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High Performance Monte Carlo Computing Projects: from HPMC to McSAFE

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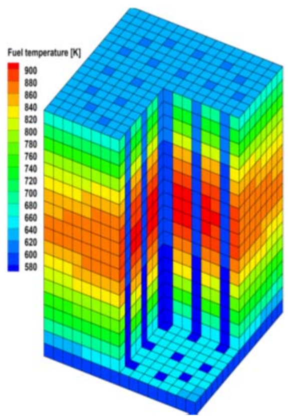
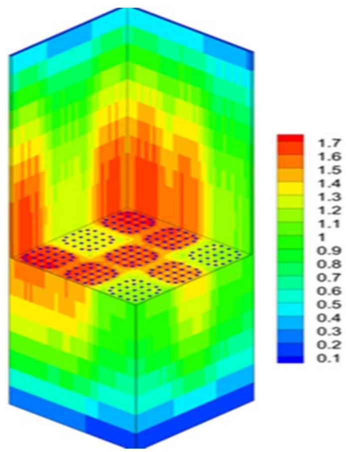
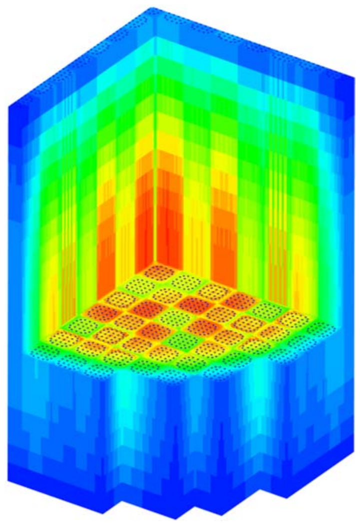


PWR Fuel Assembly



PWR 3x3 FA Cluster



PWR ¼ Core (56 FAs)

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Introduction

- **Currently mainly deterministic codes are used for reactor safety calculations**
  - Based on multiple approximations (energy, angle, homogenized geometry)
  - Pin power approximately reconstructed from 2D lattice calculations
  - SP3 and SN solvers are still under development. These methods are currently very time and memory expensive due to insufficient scalability

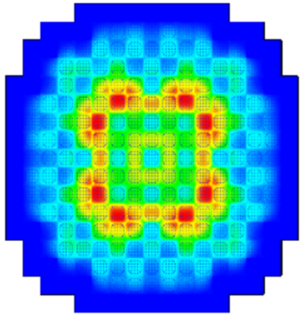
- **Experimental data at pin level is scarce and not easy to be measured**

- **Neutron transport simulations without approximations are needed as reference solutions and for validation**

- **Solution:**
  - Use MC-based multi-physics core simulations with improved depletion, time-dependent MC and massive use of HPC

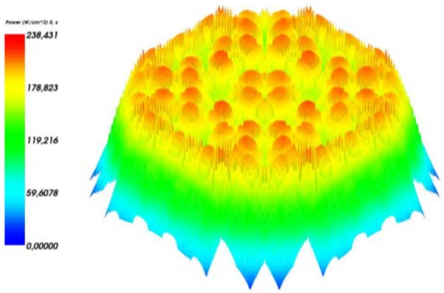
Monte Carlo Based High Fidelity Simulations

- Diffusion + Pin Power Reconstruction (PPR)



DYN3D-PPR: NURISP PWR Boron Dilution Benchmark

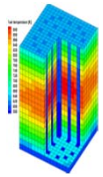
- SP3 Transport /Subchannel



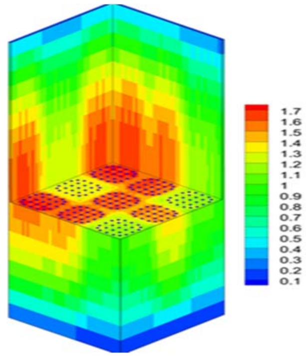
DYNSUB: 3D Avg. Pin Power Density [W/cm³]

