IMPROVED METHODS FOR PARTICLE TRACKING IN CAD-BASED MONTE CARLO RADIATION TRANSPORT

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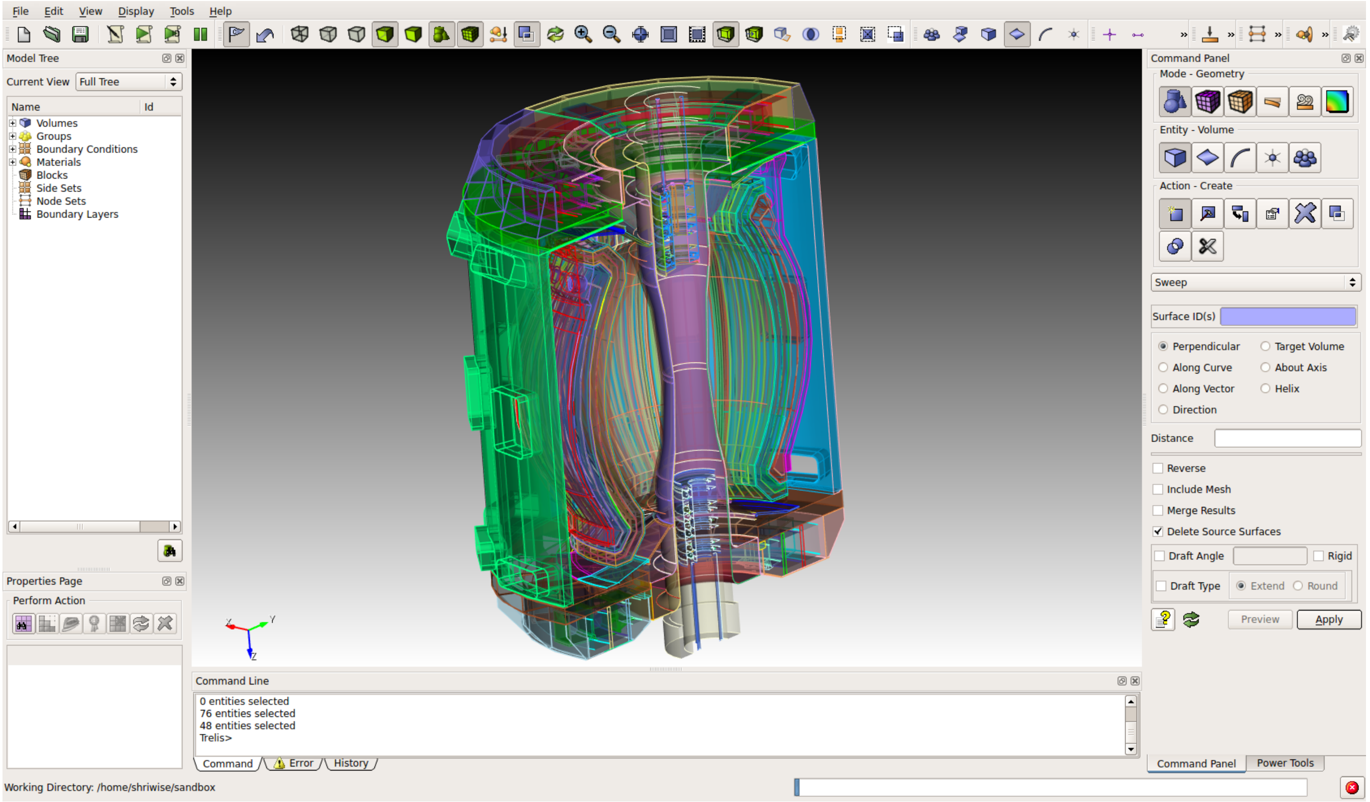
MOTIVATION

MOTIVATION

CAD-Based Monte Carlo Radiation Transport (MCRT)

- equal freedom in design and analysis
- engineering analysis on the same model



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MC GEOMETRY REPRESENTATIONS

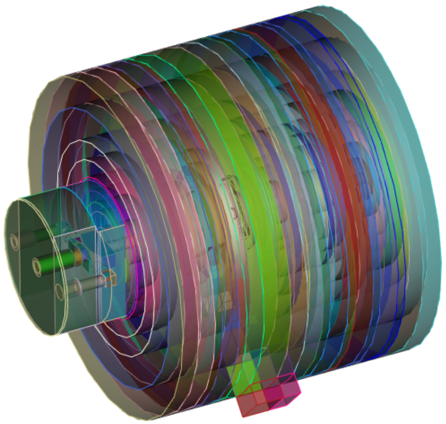
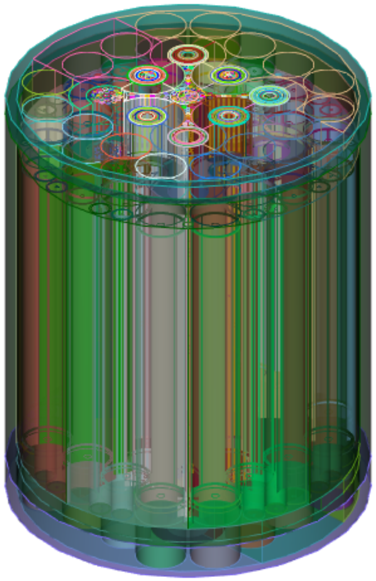
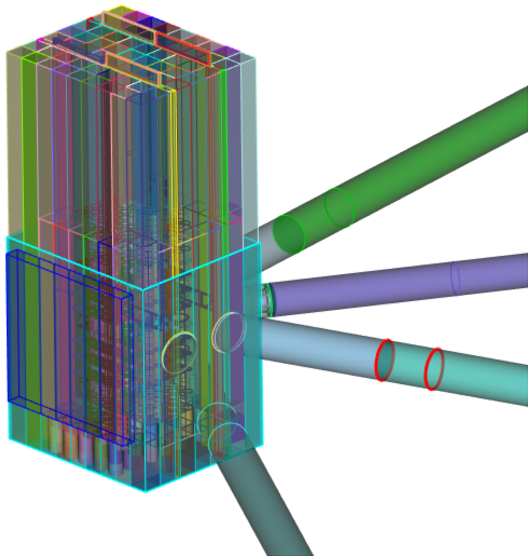
Native Geometry	CAD Geometry
• Variants of Computational Solid Geometry (CSG) • Volumes formed from Boolean combinations of simple implicit surfaces • Geometry queries are analytic in nature	• Allows for higher order surface complexity • Contains convenient design tools: ▪ extrude, sweep, loft, splines, etc. • Geometry queries are complex and sometimes impossible analytically

CAD-BASED MCRT

- A pathway for robust particle transport on CAD geometries exists.
  - Direct Accelerated Geometry Monte Carlo (DAGMC[13])
    - Relies heavily on Mesh-Oriented DataBase (MOAB[12])
- Not yet at its full potential
  - Difficult to meet CAD quality required for robust DAGMC transport
  - Long simulation times (2.5-10*x* longer than native codes) resulting in hours or even days of additional simulation run-time

RESEARCH GOAL

To provide CAD-based radiation transport performance comparable to native Monte Carlo geometry representations

FNG	ATR	UWNR
		
neutron source	criticality	criticality

These problems were run with both native & CAD geometries.[4]

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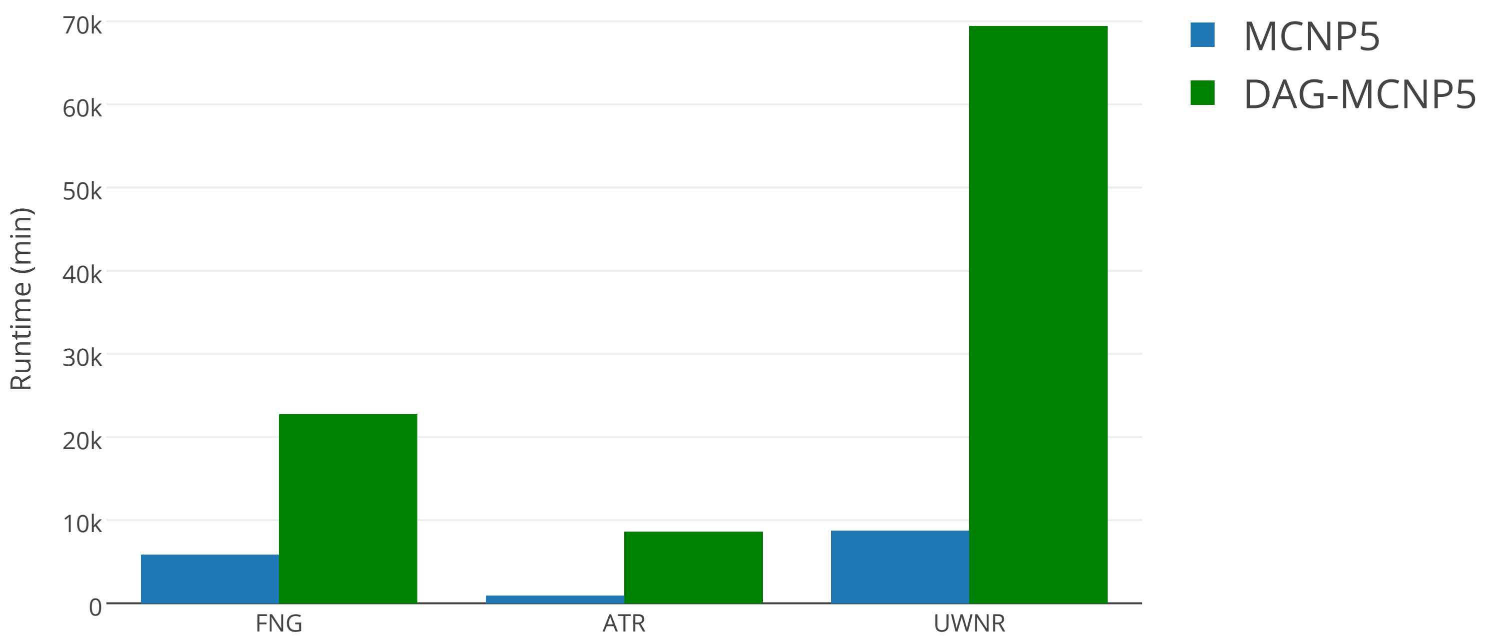
RESEARCH GOAL

To provide CAD-based radiation transport performance competitive with native Monte Carlo geometry representations



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MOTIVATION RECAP

CAD-Based MCRT:

- Allows for better geometric fidelity
- Requires less human time in model generation

Benefits of this work:

- Performance comparable to native geometry makes this more realistic/desirable for a more broad range of problems.
- Current problems requiring CAD-based MCRT will benefit from enhanced performance.
- New methods may be necessary for reasonable run-times with charged particle transport.

BACKGROUND

DAGMC GEOMETRY WORKFLOW

particle tracking

MCNP5[15]

surface faceting

CAD (Cubit/Trelis) [7] [5] → preprocessing (MOAB) → DAGMC (MOAB) ⇄ Monte Carlo

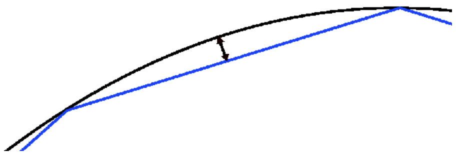
geometric design

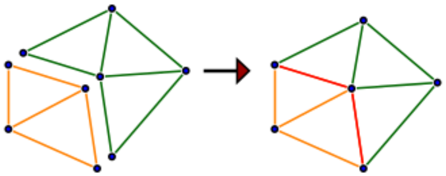
make_watertight [11]

ray tracing

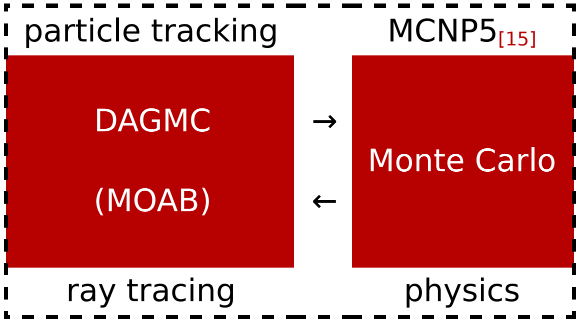
physics

Analysis

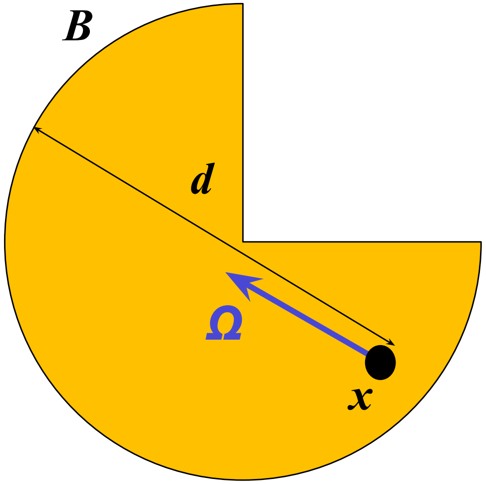




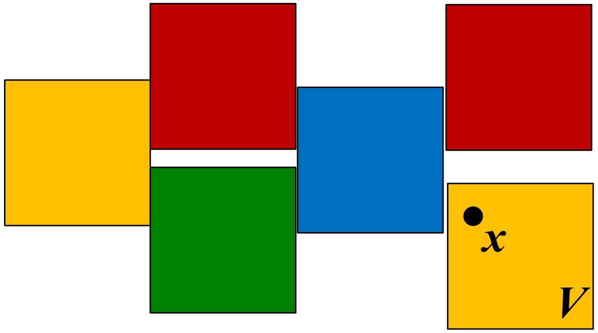
MC GEOMETRY QUERIES



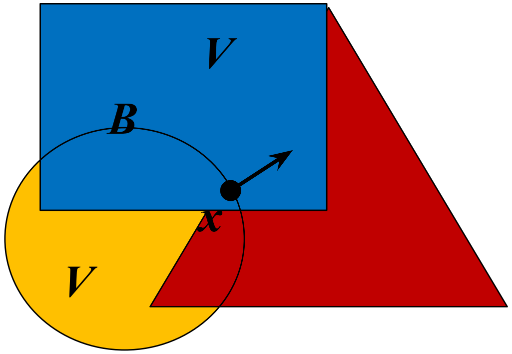
3 types of queries:



Distance to Boundary



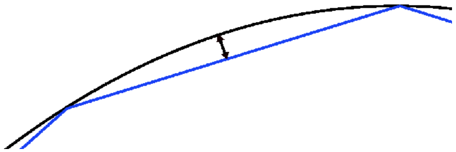
Point Location



Surface Crossing

SURFACE FACETING

Faceting Tolerance: maximum allowed distance of farthest point on the facet from the analytic surface.



