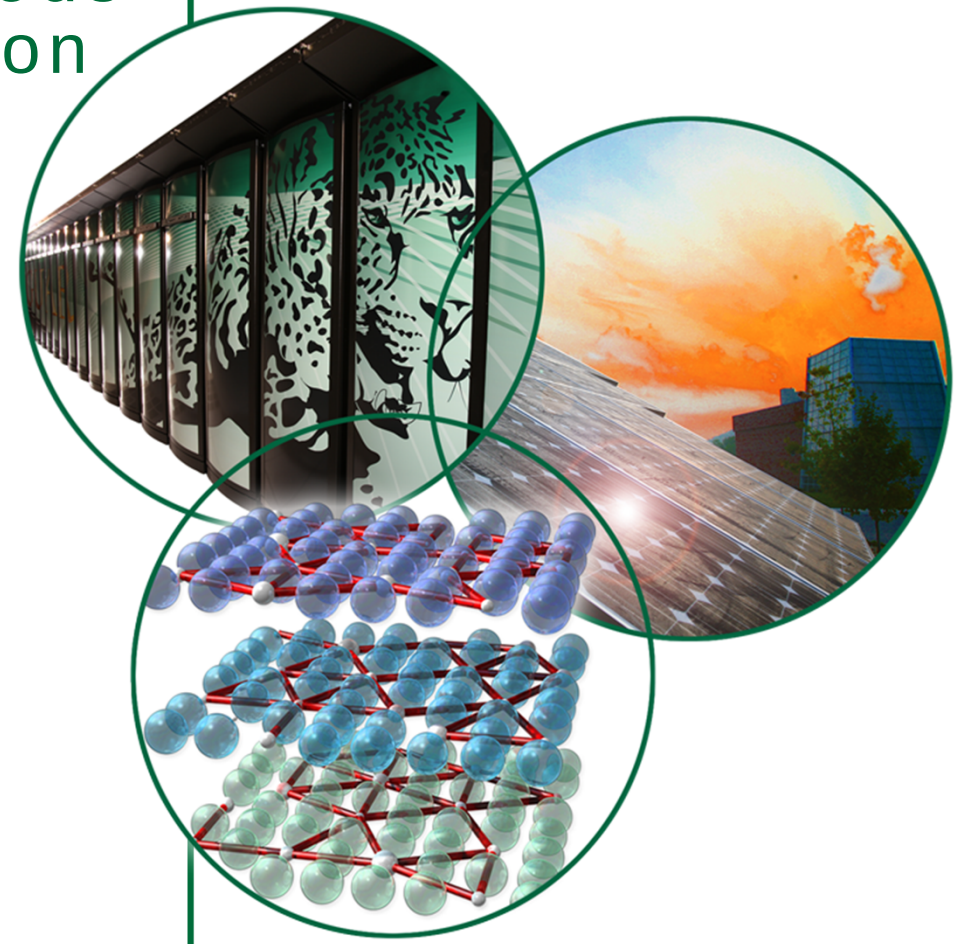
Comparison of Hybrid Methods for Global Variance Reduction in Shielding Calculations



Douglas E. Peplow
Radiation Transport Group
Reactor & Nuclear Systems Division

Tuesday, November 13, 2012
Transport and Computational Methods Session
Mathematics and Computation Division
2012 ANS Winter Meeting San Diego, CA

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Introduction

- Hybrid Methods
  - Use discrete ordinates estimates to construct variance reduction parameters for a detailed Monte Carlo calculation
  - S_N estimates: forward, adjoint or both
- Variance reduction parameters
  - Importance map for weight windows, biased source
  - Optimize the figure-of-merit (FOM) of one or more tallies
    - Single detector response
    - Flux/response over a portion of the problem
    - Flux/response over the entire problem space

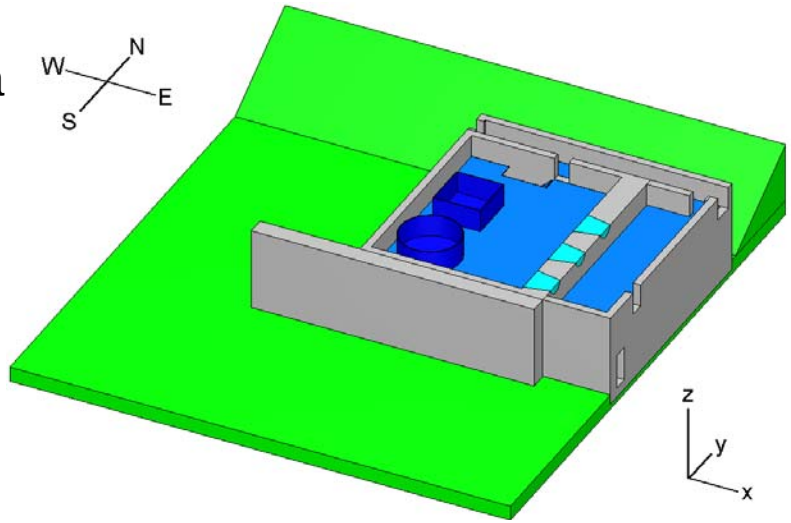
Global Problem

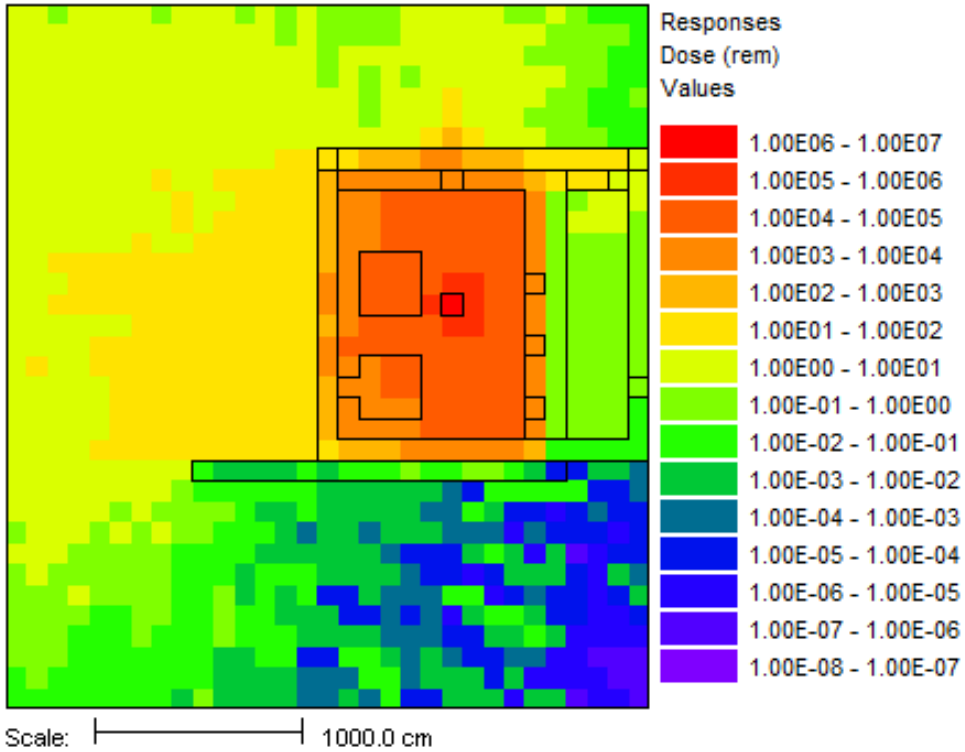
Monte Carlo for Global Solutions

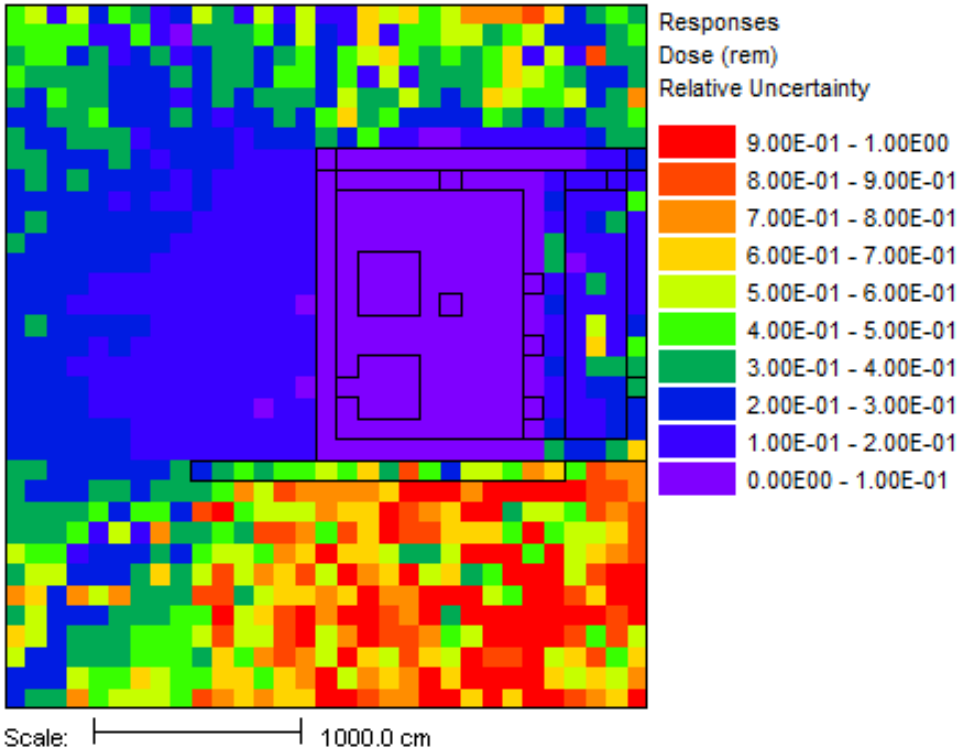
- Mesh tallies
  - Consist of I×J×K voxels
  - Range of flux values
  - Range of uncertainties

