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Title: Reactor Physics Analysis with Monte Carlo

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Intended for: ANS PHYSOR-2010 Conference Workshop
9 May 2010, Pittsburgh, PA

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LA-UR-10-02762

PHYSOR 2010 Workshop
Pittsburgh PA, 9 May 2010

Reactor Physics Analysis with Monte Carlo

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Abstract

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Reactor Physics Analysis with Monte Carlo

Workshop for PHYSOR-2010, Pittsburgh PA, 9 May 2010

Forrest Brown (LANL), William Martin (U. Mich), Jaakko Leppanen (VTT), Wim Haeck (IRSN), Bertrand Cochet (IRSN)

Monte Carlo criticality calculations are performed routinely on large, complex models for reactor physics applications. This workshop provides an introduction to some of the key issues for code developers and reactor analysts, a summary of best practices for Monte Carlo calculations, and a review of current and future Monte Carlo code capabilities. The workshop includes university, national laboratory, and industry perspectives. It should benefit both Monte Carlo practitioners and developers.

- Challenges for Large-Scale Reactor Calculations - W.Martin
- Reactor Physics Calculations with MCNP5 & Status of MCNP6 - F. Brown
- Serpent - a Monte Carlo Reactor Physics Burnup Calculation Code - J. Leppanen
- Reactor Physics Calculations Using VESTA and MORET5 - W. Haeck & B. Cochet

Agenda

William R. Martin (Univ. Michigan)

Challenges for Large-Scale Reactor Calculations

Forrest B. Brown (LANL)

Reactor Physics Calculations with MCNP5 & Status of MCNP6

Jaakko Leppanen (VTT)

Serpent - a Monte Carlo Reactor Physics Burnup Calculation Code

Wim Haeck & Bertrand Cochet (IRSN)

Reactor Physics Calculations Using VESTA and MORET5

Reactor Physics Calculations with MCNP

Forrest Brown

Monte Carlo Codes, XCP-3

Los Alamos National Laboratory

- **Best Practices Summary**
  - Convergence, Bias, Statistics
- **Adjoint-Weighted Tallies**
  - Reactor Kinetics Parameters
  - Perturbations
- **Recent Improvements to MCNP5**
  - Large Problems - Geometry, Materials, Tallies
  - General Improvements
  - "Kord Smith Challenge" & Large-scale Calculations
- **MCNP6 Status**

Best Practices

Summary

Introduction

- **Several fundamental problems with MC criticality calculations were identified in the 1960s - 1980s:**
  - **Convergence of K_{eff} & source distribution**
  - **Bias in K_{eff} & tallies**
  - **Underprediction bias in tally statistics**

(see Lieberoth, Gelbard & Prael, Gast & Candelore, Brissenden & Garlick)

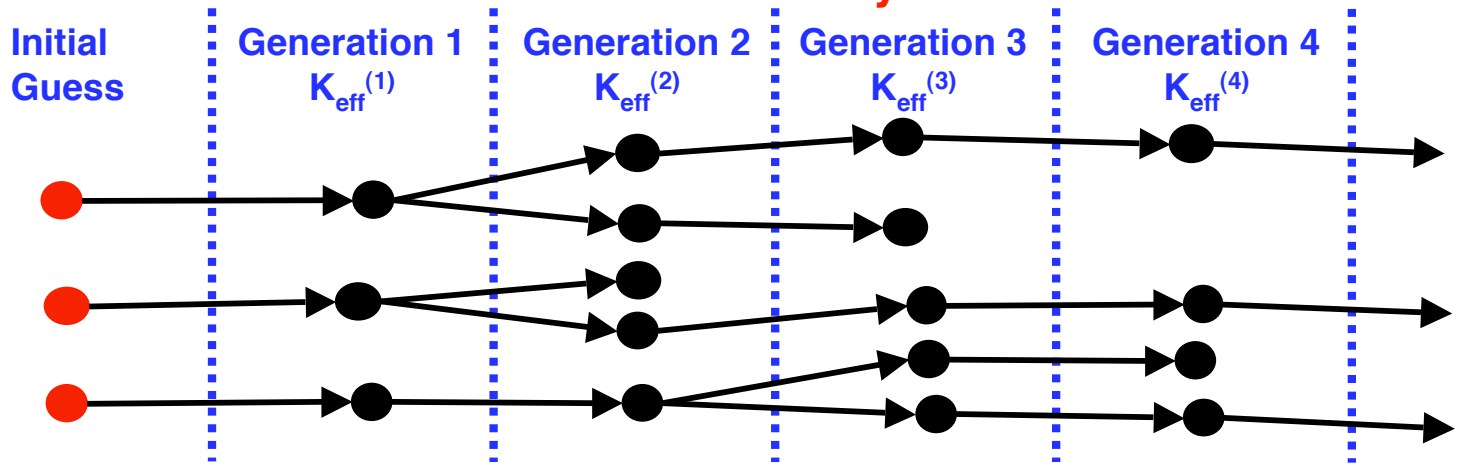
- **These problems are well-understood & can be readily avoided, if some simple "best practices" guidelines are followed**

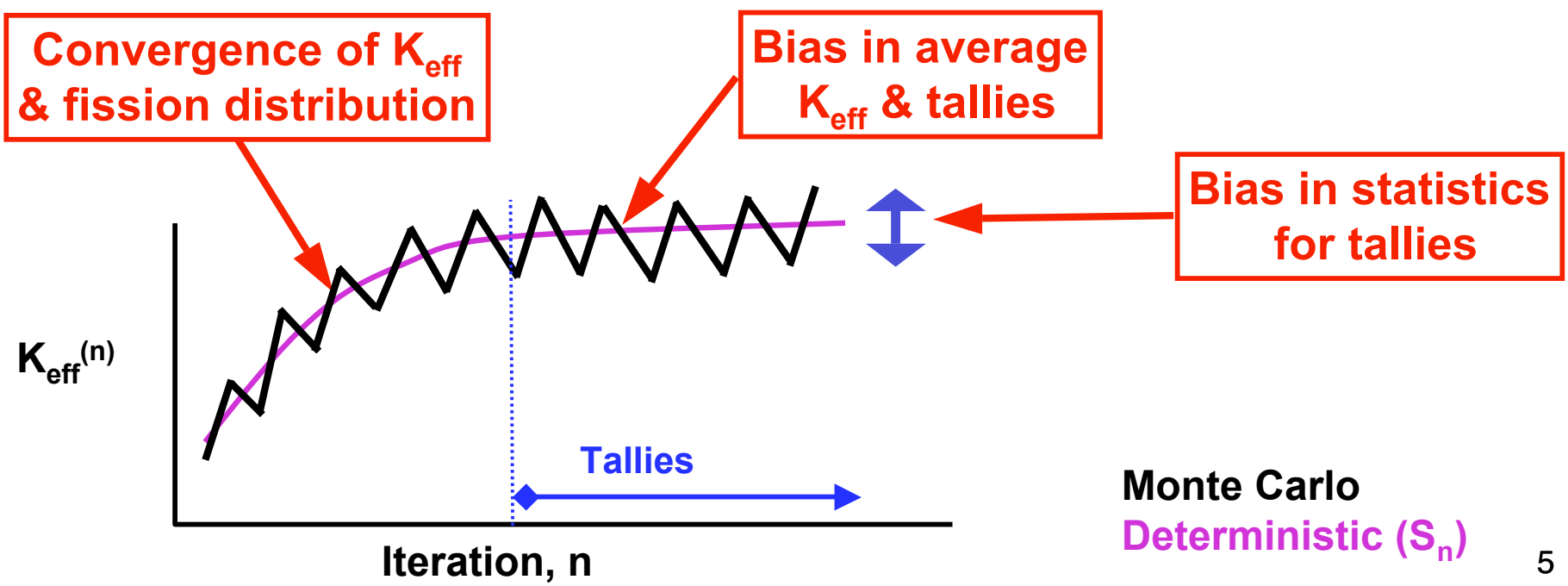
- **Previous discussion of details:**
  - **PHYSOR-2008 Monte Carlo workshop**
  - **Math & Comp 2009 Monte Carlo workshop**

Both presentations available at
http://mcnp.lanl.gov/publication/mcnp_publications.html

Concerns

Power Iteration for MC Criticality Calculations





Best Practices - Summary

- **To avoid bias in K_{eff} & tally distributions:**

  - Use 10K or more neutrons/cycle (maybe 100K+ for full-core)
  - Discard sufficient initial cycles
  - Always check convergence of both K_{eff} & the fission distribution

- **To help with convergence:**

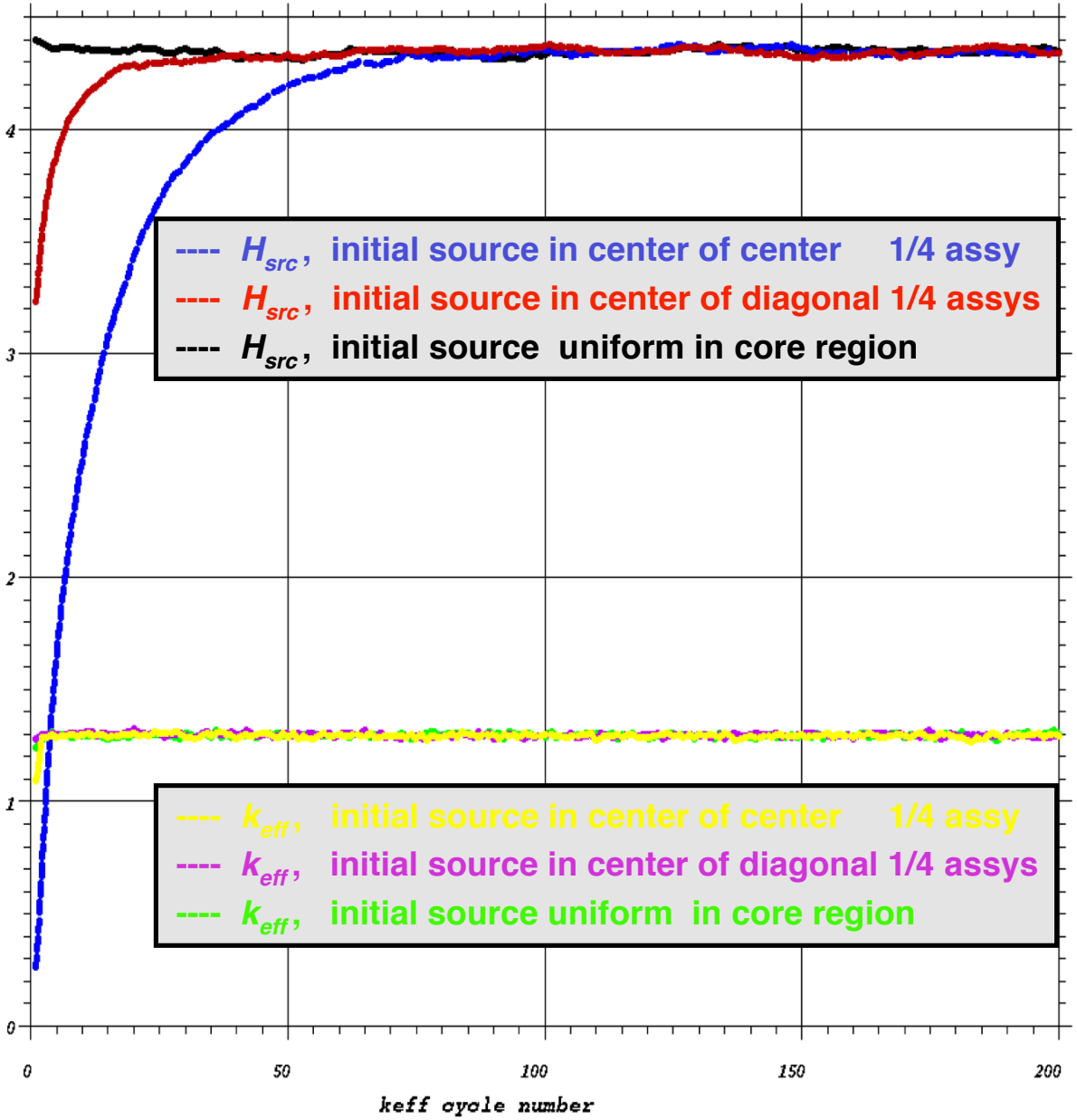
  - Take advantage of problem symmetry, if possible
  - Use good initial source guess, cover fissionable regions

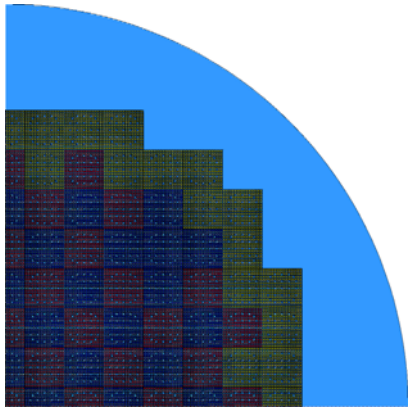
- **Run at least a few 100 active cycles to allow codes to compute reliable statistics**

- **Statistics on tallies from codes are <u>underestimated</u>, often by 2-5x; possibly make multiple independent runs**

Convergence - Reactor Example

Monte Carlo Codes
XCP-3, LANL





K_{eff} converges sooner than the fission distribution

H_{src} =

- **Shannon entropy of fission source distribution**
- **A metric for assessing convergence of the distribution**
- **Computed/plotted by MCNP**

Convergence - Guidance

- Plot K_{eff} vs cycle to check convergence of K_{eff}

- If computing any tallies (flux, fissions, dose, foils, heating, …) plot H_{src} vs cycle to check convergence of fission distribution

- Dominance ratio $\rho = k_1 / k_0$ determines the rate of convergence
  - Smaller dominance ratio ⇒ fewer cycles to converge
  - Use symmetry & reflecting BC, to eliminate higher modes & reduce ρ

PWR example:	full core	1/2 core	1/4 core	1/8 core
ρ:	.98	.97	.96	.94

  - Better initial source guess ⇒ fewer cycles to converge

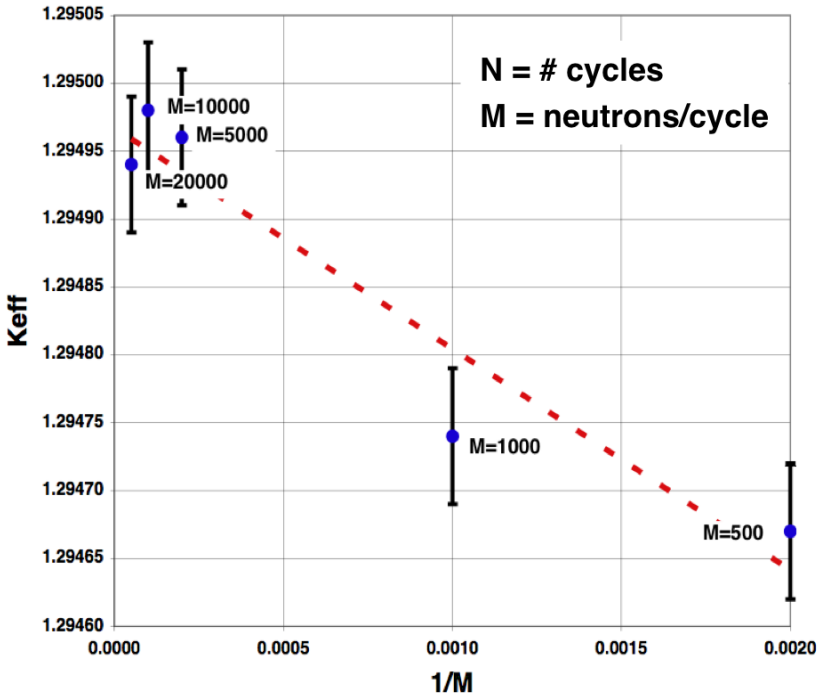
Reactor: good guess - uniform in core region

- Convergence does not depend on number of neutrons/cycle (M)