- Discretization reduces all surfaces to planar type regardless of analytic surface complexity.
- There are also now many, many more of them.

	FNG	ATR	UWNR	ITER SDDR
Surfaces	1×10^3	2.8×10^3	5.5×10^3	6.9×10^3
Triangles	1.2×10^6	4.9×10^6	3.3×10^6	4.4×10^7

A linear search of triangles is unreasonable.

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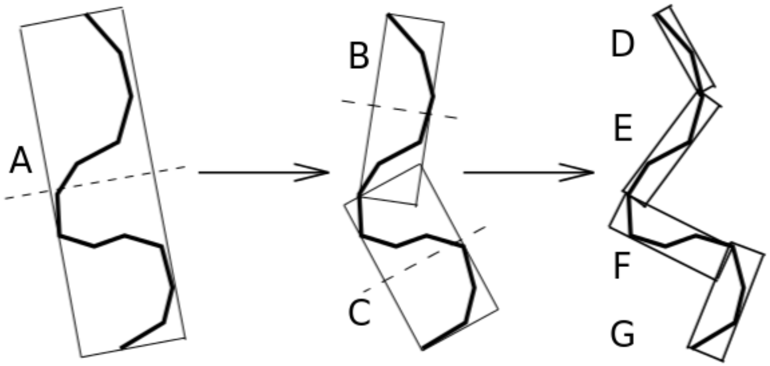
RAY TRACING ACCELERATION DATA STRUCTURES

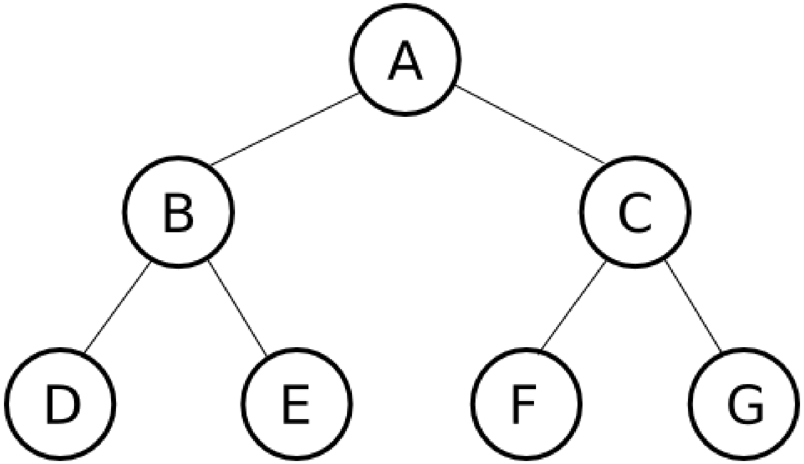
This is a field dedicated to rapid geometric queries on surface meshses of triangles.

It commonly employs a variety of hierarchical data structures:

- Bounding Volume Hierarchy (BVH)
- KDTree
- Octree
- ...

BOUNDING VOLUME HIERARCHY

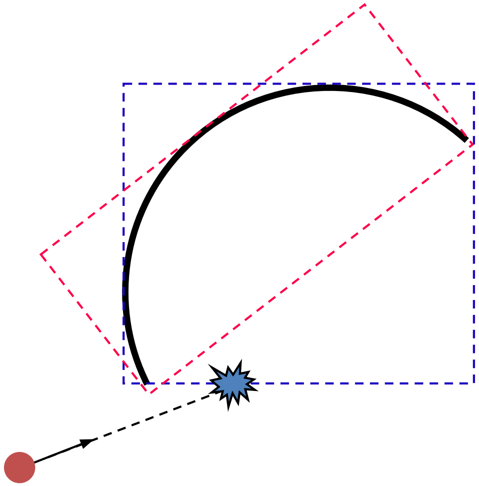




BOUNDING BOXES

Axis-Aligned Boxes

- Low storage (6 extents)
- Fast, simple intersection checks



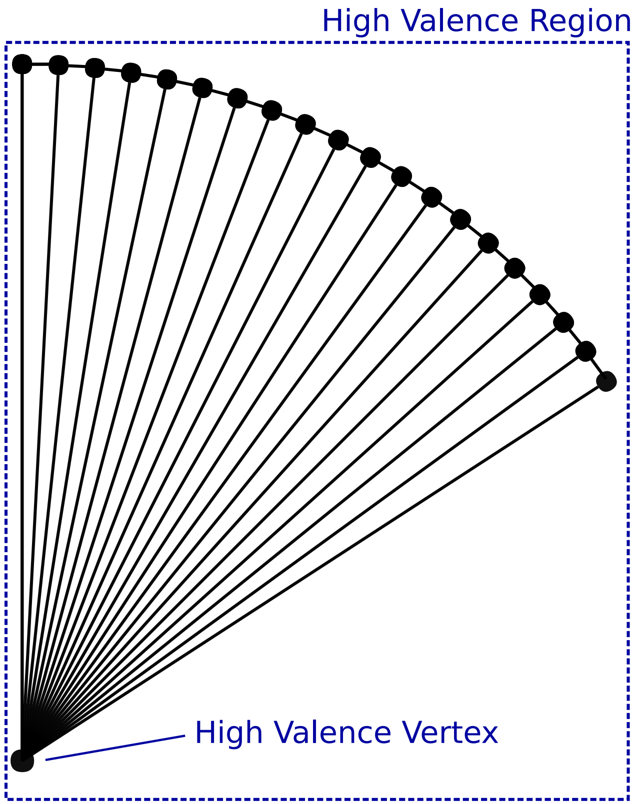
Oriented Boxes

- Higher storage (extents+axes)
- Must re-orient ray for intersection checking
- Bounds triangles well

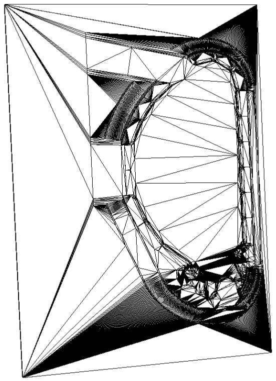
HIGH VALENCE MESH FEATURES

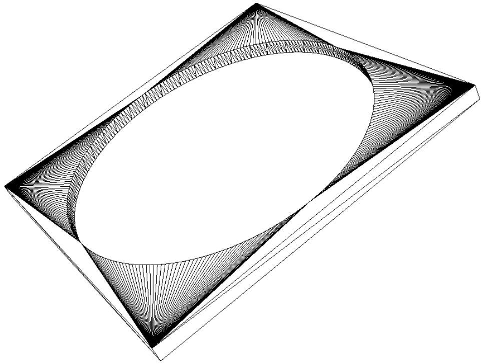
HIGH VALENCE MESH FEATURES

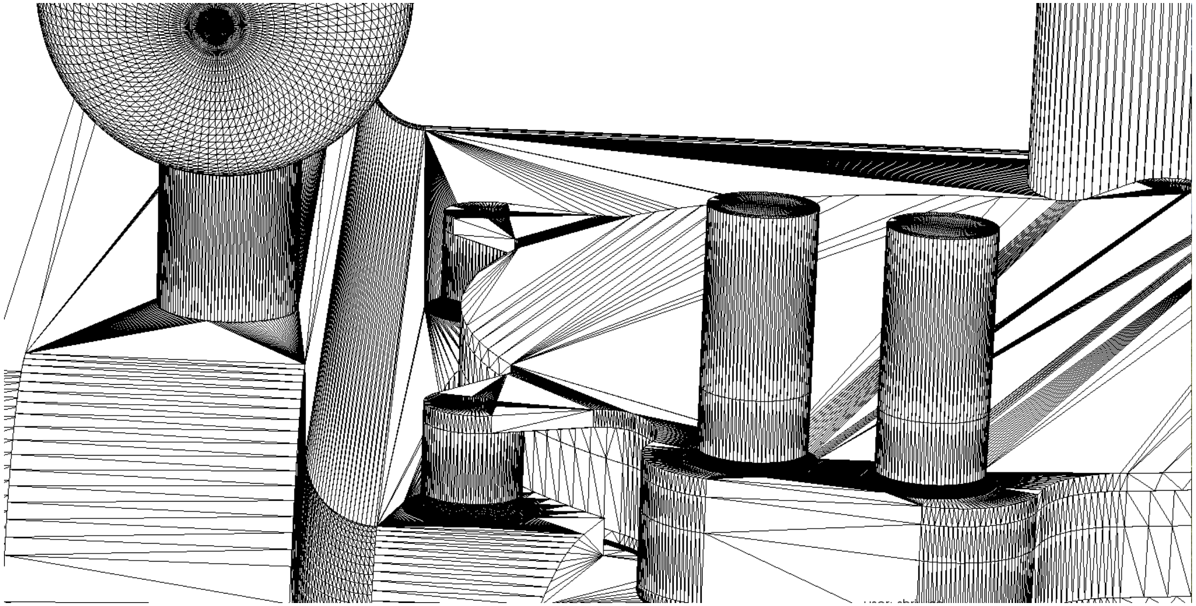
- Common feature of many faceting algorithms
- Result of trying to minimize triangles used to represent a surface
- Known to be detrimental to DAGMC performance



HIGH VALENCE IN PRODUCTION MODELS







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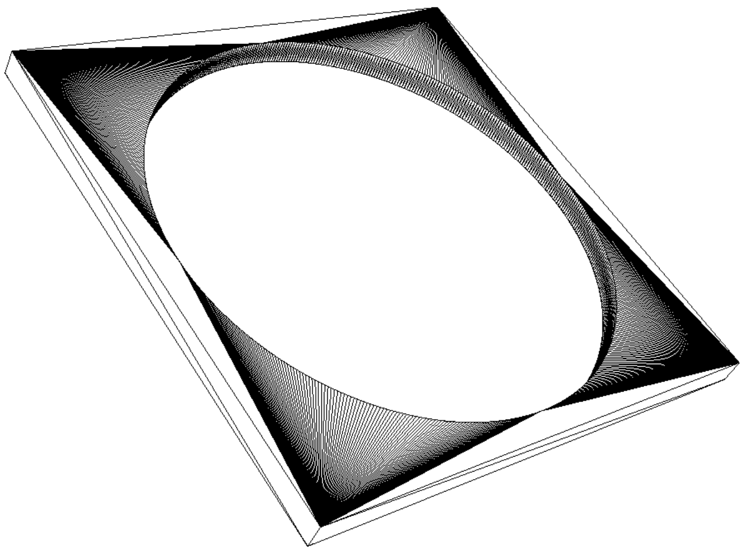
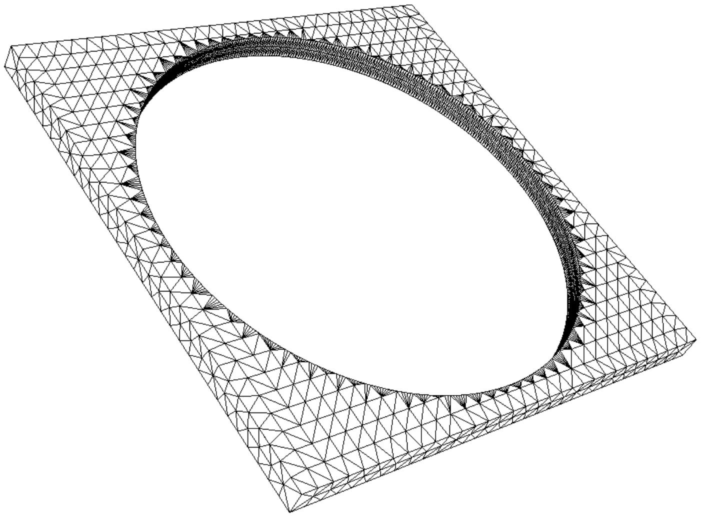
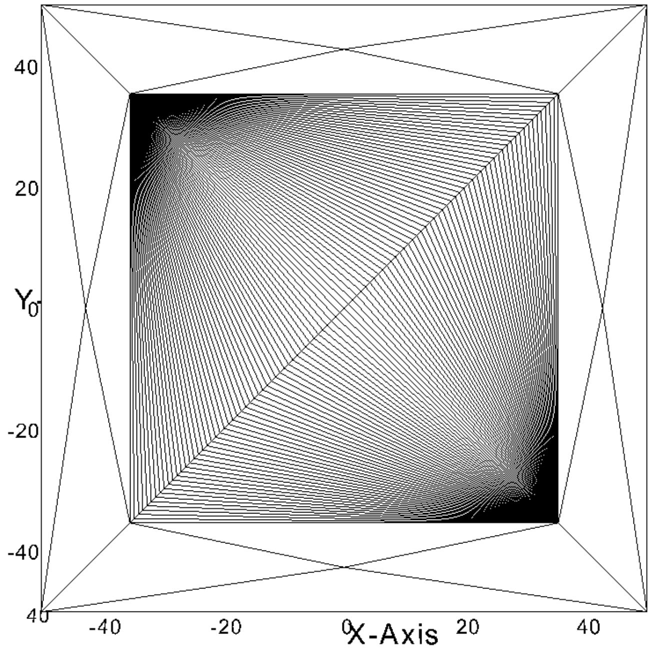
ALTERED FACETING

Length Tolerance: maximum allowed length of facet edge.

