A Three-Dimensional Simulator for Internal-Charging Effect

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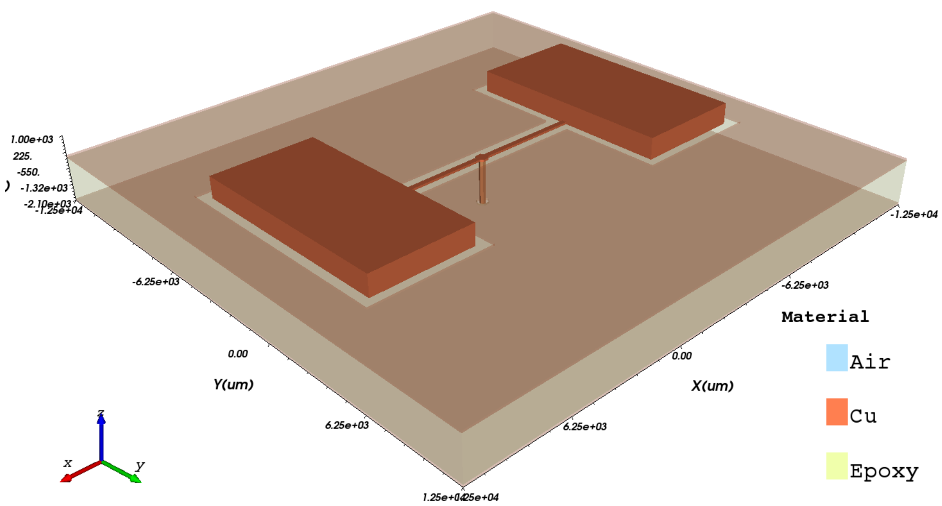
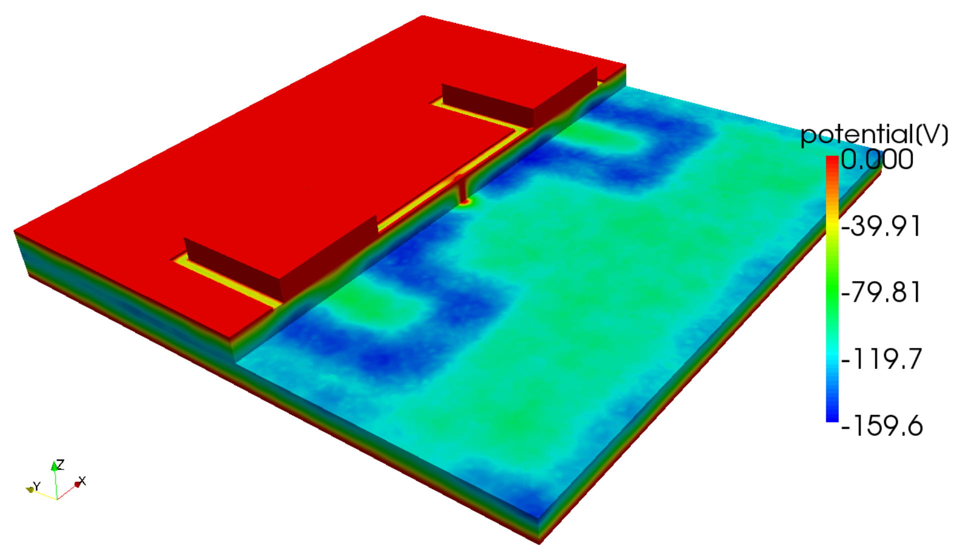
Summary

- 3D simulator of internal charging effect
  - Geant4 for tracking high-energy electrons
  - Continuum PDE solver for Poisson/continuity equations





Outline

- Description of the Simulator
  - Physics
  - Software components
- Test cases
  - 1D Slab: comparison with DICTAT
  - 3D PCB: performance bottleneck
- Proposal: Level-set in G4
  - Level-Set primer
  - Performance of level-set in G4 context
  - Road map

Physical Processes I

- Electron Physics
  - Multiple scattering / Ionization
  - Bremsstrahlung
- Photon Physics
  - Compton scattering

Physical Processes II

- Poisson's Eqn

$$\nabla\cdot\varepsilon\nabla\varphi=-\rho$$

- Charge continuity Eqn

$$-\frac{\partial\rho}{\partial t}=G-\nabla\cdot\mu\rho\vec{E}+\nabla\cdot\left[\left(\sigma_0+g\right)\vec{E}\right]$$