Advanced Deterministic Methods

Experimental Data



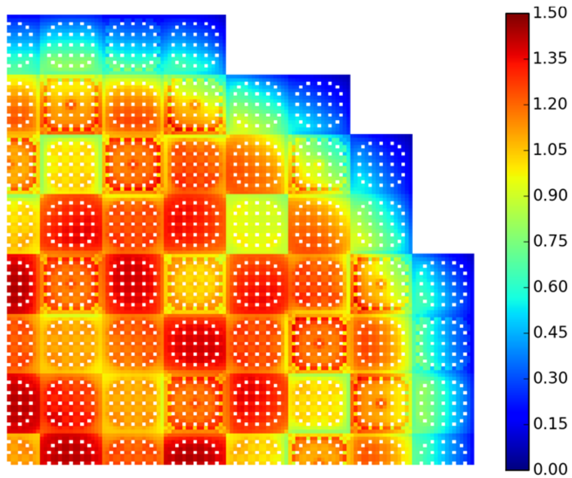
PWR FA



PWR 3x3 FA Cluster

OR

Monte Carlo with TH feedback to provide reference solutions



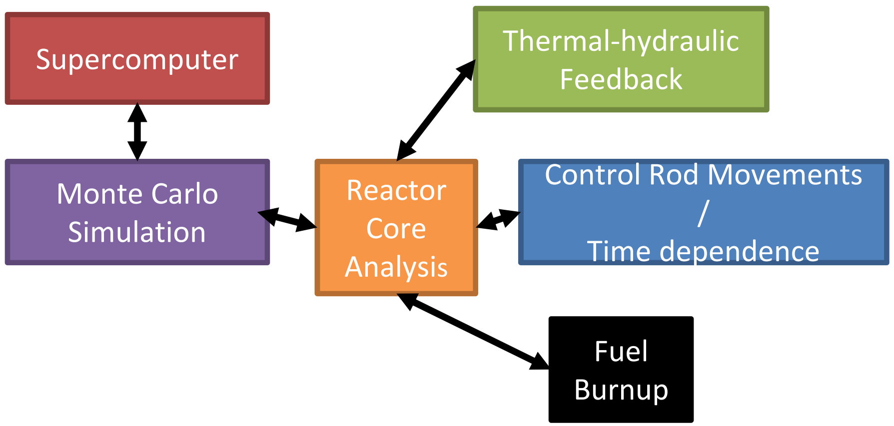
PWR UO2-MOX ¼ Core (56 FAs)

Code-to-code benchmarking

MCNP5/SUBCHANFLOW: High Fidelity Simulations at pin level

The HPMC (High Performance Monte Carlo) Project

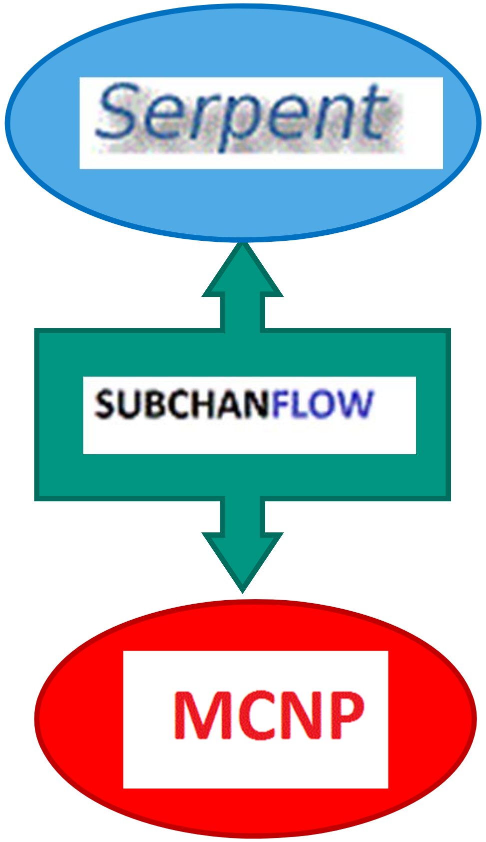
- **Develop and demonstrate (Prof of principle) the application of Monte Carlo codes to full core calculation**
  - With thermal-hydraulic feedback
  - Stable burnup
  - Time dependent
  - Massive use of High Performance Computing (HPC)
  - High-fidelity whole core solutions for safety demonstration



HPMC Project: Main Simulation Tools

- **Monte Carlo Codes:**
  - SERPENT (VTT)
  - MCNP (LANL)

- **TH Codes:**
  - SUBCHAN**FLOW** (KIT)