Faceting Tolerance Only	With Length Tolerance
	

HIGH VALENCE TEST MODEL

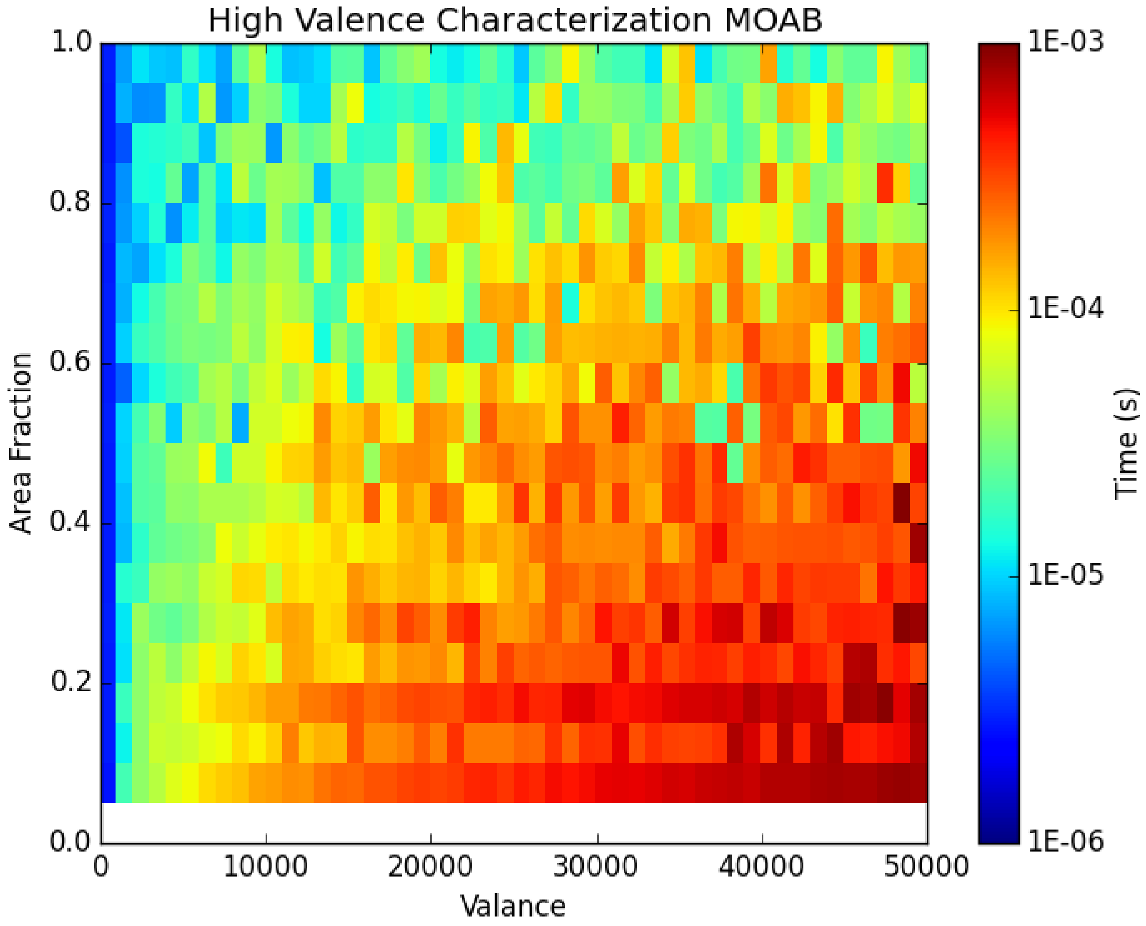
Created by manually faceting a cube surface.



Variable parameters:

- fraction of surface that high valence region occupies
- valence of corner vertices

HIGH VALENCE STUDY



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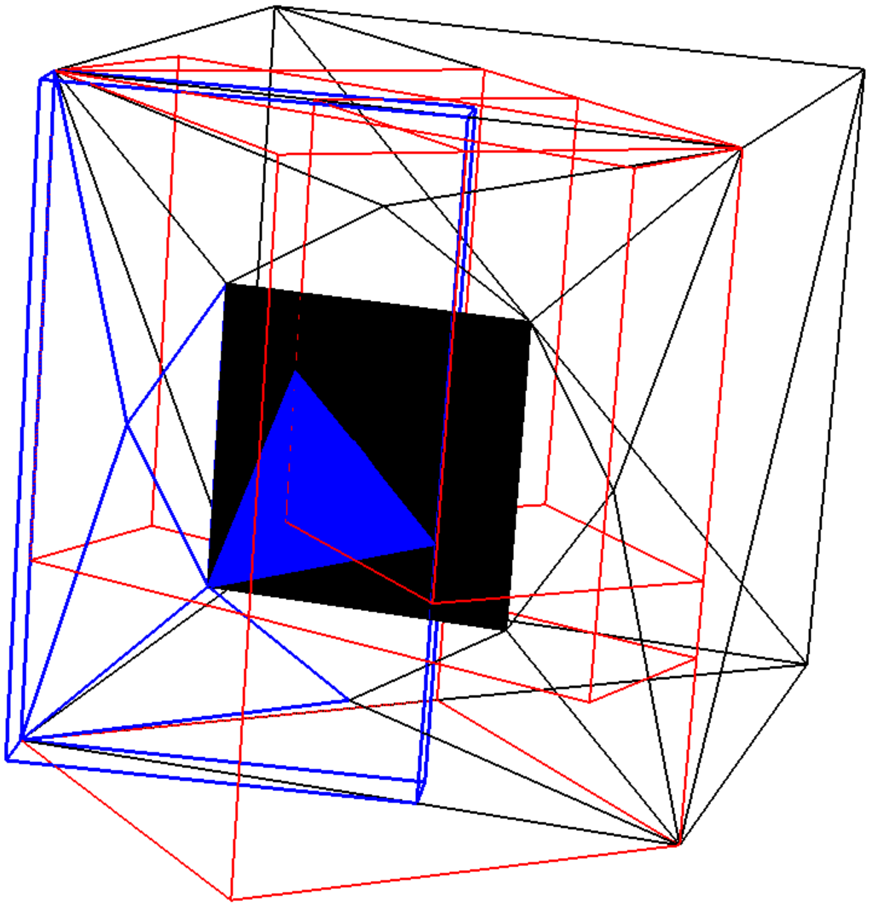
HIGH VALENCE BOUNDING BOX INVESTIGATION



MEDIAN SPLITTING ALGORITHM

CONTROLLABLE PARAMETERS

Parameter	Default Value
Max Num. Leaf Entities	8
Max Tree Depth	0
Worst Split Ratio	0.95
Best Split Ratio	0.0

$$splitting\ ratio = \frac{|left\ child\ primitives\ -\ right\ child\ primitives|}{parent\ entities}$$

Solution: Set the worst splitting ratio to 1 to force continued build of leaf nodes.

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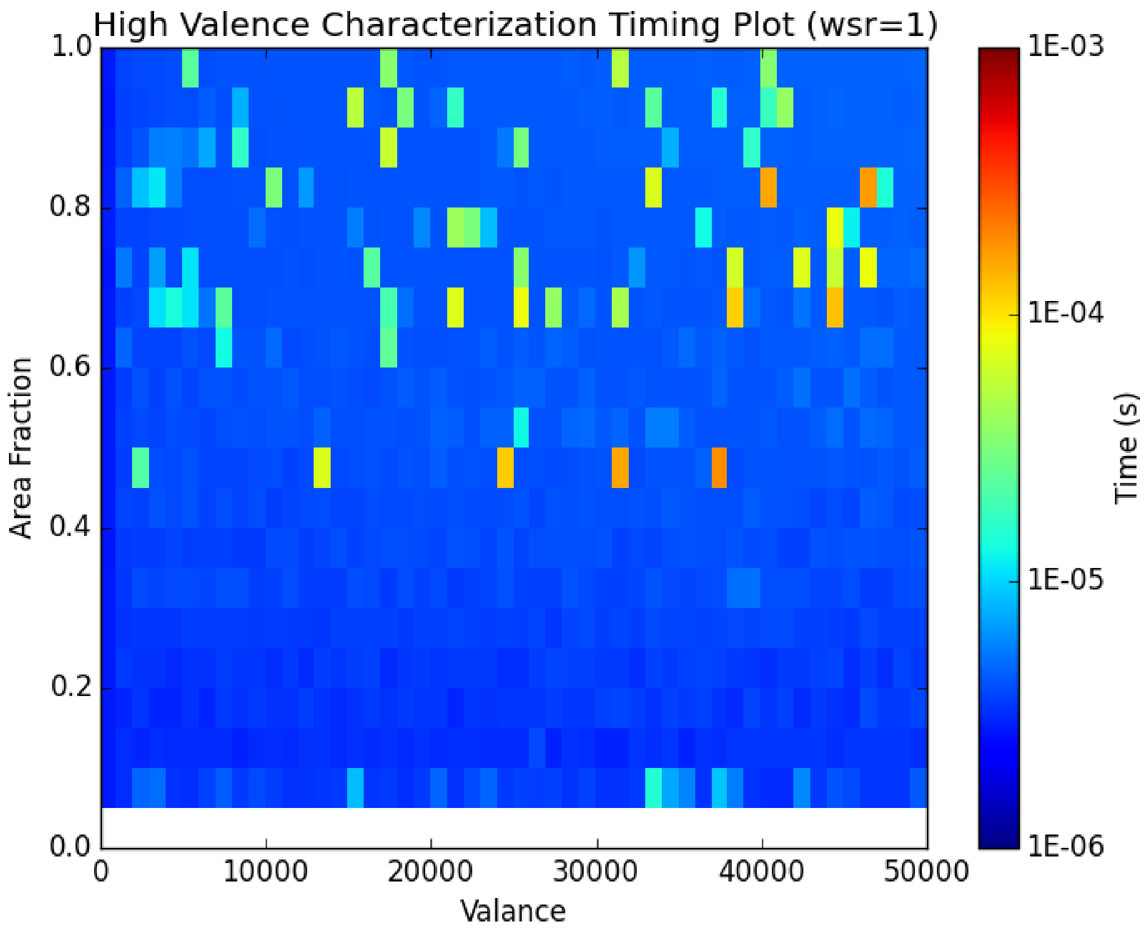
NEW HV STUDY RESULTS



Performance is maintained without need for altered faceting.

SURFACE AREA HEURISTIC

The Surface Area Heuristic (SAH) improves BVH traversal performance by 30% on average.[8]

$$C_s = C_t + \frac{A_l}{A_p}|P_l|C_i + \frac{A_r}{A_p}|P_r|C_i$$ [1]

C_s - estimated cost of split

C_t - cost of traversal to child nodes

A_l - surface area of left child

A_p - surface area of parent bounding volume

P_l - primitives contained by the left child

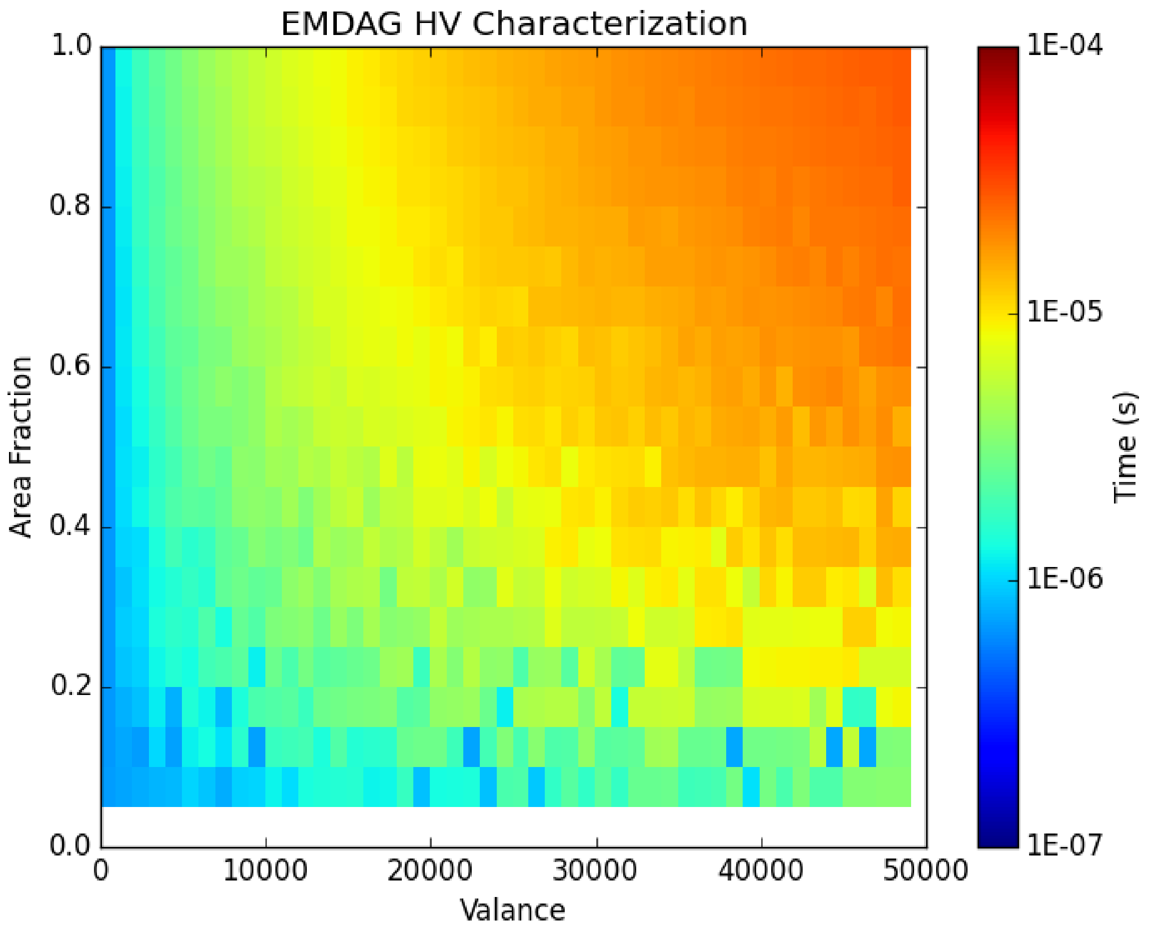
C_i - cost of primitive intersection check

A_r - surface area of right child

P_r - primitives contained by the right child

SAH APPLIED TO HIGH VALENCE

This same test was performed using the Embree ray tracing kernel. [14]



FEATURE-ADAPTIVE BVH CONSTRUCTION

FEATURE-ADAPTIVE BVH CONSTRUCTION

This process is likely of more interest to radiation transport than rendering.

Rendering	$(\sim 8\frac{rays}{px})(1024 \times 1080\, px) = 1.7 \times 10^7$ primary rays
Radiation Transport	10^9 histories $= 10^9$ primary rays

There is at least an additional order-of-magnitude in secondary rays for radiation transport.

- Higher collision density
- Secondary particle generation
- Variance reduction

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GENERAL RAY TRACING COST ANALYSIS

tts - time to solution

C - cost of other operations

T_B - acceleration data structure build time

T_T - average traversal time

N_r - ray queries required for solution

q - acceleration data structure quality

$$tts = C + T_B + \sum^{N_r} T_T$$

$$tts = C + T_B + \sum^{N_r} T_T(q, \ldots)$$

$$q(T_B) \rightarrow T_T(T_B) \rightarrow T_T \propto \frac{1}{{T_B}^x} \; (x \geq 0)$$

$$tts = C + T_B + \sum^{N_r} T_T(T_B, \ldots)$$

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PROPOSED BUILDING SCHEME

Construct BVH

- SAH
- tag poorly formed leaves

→

Resolve Tagged Leaves

Step 1:

- feature detection
- registered features
  - criterion for detection

Step 2:

- modified SAH?
- modified Median Splitting

FEATURE-ADAPTIVE BVH CONTRIBUTIONS

- Adaptive building addresses common mesh feature which is difficult for generalized heuristics to cope with and is detrimental to performance.