Deposited electron charge

Drift of deposited electrons

Radiation-induced conductance

$g=g_0 D^{\Delta}$

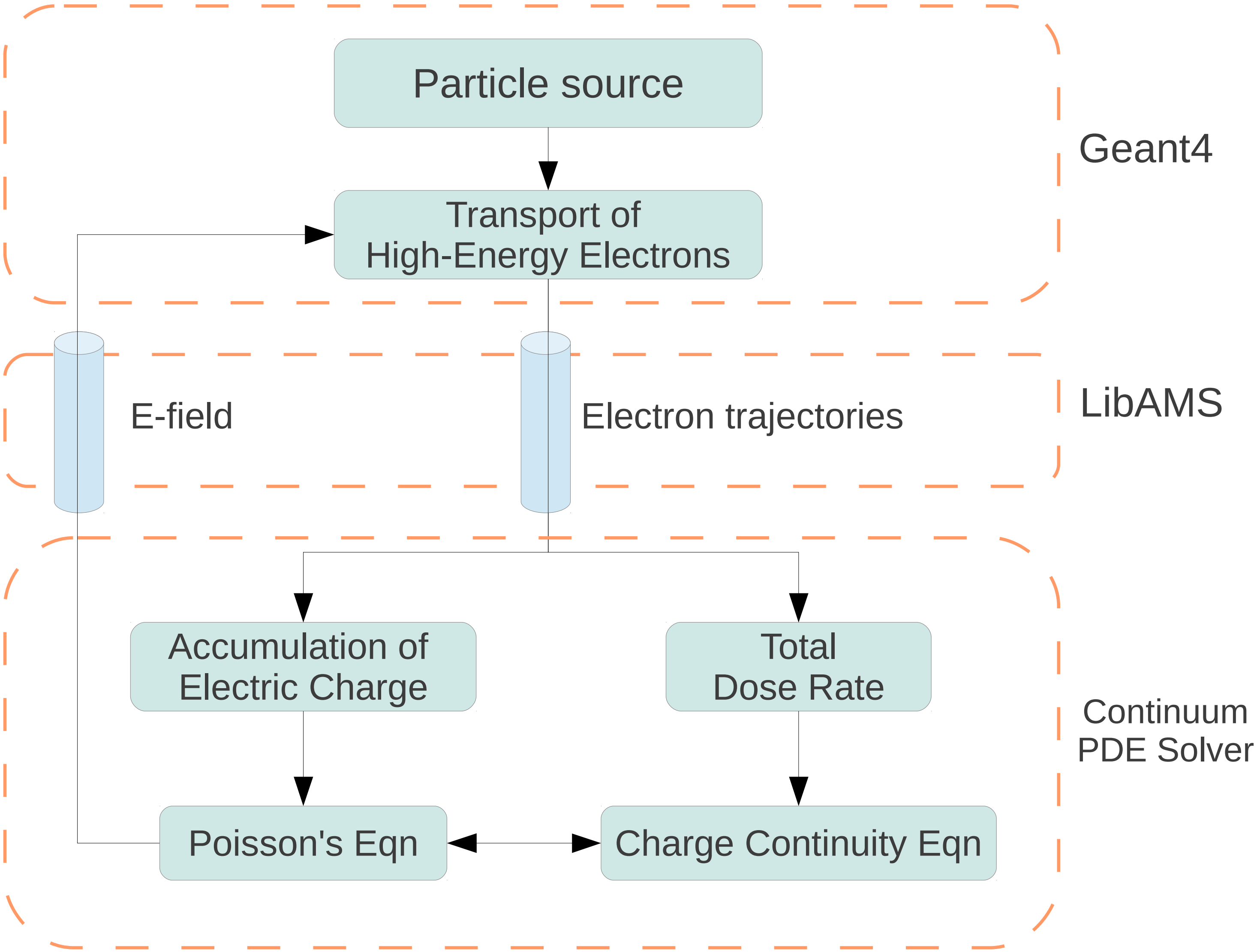
Intrinsic conductance

- Boundary Conditions
  - Dirichlet boundary at all insulator-conductor interface
    - Constant voltage, zero charge
  - Neumann boundary at insulator-vacuum interface