HPMC: Project Structure

- **WP1: Optimum Monte Carlo- Thermal Hydraulic Coupling (KIT)**
- **WP2: Optimum Monte Carlo-Burn-up Integration (KTH)**
- **WP3: Monte Carlo Time-dependence (DNC)**
- **WP4: Integration of high-performance parallel Monte Carlo (DNC)**
- **WP5: Education and training**

Connections of HPMC with NUGENIA TAs

HPMC is focused on core analysis with Monte Carlo / TH methods

- WP1: Optimize coupling of Monte Carlo with TH codes
  - Very detailed prediction of pin power as reference solution for deterministic multi-physics codes
- WP2: Optimized depletion calculation with MC codes
  - Stable depletion calculation
- WP3: dynamic Monte Carlo methods
  - Extend MC/TH coupled codes to simulate transients e.g. RIA
- WP4: Integration of high-performance parallel Monte Carlo
  - Customized MC / TH codes to run in HPC to solve whole cores at pin level in acceptable CPU time

AREA 1- Plant safety and risk

2. Plant transients: Deterministic assessment of transients
2.18 Develop and validate codes for multi-physics coupling

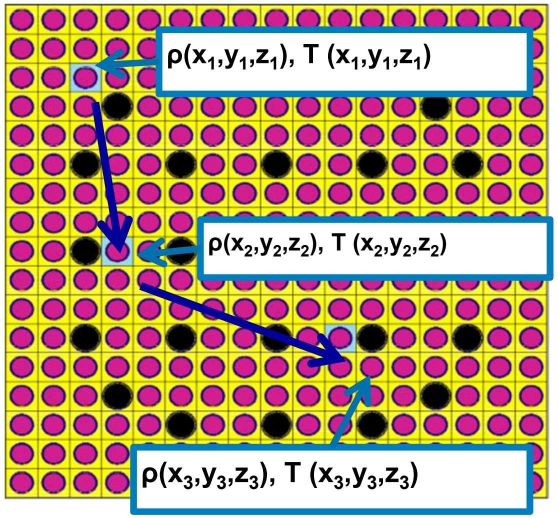
AREA 3- Core and reactor performance

3.3 Numerical modeling and core optimization (to enhance the core modeling capability using the modern method of calculation of the power distributions and of its reactivity)

WP1: Optimum MC / TH Coupling

- **Advanced internal coupling of MC/TH code:**
  - Internal coupling of MCNP5/SUBCHAN**FLOW (KIT, DNC)**
  - Internal coupling of SERPENT2/SUBCHANFLOW (**KIT**)
- **Efficient coupling scheme for whole core simulations at pin-level**
  - On-the-fly material definition
  - Modeling of complex geometries
  - Improved power and flux calculation
  - Variance reduction for criticality calculations
- **Treatment of the temperature-dependency of nuclear data**
  - Neutronic /TH feedbacks (Doppler temp. , moderator density, ..)
  - Thermal neutron scattering in water
- **Convergence of MC / TH coupling schemes: Stochastic implicit Euler**
- **Acceleration of the fission source convergence: Wieland shift**
- **Advanced Variance Reduction methods: UFS**
- **Adaptability of MC / TH coupling for massive parallel computing (HPC)**

High Fidelity MCNP/SUBCHANFLOW: Main Features



3D Online TH feedback during neutron history simulation

- Internal coupling
- Stochastic approximation convergence acceleration
- **On-the-fly** T-interpolation of XS
- **New method** for temperature dependent bound hydrogen scattering
- **Variance reduction** with newly implemented optimized UFS method.
- **Accelerated tallying** with custom written Collision Density and Track – Length estimators
- Hybrid (MPI/OpenMP) Parallelization of MCNP and SCF
- TH Solution acceleration - **BiCGStab**
- Utilization of HPC - **Blue Gene/Q**

Whole Core Simulation at pin level: The Purdue PWR UO2-MOX benchmark

PWR Core Parameter	Values
Inlet Temperature	286.85 C
Exit Pressure	15.45 MPa
Thermal Power	1034.3 MW
Highest Clad Temperature	560 K
Highest Fuel Temperature	1189 K Assembly [4,7], Pin [-5 -7 8]

