Hybrid Monte Carlo/ Deterministic Methods for Streaming/Beam Problems

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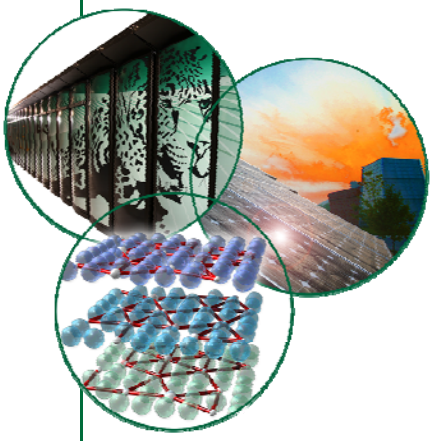

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Introduction

- Monte Carlo needs variance reduction
- One of the best VR methods is weight windows based on the adjoint of what you want to optimize
- Adding biased source to match improves MC performance
- Space/energy weight windows/biased sources have been used on many applications
- Some problems that have strong dependence on particle direction may benefit from space/energy/angle weight windows

CADIS Method

Consistent Adjoint Driven Importance Sampling

Biased source and importance map work together

Ali Haghighat and John C. Wagner, "Monte Carlo Variance Reduction with Deterministic Importance Functions," Progress in Nuclear Energy, 42(1), 25-53, (2003).

- Solve the adjoint problem using the detector response function as the adjoint source.

$$q^{+}(\vec{r},E,\hat{\Omega}) = \sigma_d(\vec{r},E)\frac{1}{4\pi}$$

- Weight window targets are inversely proportional to the adjoint flux (measure of importance of the particles to the response).

$$\overline{w}(\vec{r},E,\hat{\Omega}) = \frac{c}{\phi^{+}(\vec{r},E,\hat{\Omega})}$$

CADIS Method

- We want source particles born with a weight matching the weight window targets

$$w_0\left(\vec{r},E,\hat{\Omega}\right) \equiv \frac{q\left(\vec{r},E,\hat{\Omega}\right)}{\hat{q}\left(\vec{r},E,\hat{\Omega}\right)} = \overline{w}\left(\vec{r},E,\hat{\Omega}\right)$$

- So the biased source needs to be

$$\hat{q}\left(\vec{r},E,\hat{\Omega}\right) = \frac{q\left(\vec{r},E,\hat{\Omega}\right)}{\overline{w}\left(\vec{r},E,\hat{\Omega}\right)} = \frac{1}{c}q\left(\vec{r},E,\hat{\Omega}\right)\phi^{+}\left(\vec{r},E,\hat{\Omega}\right)$$

- Since the biased source is a pdf, solve for *c*

$$c = \iiint q(\vec{r},E,\hat{\Omega})\,\phi^{+}(\vec{r},E,\hat{\Omega})\,d\vec{r}\,dE\,d\hat{\Omega}$$

CADIS Method – Space/Energy

- Define the adjoint source

$$q^{+}(\vec{r},E)=\sigma_d(\vec{r},E)$$

- Solve for the adjoint flux $\phi^{+}(\vec{r},E)$
- Find *c* $\quad c=\iint q(\vec{r},E)\,\phi^{+}(\vec{r},E)\,d\vec{r}\,dE$
- Construct weight windows and biased source

$$\overline{w}(\vec{r},E)=\frac{c}{\phi^{+}(\vec{r},E)}$$

$$\hat{q}(\vec{r},E)=\frac{1}{c}q(\vec{r},E)\,\phi^{+}(\vec{r},E)$$

- Run the Monte Carlo

CADIS Implementation

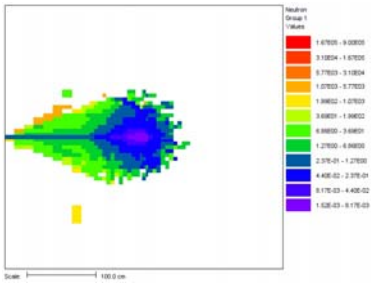
- ADVANTG code system for MCNP
- MAVRIC sequence in SCALE 6

