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Title:	Production and Depletion Calculations Using MCNP
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Production and Depletion Calculations using MCNP

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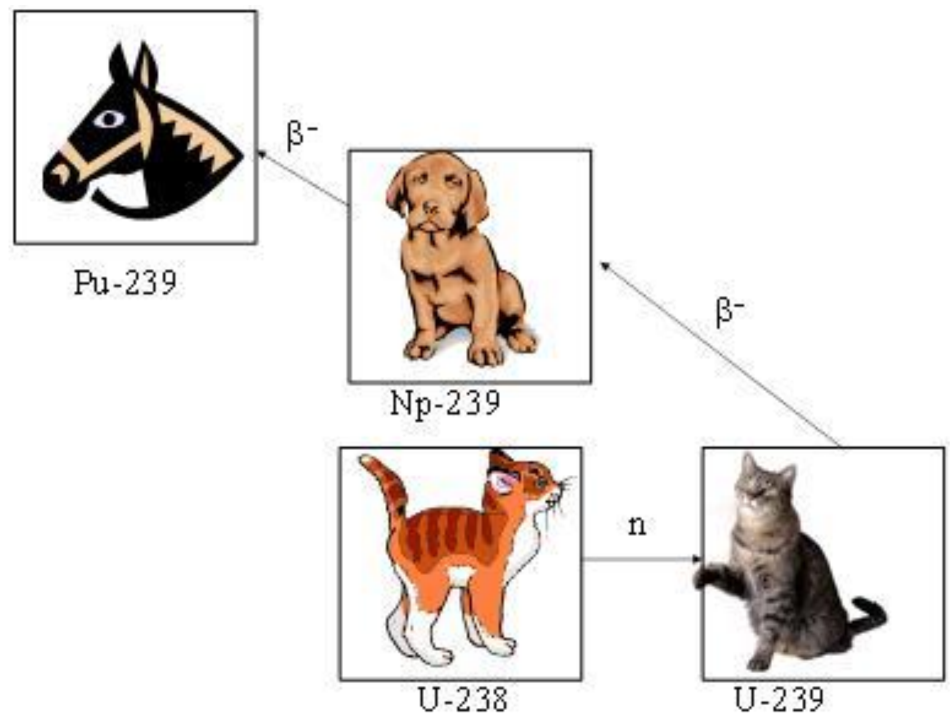
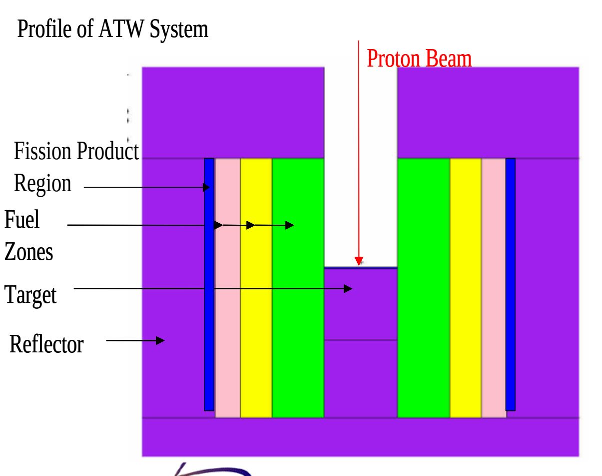
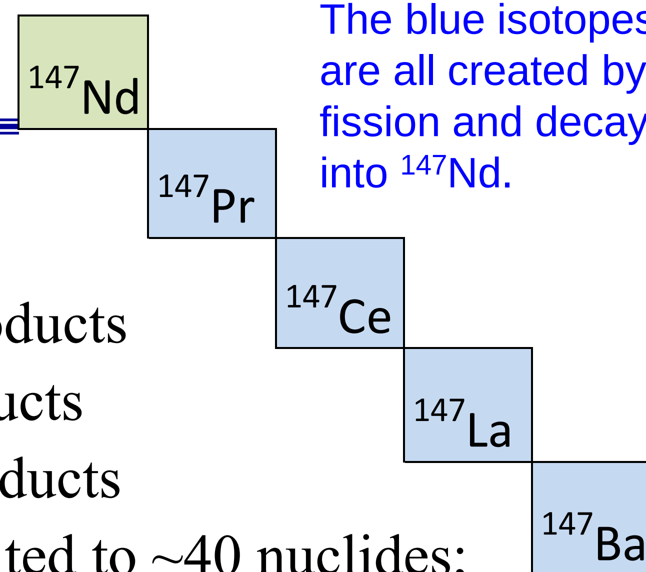


