Automatic Mesh Adaptivity for Hybrid Monte Carlo/Deterministic Neutronics Modeling of Difficult Shielding Problems

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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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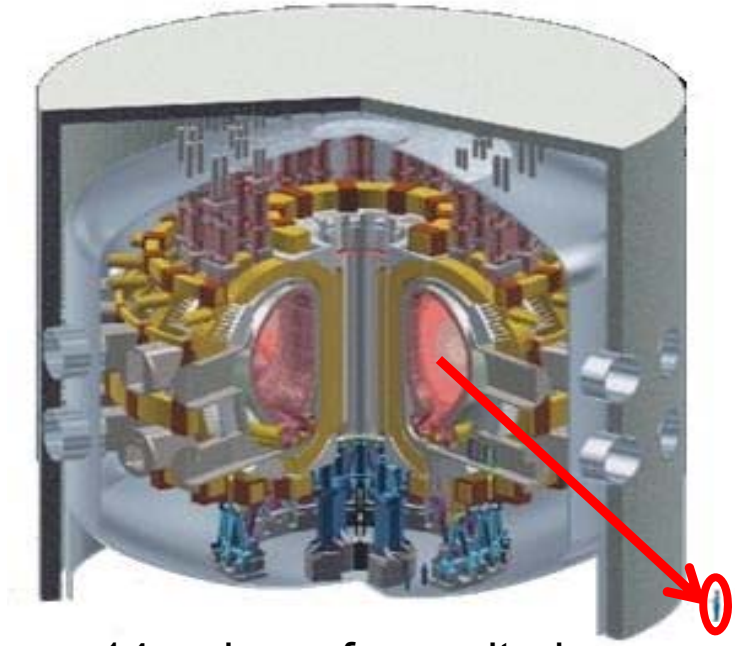
Overview

- Necessity of full-scale simulations
- ADVANTG
- Automatic mesh adaptivity
  - Macromaterials
  - Deterministic mesh refinement
  - Weight-window coarsening
- ITER prompt dose rate

Full-scale simulations

- **Optimizing design and reducing cost critical for ITER**
- **Minimizing approximations by adding more details**
- **Enabling full 3-D simulations through better computers and better modeling methods**



14 orders of magnitude prompt dose rate attenuation

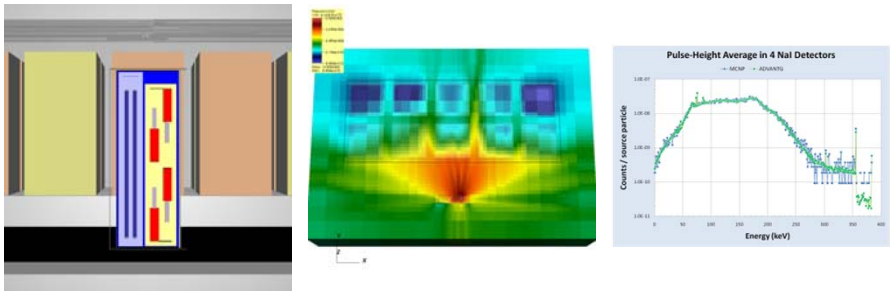
	Dose (μSv/hr)	Relative uncertainty (*R*)	Time (day)	Speed up
MC(no CADIS)	4.8	76.7%	610.0	1
MC (CADIS)	2.7	3.8%	8.6	29,000

→ Requires 393 years to reach *R* =5%

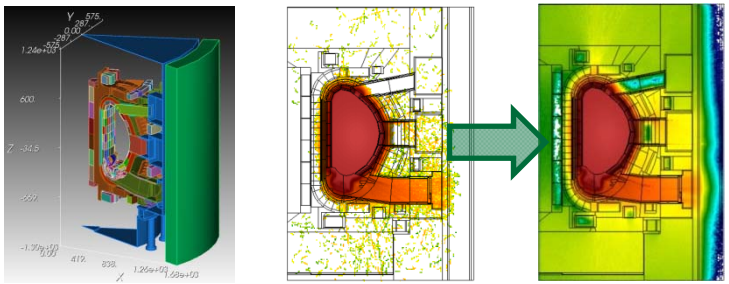
Nearly impossible without hybrid

ADVANTG (AutomateD VAriaNce reducTion Generator)

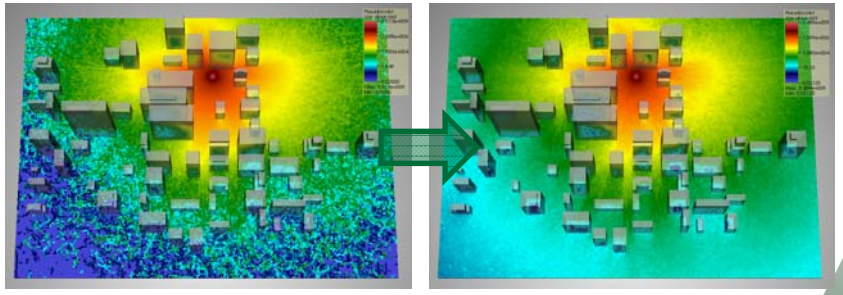
- **Generates variance reduction parameters for continuous-energy MCNP5 simulations**
- **Implements the CADIS method for accelerating single-tally estimates**
- **Implements FW-CADIS for obtaining relatively uniform uncertainties across:**
  - multiple tally cells (e.g., multiple detectors)
  - mesh tallies (over part or all of the problem)
- **Is compatible with:**
  - all MCNP geometry features
  - F1 (surface-average current), F2 (surface-average flux), F4 (cell-average flux), F6 (cell-average energy-deposition), and F8 (cell-average pulse-height) tallies, with or without tally multipliers
- **Outputs biasing parameters in a format directly readable by unmodified MCNP installations**
- **Outputs material map, fluxes, and weights in Silo-format for visualization using VisIt**