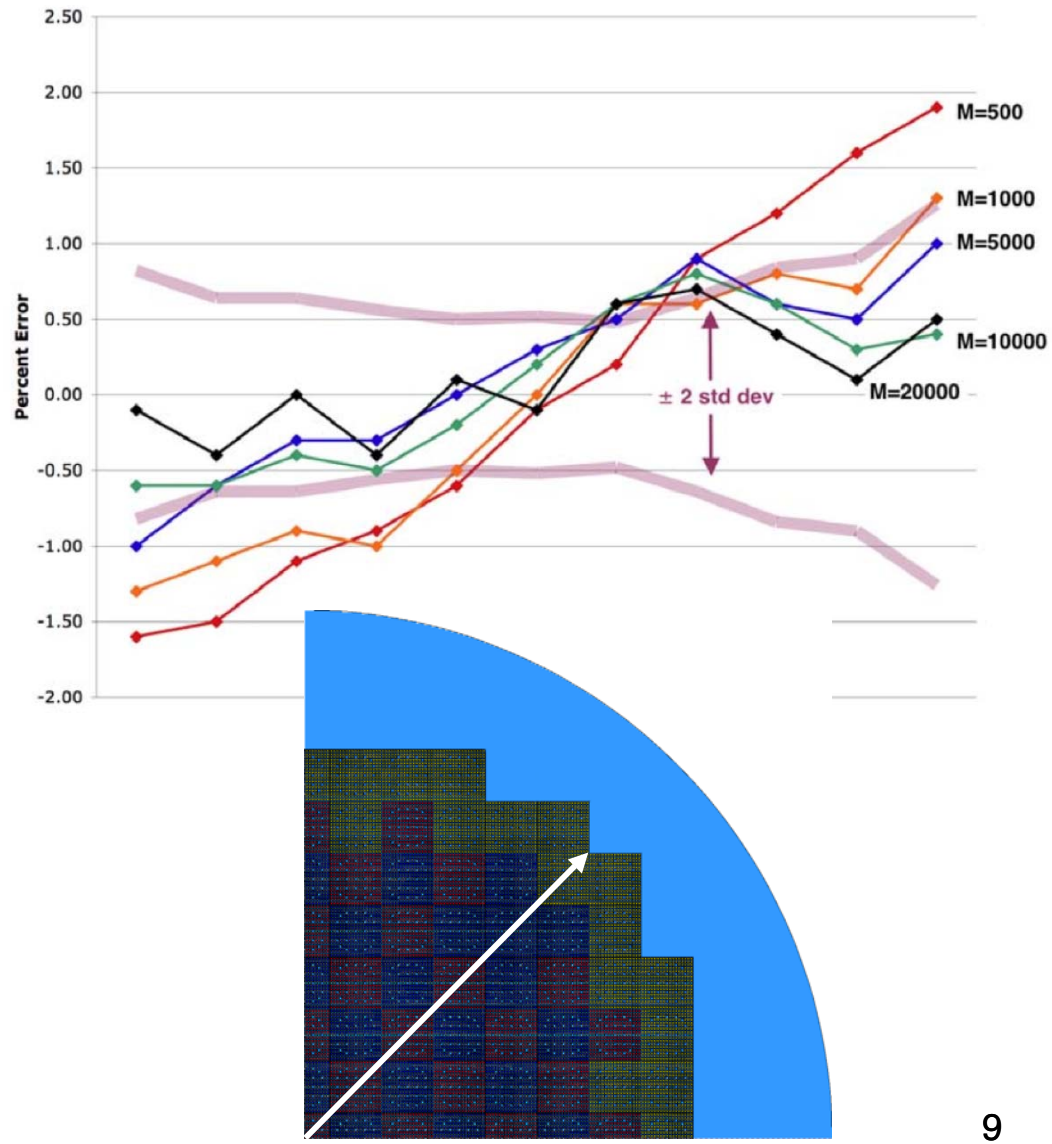
Bias in K_{eff} & Tallies - Reactor Example

Monte Carlo Codes
XCP-3, LANL

Keff vs 1/(neutrons/cycle)



Percent error in fission rates along diagonal



K_{eff} Bias ~ 1 / M

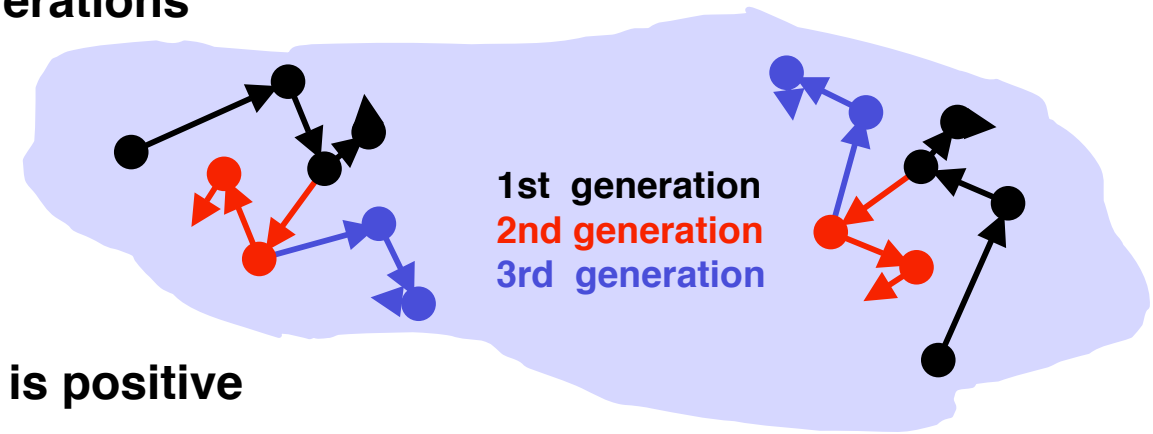
M = neutrons/cycle

Bias in K_{eff} & Tallies - Guidance

- Using too few neutrons/cycle leads to bias in K_{eff} & the fission distribution
- Bias in K_{eff} is usually small, but <u>always negative</u> (nonconservative)
- Bias in the fission distribution is generally larger than for K_{eff} & shows a significant tilt
- Practical solution - use large M (neutrons/cycle)
  - Using 10K neutrons/cycle or more $\Rightarrow$ bias negligible (100K or more for large models)
  - More neutrons/cycle $\Rightarrow$ more efficient parallel calculations

Bias in Statistics - Description

- **MC eigenvalue calculations are solved by power iteration**
  - **Tallies for one generation are <u>spatially correlated</u> with tallies in successive generations**



  - **The correlation is positive**
  - **MCNP & other MC codes ignore this correlation, hence compute statistics that are <u>smaller</u> than the real statistics**
  - **Errors in statistics are small/negligible for K_{eff}, but may be significant for local tallies (eg, fission distribution)**
  - **Running more cycles or more neutrons/cycle does <u>not</u> reduce the underprediction bias in statistics**

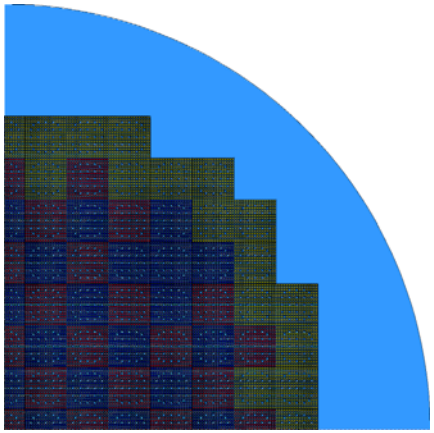
Bias in Statistics - Reactor Example

Monte Carlo Codes
XCP-3, LANL

True relative errors in 1/4-assembly fission rates, as multiples of calculated relative errors, $\sigma_{TRUE} / \sigma_{MCNP}$

3.4	3.1	2.7	2.7	2.6	2.3	2.7								
3.3	3.7	3.6	3.7	3.7	2.7	2.9								
3.8	3.8	3.9	4.0	3.6	3.3	3.0	2.9	2.5	2.5	2.2				
3.8	3.9	4.2	3.3	3.5	3.4	3.2	3.6	3.0	3.0	2.8				
3.9	3.6	3.5	3.3	3.4	3.4	4.0	3.9	3.5	3.2	3.1	2.5	1.7		
4.1	3.8	3.5	3.2	2.9	2.6	2.9	3.2	3.1	2.8	2.7	1.9	1.7		
3.4	3.4	3.2	3.5	2.6	2.4	2.6	3.0	2.9	2.9	2.8	2.3	2.1		
4.2	3.5	3.4	3.1	2.7	2.3	2.0	2.4	2.5	2.5	2.1	2.3	2.3		
3.9	3.6	3.1	2.9	2.3	1.9	1.9	2.3	2.4	2.9	2.7	2.7	2.2	2.8	2.3
3.7	3.3	3.6	2.4	2.2	2.2	2.5	1.8	2.2	2.6	2.7	2.9	2.5	2.4	2.5
3.0	3.1	3.0	2.2	2.2	2.1	2.4	2.5	2.4	2.6	2.7	2.6	2.7	3.0	2.6
2.9	3.7	3.3	2.6	2.5	2.8	3.0	2.9	3.5	3.2	3.3	3.1	3.1	3.2	3.3
3.2	3.1	2.9	3.1	3.2	3.3	3.5	3.5	3.6	3.9	3.7	3.9	3.5	3.4	2.9
3.4	3.0	3.1	3.6	3.4	3.5	3.9	3.7	4.0	4.3	4.0	4.3	3.8	4.2	3.5
3.5	3.2	2.8	3.5	3.8	3.9	3.9	3.9	4.1	4.1	4.6	4.4	4.7	4.5	3.8

Calculated uncertainties are 1.7 to 4.7 times smaller than true uncertainties



Average factor = 3.1

Best Practices - Summary

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Adjoint Weighted Tallies

Reactor Kinetics Parameters

Perturbations

Continuous-Energy Adjoint Weighting

- **MCNP now features specific adjoint-weighted tallies for criticality problems for continuous energy.**
  - **Point Reactor Kinetics Parameters** (MCNP5-1.60, summer 2010)
  - **Adjoint Perturbation Theory** (MCNP6, fall 2011)

- **Uses Iterated Fission Probability:**

  In a critical system, the importance at a point in phase space is proportional to the expected steady state neutron population resulting from a hypothetical neutron introduced into at that point in phase space.

- **No additional random walks! Slowdown only a few percent**

- **For details - see Brian Kiedrowski's section of the Math & Comp 2009 Monte Carlo workshop at**

  http://mcnp.lanl.gov/publication/mcnp_publications.html

Adjoint-Weighted Kinetics Parameters

- **Simple MCNP input card:**

```
kopts  kinetics=yes
```

- **MCNP output for the Godiva problem:**

	escape	capture	fission	removal
fraction	5.71494E-01	4.48072E-02	3.83699E-01	1.00000E+00
lifetime(abs)	1.09167E-08	1.39237E-07	1.62596E-08	6.23881E-09
lifetime(c/a/t)	1.09522E-08	1.39690E-07	1.63126E-08	6.25914E-09

the estimated adjoint-weighted point reactor kinetics parameters are:

	estimate	std. dev.	
gen. time	5.70892	0.02975	(nsec)
rossi-alpha	-1.13673E-03	4.67682E-05	(nsec-1)
beta-eff	0.00649	0.00027	

New

Adjoint-Weighted Kinetics Parameters

- Verified against analytic solutions, point solutions & multigroup discrete ordinates problems

- Validation against criticality benchmarks:

Comparison of Rossi-Alpha (ms^{-1})

Experiment	Measurement	MCNP	C/E
Godiva	-1100 ± 20	-1140 ± 2	1.04
Jezebel	-640 ± 10	-640 ± 2	1.00
BIG TEN	-117 ± 1	-115.5 ± 0.2	0.99
Flattop-233	-267 ± 5	-292.4 ± 0.8	1.09
Stacy-29	-0.122 ± 0.004	-0.122 ± 0.003	1.00
WINCO-5	-1.109 ± 0.003	-1.117 ± 0.003	1.01

Adjoint-Weighted Perturbations

- **Alternative to the differential operator technique for finding perturbed value of k_{eff}.**
  - **Greater number of perturbations possible (e.g. cross section library substitutions)**
  - **Often more accurate**

- **Example: Nuclear data library swap ENDF/B-VI to ENDF/B-VII for the Godiva benchmark (.66c to .70c xsecs):**

k_{eff}	0.99646 ± 0.00004
Ref.* Δk	0.00344 ± 0.00006
Calc. Δk	0.00358 ± 0.00006

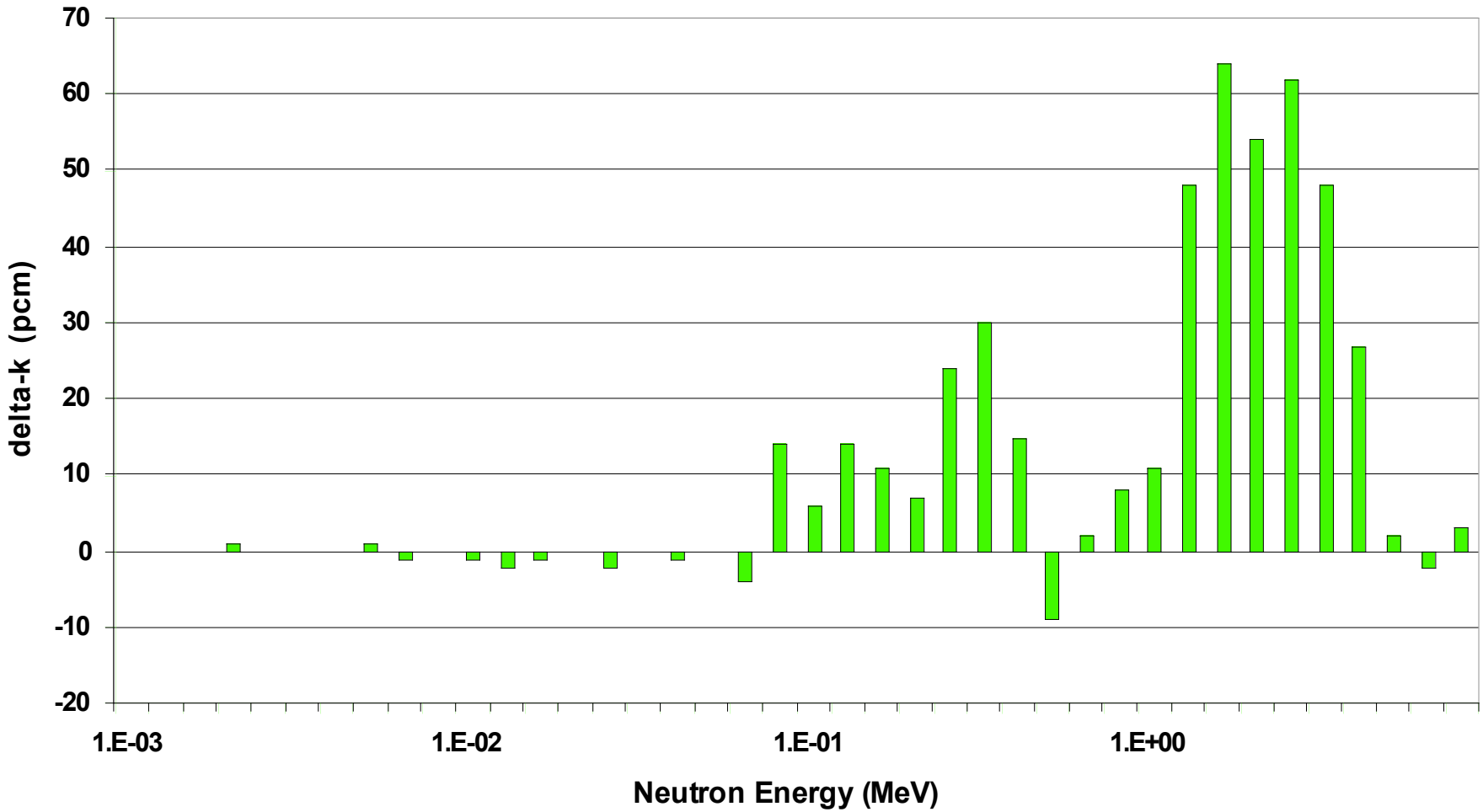
*** Reference solution obtained from subtracting results of two independent MCNP calculations.**

Adjoint-Weighted Perturbations

Monte Carlo Codes
XCP-3, LANL

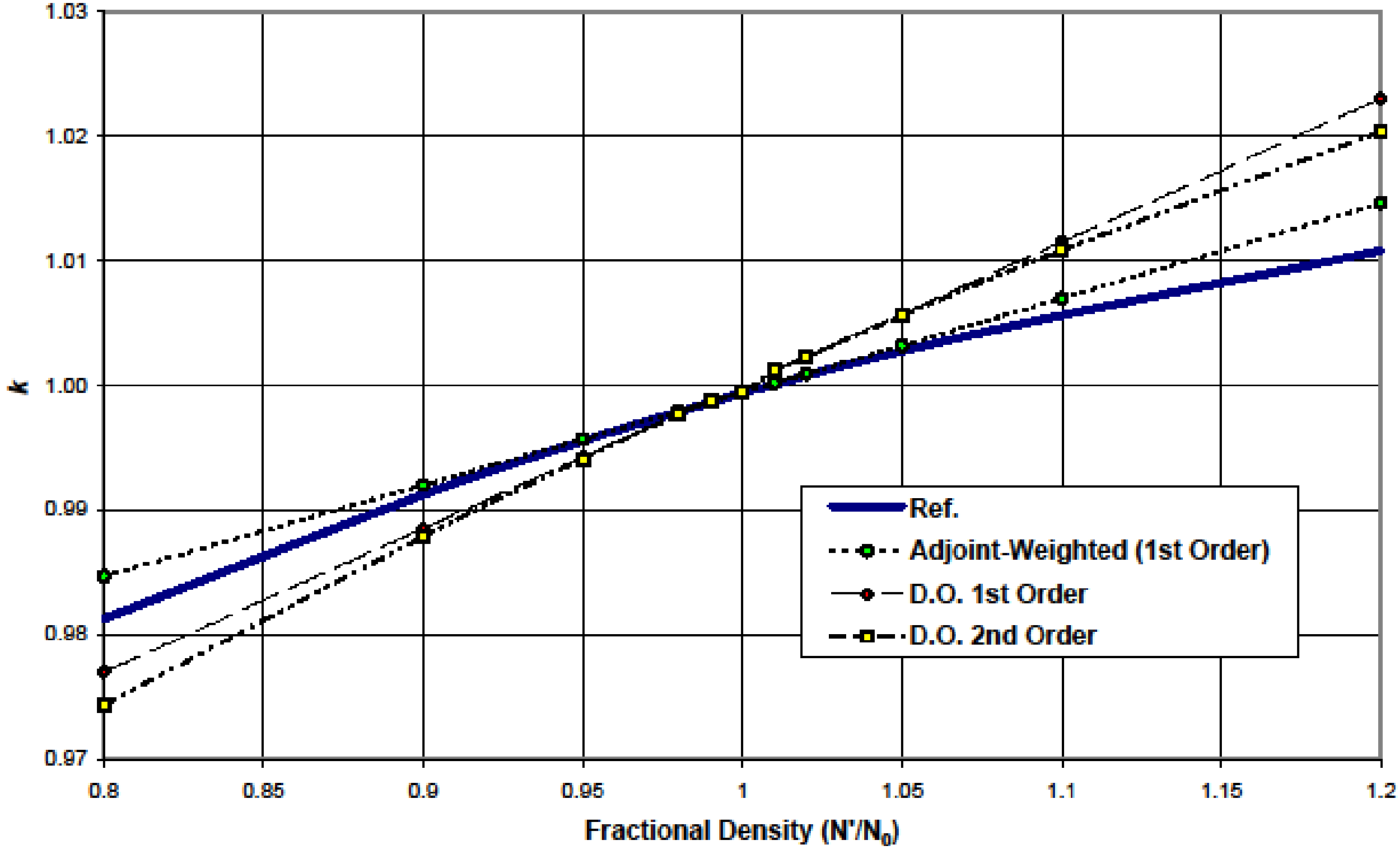
Godiva Library Perturbation (ENDF 66c to 70c)