Neutron dose from a criticality accident

Implicit capture only
18 hours





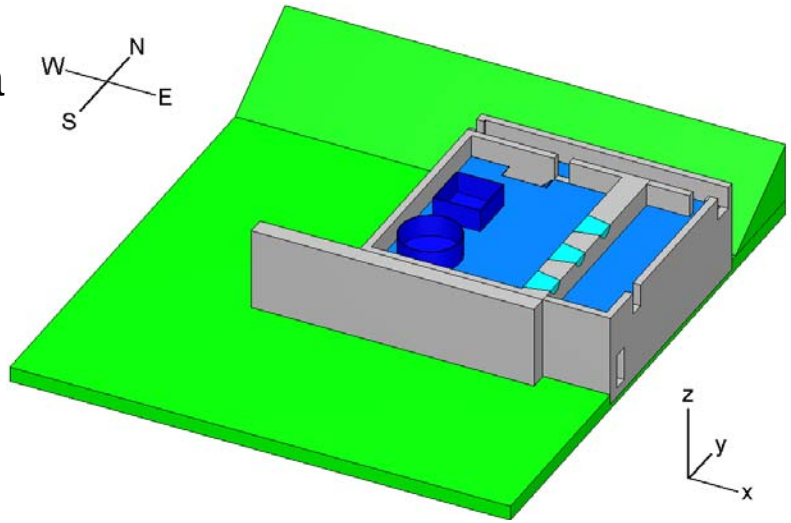


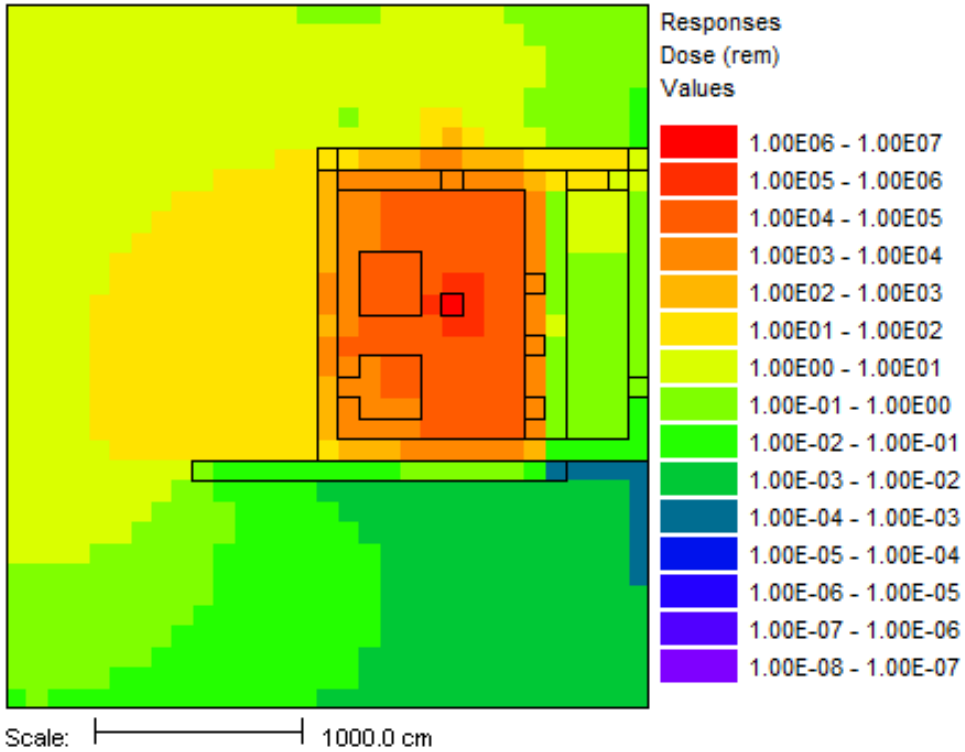
Monte Carlo for Global Solutions

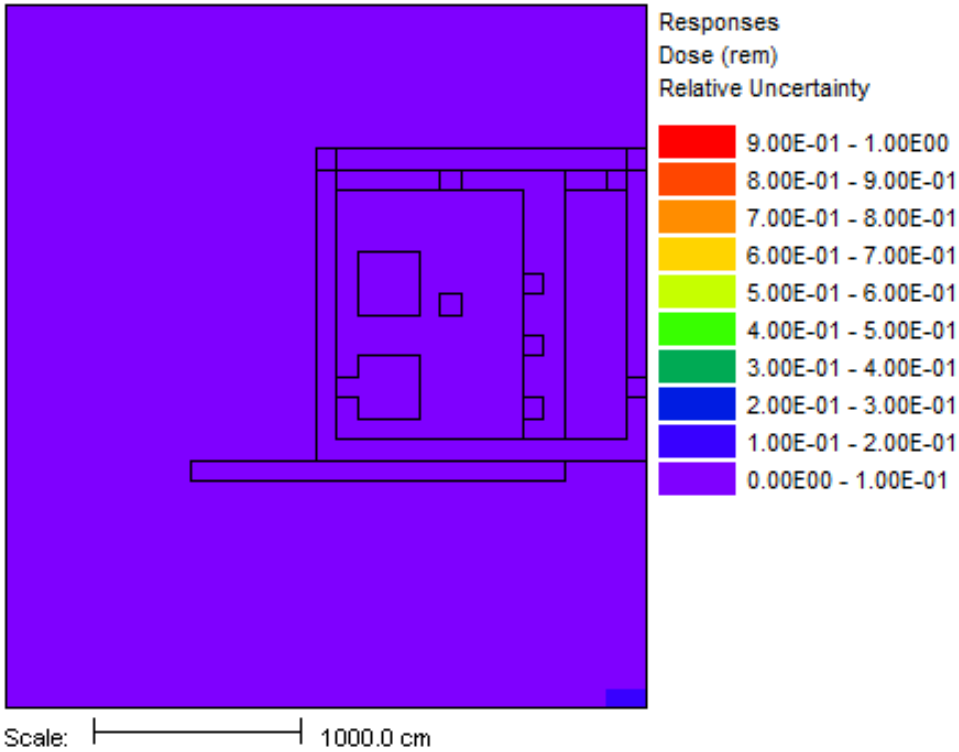
- Mesh tallies
  - Consist of I×J×K voxels
  - Range of flux values
  - Range of uncertainties

Neutron dose from a criticality accident

Hybrid
18 hours







Methods for Global Variance Reduction

- Cooper's Method
  - M. A. Cooper and E. W. Larsen, "Automated Weight Windows for Global Monte Carlo Particle Transport Calculations," *Nuc. Sci. and Eng.* **137**, 1-13 (2001).
- GFWW/GRWW
  - T. L. Becker and E. W. Larsen, "The Application of Weight Windows to 'Global' Monte Carlo Problems," ANS Math. & Comp. Top. Meeting, Saratoga Springs, New York, May 3-7, 2009.
- Van Wijk's Methods
  - A. J. van Wijk, G. Van den Eynde, and J. E. Hoogenboom, "An Easy to Implement Global Variance Reduction Procedure for MCNP," *Annals of Nuclear Energy* **38**, 2496-2503 (2011).
- Becker's Methods
  - T. L. Becker, *Hybrid Monte Carlo/Deterministic Methods for Deep-Penetration Problems*, Doctoral Dissertation, University of Michigan (2009).
- FW-CADIS
  - D. E. Peplow, E. D. Blakeman, and J. C. Wagner, "Advanced Variance Reduction Strategies for Optimizing Mesh Tallies in MAVRIC," *Transactions of the ANS* **97**, 595-597 (2007).
  - J. C. Wagner, D. E. Peplow, and S. W. Mosher, "FW-CADIS Method for Global and Semi-Global Variance Reduction of Monte Carlo Radiation Transport Calculations" submitted to *Nuc. Sci. and Eng.* (2012).