Pulse-height spectrum in portal NaI detectors



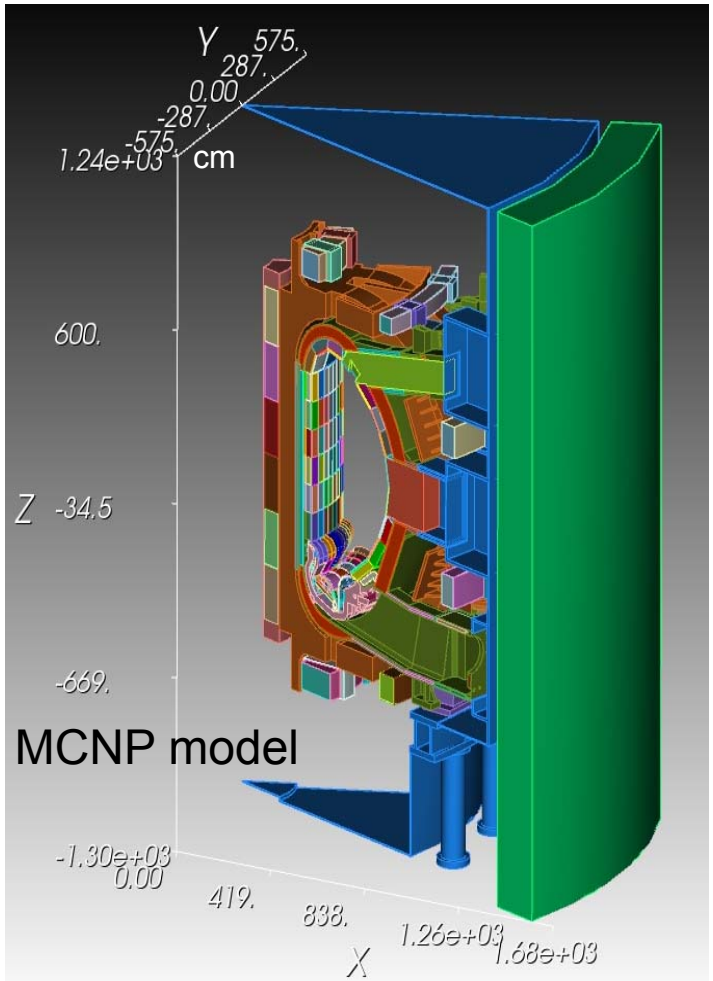
Neutron fluxes throughout ITER facility



Prompt dose rates throughout Times Square

Will be released through RSICC before tutorial in summer meeting

ADVANTG solves very difficult problems



Geometry mapping

Very complicated geometry

Denovo

Flux processing

WW (Multiple GB) and source biasing

MCNP

But needs some improvements

Automatic adaptivity

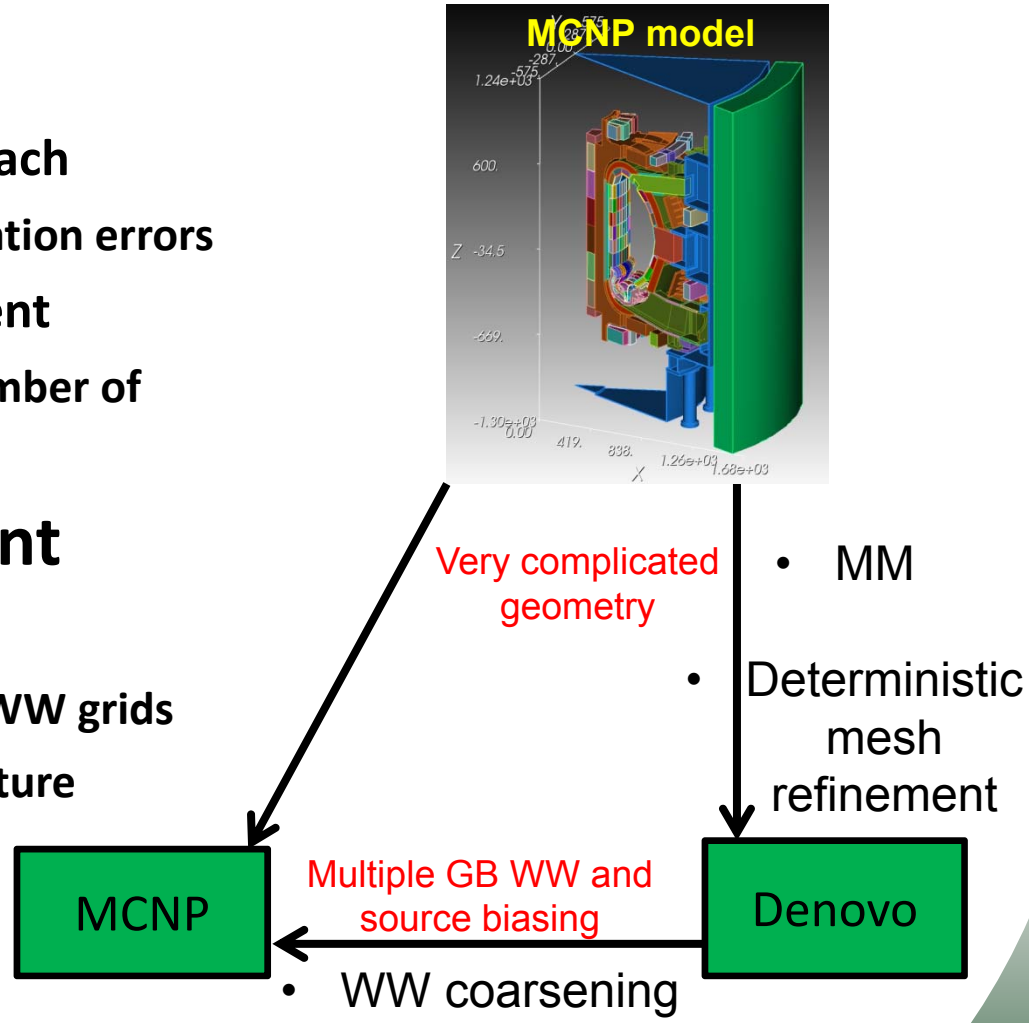
1. Improve mesh

- Macromaterials (MM) approach
  - Decrease geometry discretization errors
- Deterministic mesh refinement
  - Efficient mesh with same number of cells

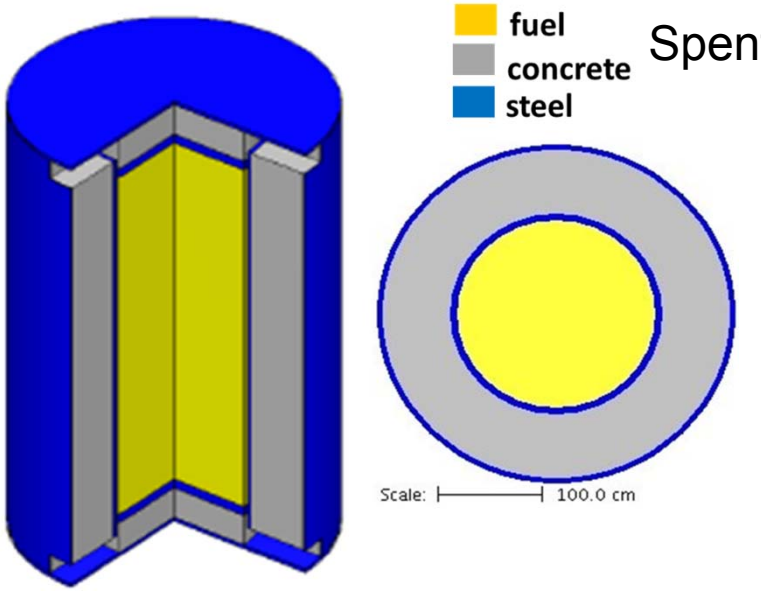
2. Allow more refinement

- WW coarsening
  - Decouple deterministic and WW grids
  - Small but efficient WW structure

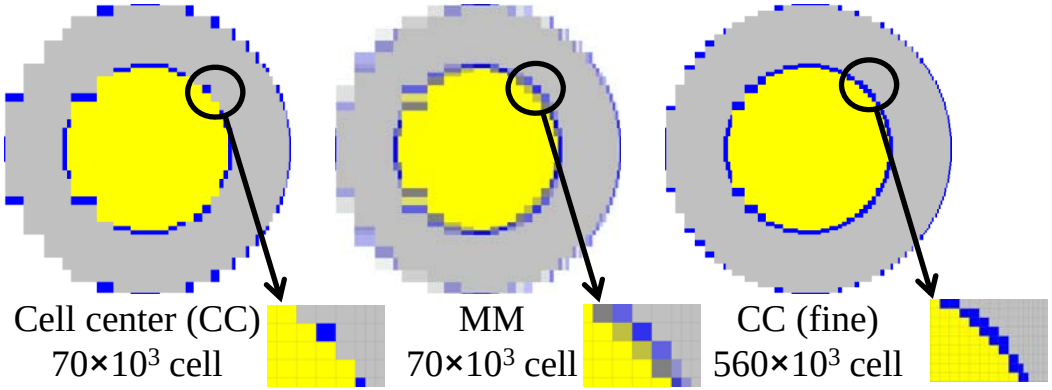
ADVANTG flowchart



More accurate fluxes with macromaterials (MM)



Spent fuel shipping cask



Denovo results

Calculation	Time (min)	Dose Rate (μSv/hr)
CC	7.6	7.2
MM	8.3	5.9
CC (fine)	62.5	3.6

→ Reference

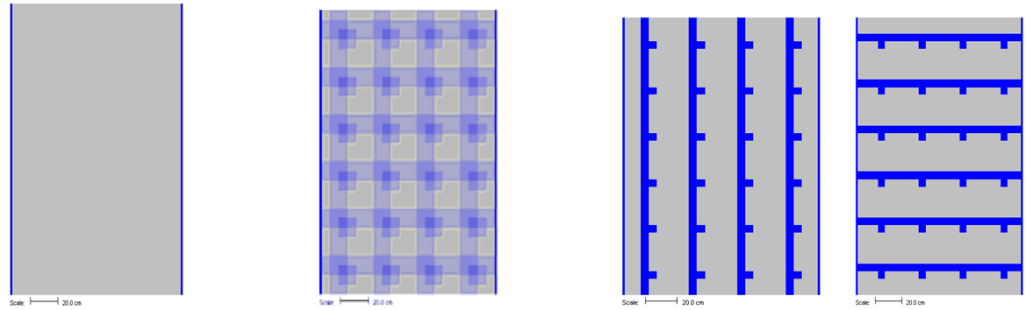
- Better answer with MM
- No time penalty

MM decreases geometry descretization errors

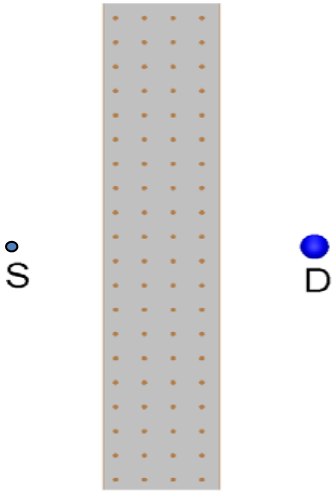
Better figure of merit (FOM) with MM

Concrete shield with steel rebar

Denovo models



CC MM Non uniform grid (CC)