(U-235 Fission Cross Section)



Adjoint-Weighted Perturbations

Example: Change moderator density in 2D PWR



Recent Improvements to MCNP5

Large Problems - Geometry, Materials, Tallies
General Improvements - MCNP5-1.60
"Kord Smith Challenge" & Large-scale Calculations

MCNP5 & MCNP6 Mods for Big Models

- **New limits for problem input [MCNP6, MCNP5-1.60]**

	Previous	New
– Cell, surface, material, universe, sdef numbers	99999 (100K-1)	99999999 (100M-1)
– Tally numbers:	999	9999
– Length of cell boundary specifiation:	1000	9999

  - Tested on problems with > 1M cells

- **Memory storage & OS issues:**
  - New limits still use 32-bit integers, same memory for existing problems
  - Even larger limits would require 64-bit integers & 2X storage for geometry
  - Problems with >10M cells need 64-bit OS, to get larger address space

- **For most problems:**
  - Hard-wired code parameters are generally not limiting
  - Practical limits arise from poor scaling of input processing algorithms
    - Problem setup times may require days/weeks
    - These scaling issues are being addressed & fixed as they are identified

MCNP5 & MCNP6 Mods for Big Models - Example

Monte Carlo Codes
XCP-3, LANL

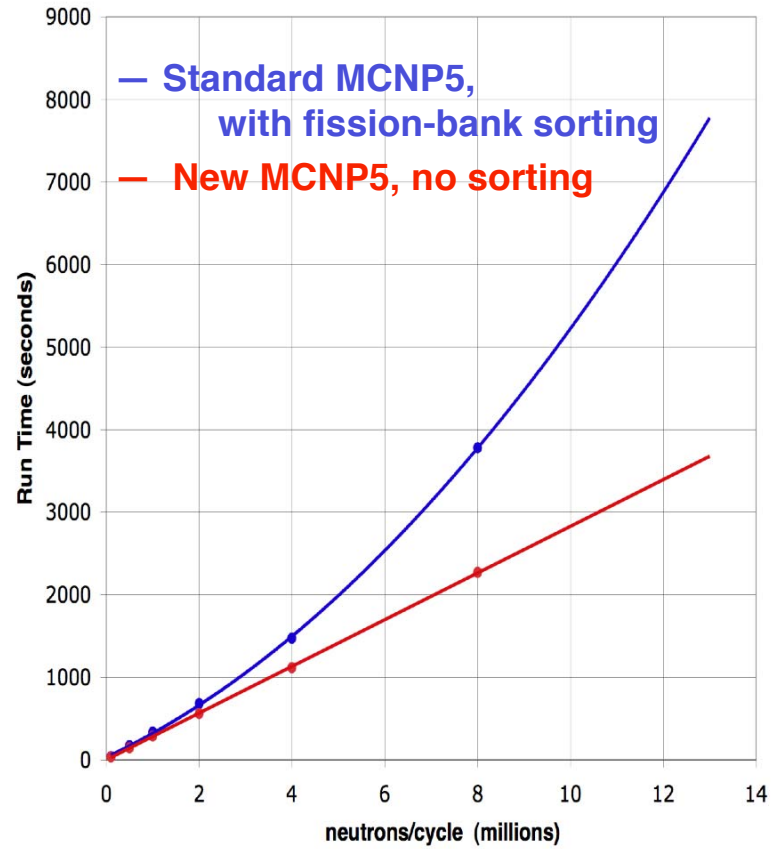
- **For criticality problems with OpenMP threading, the fission-bank needs to be reordered into a unique ordering that is independent of the number of threads or MPI processes**

- **Previous:**
  - **crude, inefficient sorting**
  - **poor scaling for large neutrons/cycle.**

  Scaling ~ $O(M^2)$ M = neutrons/cycle

- **New routine added for unique reordering WITHOUT SORTING.**
  - **FB Brown & TM Sutton, "Reproducibility & Monte Carlo Eigenvalue Calculations", *Trans Am Nuc Soc* 65, 235 (1992)**

  Scaling ~ $O(M)$ M = neutrons/cycle



General Improvements - MCNP5

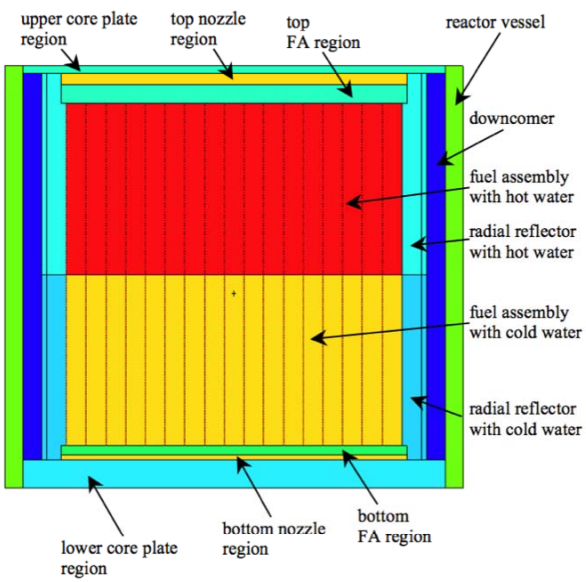
- New Verification / Validation Benchmark Suites
  - Subcritical Multiplication
  - Additional Criticality Suite (91 problems, from LANL Data Team)
  - Perturbation Verification
  - Kobayashi Benchmarks
  - Reactor Kinetics Parameter Benchmarks

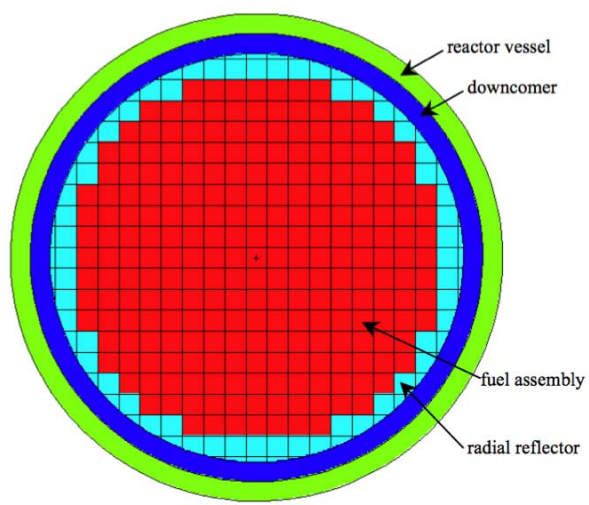
- Automated collection of results & comparison to Benchmarks

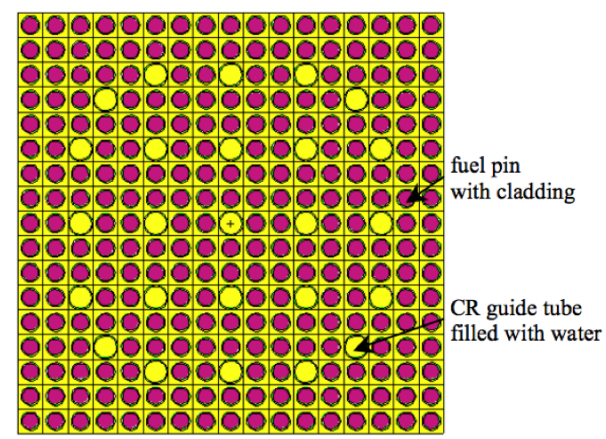
- MCNP5-1.60 is targeted for release Summer 2010
  - Numerous minor bug fixes
  - Some minor improvements for criticality problems
  - Mods for big problems (increased limits)
  - Adjoint-weighted reactor kinetics parameters
  - Additional V&V suites

MCNP & the "Kord Smith Challenge"

- **Full core, 3D benchmark for assessing MC computer performance**
  - **Specified by Hoogenboom & Martin (M&C 2009), rev for OECD 10/2009**
  - **LWR model: 241 assemblies, 264 fuel pins/assembly**
  - **Fuel contains17 actinides + 16 fission products; borated water**
  - **Detailed 3D MCNP model provided (Brown)**
    - **Mesh tallies for assembly powers, axially integrated**
    - **Mesh tallies for pin powers, (100 axial) x (264 fuel pins/assy) x (241 assy) = (63,624 pins) x (100 axial) = 6.3M pin powers**
    - **Runs easily on deskside computer (Mac Pro, 2 quad-core, 8 GB memory)**





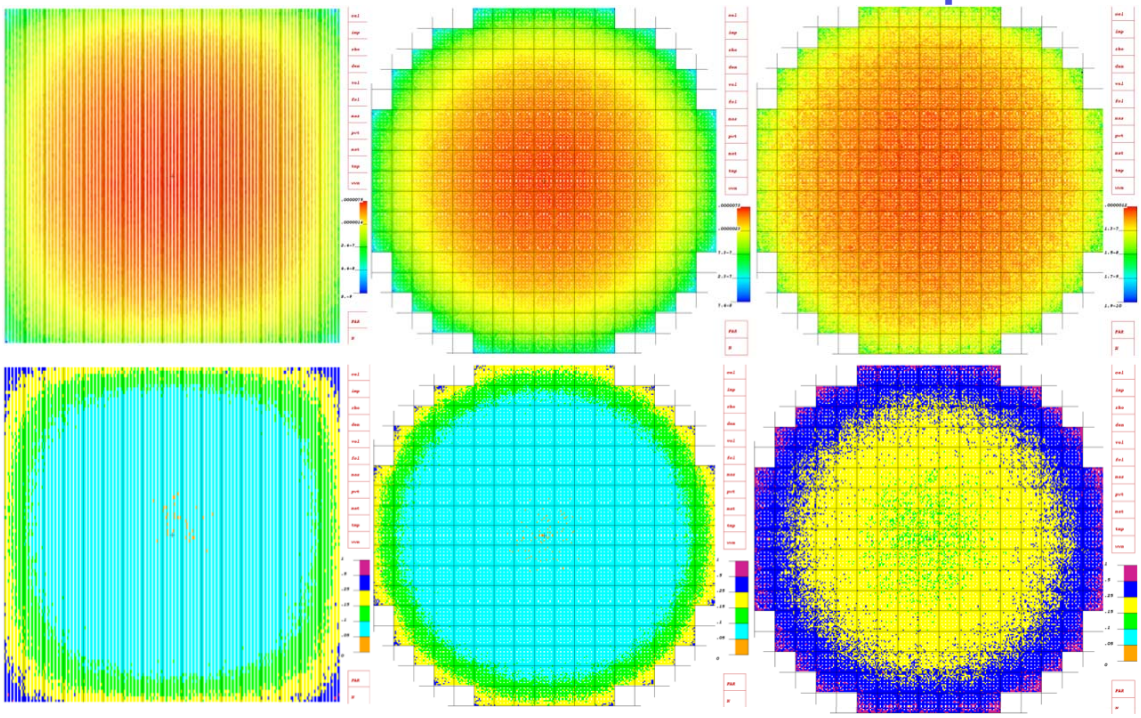


MCNP & the "Kord Smith Challenge"

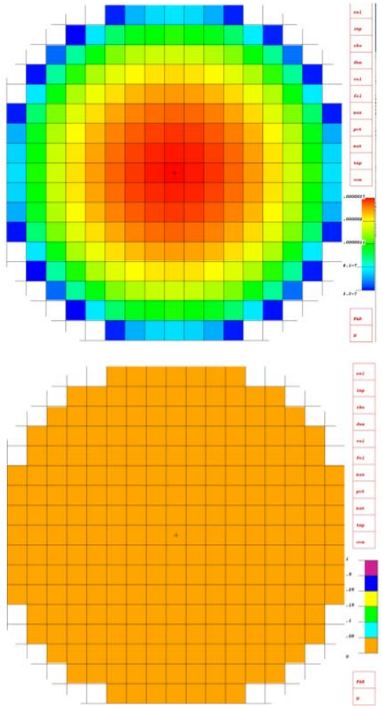
Monte Carlo Codes
XCP-3, LANL

Pin Powers & Std.Dev

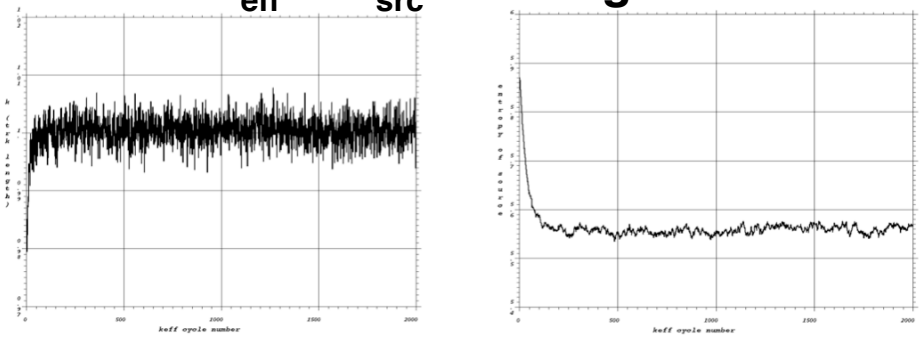
Axial | Mid | Top



Assembly Power & Std.Dev



K_{eff} & H_{src} Convergence



200M neutrons
Mac Pro, 8 cpu

- **Some preliminary findings**
  - **See talk at PHYSOR-2010 by Kelly, Sutton, Trumbull, Dobreff on KAPL/Bettis MC21 code & KS Challenge**
    - **Original spec, not the later revision …**
    - **Roughly 6M neutrons/hr per cpu on Linux cluster**
    - **69 G neutrons per day on 400-cpu Linux cluster**
  - **MCNP5**
    - **Demo calculations, to help with problem specs & MCNP input**
    - **Roughly 3M neutrons/hr per cpu on Mac**
    - **.6 G neutrons per day on 8-cpu deskside Mac**
    - **Cluster results TBD**
    - **Runs easily on laptop or deskside computer** **(just not fast enough)**

Aside: MC21 appears to be only ~2X faster than MCNP5.
SERPENT is 10-40X faster; RACER used to be 10-50X faster.

MCNP & Large-scale Reactor Calculations

Monte Carlo Codes
XCP-3, LANL

MCNP pros

- 30+ years old
- Hierarchical parallelism - threads + MPI
- Portable: Windows/Linux/Macs/Unix
- Mesh tallies for detailed power distributions
- Can model any reactor geometry
- Continuous-energy physics
- Coupled n-γ calculations
- Convergence diagnostics - K_{eff}, H_{src}, statistical checks
- Extensive documentation + V&V
- MCNP used in ENDF/B-VII development & assessment

MCNP cons

- 30+ years old
- In practice, max of ~15K fuel materials with FPs. Can't deplete full-, 1/2-, 1/4-, 1/8-core without severe spatial approximation
- Does not have: buckling search, rod search, equilibrium Xenon, equilib. Sm
- Fission energy is prompt only; need to renormalize to get total energy deposition
- Free-gas scatter ignores scattering resonances; inaccuracies in power defect
- Temperature effects not handled in-line
- Difficult to link output files to other codes
- DOE Crit-Safety & ASC support MCNP; DOE NE does not
- Export Controlled; difficult for non-US to get source code

Work in progress

- Parallel improvements: MPI + threads, distributed data model
- On-the-fly Doppler broadening (Yesilyurt/Martin/Brown)
- Links into UNIC (ANL)
- Adjoint-weighted sensitivity/uncertainty analysis
- Algorithm improvements for very large models

MCNP6 Status

MCNP6 Status

- **MCNP6 contains:**
  - MCNP6 = development version of MCNP at LANL, since 2004
  - Includes:
    - All MCNP5 1.51 & 1.60 capabilities (mpi + threads)
    - High energy protons & magnetic fields, for proton radiography
    - All MCNPX 2.7.B & new MCNPX 2.7.D capabilities (mpi)
    - New CINDER 2008
  - New Unstructured Mesh (for CAE/CAD interface)
  - Link with finite element code ABAQUS
  - Adjoint-weighted perturbation estimators
- **MCNP6 in (very) limited beta release to outside LANL**
  - Recipients are active collaborators and sponsors
  - Full beta access within LANL and LLNL

MCNP6 Status

- **Active Validation Efforts**
  - Comparisons with experiments included in test suites
  - High energy proton, Heavy Ion interactions
  - Delayed photon and neutron spectra
  - Subcritical Multiplication
  - Additional Criticality Suite (91 problems)
  - Perturbation Verification Suite
  - Kobayashi Benchmarks
  - Reactor Kinetics Parameter Benchmarks
  - Production / Depletion (CINDER) soon

- **Nightly Regression Test suites**
  - 3 Platforms (Linux 32, Linux 64, Windows 64)
  - 5 Compilers (Intel 10, Intel 11, PGI 7.2, pathscale 3.1, gfortran 4.3)
  - Serial, mpi, omp, mip+omp
  - Array bounds checking
  - 875 problem input files
  - Total: 10K runs each night

MCNP6 Status

- MCNP team has adopted MCNP6 as the base for all future development. MCNPX team will do so soon.