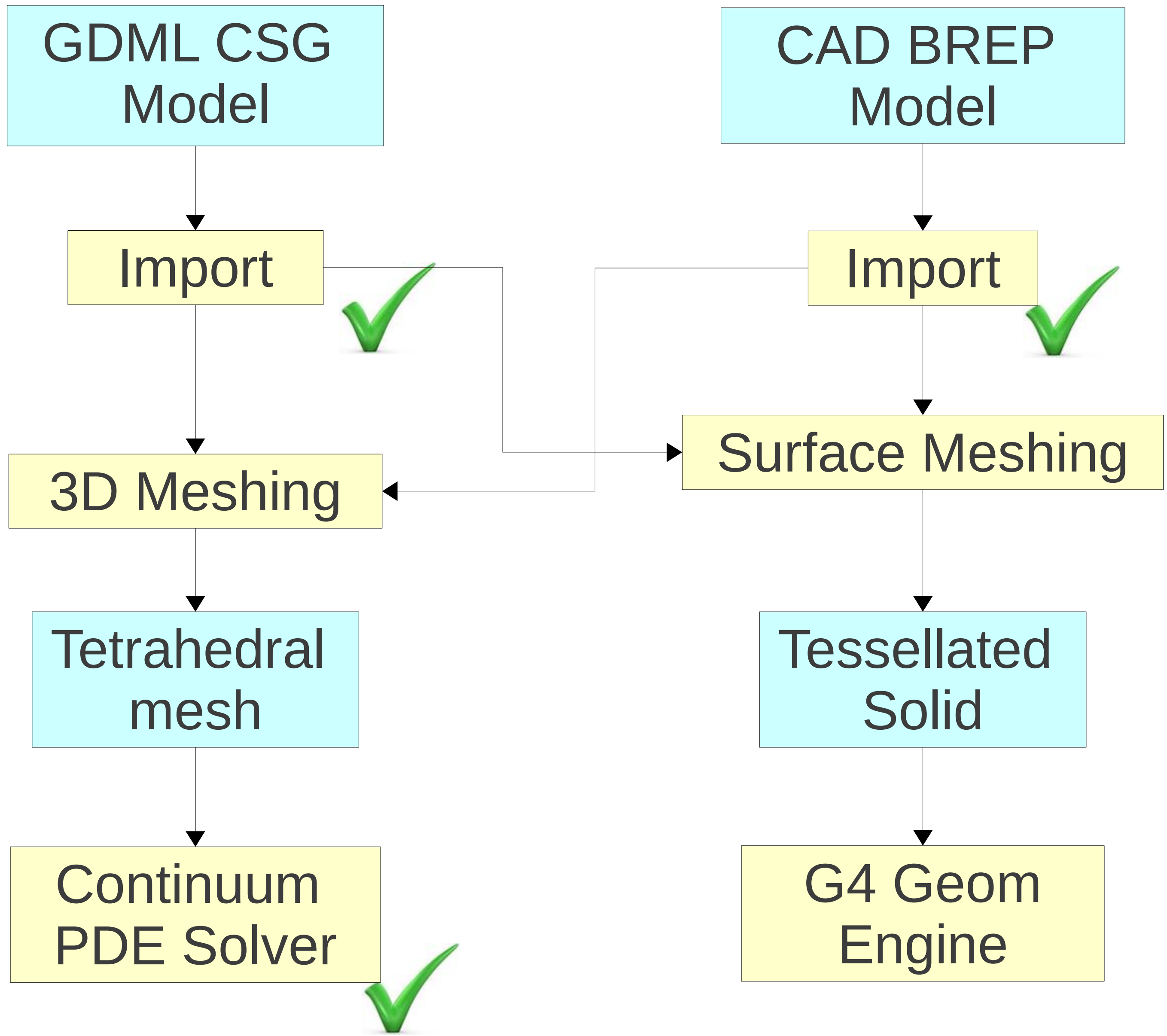
Software Components

- Two Separate Programs
  - Geant4
  - Continuum PDE solver
- LibAMS for inter-process communications
  - Developed by the Petsc team of Argonne Natl. Lab.
  - MPI-compatible
  - Socket- or File-based IPC
- Three sets of Mesh Grids
  - Tessellated solid (surface mesh) for Geant4
  - Tetrahedral mesh for continuum PDE solver
  - Oct-tree mesh for dose-rate calculation

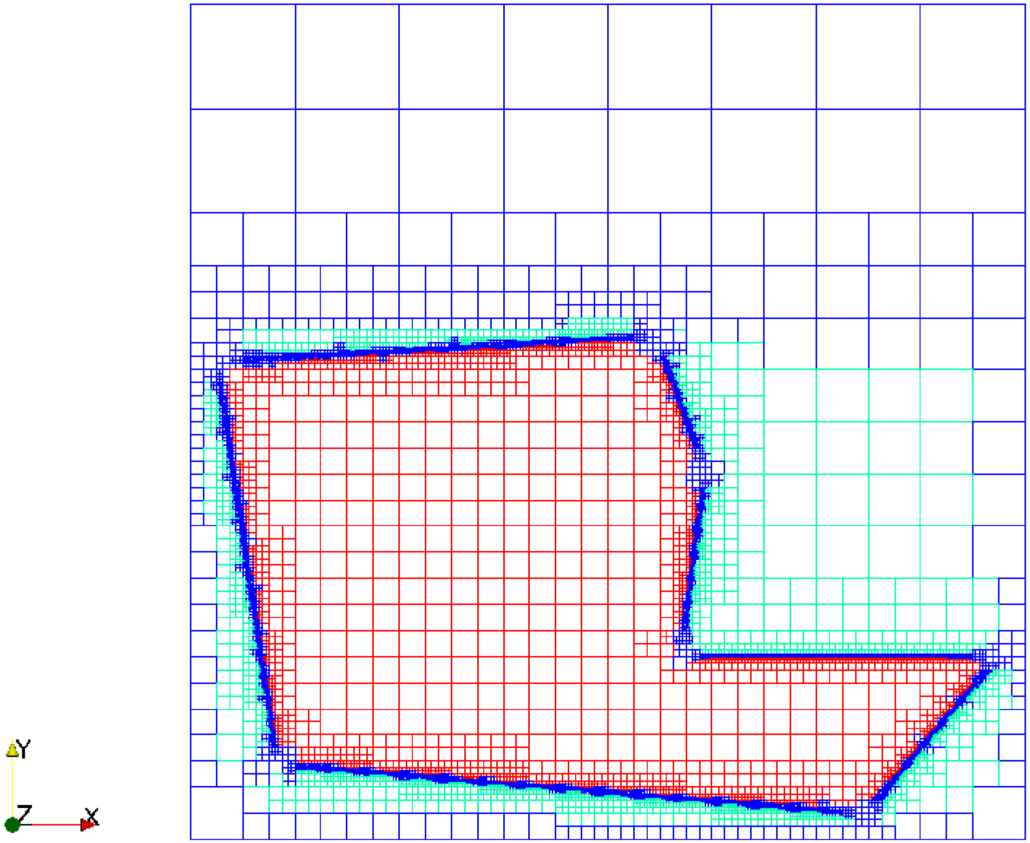
Software Components



Current Geometry Modeling

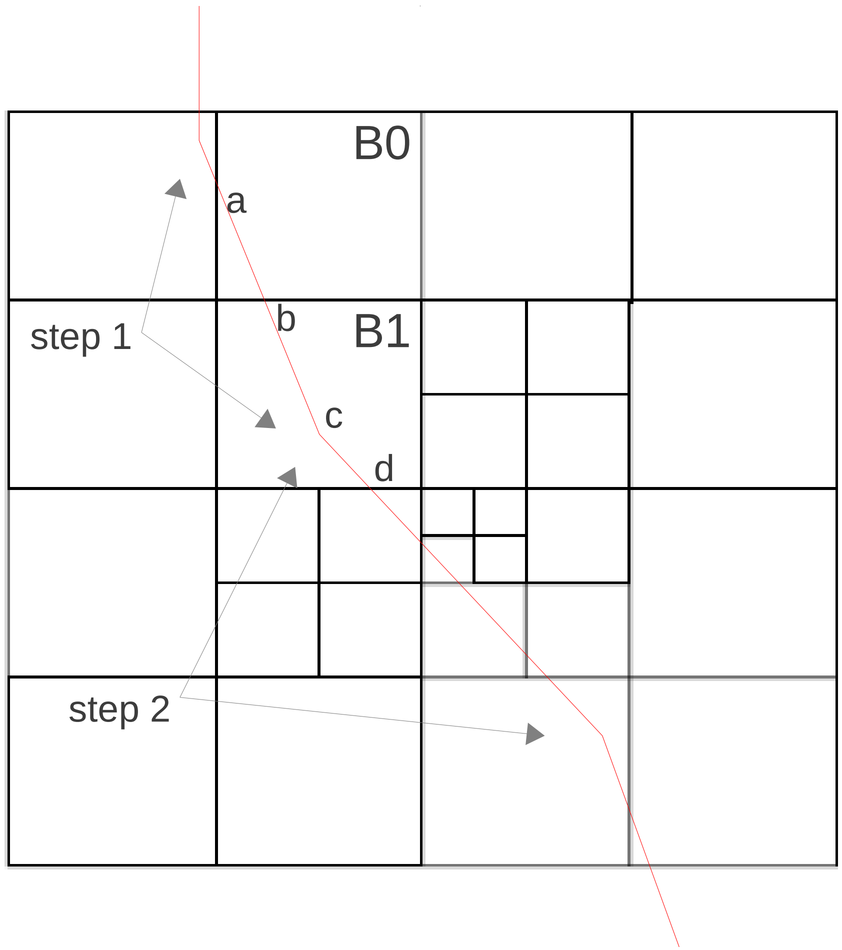


Dose Rate Calculation



- Why not do this in G4?
  - Too many detectors needed
- Hierarchical Oct-Tree mesh for dose-rate calculation
  - Mesh-size control
  - Very fast geometry operations