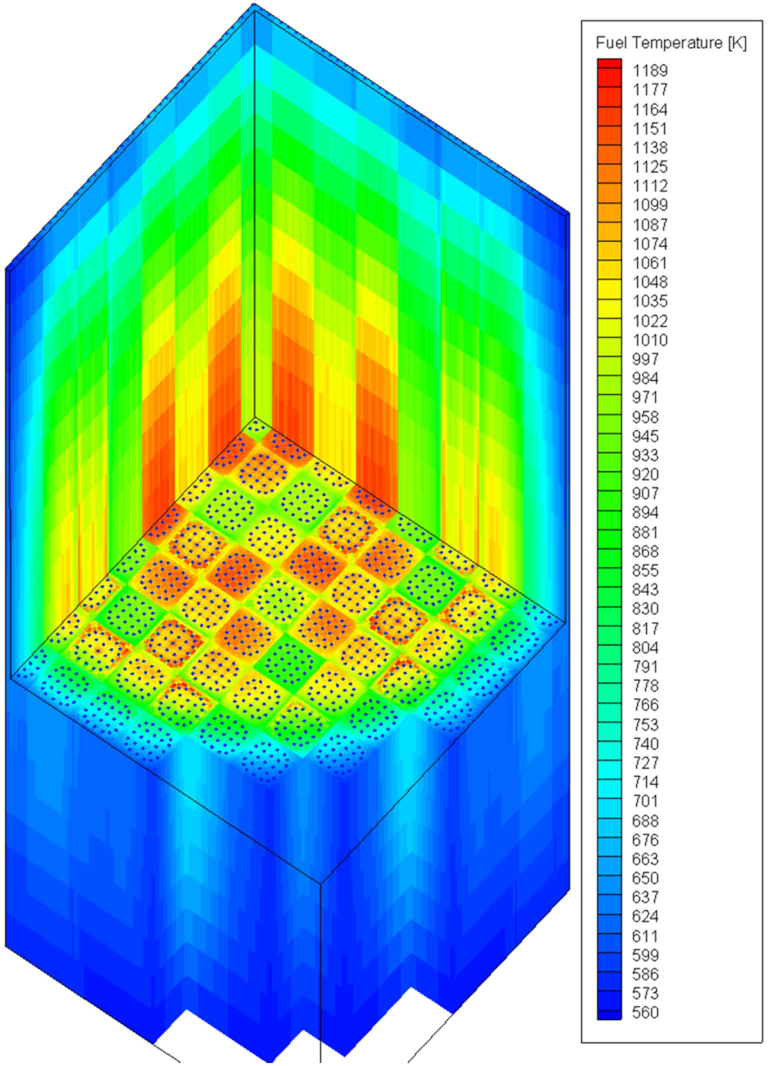
Computer Resources

- 30 dual socket - 16 cores/node – Total 240 Cores
- 2 MPI x 8 OpenMP per node
- 2.5 GB memory per MPI task!

Modeling details

Number of neutron histories:	1 E9 (kcode equivalent)
Number of tally Volumes:	369 920
Number of pins/Axial nodes:	16184 / 20
Number of TH subchannels:	18 145
TH-Neutronic Mapping:	Bijective / Pin level
Fission Source Acceleration:	Wielandt Shift
Criticality mode variance reduction	UFS method
Coupled N/TH Scheme Acceleration:	Stochastic Accelerated fixed point search

