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CAD Based Radiation Transport: DAGMC Toolkit

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Monte Carlo analysis was born in the Manhattan Project

Von Neumann, Metropolis, and Fermi

We define materials in regions of model, these regions have interaction probabilities, random numbers used to sample

Traditionally we define regions using combinations of quadratic surfaces united with boolean operations
CAD Based Workflows

- CAD is desirable as a source of geometry for Monte Carlo calculations for several reasons
  - Allows very complex models to be represented (fidelity, accuracy)
  - Produced for manufacturing purposes (provenance)
  - The model usually already exists (you don’t need to make it)
  - User friendly, easier to fix and modify than CSG (effort)
  - Faster analysis turnaround (efficiency)

- CAD model integrity - “cleanliness”

- Several routes for use:
  - Translation - MCAM, McCAD, FastRAD, CATIA-GDML
  - Directly - DAGMC
  - Hybrid - OiNK
CAD Based Workflows

- Automation (including translation) provides:
  - Reduced human effort
  - Increased quality assurance
  - Direct geometry use provides **richer surface** representation
  - Facilitates coupling to other analysis types through common geon
What is DAGMC?

- DAGMC ([http://svalinn.github.io/DAGMC](http://svalinn.github.io/DAGMC)) is an open source toolkit that allows a user to transport particles on CAD based geometries.
- Developed by the Computational Nuclear Energy Research Group (CNERG - [http://cnerg.github.io/](http://cnerg.github.io/)) at the University of Wisconsin-Madison (and since I’m at UKAEA now) and UKAEA.
- Its purpose is to enable particle transport on very detailed and complex geometries, by having a core geometry library which can be plugged into any Monte Carlo code.
20 Billion Euro Project - First Plasma 2025 / First DT Plasma 2035
Radiation analysis in Fusion calculations takes a long time:
- Depending on the geometry - 2-3 years of 10 people to generate a new reference geometry for ITER (CSG)
- Transport calculation - 3-6 months on 200-500 CPU’s typically

Clearly the bottleneck here is the geometry production time:
- Clean CAD usually only takes 1-2 months to prepare - use CAD directly as possible - no translation
- Happy to have slower calculations if overall time to produced calculation is less
- But seek to have parity in true transport time

What is DAGMC?
What is DAGMC?

- Direct Accelerated Geometry Monte Carlo (DAGMC) started in 2001 (proof of principle by 2004) integrated directly into MCNP/X and tied directly into a CAD engine

Example use, Clothes peg defined in CAD with spiral winding in clasp, Right MCNP/X radiograph
Examples of DAGMC Use

- CMS Detector - LHC
- ATR
- NASA Hab Module
- Fusion Neutron Science Facility
- Advanced Thin Ion Calorimeter
- ISS
- Spallation Neutron Source
DAGMC Theory

- Ray-tracing: fundamental operation of Monte Carlo transport
  - Ray-tracing on 2nd 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

- DAGMC has 3 main Accelerations
  1. Imprinting & merging
  2. Faceting
  3. Bounding Volume Tree
DAGMC Accelerations - Imprinting

Reduces the complexity in determining neighboring regions of space.

Surfaces A & B shared between the volumes.
DAGMC Accelerations - Merging

4 surfaces (3 new ones created during imprint), surface A imprinted upon surface B to create C,D,E

Merging surfaces F & A, now any surface can only be shared by no more than two volumes
DAGMC Accelerations - Faceting

- Reduces ray tracing to always be on planar facets
  - introduces approximation
  - millions of facets
- Axis aligned bounding box often larger than needed
  - Oriented boxes make for smaller boxes
  - OBB on facets allow for finer granularity boxes
DAGMC Accelerations - BVH Trees

Pixar’s Piper (2016)

Pixar’s WALL-E (2008)

Um… What do animated films have to do with DAGMC?

