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Title: Calculating Kinetics Parameters and Reactivity Changes with Continuous-Energy Monte Carlo

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Calculating Kinetics Parameters and Reactivity Changes with Continuous-Energy Monte Carlo

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Overview

- Theory & Current Status
- Adjoint Weighting Mechanics
- Results, Validation, and Verification

Theory & Current Status

Kinetics Parameters

- **Point reactor kinetics parameters:**
  - Neutron Generation Time

$$\Lambda = \frac{\left\langle \psi^{\dagger}, \frac{1}{v}\psi \right\rangle}{\left\langle \psi^{\dagger}, F\psi \right\rangle}$$

  - Effective Delayed Neutron Fraction

$$\beta_{\mathrm{eff}} = \frac{\left\langle \psi^{\dagger}, B\psi \right\rangle}{\left\langle \psi^{\dagger}, F\psi \right\rangle}$$

  - Rossi-Alpha

$$\alpha = -\frac{\beta_{\mathrm{eff}}}{\Lambda} = -\frac{\left\langle \psi^{\dagger}, B\psi \right\rangle}{\left\langle \psi^{\dagger}, \frac{1}{v}\psi \right\rangle}$$

- **Change in 1/*k*:**

$$\Delta\lambda = \frac{\left\langle \psi^{\dagger}, \left(\Delta\Sigma_t - \Delta S - \lambda\Delta F\right)\psi \right\rangle}{\left\langle \psi^{\dagger}, F'\psi \right\rangle}$$

- **Numerator:**
  - Change in Total Collision Rate
  - Change in Scattering Emission Rate
  - Change in Normalized Fission Emission Rate

- **Denominator:**
  - Perturbed* Fission Emission Rate

*Linear perturbation theory has fission emission rate unperturbed.

The Problem

- **All of these quantities involve the Adjoint Flux or Importance.**

- **Historically problematic for Continuous-Energy Monte Carlo.**
  - One approach: Invert random walk. Difficult in C.E. because scattering laws not easy to invert.

- **Can calculate with approaches not involving adjoints.**
  - General Issues: Approximate, problematic uncertainties, requires advanced knowledge of codes/data

Choice of Response Function

- **Fundamental adjoint mode independent of selected response function.**

- **Pick one with desirable convergence properties.**
  – Global response function is good choice

- **Iterated fission probability:**

  Importance at a location is proportional to the expected steady neutron population, after an infinite number of fission generations, caused by a neutron introduced at that location.

Adjoint Weighting Mechanics

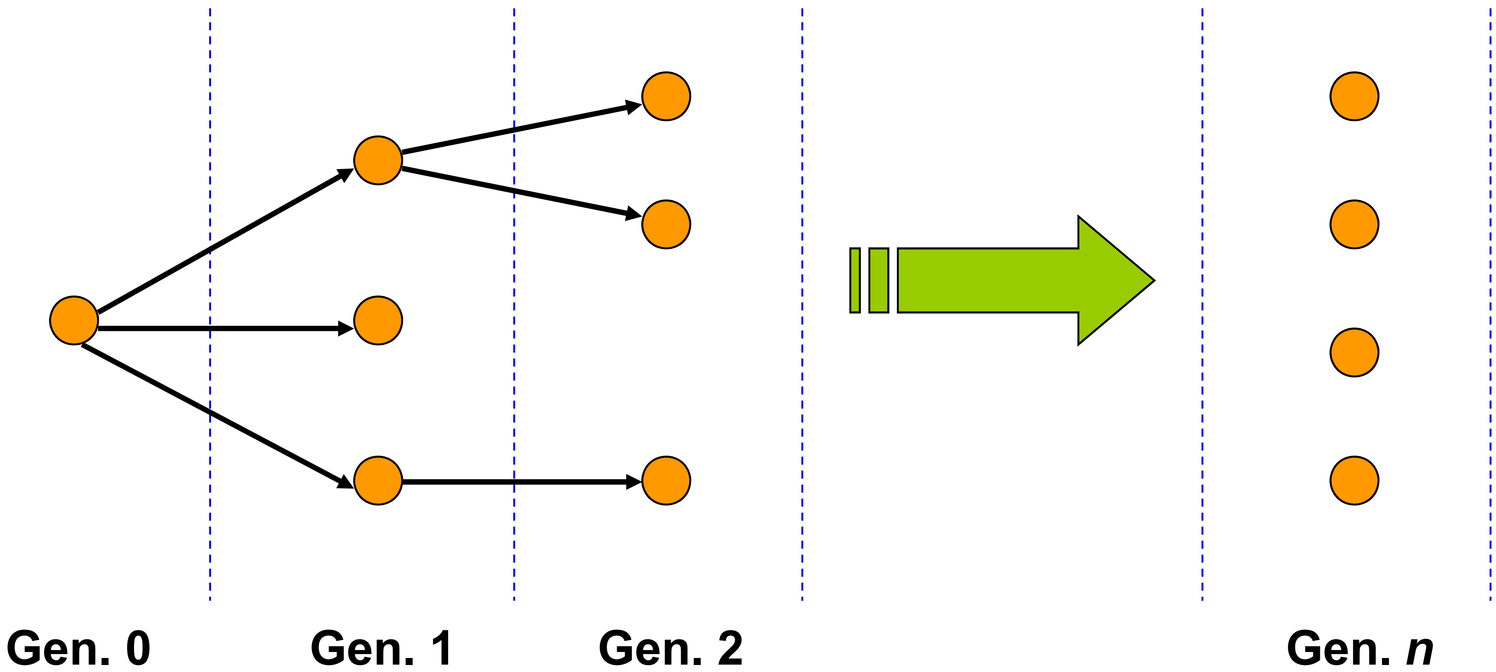
Overview

- Tag neutron ***progenitor*** and accumulate and store its ***tally contributions***.
- Follow through many generations, and measure ***asymptotic population*** in some sufficiently future generation.
- Asymptotic population is importance of tally contributions. Product of two gives ***importance-weighted score***.

Note: Only uses existing random walks.