MCNP/SUBCHANFLOW: Direct prediction of local safety parameters



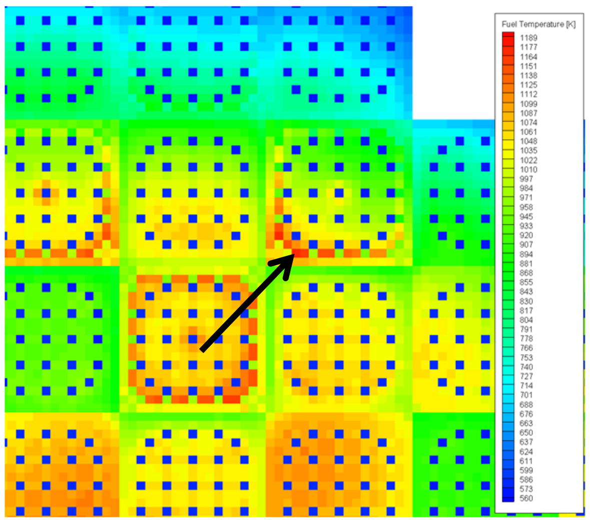
	1	2	3	4	5	6	7	8
A	U 4.2% (CR-D) 35.0	U 4.2% 0.15	U 4.2% (CR-A) 22.5	U 4.5% 0.15	U 4.5% (CR-SD) 37.5	M 4.3% 17.5	U 4.5% (CR-C) 0.15	U 4.2% 32.5
B	U 4.2% 0.15	U 4.2% 17.5	U 4.5% 32.5	M 4.0% 22.5	U 4.2% 0.15	U 4.2% (CR-SB) 32.5	M 4.0% 0.15	U 4.5% 17.5
C	U 4.2% (CR-A) 22.5	U 4.5% 32.5	U 4.2% (CR-C) 22.5	U 4.2% 0.15	U 4.2% 22.5	M 4.3% 17.5	U 4.5% (CR-B) 0.15	M 4.3% 35.0
D	U 4.5% 0.15	M 4.0% 22.5	U 4.2% 0.15	M 4.0% 37.5	U 4.2% 0.15	U 4.5% (CR-SC) 20.0	M 4.3% 0.15	U 4.5% 20.0
E	U 4.5% (CR-SD) 37.5	U 4.2% 0.15	U 4.2% 22.5	U 4.2% 0.15	U 4.2% (CR-D) 37.5	U 4.5% 0.15	U 4.2% (CR-SA) 17.5	
F	M 4.3% 17.5	U 4.2% (CR-SB) 32.5	M 4.3% 17.5	U 4.5% (CR-SC) 20.0	U 4.5% 0.15	M 4.3% 0.15	U 4.5% 32.5	
G	U 4.5% (CR-C) 0.15	M 4.0% 0.15	U 4.5% (CR-B) 0.15	M 4.3% 0.15	U 4.2% (CR-SA) 17.5	U 4.5% 32.5		
H	U 4.2% 32.5	U 4.5% 17.5	M 4.3% 35.0	U 4.5% 20.0				

Assembly Type
CR Position
Burnup [GWd/t]

Fresh
Once Burn
Twice Burn

CR-A	Control Rod Bank A
CR-B	Control Rod Bank B
CR-C	Control Rod Bank C
CR-D	Control Rod Bank D
CR-SA	Shutdown Rod Bank A
CR-SB	Shutdown Rod Bank B
CR-SC	Shutdown Rod Bank C
CR-SD	Shutdown Rod Bank D
O	Ejected Rod

Real core loading!



WP2: Optimum Monte Carlo-Burn-up Integration

- **Develop MC burnup codes that can provide reference solutions of the full-core nuclide and flux fields during the full reactor cycle**
  - Implement optimised scheme for integration of Monte Carlo and burnup calculations with **parallel execution** of the burnup calculations

- **Governing equations:**
  - Flux field ← eigenvalue (criticallity) calculation (depends on the nuclide field)
  - Nuclide field ← ordinary differential burnup equation (depend on the flux field)

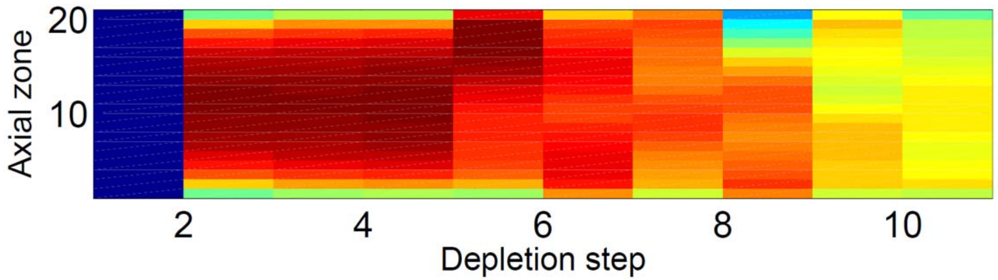
- **Solution by various numerical methods:**
  - Explicit Euler (MCB, MOCUP, ALEPH) ... numerically unstable!
  - Mid-point method (MCNPX, MONTEBURNS) ... numerically unstable!

- **Search for stable methods?**
  - Implicit Euler, modified Euler, and more advanced methods.