Introduction: Codes for Time-Dependent Isotopic Evolution

- Isotope Generation and Depletion
  - ORIGEN-S/ORIGEN2 (ORNL) – Matrix Exponential Method
  - CINDER90 (LANL) – Markovian Chains
- Depletion codes require accurate cross section and flux data
  - MCNP provides system-dependent, energy-integrated cross sections/fluxes for important isotopes
  - MCNP links to CINDER90 internally or externally through *Monteburns* to any of the 3 codes in bullet 1
  - Activation script exists for proton irradiation of a target/spallation product generation
- Deterministic Lattice Physics Methods
  - CASMO/SIMULATE - nodal 3-D simulator
  - Vendor Codes



Calculations Rely on Data



The blue isotopes are all created by fission and decay into ^{147}Nd.

- Extent of Nuclides
  - CINDER90 3400 Isotopes, 1325 Fission Products
  - ORIGEN2 1700 isotopes, 850 Fission Products
  - ORIGEN-S 1946 isotopes, 1119 Fission Products
  - Applications such as radiochemistry are limited to ~40 nuclides; could benefit from more detailed calculations.
- Fission Product Yields
  - ORIGEN includes up to 8 actinides/reactor type
  - CINDER90 includes up to 24 actinides from ENDF-B VI
  - Thermal: 18 isotopes, Fast: 22 isotopes,
    14 MeV: 11 isotopes, Spontaneous Fission: 9 isotopes

CINDER90 (Tal England, Bill Wilson)

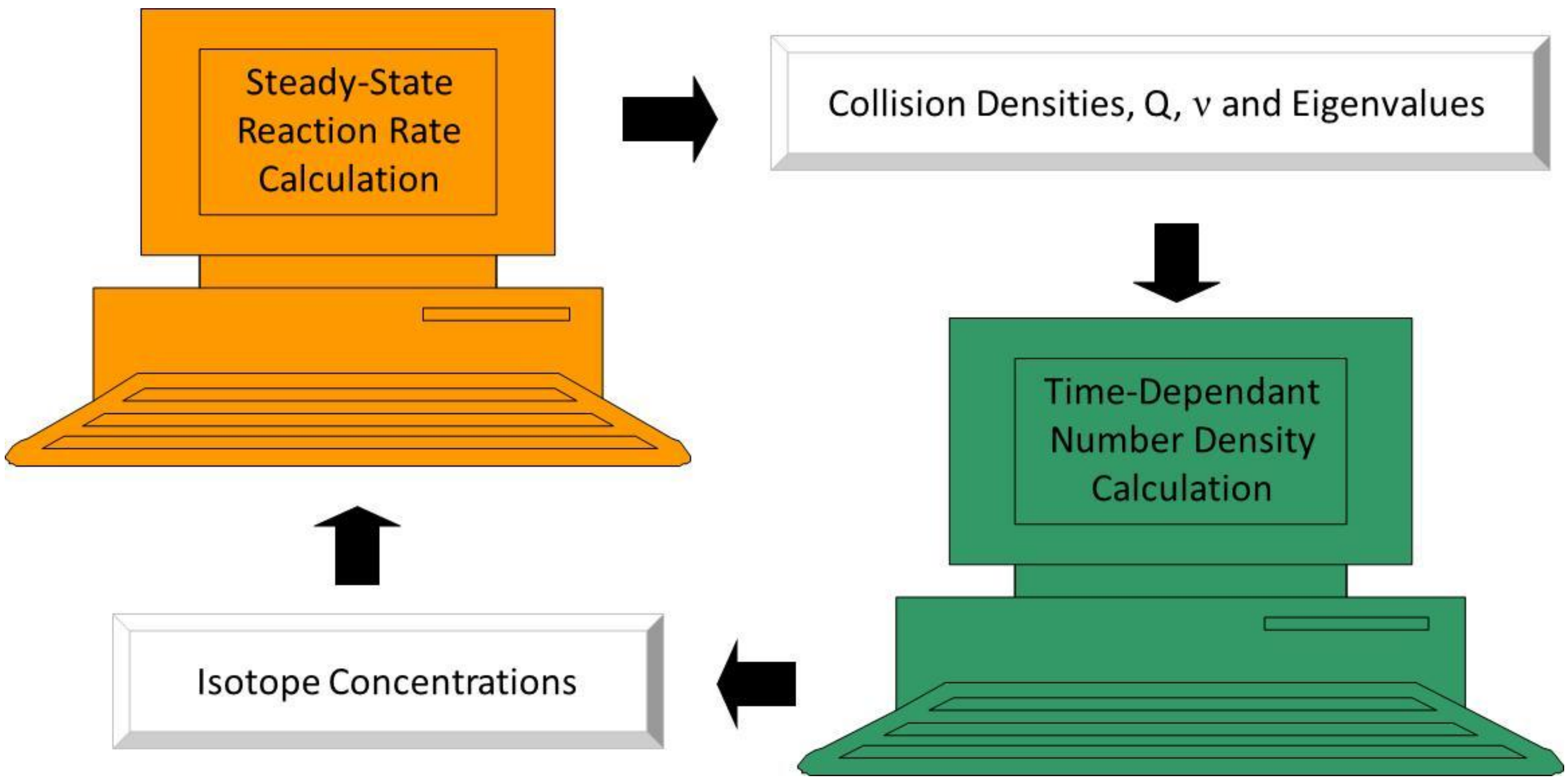
- CINDER90 constructs sequences/chains of nuclide interactions and follows all possibilities until they are smaller than a limiting value.
- Much data for the CINDER90 library came from the Evolved Netherlands Energy Research Foundation Activation File (ECNAF) but may also be calculated by ALICE or McGNASH.
  - Spontaneous fission
  - Spallation product generation
  - Radionuclide hazards (Cat 3)
  - Delayed neutrons (purpose of initial link to MCNP)
  - Ground state plus first and second isomeric state nuclides
  - Processed spectral data: υ, β^-,β^+, γ+X-ray, α emission
  - 63-group default neutron cross sections for a Power Reactor; collapsed to 1-group for actual calculations