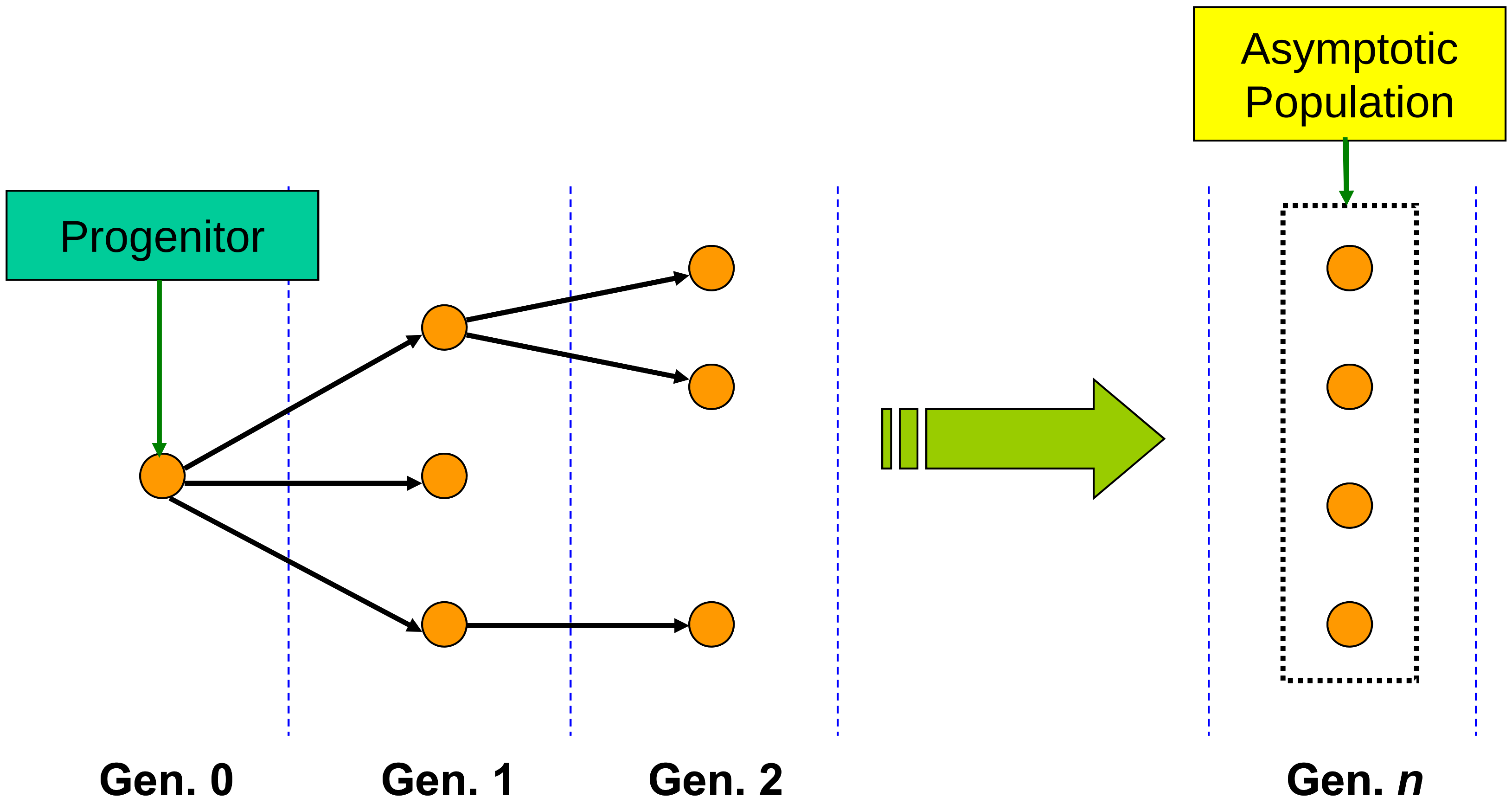
Overview

- **Method terminology:**



Overview

- **Method terminology:**



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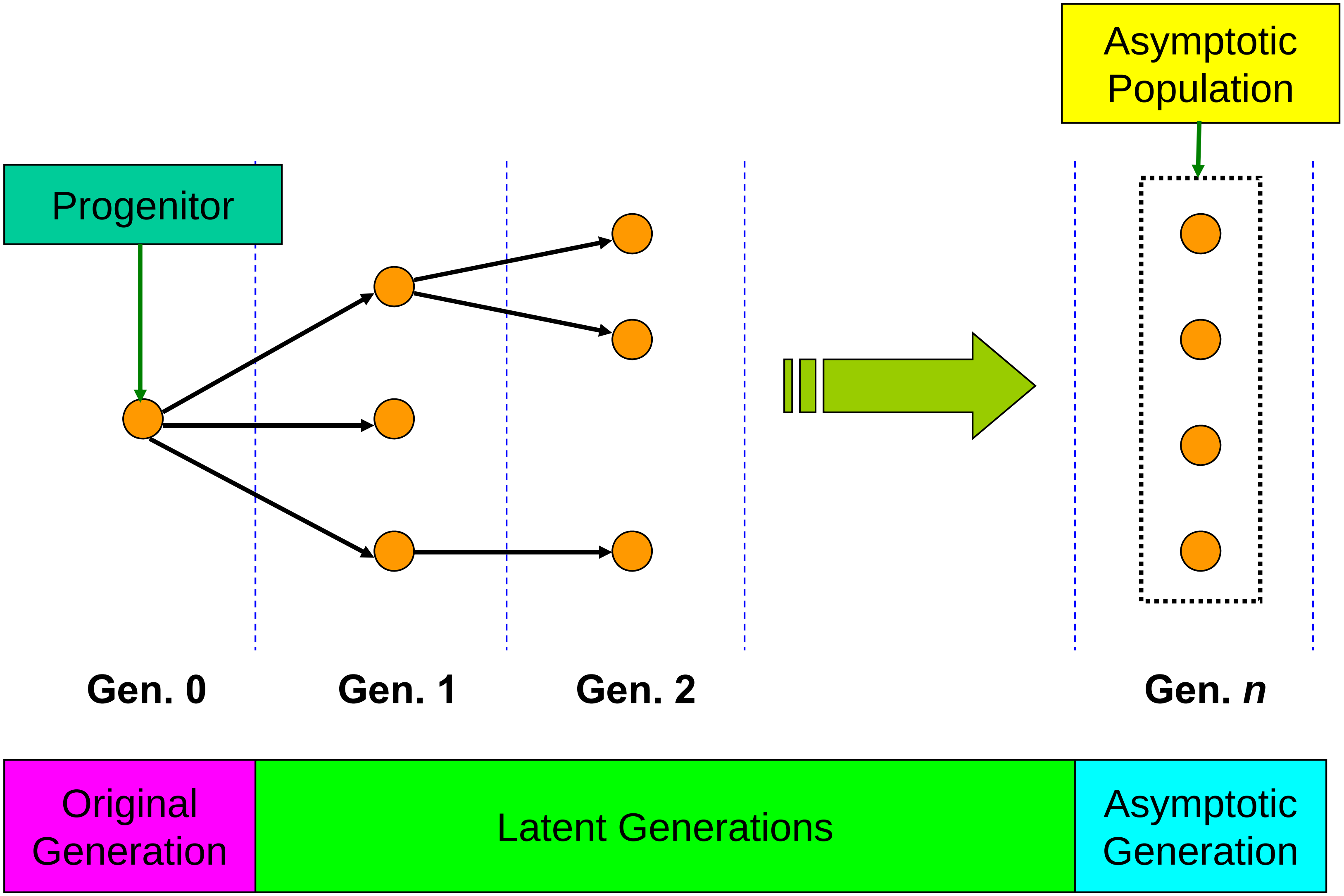
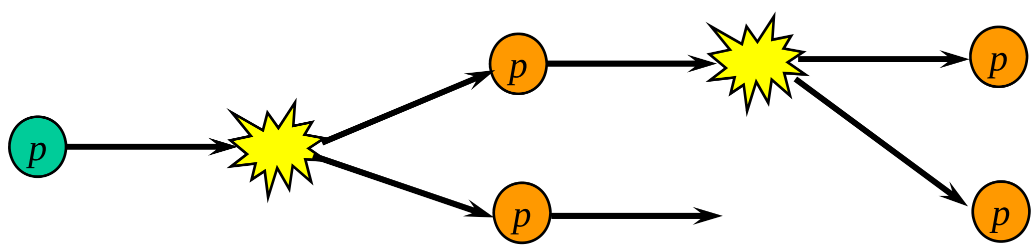
- **Method terminology:**