- To go from Beta release to Production release:
  - Assurance of reliability and accuracy for criticality
  - Assurance of reliability and accuracy for other apps
  - Comparable performance
  - Complete documentation

- Future Work
  - Cleanup Style
  - Remove duplicate features (input files backwards compatible)
  - Extend threading parallel capability to new features
  - New Features

- Release to RSICC
  - 2011 (?)

Serpent

a Monte Carlo Reactor Physics Burnup Calculation Code

Jaakko Leppänen

Business from technology

Outline

- Background
- History
- The Serpent code:
  - Overview
  - Neutron tracking
  - Physics and interaction data
  - Burnup calculation
  - Output
  - Additional features
  - Results
  - Performance
- Code distribution and maintenance
- Demo

Background

- Monte Carlo codes are traditionally used for criticality safety analyses, shielding and dosimetry calculations, detector modeling and validation of deterministic transport codes.
- ”New” applications:
  - Burnup calculation
  - Homogenization and group constant generation
- Existing general-purpose codes are not always the best solution for the above tasks.

  ⇒ Development of <u>dedicated</u> Monte Carlo reactor physics codes

Background

- Computational challenges for lattice physics calculations differ from traditional Monte Carlo applications:
  - Relatively simple assembly-level geometry (vs. detailed 3D models).
  - Large set of standard output parameters (vs. criticality eigenvalue or user-defined tallies).
  - Some of the parameters cannot be calculated using conventional tally techniques.
  - Efficient user-friendly burnup calculation routine is a necessity.
  - The main goal is to *generate a set of input parameters that represent the neutron interaction physics* in the next stage of the calculation chain (vs. replicate the neutron transport process in a realistic geometry).
- Also the advantages the Monte Carlo method are different:
  - Versatility (vs. detailed modeling of geometry and physics).

Background

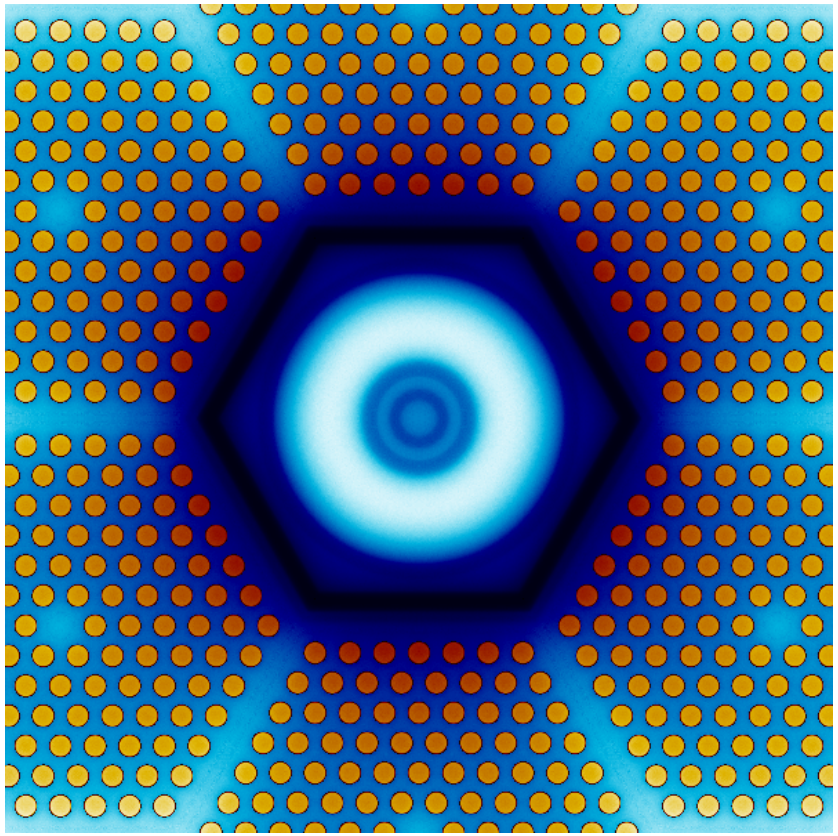
- Disadvantages of using Monte Carlo for lattice physics:
  - The method is slow compared to deterministic 2D codes
  - Results are random variables
  - Some parameters are difficult to calculate (diffusion coefficient)
  - Some features that are standard techniques in deterministic codes are just beginning to emerge in Monte Carlo:
    - Neutron leakage models
    - Continuous-energy adjoint calculation
    - Sensitivity and uncertainty analysis

History

- Development of Serpent started in 2004, under the working title ”Probabilistic Scattering Game”, or PSG.
- A related doctoral thesis published in 2007
  - Available on-line at: www.vtt.fi/inf/pdf/publications/2007/P640.pdf
  - Still the best available reference to methodology
- 200 subroutines, 60000 lines of C-code. Source code written from scratch (re-written in 2005 and 2007).
- Burnup calculation capability in 2008.
- Name changed to ”Serpent” and limited release in October 2008 (pre-release of version 1.0.0).
- NEA release (version 1.1.0) in May 2009, RSICC release (version 1.1.7) in March 2010.

Overview

- Serpent is a continuous-energy Monte Carlo reactor physics burnup calculation code.
- Built-in capabilities for lattice physics calculations, but the geometry is not restricted to 2D.
- Applications:
  - Generation of homogenized multi-group constants for deterministic reactor simulator calculations
  - Fuel cycle studies
  - Validation of deterministic lattice transport codes
  - Research reactor applications
  - Educational purposes



Neutron tracking

- Three-dimensional universe-based geometry model (similar to MCNP and KENO).
- Analog Monte Carlo game.
- *K*-eigenvalue criticality source method ⇒ applications limited to multiplying systems (external source mode under development).
- Neutron transport based on a combination of conventional surface-tracking and the Woodcock delta-tracking method[1]:
  - Tracking routine efficient in lattice calculations and especially when modeling HTGR particle fuels
  - Combination of two tracking methods overcomes efficiency problems encountered with delta-tracking with localized heavy absorbers
  - Integral reaction rates calculated using the collision flux estimator ⇒ Serpent is not the best choice for shielding applications

[1] J. Leppänen. *"Performance of Woodcock Delta-Tracking in Lattice Physics Applications Using the Serpent Monte Carlo Reactor Physics Burnup Calculation Code."* Ann. Nucl. Energy, **37** (2010) 715-722.

Physics and interaction data

- Continuous-energy cross sections read from ACE format data:
  - Data format shared with MCNP ⇒ validation by direct comparison to reference results
  - Cross sections reconstructed on a unionized energy grid used for all nuclides[2]:

    ⇒ Considerable increase in efficiency
    ⇒ Computer memory wasted for storing redundant data points

  - Interaction physics modeled according to classical collision kinematics and ENDF reaction laws
  - Bound-atom scattering libraries for important moderators
  - Probability table sampling in the unresolved resonance region

[2] J. Leppänen. *"Two Practical Methods for Unionized Energy Grid Construction in Continuous-Energy Monte Carlo Neutron Transport Calculation."* Ann. Nucl. Energy, **36** (2009) 878-885.

Burnup calculation

- Fully automated built-in depletion routines with predictor-corrector calculation.
- Transmutation cross sections calculated either using standard reaction rate tallies or micro-group spectrum.
- Radioactive decay and fission yield data read from ENDF format files.
- Two methods for solving the Bateman depletion equations:

1. Transmutation Trajectory Analysis (TTA):
   - Analytical solution of linearized depletion chains
2. Chebyshev Rational Approximation Method (CRAM):
   - An advanced matrix exponential solution developed at VTT[3]

[3] M. Pusa and J. Leppänen. *"Computing the Matrix Exponential in Burnup Calculations."* Nucl. Sci. Eng., **164** (2010) 140-150.

Lattice physics capabilities

- All numerical output written in matlab m-format files.
- Serpent calculates by default:
  - Effective multiplication factors using different methods
  - Homogenized few-group cross sections
  - Group-transfer probabilities and scattering matrices
  - Diffusion coefficients using two fundamentally different methods
  - P_n scattering cross sections up to order 5
  - Assembly discontinuity factors (surface and corner)
  - Assembly pin-power distributions
  - Point-reactor kinetic parameters
  - Physical and effective delayed neutron parameters
- Few-energy group structure defined by user.
- Experimental leakage models (”B_1 fundamental mode calculation” or iteration of Albedo boundary conditions).

Additional output and tallies

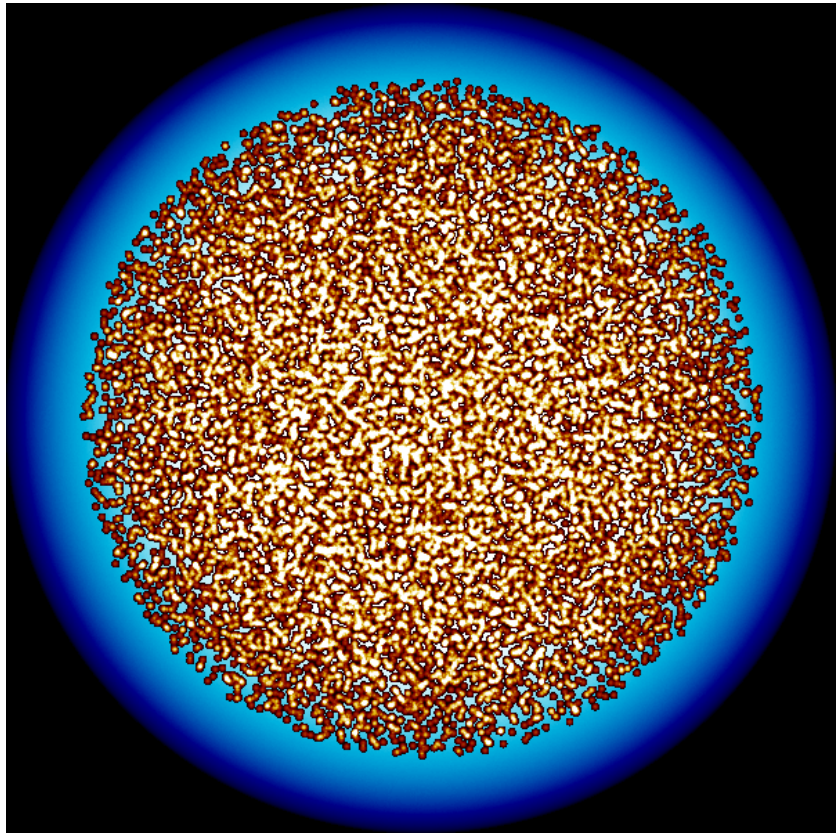
- Fission source entropy calculated automatically (total and x-, y- and z-components).
- User-defined detectors (tallies) for calculating volume-integrated reaction rates:
  - Spatial domain defined by a combination of cells, universes, lattices and materials or using a super-imposed 3D mesh
  - Arbitrary energy bin structure
  - Various response functions (material total and isotopic reaction cross sections, ACE format dosimetry data)
  - Differential and integral flux and reaction rate spectra
- Geometry and thermal flux / fission rate plotter producing png-format graphical output.

Output in burnup calculation mode

- Standard output in burnup calculation mode:
  - Isotopic compositions
  - Transmutation cross sections
  - Activities
  - Decay heat data
- All results given as both material-wise and total values.
- Group constants and other output printed for each step.
- Capability to run depletion steps without transport simulation.

HTGR capabilities

- The Woodcock delta-tracking method works exceptionally well in HTGR particle fuel geometries:
  - Small dimensions compared to neutron mfp
  - Speed-up in tracking up to a factor of 20
- Explicit particle fuel model for stochastic geometries:
  - Coordinates read from a separate file
  - Works at several levels (TRISO particles and fuel pebbles)
  - Pebble-wise power distributions printed in a separate output file
  - Tested with over 2 million random units
  - No major increase in running time compared to a regular lattice calculation



Additional features

- Built-in Doppler-broadening preprocessor routine[4]:
  - Works for small (< 300K) temperature adjustments
  - No significant increase in calculation time
- Iteration of equilibrium xenon concentration (in both transport and burnup calculation modes).
- Iteration of soluble absorber concentration (in both transport and burnup calculation modes).
- Serpent installation package contains ACE format cross section libraries for 432 nuclides at 6 temperatures based on ENDF/B-VI.8, ENDF/B-VII, JEF-2.2, JEFF-3.1 and JEFF-3.1.1 evaluated data files.

[4] T. Viitanen. *"Implementing a Doppler-Preprocessor of Cross Section Libraries in Reactor Physics Code Serpent."* M.Sc. Thesis, Helsinki University of Technology (2009).

Results

- Serpent is extensively validated by comparing to MCNP results in infinite lattice calculations:
  - Capability to use the same ACE format cross section libraries
  - Differences generally within the range of statistical accuracy
- Validation of burnup calculation routines is more complicated:
  - No ”perfect” reference code
  - More uncertainties resulting from approximations (data, methods, implementation)
  - Reasonably good results so far (comparison to CASMO-4E and TRITON / NEWT).

Results

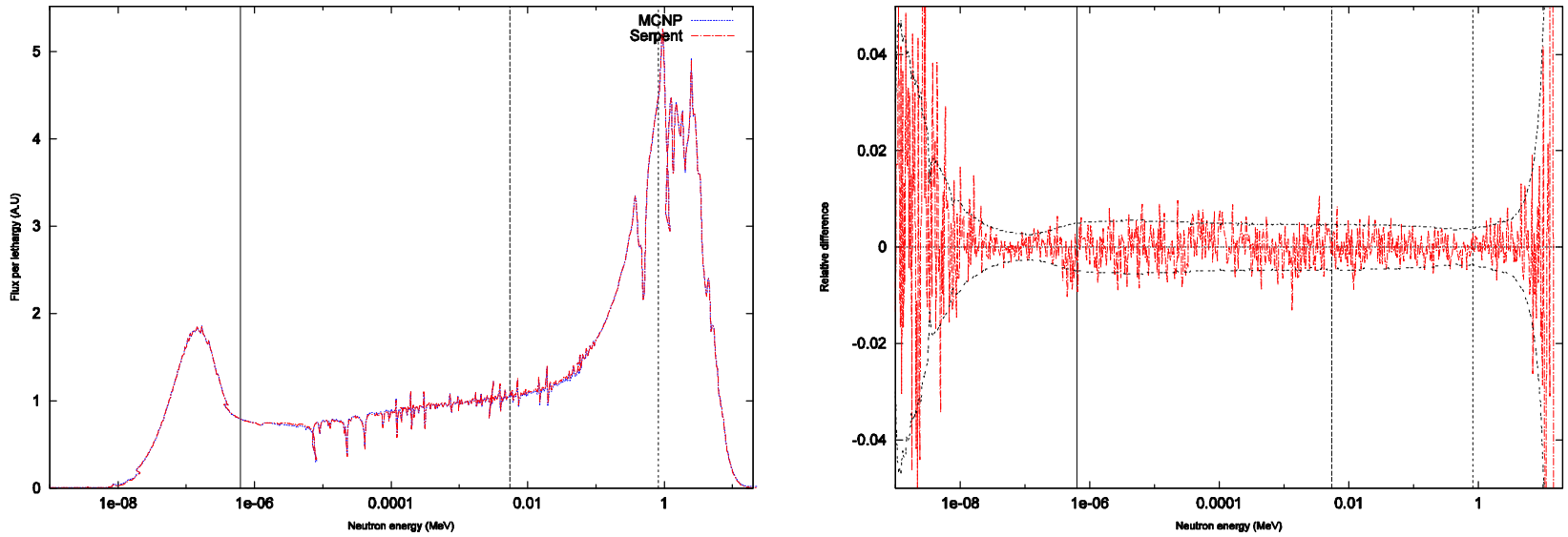
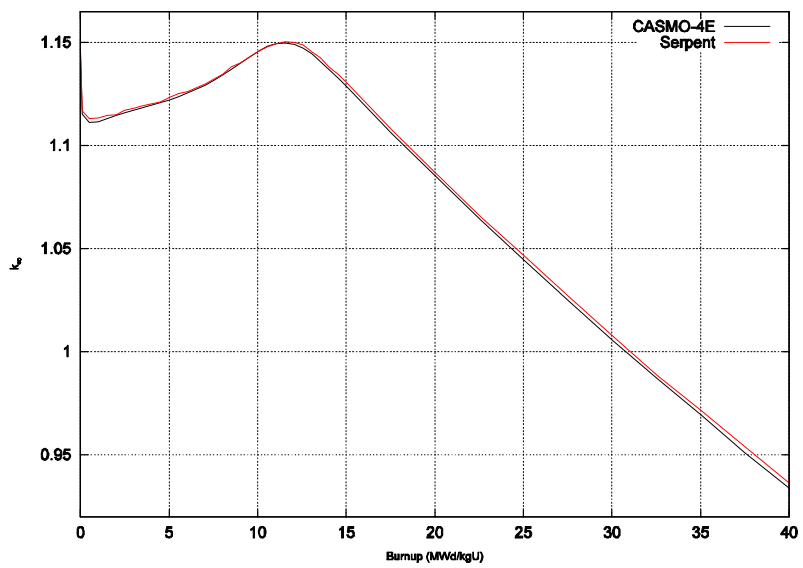


Figure 1: Comparison of LWR flux spectra. Steady-state calculation, Serpent vs. MCNP5.