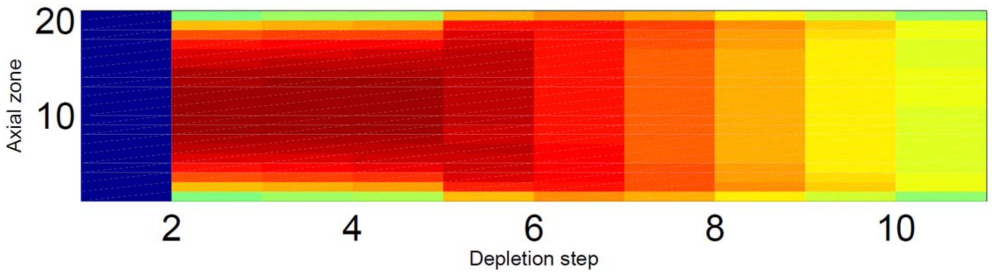
  ➔ **What is the ideal method for MC burnup?**

WP2: Selected Results
Optimal Monte Carlo Depletion Integration

- Numerical instability of the commonly used predictor-corrector method was demonstrated in MC burnup calculations
- New **S**tochastic **I**mplicit **E**uler (**SIE**) based MC burnup scheme was suggested.
- The SIE-based scheme was proved to be stable for any time step length, which was also demonstrated on a PWR-FA MC burnup calculations



Predictor-corrector based MC burnup: Spatial distribution of Xe-135 for a PWR-FA with 10.0 MWd/kgU step.



SIE-based MC Burnup: Spatial distribution of Xe-135 for a PWR-FA with 10.0 MWd/kgU step (same statistics in all calculations).

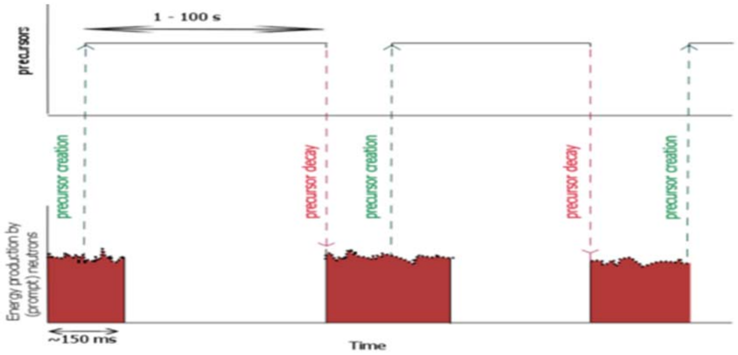
WP3: Monte Carlo Time-dependence

- **Develop dynamic MC-Codes capable of dealing with time-dependent problems including TH feedback for safety assessment**
  - Envisaged time domain: seconds and minutes
  - Describe behaviour of delay neutrons precursors (generation and decay)
  - Efficient implementation ➔ Variance reduction techniques for decay precursors
  - Describe movement of control rods
  - Full parallel implementation needed
- **Implement developed methods in MCNP5**
- **Demonstrate POTENTIALS for safety analysis**
- **Major challenges in the statistics of predicted power as a function of time:**
  - The inherent statistics in the chain length of prompt neutrons
  - Large difference in lifetime of a prompt neutron chain (< 1 ms) and decay time of neutron precursors (0.1 to 100 s)

Dynamic MC: Solutions Approach

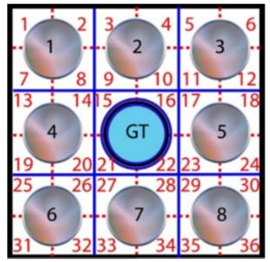
- Introduction of innovative techniques e.g.
  - Use cycle methodology for time interval
  - Use of concept of storing precursors for next time interval
  - Add prompt neutrons that reach the time interval boundary
  - Distinguish precursors by negative weight
  - forced decay of precursors in each time interval (to reduce variance)
  - branchless collision method: allows always a single neutron continuing after a collision (either from scattering or fission)
  - Novel and accurate technique to describe the movement of control rods or control rod banks