Overview

- In original generation store contribution for each progenitor of index *p*:
  - Ex. Track-length flux: $$T_p = \sum_{\tau \in p} d_\tau$$
- Progenitor index *p* inherited by all progeny:

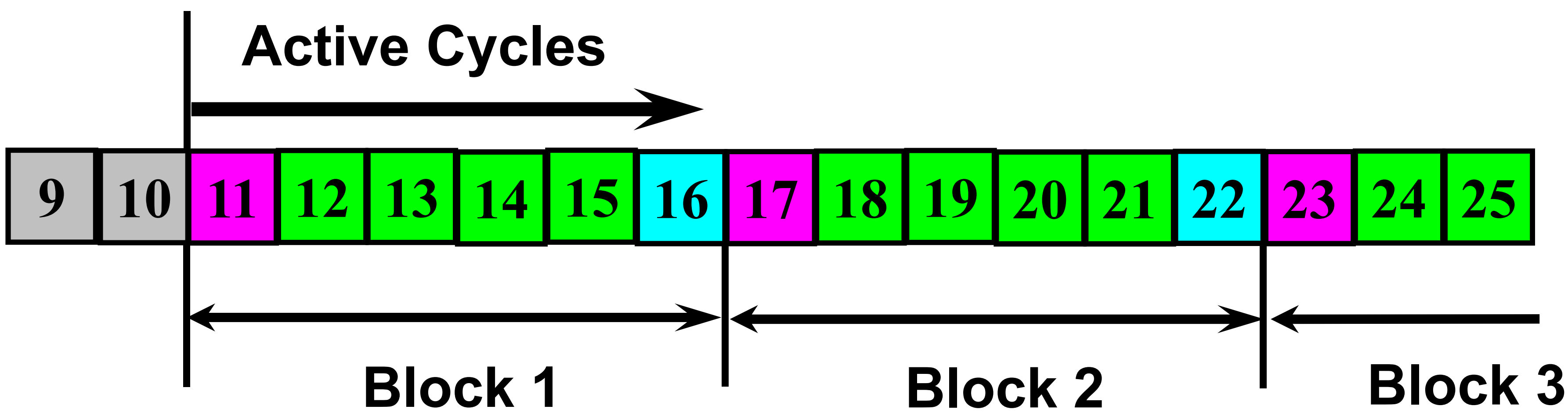


- Tally asymptotic population in asymptotic generation:

$$R_p = \sum_{\tau \in p} \nu \Sigma_f w d_\tau \qquad \text{Tally} = \sum_p R_p T_p$$

Overview

- Active cycles in the power iteration are broken into ***blocks***.



Note: Could overlap blocks, but memory becomes an issue.

Kinetics Parameter Tallies

- **Adjoint-weighted neutron density:**

$$\left\langle \psi^{\dagger}, \frac{1}{v}\psi \right\rangle = \frac{1}{W}\sum_{p} R_p \sum_{\tau \in p} \frac{d_\tau}{v_\tau}$$

- **Adjoint-weighted total fission source:**

$$\left\langle \psi^{\dagger}, F\psi \right\rangle = \frac{1}{W} k \sum_{p} R_p$$

- **Adjoint-weighted delayed fission source:**

$$\left\langle \psi^{\dagger}, B\psi \right\rangle = \frac{1}{W} k \sum_{p} R_p \left(1 - \delta_i\right)$$

Perturbation Tallies

- **Adjoint-weighted collision rate perturbation:**

$$\left\langle \psi^{\dagger}, \Delta\Sigma_t \psi \right\rangle = \frac{1}{W} \sum_{p} R_p \sum_{\tau \in p} \Delta\Sigma_{t,\tau} d_{\tau}$$

- **Adjoint-weighted scattering source perturbation:**

$$\left\langle \psi^{\dagger}, \Delta\mathbf{S}\, \psi \right\rangle = \frac{1}{W} \sum_{p} R_p \sum_{s \in p} \frac{\Delta\Sigma_s}{\Sigma_s}$$

- **Adjoint-weighted fission source perturbation:**

$$\left\langle \psi^{\dagger}, \lambda \Delta\mathbf{F}\, \psi \right\rangle = \frac{1}{W} \sum_{p} R_p \frac{\Delta \nu\Sigma_f}{\nu\Sigma_f}$$

Results, Validation & Verification

Adjoint-Weighted Kinetics Parameters

- **Simple MCNP5 v1.60 (June 2010) 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	

Kinetics Parameters: Analytic Solution

- Infinite-medium problem with cross-section data:

g	Σ_{tg}	$\nu\Sigma_{fg}$	Σ_{sg1}	Σ_{sg2}
1	2	0	1/2	1/2
2	3	5/24	0	1

- Other data:

g	v_g (ns)	χ_{pg}	χ_{1g}	χ_{2g}	ξ_g
1	10	1	3/4	1/2	1/4
2	5	0	1/4	1/2	1/8

$$\xi_g = \sum_i \beta_i \chi_{ig}$$

Note: Custom version of MCNP used.

- **Solutions:**

$$\Lambda = \frac{\frac{1}{v_1}\frac{\Sigma_{s12}}{\Sigma_{R2}} + \frac{1}{v_2}\frac{\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}}{\left\{\frac{\Sigma_{s12}}{\Sigma_{R1}}\left[(1-\beta)+\xi_1\right]+\xi_2\right\}\frac{\nu\Sigma_f\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}} = 44/3 \ \ \text{ns}$$

$$\beta_{\text{eff}} = \frac{\frac{\Sigma_{s12}}{\Sigma_{R1}}\xi_1 + \xi_2}{\frac{\Sigma_{s12}}{\Sigma_{R1}}\left[(1-\beta)+\xi_1\right]+\xi_2} = 1/2$$

$$\alpha = -\frac{\left[\frac{\Sigma_{s12}}{\Sigma_{R1}}\xi_1 + \xi_2\right]\frac{\nu\Sigma_f\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}}{\frac{1}{v_1}\frac{\Sigma_{s12}}{\Sigma_{R2}} + \frac{1}{v_2}\frac{\Sigma_{s12}}{\Sigma_{R2}-\xi_2\nu\Sigma_f}} = -3/88 \ \ \text{ns}^{-1}$$