Cooper's Method

- Goal: uniform relative uncertainties
  - Make the Monte Carlo particle density $m(\vec{r})$ constant
  - Physical density $n(\vec{r})$ is related to the average weight $\overline{w}(\vec{r})$ by

$$n(\vec{r}) = \overline{w}(\vec{r})\, m(\vec{r})$$

- So, use forward deterministic estimate of flux $\phi(\vec{r})$
  - and make $\overline{w}(\vec{r}) \propto \phi(\vec{r})$

$$\overline{w}(\vec{r}) = \frac{\phi(\vec{r})}{\max\left(\phi(\vec{r})\right)}$$

  - Space-only method

Global Flux/Response Weight Windows

- Extension of Cooper's method to space/energy
- Use forward discrete ordinates estimate of $\phi(\vec{r}, E)$
- To optimize MC $\phi(\vec{r}, E)$ everywhere

$$\bar{w}(\vec{r}, E) \propto \phi(\vec{r}, E)$$

- To optimize MC $D(\vec{r}) = \int_E f(E)\, \phi(\vec{r}, E) dE$ everywhere

$$\bar{w}(\vec{r}, E) \propto \frac{\int_E f(E)\, \phi(\vec{r}, E) dE}{f(E)} = \frac{D(\vec{r})}{f(E)}$$

Van Wijk's Methods

- Developed an iterative scheme with MCNP
- Estimates could be found using deterministic solution

- Flux-based method: $\bar{w}(\vec{r}) = \dfrac{\phi(\vec{r})}{\max\left(\phi(\vec{r})\right)}$

- Relative error is $Re(\vec{r}) \propto 1/\sqrt{\phi(\vec{r})}$
- Re-based method:

$$\bar{w}(\vec{r}) = \frac{\min\left(Re(\vec{r})\right)}{Re(\vec{r})}$$

Becker's Methods

- Uses forward and adjoint estimates
- Different for detector, region, or global problems
- Optimize either $\phi(\vec{r}, E)$ or response function $f(E)$

Compute the forward flux estimate	$\phi(\vec{r}, E)$
Construct the adjoint source - for optimizing flux use	$q^{+}(\vec{r}, E) = {}^{1}/_{\phi(\vec{r}, E)}$
or for optimizing response use	$q^{+}(\vec{r}, E) = \dfrac{f(E)}{\int_0^\infty f(E)\,\phi(\vec{r}, E)\,dE}$
Compute the adjoint flux estimate	$\phi^{+}(\vec{r}, E)$
Construct the contributon flux	$\phi^{c}(\vec{r}, E) = \phi(\vec{r}, E)\,\phi^{+}(\vec{r}, E)$
Find the space-only contributon flux	$\phi^{c}(\vec{r}) = \int_0^\infty \phi^{c}(\vec{r}, E)\,dE$
Construct the weight windows	$\bar{w}(\vec{r}, E) = \dfrac{\phi^{c}(\vec{r})}{\phi^{+}(\vec{r}, E)}$

FW-CADIS

- Uses forward and adjoint estimates
- Same for detector, region, or global problems
- Optimize either $\phi(\vec{r}, E)$ or response function $f(E)$

Compute the forward flux estimate	$\phi(\vec{r}, E)$
Construct the adjoint source - for optimizing flux use	$q^{+}(\vec{r}, E) = g(\vec{r}) \big/ \phi(\vec{r}, E)$
or for optimizing response use	$q^{+}(\vec{r}, E) = \dfrac{g(\vec{r})\, f(E)}{\int_0^\infty f(E)\, \phi(\vec{r}, E)\, dE}$
Compute the adjoint flux estimate	$\phi^{+}(\vec{r}, E)$
Compute the response estimate	$R = \iint q(\vec{r}, E)\, \phi^{+}(\vec{r}, E) dE\, d\vec{r}$
Construct the weight windows	$\bar{w}(\vec{r}, E) = \dfrac{R}{\phi^{+}(\vec{r}, E)}$
Construct the biased source	$\hat{q}(\vec{r}, E) = \dfrac{q(\vec{r}, E)\, \phi^{+}(\vec{r}, E)}{R}$

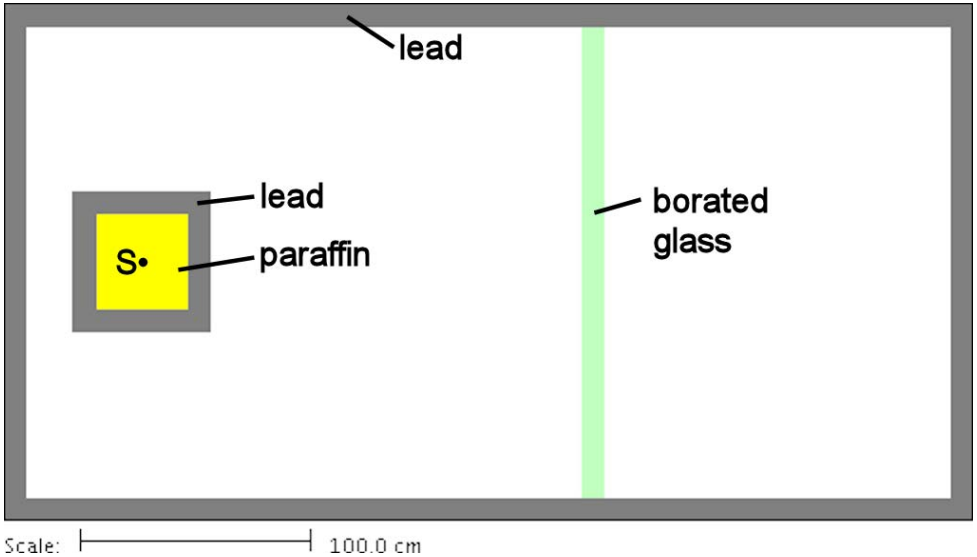
Mesh Tally Metrics

- Look at the relative error, r_i, in each of the V voxels
- Form a distribution of relative uncertainties
- Mean relative uncertainty $\bar{r} = \frac{1}{V}\sum r_i$
  - Should be $\propto 1/\sqrt{N}$ if each voxel is $\propto 1/\sqrt{N}$
- Tests:
  - Is the fraction of voxels with score, ζ, constant?
  - Is $\bar{r} \propto 1/\sqrt{N}$?
  - Is the variance of $\bar{r} \propto 1/N$?
  - Is the FOM, $1/(\bar{r}^2 T)$, constant?

Based on:
B. C. Kiedrowski and C. J. Solomon, "Statistical Assessment of Numerous Monte Carlo Tallies," ANS Math. & Comp. Top. Meeting, Rio de Janeiro, Brazil, May 8-11, 2011.

Simple Shielding Problem

- 420 × 220 × 240 cm lead rooms
- Source: 1 Ci, 14 MeV, point
- Optimize $D(\vec{r})$ everywhere

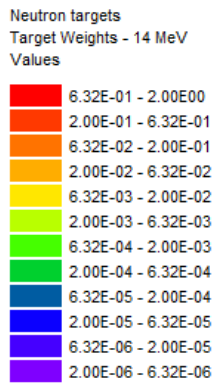


	Time (min)			
	for	adj	MC	Total
Analog			420	420
Cooper	8.9		50.9	60
van Wijk (Re)	8.9		50.1	59
GRWW	8.9		51.0	60
Becker	8.9	7.4	40.8	57
FW-CADIS	8.9	7.4	40.3	57

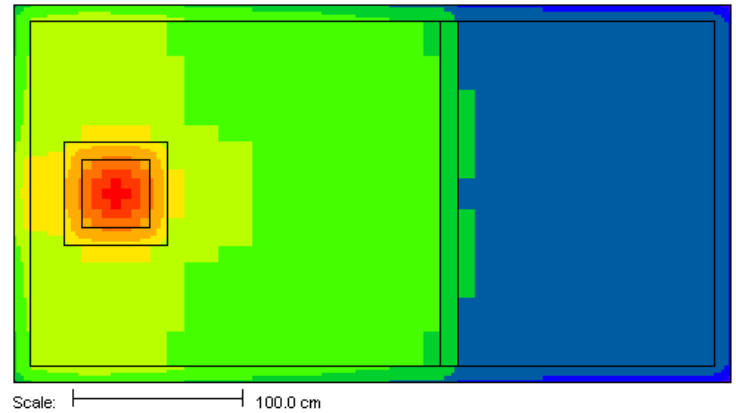
- Mesh Tally:
  - 84 × 44 × 48 uniform
- Deterministic
  - grid: 51 × 35 × 37 non-uniform
  - S_8, P_3
  - 27 groups