- Both use the new Denovo S_N code for the adjoint
- Both use just the space and energy components

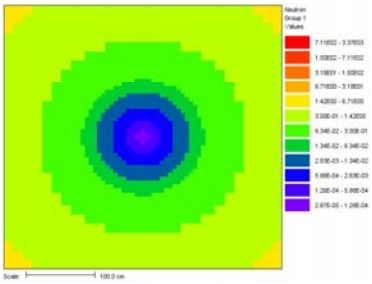
- Used on a variety of problems:
  - Spent fuel casks, Doses in a PWR, Doses in ITER, Doses from nuclear detonation and fallout, CAAS modeling, etc.

Idealized Active Interrogation Problem

- Spherical boat with HEU center



Importance map from MCNP WWG



Importance map from CADIS

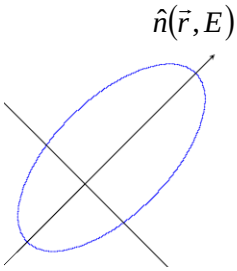
- Space/energy CADIS finds the importance for a particle going in *any* direction, not a *specific* direction

Direction in the Importance Map

- Using every quadrature direction:
  - Very large importance map $\propto I \times J \times K \times G \times \left(S^2 + 2S\right)$
  - Need to interpolate between quadrature directions
- AVATAR P_1 Approximation (Van Riper et al, 1997)
  - Assume adjoint flux is separable in angle and symmetric about the average adjoint current direction

$$\psi^+(\vec{r}, E, \hat{\Omega}) \cong \phi^+(\vec{r}, E)\, f(\hat{\Omega} \cdot \hat{n})$$

$$f(\mu) = \frac{\lambda e^{\lambda\mu}}{2\sinh(\lambda)}$$

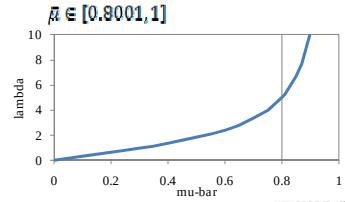


Direction in the Importance Map

- Angular distribution
  - direction of the adjoint current $$\hat{n}(\vec{r},E) = \frac{\vec{J}(\vec{r},E)}{\|\vec{J}(\vec{r},E)\|}$$
  - average cosine of flux about the adjoint direction is the ratio of the adjoint current to the scalar adjoint flux $$\bar{\mu}(\vec{r},E) = \frac{\|\vec{J}(\vec{r},E)\|}{\phi^{+}(\vec{r},E)}$$
  - information theory and the maximum entropy

$$\lambda = \begin{cases} \dfrac{2.99821\bar{\mu} - 2.2669248\bar{\mu}^2}{1 - 0.769332\bar{\mu} - 0.519928\bar{\mu}^2 + 0.2691594\bar{\mu}^3} & \bar{\mu} \in [0, 0.8001) \\ \dfrac{1}{1-\bar{\mu}} & \bar{\mu} \in [0.8001, 1] \end{cases}$$

$$f(\mu) = \frac{\lambda e^{\lambda\mu}}{2\sinh(\lambda)}$$



Space/Energy/Angle CADIS

- Use a similar approximation for angle as AVATAR

$$\psi^{+}(\vec{r},E,\hat{\Omega}) \cong \phi^{+}(\vec{r},E)\ \frac{1}{2\pi} f(\hat{\Omega}\cdot\hat{n})$$

- Assume true source is $q(\vec{r},E,\hat{\Omega}) = q(\vec{r},E)\ \frac{1}{2\pi} q(\hat{\Omega}\cdot\hat{d})$
- Create weight window target values inversely proportional to the approximation of adjoint flux

$$\bar{w}(\vec{r},E,\hat{\Omega}) = \frac{2\pi\, k}{\phi^{+}(\vec{r},E)\ f(\hat{\Omega}\cdot\hat{n})}$$