    - 25-group photon spectra

Cross Sections:

- Fission, (n,γ),
- (n,α), (n,t)
- (n,2n), (n,3n)
- more

Methodology:
System-Dependent Depletion Process



Result is neutron fluence, or commonly

Burnup (BU) = Power*Time/Tons Heavy Metal

Non-Linear Problem

- **The depletion equation uses time-dependent fluxes, interaction rates, and number densities to determine inventories as a function of time.**
  - Unfortunately, the time-dependent flux also is dependent on the time-dependent nuclide density, thus making the depletion equation NONLINEAR

- **Reaction rates must be reevaluated as spectrum alters further calculations**
  - More time intervals = More computational cost

- **MCNP6 approximate reaction rates over time**

Steady State
Flux Calculation (Predictor – may be optional in Monteburns)

↓

Time Dependant Number Density Calculation (Predictor)

↓

New Steady State
Flux Calculation (Corrector)

↓

Time Dependant Number Density Calculation (Corrector)

↓

Final Result
Based on Average Behavior

Flux Normalization/Power

$$C = \frac{P * \nu}{k_{eff} * Q_{rec}}$$

$$\emptyset = C * f4tally$$

$$P = Q_{rec} * \varphi * \Sigma_f * V$$

P	=	thermal power,
k_{eff}	=	effective multiplication factor,
υ	=	average number of neutrons produced per fission
		$= fsrc/floss$ or $k_{eff} * src/floss$ ("nps" vs. "ksrc" definition),
$floss$	=	weight of neutrons lost to fission (from MCNP),
src	=	weight of source neutrons (~1),
$fsrc$	=	weight of source neutrons gained in fission,
Σ_f	=	the macroscopic fission cross section,
V	=	volume of material, and
φ	=	neutron flux.

