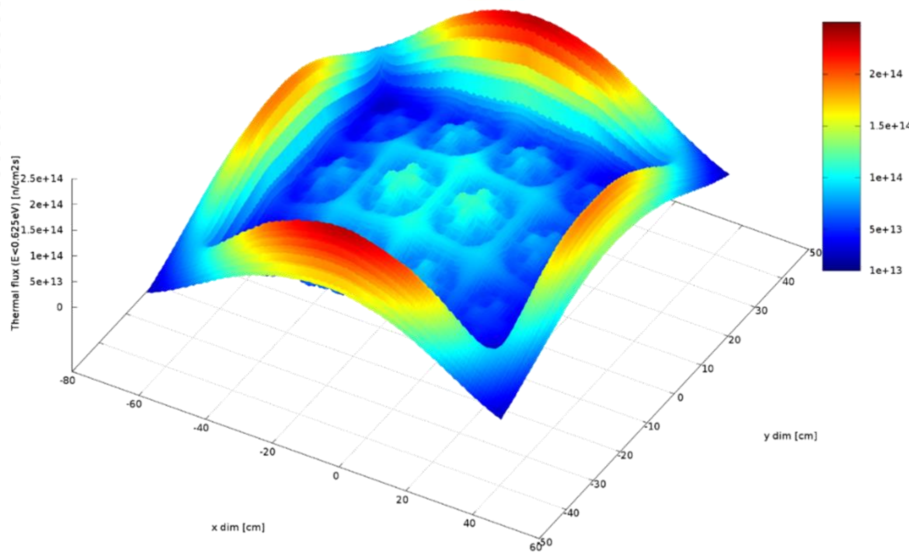
3. Testing in a HPC environment: Resources

- Main results (qualitative):

Power x-y profile midplane:



Thermal neutron flux x-y midplane:



- Main run parameters:

Parameter	Value	Comment
RAM memory (Total)	50.456 GB	Includes all. The node limit is 64GB. Additional memory is to be used by other codes in coupling
RAM memory (materials)	**46.063** GB	*~1e5 burnable zones*
Running time @ 2.6 GHz CPU	~8e4 mins [1]	Per Iterator or corrector step
Running time @ 2.6 GHz CPU w/o MP	~5e4 mins[1]	Per Iterator or corrector step
Calculation time overhead due to MP	~**60**%	
Total active histories	2e9	2000 active cycles of 1e6 histories each

[1] 4.4E4 mins ~1 month CPU

3 – Screening of capabilities & limitations

3. Testing in a HPC environment: Convergence & scalability

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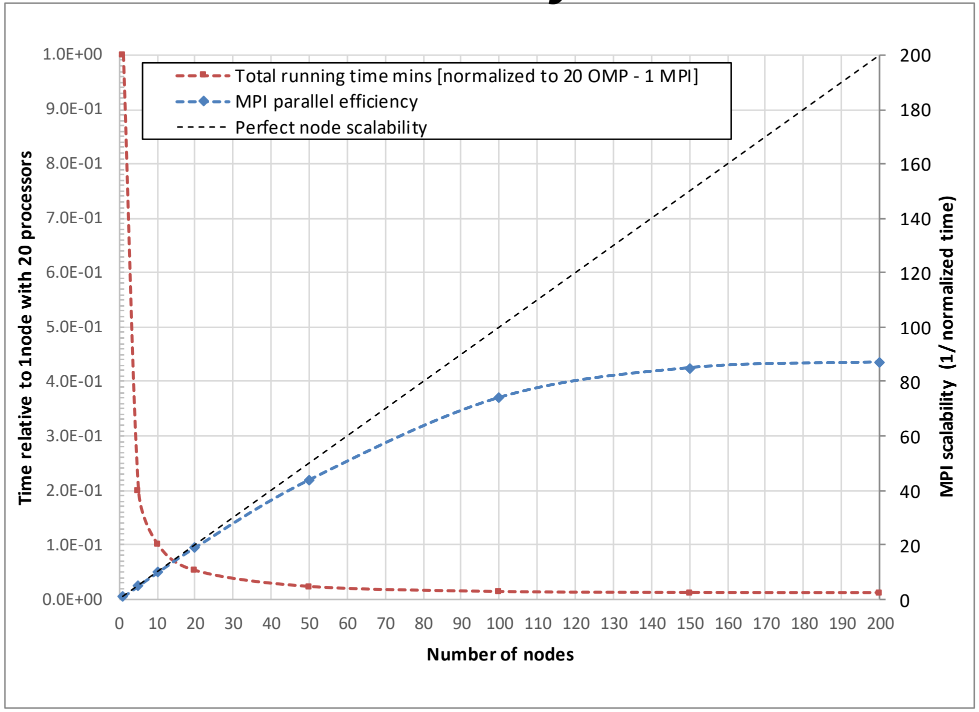
- ***Statistical convergence reached:***