Kinetics Parameters: Analytic Solution

- **Comparison of Analytic Solution to Monte Carlo (MCNP):**

	Analytic	Monte Carlo	C/R
Λ (ns)	14.66667	14.66548 +/- 0.00110	0.99992
β_{eff}	0.50000	0.50003 +/- 0.00005	1.00006
α (ns^{-1})	-3.40909×10^{-2}	-3.40955 +/- 0.00044×10^{-2}	1.00013

Kinetics Parameters: Discrete Ordinates

- Neutron generation time computed for various 1D problems:

#	G	Description
1	4	Bare Metallic Slab (Fast)
2	4	Metallic Slab w/ Moderating Reflector (Thermal)
3	2	Metallic Slab, Strong Thermal Abs., Mod. Reflector
4	8	Homogenous Slab (Intermediate)
5	4	Bare Metallic Sphere (Fast)
6	4	Reflected Metallic Sphere (Fast)
7	4	Subcritical Bare Metallic Slab (Fast, k = 0.78)
8	4	Supercritical Bare Metallic Slab (Fast, k = 1.14)

Kinetics Parameters: Discrete Ordinates

- Comparisons of Generation Time between Discrete Ordinates (Partisn) and Monte Carlo (MCNP).

#	I	Discrete Ordinates	Monte Carlo	C/R
1	0.99021	9.79325 ns	9.79675 +/- 0.00188 ns	1.00036
2	1.14537	135.19020 μs	135.22164 +/- 0.03384 μs	1.00023
3	0.00488	49.16822 ns	49.20663 +/- 0.01863 ns	1.00078
4	1.11580	112.05232 μs	112.29905 +/- 0.13692 μs	1.00220
5	0.86498	1.72115 ns	1.72121 +/- 0.00032 ns	1.00003
6	0.56477	10.18997 ns	10.18794 +/- 0.00233 ns	0.99980
7	1.05365	10.17161 ns	10.17110 +/- 0.00230 ns	0.99995
8	0.96534	9.67254 ns	9.67168 +/- 0.00166 ns	0.99990

- Comparison of measured values of Rossi-α (ms^{-1}) to Monte Carlo (MCNP) Calculations:

	Measured	Monte Carlo	C/R
Godiva	-1100 +/- 20	-1139.57 +/- 2.35	1.036
Jezebel	-640 +/- 10	-640.238 +/- 2.374	1.000
BIGTEN	-117 +/- 1	-115.518 +/- 0.219	0.987
Flattop-233	-267 +/- 5	-292.401 +/- 0.808	1.095
Stacy-29	-0.122 +/- 0.004	-0.122155 +/- 0.00296	1.001
WINCO-5	-1.109 +/- 0.003	-1.11723 +/- 0.00311	1.007

< 1 Std. Dev.

> 1 Std. Dev. and < 2 Std. Devs.

> 2 Std. Devs.

Adjoint Perturbation Theory

- Input and output format under review.

- Will be very similar to the existing `pert` card in MCNP:

```
kpert5  cell=17  mat=4  rho=-18.0  rxn=-6
```

- Plan is to release in MCNP6 (2011).

Perturbation V&V

- **Discrete Ordinates comparisons**

- **Direct Monte Carlo comparisons**
  - Godiva: Edge Density, Cross-Section Library
  - PWR: Xenon Concentration, Moderator Density, Rod Worth

Discrete Ordinates Comparison

4-Group Bare Slab with modified cross sections

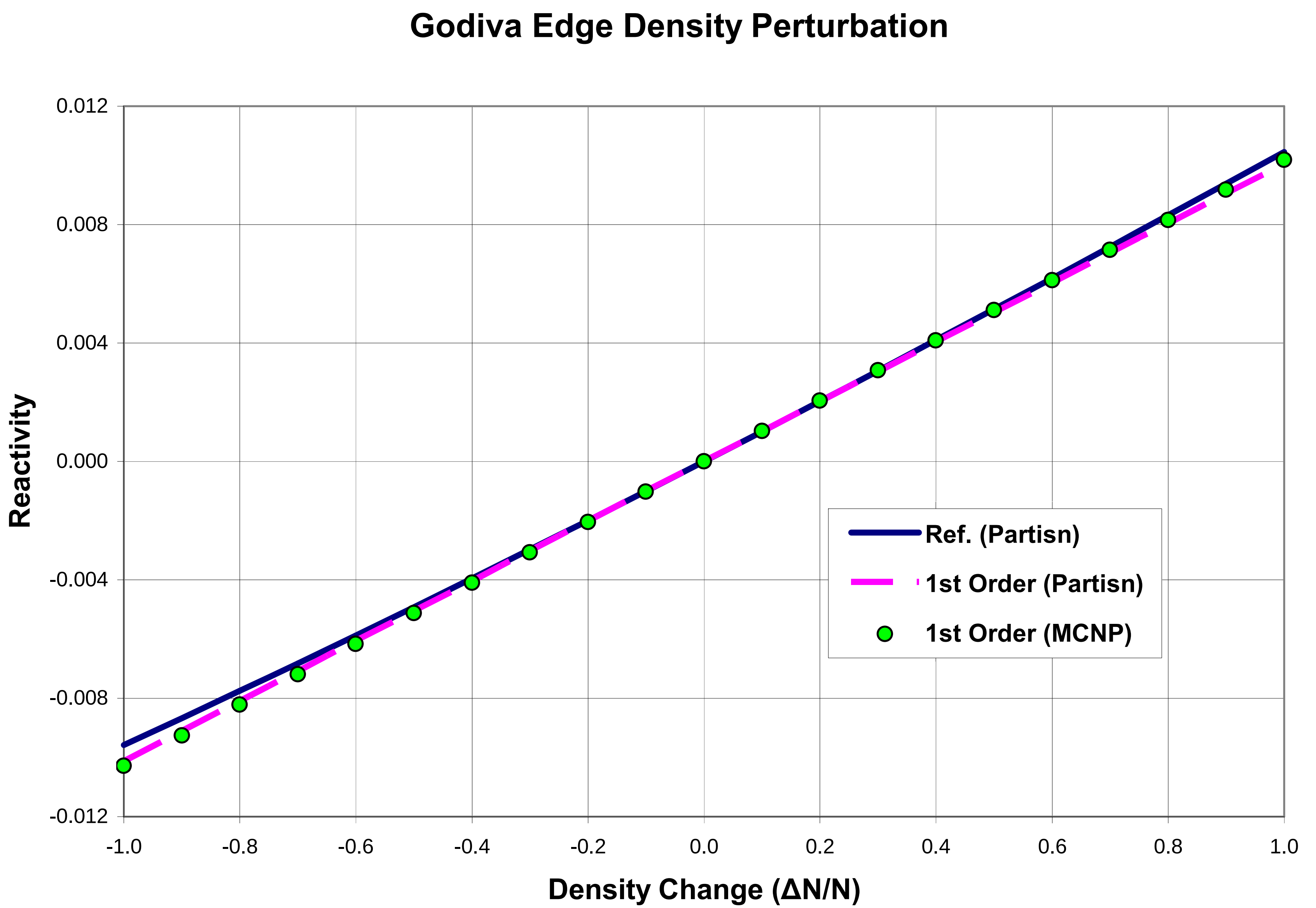
#	Σ_{c4}	Σ_{f4}	Σ_{s44}	ν_4
1	+0.05 b			
2		+0.05 b		
3	+0.05 b	+0.05 b		
4				+0.01
5	+0.05 b	+0.05 b		+0.01
6			+0.05 b	

