Acceleration of Monte Carlo Criticality Calculations Using Deterministic-Based Starting Sources

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American Nuclear Society
2011 Winter meeting
Washington, DC
11/3/2011

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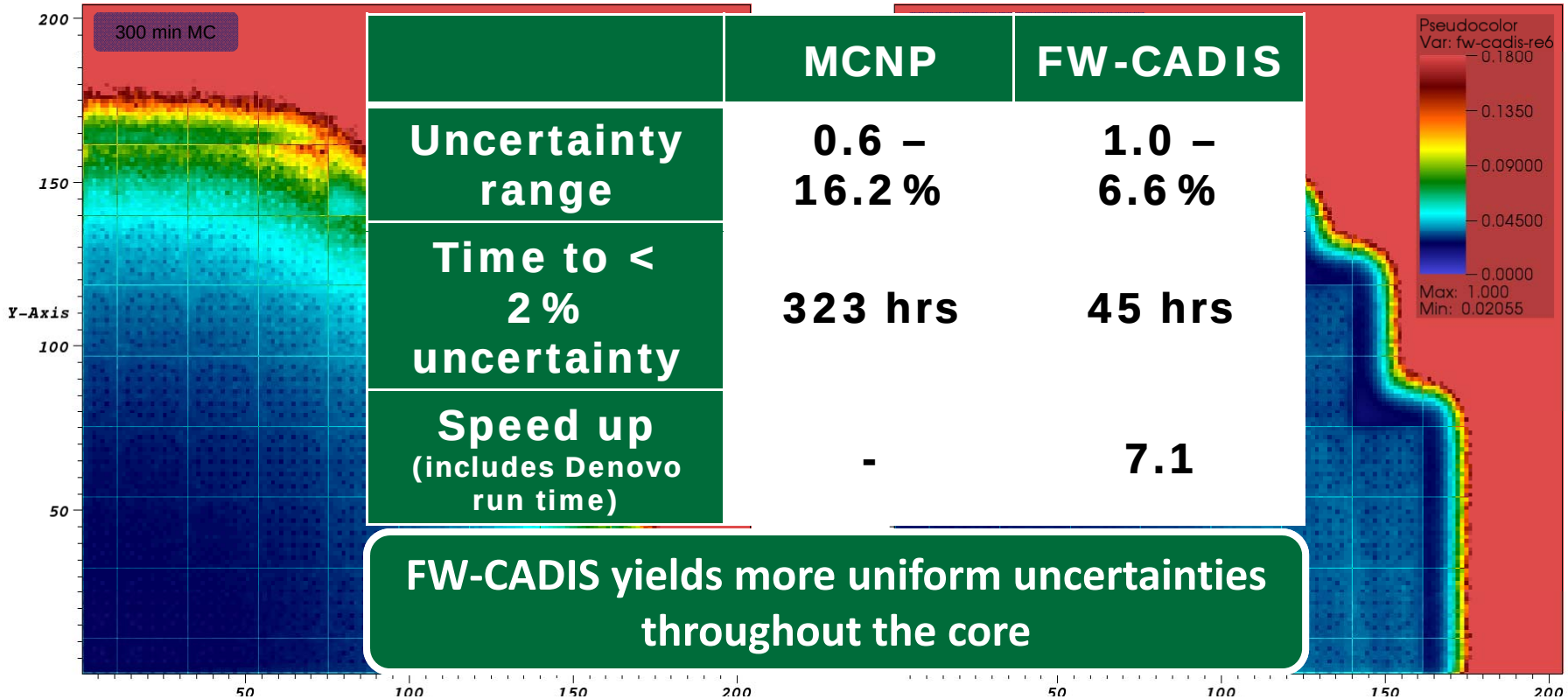
Outline

- Forward-Weighted (FW) CADIS for criticality analysis in Scale
- Deterministic starting sources for Monte Carlo (MC) eigenvalue calculations
  - Efficiency enhancement
  - Reliability improvement
- Conclusion

Coupling with depletion/decay calculation needs precise space- and energy- dependent fluxes

Statistical uncertainties in group 6 fluxes (0.15 to 0.275eV)



	MCNP	FW-CADIS
Uncertainty range	0.6 – 16.2 %	1.0 – 6.6 %
Time to < 2 % uncertainty	323 hrs	45 hrs
Speed up (includes Denovo run time)	-	7.1