Recoverable Energy per Fission (Q_{rec})

$$Q_{recoverable} = Q_{prompt} + Q_{delayed} + (\bar{\nu}(E) - k_{eff})*Q_{capture\gamma} - Q_{neutrino}$$

Emitted and recoverable energy for fission of U-235

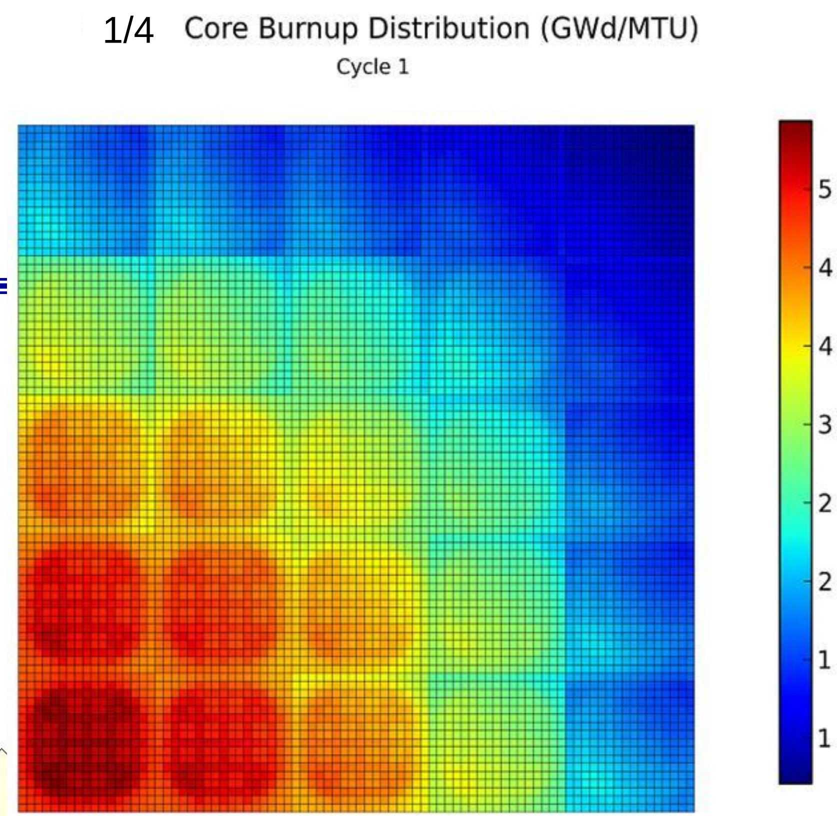
Form	Emitted Energy (MeV)	Recoverable Energy (Mev)
Fission Fragments	168	168
Fission Product Decay		
γ -rays	8	8
β-rays	7	7
neutrinos	12	--
Prompt gamma rays	7	7
Fission neutrons (kinetic energy)	5	5
Capture γ-rays	**--**	**3-12**
Total	**207**	**198-207**

- CINDER90 gives Q_{rec} for 36 actinides
- Prompt Q value is determined from ENDF or other sources.
  - File 1 MT 458
  - MCNP6 has data for ~23 actinides
  - Additional Q values desired!
- Delayed Q value may be estimated assuming local energy deposition
  - General 11% increase may be applied.
  - Total Q increases with BU as higher actinides build in.
  - 207 of 390 isotopes contain capture gamma data in ENDF VII.0; deposited gamma energy may be calculated.