Dose Rate Calculation



- Track's contribution to the dose-rate in
  - Box B0: $E_a – E_b$
  - Box B1: $E_b – E_d$
- Particle energy linearly interpolated along each step of the track

Continuum PDE Solver

- Using the framework of Cogenda's TCAD
  - Unstructured Mesh Elements
  - Finite-Volume Discretization
  - Newton's method for nonlinear equations
- Capability
  - Fully-parallel computation
  - Able to handle up to a few million mesh points

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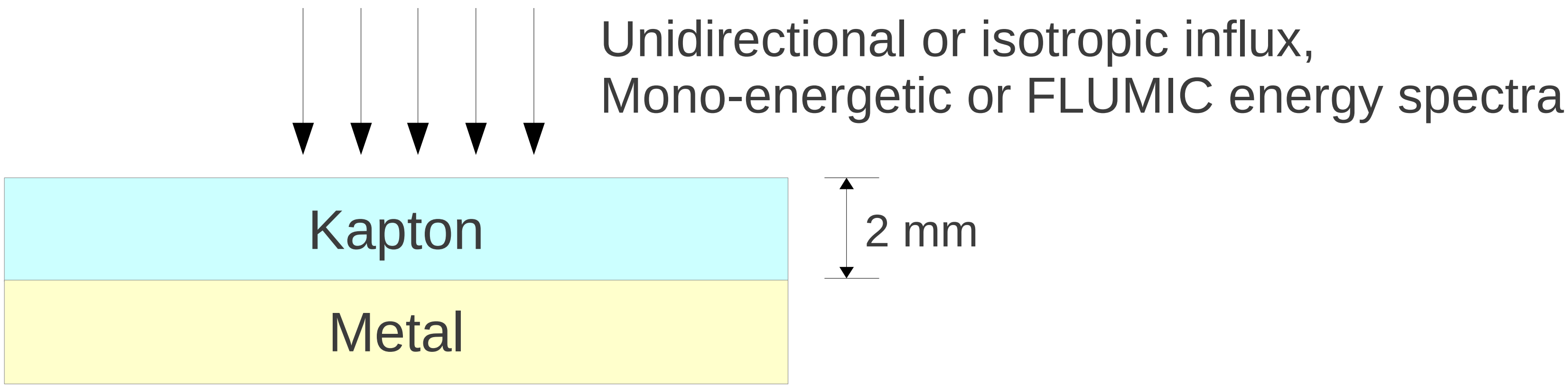
Test Case: 1D Slab



- Compare with the maximum voltage computed by DICTAT (SPENVIS)

Test Case: 1D Slab

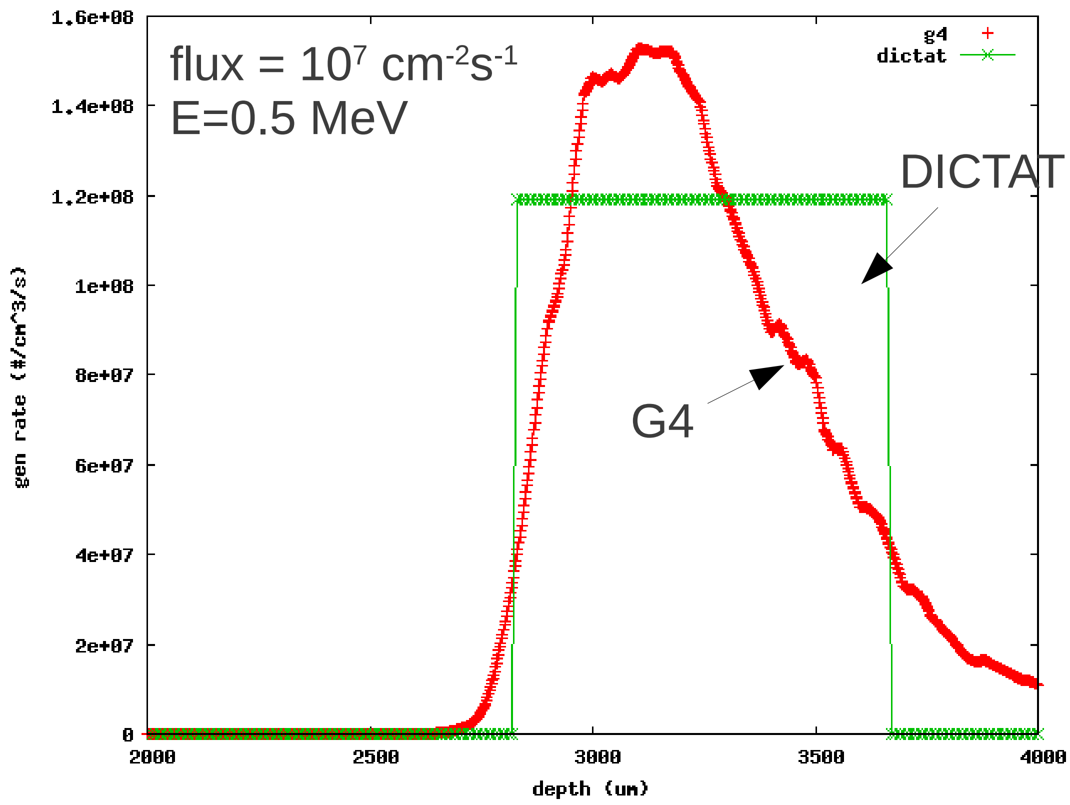
- Maximum Voltage under a high flux of 10^7 $cm^{-2}s^{-1}$