	Denovo time (min)	Dose rate per curie (10^{-5} µSv/hr)/Ci	*R*	Monaco time (min)	Normalized FOM
CC	18.01	2.5	0.3%	185.24	1.00 ±0.8%
MM: 2^3	18.22	2.5	0.2%	185.18	2.08 ±0.6%
MM: 3^3	18.72	2.5	0.2%	183.99	1.77 ±0.6%
MM: 4^3	17.65	2.5	0.2%	187.97	2.00 ±0.6%
MM: 5^3	18.34	2.5	0.2%	181.16	1.94 ±0.6%
Non-uniform grid	17.12	2.5	0.2%	188.03	1.67 ±0.6%

MM increases FOM for free

Deterministic mesh refinement

- **Goal**
  - **Automatically capture geometric details**
- **MM data**
  - **Materials fractions stored in 1-D vector**
- **Heterogeneity parameter**
  - $h_{ijk} = (\sigma_{max} - \sigma_{ijk})V_{ijk}$
    - $\sigma \equiv$ **standard deviation of materials fractions**
    - $\sigma_{max} - \sigma_{ijk}$
      - **Dispersion factor**
    - $V_{ijk} \equiv Volume\ of\ cell\ ijk$

Dispersion factor calculation

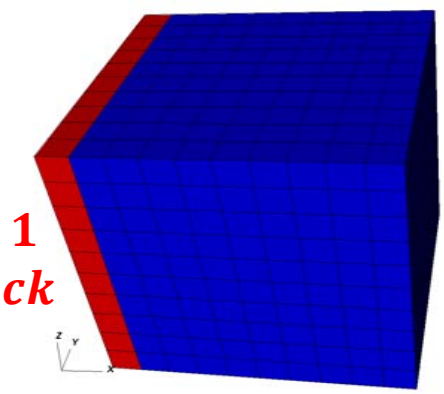
Materials\Cells	Cell 1	Cell 2	Cell 3	Cell 4
vacuum	0.25	0.33	0.50	1.00
Mat 1	0.25	0.33	0.50	0.00
Mat 2	0.25	0.33	0.00	0.00
Mat 3	0.25	0.00	0.00	0.00
σ	0.00	0.17	0.29	0.50
σ_{max}-σ	**0.50**	**0.33**	**0.21**	**0.00**

- Block heterogeneity parameter
  - Denovo only allows continuous mesh

$$H_i = \sum_{jk} h_{ijk}$$

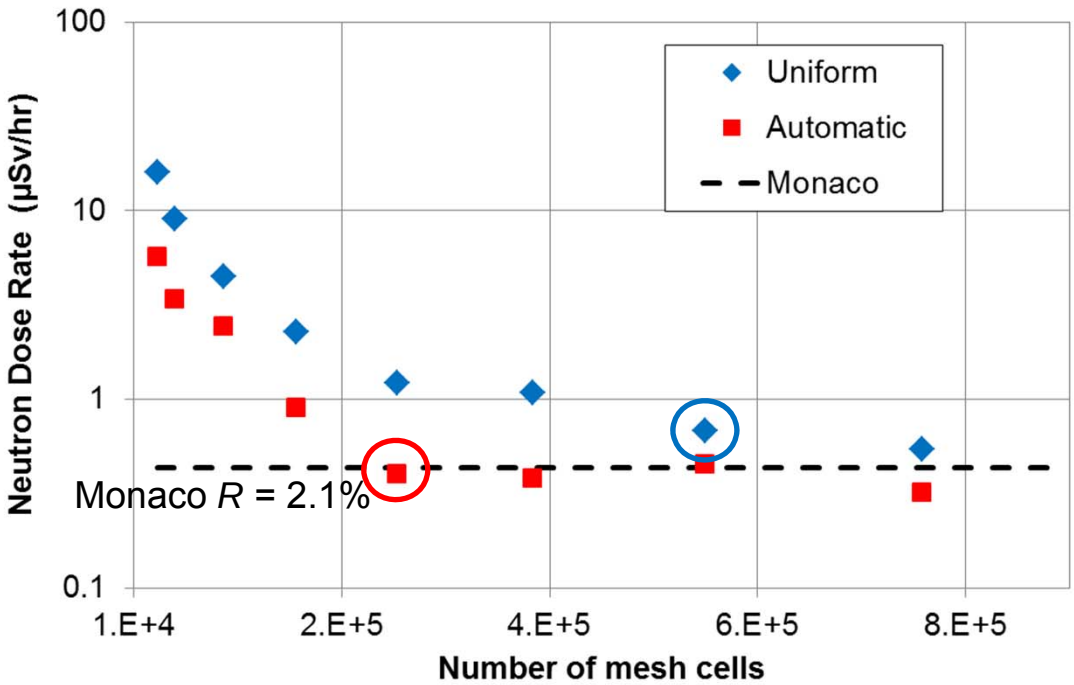
$$H_j = \sum_{ik} h_{ijk}$$

$$H_k = \sum_{ij} h_{ijk}$$

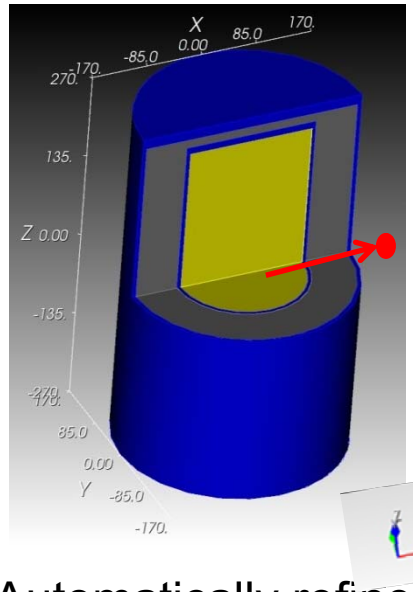


More accurate fluxes with automatic mesh

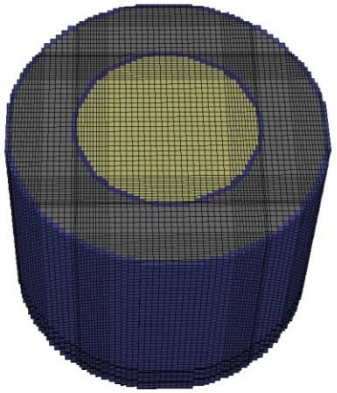
Neutron dose rate outside shipping cask



Shipping cask model



Automatically refined mesh with 7.7×10^5 cell

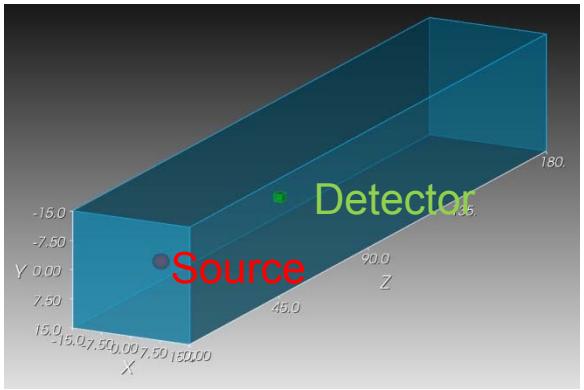


- Denovo starts converging at half number of mesh elements with automatic refinement
- < 27 % difference between Denovo and Monaco (exact geometry) with automatic refinement

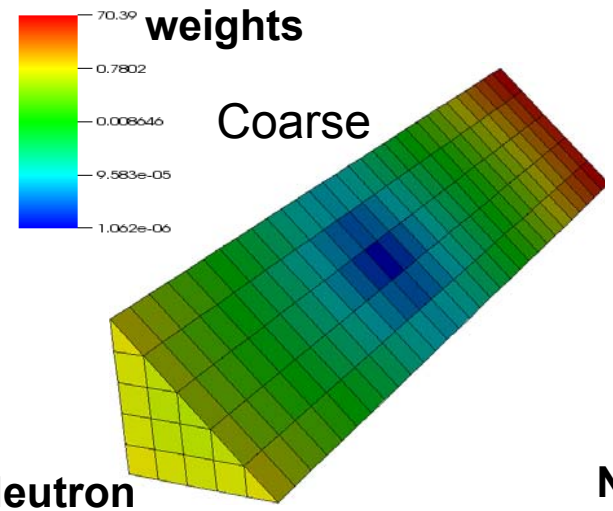
Better (automatic) deterministic models

Weight-window (WW) coarsening reduces size of WWINP without collapsing important regions