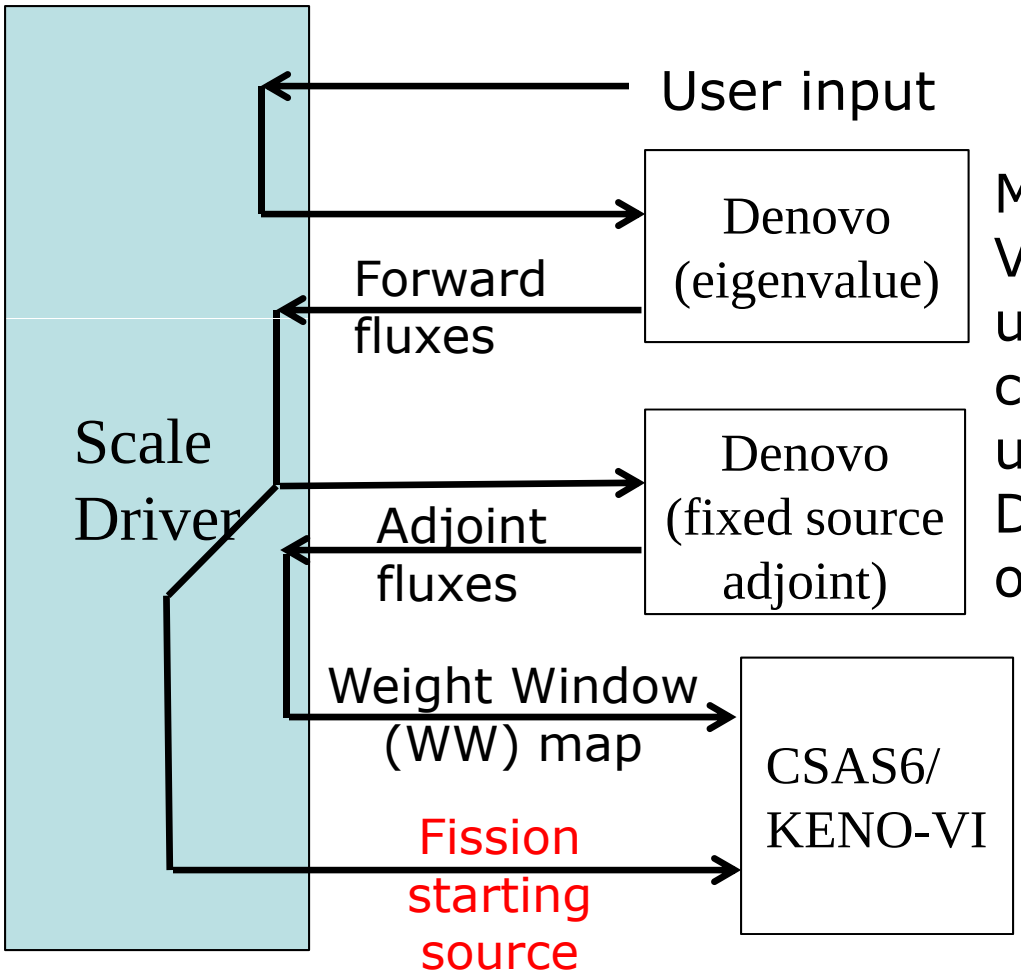
FW-CADIS yields more uniform uncertainties throughout the core

Conventional MC simulation

MC with FW-CADIS

J. Wagner, S. Mosher, "Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Reactor Analyses," *Trans. Am. Nucl. Soc.*, **103**, 342 (2010).

New sequence in **Scale** for FW-CADIS criticality analysis



Monaco with Automated Variance Reduction using Importance calculation (**MAVRIC**) used for processing Denovo input and output

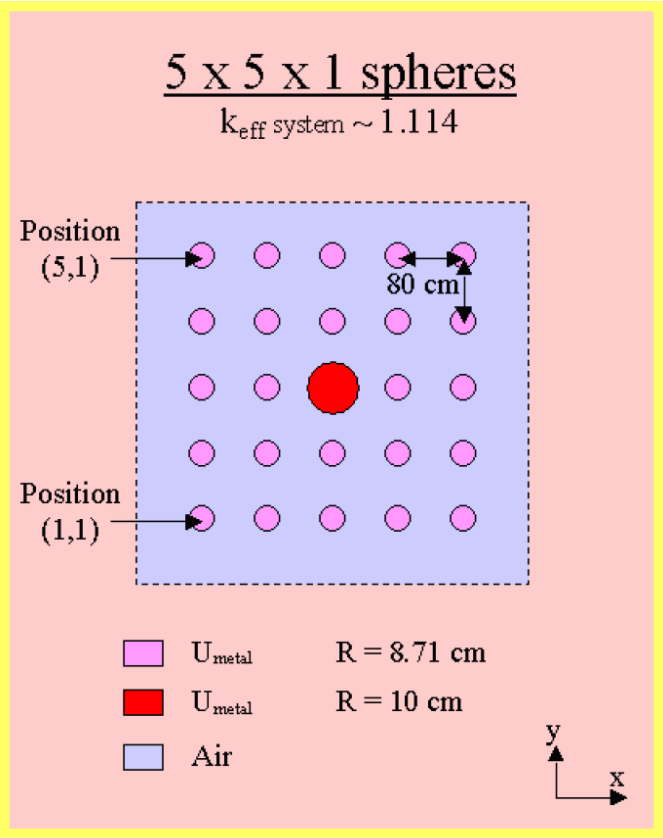
For deterministically generating WW, fission starting source will be available for free

$$s(\vec{r},E) = \chi(E)\int_{E'=0}^{\infty} \upsilon(E')\Sigma_f(\vec{r},E')\phi(\vec{r},E')dE'$$