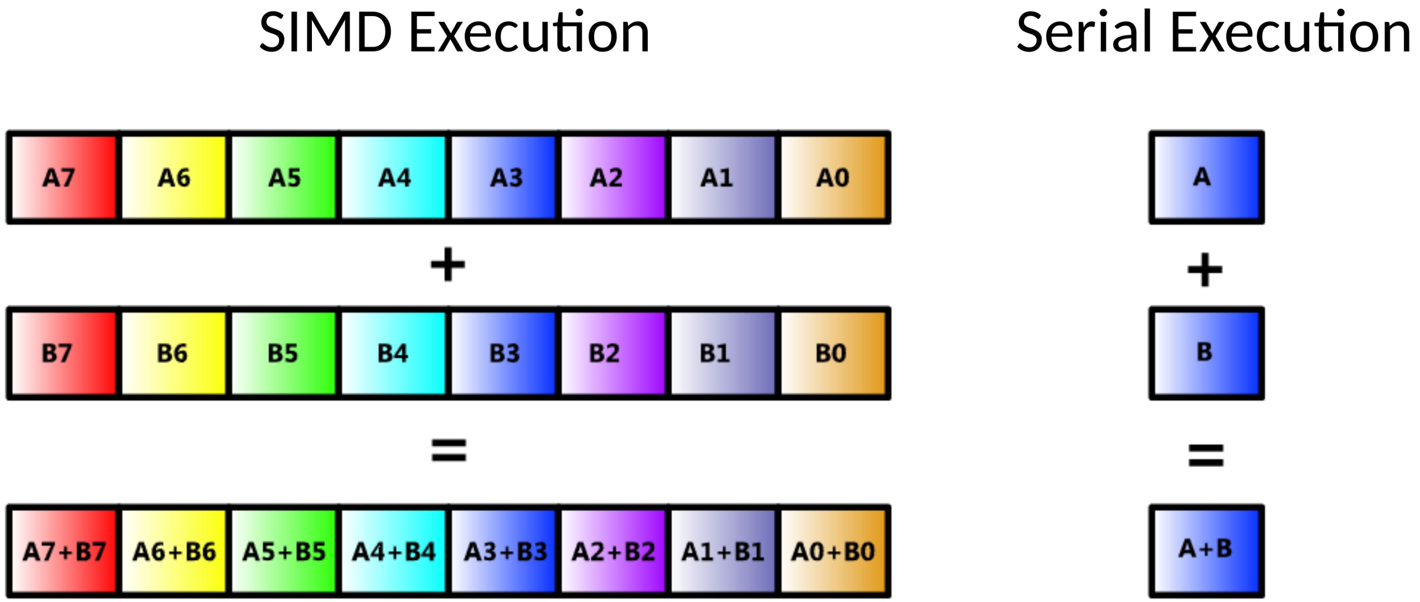
- BVH heuristic adaptation maintains expected O(logN) performance without the need for additional triangles or mesh alteration.

$$tts = C + T_B + \sum^{N_r} T_T \left(T_B , \ldots \right)$$

EMDAG

ARCHITECTURE BASED ACCELERATION

- Embree was not selected only for its use of the SAH.
- It employs Single Instruction Multiple Data (SIMD) commands, performing multiple ray-box and ray-triangle intersection checks at once in single-precision.

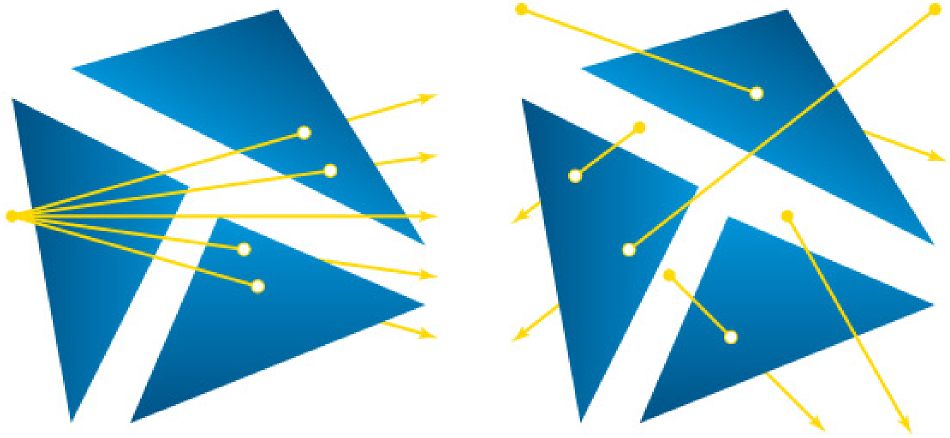


SOME HISTORY

Two approaches to using SIMD in ray tracing:

- N:1 - test many rays against a single box at once
- 1:N - test one ray against many boxes at once

Performance of selected method will depend on *ray coherence*.



coherent incoherent

* image courtesy of Intel

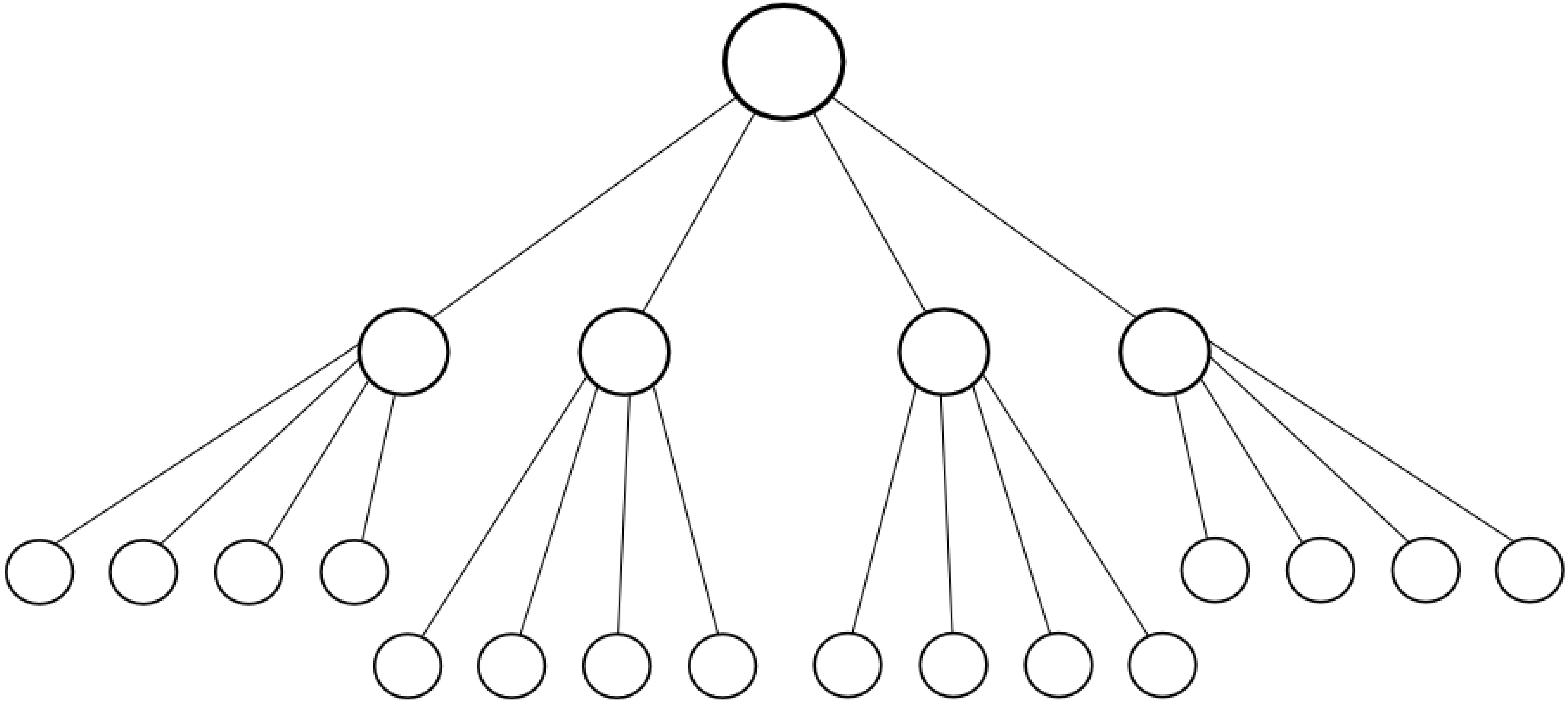
QUASI-MONTE CARLO RAY TRACING

photo-realism (rendering based on realistic photon physics)

N:1		**1:N**
(ray packets)		(single-ray SIMD traversal)
ray coherence	→	ray incoherence
visualization	→	physical rendering/simulation
		MCRT

SIMD BVH TOPOLOGY

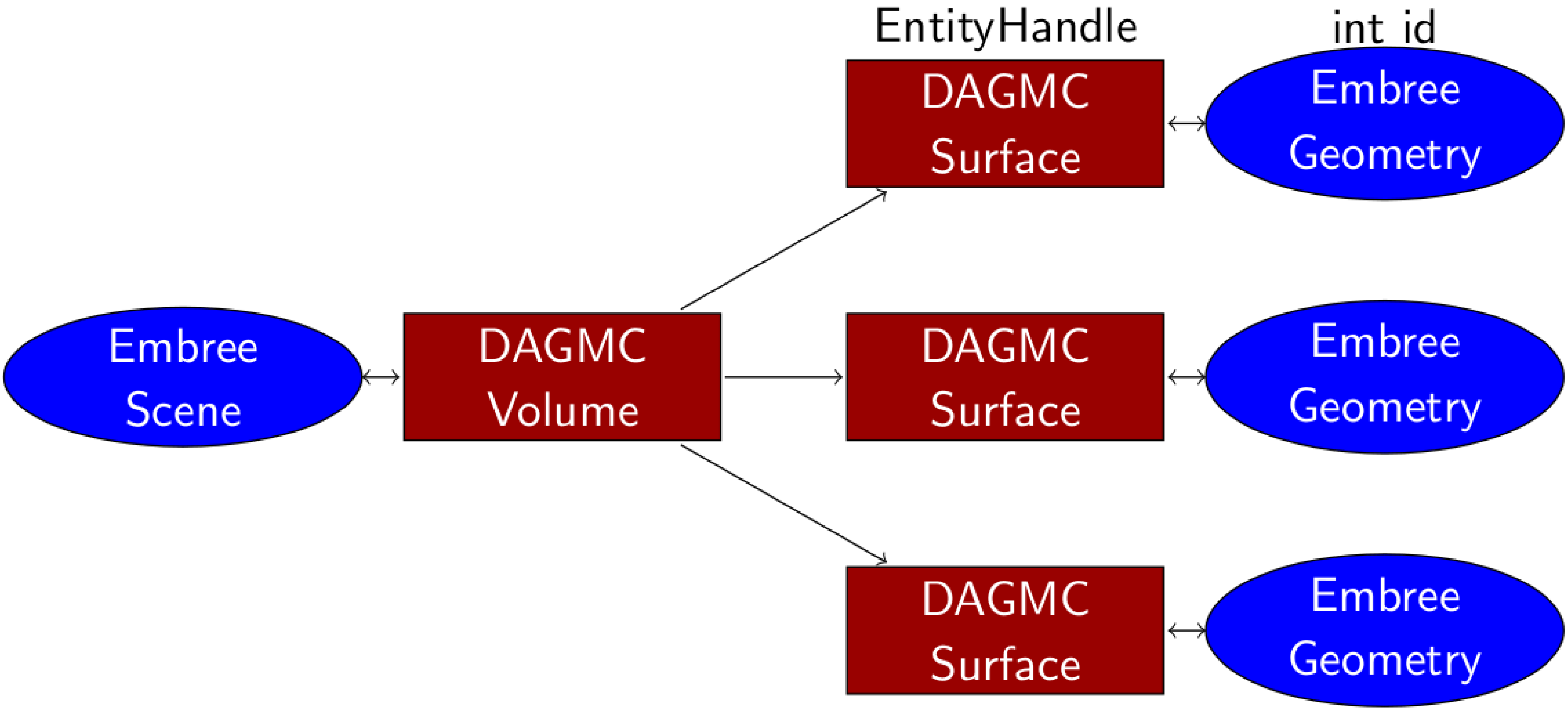
In order to take advantage of SIMD register widths BVH topologies are altered.



This is accomplished by collapsing a binary tree into an n-ary tree.