MOAB OBBs

Embree AABB
DAGMC Convenience - Implicit Compliment

- CAD models generally do not define “void space”, including:
  - Coolants
  - Vacuum
  - Air

- DAGMC
  - Any surface that does not associate with 2 volumes must bound this compliment space (due to imprinting a surface can only be associated with 1 or 2 volumes)

- Is **automatically** generated

- On going work to have multiple logically derived implicit complements
DAGMC Advantages

- Richer surface description
  - Stellarator only possible to model in DAGMC - Andre Haussler (KIT)
- Implicit Complement
  - Complex negative space geometry not needed to be defined
- All volumes implicitly derived from triangle surface representation

- Tighter coupling to other physics
  - Facet based model can be deformed due to external input
Access to DAGMC

- Fundamentally open source
  - http://svalinn.github.com/DAGMC

- Software stack:
  - Free & Open: MOAB, HDF5, (optional PyNE), DAGMC
  - Licensed: Cubit/Trelis
    - Maybe use Attila mesher?
  - Working on OS solution for geometry

- Community forum:
  - dagmc-users@groups.google.com

- Please try it!
DAGMC - Integration

Complete and Available

- FLUKA
- MCNP5
- Tripoli4

In Progress

- MCNP6
- GEANT4
- Shift

Proposed

- OpenMC
- EGSnrc
- PHITS
- Serpent2

Not Currently Planned

- Penelope
- Mercury
- MARS
DAGMC Workflow

CAD File → SpaceClaim → ACIS File

MaterialLib builder → MaterialLibrary

Trelis/Cubit Plugin for Desktop Model Preparation:
- Cubit/Trelis → DAGMC H5M File
- Make Watertight → Watertight DAGMC H5M File

(UW)^2 → DAGMC H5M* File (with compositions)

DAG* (physics) → H5M Mesh Tally File
Geometry as a Service

- We have MC code agnostic workflow where materials are encoded in generic form

- Deploy the literal same geometry in supported codes - no changes needed
DAGMC Software Testing

● Fundamental library tests within MOAB
  ○ Run nightly
  ○ Run on demand with pull requests

● Fundamental DAGMC Code Interface tests
  ○ Run nightly on the baseline branch
  ○ Run on demand with Github pull requests

● DAG-MCNP5/MCNP6 Verification and Validation
  ○ Sinbad, Several code comparisons, MCNP5 test suite

● FluDAG
  ○ Sinbad, Several code comparisons, bespoke test suite
DAGMC Examples - ITER NBI Sector

- A detailed, updated model of the NB port region was integrated into the BL-Lite model (40° model) - 2646 volumes, 72019 surfaces, 171361 curves

Calculations run using DAG-MCNP5 and FENDL-2.1 cross section library
DAGMC Examples - ITER NBI Sector

- A lot of detail in the BM13-16 region:
  - ELM coils, manifolds, brackets
  - Water coolant channels
  - VV (top view)
  - SB (rear view)
ITER lifetime is 0.54 FPY (1.7e7 sec) so 2.94e-8 dpa/sec corresponds to 0.5 dp
Detailed Blanket Module Heating

- Entire BM08 model covered with a rectangular (non-conformal) mesh tally

Slice through mid-plane
Detailed Blanket Module Heating

- The IO requested nuclear heating mapped onto an ANSYS mesh of the BM08 beam with units of W/mm³
- The nuclear heating generated with the Cartesian mesh was used for this mapping:
SNL Space Reactor

- CAD geometry of the SNL Space reactor was meshed, structural mechanics of the FE mesh used to determine deformation of the geometry when the reactor was dropped ‘during launch conditions’
- Need to determine the $k_{\text{eff}}$ of the system under various failure modes, drop angles
SNL Space Reactor

Neutron Multiplication Factor vs. Time

- ▲ 0 Degree SPH
- □ 0 Degree
- • 45 Degree

Time [ms]

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

$K_{\text{eff}}$

0.865 0.875 0.885 0.895 0.905 0.915 0.925 0.935 0.945
DAG-MCNP6 SNS

- Oak Ridge National Laboratory (ORNL) Spallation Neutron Source (SNS) are interested in shifting to a complete CAD based workflow
  - They have extensive CAD models of the facility and a planned upgrade

- SNS 1 GeV proton beam impinges on liquid mercury target delivering 1 MW of heat into the target, producing around 20 spallation neutrons for each source neutron
  - The neutrons are then ‘encouraged’ along beamlines to target stations
DAG-MCNP6 SNS

- Oak Ridge National Laboratory (ORNL) provided native MCNPX model
- Converted to CAD geometry using the mcnp2cad tool (automatic)
- The native MCNP model was created by hand at great expense of time and effort (6 months)
DAG-MCNP6 SNS