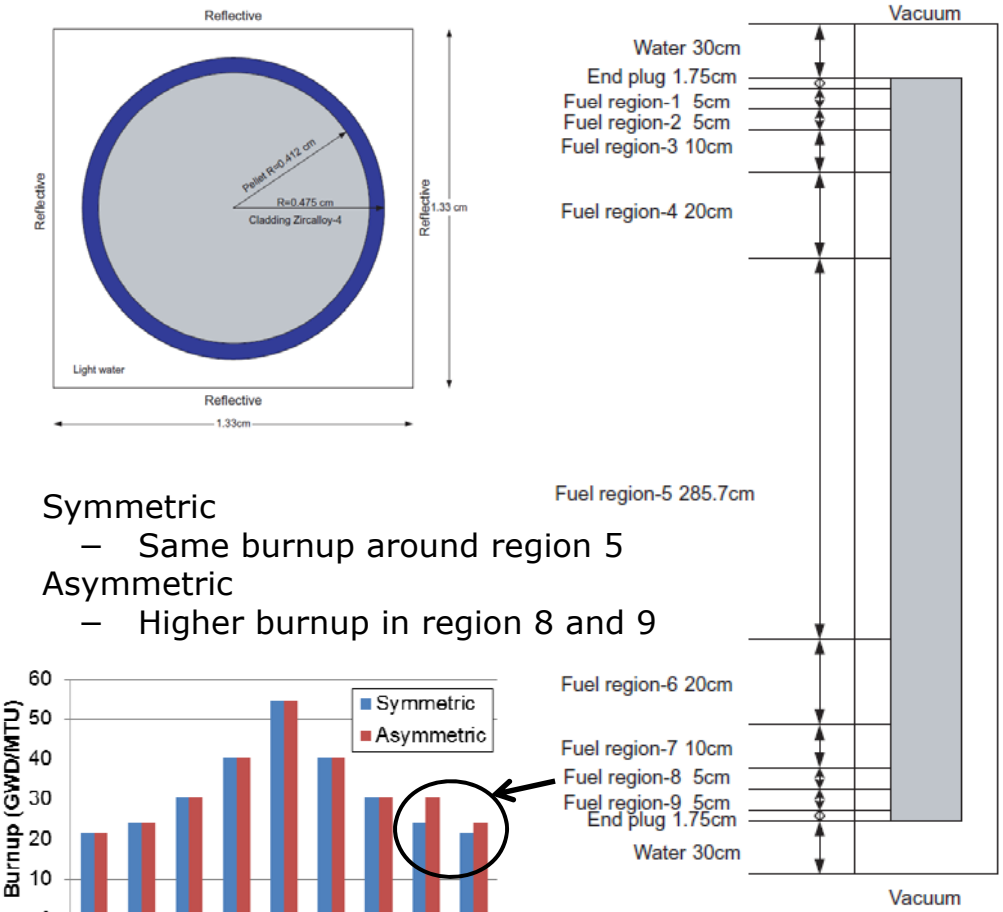
MC eigenvalue with deterministic starting source

- Problem-dependent
  - User does not have to guess
- Efficiency
  - Computational effort with and without deterministic starting source
- Reliability
  - Replicated independent MC calculations with different random number seeds
  - Probability of calculating correct eigenvalue

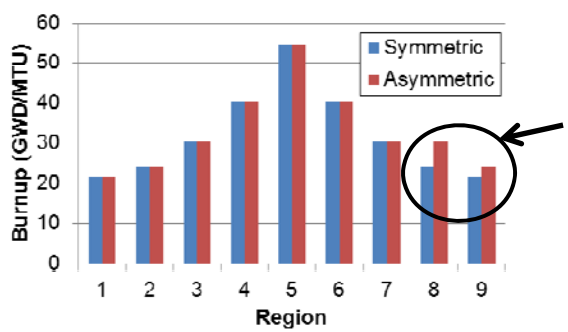
OECD/NEA Expert Group standard test problems



Array of interacting (Spheres)



- Symmetric
  - Same burnup around region 5
- Asymmetric
  - Higher burnup in region 8 and 9



(Pin-cell) array with irradiated fuel

Best practices

- Sufficient initial cycles (skipped cycles) must be discarded prior to beginning the tallies*
- Essential to monitor convergence of both **source distribution** and k_{eff}, not just k_{eff}*
- **Shannon entropy**† was shown to be effective in characterizing convergence of source distribution*
  - Used to **determine number of skipped cycles**

- *F. Brown, "A Review of Best Practices for Monte Carlo Criticality Calculations," LANL report, LA-UR-09-3136 (2009).
- †Taro Ueki, "Stationary Modeling and Informatics-Based Diagnostics in Monte Carlo Criticality Calculations," *NSE*, **149**, 38(2005).

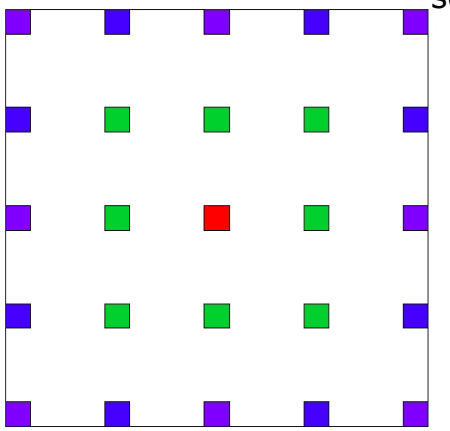
How we measure efficiency

- k_{eff} and Shannon entropy plots investigated before calculating efficiency
  - Determine number of skipped cycles
- Stop MC calculation at certain threshold ($1\sigma_{k_{eff}} = 2.0 \times 10^{-4}$)
- Efficiency in computer time saving

