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The New MCNP6 Depletion Capability

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Abstract –*The first MCNP based inline Monte Carlo depletion capability was officially released from the Radiation Safety Information and Computational Center as MCNPX 2.6.0. Both the MCNP5 and MCNPX codes have historically provided a successful combinatorial geometry based, continuous energy, Monte Carlo radiation transport solution for advanced reactor modeling and simulation. However, due to separate development pathways, useful simulation capabilities were dispersed between both codes and not unified in a single technology. MCNP6, the next evolution in the MCNP suite of codes, now combines the capability of both simulation tools, as well as providing new advanced technology, in a single radiation transport code. We describe here the new capabilities of the MCNP6 depletion code dating from the official RSICC release MCNPX 2.6.0, reported previously, to the now current state of MCNP6. NEA/OECD benchmark results are also reported.*

The MCNP6 depletion capability enhancements beyond MCNPX 2.6.0 reported here include: (1) new performance enhancing parallel architecture that implements both shared and distributed memory constructs; (2) enhanced memory management that maximizes calculation fidelity; and (3) improved burnup physics for better nuclide prediction.

MCNP6 depletion enables complete, relatively easy-to-use depletion calculations in a single Monte Carlo code. The enhancements described here help provide a powerful capability as well as dictate a path forward for future development to improve the usefulness of the technology.

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Overview

- Introduction
- Parallel Architecture
- Memory Management
- Physics Enhancements
- H. B. Robinson Benchmark
- Further Considerations

The Way I See It

- **Monte Carlo linked burnup strategies still exist!**
  - Link MCNP, TRIPOLI, MVP, etc. to ORIGEN, CINDER, PEPIN, etc.
- **Advantages**
  - Self Shielding
  - Continuous Energy
  - Combinatorial Geometry
  - “Details”
- **Disadvantages**
  - Size
  - Speed

“Details”

- **Details**
  - When cross section fidelity is extremely important
  - High degree of anisotropy
  - Large streaming effects
- **Examples**
  - **Nonproliferation and Process Monitoring**
    - Low σ_c, high decay yield nuclides used in a material characterization
  - **High Burnup and Advanced Clads and Coatings**
    - Appreciable spectra over varying significant resonances
  - **SMRs, Fast Reactors and Test Reactors**
    - Fuel reflector interface and highly leaky systems
- **Best Fit**
  - **Compliment deterministic solutions by qualifying the design space**

MCNP6 Burnup History

- **First official release to RSICC as MCNPX 2.6.0**
  - Easy-to-use interface and linked to CINDER90
  - Reactor-wide and region-specific isotopics and power distributions
  - Isotope Generator Algorithm
  - (n,f), (n,γ), (n,2n), (n,3n), (n,p), and (n,α) with error printing
  - Automatic fission yield selection
  - Repeated structures
  - Predictor-Corrector
  - Time dependent material modification
- **Second official release to RSICC as MCNPX 2.7.0 → MCNP6**
  - MPI Parallel architecture
  - First cut memory savings
  - "Other Physics Enhancements"

Parallelization Considerations

$$\frac{dN_m(\vec{r},t)}{dt} = -N_m(\vec{r},t)\beta_m + \overline{Y}_m + \sum_{k \neq m} N_k(\vec{r},t)\gamma_{k\to m}$$

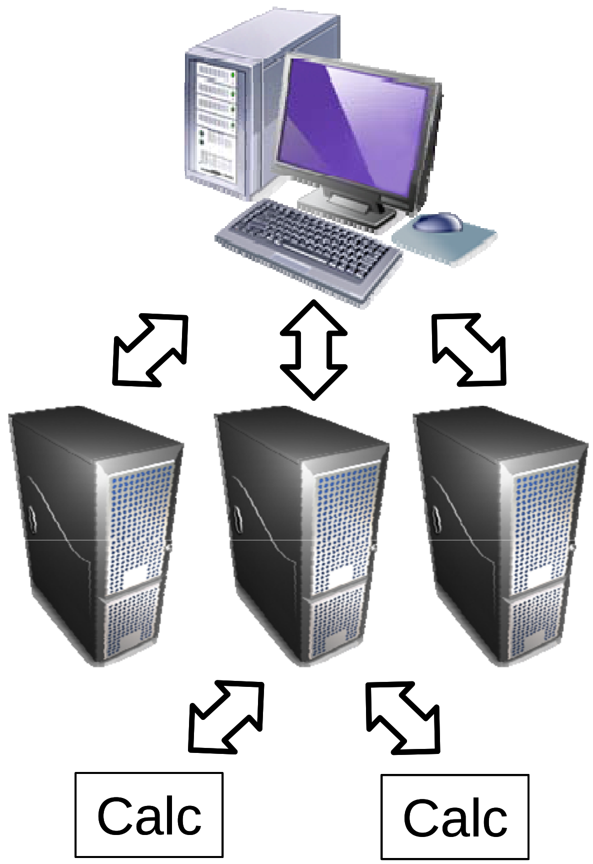
$$\beta_m = \lambda_m + \sum_r \int \sigma_{m,r}(E)\Phi(r,E,t)dE$$