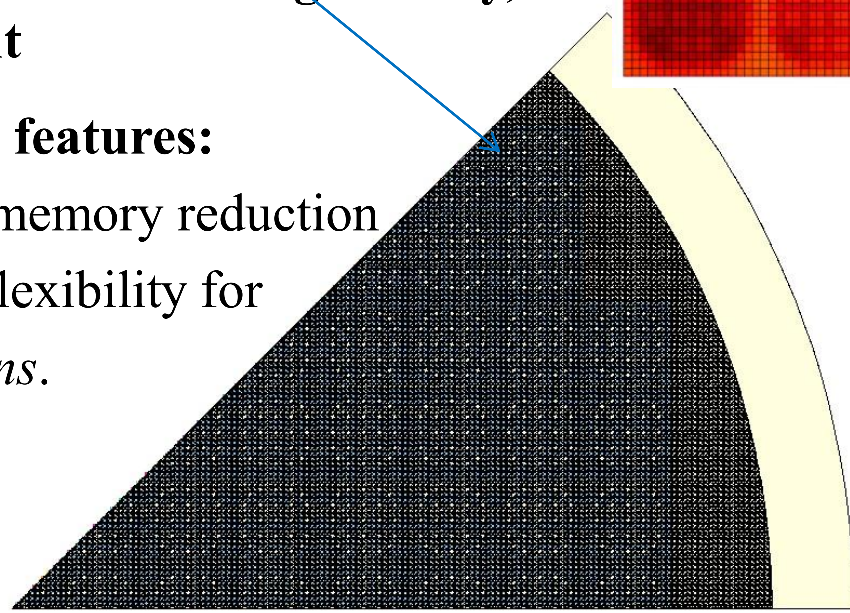
Applications

- Modeling of Full Reactor Cores
- Radiochemistry diagnostic calculations and nuclear detonation simulations
- Nonproliferation: determination of Pu, fission products, and more from irradiated nuclear fuel
  - Varies with reactor type
  - Process-dependent
- Innovative Reactor Concepts/Fuel Cycles
- Accelerator-Driven Systems

MCNP Full Reactor Core Modeling



- **With increased computing power and memory reduction techniques, we can now model individual pins in a Pressurized Water Reactor core using Monte Carlo burnup simulations.**
- **6,447 fuel pins in 1/8th core geometry, 1 axial segment**
- **Desired future features:**
  - Even more memory reduction
  - More tally flexibility for *Monteburns*.



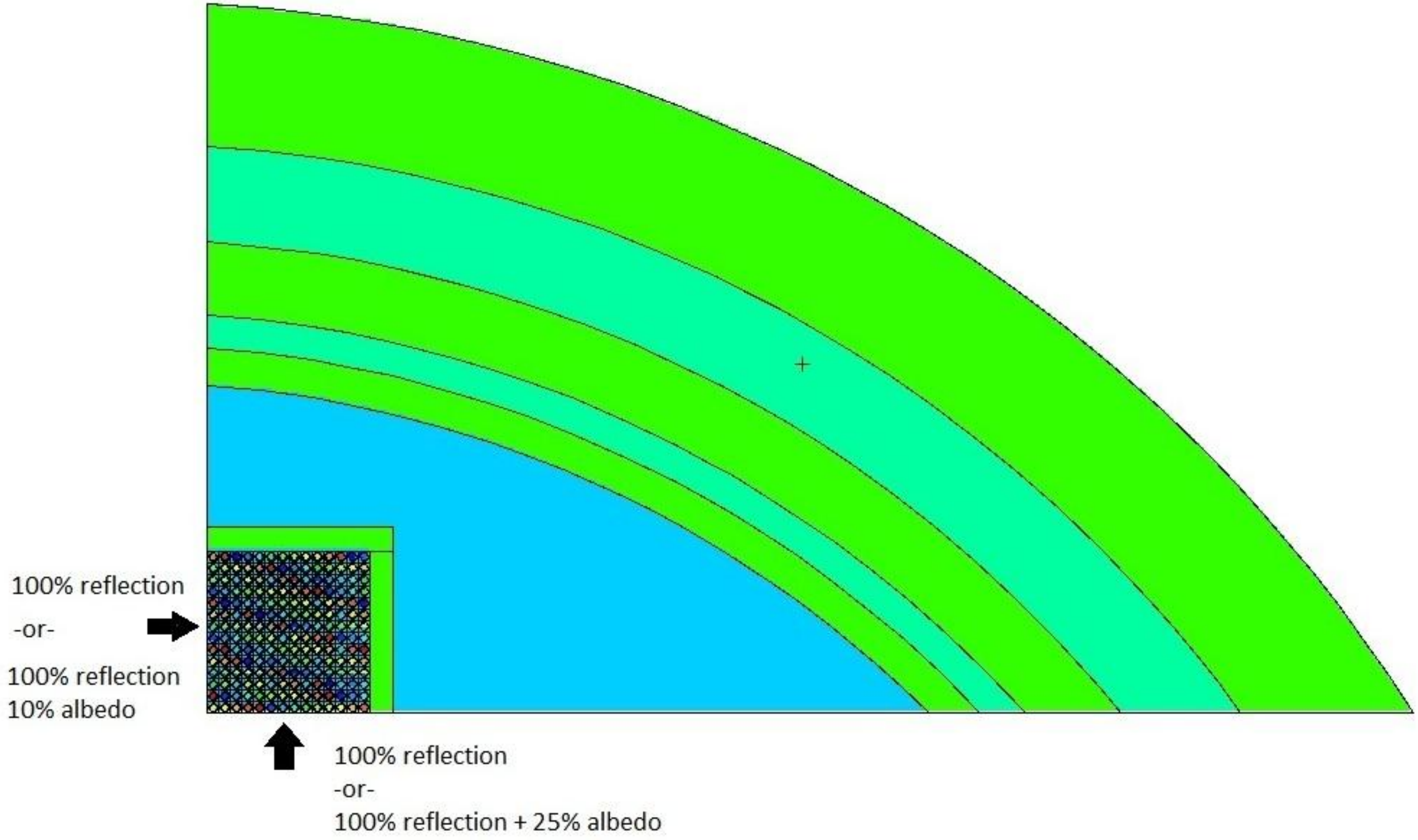
Comparison to Destructive Analysis (DA)