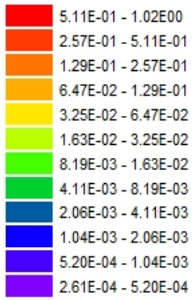
$$Speedup = \frac{MC\ time\ with\ uniform\ starting\ source}{MC\ time\ with\ deterministic\ starting\ source + Deterministic\ time}$$

Spheres

Denovo

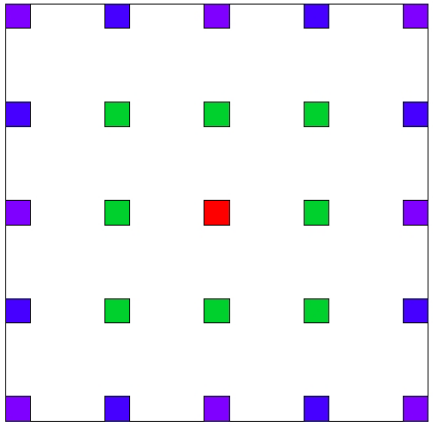


Normalized source

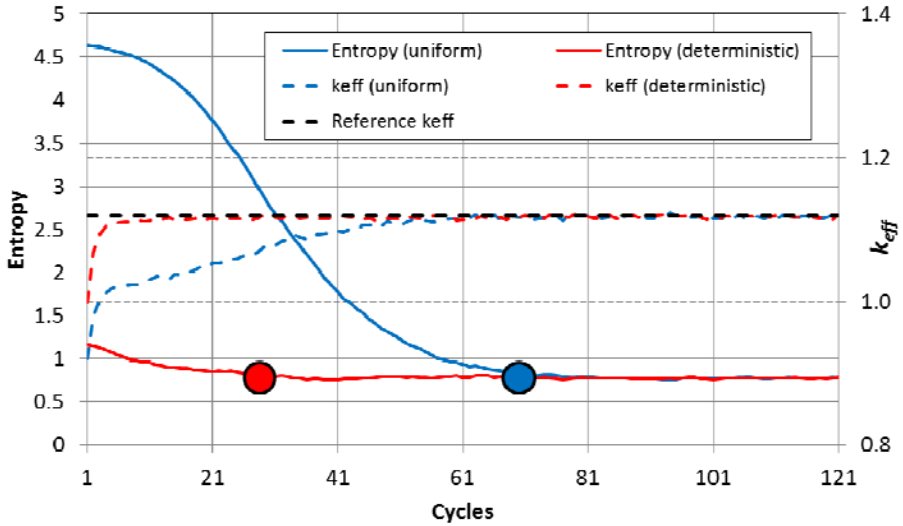


Reference
k_{eff}=1.11768±0.00003
4k skipped cycles
10k active cycles

KENO



Convergence of k_{eff} and Shannon Entropy



Starting source	Cycles		Time (min)	
	Skipped	Active	Denovo	Keno
Uniform	69	139	0.00	9.43
Deterministic	26	133	0.91	7.67

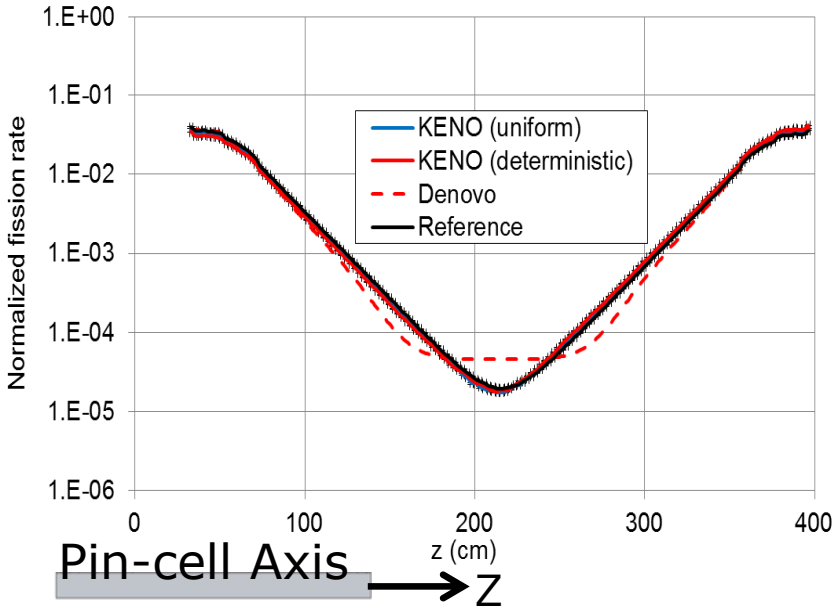
Starting source	k_{eff}	Speedup*
Uniform	1.11707 ± 0.00019	1.0
Deterministic	1.11758 ± 0.00019	1.2