- Develop a consistent biased source

Space/Energy/Angle CADIS

- Method 1 – biased source *without* direction biasing

$$\hat{q}(\vec{r},E,\hat{\Omega}) = \frac{1}{R}\left[q(\vec{r},E)\ \frac{1}{2\pi}q(\hat{\Omega}\cdot\hat{d})\right]\ \phi^{+}(\vec{r},E)$$

$$R = \iint q(\vec{r},E)\ \phi^{+}(\vec{r},E)\ dE\ dr\ \int \frac{1}{2\pi}q(\hat{\Omega}\cdot\hat{d})\ d\hat{\Omega}$$

- Make map and source consistent at one point $(\vec{r}_0, E_0, \hat{\Omega}_0)$

$$\hat{q}(\vec{r},E,\hat{\Omega}) = \hat{q}(\vec{r},E)\ \frac{1}{2\pi}q(\hat{\Omega}\cdot\hat{d})$$

$$\overline{w}(\vec{r},E,\hat{\Omega}) = \overline{w}(\vec{r},E)\frac{f\left(\hat{\Omega}_0\cdot\hat{n}(\vec{r}_0,E_0)\right)}{f\left(\hat{\Omega}\cdot\hat{n}\right)}$$

Space/Energy/Angle CADIS

- Method 2 – biased source *with* direction biasing

$$\hat{q}(\vec{r},E,\hat{\Omega}) = \left[\frac{1}{R}q(\vec{r},E)\ \phi^{+}(\vec{r},E)\right]\times\left[\frac{1}{c}\frac{1}{2\pi}q(\hat{\Omega}\cdot\hat{d})\frac{1}{2\pi}\ f(\hat{\Omega}\cdot\hat{n}_0)\right]$$

$$c = \int \frac{1}{2\pi}q(\hat{\Omega}\cdot\hat{d})\frac{1}{2\pi}\ f(\hat{\Omega}\cdot\hat{n}_0)\ d\hat{\Omega}$$

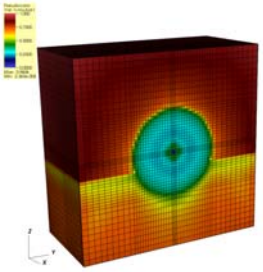
- Make map and source consistent at one point $(\vec{r}_0, E_0, \hat{\Omega}_0)$

$$\hat{q}(\vec{r},E,\hat{\Omega}) = \hat{q}(\vec{r},E)\ \frac{1}{c}\ \frac{1}{2\pi}q(\hat{\Omega}\cdot\hat{d})\ \frac{1}{2\pi}f(\hat{\Omega}\cdot\hat{n}_0)$$

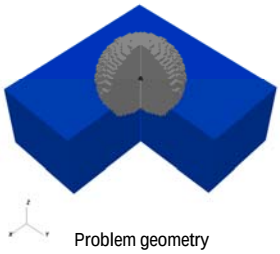
$$\overline{w}(\vec{r},E,\hat{\Omega}) = \overline{w}(\vec{r},E)\frac{2\pi c}{f(\hat{\Omega}\cdot\hat{n})}$$

Spherical Boat Test Problem (ADVANTG)

- Homogenized "boat" (steel, aluminum, PVC, etc.) holding a 19.64 kg sphere of 93% enriched uranium
- 14.1 MeV neutron interrogation source collimated into a 1° (half-angle) beam at 1.05 m distance
- Objective is to estimate fission rate in the HEU sphere
- Denovo adjoint calculation: 132,651 cells, 27 groups, S_8/P_3 in 15 - 17 minutes
- Angular CADIS is 10.2x faster than no WW and 2.3x faster than isotropic CADIS (based on FOM)