Flux type	DICTAT	This work
Isotropic flux with FLUMIC spectra	2560 V	882 V
Unidirectional flux 0.5 MeV energy	6924 V	3447 V
Unidirectional flux 1.0 MeV energy	157 V	69.3 V

- Maximum Voltage under different flux (0.5 MeV unidirectional)

Flux	DICTAT	This work
10^3 $cm^{-2}s^{-1}$	2.38 V	1.42 V
10^4 $cm^{-2}s^{-1}$	21.2 V	12.6 V
10^5 $cm^{-2}s^{-1}$	186 V	87 V
10^7 $cm^{-2}s^{-1}$	6924 V	3447 V

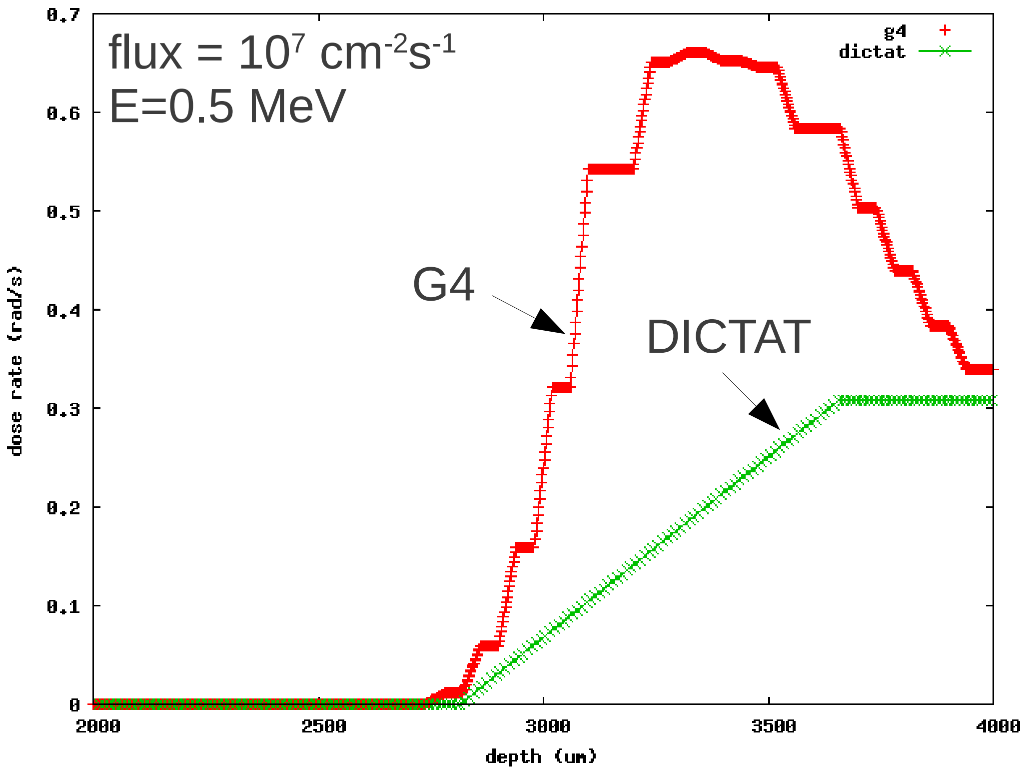
Comparison of Electron Deposition Profile



- Difference is obvious
- At low flux, this should be the main source of error.
- Improved model in DICTAT already *

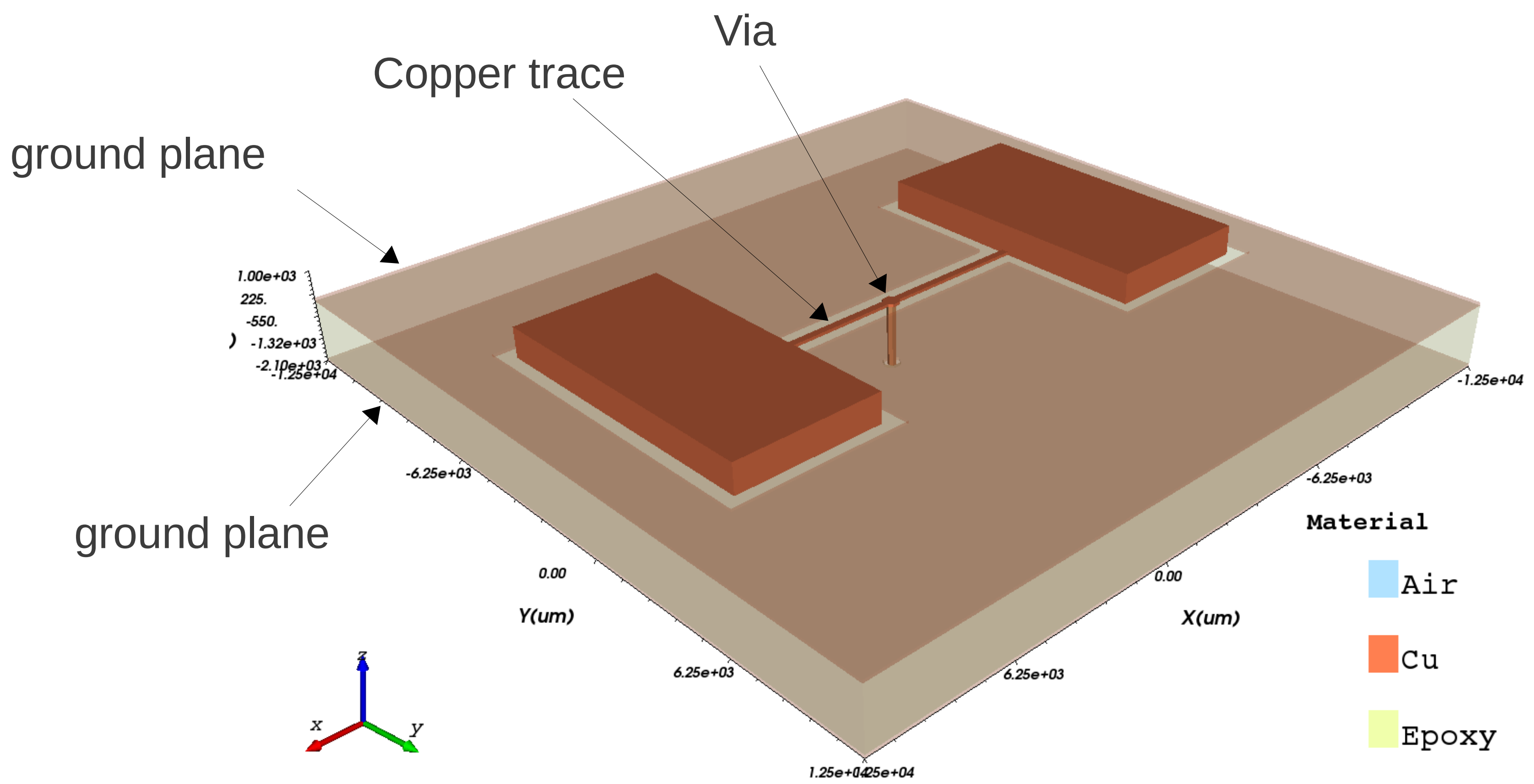
* D. J. Rodgers, et al, “DICTAT internal charging code for the Jovian environment,” SCTC 2012