Discrete Ordinates Comparisons

- **Comparisons of reactivity changes (in pcm) Discrete Ordinates (Partisn) to Monte Carlo (MCNP):**

#	Discrete Ordinates	Monte Carlo	C/R
1	-32.839	-32.748 +/- 0.152	0.99723
2	+49.517	+49.465 +/- 0.308	0.99786
3	+16.644	+16.744 +/ 0.405	1.00601
4	+33.068	+32.891 +/- 0.107	0.99464
5	+49.767	+49.931 +/- 0.483	1.00330
6	+2.166	+2.192 +/- 0.283	1.01200

Godiva: Density, Outer 0.1 cm



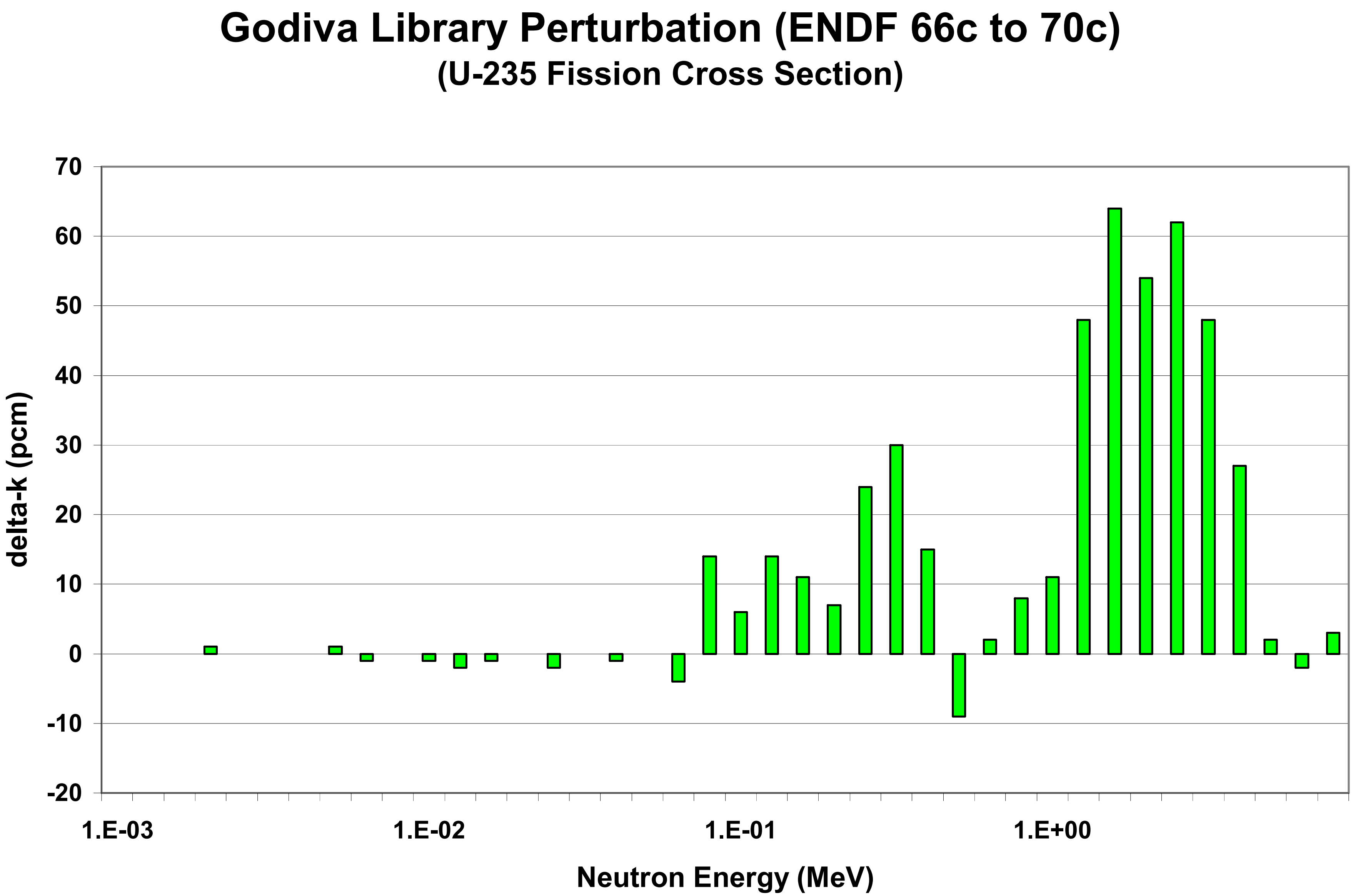
Godiva: Cross Section Library

- **Change cross section library from ENDF/B-VI.5 to ENDF/B-VII.0**

k_{eff}	**0.99646 +/- 0.00004**
Ref. Δ*k*	**0.00344 +/- 0.00006**
Calc. Δ*k*	**0.00358 +/- 0.00006**

Ref. obtained by comparing k_{eff} for two separate MCNP runs.

