Direct Use of CAD Geometry in Monte Carlo Radiation Transport

Paul Wilson
CNERG/FTI Neutronics Team
U. Wisconsin-Madison
Nuclear Design & Analysis

Enhancements

Radiation Transport & Effects Code Development

L. El-Guebaly
(M. Cusentino)
(L. Mynsberge)

T. Bohm
(M. Sawan)
(A. Ibrahim)

M. Sawan
(A. Jaber)

E. Marriott

Nuclear Design & Analysis

3-D Geometry Capability Enhancements

T. Tautges
(ANL)

P. Wilson
(S. Slattery)
(K. Dunn)

D. Henderson
(A. Robinson)

S. Jackson
(M. Klebenow)

8 Research Staff
1 Visiting Scientist
7 Graduate Students
3 U/G Students

CNERG/FTI Neutronics Team

03.27.2012

P. Wilson: Direct use of CAD in Monte Carlo
Overview

• Motivation

• Developer’s Perspective
  – Core Software Infrastructure
  – Fundamental Geometry Operations
  – Methods & Accelerations
  – Performance
  – Robustness

• User’s Perspective
  – Workflow
  – Examples

• Current Research

03.27.2012
Monte Carlo Transport in Fusion Neutronics

- Complex shielding problems
  - Monte Carlo preferred
  - Intricate geometries created by hand
- Complex cell boundaries
  - Especially tori
- Small numerical gaps in geometry
- Lost particles accepted as necessary
Three Motivations for CAD-Based Monte Carlo Tools

• Faster
  – Reduce human effort – faster design iteration
  – Provide common domain for coupling to other analyses

• Cheaper
  – Reduce human effort

• Better
  – Avoid human error in conversion
  – Include higher-order surface descriptions in analysis
Promise of CAD-based Monte Carlo Transport

Robustness vs Human Efficiency

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
Developer’s Perspective
Developers Perspective: Software Infrastructure

Direct Accelerated Geometry Monte Carlo

Monte Carlo Application

Geometry Representation A

DAGMC Geometry Representation

Geometry Representation B

Mesh Oriented datABase [MOAB]

Common Geometry Module [CGM]

ACIS Solid Modeling Engine

OpenCascade Solid Modeling Engine

Other Solid Modeling Engine

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
Demonstrated Implementations

- **MCNP5 (LANL)**
  - Main development & testing platform
- **Tripoli 4 (CEA/France)**
  - UW implementation
- **GEANT4**
  - Implementation by S. Korean researchers
- **FLUKA**
  - Interest by NASA users and FLUKA developers
- **MCNPX 2.x (LANL)**
  - Initial development platform
  - Being merged with MCNP5 ⇒ MCNP6
Developers Perspective: Software Infrastructure

Geometry & Mesh Infrastructure

- CGM
  - Common API to many solid modeling engines
  - Virtual geometry capabilities for merging and metadata

- MOAB
  - Robust & efficient mesh representation
  - Common API to many mesh formats

- Both are under independent with ongoing improvements
  - Access to other mesh operations/services
  - Other users benefit from developments
For a given point, $x$, and direction, $\Omega$, find

- the nearest boundary, $B$, and
- the distance, $d$, to that boundary
Developers Perspective: Fundamental Geometry Queries

POINT LOCATION

- For a given point, $x$, find
  - the unique volume, $V$, containing that point
• For a given point, $x$, on the boundary, $B$, of volume, $V$, find
  – which volume, $V'$, will be entered next
• For a given point, $x$, on the boundary, $B$, of volume, $V$, find
  – the unit normal, $n$, to that surface
• Metadata can be added to geometry to facilitate
  – Material assignment
  – Boundary conditions
  – Source definition
  – Tally/response definition
  – Variance reduction
• Ray-tracing: fundamental operation of Monte Carlo transport
  – Ray-tracing on 2\textsuperscript{nd} order analytic surfaces is efficient
  – Ray-tracing on arbitrary high-order surfaces requires high-order root finding
  – Also need to detect curves where surfaces meet
  • More complexity with high-order surfaces
Accelerations

• Imprint & merge
  – Reduce complexity of determining neighboring regions in space
  – Reduce number of ray-firing operations