Results



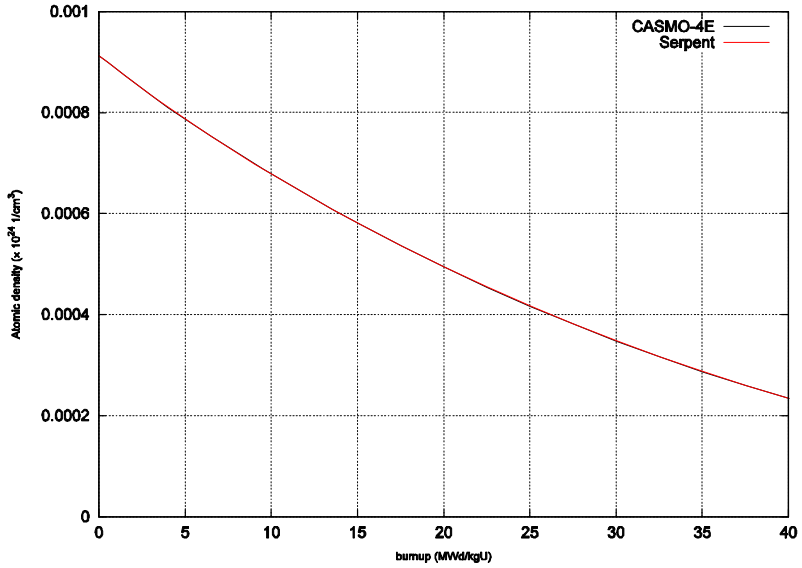


Figure 2: Comparison of k-eff and U-235 concentration in PWR assembly burnup calculation. Serpent vs. CASMO-4E.

Results

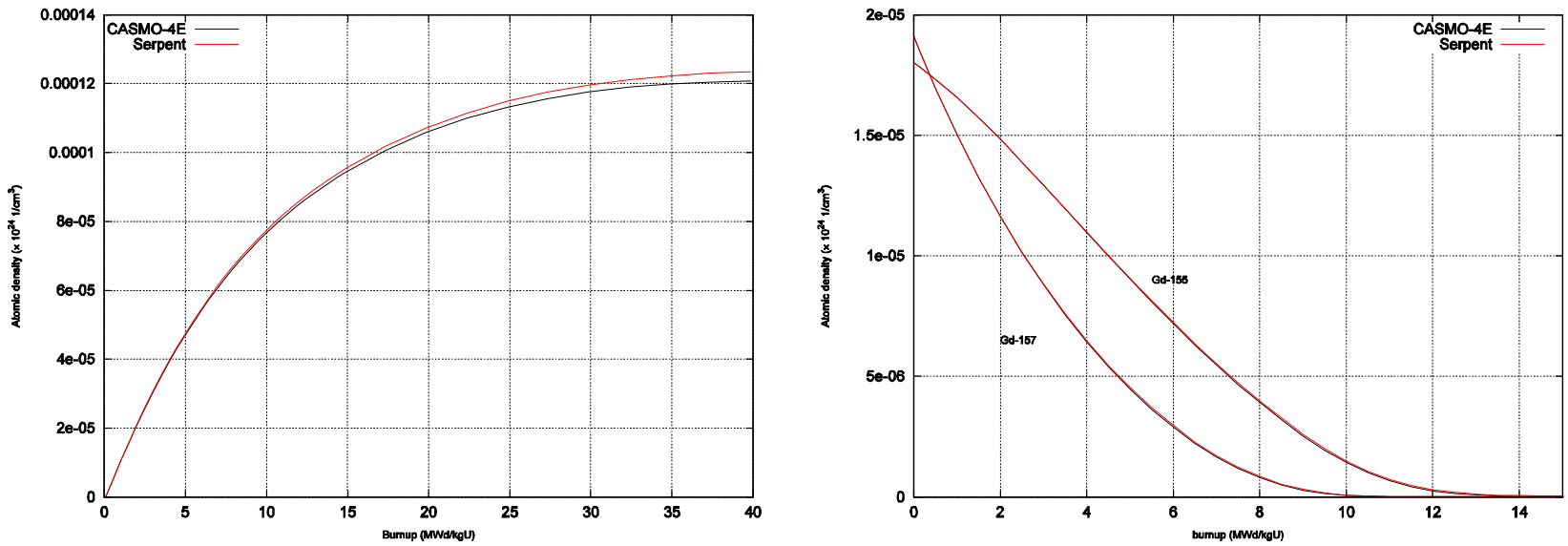


Figure 3: Comparison of Pu-239 and gadolinium concentrations in PWR assembly Burnup calculation. Serpent vs. CASMO-4E.

Results

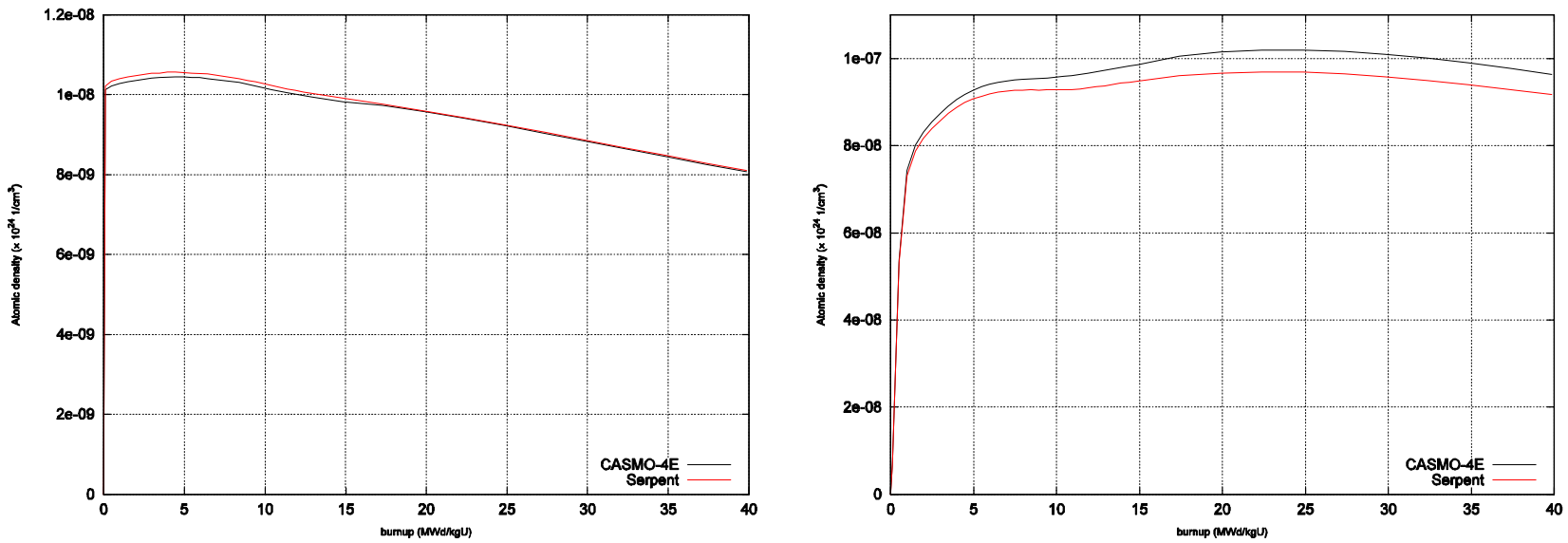


Figure 4: Comparison of Xe-135 and Sm-149 concentrations in PWR assembly burnup calculation. Serpent vs. CASMO-4E.

Performance

- Serpent is optimized for performance (at the cost of memory usage).
- Typical running time for an LWR lattice calculation is less than 10 minutes (3.0 GHz PC workstation, 3 million neutron histories).
- Burnup calculations are usually completed within 24 hours.
- Code performance results from two factors:

  1. Woodcock delta-tracking method
  2. Internal unionized energy grid format

- *Overall calculation time is not strongly dependent on the number nuclides included in burnup calculation*.
- Parallel calculation with MPI.

Distribution and maintenance

- Free software license for non-commercial research and educational use.
- Main distributors are the OECD / NEA Data Bank and RSICC.
- Updates in source code distributed to registered users by e-mail.
- Serpent user community consists of some 25 organizations in 15 countries around the world.
- Serpent website: http://montecarlo.vtt.fi
  - The most up-to-date description of methodology
  - User's manual
  - References, examples, etc.
  - Serpent discussion forum

Reactor Physics Calculations using VESTA and MORET5

May 9, 2010

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Loïc Heulers, Yann Richet, Alexis Jinaphanh, IRSN

Olivier Jacquet, Independent consultant

Outline

- **VESTA – Generic Monte Carlo depletion**
- **MORET – Monte Carlo transport simulation**
- **Reactor physics applications using VESTA and MORET5**
  - ARIANE program
  - Fuel performance applications
  - A 3D reactor application
- **Conclusions**

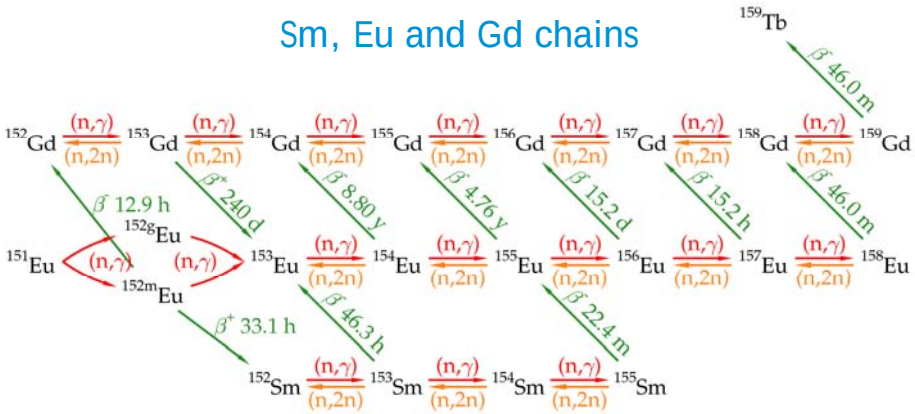
VESTA – Generic Monte Carlo depletion

vesta

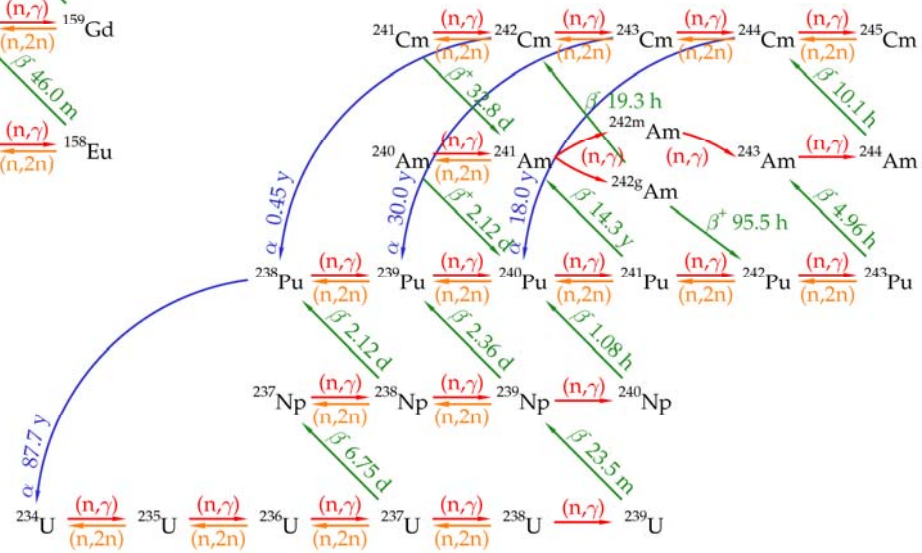
Introduction: depletion calculations

- **The time dependence in any depletion problem is not linear:**
  - Every change in composition has its effect on the neutron spectrum
  - One can go very far in this: influence of temperature, etc.

Sm, Eu and Gd chains

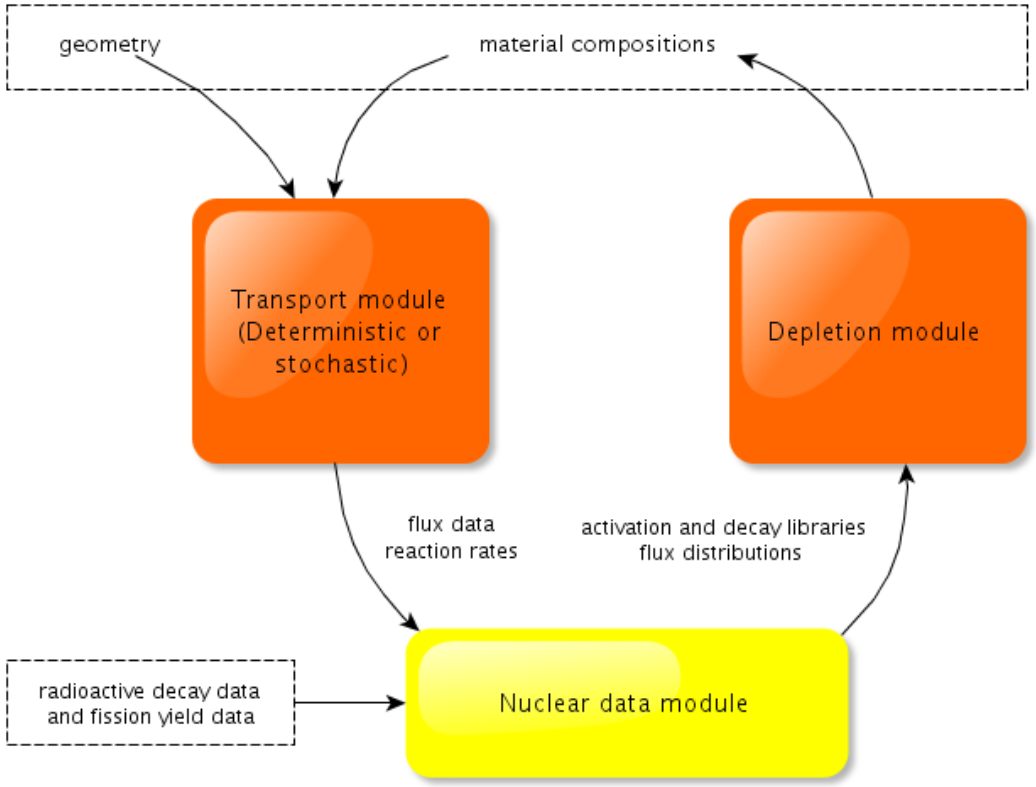


Actinide chains



Introduction: depletion calculations

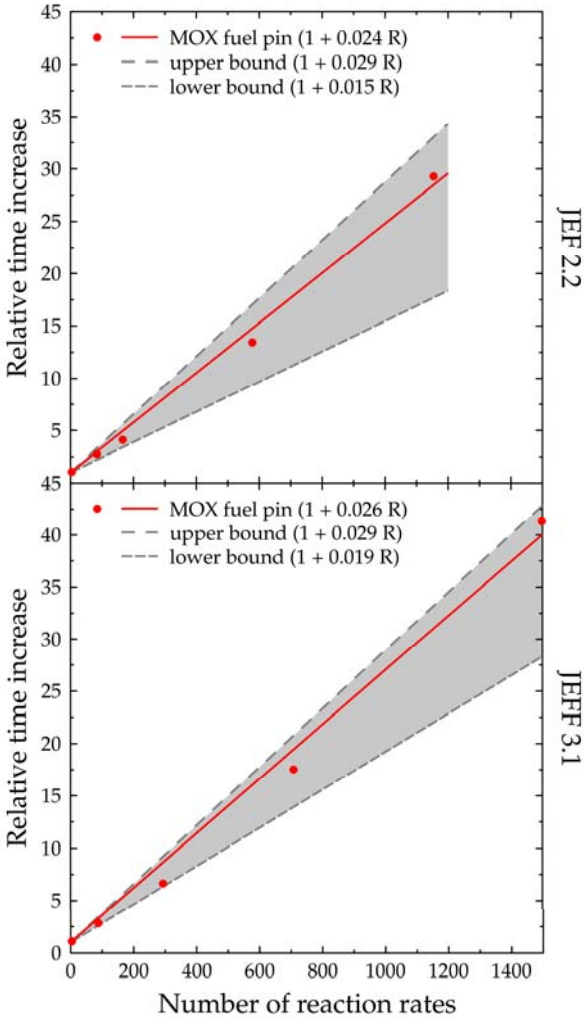
- **Any depletion code will approximate this time dependence by splitting up the irradiation history into small constant steps**



Introduction: Monte Carlo depletion codes

- **Advantages:**
  - Accurate spectra and flux values
  - From simple 1D to realistic 3D
  - Exotic and standard applications
  - Nuclear data (continuous energy, multi-particle physics, detailed energy-angle treatment, etc.)