Godiva: Cross Section Library



PWR: Xenon-135 Buildup

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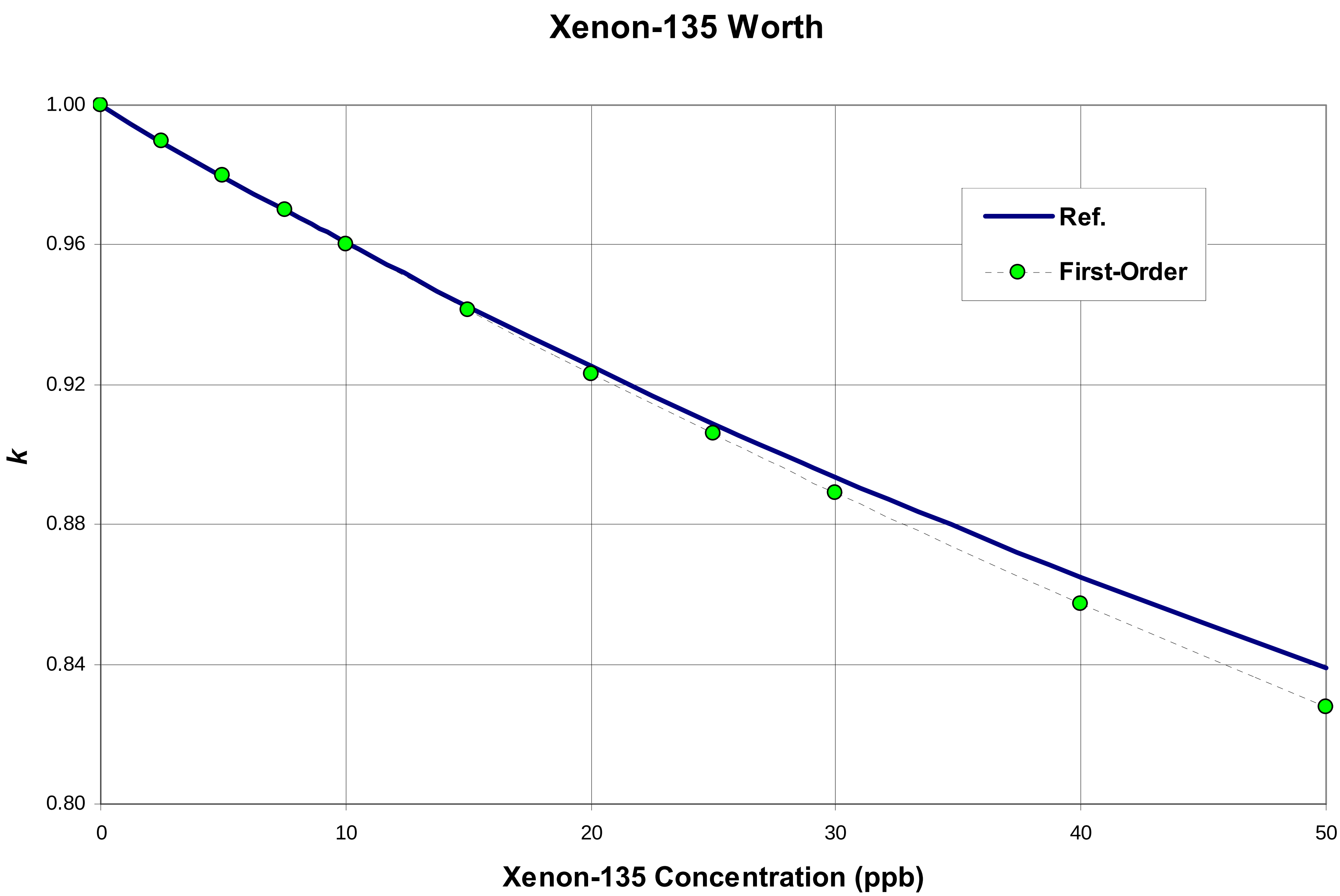
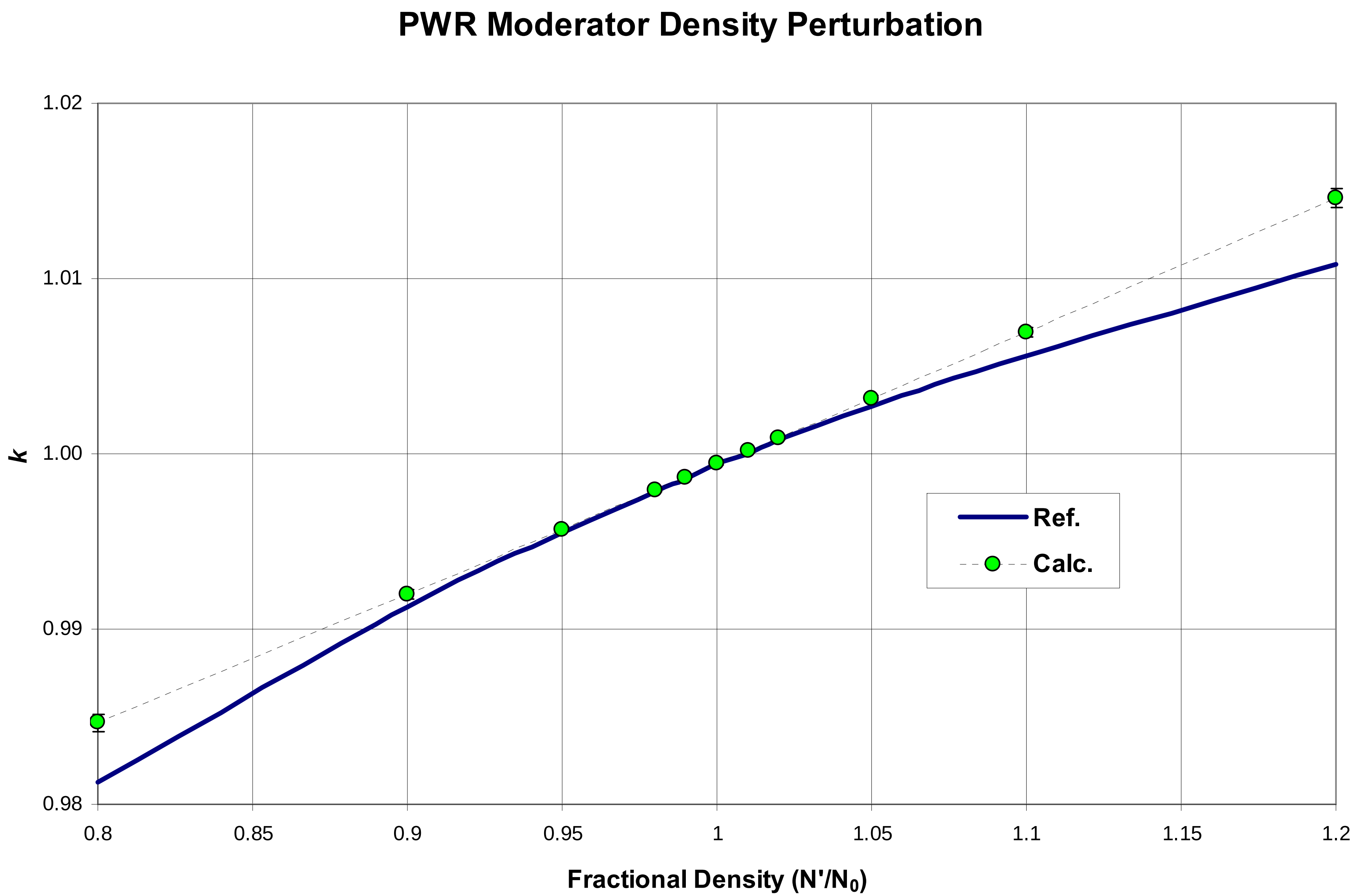
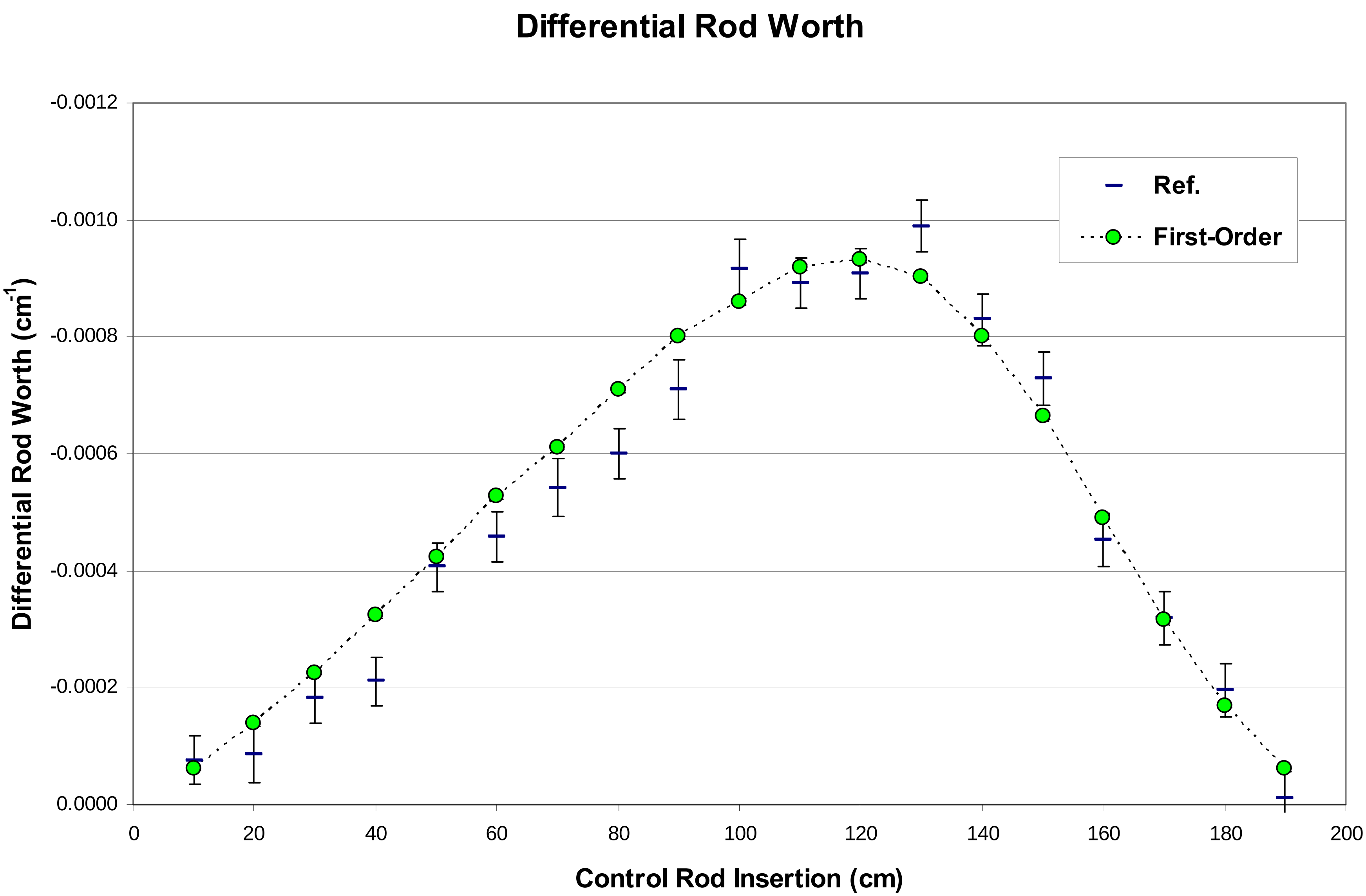