• Faceting
  – Reduce ray-tracing to always be on (planar) facets, but
    • introduce approximations
    • millions of individual facets

• Oriented Bounding Box Tree
  – Accelerate search of millions of surfaces
  – Reduce number of surface tests
Imprint & Merge

• Imprinting

• Merging

• Each surface in max. 2 cells
Avoiding the Explicit Calculation of the “Complement”

• CAD-based solid models do not typically represent non-solid regions
  – e.g. voids, coolants

• Explicit calculation
  – Boolean operations in CAD (or CUBIT)
  – Often computationally expensive

• Implicit determination
  – Volume bounded by surfaces with only 1 cell following imprint & merge
• Simple (inexpensive) bounding box test
  - Streaming distance to closest approach
  - Collision distance to closest approach
Oriented Bounding Box on Facets as Nodes in a Tree

- Axis-aligned bounding box often larger than necessary
- *Oriented* bounding box makes smaller boxes
- OBB on facets allows finer-granularity boxes to be arranged in tree
Tree Traversal Could Have $O(\log_2(n))$ Bounding Box Tests

- Distance limit should guarantee improved performance
- Tree root for each cell/volume
  - Accelerate ray-tracing in implicit complement

03.27.2012
P.Wilson: Direct use of CAD in Monte Carlo
OBB-Tree Traversal Performance Tested on 3 Geometries

Sphere

“Deathstar”

ITER Benchmark Complement
Performance does not meet expectations

Average Ray-Tracing Time (µs)

Number of Triangles in Model

- Sphere (No Edge Length)
- DeathStar (No Edge Length)
- ITER Volume (No Edge Length)

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
High Valence Vertices
Edge Length Guidance
Improved Performance with Better Faceting

![Graph showing average ray-tracing time vs. number of triangles in model for different models and edge lengths. The graph highlights that the most time is spent traversing an OBB tree and in ray-triangle intersection.]

- Sphere (No Edge Length)
- Sphere (Edge Length)
- DeathStar (No Edge Length)
- DeathStar (Edge Length)
- ITER Volume (No Edge Length)
- ITER (Edge Length)

03.27.2012
P.Wilson: Direct use of CAD in Monte Carlo
• Facilitates even more complex geometry
• More opportunity for
  – Small features and geometrical gaps
  – Automated precision to close gaps
• Impact on lost particles unclear
• Lost particle rate used as one performance metric ($< 10^{-5} - 10^{-6}$)
Initial Impact of DAGMC

Robustness vs. Human Efficiency

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
New Problems with CAD-based Monte Carlo

• Quality of CAD geometry
  – Small gaps & overlaps
  – Previous applications of CAD less sensitive

• Human efficiency gains reduced
  – New skills required

• DAGMC-specific challenges/opportunities
  – Inconsistent faceting
  – Robustness of tracking algorithm
Lost Particle Risk

Human Efficiency

Robustness

P. Wilson: Direct use of CAD in Monte Carlo
Lost Particle Risk

- Intrinsically shielding/deep penetration
- Intense variance reduction necessary
- Some lost particles have high weight

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
Implicit Complement

Handle small modeling gaps

Robustness

Human Efficiency

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
Implicit Complement

• Merging of adjacent surfaces accelerates ray-tracing

• Complex volume defined by all unmerged surfaces
  – Inefficient definition in native MCNP
  – OBB-tree preserves efficiency in DAGMC

• Small gaps between volumes are automatically captured in implicit complement
Avoid modeling holes

Robustness

Human Efficiency
• Watertight faceting not guaranteed in merged geometry

Unsealed  
Sealed
Robust Tracking

Avoid numerical holes

Robustness

Human Efficiency

03.27.2012
Robust Tracking

• Ray-tracing failure modes

- Behind previous surface (numerical)
- Ahead of next surface (numerical)
- Tangent to Surface (numerical)
- Edge/Point Intersection (logical)
- Leak Between Triangles (numerical)
- Oscillate Between Triangles (logical)

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
Robust Tracking

- Plücker ray-triangle test
- Edge/Point Post-processing
- Ray Intersect Facets
- Point Inclusion Test
- Tracking Algorithm
- Physics Application