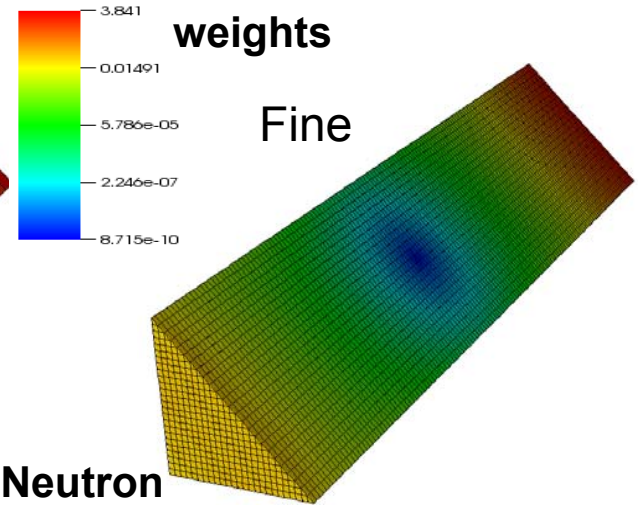
MC model



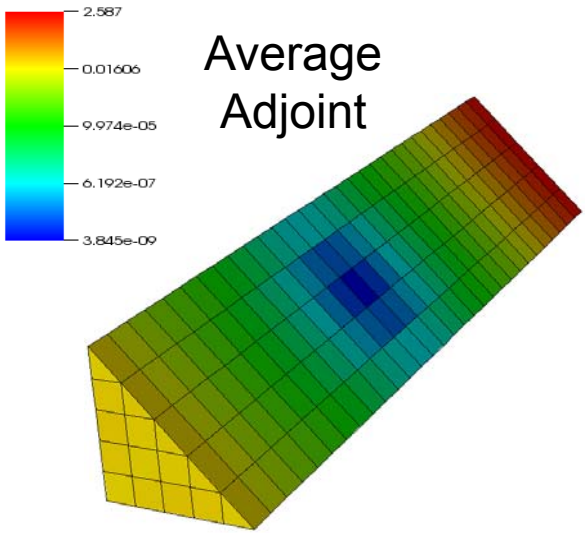
Neutron weights



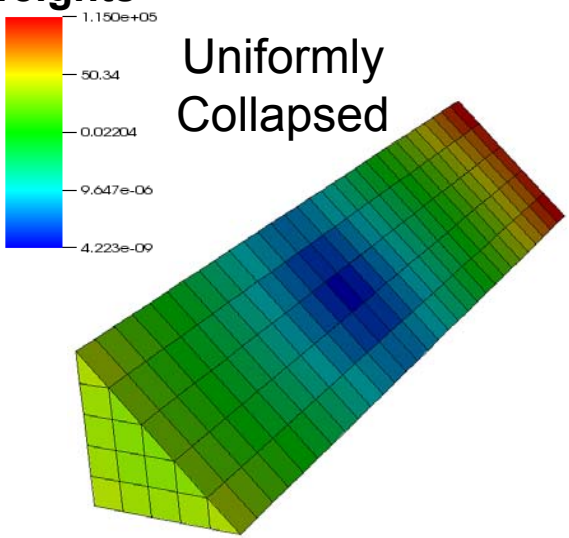
Neutron weights



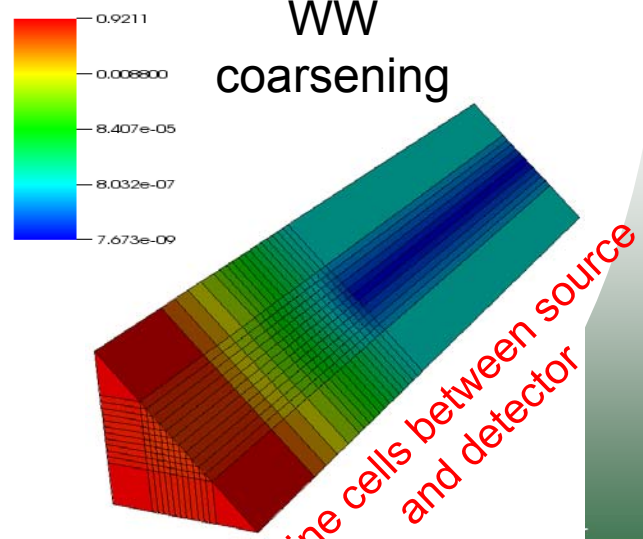
Neutron weights



Neutron weights

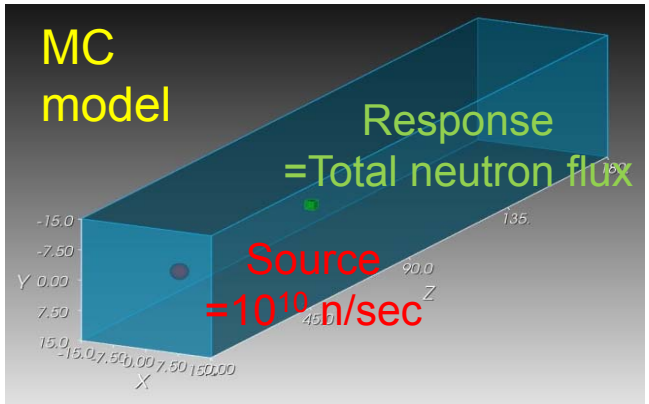


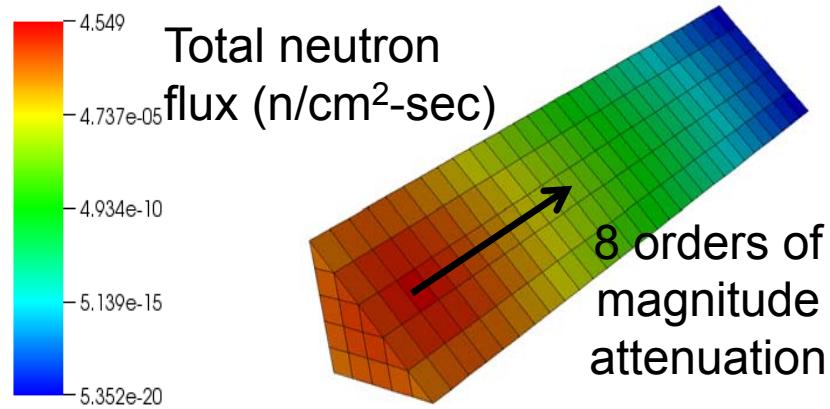
Neutron weights



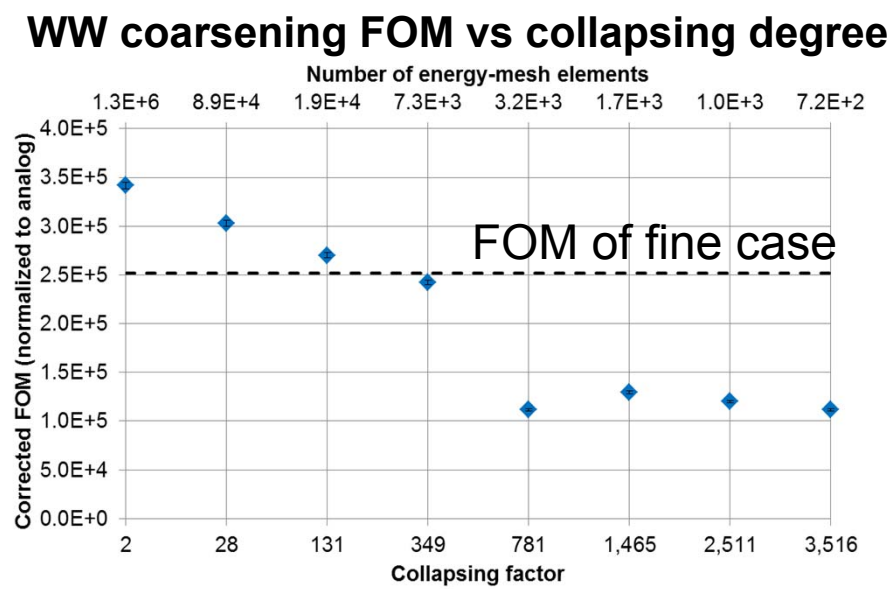
Fine cells between source and detector

Minor (to no) decrease in FOM





Calculation	Number of space-energy cells (Thousands)	Neutron flux (n/cm^2-sec)	Normalized FOM (deterministic correction)
Analog	n/a	16.00 ± 48.56%	1.00 ± 56%
Coarse	20	10.91 ± 1.73%	**3.15E+03** ± 3.2%
Fine	2531	10.85 ± 0.19%	2.52E+05 ± 1.0%
Average	20	10.89 ± 0.21%	2.06E+05 ± 1.0%
Uniform	20	10.88 ± 0.20%	2.19E+05 ± 1.0%
WW coarsening	19	10.90 ± 0.18%	**2.70E+05** ± 1.0%