*Speedup **accounts for deterministic** time too

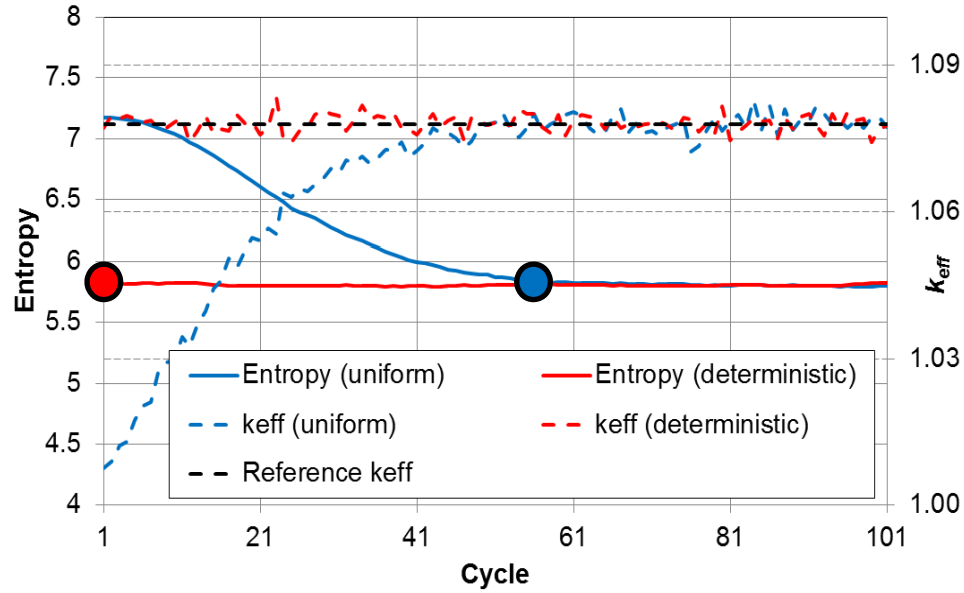
- Easy to converge
- Slight speedup

Symmetric Pin-cell

Final source distribution



Convergence of k_{eff} and Shannon entropy



Starting source	Cycles		Time (min)	
	Skipped	Active	Denovo	Keno
Uniform	56	79	0.00	60.20
Deterministic	1	74	3.69	33.75

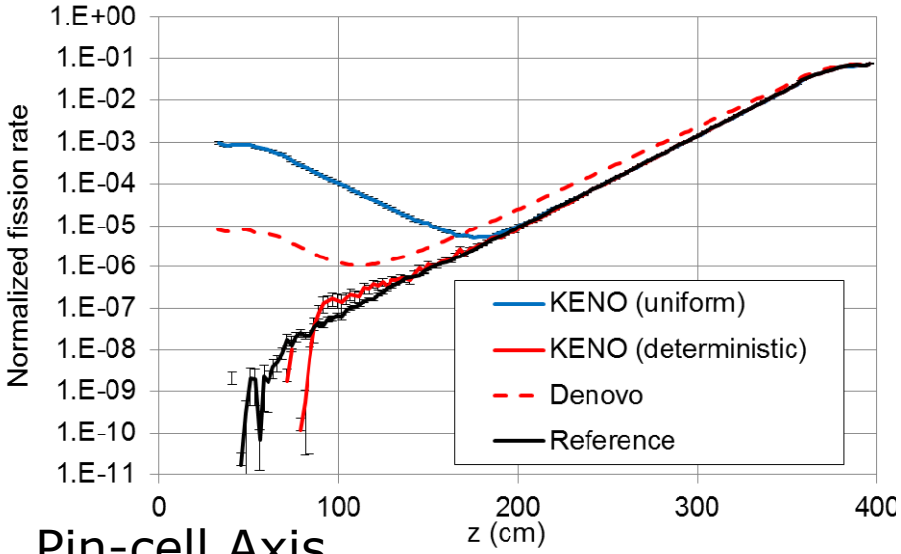
Starting source	k_{eff}	Speedup
Uniform	1.07783 ± 0.00019	1.0
Deterministic	1.07807 ± 0.00019	**1.6**