$$\gamma_{k\to m} = \sum_{m\neq k} L_{km}\lambda_k + \sum_{m\neq k}\sum_r \int Y_{km,r}(E)\sigma_{k,r}(E)\Phi(r,E,t)dE$$

- **ANFM 2009**
  - "*CINDER90 takes seconds to run, but running 100s of calculations in serial causes the burnup to take longer than the transport*"
- **No transverse leakage terms in Bateman equations!**
  - MPI method implemented in MCNPX 2.7.A

OPENMP and MPI

- **Message Pass Interface – Distributed**
  - **Advantages**
    - Amdahl's Law → $S(N) = \frac{1}{(1-p)+\frac{P}{N}}$
    - Independent work → No locks for race conditions
  - **Disadvantages**
    - Memory
    - Bottleneck with collection as N → large
- **OPENMP – Shared Memory**
  - **Advantages**
    - Shared memory usage
    - Reduced bottleneck from minimal collection
  - **Disadvantages**
    - Locks required to sweep global variables



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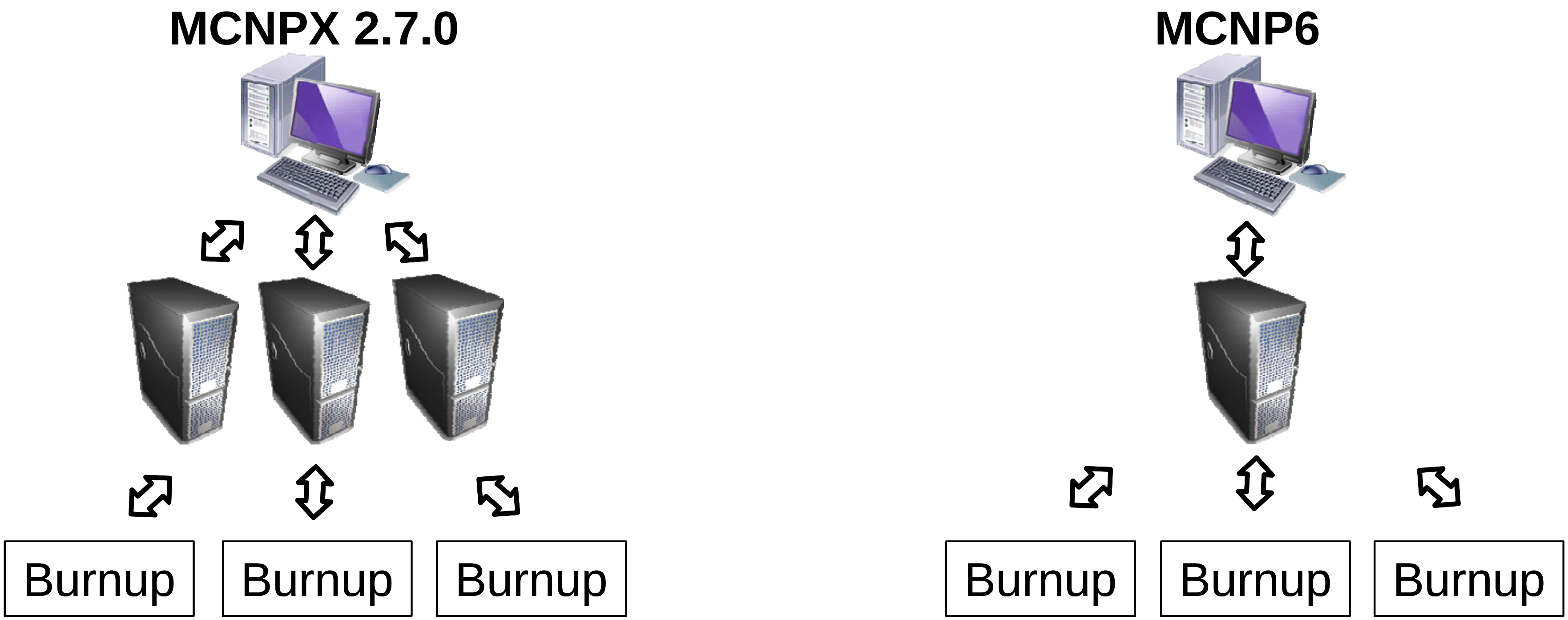
Work Distribution Algorithm