PWR: Moderator Density



PWR: Differential Rod Worth



PWR: Integral Rod Worth

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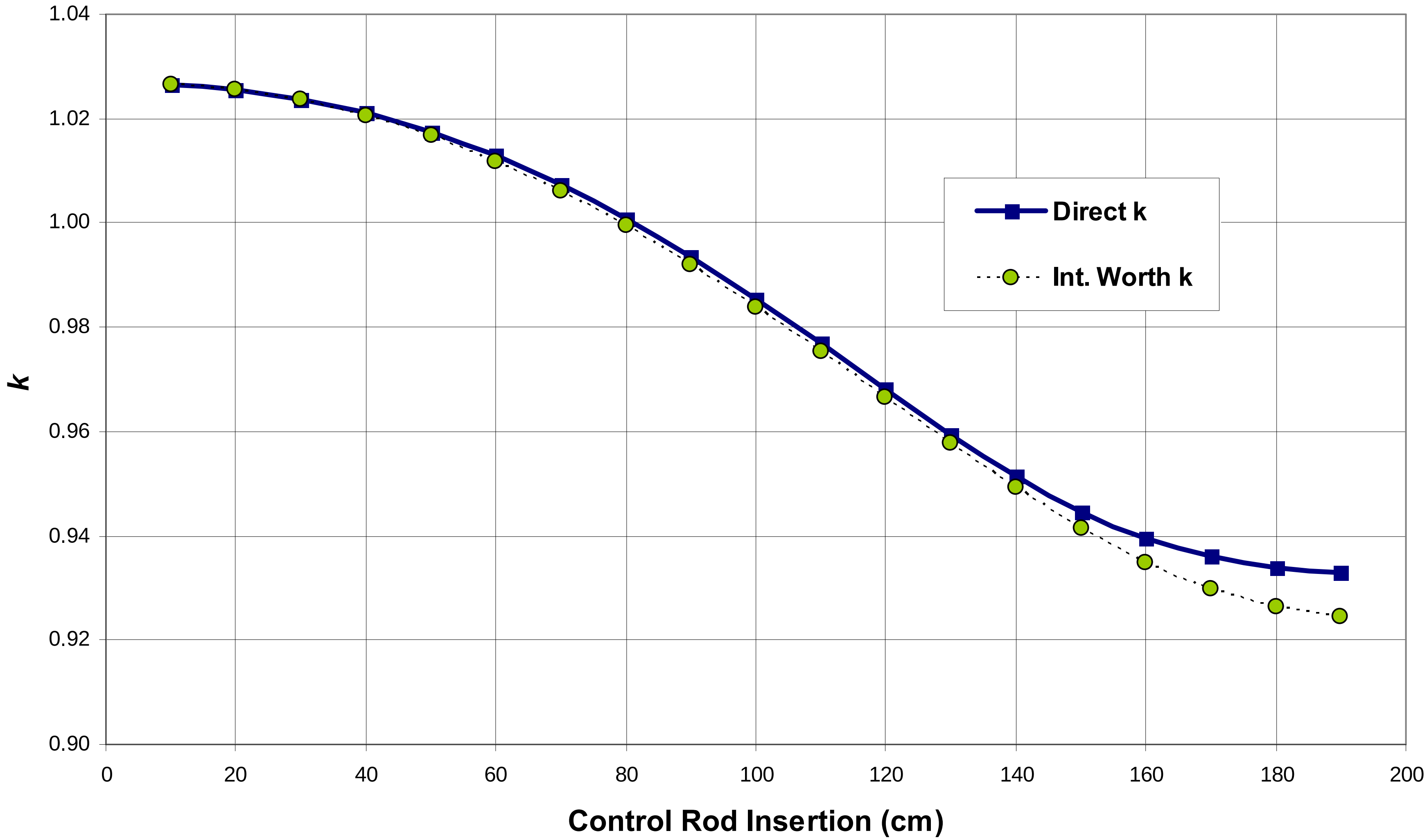
k_{eff} Estimated by Integral Worth Curve