<table>
<thead>
<tr>
<th>Model</th>
<th>Particles Simulated [millions]</th>
<th>Lost Particles</th>
</tr>
</thead>
<tbody>
<tr>
<td>UW Nuclear Reactor</td>
<td>41</td>
<td>5649 ± 178</td>
</tr>
<tr>
<td>Advanced Test Reactor</td>
<td>74</td>
<td>141 ± 32</td>
</tr>
<tr>
<td>40° ITER Benchmark</td>
<td>225</td>
<td>67 ± 39</td>
</tr>
<tr>
<td>ITER TBM</td>
<td>205</td>
<td>665 ± 184</td>
</tr>
<tr>
<td>ITER Module 4</td>
<td>59</td>
<td>59 ± 19</td>
</tr>
<tr>
<td>ITER Module 13</td>
<td>79</td>
<td>450 ± 60</td>
</tr>
<tr>
<td>FNG Benchmark</td>
<td>1310</td>
<td>31273 ± 989</td>
</tr>
<tr>
<td>ARIES First Wall</td>
<td>4070</td>
<td>25 ± 18</td>
</tr>
<tr>
<td>HAPL IFE</td>
<td>286</td>
<td>65 ± 19</td>
</tr>
<tr>
<td>Z-Pinch Fusion</td>
<td>409</td>
<td>2454 ± 317</td>
</tr>
</tbody>
</table>
Overlap Tolerance

Handle small overlaps

Robustness vs. Human Efficiency

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
Overlap Tolerant Tracking

• User specifies an overlap tolerance
  – Only numerical tolerance in DAGMC ray tracing
• Search behind current point for intersection within tolerance
• Update logical location if in overlap
• Does NOT preserve exact physics in overlap region
User’s Perspective
Workflow Includes a Variety of New Tools and Skills

Generate CAD Geometry

Annotate CAD Geometry

Prepare Input File

Standard CAD software tools are used to define the solid model.

Models are exported to a standard geometric-model file format supported by Common Geometry Module (CGM).

DAG-MCNP5

Read Model and Initialize Search Tree

Perform Random Walks

Report Tally Results
Workflow Includes a Variety of New Tools and Skills

Generate CAD Geometry

Allocate materials and densities

Define boundary conditions

Define tally locations

Imprint & Merge

(CURRENTLY USE CUBIT MESH GENERATION TOOL FOR THIS STEP)

Annotate CAD Geometry

Prepare Input File

DAG-MCNP5

Read Model and Initialize Search Tree

Perform Random Walks

Report Tally Results

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
Workflow Includes a Variety of New Tools and Skills

- Generate CAD Geometry
- Annotate CAD Geometry
- Prepare Input File
- DAG-MCNP5
  - Read Model and Initialize Search Tree
  - Perform Random Walks
  - Report Tally Results

Skip cell definitions
Skip surface definitions
Provide data cards
- Material definitions
- Tally modifiers
- Source definition
- etc...
Workflow Includes a Variety of New Tools and Skills

Generate CAD Geometry

Annotate CAD Geometry

Prepare Input File

Generate *tree-based decomposition* of facets on model surfaces

DAG-MCNP5

Read Model and Initialize Search Tree

Perform Random Walks

Report Tally Results

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
Workflow Includes a Variety of New Tools and Skills

Generate CAD Geometry

Annotate CAD Geometry

Prepare Input File

**DAG-MCNP5**

Read Model and Initialize Search Tree

Perform Random Walks

Report Tally Results

Circumvent standard functions involved in ray-tracing, esp.
- ray-surface intersection
- point-in-volume determination
- neighboring cell determination
ITER Benchmark

• Comparing 4 problems
  – Neutron wall loading
  – Divertor fluxes and heating
  – Magnet heating
  – Midplane port shielding/streaming

• Participants
  – UW, FZK, ASIPP, JAEA
  + ATTILA (UCLA/PPPL)
IB TFC heating

Nuclear Heating (kW)

Distance from top of IB TFC (cm)

- ASIPP
- FZK
- JAEA
- UW (geometry fixed)

03.27.2012
P.Wilson: Direct use of CAD in Monte Carlo
Performance Compared Using Translated Models

ITER Benchmark Model: >800 cells, ~10,000 surfaces

MCAM
Translation

McCad
Translation

DAGMC
Solid Model

P.Wilson: Direct use of CAD in Monte Carlo
Overall Performance Less than 3x Slower than Native Geometry