- H.B. Robinson infinitely-reflected assembly simulation.
- Plutonium isotopics can be predicted within 2-4% of measured values.
- Better benchmark data is desirable:
  - DA for multiple pins across the assembly,
  - Detailed operating history, and
  - Information on surrounding assemblies.

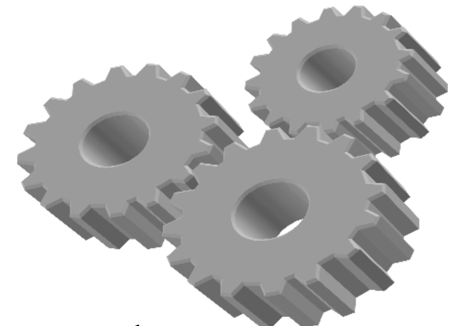
% Error = 100%*
(Calculated – Measured)/Measured

	MCNP6	SCALE
U235	-0.08	1.97
U236	0.17	0.52
U238	-0.73	-0.07
Pu238	-8.58	-11
Pu239	-0.20	4.21
Pu240	1.32	3.94
Pu241	-2.56	-1.72
Np237	1.58	1.46
Tc99	7.79	14.1
Cs137	-2.45	0.42

New Albedo Boundary Capability Assists Ability to Match DA



Desired Future Work:
Memory Limitations Increase with:



- Isotopes tracked
  - Fission Products
  - Decay Chains
- Reaction rates calculated
  - The more reaction rates that are calculated, the larger the storage requirements.
  - Only most probable reaction rates should be tracked.
- Time steps calculated
- Geometrical size
  - Physical problem size
  - Giant systems may endure large temperature and material density variations leading to complicated meshing procedures to accurately calculate spatial reaction rates

Irradiation Creates Fission Products and Isomers

- ENDF/B-VII has 323 non-actinides and 70 actinides that can be included in irradiation, ~220 FPs, 3 elements, and 9 metastable isotopes.
- TENDL provides ~2000 isotopes but has not been tested for burnup.
- Lumped fission products may increase accuracy.
  - Fission products lacking data could be lumped into a problem-dependent material for particle transport.
    - Improved computational cost, but
    - Results are sensitive to choice of fission products.
    - Lumped cross sections would be burnup-dependent.
  - How do we determine what worth value is an acceptable cutoff for lumping?
- Isomer branching following capture currently uses established fractions but should be energy-dependent.

Calculating Number Density Error and Error Propagation

- Toshikazu Takeda, Naoki Hirokawa and Tomohiro Noda "*Estimation of Error Propagation in Monte-Carlo Burnup Calculations*" Journal of Nuclear Science and Technology, Vol 36, No. 9, September 1999.

- Number density in depletion calculation satisfies the following equation:
  - M(t) = burnup matrix of group collapsed reaction rates
  - N(t) = number density

$$\frac{dN(t)}{dt} = M(t)N(t)$$

- If $N_0(t_0)$ is the true number density then $N(t_0) = N_0(t_0) + \delta N(t_0)$

- If $M_0(t_0)$ is the true reaction rate then $M(t_0) = M_0(t_0) + \delta M(t_0)$