MCNP6

Proton Flux

DAG-MCNP6
DAG-MCNP6 SNS

MCNP6

Neutron Flux

DAG-MCNP6
DAG-MCNP6 SNS

MCNP6

Photon Flux

DAG-MCNP6
Specific Tally Comparison in SNS

Tally 6: top upstream moderator hydrogen heating

Tally 14: tu poison plate neutron absorption rate
SNS Calculation - FluDAG/DAG-MCNP6 - Protons

Same SNS geometry used as in the previous validation cases - if using the UWU one can run the literal same geometry in any of the codes. The only difference between this and the previous calculations was a more simplified source description used, 1 GeV proton beam gaussian profile in X,Y directions 3 cm FWHM.
SNS Calculation - FluDAG - DAG-MCNP6

Neutrons

![Graph showing neutron distribution with DAG-MCNP6 and FluDAG results.](image)
Human Mesh Phantom

- Adult female Mesh-type ICRP Reference Computational Phantom
- Created by HUREL @ Hanyang University
- 2.6 million triangular facets
- Tet mesh originally - extract surface triangles
Human Mesh Phantom

Results: 0.1 MeV Photon Source

Photon Flux
[p/cm² src]
Human Mesh Phantom

Photon Flux
[p/cm² src]

0.0002000
0.0001750
0.0001500
0.0001250
0.0001000
Human Mesh Phantom

Comparison of Organ Dose

Dose Ratio

Absorbed Dose MeV/g

DAG-MCNP5/FLUDAG
DAG-MCNP5/DAG-MCNP6.1
ATIC Benchmark

NASA Radiation Detector flown on high altitude balloon Advanced Thin Ionization Calorimeter (ATIC), used to measure cosmic ray spectra

Relatively complex & intricate geometry

~ 6200 volumes

Used as acceptance case to validate FluDAG

Results expected to match exactly with Fluka results.

Layers of Silicon, Mylar, Aluminium, BiGeO

1 GeV protons incident from above the geometry

Interested in Proton Flux, Neutron Flux, Photon Flux, Energy Deposition and a few others
Proton Flux

FLUKA Proton Flux

FludAG Proton Flux
Proton flux lineout
Energy Deposition Profile
Energy Deposition lineout
Neutron Flux Profile

FLUKA Neutron Flux

FluDAG Neutron Flux
Neutron flux lineout

![Graph showing neutron flux lineout with FLUKA and FLUDAG datasets. The graph plots neutron flux (1/cm² s/ nc) against Z position (cm). The ratio FLUKA/FLUDAG is also shown with a +/- 3σ uncertainty.](image-url)
High Energy Physics Example

- 20 (ish) GeV proton beam onto a largely lead target
  - For a STEP file CAD was very clean :) 
  - Needed some repairs in the spiral section
  - Model was rotated to the appropriate coordinate system and shifted

SS316LN

WB128HP

Water
nTOF Geometry

Slice through x=0

$\theta = 15^\circ$
nTOF Comparisons - Neutron Flux (per src)
nTOF Comparisons - Neutron Spectrum
Space Radiation Example

- NASA wanted to simulate the RAD detector that flies on the ISS
- CAD model taken from drawing office
  - Simplified in SpaceClaim (2 weeks)
  - Running in FLUDAG & DagGeant4
Space Radiation Example

This work performed by SRAG - NASA
Space Radiation Example

DagGeant4

FluDAG
**The Future**

- DAGMC is approaching being a finished project
- Work in progress
  - DAGMC ‘parallel’ universe
  - Cubitless workflow
  - MC code integration(s)
  - Integration of DAGMC like workflow using NVidia OPTIX as ray fire engine
- CERN are interested in integration of DAGMC directly into Geant4 as a prime geometry member
- Argonne National Lab want the same for OpenMC
Advantages of DAGMC

- Faster model creation time
- Easier integration with existing CAD models
- MC Code independence
- Not native MCNP
- Stresses the right part of the workflow (CAD)
- Simple coupling with other multiphysics analysis
- Represents the boundary of the volume only
  - no expensive extraneous boundary crossings
Questions

Any questions, sorry for all the slides :)

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https://github.com/svalinn/dagmc