- **Disadvantages and problems:**
  - Time consuming
    - Needs to follow thousands of nuclides
    - Reaction rate tallies for the depletion calculation are CPU time intensive
  - Approximations jeopardise accuracy
    - Less nuclides and depletion zones, longer time steps, etc



The philosophy behind VESTA

- **A generic Monte Carlo evolution interface**
  - Provide a generic software framework for depletion calculations
  - Highly customisable to a user's needs
    - Monte Carlo code: which code to use, etc.
    - Depletion module: type of reactions, decay modes, etc.
    - Various predictor-corrector options
    - Nuclear data (JEF 2.2, JEFF 3.1, ENDF/B, JENDL)

- **Provide maximum precision for the smallest computing effort possible**
  - The Monte Carlo simulation time should be as low as possible
  - Reaction rate calculation should be negligible compared to the simulation

- **Efficient, flexible and easy to use**
  - Provide default values for every option
  - Logical input options

VESTA today

- **Any version of MCNP(X) or MORET5 as Monte Carlo module**
  - Both fixed source (with MCNP(X) only) and criticality
  - Parallel capability using MCNP(X)

- **Use ORIGEN 2.2 or the built-in PHOENIX module (under development)**

- **Predictor-corrector algorithms:**
  - Predictor only (explicit forward Euler method)
  - Predictor-corrector
  - Middle step approach (MONTEBURNS, SCALE)

- **Irradiation history modeling capabilities**
  - Constant power, constant flux and normal radioactive decay

VESTA today

- **Material and geometry modelling**
  - Non-burnable materials (changes on cell level):
    - Change the temperature in a cell
    - Change the density of a material in a cell
  - Burnable materials (changes on burn-up zone level):
    - Change the temperature in a burn-up zone
    - Change the material in a depletion zone: material reshuffling
  - Geometry changes using translation and rotation transformations:
    - Moving components like slow moving control rods/plates
    - Using user defined positions in the irradiation history
    - Using an automated search algorithm with a target k_{eff} value

- **ENDF data compatibility**
  - Decay data
  - Fission yield data

Accelerating Monte Carlo depletion codes

- **There are a number of solutions to overcome the CPU time problem:**
  - The easy way out: apply brute calculation power (parallel processing)
  - The intelligent way out: achieve the optimal situation

- **This can be achieved by calculating reaction rates after the simulation**
  - Using a hybrid method like the multi-group binning approach
  - Using an intelligent Monte Carlo estimator:
    - Store and sort energy, track length and particle weight
    - Go over the cross section data interval by interval

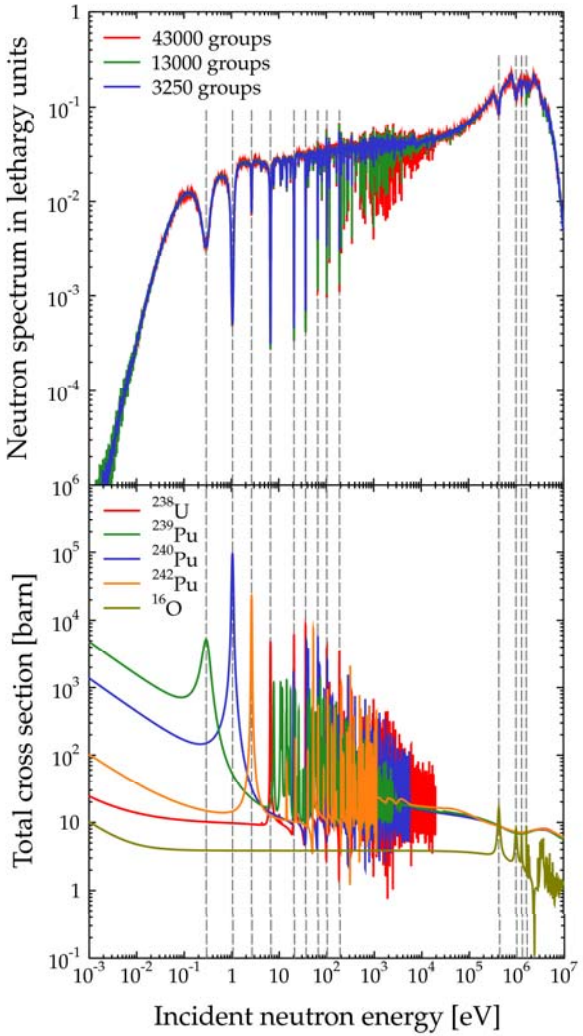
- **Optimised Monte Carlo simulation using a universal energy grid:**
  - Almost as performant as multi-group Monte Carlo but with more detail
  - Optimised reaction rate calculation *by default*
  - This is the continuous energy version of MORET5

The multi-group binning approach

- **Calculate an ultra-fine neutron spectrum instead of all reaction rates:**

$$\sigma = \frac{\lim_{g\to\infty}\sum_g \sigma_g \phi_g}{\lim_{g\to\infty}\sum_g \phi_g} \qquad \sigma_g = \frac{\int_{E_{g-1}}^{E_g} \sigma(E)\,dE}{E_g - E_{g-1}}$$

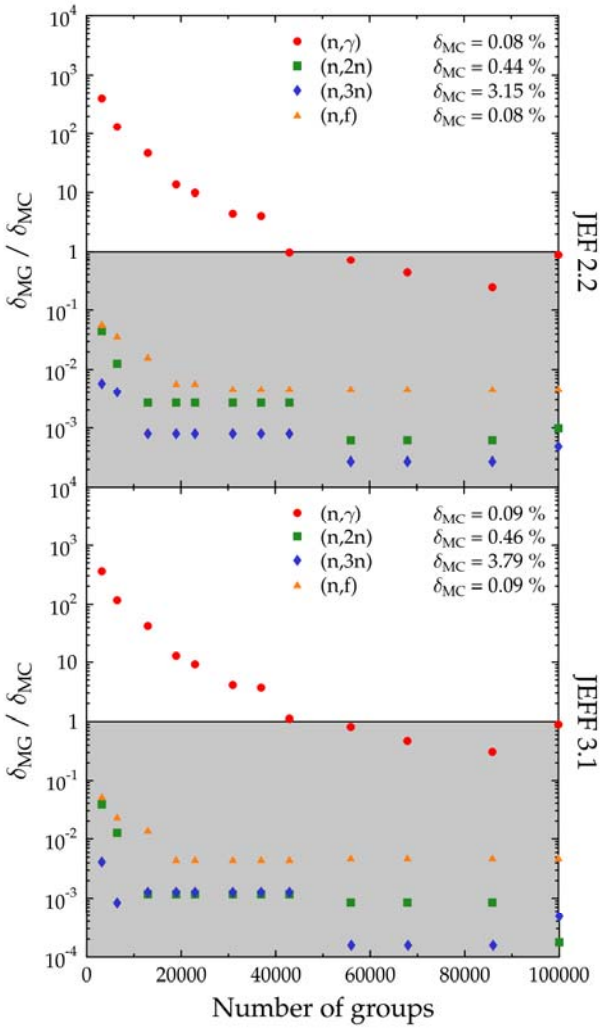
- **Precision is achieved by default:**
  - Calculating 1 or 1000 reaction rates takes about the same amount of time
  - We can be as precise as we want
- **There are of course some requirements:**
  - Accuracy & Stability
  - Nuclear data consistency



The multi-group binning approach

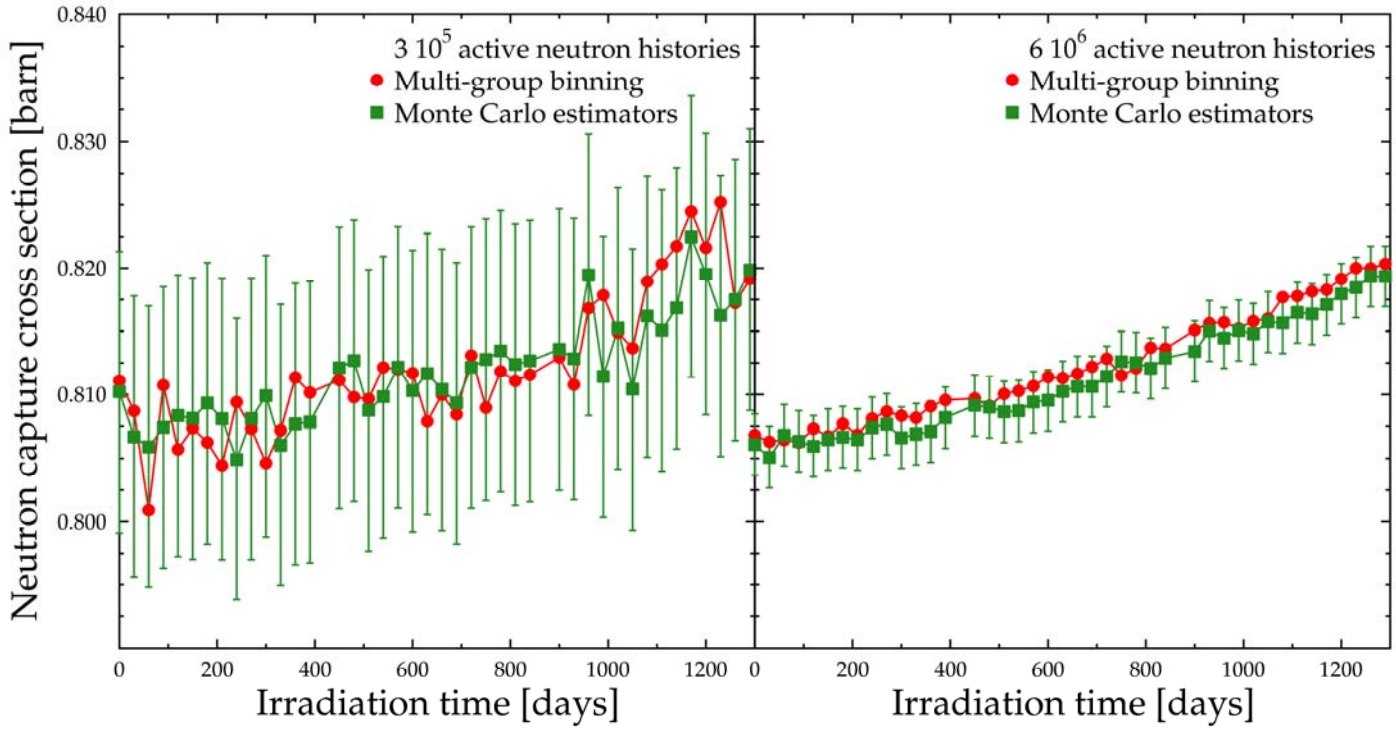
- **To be as accurate as standard Monte Carlo, we use an optimized binning group structure:**
  - To take into account the resonance self-shielding effect by placing more groups in the resonance region (between 1 eV and 1 MeV)
  - This is possible for every type of problem and every evaluation

- **A good test case: ^{238}U**
  - Large amount of resonances
  - Agreement for all reactions except neutron capture is reached quickly
  - Neutron capture requires at least 30000 binning groups in the resonance region



VESTA today

- **Two reaction rate calculation methods:**
  - Calculate reaction rates directly using a Monte Carlo estimator
  - Use a multi-group approach to significantly accelerate the calculation



^{238}U microscopic capture cross section calculated by VESTA for a MOX fuel pin

MORET – Monte Carlo transport simulation

What is MORET ?

- **Monte Carlo code developed for criticality and reactor safety assessment**
  - Neutron population characterization for a given geometry
  - Calculation of several physical quantities
    - Multiplication factor k_{eff} , fluxes, reaction rates, reactor kinetics parameters
    - See also:
      A. Jinaphanh et al., Calculating The Kinetic Parameters In The Continuous Energy Monte-Carlo Code Moret, this conference (Tuesday May 11, session 3C)

- **Optimized for industrial applications**
  - High precision and low calculation time

- **Experimental validation program**
  - Over 2000 experiments (mostly coming from the ICSBEP criticality benchmark compilation)

How to perform calculations with MORET ?

- **Create input file and launch the code with it**
  - Nuclear data reference in a data file

- **How to write an input file?**
  - Only one ASCII file
  - Sequence of instructions with formatted syntax
    - Predefined structure
    - User friendly
    - Easily interpretable by the code

Input file structure

```
"Title line"

Materials   MATE
                <material description>
            ENDM

Geometry    GEOM
                <geometry description>
            ENDG

Sources     SOUR
                <initial distribution for neutrons>
            ENDS

Simulation  SIMU
                <calculation options>
            ENDS

Output      OUTP
                <output options>
            ENDO

[ Other options ]

ENDData
```

Materials

- **Multi-group approach**
  - Use calculated cross sections for “ macroscopic ” regions - homogenization
  - Coupled with several deterministic codes
    - APOLLO2
    - DRAGON
    - SCALE

- **Continuous energy code**
  - Use cross section data files directly (ace format)
  - Unified energy grid
    - Correspondence tables
  - Coupled with VESTA (under development)

Geometry (1/2)

- **3D "modular" geometry**
  - made from building blocks called "modules"
  - Set of independent geometric sub-systems containing volumes

- **Predefined shapes**

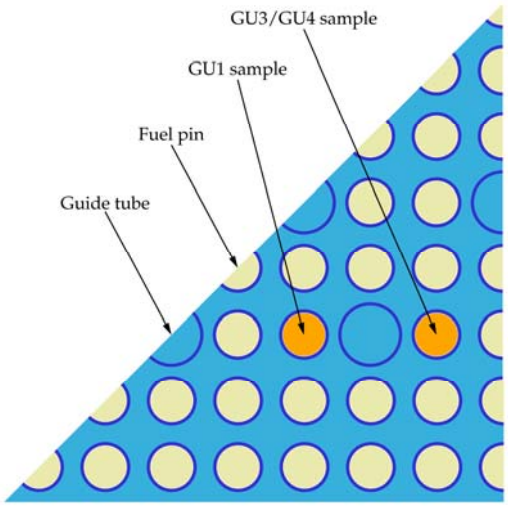
```
BOX, SPHERE, CYL{X|Y|Z|Q}, HEX{X|Y|Z}, CON{X|Y|Z}, PLA{X|Y|Z}, Multiple PLAnes …
```

- **Combinatorial operators**
  - Override, Union, Intersection, Subtraction
  - Rotation (under development)

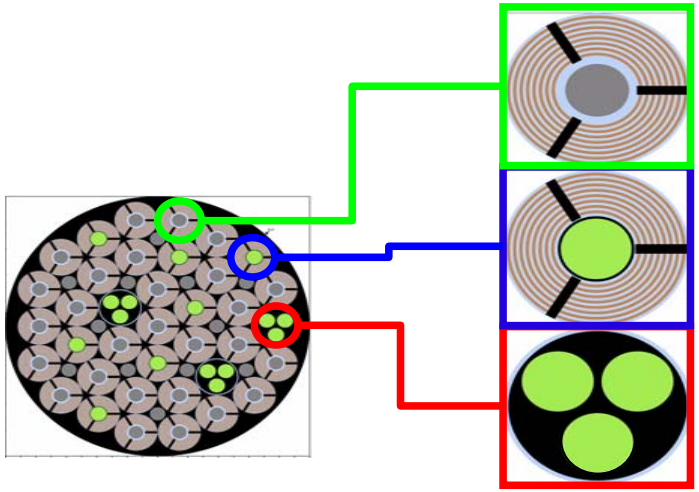
- **Lattices (and lattices of lattices)**

Geometry (2/2)

- **Examples**



ARIANE program



RJH

Simulation (1/3)

- **Analog (or natural or conventional) method**
  - Calculation of the proportion of neutrons for each fissile zone to be emitted in the following step
  - Default simulation method (widely used in Monte Carlo criticality codes)

- **Stratified sampling**
  - Similar to analog method
  - Each fissile zone contains at least one source neutron at each generation
    - If necessary, an additional neutron is generated with a reduced weight
  - Useful for tracking in zones that are weakly coupled with the rest of the system

- **Superhistory powering**
  - Tracking of source neutrons and its progeny over several generations
    - Avoid recalculating the source distribution at each generation
  - Useful to reduce correlations between steps

Simulation (2/3)

K_{ij} matrix : neutrons produced by fission in volume i based on one neutron emitted in volume j

- Multiplication factor k_{eff} = largest eigenvalue
- Neutron distribution = associated eigenvectors

- **K_{ij} (or fission matrix) method**
  - Similar approach as stratified sampling
  - Use of K_{ij} matrix
    - Eigenvectors of the K_{ij} matrix simulate the distribution of source neutrons for the following step in order to accelerate source convergence

- **Importance method**
  - Similar approach as stratified sampling
  - Use of "importance function" based on eigenvectors of the adjoint K_{ij} matrix
    - Inhibits the creation of neutrons in lower reactivity volumes

Simulation (3/3)

- **Wielandt method** (under validation)
  - Accelerate source convergence by modifying the transport equation to be solved, by subtracting the same fission source term in each side
    - Same eigenfunctions
    - k-eigenvalues are shifted : the dominance ratio is decreased

- **Alternative tracking approach : Woodcock method**
  - Introduction of new concept : fictive collisions
  - Only one homogeneous cross section in “woodcock” zone
    - Fictive cross section for each material in “woodcock” zone
  - Useful for tracking in (heterogeneous) systems with a high number of volumes and/or volumes with complex shapes

Output

- **Flexible**
  - User can define his own output quantities
- **Integrated graphical output**
  - Simulation
  - Geometry
- **Includes specific predefined output for coupling with VESTA**

Reactor physics applications

Application areas

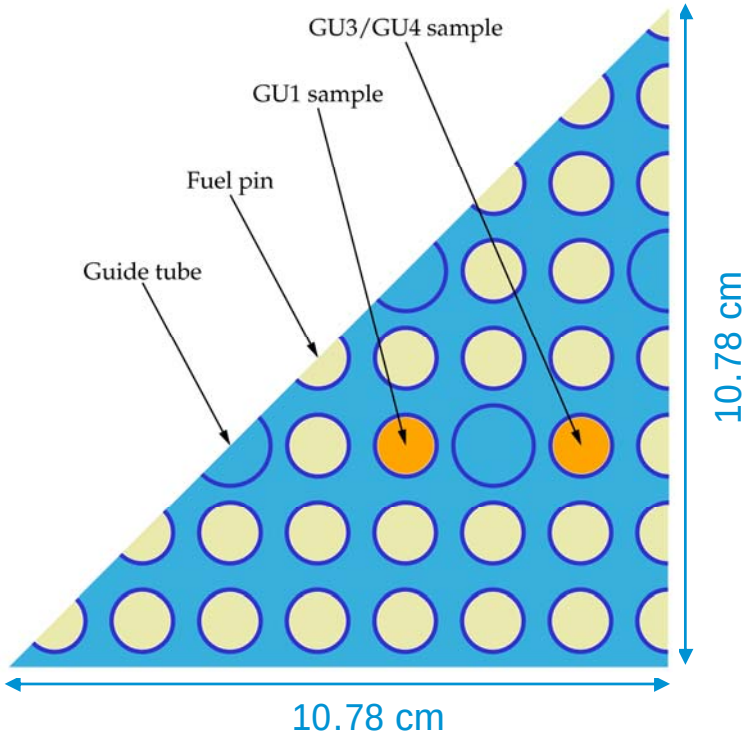
- **Current reactor applications:**
  - Burn-up credit calculations (fuel pin or assembly level)
  - Standard applications: PWR – BWR

- **New and « exotic » applications:**
  - Research reactors: ILL's RHF, Réacteur Jules Horowitz (RJH, France)
  - Advanced nuclear systems: GEN IV, hybrid systems, etc.
  - Fusion systems (ITER, DEMO, etc.)