- Then we have an equation to explain change in error of the number density as a function of time step:

$$\frac{d\delta N(t)}{dt} = M_0(t_0)\delta N(t) + \delta M(t_0)N_0(t)$$

Optimization of Hardware/Parallelization

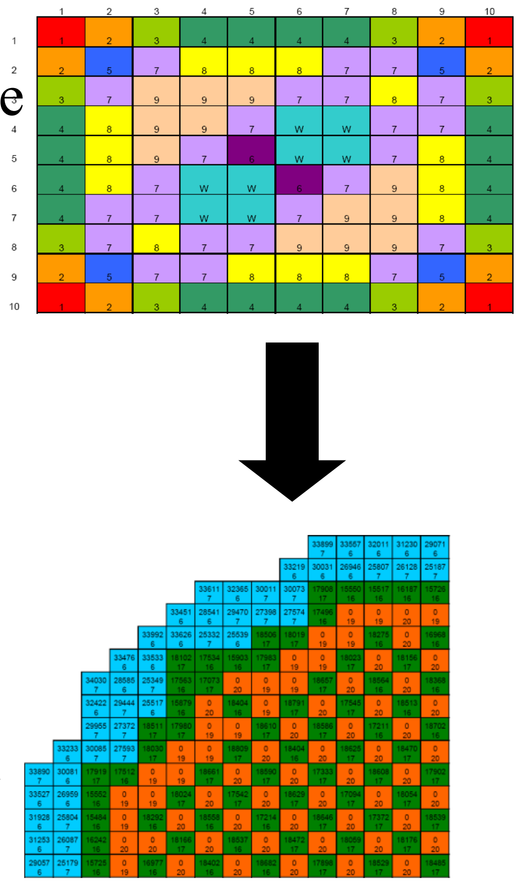
- Continuously improving hardware is always desired!
- Calculations with large numbers of materials possible using:
  - OpenMPI parallel processing implementation for both transport and depletion
  - Infiniband
  - Nodes with lots of memory (256 GB - 16 cores), and SSDs for swap space
- Example of large problem run: 3,960 materials to burn, ~25 seconds per material
  - Serial mode, 3,960*25 seconds = ~27 hours per production/depletion calc.
  - Parallel mode with ~200 processors scales by ~200, thus 27 hours → ~10 min.
- Ability to choose different machinefile (hostfile) for parallel run
  - MCNP has optimum curve for selection of number of CPUs in kcode calculation
    - Too many will slow down calculation in communication
  - For production/depletion want to use as many CPUs as possible

Conclusions/Areas of Improvement

- Monte Carlo burnup capability has made HUGE progress!
- Full nuclear core modeling with MCNP now possible with limited axial fidelity.
- Future Work
  - More memory reduction
  - Incorporate full isotope chains into a range of calculations
    - Increase in products given detailed geometry/fluxes
    - Lumped fission products
  - *Monteburns* would benefit from tally flexibility; internal MCNP burn capability avoids the necessity
  - Need Q_{rec} values for more actinides
  - Energy-dependent isomer branching ratios
  - Other predictor-corrector methods should be explored

Applications: Large Reactor Core Design

- Traditional technique: deterministic
  - Solve lots of smaller calculations to get average parameters to solve the larger calculation.
  - Fuel bundle calculation generates collapsed group constants for the full core solution.
  - Utilize collapsed group cross sections to run a large-scale nodal calculation of reactor behavior.