Simple Shielding Problem

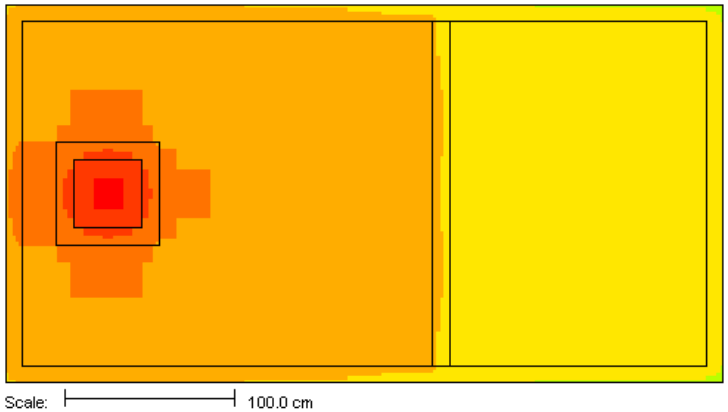
analog



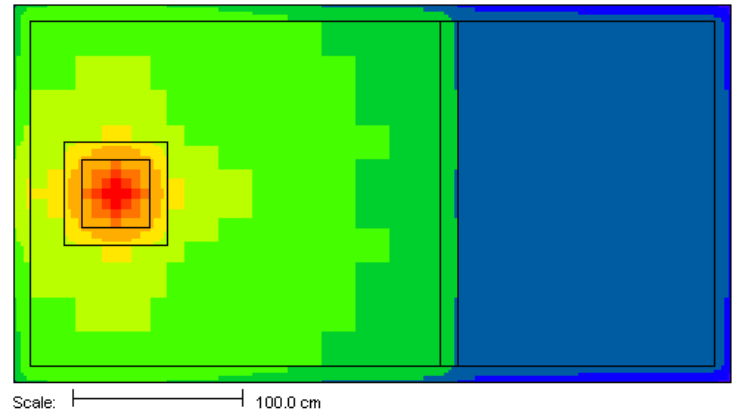
Cooper



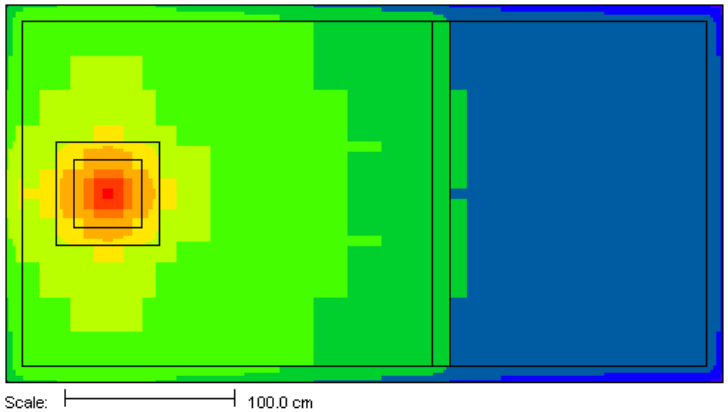
Van Wijk



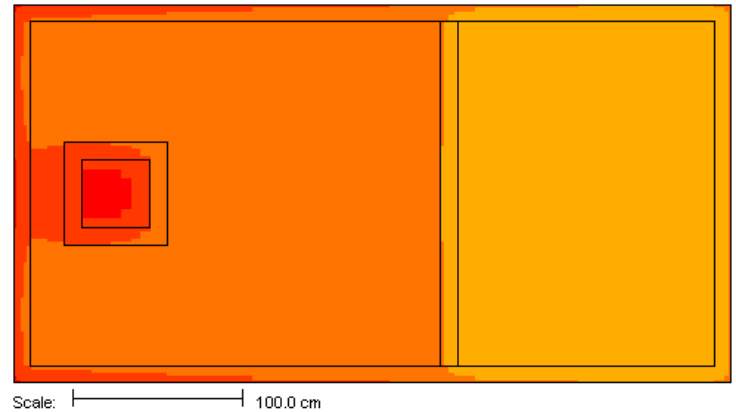
GRWW



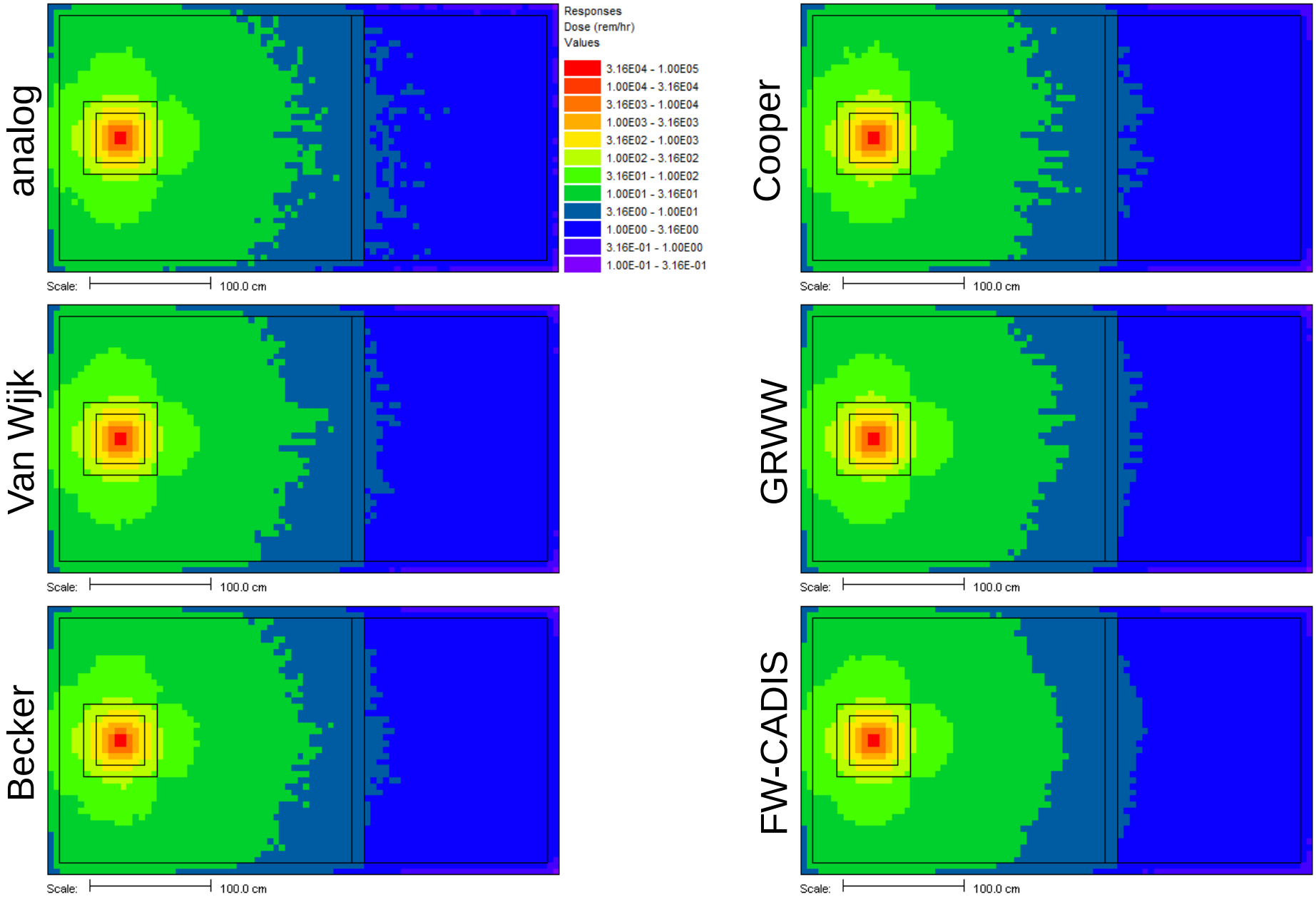
Becker



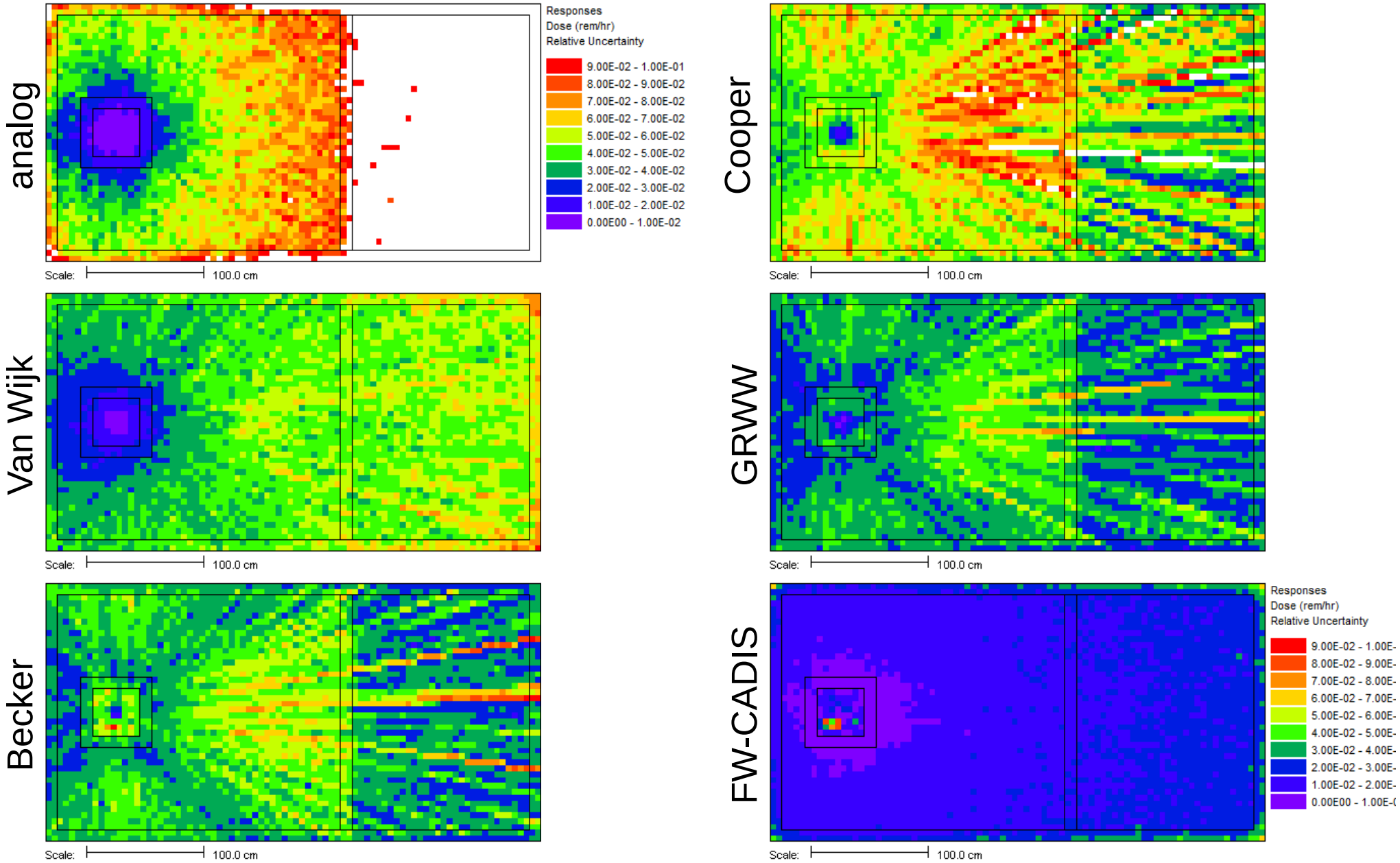
FW-CADIS



Simple Shielding Problem



Simple Shielding Problem

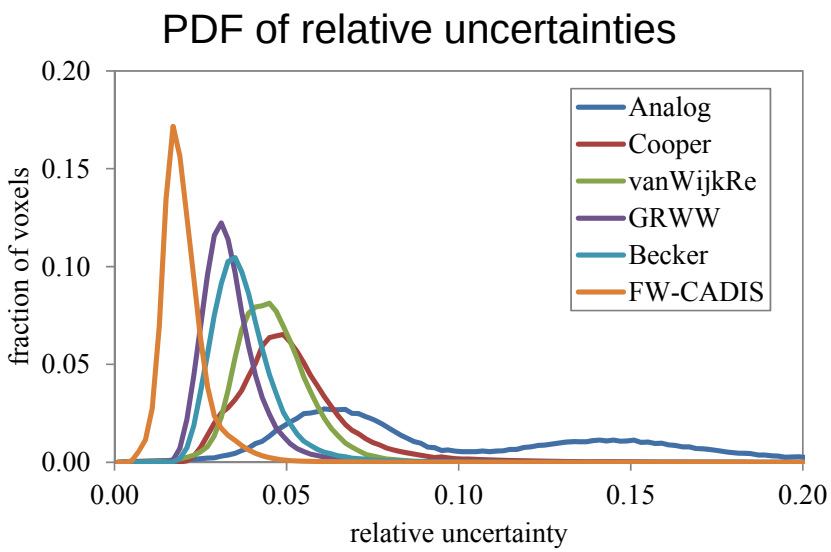


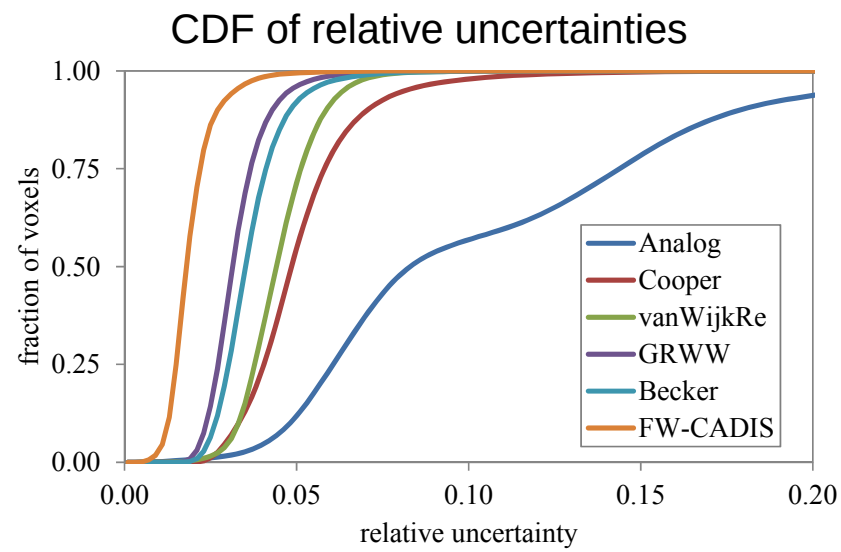
Simple Shielding Problem