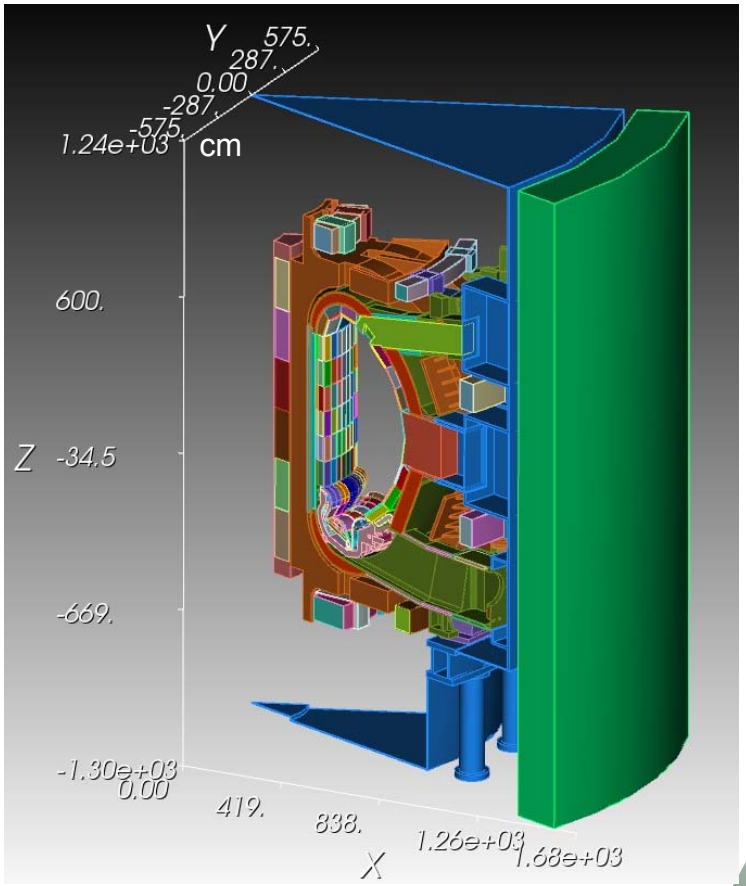
Adaptive collapsing has 86 times higher FOM for fixed map size

WW coarsening enables substantial size reduction

ITER global prompt dose rate calculation

- Necessary for
  - Personnel accessibility
  - Occupational safety
  - Guide possible design changes
- Only analyzed by coupling 1-D with 3-D analyses*
  - Ignore important details
    - Ports effect

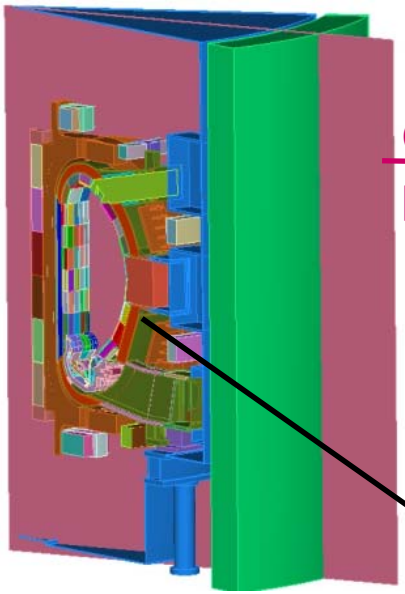
MCNP model



19,945 lines of geometry (cells + surfaces) cards

* ITER-IO Nuclear Analysis Report (2004)

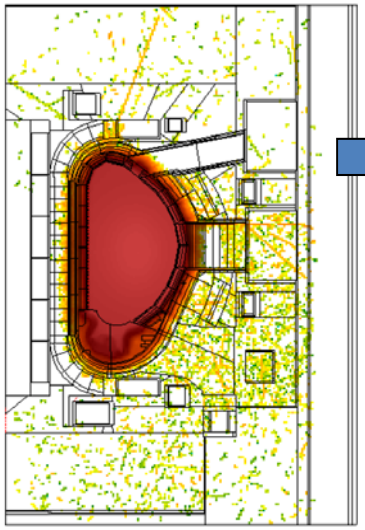
FW-CADIS increases regions with MC answers



Central plane

20° plane

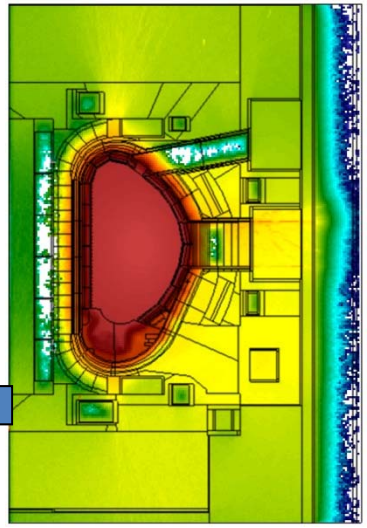
Prompt dose rate maps



10 days analog

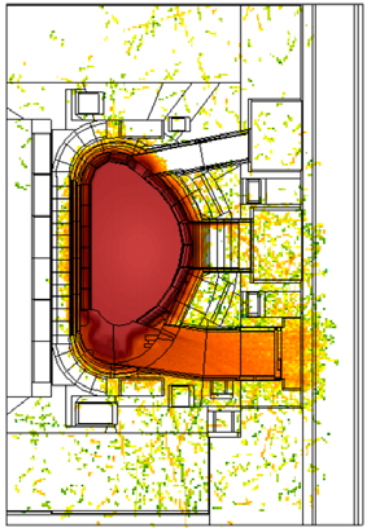
Answers in 25.8%

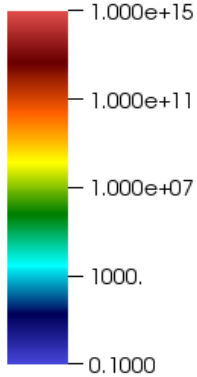
Answers in 95.6%

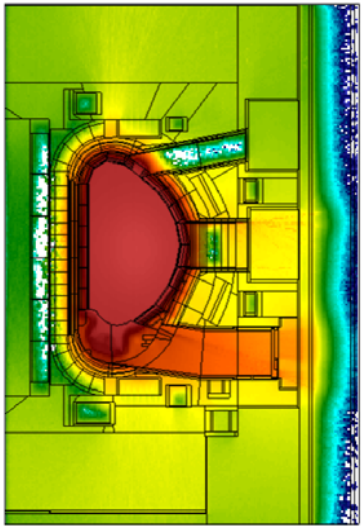


10 days FW-CADIS

Ports plugs in VV

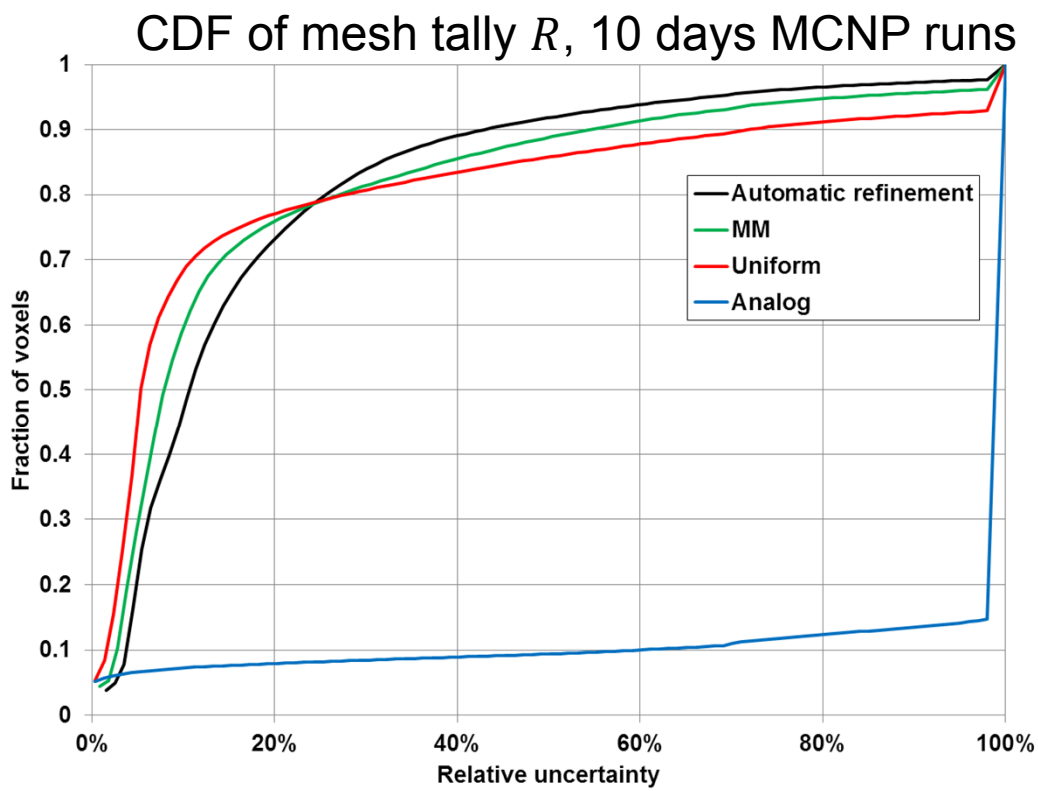






Answers in 2.7 times more regions with FW-CADIS

Effect of MM and deterministic refinement



- All deterministic models
  - 7.9 million cell
  - 67 groups
- WW file
  - 6.5 GB