$\vec{\phi}$ in group 1

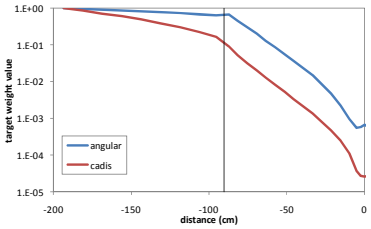


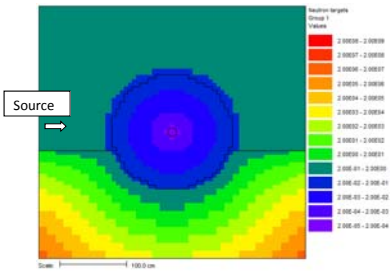
Problem geometry

	No WW	Isotropic CADIS	Angular CADIS
run time (min)	30.0	30.0 (45.28)[1]	30.0 (46.50)
# particles	3,779,173	30,663	469,840
mean	1.4367E-05	1.4810E-05	1.4872E-05
rel. uncertainty	1.81%	0.70%	0.46%
VOV	0.0031	0.0002	0.0001
PDF slope	10.0	10.0	10.0
FOM (1/min)	102	680 (451)	1,575 (1,039)

[1] Values in () include Denovo run time

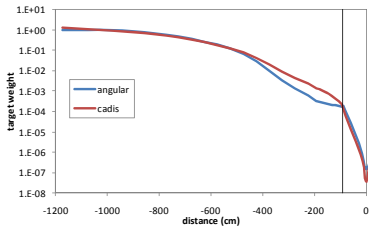
Spherical Boat Test Problem

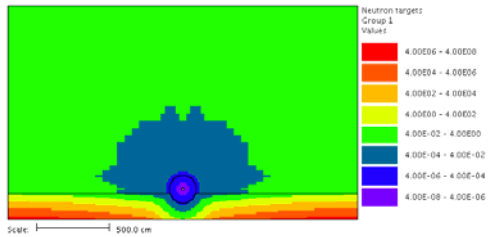




method	Time (min) S_N	Time (min) MC	Fission rate /sec	Fission rate rel unc	MC FOM (/min)
analog		724	2.61E+26	0.50%	54.7
standard CADIS	12	121	2.60E+26	0.43%	445
angular CADIS (1)	13	128	2.59E+26	0.27%	1060

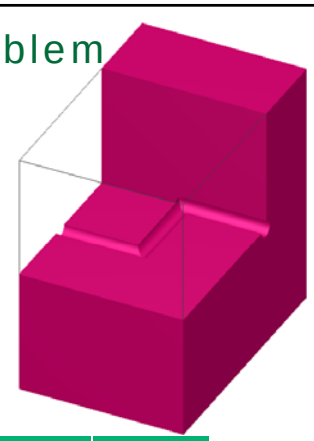
Sph. Boat Test with a Distance Source





method	Time (min) S_N	Time (min) MC	Fission rate /sec	Fission rate rel unc	MC FOM (/min)
analog		607	1.55E+26	0.61%	44.5
standard CADIS	48	125	1.44E+26	5.87%	2.3
angular CADIS (1)	50	91	1.51E+26	3.62%	8.4

Simple Duct Streaming Problem



- Source: Watt spectrum, isotropic
- Find dose rate at exit

- Angular biasing of source:

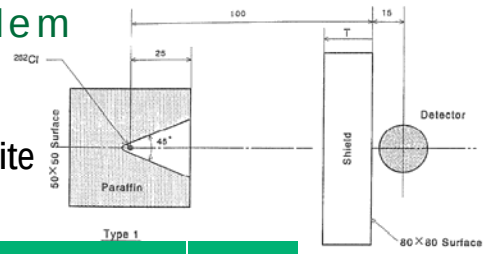
$\lambda = 2.1$

$$\hat{q}(\hat{\Omega} \cdot \hat{d}) = \frac{\lambda e^{\lambda \mu}}{4\pi \sinh(\lambda)}$$

method	Time (min) S_N	Time (min) MC	Dose rate rem/hr	Dose rate rel unc	MC FOM (/min)
analog		1080	4.65E-14	16.5%	0.0341
standard CADIS	10	1080	5.04E-14	0.9%	12.6
angular CADIS (1)	10	1080	5.02E-14	0.6%	25.5