177,408 voxels

	Time (min)			
	for	adj	MC	Total
Analog			420	420
Cooper	8.9		50.9	60
van Wijk (Re)	8.9		50.1	59
GRWW	8.9		51.0	60
Becker	8.9	7.4	40.8	57
FW-CADIS	8.9	7.4	40.3	57

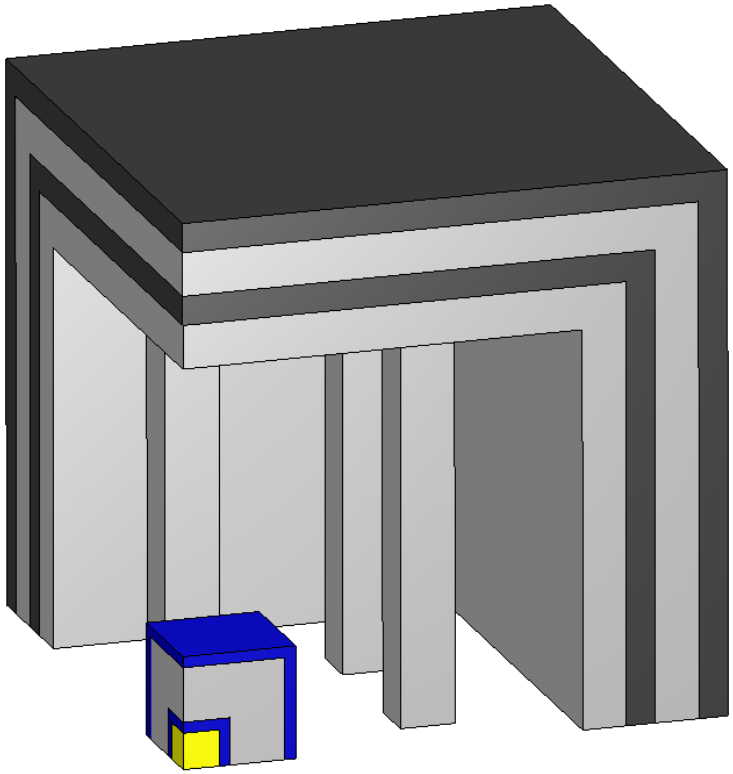
			FOM	Stat. Test			
	ζ	$\bar{r}$	(/min)	1	2	3	4
Analog	1.0000	1.07E-01	0.21	X	X	X	X
Cooper	1.0000	5.23E-02	6.11	X	-	X	-
van Wijk (Re)	1.0000	4.61E-02	7.97	X	X	X	X
GRWW	1.0000	3.38E-02	14.60	X	-	-	-
Becker	1.0000	3.77E-02	12.32	X	-	X	-
FW-CADIS	1.0000	2.03E-02	42.83	X	X	X	X