- **But also for radiation protection related applications:**
  - Assessment of material activation:
    - Shielding design (particle induced neutron sources)
    - Production of medical isotopes
  - Radioactive waste characterisation

The ARIANE program: modelling a PWR assembly

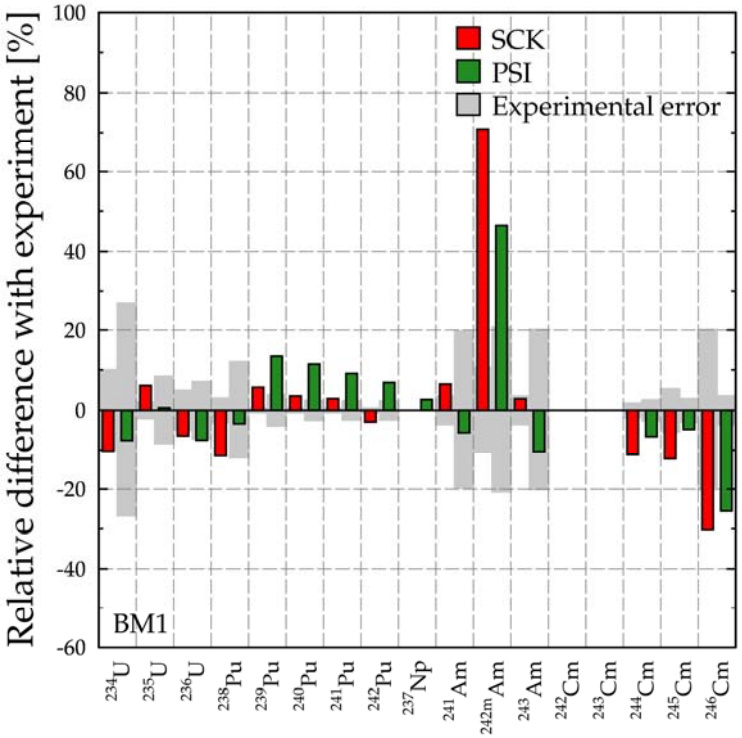
- **Model characteristics:**
  - 2D model (no rod end effects)
  - Use symmetry :
    - 1/8 assembly for the UO_2 samples
    - 1/2 assembly for the MOX samples
  - Average boron concentration
  - Individual pins are being depleted:
    - 32 pins for the UO_2 samples
    - 94 pins for the MOX samples
  - Tmod = Tclad = 600 K
  - Tfuel = 900 K
  - Nuclear data: JEFF 3.1



- **See also:**
  - L. Cousin, W. Haeck, B. Cochet, Validating the VESTA Monte Carlo Depletion Interface using ARIANE Chemical Assay Data for Pressurised Water Reaction Applications, this conference (Monday May 10, session 3B)

Some actinide results

- **U isotopes**
  - Overestimation of ^{235}U by 5-10 %
  - ^{234}U and ^{236}U are generally below the experimental values
- **Pu isotopes:**
  - Differences rarely larger than 5-10 %
  - Underestimation for ^{238}Pu and ^{242}Pu
  - Overestimation for ^{239}Pu, ^{240}Pu and ^{241}Pu
- **Am and Cm isotopes:**
  - Am overestimated
  - Cm underestimated by at least 10 %
  - Large overestimation for ^{242m}Am due to branching ratio data

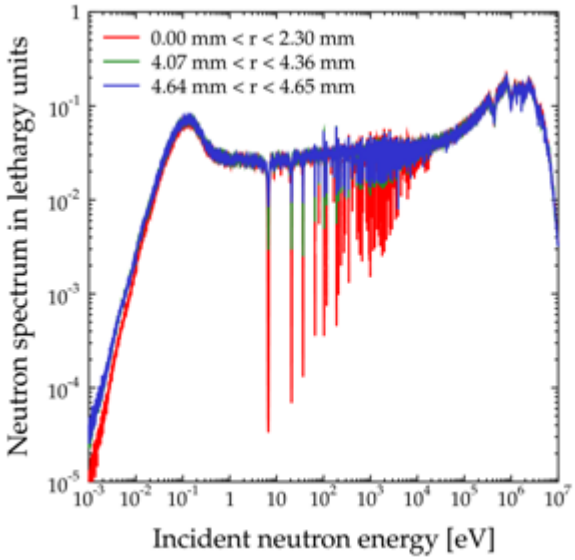


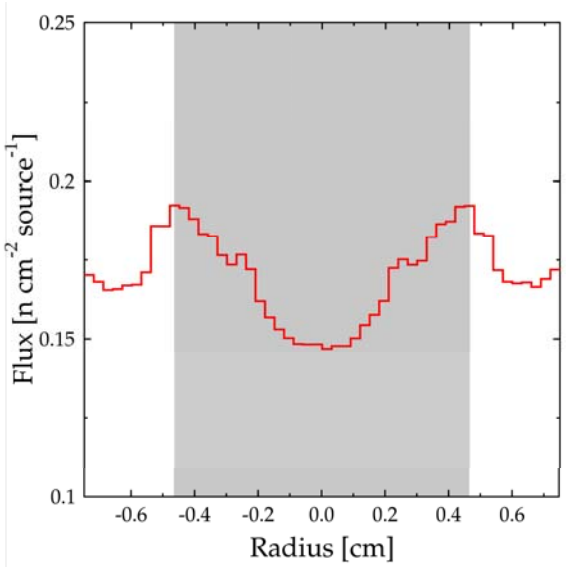
Fuel performance

- **Self-shielding in a nuclear reactor**
  - A spatial effect due to the heterogeneity of the reactor
  - An energetic effect due to cross section resonances

- **This leads to a radial dependance of the composition of the fuel pellet**

Neutron spectra and the radial flux distribution in a fuel pellet

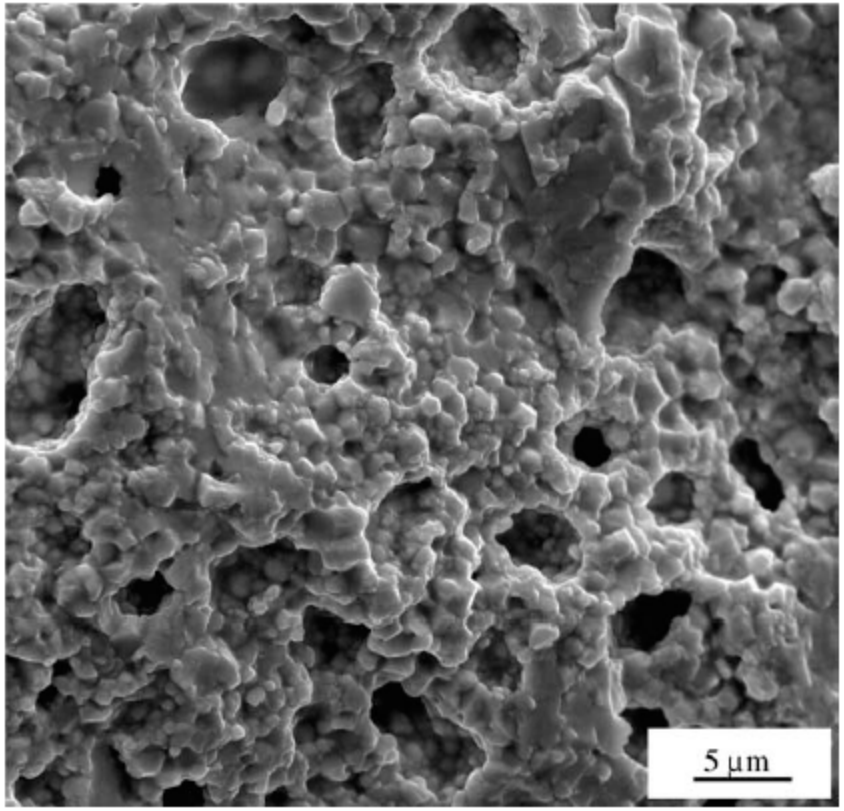




Fuel performance

- **Self-shielding and its effect on the material composition has an impact on fuel performance:**
  - Thermal properties, retention of fission products inside the fuel, etc.
  - Local recristalisation of the pellet above 60 MWd/kgHM

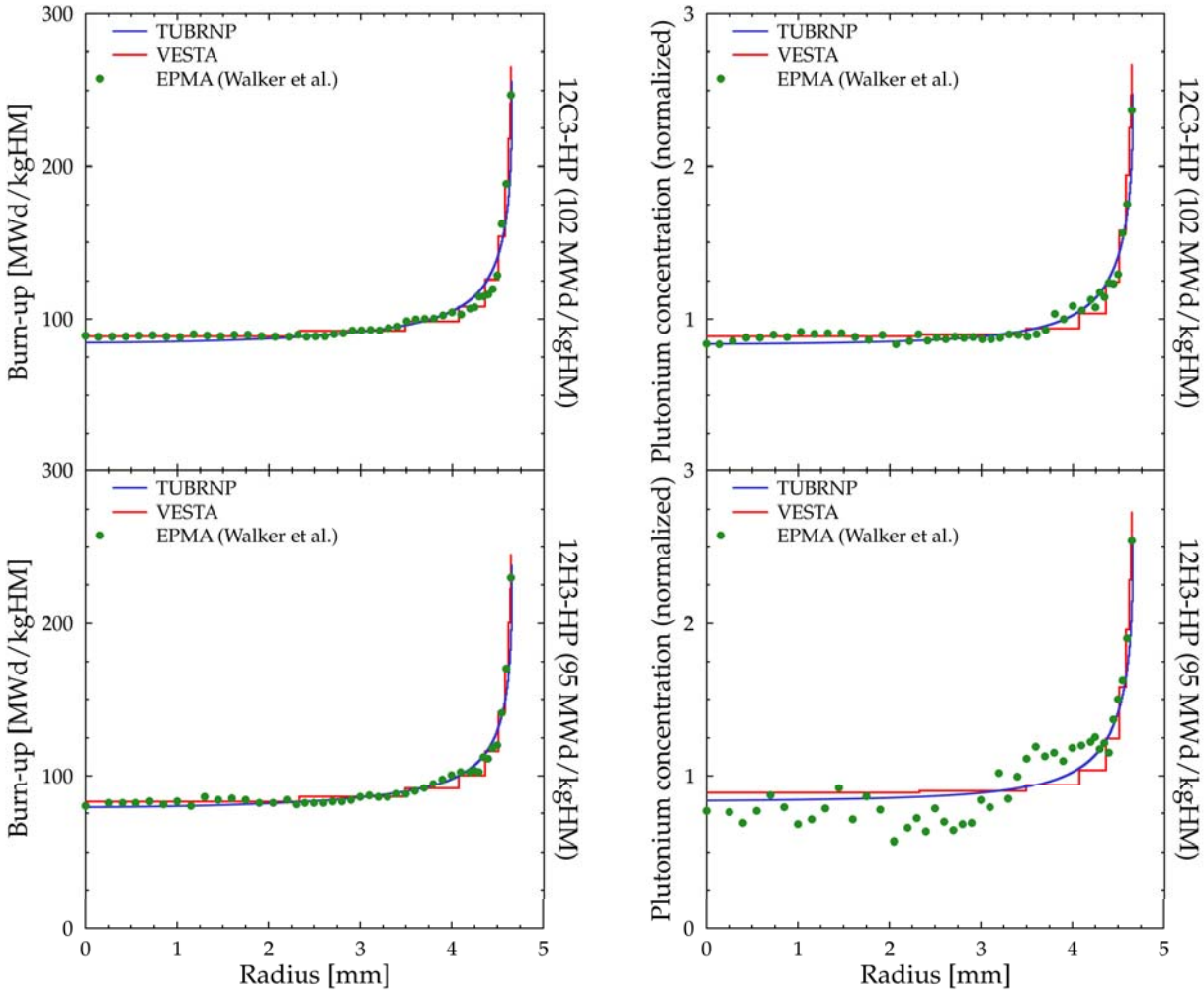
- **High burnup structure:**
  - Small grains with an average size of around 0.15 µm
  - Pores with a typical diameter of 1 to 2 µm
  - Characterised by Xe loss



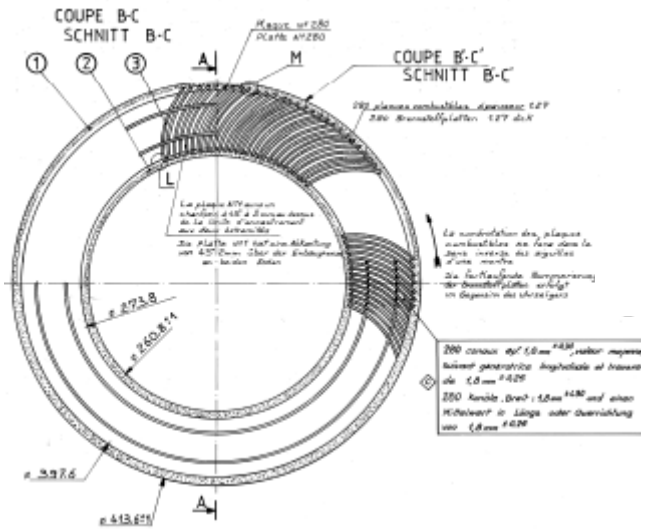
Picture taken from C. T. WALKER, D. STAICU, M. SHEINDLIN, D. PAPAIOANNOU, W. GOLL, F. SONTHEIMER, "On the thermal conductivity of UO2 nuclear fuel at a high burn-up of around 100 MWd/kgHM", *J. of Nucl. Mat.* **350**, 19-39 (2006)

Fuel performance

Radial burn-up and plutonium profiles in a fuel pellet

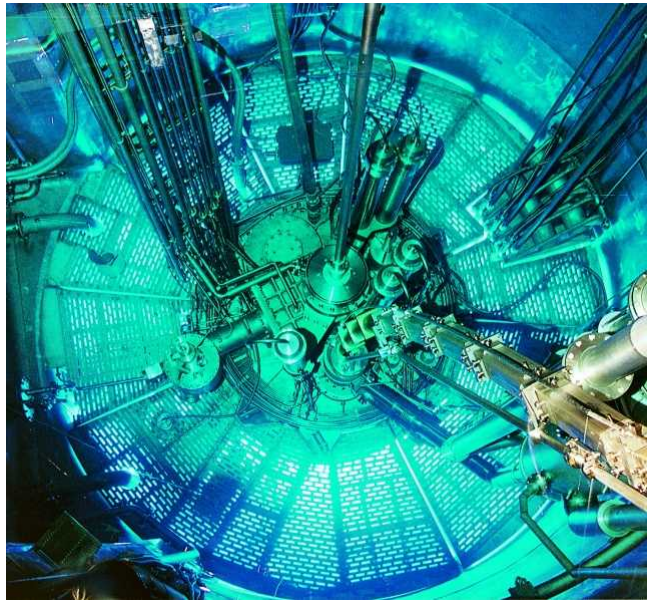


The High Flux Reactor at ILL



- **A very interesting test case:**
  - An atypical reactor designed to obtain high flux levels
  - Very high burn-up of 250-300 MWd kg^{-1}
  - Slow moving control element: a few cm day^{-1}
  - High enriched uranium fuel

- **VESTA calculations:**
  - Using the MCNP model provided by ILL
  - One 50 day cycle at 55 MW
  - Using single day time steps
  - ENDF/B-VII at 293.6 K



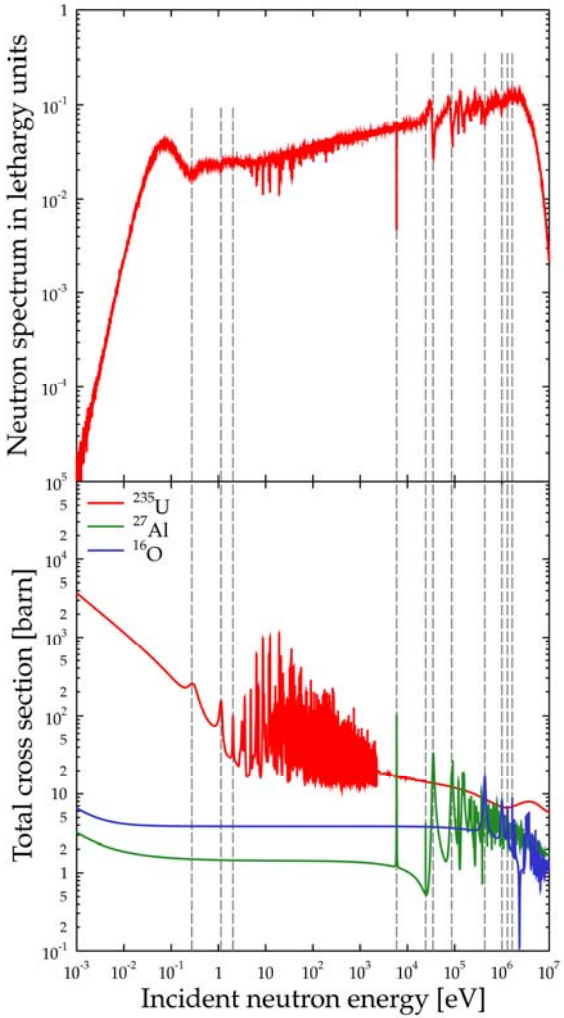
- **See also:**
  - A. Bergeron, Y. Calzavara, W. Haeck, B. Cochet, Study of RHF Conversion in LEU Fuel Neutronic Calculations with MCNPX and VESTA, this conference (Wednesday May 12, session 9C)