Reference
k_{eff}=1.07790±0.00002
1k skipped cycles
9k active cycles

- Source convergence still easy
- Moderate speedup

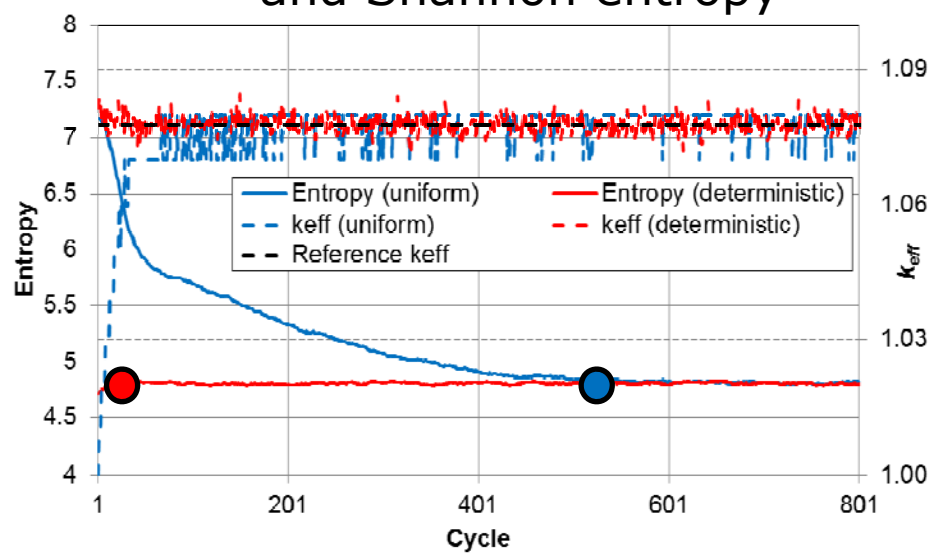
Asymmetric Pin-cell

Final source distribution



Pin-cell Axis → Z

Convergence of k_{eff} and Shannon entropy



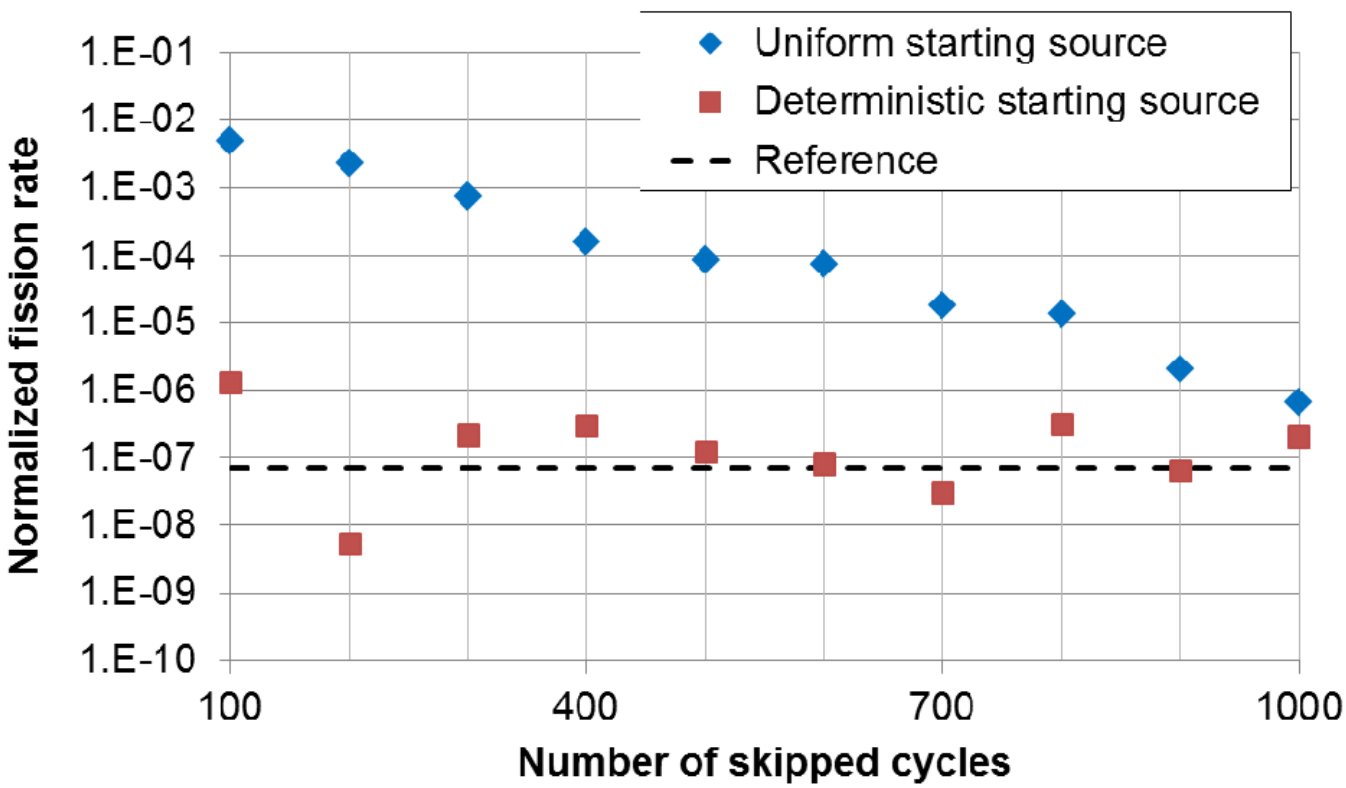
Starting source	Cycles		Time (min)	
	Skipped	Active	Denovo	Keno
Uniform	490	138	0.00	278.25
Deterministic	10	140	25.28	68.28

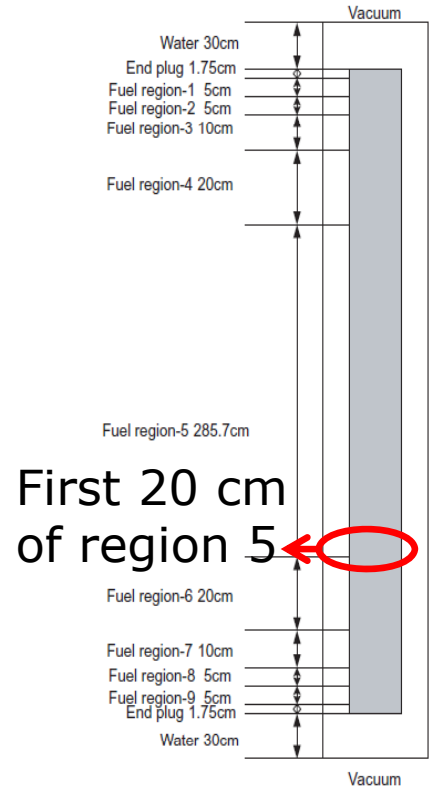
Reference
k_{eff}=1.07792±0.00002
1k skipped cycles
9k active cycles