Becker's Challenge

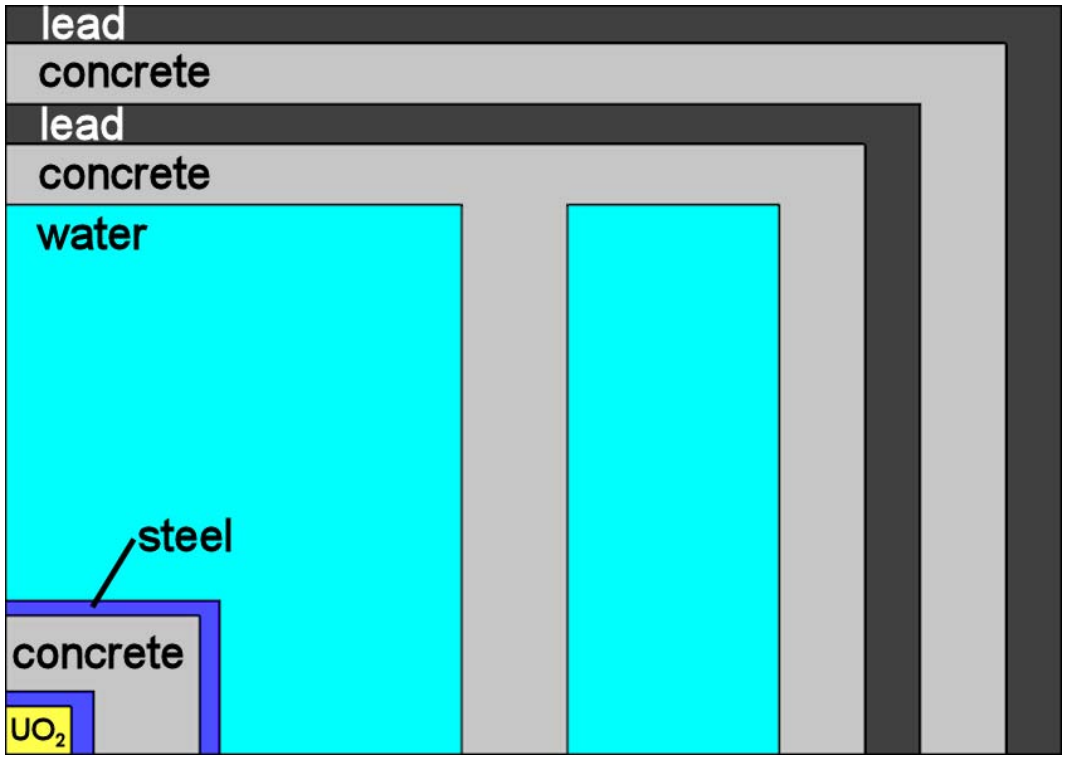
- 300 × 300 × 300 cm
- Source: fission neutrons
- Optimize $\phi(\vec{r})$ everywhere



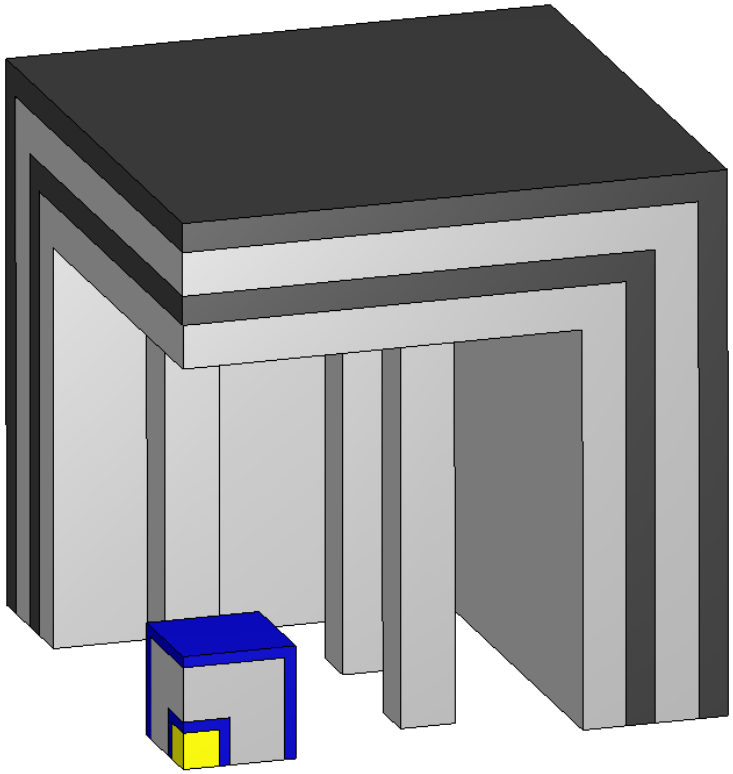
	Time (min)			
	for	adj	MC	Total
Analog			1203	1203
Cooper	38.6		1173	1212
van Wijk (Re)	38.6		1163	1202
GRWW	38.6		1184	1222
Becker	38.6	48.6	1118	1205
FW-CADIS	38.6	48.7	1117	1204

- Mesh Tally:
  - 30 × 30 × 30 uniform (1/8th)
- Deterministic
  - grid: 68 × 68 × 68 non-uniform
  - S_8, P_3
  - 27 groups