INTEGRATING EMBREE WITH DAGMC

(EmDAG)



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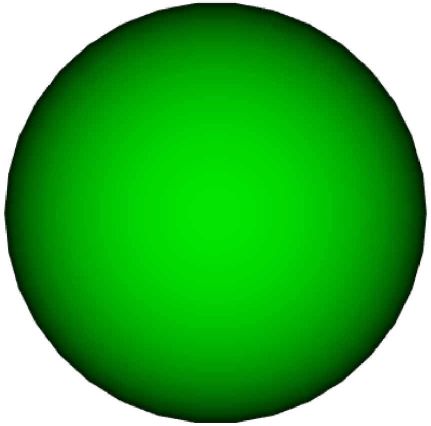
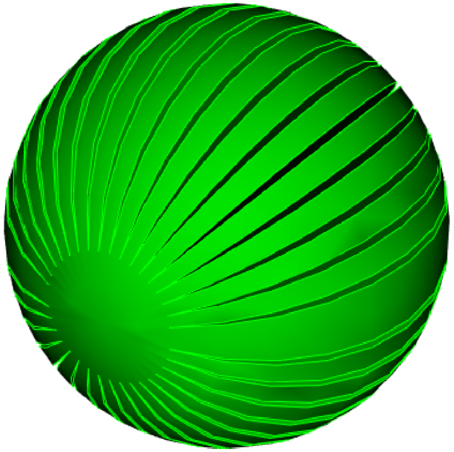
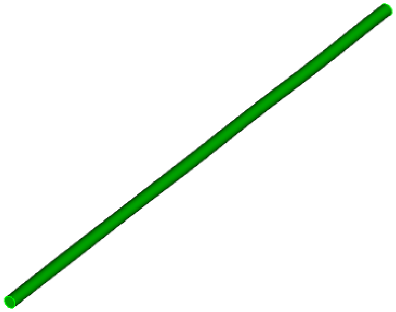
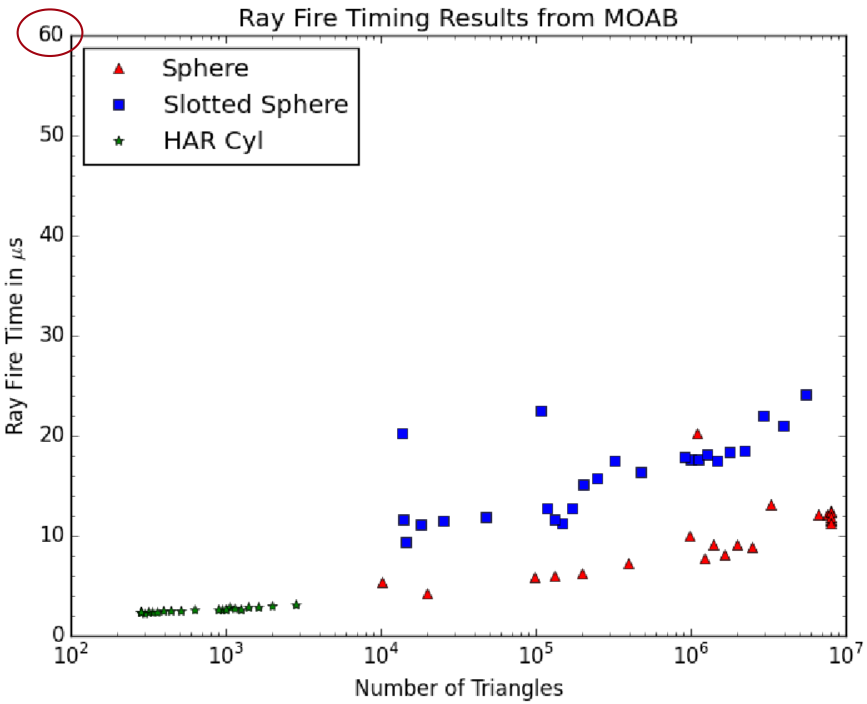
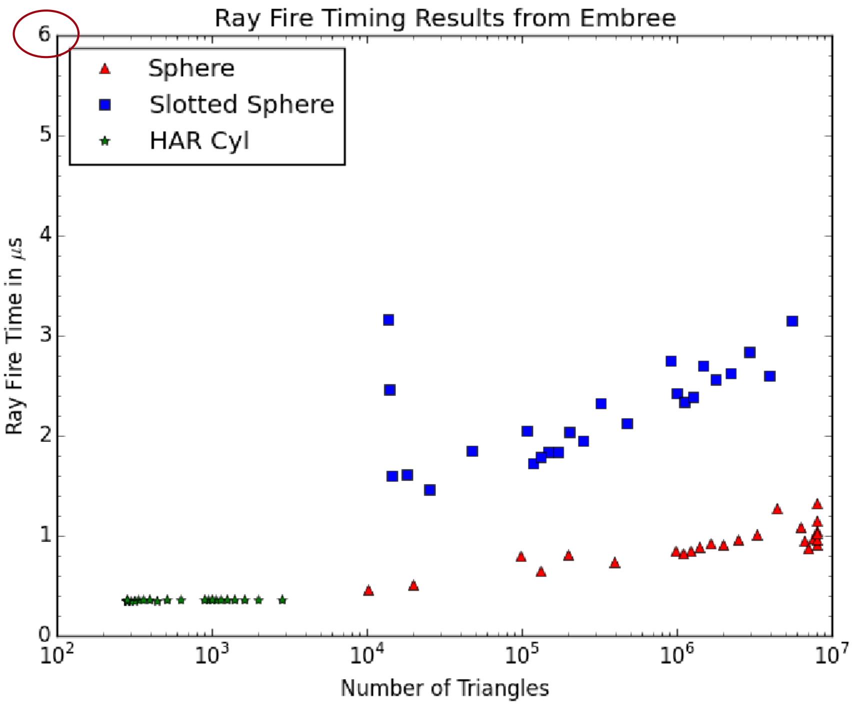
RAY FIRE TESTING ZOO







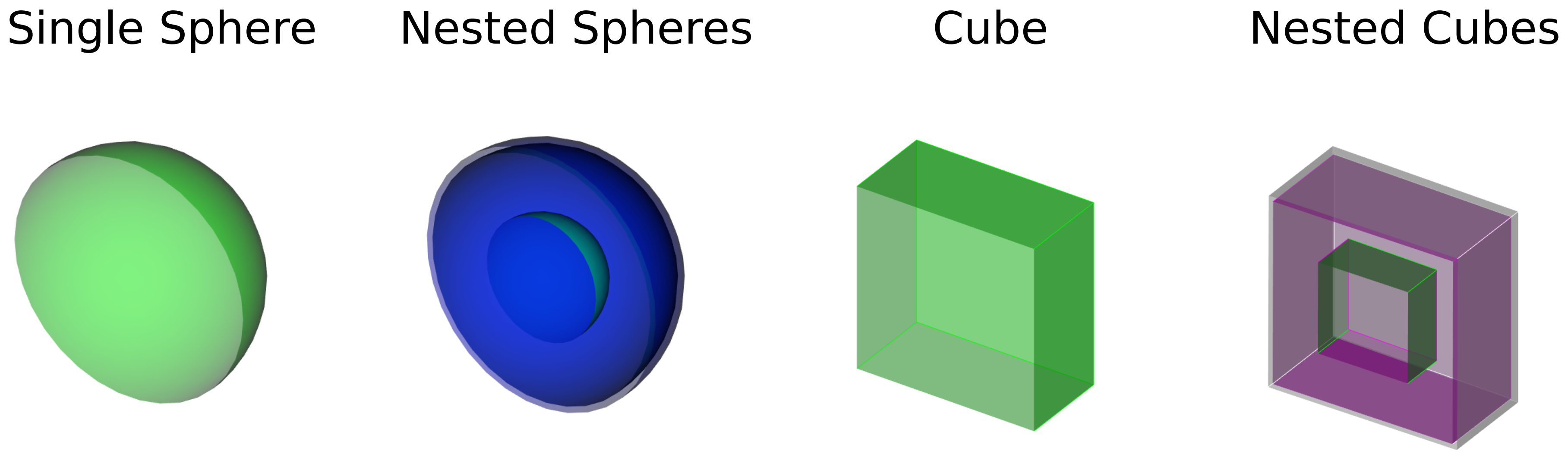
PERFORMANCE COMPARISON

DAGMC (MOAB)	EmDAG (Embree)
	

TRANSPORT TESTING

EmDAG was applied to a few simple models:

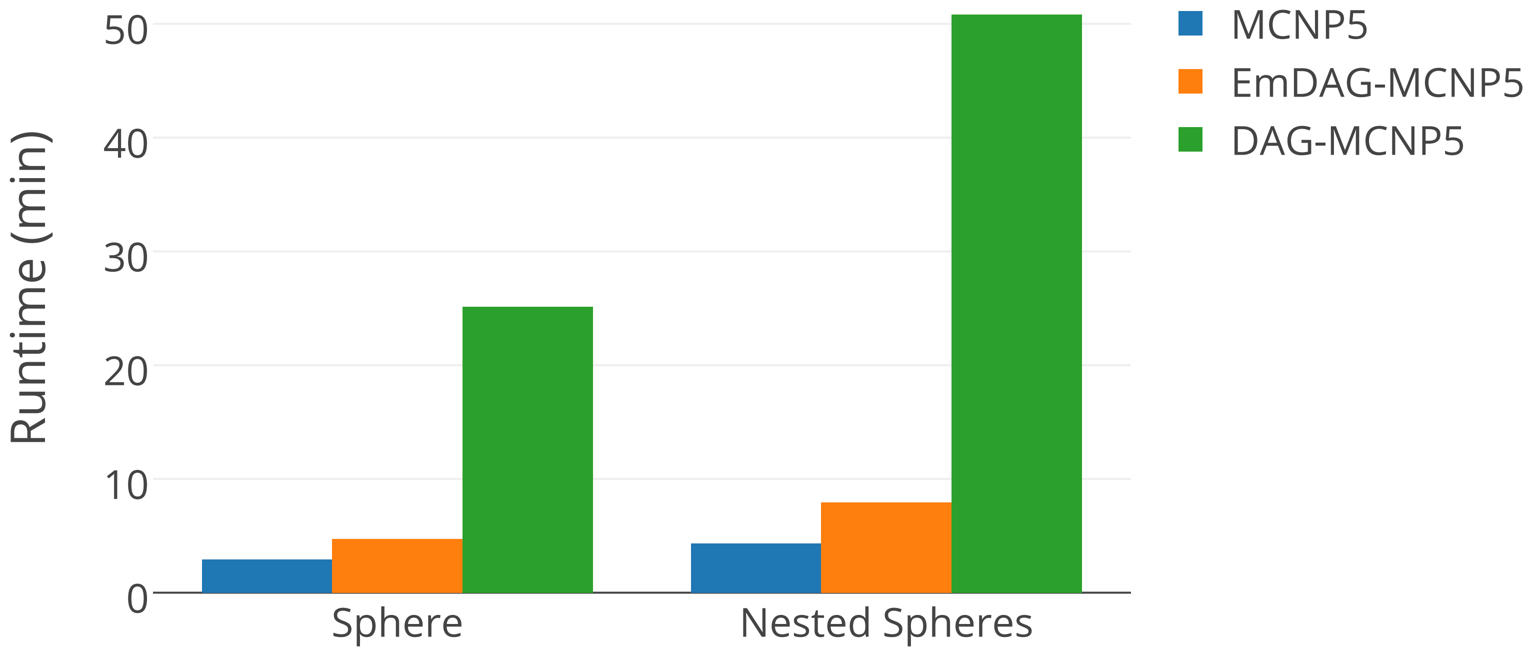
- 5 MeV isotropic neutron point source at model origin
- All volumes are water-filled (ρ = 1 g/cc)
- Faceting tolerance: 10^{-4}cm
- 1M histories



Flux and energy tallies were applied in all cells.