Comparison of Dose Rate Profile



- When flux is high, significant difference in induced conductance
- Could be a major source of error at high flux

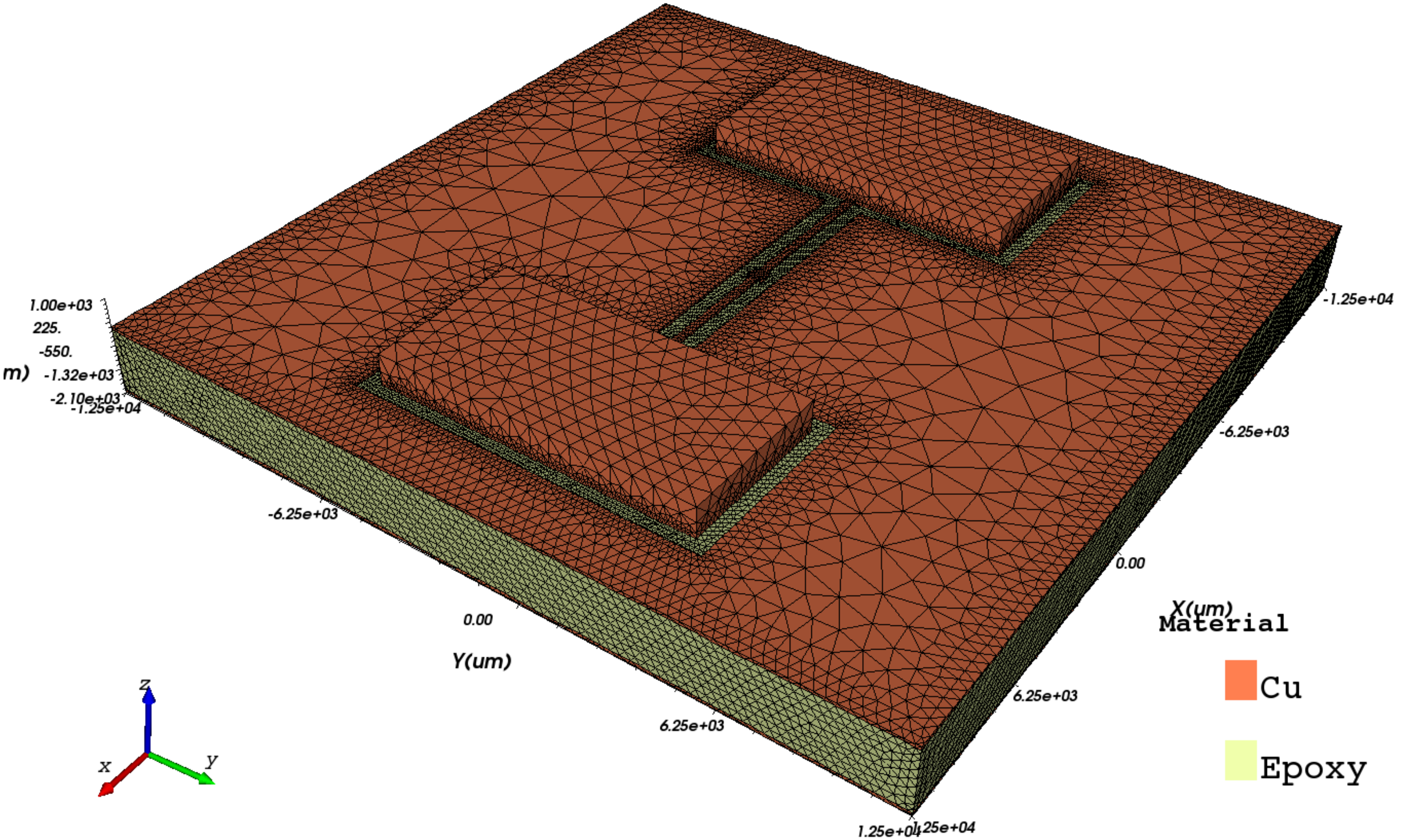
Test Case: 3D PCB Board



Tessellated solid for Geant4.
After simplification, the surface mesh contains 256 triangular facets.