Parameter	Value			
	Max	Min	Average	Stdev
Effective multiplication factor statistical convergence	-	-	-	2.9e-5
Thermal flux detector (tally) statistical convergence	0.0723	0.0032	**0.0071**	0.0040
power flux detector (tally) statistical convergence	0.0260	0.0000	**0.0075**	0.0035

- ***Massive parallelization scalability***:



→ ***Very Good scalability (up to 2000 cores)***

3 – Discussion of main findings

- Burnup instabilities found: face this issue with improved algorithms and methodologies (under development). Specific criteria for some isotopes to be applied.
- Memory bottlenecks:
  - ✓ Improve RAM management for each burnable zone (under development).
  - ✓ Implement Domain Decomposition (collision based) → Please refer to “Development of a spatial domain decomposition scheme for Montecarlo neutron transport” - **ICONE26-82144.**
- Scalability to HPC preliminary results are promissory.
- High fidelity MC calculations with burnup is feasible.

5 – Conclusions

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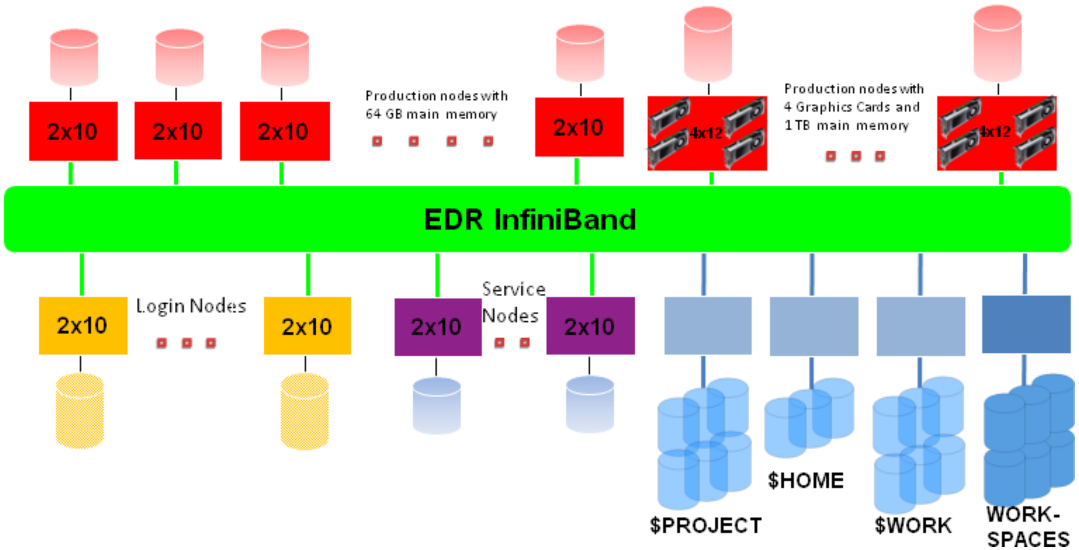
- Increasing demand from designers, operators, regulators and other stakeholders of advanced tools and methods in reactor analysis.
- Several projects around the world oriented to tackle this demand → McSAFE (EU Horizon 2020) started 2017.
- Main aspects of capabilities and bottlenecks of using High performance MC codes (Serpent) for large-scale burn-up calculation problems have been discussed.
- Main aspects analyzed:
  - ✓ *Xenon oscillations (induced by MC approach).*
  - ✓ *CPU and RAM requirements for large scale burnup problems.*
  - ✓ *Resource estimation for the big burnup problems.*
- Solutions to deal with detected issues are under development in McSAFE
- ***Outlook***: Domain Decomposition → Implementation & testing

Questions?
Thank you for your attention!!!

HPC architecture

- HPC used is FH2



- ✓ 1152 20-way Intel Xeon compute nodes.
- ✓ Each w / two Intel Xeon E5-2660 v3 (Haswell)@ 2.6 GHz + 64 GB RAM + 480 GB local SSD.
- ✓ FDR adapter to connect to the InfiniBand 4X EDR interconnect.

Close-up of ForHLR II © KIT (SCC) - https://wiki.scc.kit.edu/hpc/index.php/Category:ForHLR

- MPI+OMP hybrid calculations are mandatory
- RAM is a bottleneck