- Performance of translation approaches vary by 60%

<table>
<thead>
<tr>
<th>Model</th>
<th>Number of Volumes</th>
<th>Number of Surfaces</th>
<th>Relative CPU-Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCAM translation</td>
<td>4148</td>
<td>3192</td>
<td>1</td>
</tr>
<tr>
<td>McCad translation</td>
<td>6031</td>
<td>3800</td>
<td>1.63</td>
</tr>
<tr>
<td>DAGMC</td>
<td>802</td>
<td>9834</td>
<td>2.46</td>
</tr>
</tbody>
</table>
Analysis for an Initial Mod 13 Design

03.27.2012

P. Wilson: Direct use of CAD in Monte Carlo
Detailed 3-D Neutronics for DCLL TBM

Mid-plane nuclear heating

Mid-plane T production

Source Input Table

DCLL TBM

Steel damage at section X2

03.27.2012
P.Wilson: Direct use of CAD in Monte Carlo
Surface Source Approach Applied to ITER FWS Mod. 4

Overestimate in nuclear heating (MW) resulting from surface source.

<table>
<thead>
<tr>
<th>Material</th>
<th>Full ITER Model</th>
<th>Surface Source Model</th>
<th>% Overestimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beryllium</td>
<td>0.0535</td>
<td>0.0543</td>
<td>1.50%</td>
</tr>
<tr>
<td>CuCrZr</td>
<td>0.0350</td>
<td>0.0356</td>
<td>1.71%</td>
</tr>
<tr>
<td>Steel</td>
<td>0.757</td>
<td>0.790</td>
<td>4.36%</td>
</tr>
<tr>
<td>Water</td>
<td>0.150</td>
<td>0.157</td>
<td>4.67%</td>
</tr>
</tbody>
</table>
Assessment of Accuracy of Surface Source Approach
Assessment of Accuracy of Surface Source Approach

Heating Ratio Module 4 (x=404.5 cm)

- Case 1 (ext=0 cm)
- Case 2 (ext=10 cm)
- Case 3 (ext=25 cm)
- Case 1 (ext=0 cm, offset=0 cm)

Heating Ratio (vs baseline case)

Z (cm)
Application to ARIES-CS Compact Stellarator

- Geometry complex
- FW shape and plasma profile vary toroidally within each field period
- Cannot be modeled by standard MCNP

Examined effect of helical geometry and non-uniform blanket and divertor on NWL distribution and total TBR and nuclear heating
Source Probability Map

Increasing Poloidal Angle
(0° at O/B midplane)
NWL Maps (colormaps in MW/m²)

5 cm SOL

uniform src

30 cm SOL

Radiative heating

Poloidal Angle (degrees)

Toroidal Angle (degrees)
Multi-Physics: Coupling to CFD

- Fine mesh DAG-MCNP5 results
  - 1-3 mm Cartesian mesh overlay
  - Total nuclear heating
- Arbitrary mesh on CAD geometry
  - Tetrahedral
  - Polyhedral (Star-CCM+)
- Automated interpolation using MOAB
Multi-Physics: Coupling to CFD

- 1 of 40 fingers in ITER First Wall concept
- Beryllium plasma facing component
- CuCrZr heat sink into pressurized water
- Steel backing for structural support
- 0.2 MW/m^2 heat flux onto Beryllium
- Inlet: 0.2 kg/s water. 373 K. 3 Mpa

03.27.2012
P.Wilson: Direct use of CAD in Monte Carlo
Notice “hot spot” at elbow and center due to nuclear heating.

These temperatures are ~30C higher than UCLA results, perhaps due to nuclear heating.
Fission Applications
ATR National Science User Facility

AFIP Experiment In CFT

P. Wilson: Direct use of CAD in Monte Carlo
Fission Applications
Irradiation Experiment Design

Geometry File

Solid Modeling Software

Geometry Model

ABAQUS CAE

ABAQUS Input File

ABAQUS

ABAQUS Output File w/ thermal response

MCNP5 Output

DAG-MCNP5

Automated Conversion

Simplified MCNP5 Input

MCNP5 Output File w/ thermal response

Geometry File

Fission Applications
Irradiation Experiment Design
Neutron Transport in Deformed Geometries

- Space reactor launch accidents may result in reactor return to earth
- Criticality of intact reactor well understood
- Impact likely to deform reactor
- Is criticality possible?
The single pin $k_{eff}$ increases with deformation.