Time

Case	Time (hr)		
	Initialization	Deterministic	MC
Uniform	0.6	195.2	240.5
MM	16.6	1514.7	240.5
Automatic	14.1	222.6	240.5

FOM (normalized to analog)

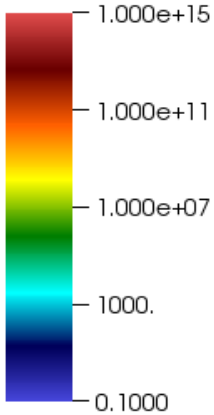
Case	Fraction of nonzero voxels	$\frac{1}{\overline{R^2}T}$
Uniform	95.5%	7.2
MM	97.5%	9.1
Automatic	**98.3%**	**11.1**

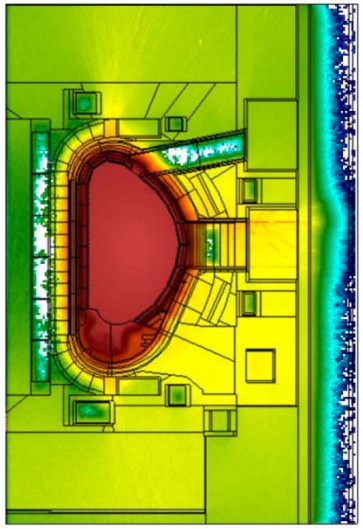
54% increase in MC FOM and (more importantly) 2.8% (74,000 mesh elements) increase in fraction of voxels with MC scores

Where is the 2-3% difference in nonzero voxels?

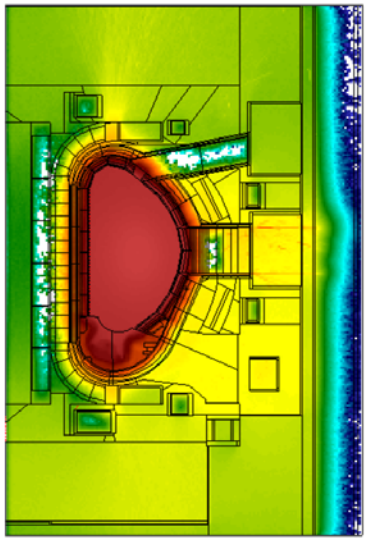
Central plane

Dose rate (μSv/hr)

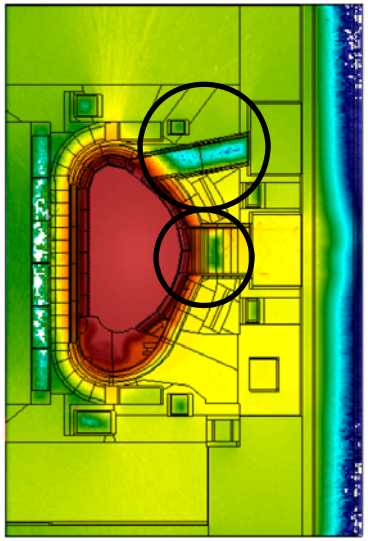




Uniform

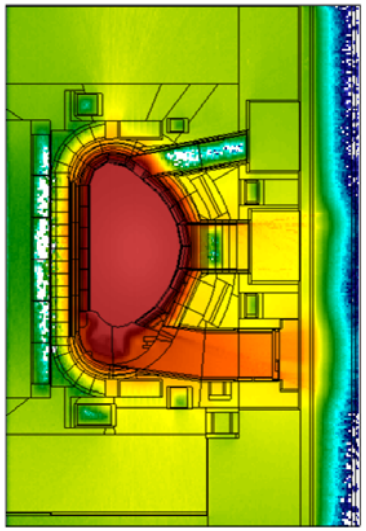


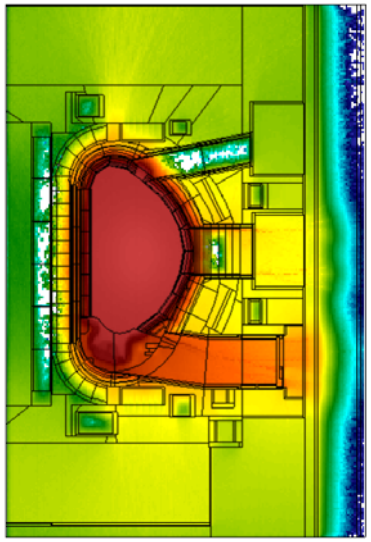
MM

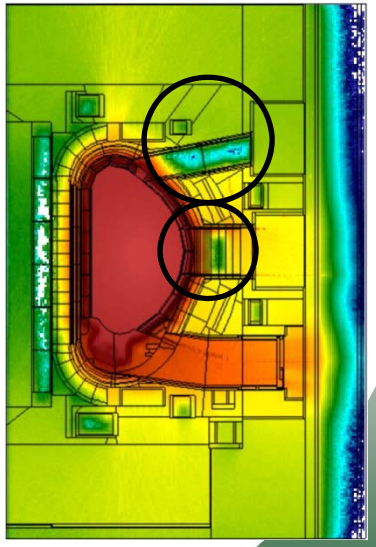


Automatically refined

20° plane



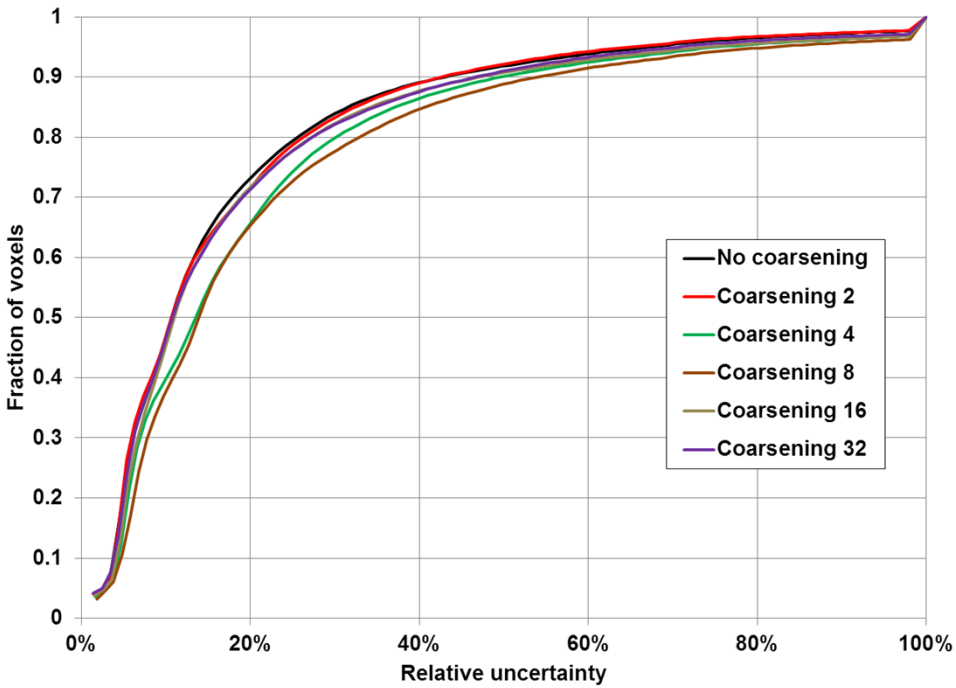




Enhanced efficiency in **difficult** (high attenuating) regions

WW coarsening

CDF of mesh tally R, 10 days MCNP runs



All coarsening times <20 hrs

FOM (normalized to analog)

Case	Size of WW file (GB)	Fraction of nonzero voxels	$\frac{1}{R^2T}$
No coarsening	6.5	98.3%	11.1
Coarsening 2	3.3	98.3%	11.2
Coarsening 4	1.7	97.8%	9.0
Coarsening 8	0.8	97.5%	8.2
Coarsening 16	0.4	97.6%	9.7
Coarsening 32	0.2	97.8%	10.1