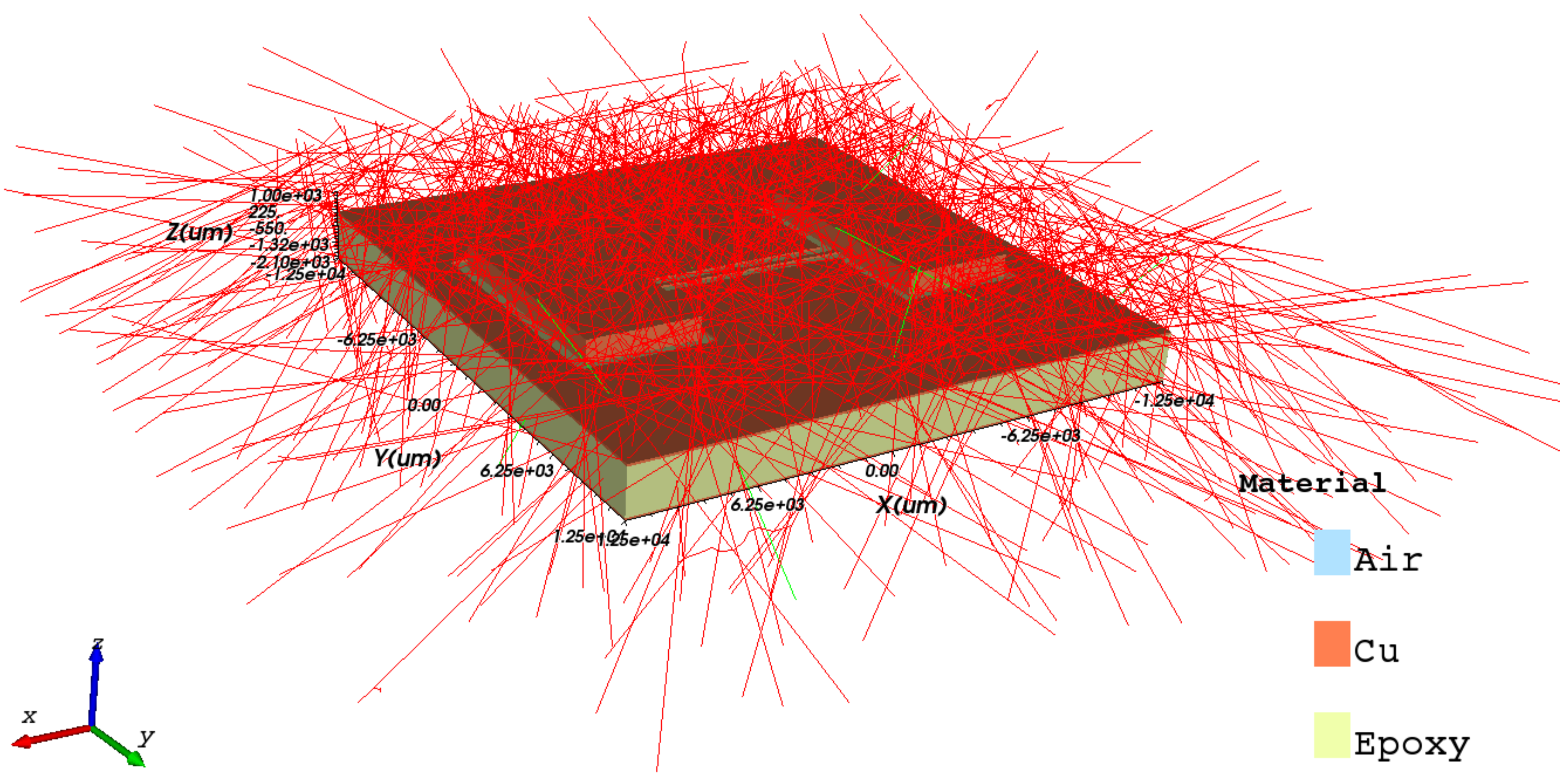
Test Case: 3D PCB Board

Tetrahedral mesh for continuum PDE solver



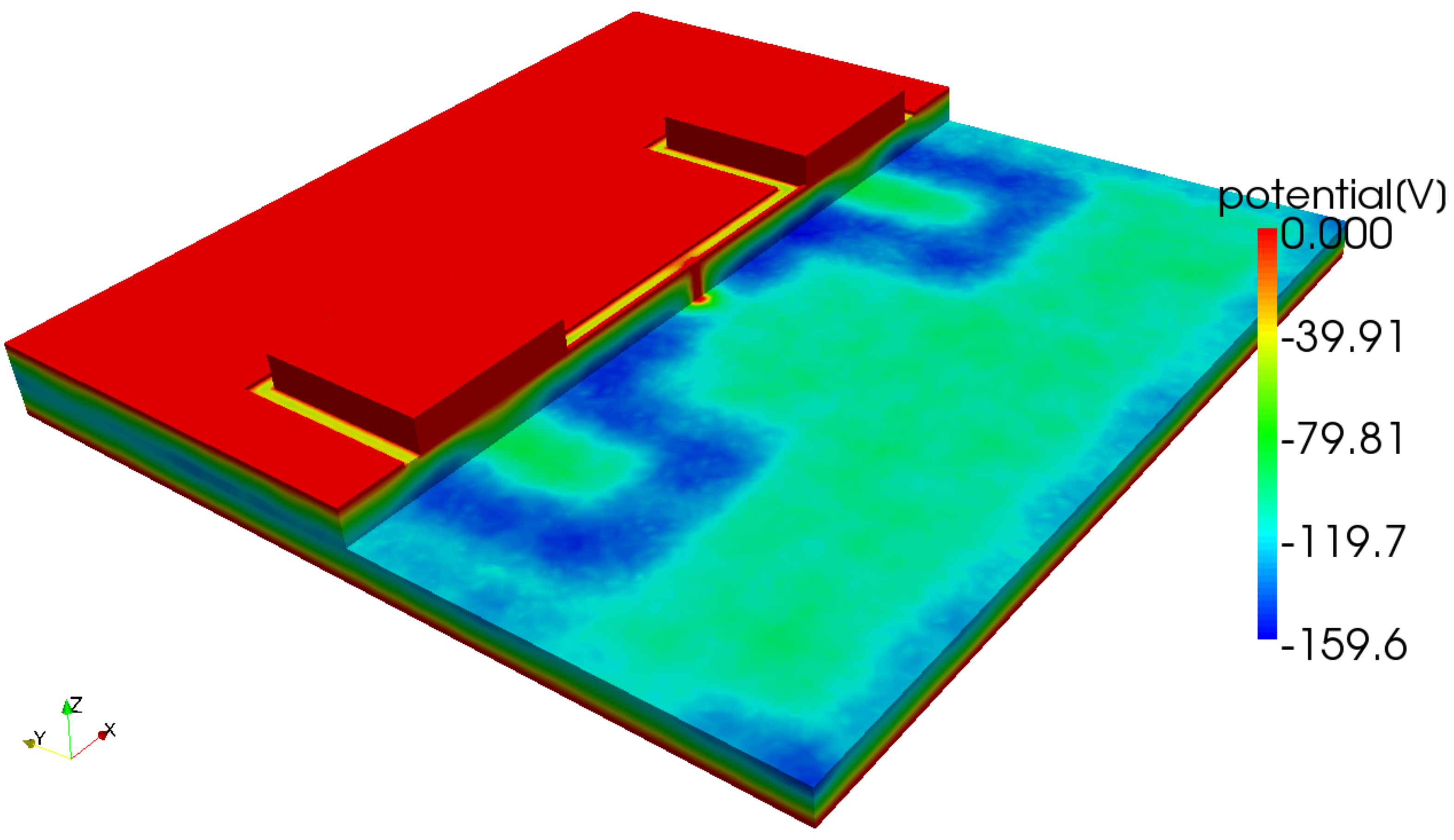
Test Case: 3D PCB Board

- Isotropic incident electrons (General Particle Source in G4)
- FLUMIC worst-case energy spectra at GEO orbit
- 10^7 particles



Test Case: 3D PCB Board

Solution: Potential distribution in the structure



Computation Time

Structure	PCB board	Structure A
GDML	Tessellated solid 256 facets	Intrinsic G4 CSG solid 98 physical volumes
Number of mesh points (for continuum PDE solver)	110,313	97,963
Number of electrons	10^7	10^8
Particle Tracking in G4 *	2 hours (serial)	12 hours (serial)