Starting source	k_{eff}	Speedup
Uniform	1.07806 ± 0.00018	1.0
Deterministic	1.07809 ± 0.00017	**3.0**

- Difficult to converge
- High speedup

Fission rate in low reactive region





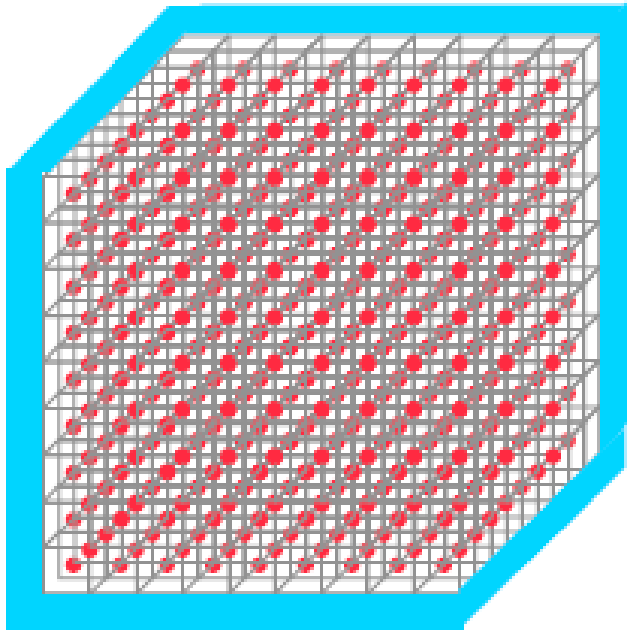
Notes

- Reference calculation
  - 10k skipped cycles
  - 10k active cycle
- Uniform uncertainties <10%
- Deterministic uncertainties <25%

- Tally estimates are **much better with deterministic** starting sources
- MC tallies **not reliable** in low reactive regions
  - May need FW-CADIS WW

k_{eff} of the world

- Introduced in 1971 to show limitations of MC methods*
  - Undersampled results unless correct fission distribution is achieved
- In 2010, original "k_{eff} of the world" was proven not to be difficult using
  - Today's computers
  - Best practice
    - 150 or more skipped cycles
    - 10K or more neutrons/cycle†



- 9×9×9 array of Pu^{239} spheres
- Only center sphere is critical (by itself) and rest is subcritical

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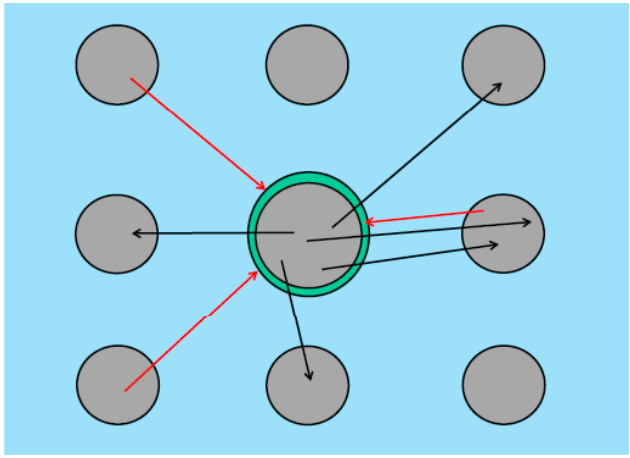
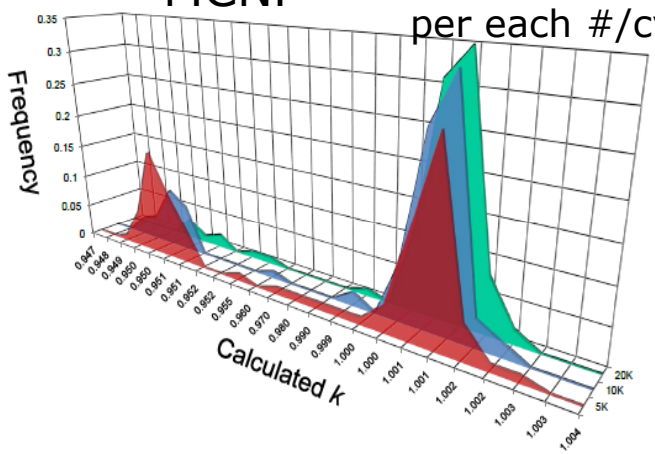
- *G. Whitesides, "A Difficulty in Computing the k-effective of the World," *Trans. Am. Nucl. Soc.*, **14**, 680 (1971).
- †F. Brown, "Revisiting the K_{eff} of the World Problem," LANL report, LA-UR-10-03745 (2010).