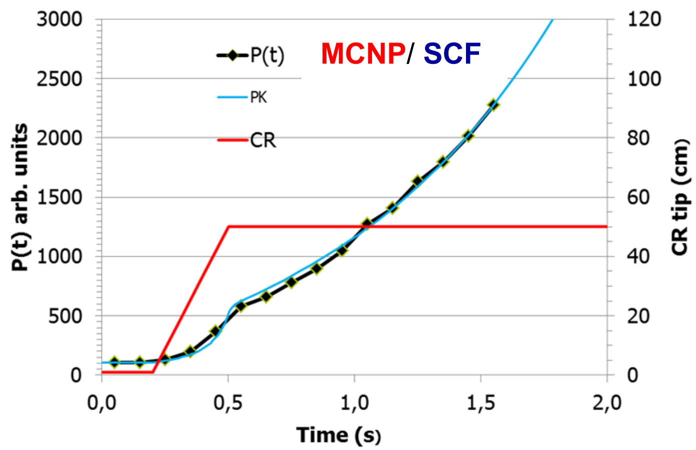
- Status: Methods are about ready to demonstrate the calculation of time dependence in the time domain of seconds with a Monte Carlo code without any approximation to the physical modelling



Dynamic MC: Concept of time intervals

- **Test problem:**
  - Pin cluster with 3x3 rods
  - Centre rod replaced by moveable CR
  - Boron concentration tuned for criticality
  - From criticality run special "wssa" file prepared to start time dependence





Code-to-code Benchmarking

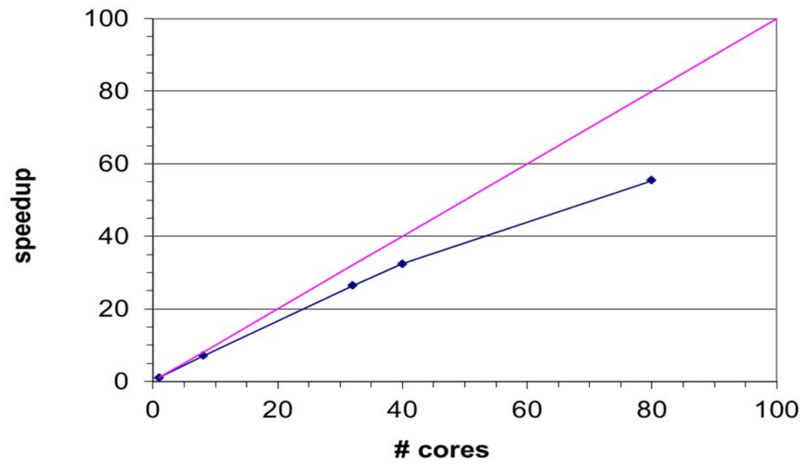
WP4: Integration of high-performance parallel Monte Carlo

- **Demonstration of full core MC based on dynamic safety analysis with ultimate efficiency in parallelisation**
  - Requires several demo problems
  - Very challenging
  - Massively parallel calculation on supercomputers

- **Main tasks for this purpose:**
  - Minimisation of data exchange between processors in parallel Monte Carlo criticality calculations
  - Implementation of optimum (hyper)threading and load balancing in SERPENT and MCNP
  - Demonstration of efficient massive parallelisation of SERPENT and MCNP on a supercomputer
  - Demonstration of the capabilities of the final product for a full-core reactor system after control rod ejection

WP4: Selected Results for MCNP5.1.51

- Effective utilization of HPC
  - Use master tool for simulations
  - Send only relevant part of fission bank to each slave
  - Exclude unwanted stops for rendezvous points
  - **Even using small number of processors the speedup if far from the theoretical maximum**
  - **Cause: Extensive master-slave communication overhead**
  - **Significant improvements needed to effectively run on large scale computers.**