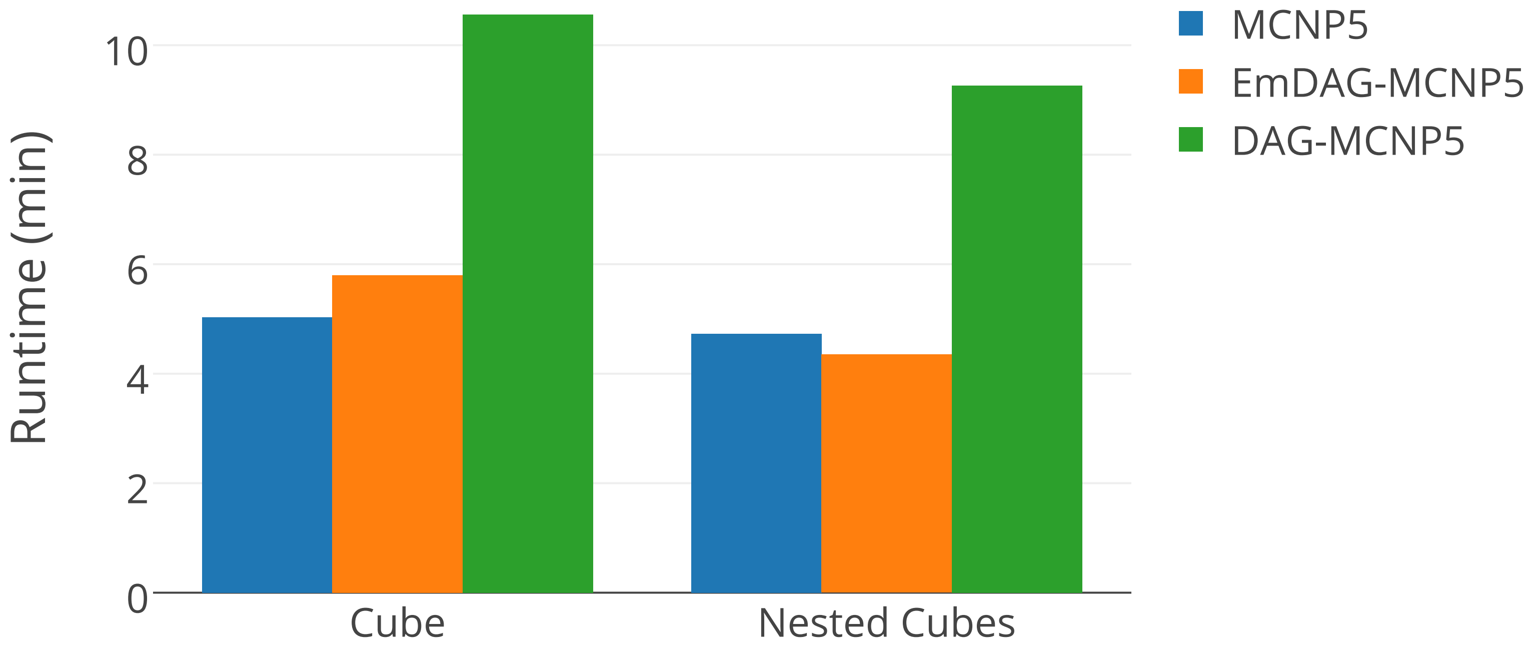
TRANSPORT PERFORMANCE

SPHERE MODELS



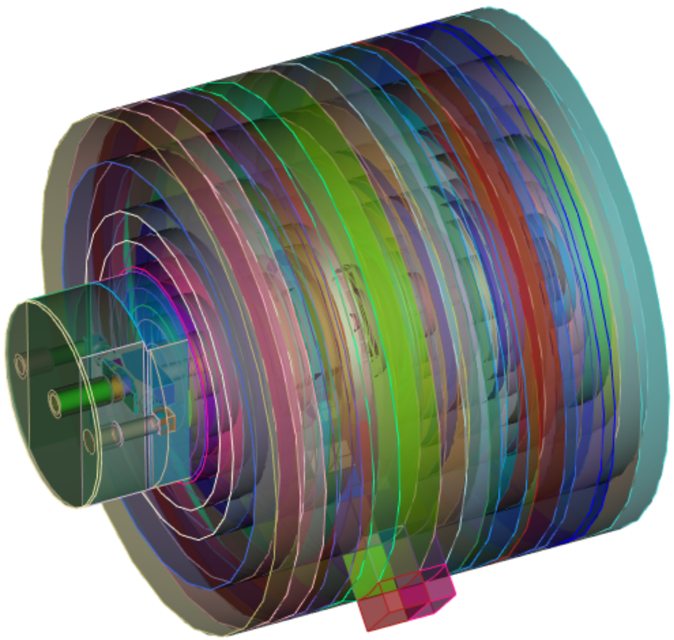
TRANSPORT PERFORMANCE

CUBE MODELS



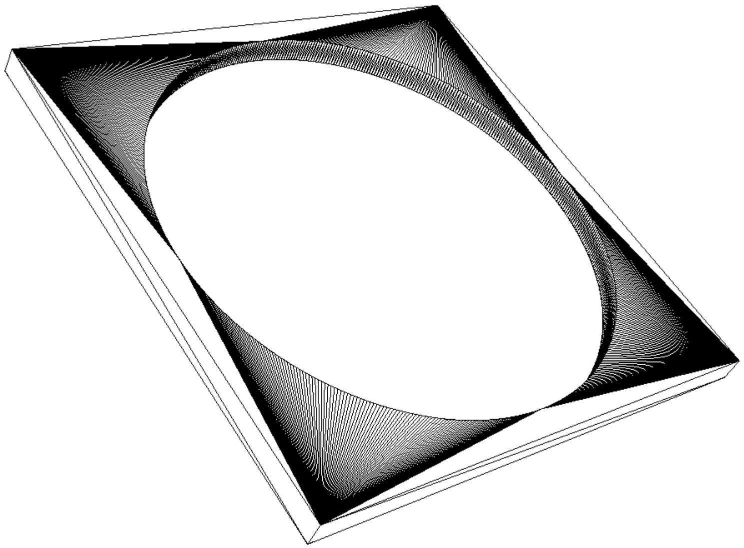
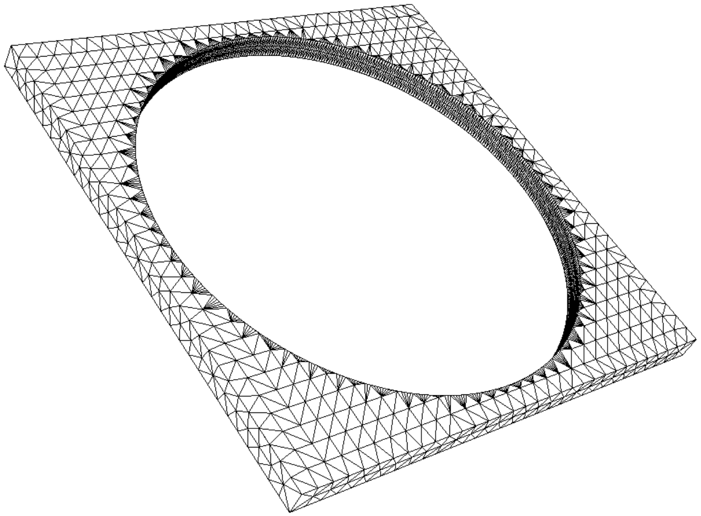
FNG TRANSPORT TEST

- The original source was replaced with 14.1 MeV neutron isotropic volume source.
- 100M histories
- Facet tolerance: 1e-04cm
- Length tolerance: 5cm

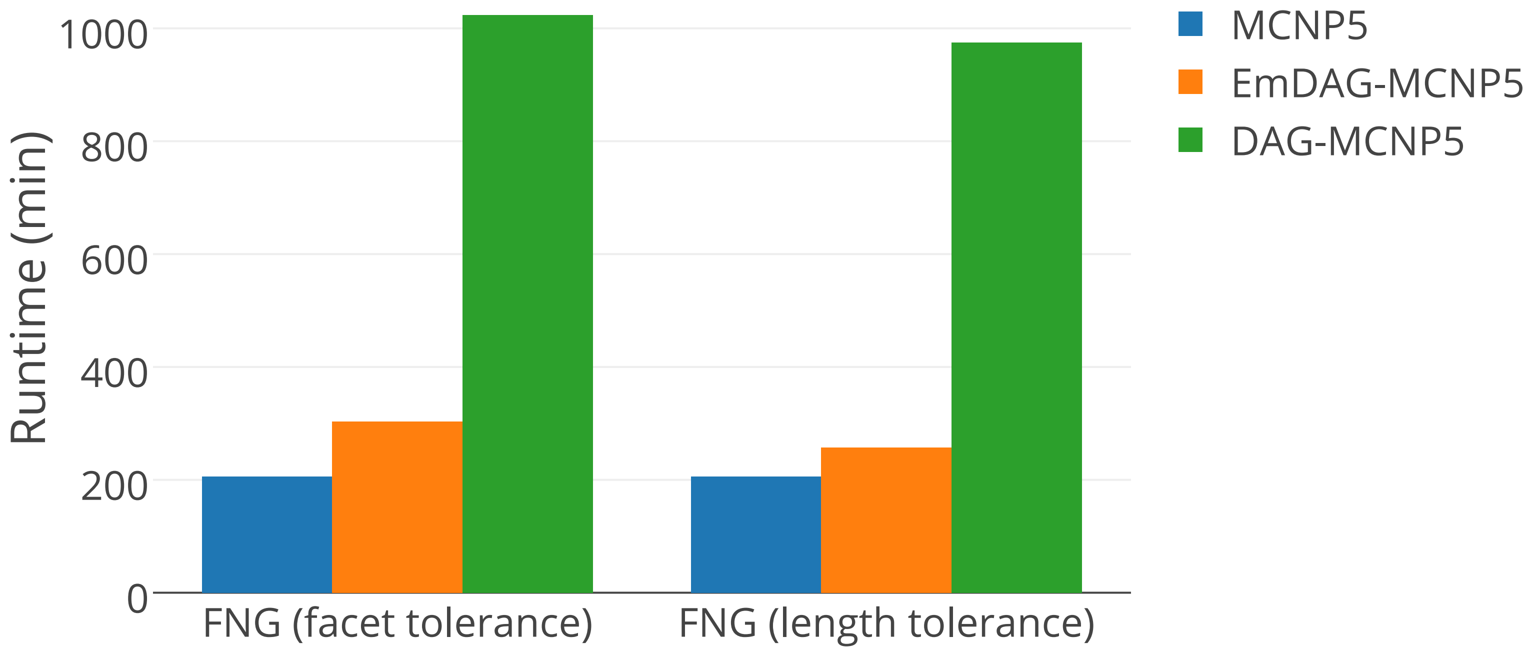


A flux mesh tally was applied over the entire problem.

FNG FACETING

Faceting Tolerance Only	With Length Tolerance
	

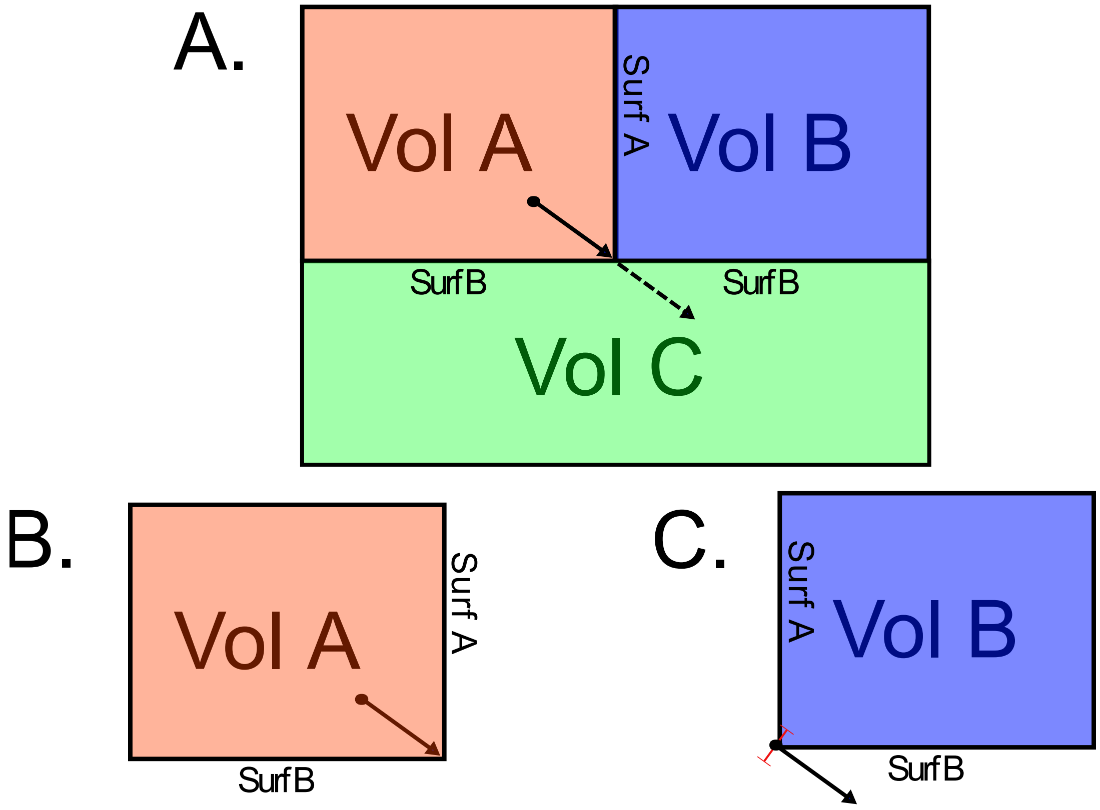
FNG TRANSPORT RESULTS



15% improvement in EmDAG performance with length tolerance applied

EMDAG LIMITATIONS

Tolerance(s)	Lost Particles
Faceting Tolerance	255
Faceting & Length Tolerance	247



Cause: Conversions from single to double precision and vice versa.

ENHANCED SIMD BVH TRAVERSAL FOR MCRT

ENHANCED SIMD BVH TRAVERSAL FOR MCRT

Embree does not meet the requirements of the robust tracking algorithm used by DAGMC as it currently exists.

- Single to double precision conversion decouples logical and numerical position of particles.
- Embree has no known capability for deeper mesh interrogation for enhanced logical tracking.
- No closest to location capability is implemented.

KERNEL COMPARISON

MOAB	Embree
Pros: • designed for interrogation/manipulation of mesh • mesh data in contiguous memory	**Pros:** • SIMD BVH ray tracing framework relevant to MCRT • mesh data provision design
Cons: • double-precision • kernel impeded by database context	**Cons:** • single-precision • limited mesh data interface

HIGHER PRECISION SIMD KERNEL

- The natural inclination might be to make Embree double precision
- This is doubly disadvantageous:
  - slower double precision calculations
  - increased box memory means fewer entities can fit in lower level caches

MIXED-PRECISION CONCEPT

PROPOSED DESIGN OF SIMD BVH FOR MCRT

MOAB

- generate single-precision bounding boxes around double-precision primitives

→

RT Kernel

- mesh provision via MOAB's direct access
- SIMD traversal in single-precision hierarchy
- SIMD double-precision triangle intersections

↘ ↖

DAGMC

- RT Kernel for numerical position
- MOAB for logical position when necessary

↗ ↙

ENHANCED SIMD BVH FOR MCRT CONTRIBUTIONS

- SIMD oriented closest to location algorithm
- Single-precision allows much of Embree's speed to be retained as majority of time is spent in BVH traversal.[3]
- Takes advantage of MOAB's direct access methods to provide a spatial hierarchy traversal suitable for engineering analysis purposes with comparable performance to that of analytic geometry methods such as CSG on common CPU architectures.

IMPLICIT SURFACES AND SIGNED DISTANCE FIELDS

IMPLICIT SURFACES

(LEVEL-SET METHODS)

An implicit surface is a multivariate function defined over an R^3 domain

$$\Omega(R^3) \to R$$

where points on the surface are represented by the isocontour $v = 0$.[9]

$$\Omega(\vec{x}) - v = 0$$

Important geometric properties can be easily recovered from this representation.

Surface Normal

$$< \Omega_x(\vec{x}), \Omega_y(\vec{y}), \Omega_z(\vec{z}) >$$

Distance to Nearest Intersection

$$|\Omega(\vec{x})|$$

Interior vs. Exterior Locations

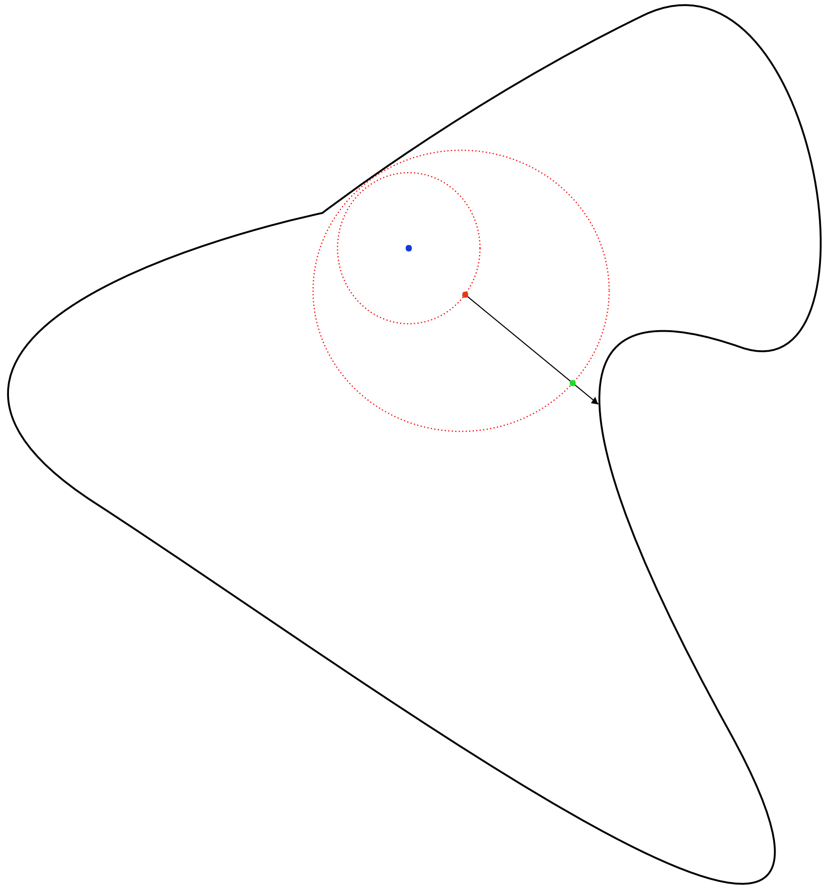
$$sign(\Omega(\vec{x}))$$

IMPLICIT SURFACES

Implicit surface uses:

- modeling (CSG), simulation, triangulation
- rendering of dynamic surfaces like smoke or fire ($\Omega(\vec{x}, t)$) [6]