Becker's Challenge

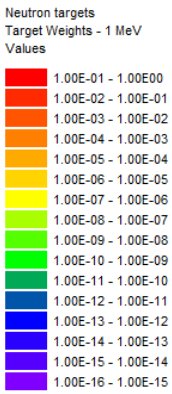


Along the $x = y$ plane

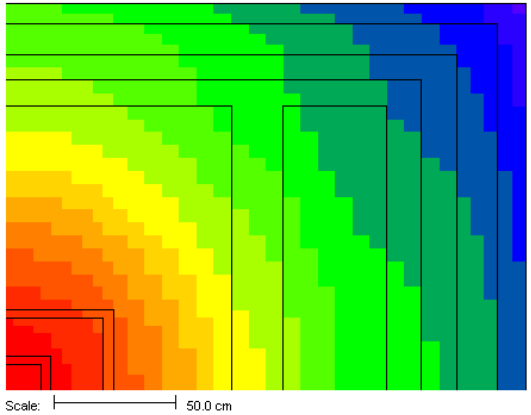


Becker's Challenge Problem

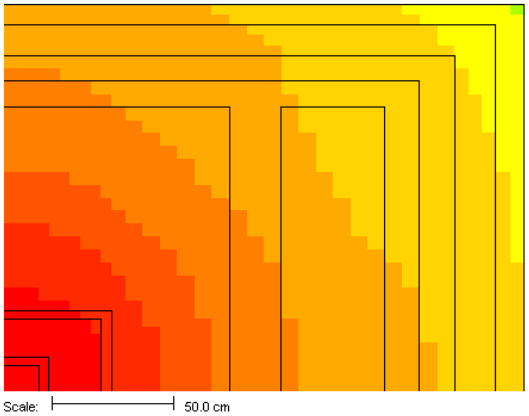
analog



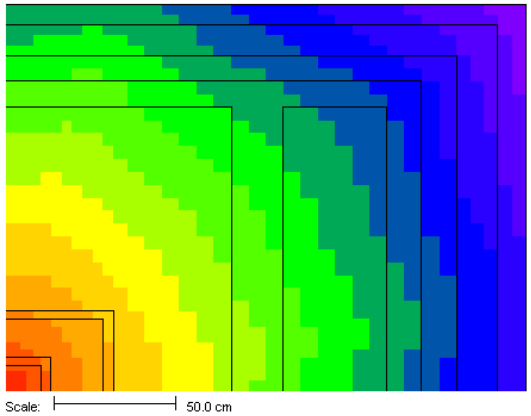
Cooper



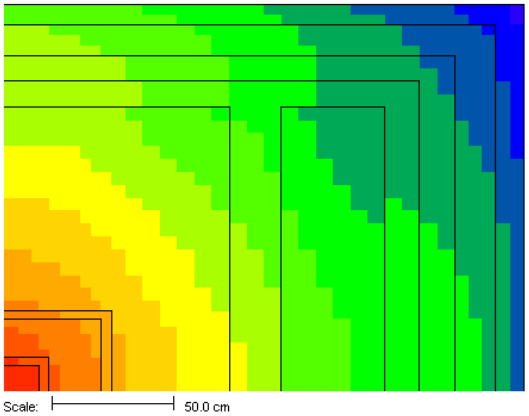
Van Wijk



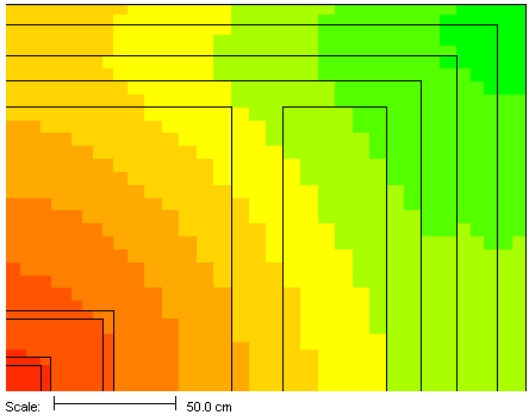
GRWW



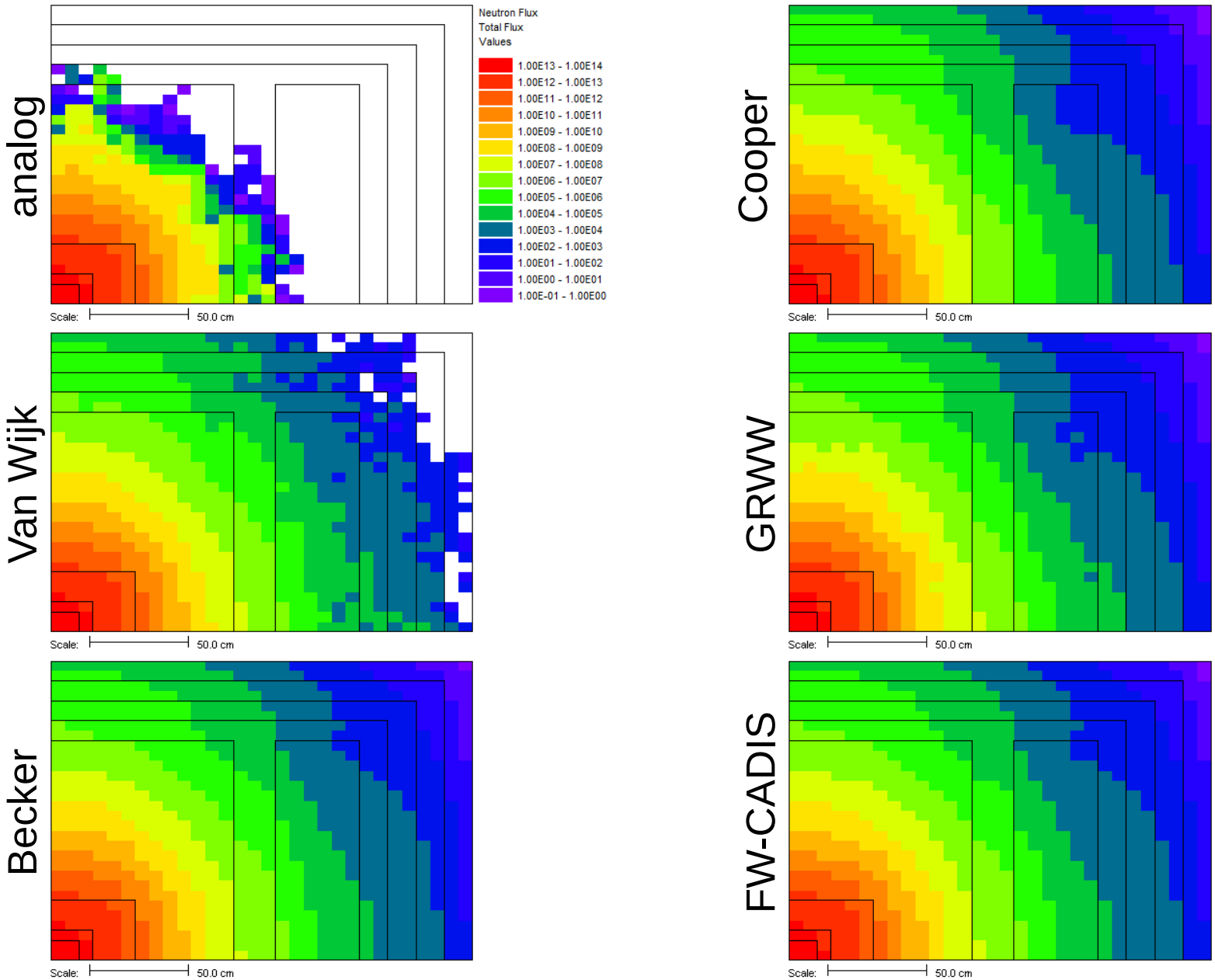
Becker



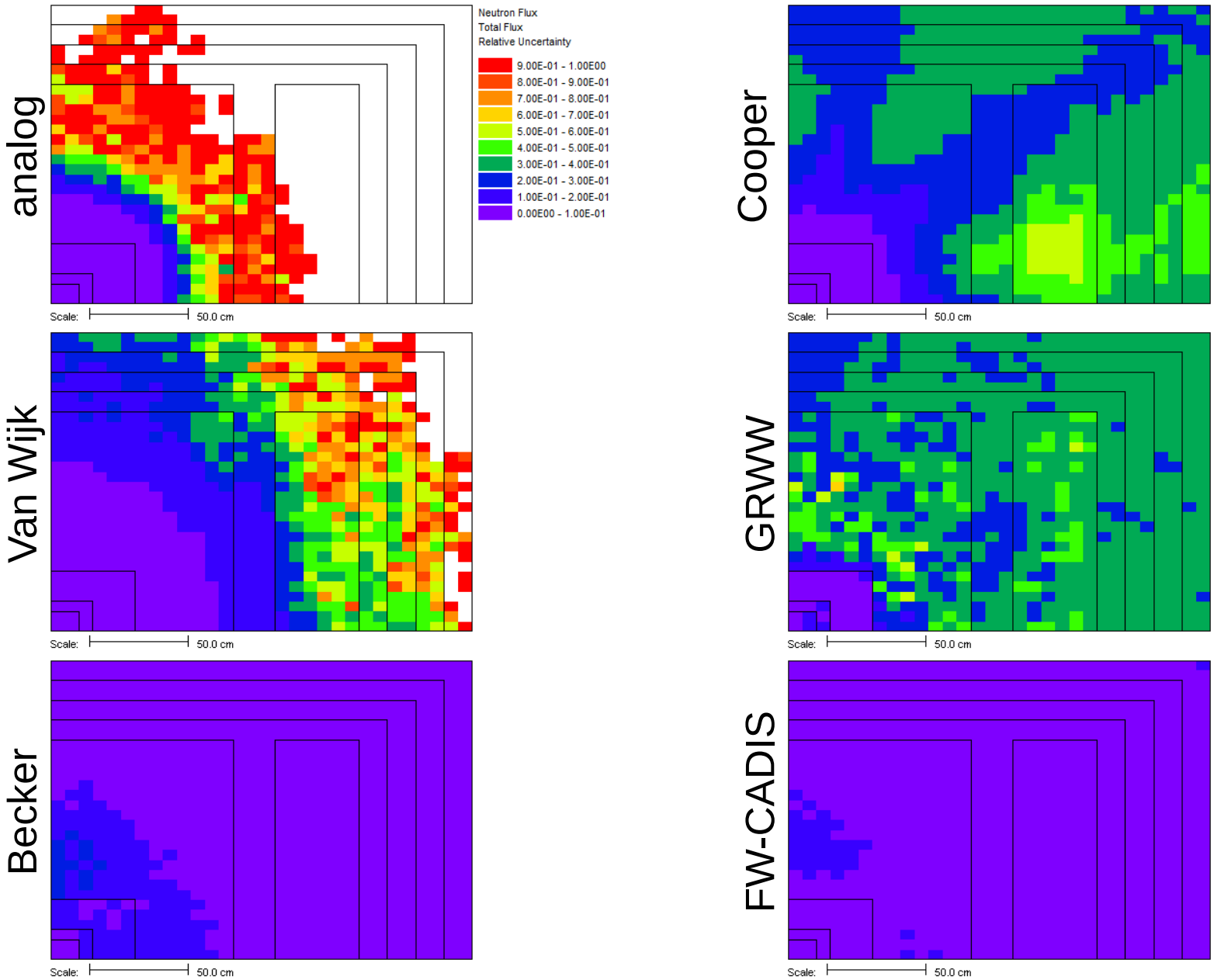
FW-CADIS



Becker's Challenge Problem



Becker's Challenge Problem

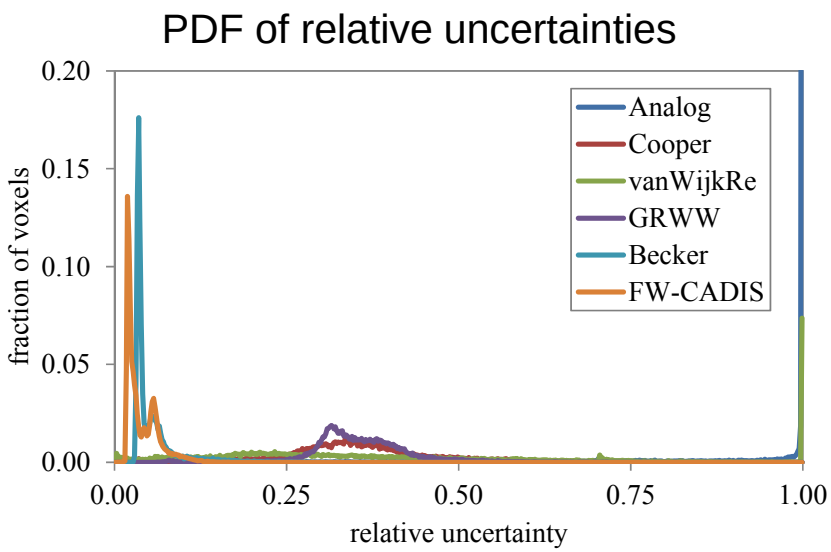


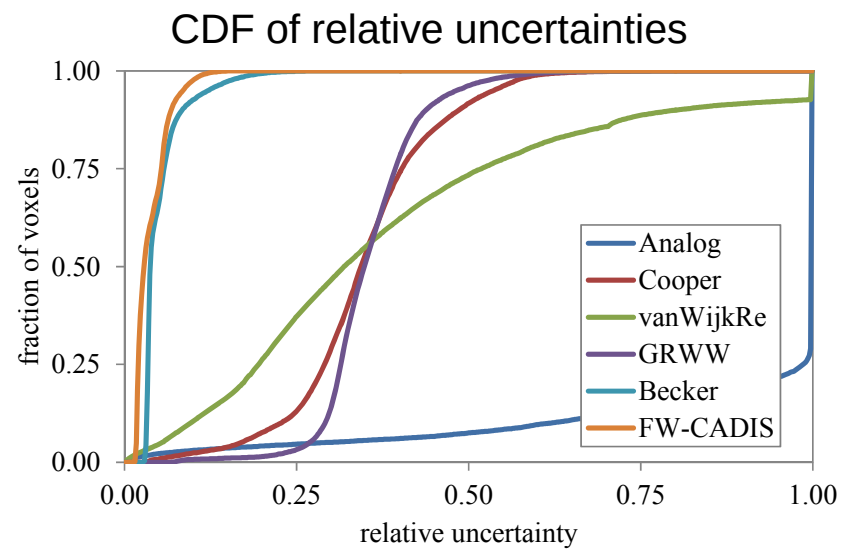
Becker's Challenge Problem

27,000 voxels

	Time (min)			
	for	adj	MC	Total
Analog			1203	1203
Cooper	38.6		1173	1212
van Wijk (Re)	38.6		1163	1202
GRWW	38.6		1184	1222
Becker	38.6	48.6	1118	1205
FW-CADIS	38.6	48.7	1117	1204

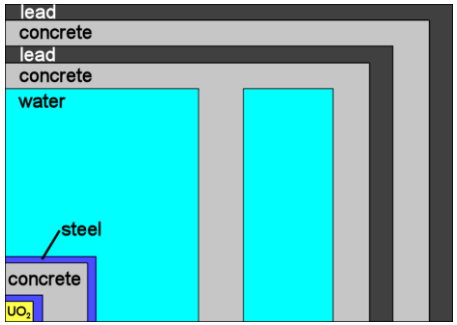
			FOM	Stat. Test			
	ζ	$\bar{r}$	(/min)	1	2	3	4
Analog	0.3428	2.64E-01	0.012	-	-	-	-
Cooper	1.0000	3.49E-01	0.007	X	-	-	-
van Wijk (Re)	0.9675	3.54E-01	0.007	X	-	-	-
GRWW	1.0000	3.58E-01	0.007	X	-	-	-