- **Larger sends to fewer nodes**
- **Using sections of coefficient and density arrays on each thread**

Speedup Tests

- **Simple Test**
  - 28 burn regions
  - 76 total nuclides per region
  - 5000 p/c, 33 c skipping 2 c
- **Results**
  - 1N8T ~50% speedup from 8N1T
  - 3N1T almost linear speedup
  - 8N1T not linear speedup
  - 3N8T ~33% speedup from 24N1T
  - KCODE is less parallel friendly than SDEF → communication at the itteration

Nodes	Threads	Computational Speedup*
1	1	na
1	8	7.66
8	1	4.88
3	1	2.28
24	1	9.00
3	8	13.38

Performance -- What is going on?

- **Using MPI initiates communication logic**
  - **Bottleneck**
- **Collection is linear**
  - **Bottleneck**
- **CINDER90 involves minimal file I/O**
  - File I/O requires locking → only minimal locking
- **Symbiotic relationship between MPI and OPENMP**
  - Leverage MPI to talk to nodes that use OPENMP to talk to cores
  - Sends between threads on common RAM is faster than sends between separate computers → **Reduce Bottleneck**
  - Coefficient/density arrays are THREADSHARED → **Decrease Memory**

Memory Management Considerations

- **MCNP is too robust!**
  - MCNPX merged MCNP4B and LAHET 2.8 codes, to transport all particles at all energies, in support of the Accelerator Production of Tritium (APT)
  - No ENDF/B greater than ~100 MeV → mix and match cross section models
    - **Arrays allocated regardless of use due to potential of use**
- **Too robust = defaults not best for every application**
  - Particle bank → **Too high memory restrictions; Too low performance restrictions**
- **Better guessed defaults and removing not unused capability (MCNPX 2.7.D good → MCNP6 better)**
  - dbcn(28) = amount of particles saved in the bank
  - MCNPX → phys:n A 3j B where B > A; MCNP6 → phys:n A 6j B where B > A
    - Turn off photonuclear
  - MCNP6 eliminates more non-neutron transport stuff (Heavy ions and electrons)
  - MCNP6 also expunges all cross sections not used for burnup or in transport (~8%)

Memory Savings

- **Simple Test**
  - 600 concentric spheres
  - 600 burnable regions containing
  - 277 total nuclides per region

Case	RAM usage during runtime [GB]*	Savings [GB]	% Savings*
MCNPX 2.7.D	3.80	na	na
MCNPX 2.7.D M	0.78	3.02	79.47%
MCNP6 M	0.43	3.37	88.68%

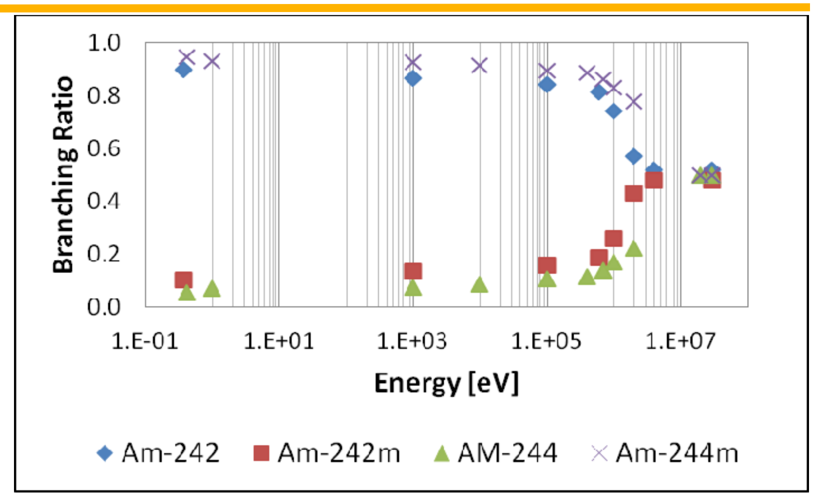
- **Results**
  - Savings is ~order of magnitude from base case in MCNP6
  - MCNP6 saves about 10% more memory than MCNPX
  - As problem size increases savings increases
    - $Size = \left(\sum_i^I Isotopes_i\right) \times \left(\sum_j^C Cells_j\right) \times \left(\sum_k^S Stuff_k\right)$
    - MORE BURN MATERIALS PER MEMORY