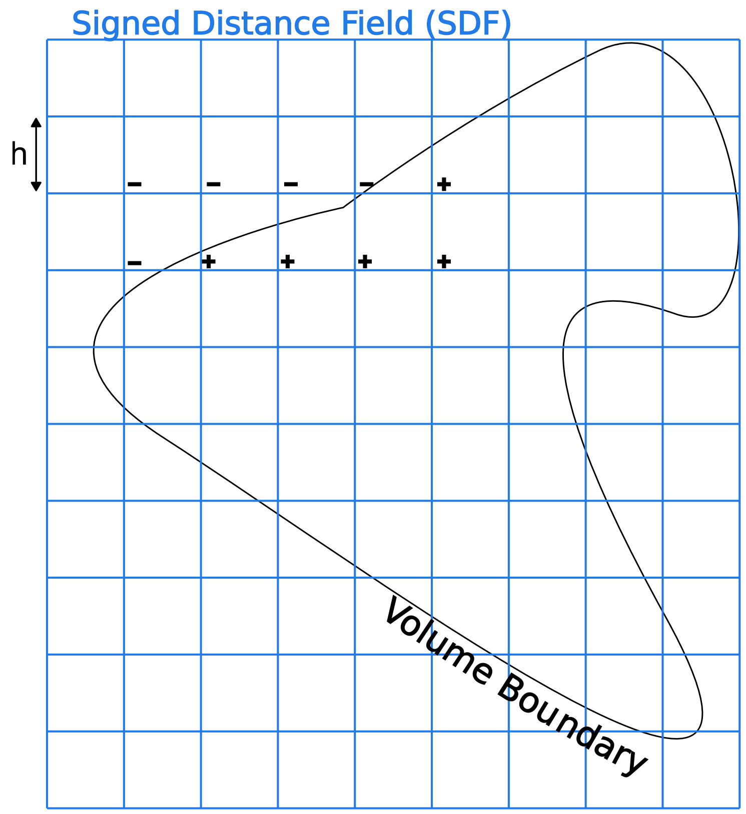
Ray Marching:



SIGNED DISTANCE FIELDS

- $d(\vec{x}) = 0$ for all $\vec{x}$ on the surface boundary
- $d(\vec{x}) > 0$ for all $\vec{x}$ inside the surface boundary
- $d(\vec{x}) < 0$ for all $\vec{x}$ outside the surface boundary

$$d(\vec{x}) = sign(\Omega(\vec{x}))|\Omega(\vec{x})|$$



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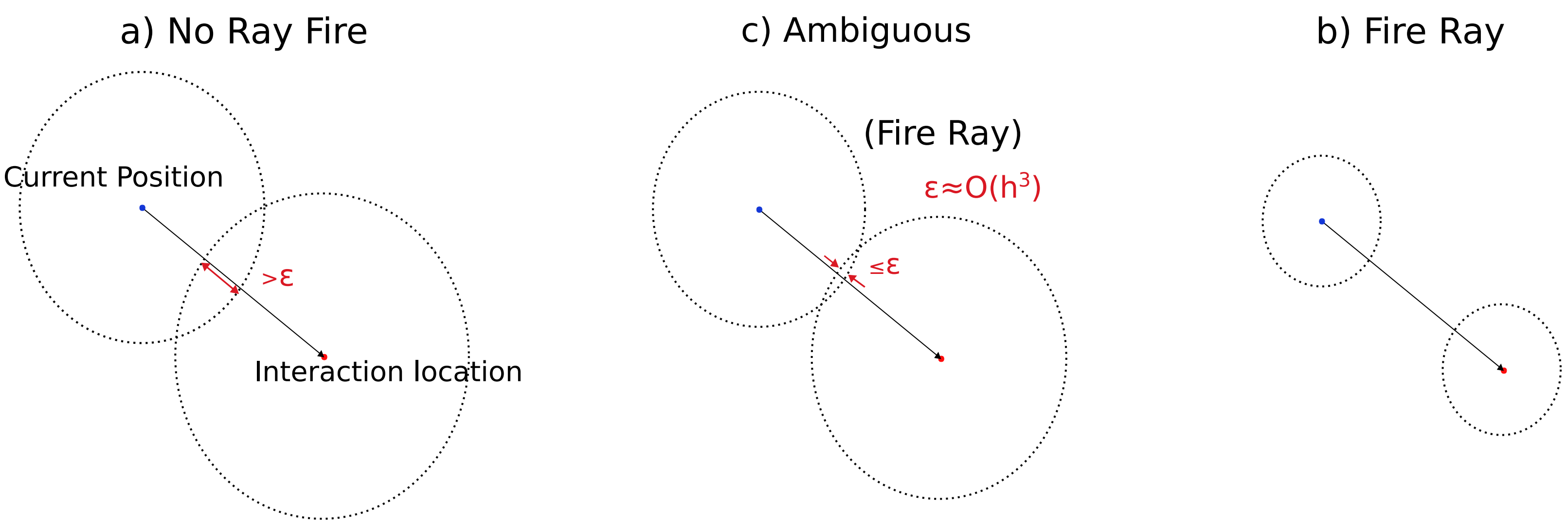
PARTICLE TRACKING PRECONDITIONER

Concept: Use interpolated signed distance values to rule out surface crossing between current position and next event location.

- avoids O(log(N)) in favor of O(1) process
- best for particles traveling far from surfaces



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PARTICLE TRACKING PRECONDITIONER

- Signed Distance Values (SDVs) can be used to precondition closest to location calls or determine point containment in O(1) complexity as well.

Simple condition for these operations:

$$|SDV| > \epsilon$$

INTERPOLATION ERROR ESTIMATE

(A 2D LINEAR EXAMPLE)

$$\epsilon = \frac{1}{2}\Delta x(h - \Delta x)\frac{\partial^2 u}{\partial x^2} + \frac{1}{2}\Delta y(h - \Delta y)\frac{\partial^2 u}{\partial y^2}$$

ϵ	- interpolation error
Δx	- x distance to interpolation point from data point
h	- mesh interval size
$u(x, y)$	- sampled function on mesh
Δy	- y distance to interpolation point from data point

curvature terms are problematic

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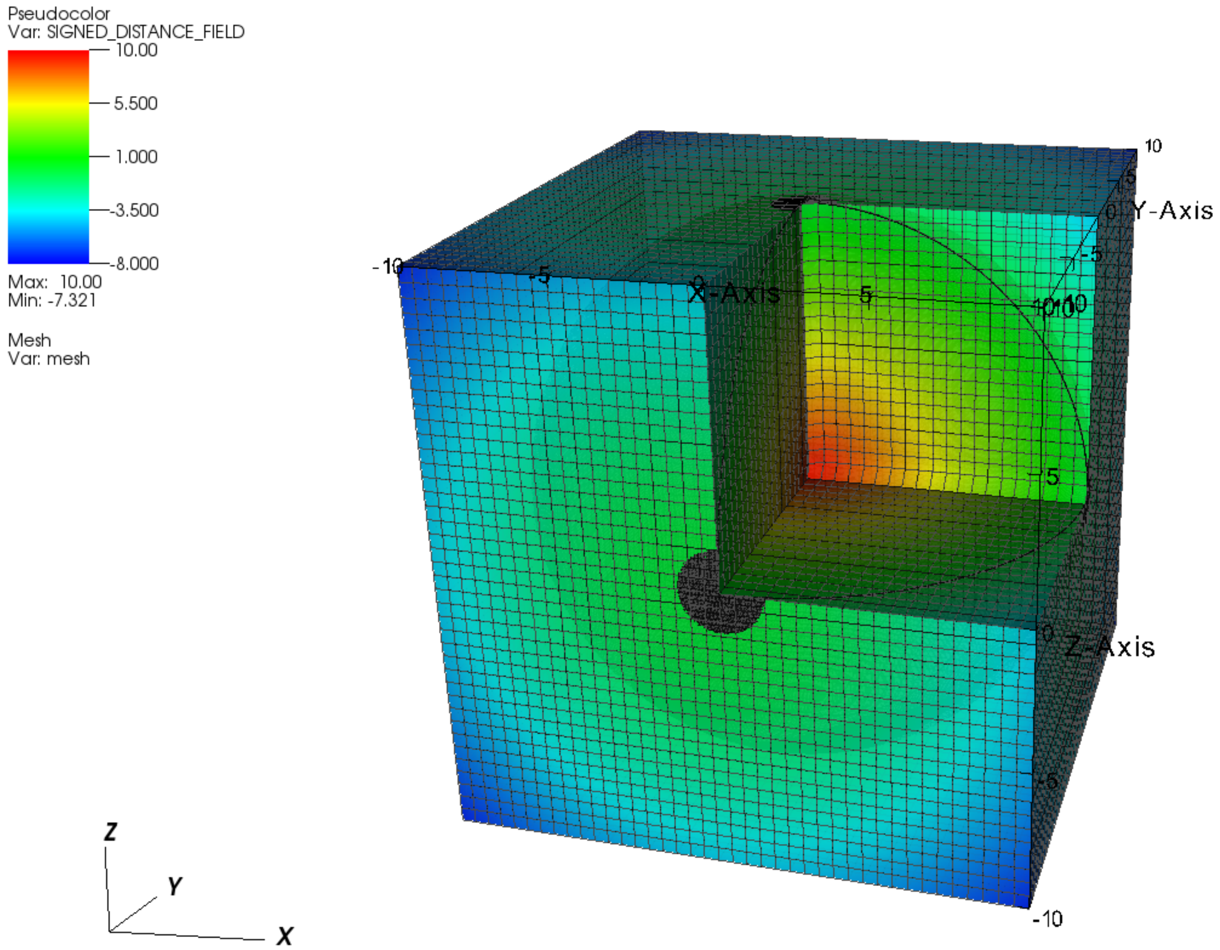
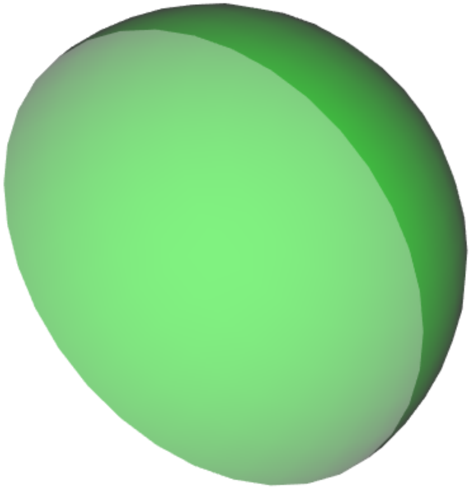
INITIAL IMPLEMENTATION

- uses MOAB's structured mesh interface
- populated using MOAB's ray tracing interface (closest to location)
  - disambiguate distance value signs using DAGMC's point containment algorithm



PRECONDITIONER TEST

- 10cm radius sphere
- 5 MeV isotropic neutron point source at origin
- density varied from 0 to 1 (g/cc)
- faceting tolerance: 10^{-4}cm
- 1M histories (100k for profiling)
- Mesh step size: $h = 0.5cm$
- Error evaluation: $\sqrt{3}h$



Flux and energy cell tallies were applied.