Becker	1.0000	5.26E-02	0.323	X	X	X	X
FW-CADIS	1.0000	3.92E-02	0.582	X	X	X	X

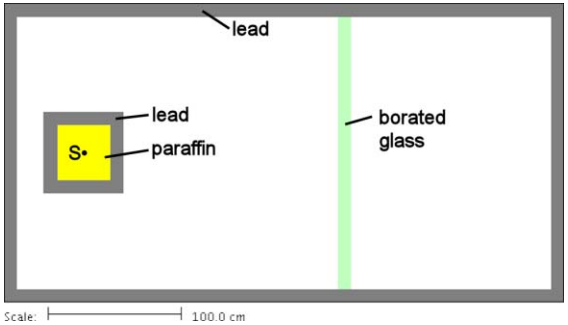




What about Semi-global?

- Note that most problems are not global
  - Need to specify where to get "good" results
    - Based on geometry, material
    - Based on result value
  - Adjoint methods more flexible





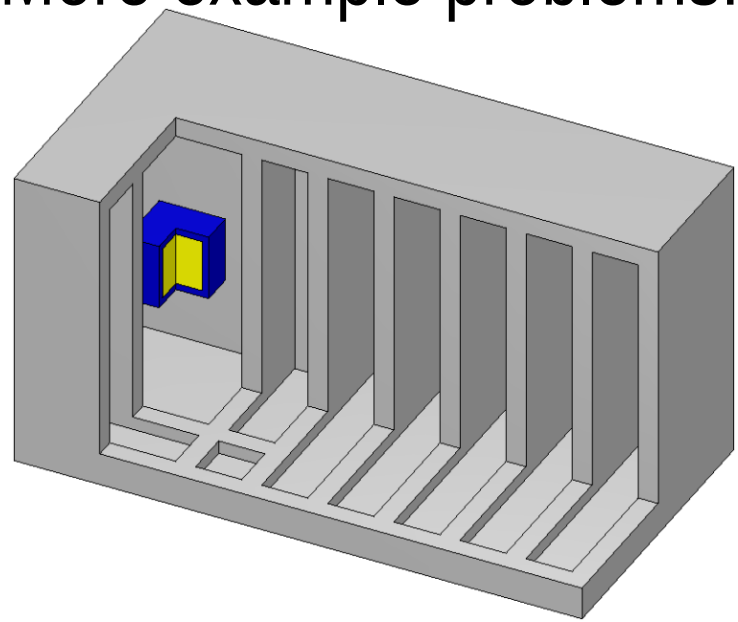
  - Forward-based methods spread particles around evenly
    - Difficult to optimize a specific portion of phase space

Summary

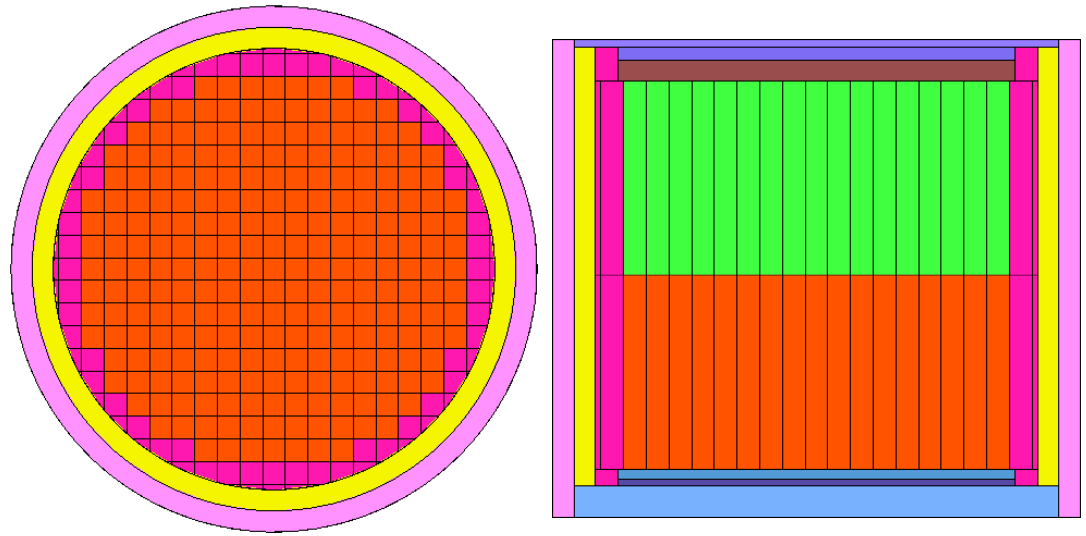
- Forward/adjoint methods far superior to forward-only
  - Adjoint contains importance information
  - Forward-based methods spread particles around evenly
- FW-CADIS
  - Higher FOM's than Becker's global method on both problems
  - More flexible (same method for semi-global problems)

Coming Attraction

- More example problems:



Deep Penetration Demo
Optimize $\phi(\vec{r}, E)$ everywhere



Monte Carlo Performance Benchmark
Optimize $\phi(\vec{r})$ everywhere

- Presentation in Sun Valley (May 2013)