↓ Large size reduction

Small FOM decrease

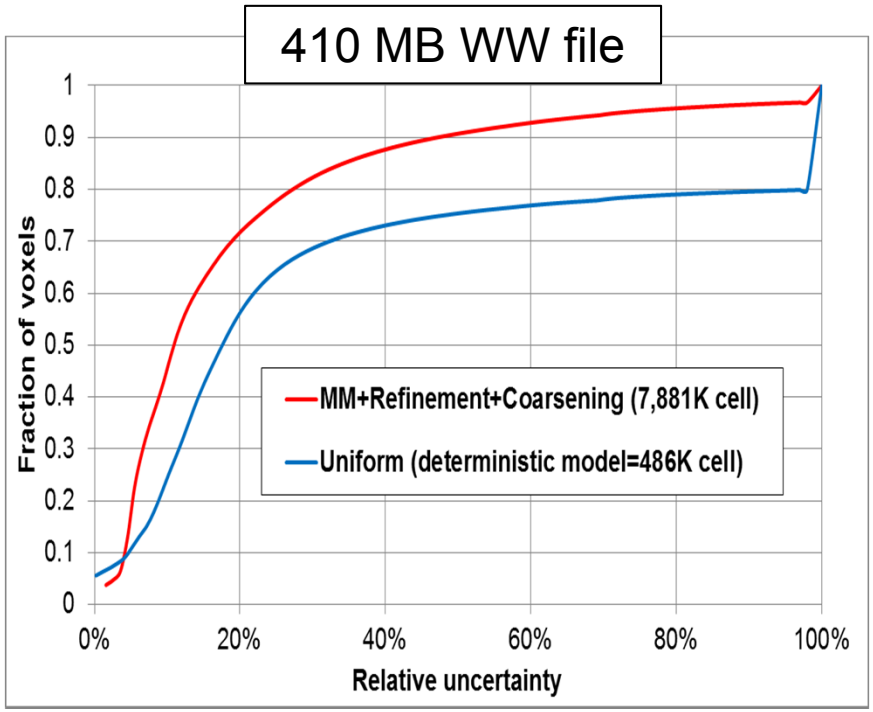
- Large reduction in size
- Small (~0.5%) systematic decrease in nonzero regions and (<10%) in FOM

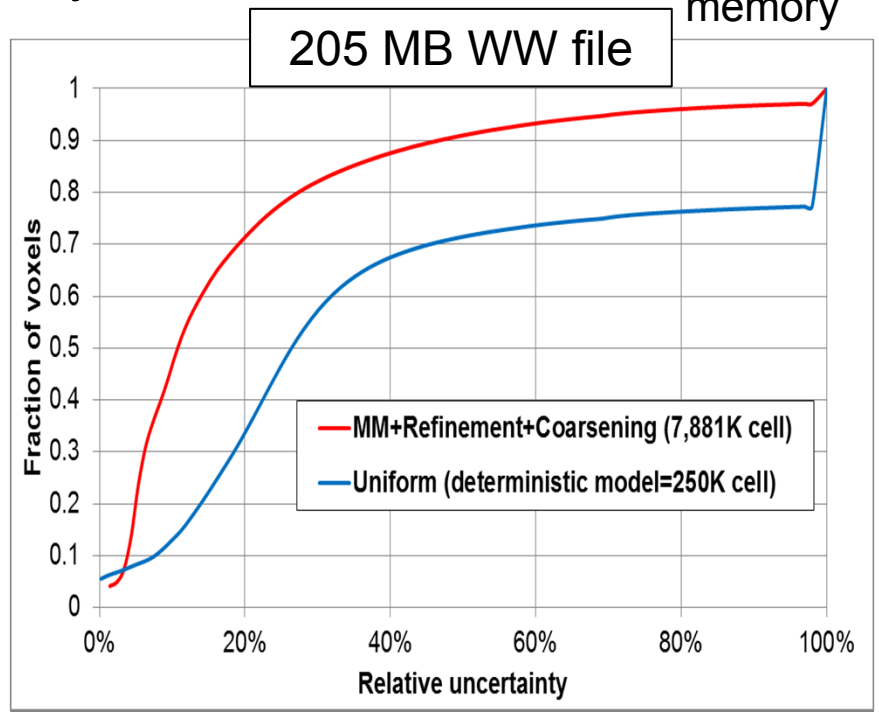
Now we can run 100s of jobs in parallel without worrying about memory

Combined effect (MM+ refinement+ coarsening)

CDF of mesh tally R, 10 days MCNP runs

Small memory



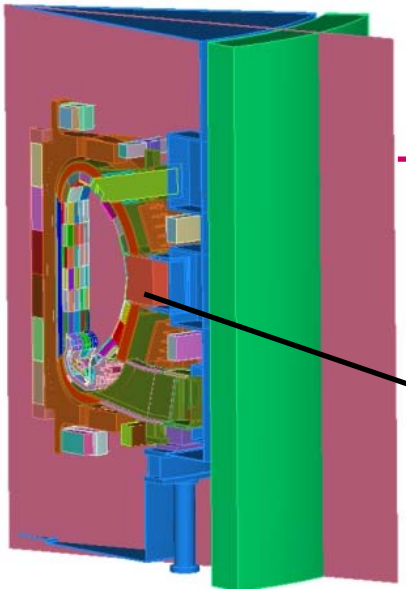


Case	Fraction of nonzero voxels	$\frac{1}{\overline{R^2T}}$
No adaptivity	81.9%	3.5
Adaptivity	97.6%	9.7

Case	Fraction of nonzero voxels	$\frac{1}{\overline{R^2T}}$
No adaptivity	79.3%	3.0
Adaptivity	97.8%	10.1