2011 k_{eff} of the world problem

- Flood area between spheres, reduce radii to maintain criticality
  - Decreases spheres' coupling
- Coat central (critical) sphere with Cd
  - Create asymmetry in coupling*



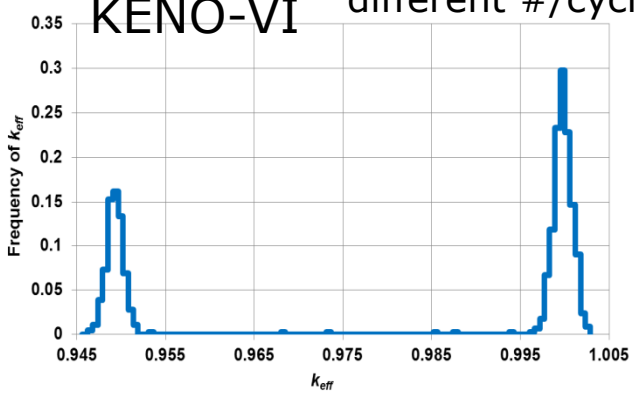
MCNP* 100 independent run per each #/cycle



Numerous independent MC simulations give clearly undersampled k_{eff} with nontrivial probability*

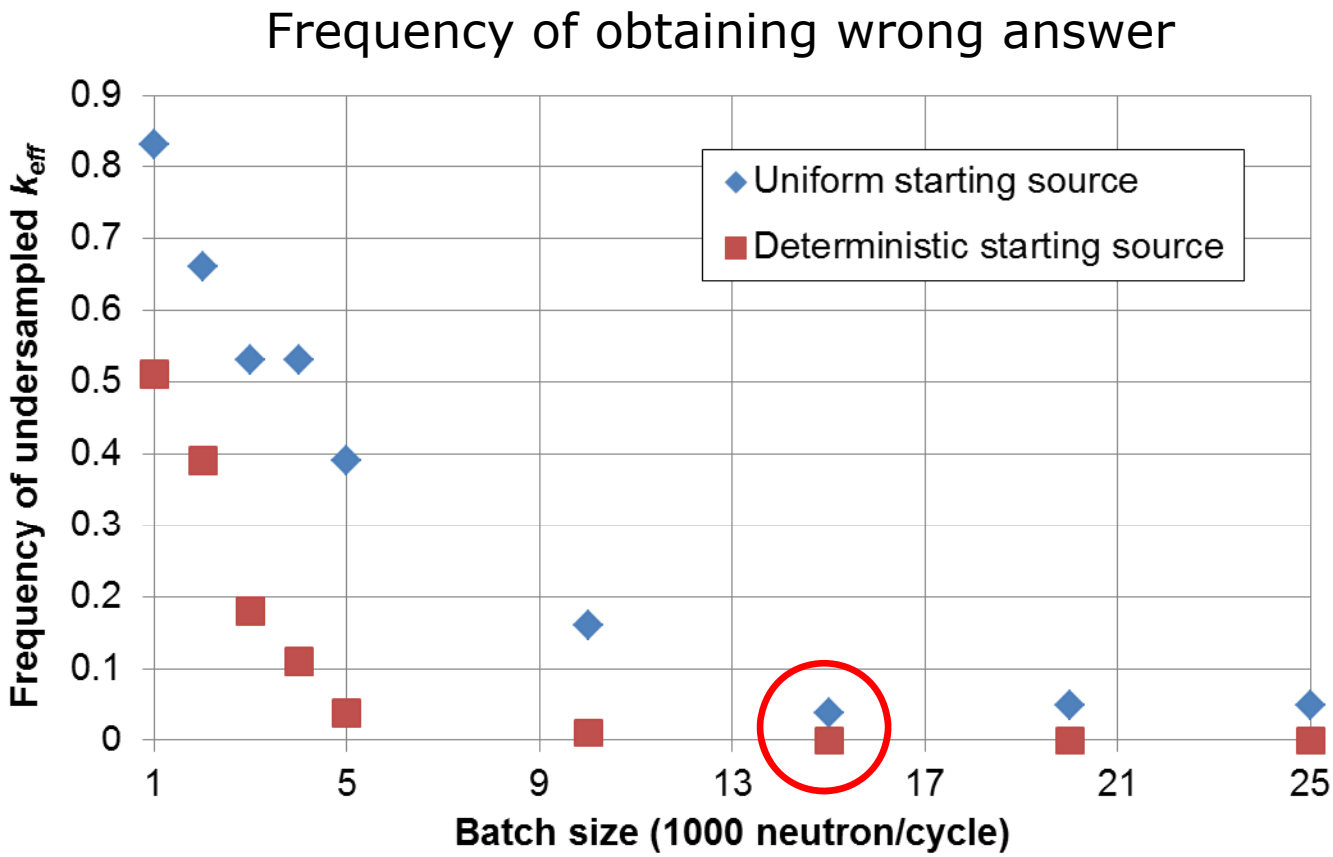
900 runs with different #/cycle

KENO-VI



*B. Kiedrowski, "Statistical Coverage Concerns in a Revised k-Effective of the World Problem", LANL report, LA-UR-11-03593 (2011).

2011 k_{eff} of the world with deterministic-based starting source



Starting from 15k neutrons/cycle, probability of obtaining incorrect answer reaches **zero** (100% reliable answer) with deterministic starting sources but remains around 5% with uniform starting source

Conclusion

- Automating the coupling between deterministic and MC eigenvalue calculations is under development in Scale
- For FW-CADIS, deterministically calculated fission starting source will be available for free
- Deterministic starting sources
  - Easier for users
    - Take guess-work out of defining problem-dependent starting sources
  - Increase efficiency
    - Significant decrease in number of skipped cycles
  - Increase reliability
    - Decrease probability of getting wrong answer due to improper source convergence