Validating the group structure for the RHF

- **The standard group structure appears to be appropriate for the RHF:**
  - The spectrum inside the fuel plates passes the ^{238}U test case
  - The differences of the values calculated by VESTA are negligible compared to the standard deviation given by MCNP5

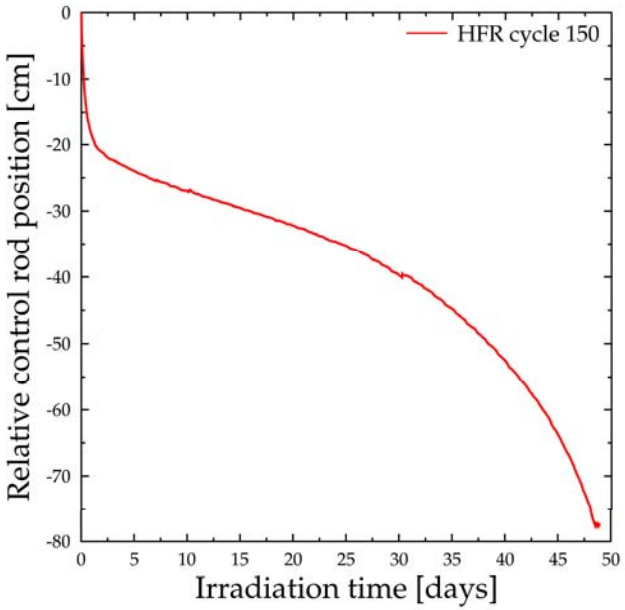
^{238}U single group cross sections as calculated by MCNP5 and VESTA using multi-group binning

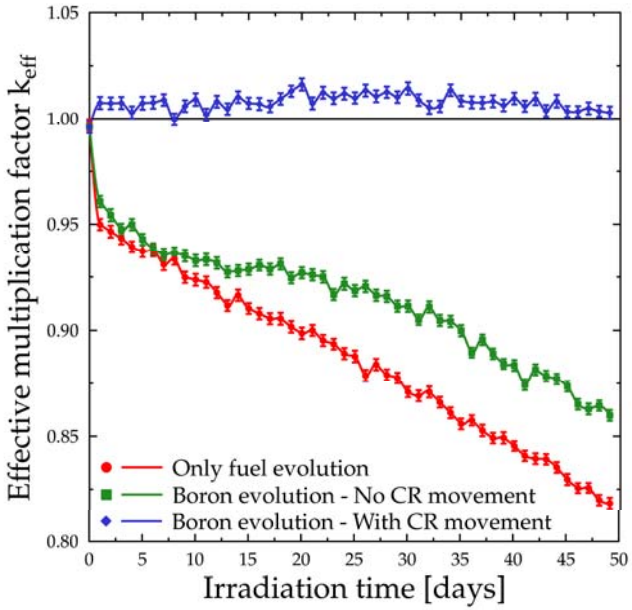
Reaction	MCNP5	VESTA
Neutron capture	5.7893E+00 (2.29 %)	5.7913E+00 (0.03 %)
n,2n	3.4130E-03 (2.81 %)	3.4127E-03 (0.01 %)
n,3n	1.4335E-05 (28.23 %)	1.4338E-05 (0.02 %)
Fission	7.6407E-02 (0.61 %)	7.6408E-02 (0.001 %)



Reactor operation

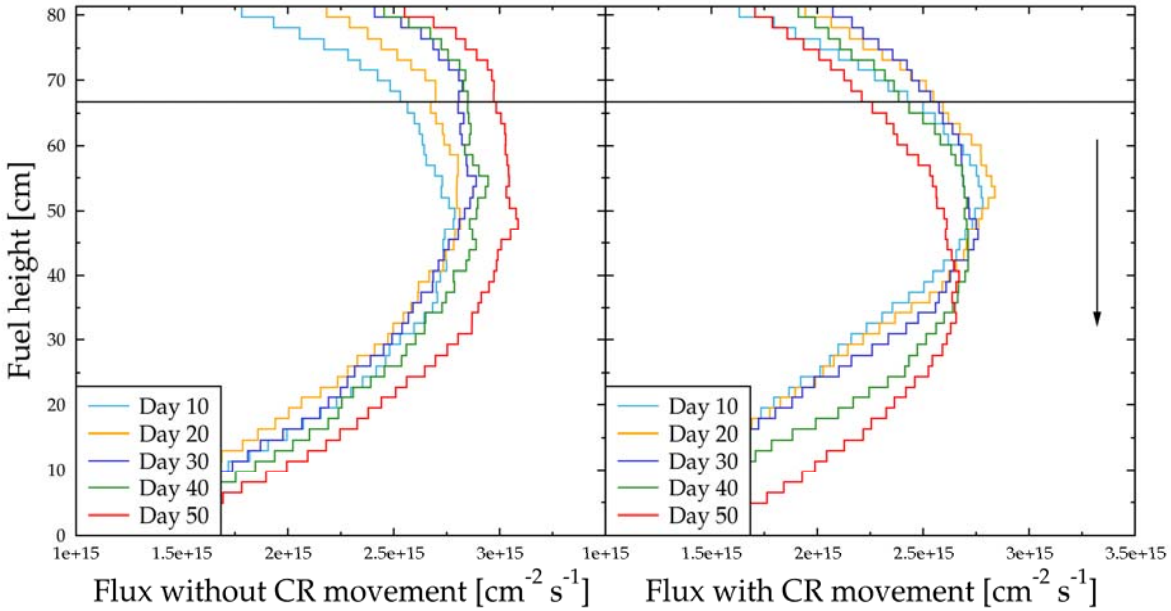
- **Due to fuel burn-up it is impossible to maintain the criticality of a reactor without external effort:**
  - ^{10}B burnable absorber included at the top and bottom of the fuel plates
  - The control element in the middle of the core
- **Taking these control mechanisms into account, results in a constant k_{eff}**





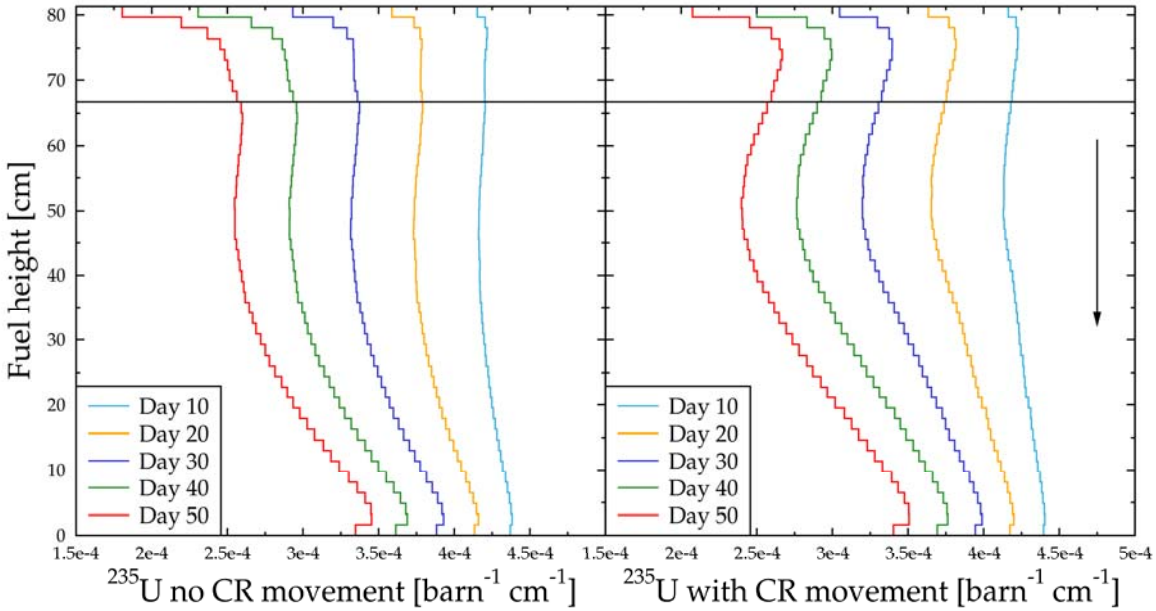
Flux distributions

- **Without control rod movement:**
  - An artificial increase of the flux to obtain the same power level
- **With control rod movement:**
  - A (relative) stable distribution with a maximum that moves with the control rod



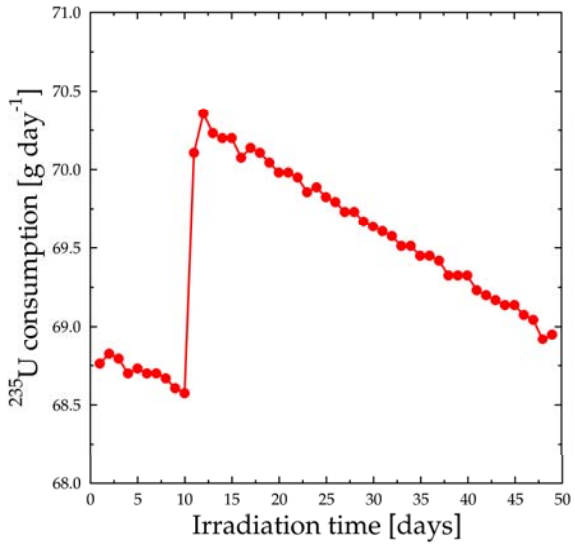
Fissile material consumption

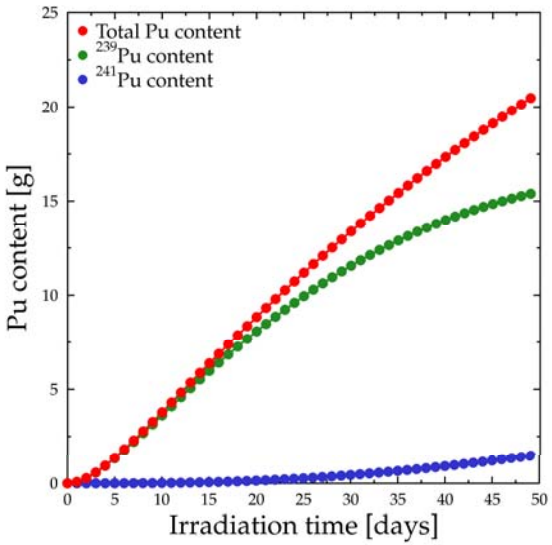
- **Without control rod movement:**
  - High ^{235}U consumption at the top of the fuel element
- **With control rod movement:**
  - More ^{235}U consumption in the middle of the fuel element
  - A local minimum that moves with the control rod



Uranium consumption and plutonium production

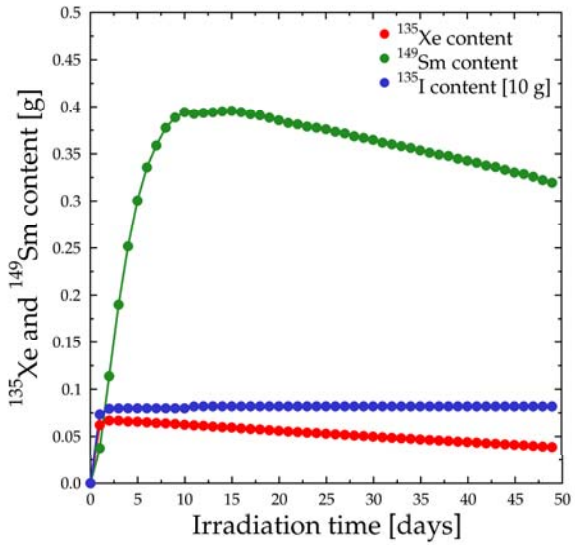
- **For a typical cycle, the HFR is loaded with 8.58 kg of ^{235}U:**
  - The ^{235}U consumption is slightly constant at 71 to 68 g day^{-1} with an increase after day 10 due to a power increase from 53.6 to 55 MW
  - At the end of the cycle, 3.40 kg of ^{235}U has been consumed
  - This is "compensated" with Pu production and consumption:
    - Steady buildup of ^{239}Pu up to day 15
    - Buildup slows down afterwards due to increased consumption

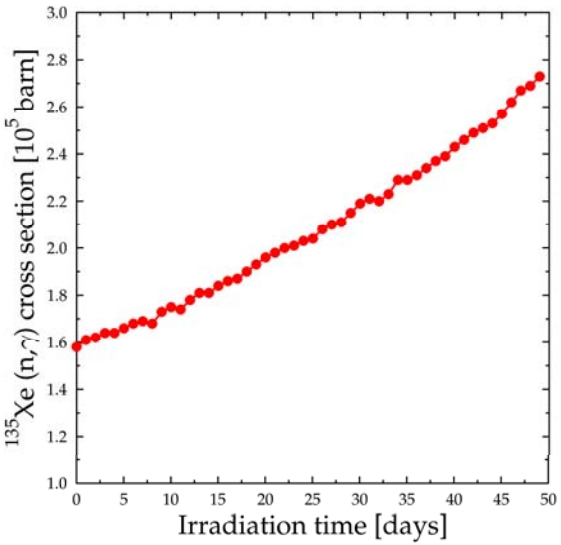




Fission product equilibrium in the HFR core

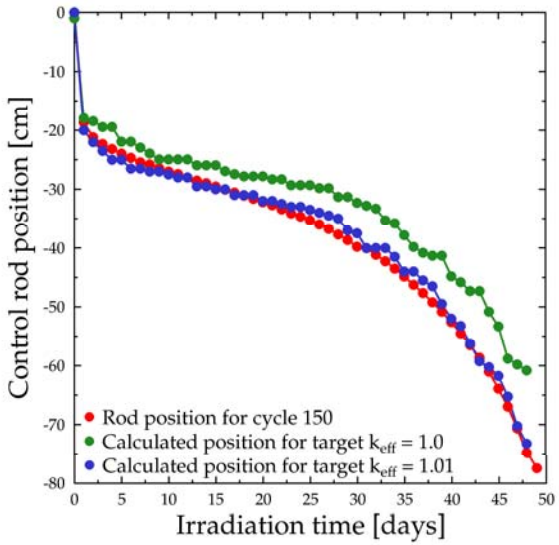
- **The ^{135}Xe and ^{149}Sm content never reach equilibrium:**
  - A global equilibrium in ^{135}Xe production as evidenced by the constant ^{135}I content
  - An ever increasing ^{135}Xe (n,γ) cross section due to significant spectral changes (thermalisation) of the HFR core
  - This results in a decreasing ^{135}Xe content as a function of irradiation time

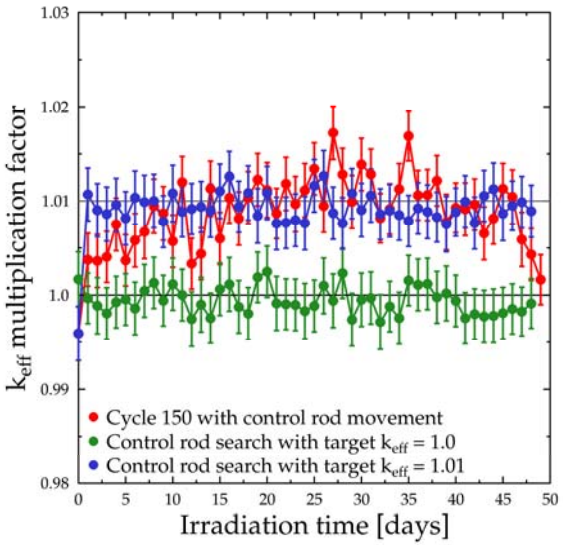




Automated control rod position search for the RHF

- **For some applications the control rod position is not known and requires an automated control rod position search**
  - Determination of cycle length in the HFR's fuel conversion program
- **Differences in control rod positions for HEU cycle 150:**
  - Control rod ageing (systematic bias on the control rod position)
  - Nuclear data uncertainty for fission products

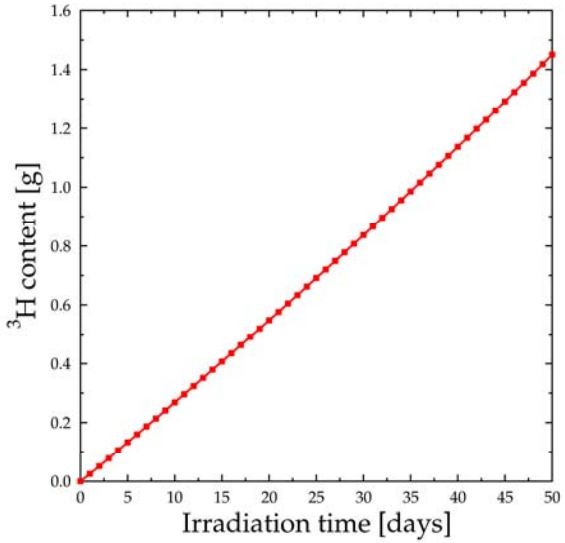




Some radiological issues

- **Due to the high neutron flux in the HFR, the deuterium in the heavy water used in the HFR is transformed into tritium ($T_{1/2}$ = 12.33 years)**

- **In a total volume of 11.5 m^3 of heavy water, about 1.4 g of tritium has been produced during a single 50 day cycle:**
  - Density of 0.0244 atoms $barn^{-1}$ m^{-3}
  - Activity of 43.5 MBq cm^{-3}



Conclusions

- **VESTA and MORET5:**
  - Efficient and accurate
  - Flexible and easy to use

- **Good agreement between calculations and experiments for realistic applications:**
  - PWR applications
  - RHF reactor

- **A code for reactor physics calculations should always be qualified and should not be used as a black box**
  - Never ending work in progress!

If you can model it, we can burn it!