Physics Enhancements

- **Automatic Fission yield selection**
  - Fast fission band changed from 1-14 MeV to 1e-6-14 MeV
- **Actual (n, γ) instead of summed capture for computing (n, γ) collision rates for CINDER90**
  - Greatly improves B-10 burnuout
- **Corrected Isomer Branching**
  - Combination of continuous energy integrated (n, γ) from MCNP and computed 63-group energy integrated (n, γ*) from CINDER90

Isomer Branching

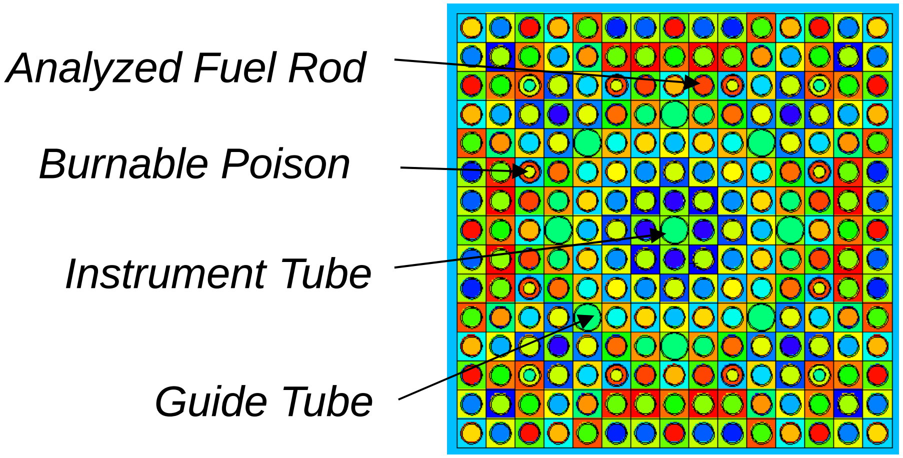
- **MCNPX 2.6.0 over predicted (n, γ) by Tallying total (n, γ)**
- **At ICAPP 2008 → *"future focus… include ENDF/B File 9 MT 102 and File 10 in ACE…"***
  - W. HAECK, B. Cochet, L. Aguiar, "Isomeric Branching Ratio Treatment for Neutron-Induced Reactions," *Trans ANS*, **103**, pg 693-695 (2010) – **Memory Increase**
- **Isomer Branching in MCNP**
  - **Less memory and faster!**



$$(n,\gamma)_{Corrected} = \left(1 - \frac{\left(\sigma_{n,\gamma^*} * \Phi\right)_C}{\left(\sigma_{n,\gamma} * \Phi\right)_M}\right) \times \left(\sigma_{n,\gamma} * \Phi\right)_M$$

H. B. Robinson

- **15 X 15 Westinghouse fuel assembly from H. B. Robinson Unit 2**
  - ORNL/TM-12667
  - ENDF/B VII.0 temperature dependent library
  - 16.02, 23.8, 28.47, and 31.66 GWD/MTU



Cycle	1	2	3	4
Operating Interval (days)	243.5	243.5	156	156
Downtime (days)	40	64	39	--**
Average Soluble Boron Concentration (ppm)	625.5	247.5	652.5	247.5

** 3936 for Cases A-B or 3637 for Cases C-D

Results

	Case A 16.02 GWD/MTU			
Isotope	MCNP6	MCNPX	SCALE	MONTEBURNS
235U	3.73	0.42	0.60	2.62
236U	-3.43	-1.76	-1.50	-3.37
238U	0.06	0.12	0.10	0.17
238Pu	-2.69	-3.41	1.50	2.29
239Pu	5.59	0.27	7.00	2.01
240Pu	2.66	3.32	-1.50	4.22
241Pu	7.68	3.57	5.90	7.04
237Np	-3.23	-6.13	6.00	-2.76
99Tc	8.49	10.91	12.40	11.35
137Cs	-3.06	-1.12	0.20	-1.64