Ueki Shielding Problem

- Source: ^{252}Cf, isotropic
- Find dose rate behind graphite



20 cm

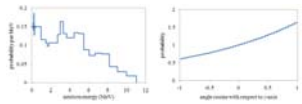
method	Time (min) S_N	Time (min) MC	Dose rate rem/hr	Dose rate rel unc	MC FOM (/min)
analog		600	1.50E-02	0.7%	35.8
standard CADIS	0.2	60	1.49E-02	0.3%	1740
angular CADIS (1)	0.25	60	1.49E-02	0.4%	3160
angular CADIS (2)	0.25	60	1.49E-02	0.2%	4370

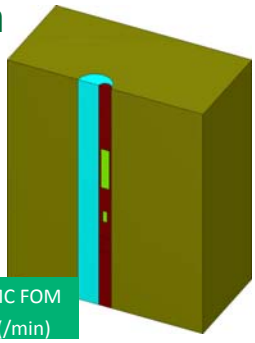
35 cm

method	Time (min) S_N	Time (min) MC	Dose rate rem/hr	Dose rate rel unc	MC FOM (/min)
analog		1080	4.65E-14	16.5%	0.0341
standard CADIS	10	1080	5.04E-14	0.9%	12.6
angular CADIS (1)	10	1080	5.02E-14	0.6%	25.5

Neutron Well-Logging Problem

- Source: neutron, slightly upward peaked
- Two ^{3}He detectors
- Find count rate





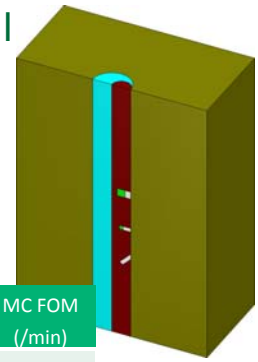
Near

method	Time (min) S_N	Time (min) MC	Dose rate rem/hr	Dose rate rel unc	MC FOM (/min)
standard CADIS	19	61	6.66E+08	0.30%	1860
angular CADIS (1)	23	64	6.67E+08	0.31%	1670
angular CADIS (2)	23	63	6.69E+08	0.31%	1700

Far

method	Time (min) S_N	Time (min) MC	Dose rate rem/hr	Dose rate rel unc	MC FOM (/min)
standard CADIS	20	121	1.51E+08	0.34%	710
angular CADIS (1)	27	120	1.51E+08	0.35%	691
angular CADIS (2)	27	120	1.50E+08	0.34%	702

Gamma-Ray Lithodensity Tool



- Source: ^{137}Cs
- Two NaI detectors
- Find total photon flux

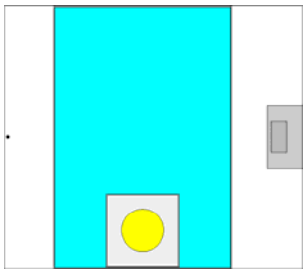
Near

method	Time (min) S_N	Time (min) MC	Total Flux /cm s²	Total Flux rel unc	MC FOM (/min)
standard CADIS	15	60	1.62E+03	0.72%	317
angular CADIS (1)	15	60	1.58E+03	1.34%	93
angular CADIS (2)	15	60	1.62E+03	1.56%	68

Far

method	Time (min) S_N	Time (min) MC	Total Flux /cm s²	Total Flux rel unc	MC FOM (/min)
standard CADIS	15	120	5.90E+01	0.40%	523
angular CADIS (1)	15	120	5.90E+01	0.30%	939
angular CADIS (2)	15	120	5.92E+01	0.27%	1120

Active Int. Barrel Problem



- Source: D-T neutrons, isotropic
- Detector: ^{3}He
  - Step 1: Find fission rate in HEU
  - Step 2: Find total detector response

Step 1

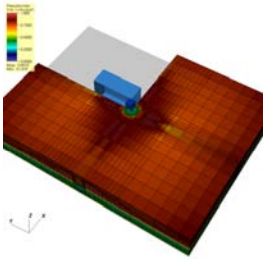
method	Time (min) S_N	Time (min) MC	Fission rate /sec	Fission rate rel unc	MC FOM (/min)
standard CADIS	2.8	61	4.22E+07	0.94%	189
angular CADIS (1)	2.7	61	4.17E+07	0.54%	566
angular CADIS (2)	2.9	61	4.18E+07	0.51%	626