Summary and Future Work

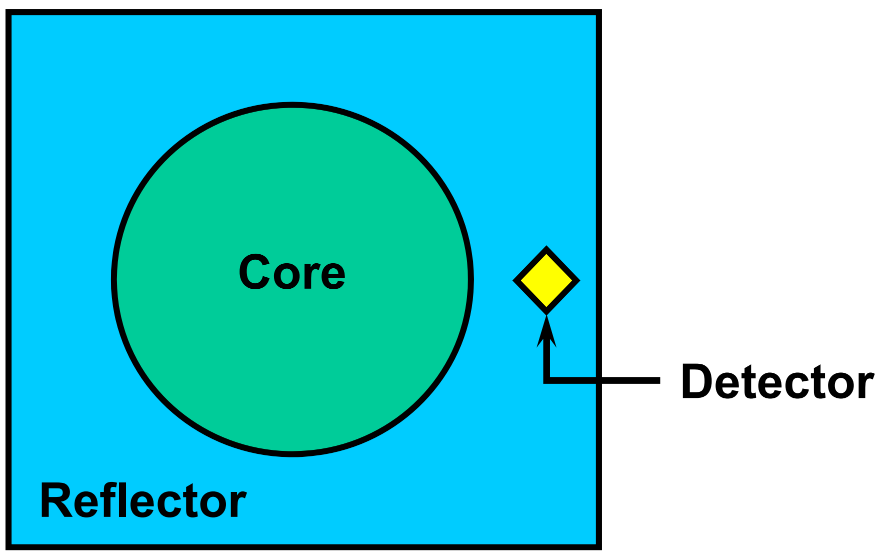
- **MCNP can now perform adjoint-weighting in k-eigenvalue problems.**
  – Point Kinetics Parameters (MCNP5 v1.60, June 2010)
  – Adjoint Perturbations (MCNP6, 2011)

- **Future Work:**
  – Adjoint-weighted mesh tallies
  – Sensitivity coefficients
  – Fixed source adjoint-weighted quantities
  – Generalized perturbation theory

Questions?

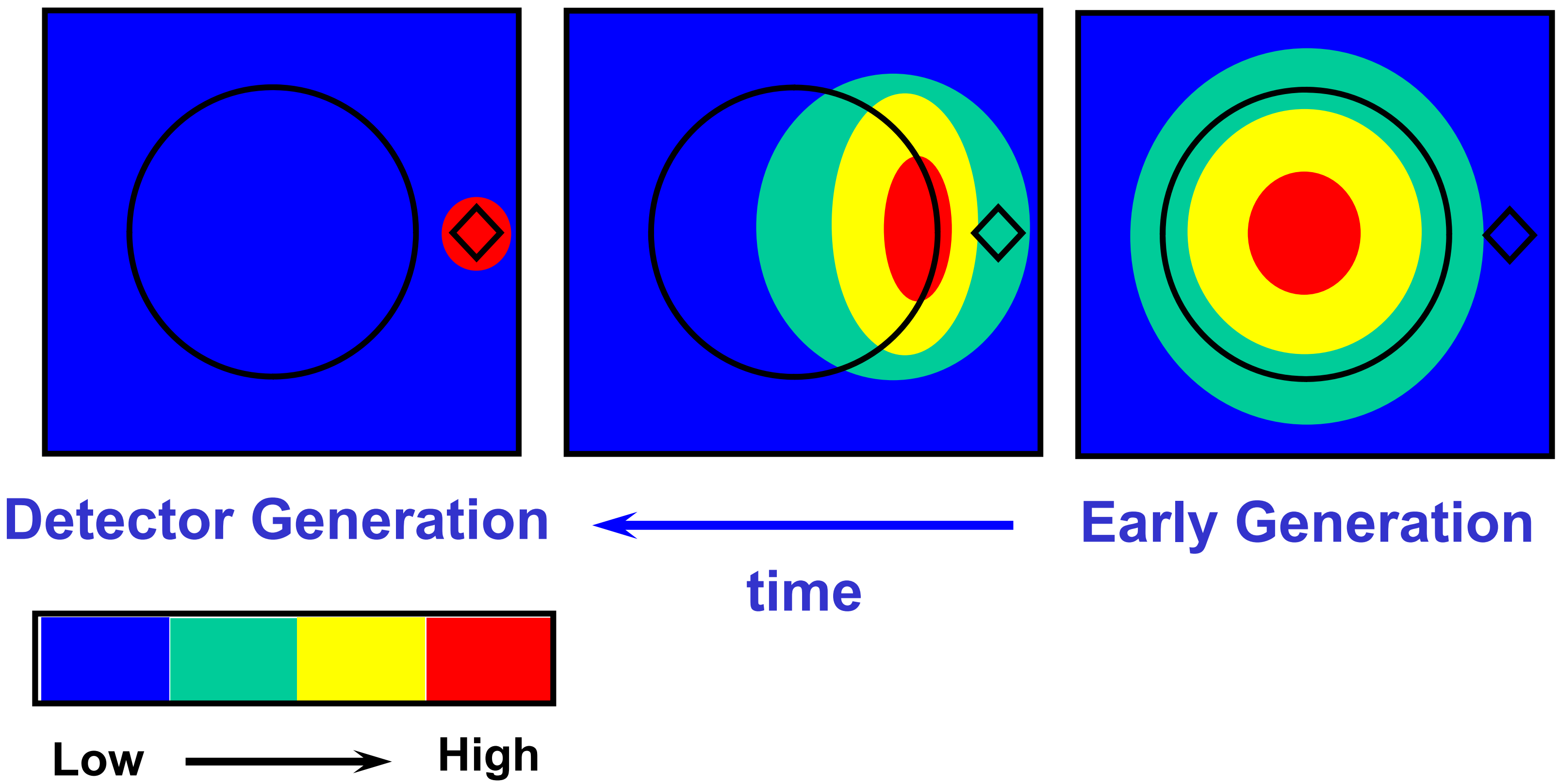
The Adjoint Flux: A Step Back

- A detector response existing only in one distant generation is prescribed.
- The adjoint flux measures the importance of neutrons within the current generation to the detector.
- Let's consider an example…



The Adjoint Flux: A Step Back

- Evolution of the adjoint function:



Subtle Pitfalls

1) Progenitors must be tagged in a way to ensure tally contributions are of the same causal chain within the original generation. (Ex. n,2n, splitting, etc.)

    Result: Individual history may have many progenitor tags.

2) Expected value methods of computing fission source for next iteration biases neutron production by particle weight. Importance should be for a unit weight neutron introduced at the point of sampling the tally contribution.

    Result: Tally contributions are unweighted.