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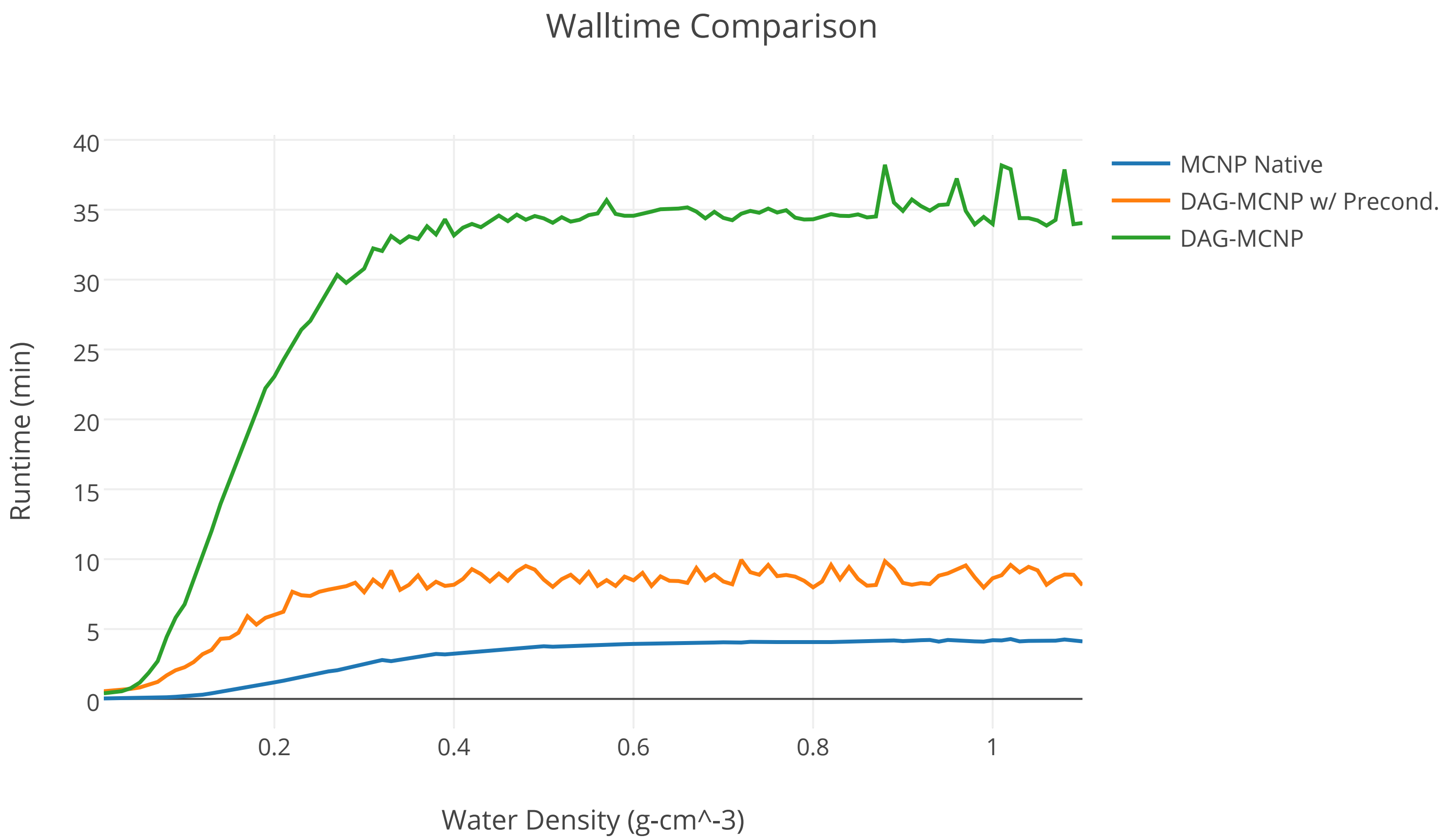
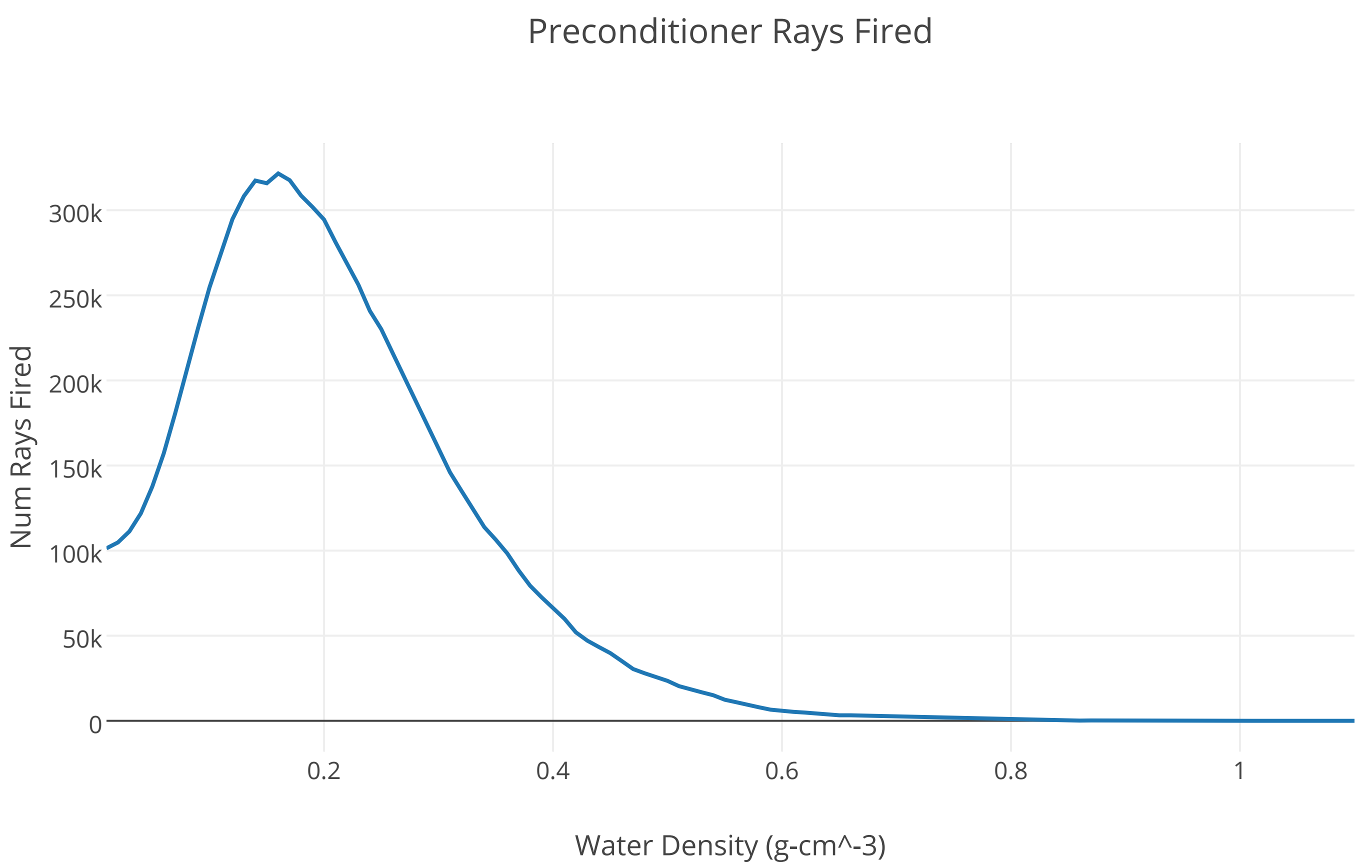
INITIAL RESULTS

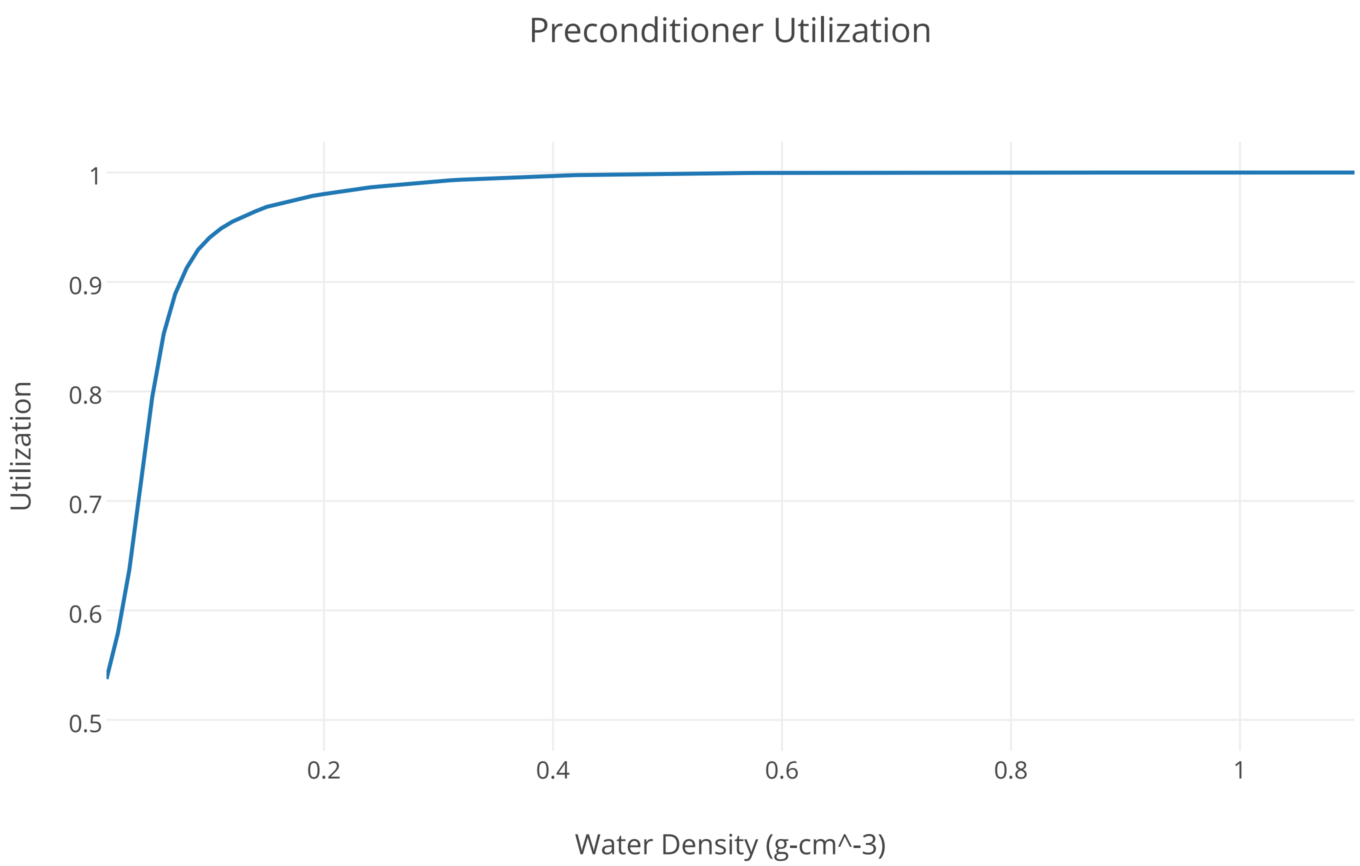


INITIAL RESULTS



INITIAL RESULTS

$$u = \frac{DAGMC\,rays - DAGMC\,w/\,precond.\,rays}{DAGMC\,rays}$$



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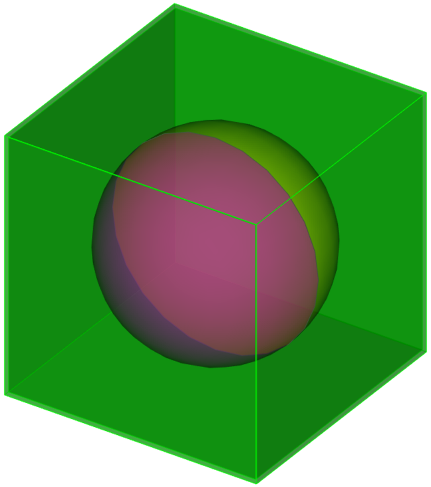
CHARGED PARTICLE TRANSPORT

- Particles take many small steps in space to approximate their straggling paths.
- Each step requires a geometry check for surface crossing.

A sample problem of electron transport from MCNP6 tests:

- Fluorescence test of 1 keV - 100 keV photons on Fe/W target
- 5,000 histories
- single-event electron physics



INITIAL RESULTS

	MCNP6[2]	DAG-MCNP6 w/ Precond.	DAG-MCNP6
Run Time (min)	0.16	0.46	1413.94

SIGNED DISTANCE FIELD PRECONDITIONER

SIGNED DISTANCE FIELD PRECONDITIONER

- The SDF preconditioner has already been shown to be a powerful acceleration tool given the proper conditions.
- The identification of proper conditions for this data structure is important.
- Memory usage is a concern:
  - Adaptive mesh refinement or octree may be useful.
  - Error estimation becomes more difficult with non-uniform techniques.
  - Other global mesh methods will be explored.[10]
- Predictive model of utilization will be important if global uniform mesh is not an option.

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SIGNED DISTANCE FIELD PRECONDITIONER CONTRIBUTIONS

- Population of signed distance field with ray tracing kernel rather than generating an implicit surface representation for static mesh application.

- When applied in a robust manner, this method can decrease lost particle rate in unsealed models.

- Coupling of the signed distance field to the BVH may provide insight for further accelerations.

- When well utilized, this data structure can bring particle tracking closer to an O(1) process than the O(logN) process relied upon in the past.

$$u\,O(1) + (1-u)\,O(logN)$$

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SUMMARY

FEATURE-ADAPTIVE BVH CONTRIBUTIONS

- Adaptive building addresses common mesh feature which is difficult for generalized heuristics to cope with and is detrimental to performance.
- BVH heuristic adaptation maintains expected O(logN) performance without the need for additional triangles or mesh alteration.

$$tts = C + T_B + \sum^{N_r} T_T\left(T_B, \ldots\right)$$

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FEATURE-ADAPTIVE BVH OBJECTIVES

- Implement feature-adaptive BVH builder in MOAB as proposed
- Establish conditions for leaf nodes expected to have a significant impact on performance
- Characterize and address any other detrimental mesh features discovered along the way
    - These additional mesh features may only be elucidated by a higher-performance system.
- Demonstrate effectiveness for transport on HV test model and other production models known to contain HV features.

ENHANCED SIMD BVH FOR MCRT CONTRIBUTIONS

- SIMD-oriented closest to location algorithm
- Single-precision allows much of Embree's speed to be retained as majority of time is spent in BVH traversal.[3]
- Takes advantage of MOAB's direct access methods to provide a spatial hierarchy traversal suitable for engineering analysis purposes with comparable performance to that of analytic geometry methods such as CSG on common CPU architectures.
- Allows DAGMC's robust particle tracking to be coupled to a high-performance ray tracing kernel for improved CAD-Based radiation transport performance.

ENHANCED SIMD BVH FOR MCRT OBJECTIVES

- Implement a SIMD-oriented BVH builder in MOAB which generates memory contiguous single-precision bounding boxes around double-precision primitives (triangles).

- Develop or extend a ray tracing kernel which is capable of SIMD traversal on the MOAB-provided BVH and associated double-precision triangles.
  - Kernel should have no more lost particles than would be seen in the current version of DAGMC for the same triangle mesh.
  - Kernel should provide comparable performance to the EmDAG system.

- Compare performance and robustness to EmDAG system for simple transport problems

- Demonstrate effectiveness for production models as well

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SIGNED DISTANCE FIELD PRECONDITIONER CONTRIBUTIONS

- Population of signed distance field with ray tracing kernel rather than generating an implicit surface representation for static mesh application.

- When applied in a robust manner, this method can decrease lost particle rate in unsealed models.

- When well utilized, this data structure can bring particle tracking closer to an O(1) process than the O(logN) process relied upon in the past.

$$u\,O(1) + (1 - u)\,O(logN)$$

SIGNED DISTANCE FIELD PRECONDITIONER OBJECTIVES

- Create a predictive model for preconditioner utilization, u, based on three problem-specific factors:

$$u(\lambda, v, h)$$

  - λ - average mean free path
  - v - characteristic volume size
  - h - preconditioner mesh step size

- Explore global mesh preconditioner solutions for production DAGMC models.

- Demonstrate effectiveness of the utilization model and resulting data structure in toy and production models for neutron, photon, and charged particle transport.

PRELIMINARY PLAN AND TIMELINE

Short-term (next 3 months):

- Feature-adaptive BVH construction implementation in MOAB
- Predictive model development for SDF Preconditioner
  - Obtain and modify one-group cross-sections for control of λ
- Evaluate Feature-Adaptive BVH on HV test model and production models

Mid-term (next 6-8 months):

- Explore global mesh options for SDF preconditioner
  - Either ARM or SPGrid
- Begin R&D of SIMD BVH for MCRT
  - Single-precision BVH construction in MOAB
  - Robust single-precision BVH traversal w/ double-precision triangle intersections

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PRELIMINARY PLAN AND TIMELINE

End-term (8-12 months):

- Demonstrate new ray tracing kernel effectiveness in comparison to native codes and EmDAG
- Finalize form of SDF Preconditioner
  - Global solution application
  - Selective application based on predictive model
- Demonstrate SDF preconditioner effectiveness on toy and production models

Complete data collection & write

COMPLEMENTARY EFFECTS

- A SIMD-based closest to location algorithm
- A SIMD-based closest to location algorithm may allow avoidance of other, more costly methods of populating the SDF data structure.
- Coupling of the signed distance field to the BVH may provide insight for further accelerations.
- Feature-adaptive BVH construction will improve performance of both signed distance field population and transport queries during simulation.

The combined effect provides a more efficient pathway for CAD-Based Monte Carlo Radiation Transport analysis.

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