Step 2

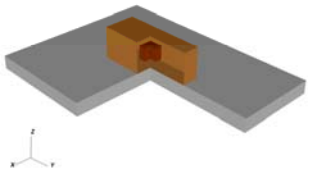
method	Time (min) S_N	Time (min) MC	Count rate rem/hr	Count rate rel unc	MC FOM (/min)
standard CADIS	3.6	121	7.76E+03	0.56%	260
angular CADIS (1)	3.7	120	7.75E+03	0.40%	511
angular CADIS (2)	3.8	121	7.76E+03	0.43%	447

Cargo Container A Problem (ADVANTG)

- Cargo container holding 1 m cube of polyethylene containing a 10 kg sphere of 95% enriched uranium
- 14.1 MeV neutron interrogation source collimated into a 5° (half-angle) beam at 20 cm distance
- Objective is to estimate fission rate in the HEU sphere
- Denovo adjoint calculation: 38,976 cells, 27 groups, S_8/P_3 in 8 - 9 minutes
- Angular CADIS is 3.6x faster than no WW and 3.2x faster than isotropic CADIS



$\vec{\Omega}$ in group 1



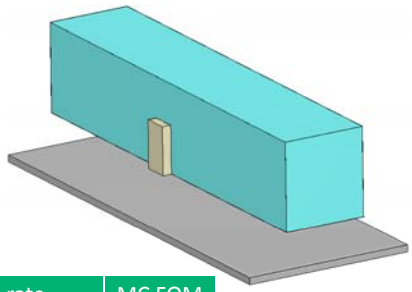
Problem geometry

	No WW	Isotropic CADIS	Angular CADIS
run time (min)	30.0	30.0 (38.63)[1]	30.0 (38.69)
# particles	3,262,156	6,555	82,070
mean	7.5223E-05	7.4956E-05	7.4788E-05
rel. uncertainty	1.16%	0.96%	0.54%
VOV	0.0009	0.0010	0.0002
PDF slope	10.0	10.0	10.0
FOM (1/min)	248	382 (281)	1,143 (886)

[1] Values in () include Denovo run time

Cargo Container B

- Source: D-D neutrons
- Detector: HP-Ge



No HEU

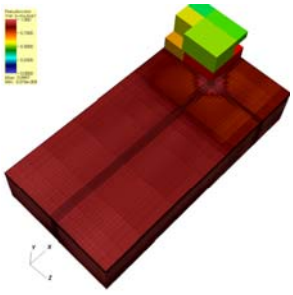
method	Time (min) S_N	Time (min) MC	Count rate rem/hr	Count rate rel unc	MC FOM (/min)
analog		961	8.49E+04	7.9%	0.17
standard CADIS	76	848	9.74E+04	1.3%	6.8
angular CADIS (2)	78	842	9.83E+04	0.7%	22.2

With HEU

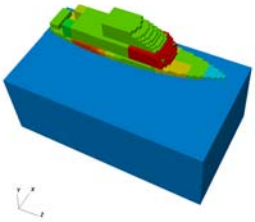
method	Time (min) S_N	Time (min) MC	Count rate rem/hr	Count rate rel unc	MC FOM (/min)
fis rate - CADIS	86	61	7.30E+07	0.5%	750
fis rate - ang. (2)	85	61	7.26E+07	0.4%	870
resp - CADIS	95	722	2.84E+03	1.0%	14.3
resp - angular (2)	104	725	2.85E+03	0.6%	39.6

Yacht Problem (ADVANTG)

- Yacht (32 m long, 7 m wide) holding a 25 kg sphere of 93% enriched uranium
- Bremstrahhlung source (from 25 MeV electrons) collimated into a 0.3° (half-angle) beam at 13.34 m distance
- Objective is to estimate photon flux in the HEU sphere
- Denovo adjoint calculation (on a reduced model): 167,904 cells, 19 groups, S_8/P_3 in 4 - 5 minutes
- Angular CADIS performs better than isotropic CADIS, but rather poorly overall