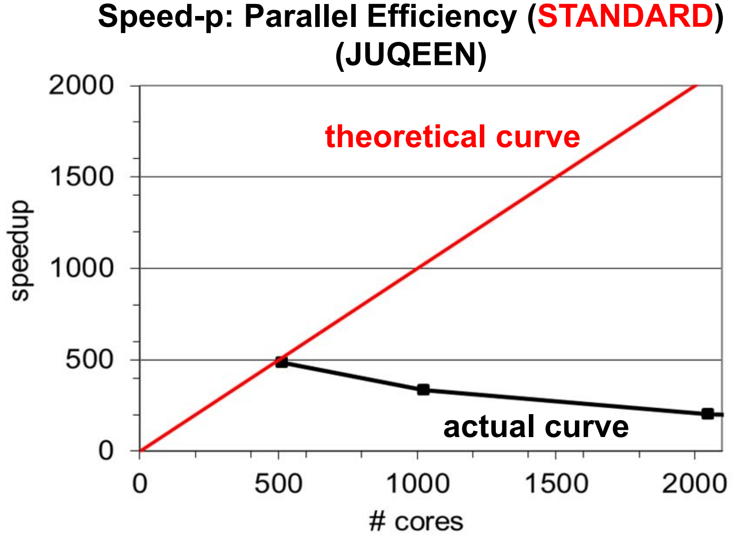


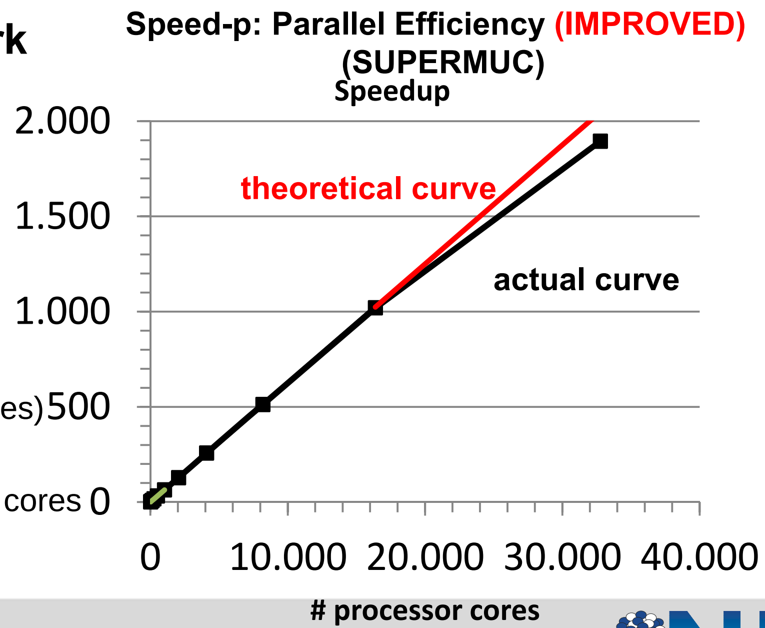
Speed-up on small Cluster

WP4: Selected Results for MCNP5.1.60

- **MCNP5.1.60**
  - Full fission bank is sent at the start
    - only necessary when “srctp” file is used
    - then only relevant part per slave
  - Former tallying improvement was made for fixed core of Performance Benchmark
  - Now input file is reread to determine FA and core layout -> much more general
  - Tricky parallelisation

- **Full-core problem from Performance benchmark**
  - 241 FAs of 17x17-25 fuel pins
  - 100 axial zones per fuel pin
    - about 7×10^6 tally bins
  - No TH feedback
  - Needs at least 10^9 neutron histories
  - Execution:
    - Preliminary preparation of converged source (100 cycles)
    - 1000 cycles of 10^6 histories for power tallying
    - Parallel execution on supercomputer with nodes of 16 cores





Main Outcome of HPMC

- **New innovative coupling approaches for MC and Subchannel codes developed and applied for full core pin/by/pin solutions**
  - On-the-fly thermal-hydraulic feedback
  - Improved physics
- **New DynMCNP time-dependent coupled code for transient analysis developed**
  - Delay neutrons and control rod movement included
  - Rod ejection of a 3x3 pin clusters simulated
- **New implicit unconditionally stable Monte Carlo depletion method was implemented**

→ **Very promising developments**

The McSAFE Project Goals

- Validation of coupled MC/TH Codes using experimental data (VVER/1000, SPERT)
- Further development of dynamic Monte Carlo codes (MCNP, SERPENT, TRIPOLI) to be able to simulate real cores (safety cases)
- Implementation of fuel pin mechanics solvers in the coupled MC / TH codes
- Optimization of MC and TH codes for HPC-applications for safety for LWR, FR and research reactors
- Education and Dissemination of knowledge
- Partners: KIT, CEA, KTH, VTT, DNC, UJV Řež
- McSAFE got a NUGENIA LABEL
- H2020 evaluation: 14 point (but no budget due to big competition)
- McSAFE partners will improve proposal and resend it to next H2020 call (in 2015?)

Thank you for your attention

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