MC results in 18.5% more elements and **3.4** efficiency increase

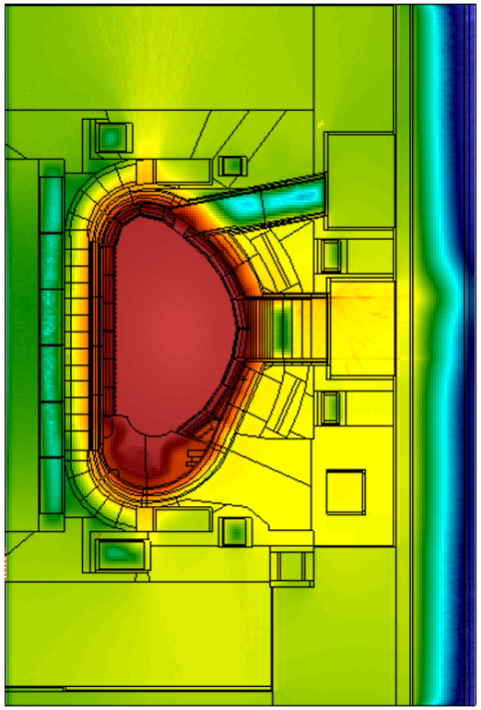
ITER dose rates with new algorithms

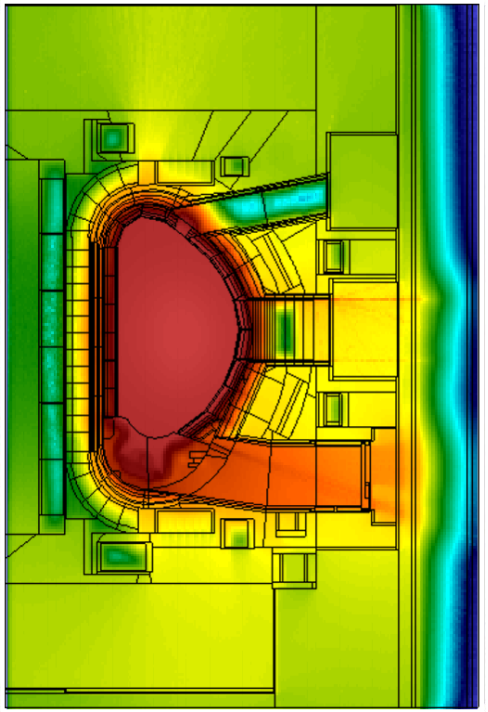


Central plane

20° plane

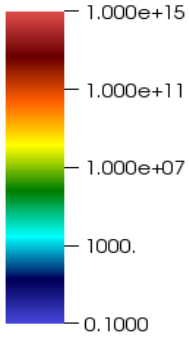
Prompt dose rate maps 2012





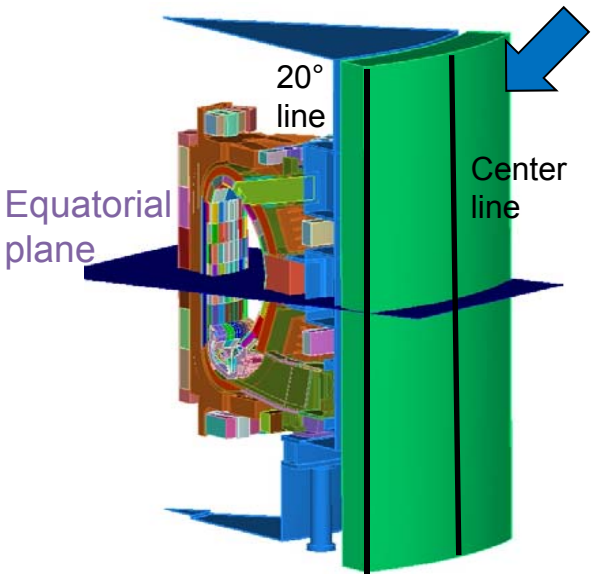
Ports plugs in VV

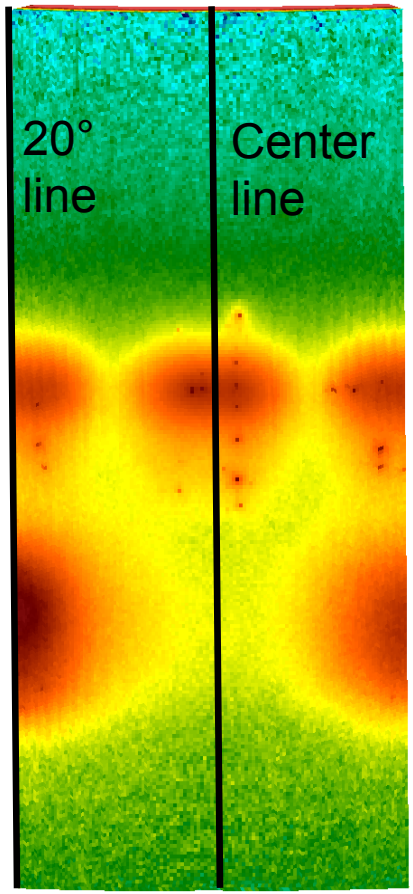
Dose rates µSv/hr

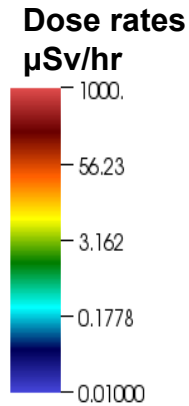


Diagnostics ports are very effective

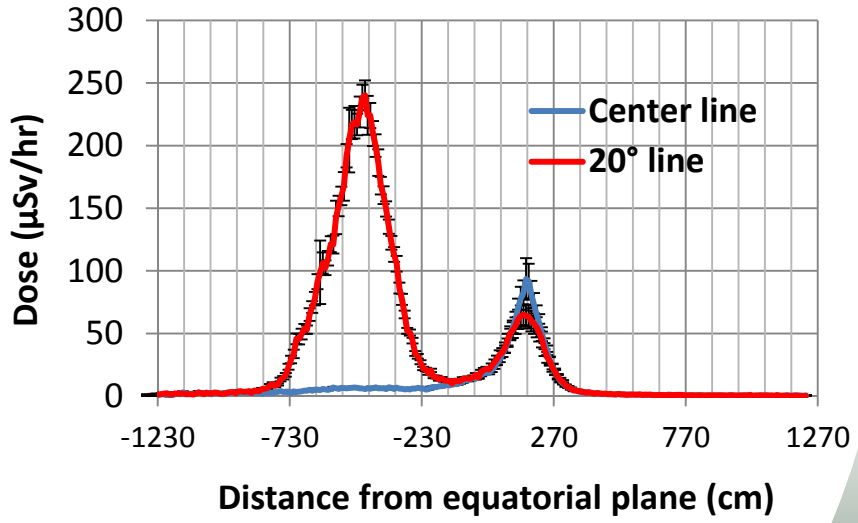
Dose rates at back surface of bioshield







Dose rates along two lines behind bioshield

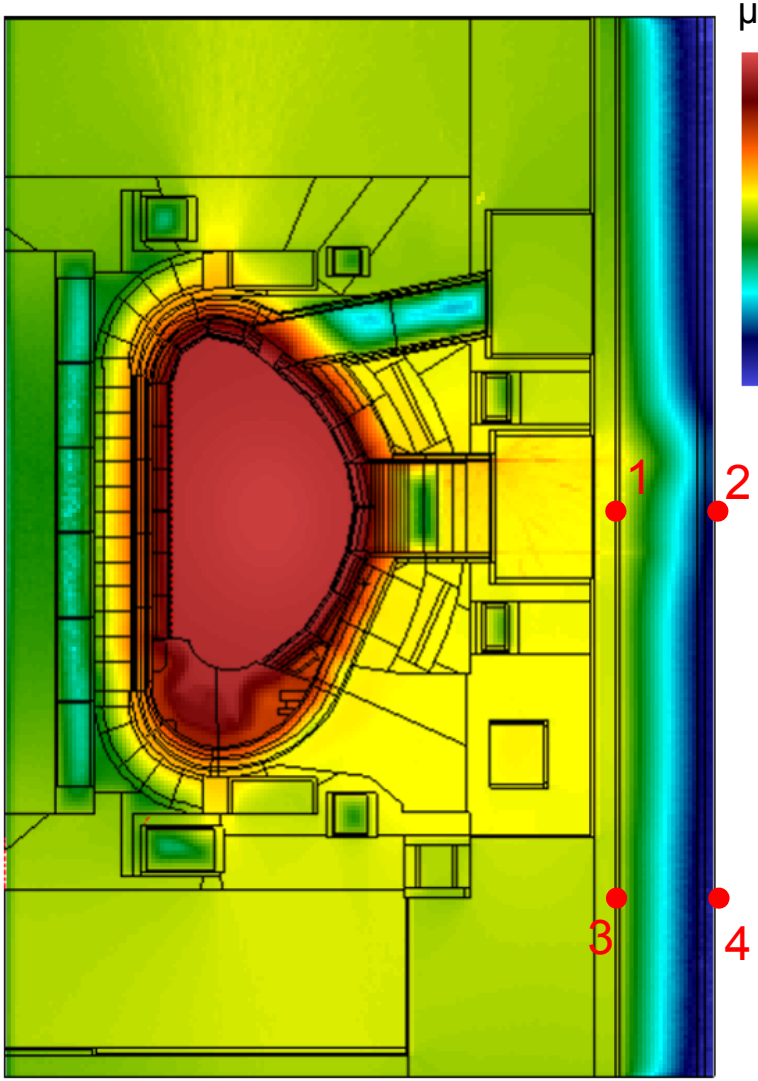


Ports openings in VV

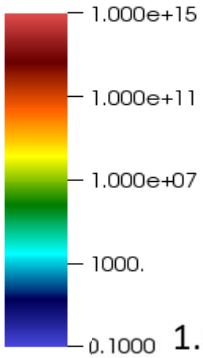
- Factor of 1000 because of ports
- **Hybrid averts** over-conservative design

Reliability of global dose rate calculation

Dose rate at ITER central-plane

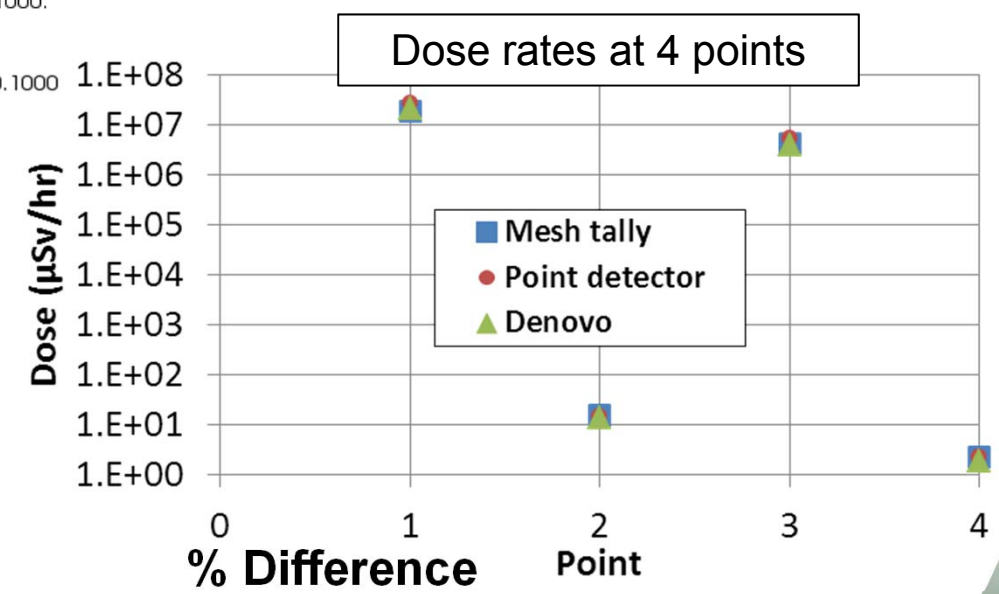


Dose rate
μSv/hr



Parameters of HPC Denovo calculation

Cells	1.34×10^{9}
Groups	67
Unknowns	3.62×10^{15}
Cores	4.02×10^{4}
Time	7.6 hr
Total time	35 years



% Difference

Mesh tally and Pt. Det.	1%-29%
Mesh tally and Denovo	4%-19%
Pt. Det. and Denovo	5%-25%

Excellent agreement