$\vec{\mu}$ in group 1



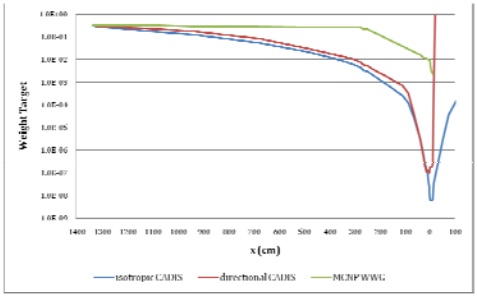
Problem geometry

	No WW	Isotropic CADIS	Angular CADIS
run time (min)	30.0	30.0 (34.02)[1]	30.0 (34.29)
# particles	63,742,673	151	1,470
mean	2.2835E-05	2.1330E-05	2.3164E-05
rel. uncertainty	0.14%	8.35%	2.66%
VOV	0.0000	0.0105	0.0016
PDF slope	10.0	0.0	7.9
FOM (1/min)	17,007	5 (4)	47 (41)

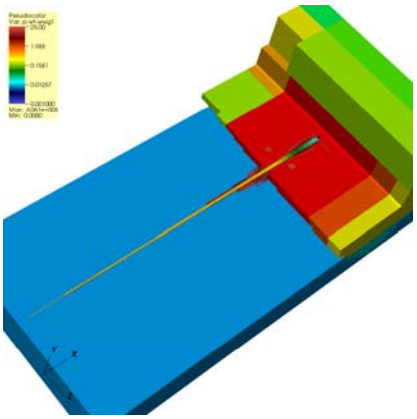
[1] Values in () include Denovo run time

Yacht Problem

- MCNP WWG targets vary over about 2 orders of magnitude; Angular CADIS targets vary by 6 – 8
- MCNP targets are computed as expected score of forward histories (average over histories that actually occur)
- ADVANTG targets are computed from deterministic scalar adjoint fluxes (average over all paths through a cell)



Group 1 weight targets along beam axis



MCNP WWG group 1 weight targets from 8,000 minute simulation

Improvement over Space/Energy

Problem	Code	Method 1: Without Source Dir. Bias	Method 2: With Source Dir. Bias
Spherical boat test problem, source at 2 m	ADVANTG	2.3	
Spherical boat test problem, source at 2 m	MAVRIC	2.4	
Spherical boat test problem, source at 10 m	MAVRIC	3.6	
Simple duct streaming problem	MAVRIC		2
Ueki shielding problem, 20 cm C	MAVRIC	1.5 – 2.2	2.5
Ueki shielding problem, 35 cm C	MAVRIC		2.1 – 2.6
Neutron porosity tool, near detector	MAVRIC	0.9	0.9
Neutron porosity tool, far detector	MAVRIC	0.97	0.99
Gamma-ray litho-density tool, near detector	MAVRIC	0.15	0.09
Gamma-ray litho-density tool, far detector	MAVRIC	1.6	2
Interrogation of barrel, step 1	MAVRIC	3	3.3
Interrogation of barrel, step 2	MAVRIC	2	1.7
Cargo container A	ADVANTG	3.2	
Cargo container B, active background	MAVRIC		3.3
Cargo container B, determine fission source	MAVRIC		1.2
Cargo container B, total response	MAVRIC		3.1
Cargo container B, fission-only response	MAVRIC		2.8
Yacht problem	ADVANTG	9	

Summary

- Angular CADIS does provide significant speed-up over standard CADIS for many common problems.
- The approximation used here is essentially a P_1 approximation to the true angular importance function. It may not be sufficient for problems with more peaked angular fluxes.
- Difficult to say *a priori* which problems will benefit from angular biasing.

Future Work

- Using S_N methods to compute what the WWG computes may be the best approach – fast, each voxel in imp map represents the importance for particles that will travel through that voxel.

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