- 33 volumes, 113 surfaces, 103k hex elements
- Clad is not explicitly modeled
  - Clad is homogenized with fuel
- Fuel pin is surrounded by void
- Same MCNP material density was used pre/post deformation

<table>
<thead>
<tr>
<th>Time Step</th>
<th>Stage</th>
<th>$k_{eff}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Undeformed</td>
<td>0.84479 (0.00041)</td>
</tr>
<tr>
<td>29</td>
<td>Last deformed step w/out dead elements</td>
<td>0.92412 (0.00045)</td>
</tr>
<tr>
<td>50</td>
<td>Last deformed step</td>
<td>0.96939 (0.00046)</td>
</tr>
</tbody>
</table>
Fission Applications
85-Pin Full-Scale Space Reactor Impact

40 m/s on concrete
Neutron Transport:
85-Pin Full-Scale Space Reactor Impact

Neutron Multiplication Factor vs. Time

- Δ 0 Degree SPH
- [] 0 Degree
- ○ 45 Degree

K_{eff}

0.865 0.875 0.885 0.895 0.905 0.915 0.925 0.935 0.945

0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0 2.2

Time [ms]
Research Directions
Advanced Mesh Tallies

• Perform track length tallies on arbitrary polyhedral mesh
  – Prototype exists for tetrahedral mesh
• Develop alternative tally estimators
  – Functional expansion tallies
  – Kernel density estimators
• Explore $hp\sigma$-adaptivity of advanced mesh tallies
Next Steps: Human Efficiency

- Unstructured mesh tallies
  - Small volume fraction tallies
  - Multi-physics coupling
Next Steps: CPU Efficiency

• Hybrid Transport
  – Automated mesh generation based on CAD model

- CAD Geometry
  - Geometry/materials
- \( S_N \) Calculation
  - Geometry/materials
  - Source region
  - Tally regions
- WW Calculation
  - Forward Fluxes
  - Adjoint Fluxes
- MC Calculation
  - Geometry/materials
  - Source region
  - Tally regions
  - Variance Reduction

03.27.2012
P.Wilson: Direct use of CAD in Monte Carlo
• Monte Carlo not well-suited to deep penetration problems
• Deterministic methods not well suited to gap streaming problems
• Use deterministic methods to develop importance maps for Monte Carlo problems
Research Directions
Hybrid Methods

50 CPU-days

Neutrons

Analog

FW-CADIS (ORNL)

Photons

03.27.2012
P.Wilson: Direct use of CAD in Monte Carlo
Total neutron flux cumulative distribution functions (50 days)

Fraction of voxels

Relative uncertainty

0.1
0.78
0.99
0.59
0.1

FW-CADIS

Analog

03.27.2012

P.Wilson: Direct use of CAD in Monte Carlo
Total gamma flux cumulative distribution functions (50 days)

Fraction of voxels

Relative uncertainty

FW-CADIS

Analog

0.1

0.6

0.95

0.3

0.1

0.3

0.0

0

20%

40%

60%

80%

100%
Next Steps: Human Efficiency

• 3-D Activation
  - Automated material mesh generation from CAD
  - Efficient mesh-based photon source sampling
Summary of Research Directions

• Common Domain Solution Coupling
  – Neutronics-Neutronics coupling
    • Hybrid acceleration of shielding
    • Hybrid acceleration of source convergence
  – Neutronics-”other physics” coupling
    • N source term
    • N feedbacks
    • Activation dose/depletion
    • Uncertainty propagation

• Advanced mesh tallies
  – Alternative tally estimators
  – $hp_\sigma$-adaptivity
• Fundamental capability in production use for fusion shielding applications
  – Robustness improvements
    • Goal: Guarantee no lost particles
  – Performance improvements
    • Goal: Users don’t care about performance penalty
  – Feature enhancement
    • Goal: Extend utility of Monte Carlo radiation transport
Questions?

wilsonp@engr.wisc.edu

cnerg.engr.wisc.edu