	Case B 23.8 GWD/MTU			
Isotope	MCNP6	MCNPX	SCALE	MONTEBURNS
235U	3.71	-0.58	1.40	4.11
236U	-2.70	-1.90	-2.20	-3.09
238U	-0.60	-0.54	-0.60	-0.53
238Pu	-4.22	-3.86	0.90	0.83
239Pu	2.50	-0.37	7.70	1.31
240Pu	1.62	0.59	-4.20	1.61
241Pu	5.44	2.82	6.00	4.97
237Np	-4.88	-7.31	5.50	-5.55
99Tc	5.70	6.76	8.60	8.34
137Cs	-2.82	-1.88	-0.80	-2.22

% Difference from Measured Data

Results

	Case C 28.47 GWD/MTU			
Isotope	MCNP6	MCNPX	SCALE	MONTEBURNS
235U	-3.27	-11.80	-4.90	-2.44
236U	1.84	3.72	2.20	1.24
238U	0.47	0.47	0.50	0.54
238Pu	-11.04	-14.72	-6.50	-7.01
239Pu	-0.64	-9.22	5.30	-1.77
240Pu	2.09	-5.42	-4.90	1.14
241Pu	-5.08	-11.03	0.50	-4.72
237Np	3.03	2.43	14.30	2.45
99Tc	11.45	9.58	14.60	14.94
137Cs	0.11	-0.38	3.90	0.70

	Case D 31.66 GWD/MTU			
Isotope	MCNP6	MCNPX	SCALE	MONTEBURNS
235U	-0.08	-9.66	3.30	5.98
236U	0.17	1.18	-0.40	-1.51
238U	-0.73	-0.73	-0.80	-0.89
238Pu	-8.58	-10.69	2.60	1.97
239Pu	-0.20	-8.66	12.80	6.00
240Pu	1.32	-6.52	-4.10	2.65
241Pu	-2.56	-8.79	9.10	2.71
237Np	1.58	3.08	18.40	7.91
99Tc	7.79	5.53	11.20	11.90
137Cs	-2.45	-3.09	1.50	-1.44

% Difference from Measured Data

Notes on Results

- **Assumptions**
  - Geometry
  - Data
- **Results**
  - **No code best predicts all isotopes at all burnups**
  - Creation and destruction is dictated by spectrum and geometry self- shielding; it is difficult to determine the specific reaction where the methods differ
  - **The difference in data or calculation setup may be generating the largest difference**
- **Conclusions on MCNP6 burnup**
  - Each actinide and Cs-137 was computed to within a few %
  - Tc-99 was computed to within 12%
  - The physics updates in MCNP6 do not produce worse results; and **since these physics enhancements help to better represent the actual model, these improvements should improve accuracy in more complicated calculations**.

Conclusions

- **MCNPX + MCNP5 = MCNP6**
- **MPI with OPENMPI offers significant speedup**
  - Particle transport and the burnup calculation
  - Tests show speedups of 30%-50% as compared to using MPI alone
- **New memory management capability significantly reduces memory footprint**
  - More burn regions per gig of RAM → more fidelity
  - 600 region test case → Mem Usage improved by ~order of magnitude
- **New physics enhancements provide a more correct representation of the burnup physics**
- **H.B Robinson**
  - At 16-28 GWD/MTU → SCALE/SAS2H, MCNPX 2.6.0, MONTEBURNS and MCNP6 produces similar results
  - 31.66 GWD/MTU → MCNP6 produces “superior” results

Future Work

- **Memory reduction**
  - Eliminates 22 large dynamically allocated arrays
  - Over 64 subroutines/ modules allocate variables in MCNP6
  - Large book keeping arrays for tracking variance reduction summary information are dimensioned by $Size = \left(\sum_i^I Isotopes_i\right) \times \left(\sum_j^C Cells_j\right) \times \left(\sum_k^S Stuff_k\right)$
  - Preliminary capability to remove these arrays was tested, and resulted in a further >200 MB of savings for the 600 burn region test case
  - Performance hit!
- **Data decomposition**
  - As problem size increases, data allocation increases so large that storing a complete array on a single node may become impractical
  - Burnup may require data decomposition across several nodes

MCNP6 Release Information

- **MCNP6 Beta 2 released from RSICC in February 2012**
  - Request rate doubled after release announced
- **MCNP6 Beta 3 code now frozen**
  - Perhaps a few bug fixes
- **MCNP6 Beta 3 release expected at the end of summer 2012**
- **MCNP6 Beta 3 expected to have all the code capabilities of production release**
- **MCNP6 Production release in early 2013.**