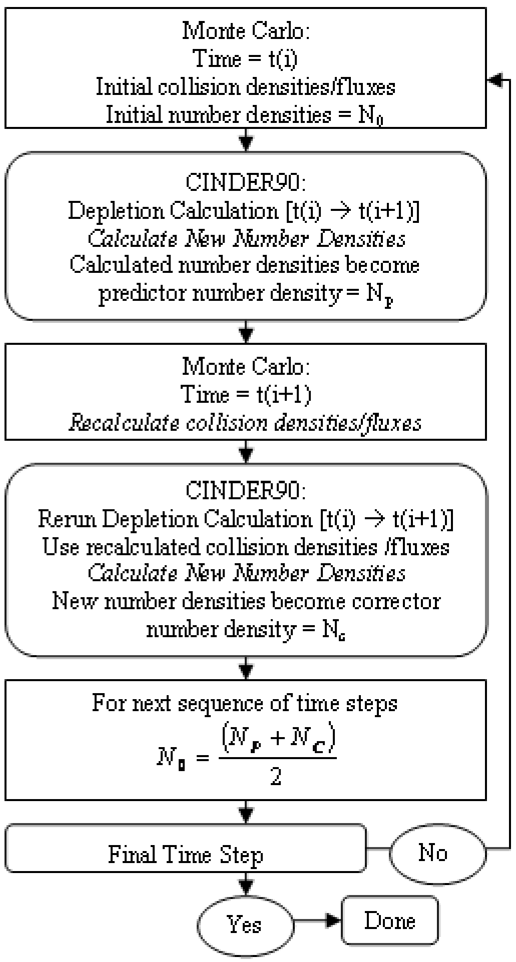


- Increases in computational power now improve calculations!
  - Time-dependent behavior of every fuel pin is important.
  - MCNP can handle detailed, complex geometry with continuous-energy data.

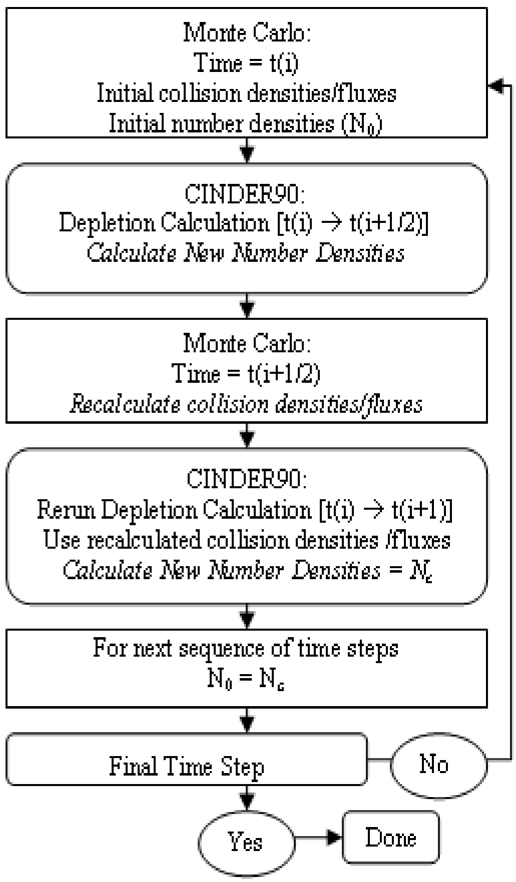
Data Requests

- Two categories
  - CINDER90
    - Fission Yields → England/Rider Data is from 1992
      - Data only exists for 0.025 eV,500 KeV, and 14 MeV
      - Does better fission yield data, at more energies, exist?
    - Proton libraries for minor nuclides
      - There are no proton libraries in CINDER90 for minor nuclides... This is important for proton target based interrogation
  - MCNPX
    - Lack of photon production data
    - Examine Am-241 capture xn to improve Cm-242 prediction

Traditional Predictor-Corrector

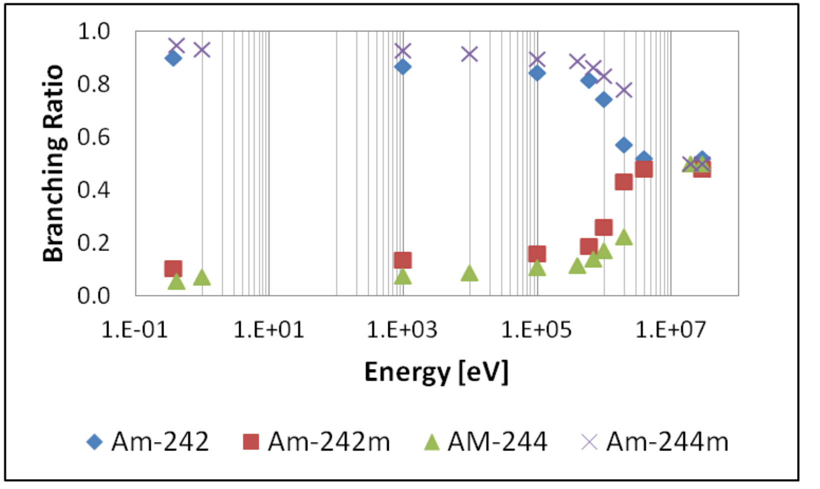


MCNP6 Predictor-Corrector



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!**

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