Dose-Rate *	30 minutes (serial)	20 minutes (serial)
Poisson/Continuity Eqn	3 minutes (parallel)	3 minutes (parallel)

* both components are very easy to parallelize

Bottleneck in Computation

- Bottleneck
  - Particle tracking dominates computation time
  - 95% time in 4 geometry predicate routines
    - Tessellated solids with 10k facets
- Solutions
  - Minimize # of facets in tessellated solids
  - Voxelized tessellated solids (available in 4.9.6)
  - Level-set geometry engine?

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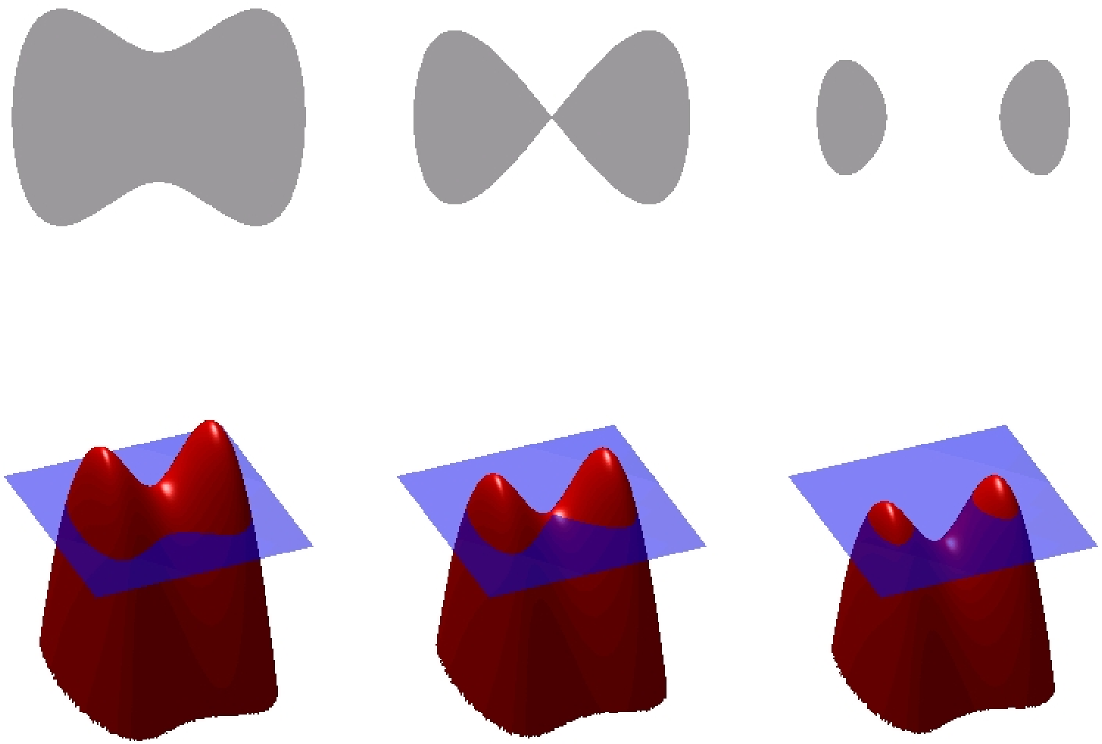
Level-Set Method: a Primer



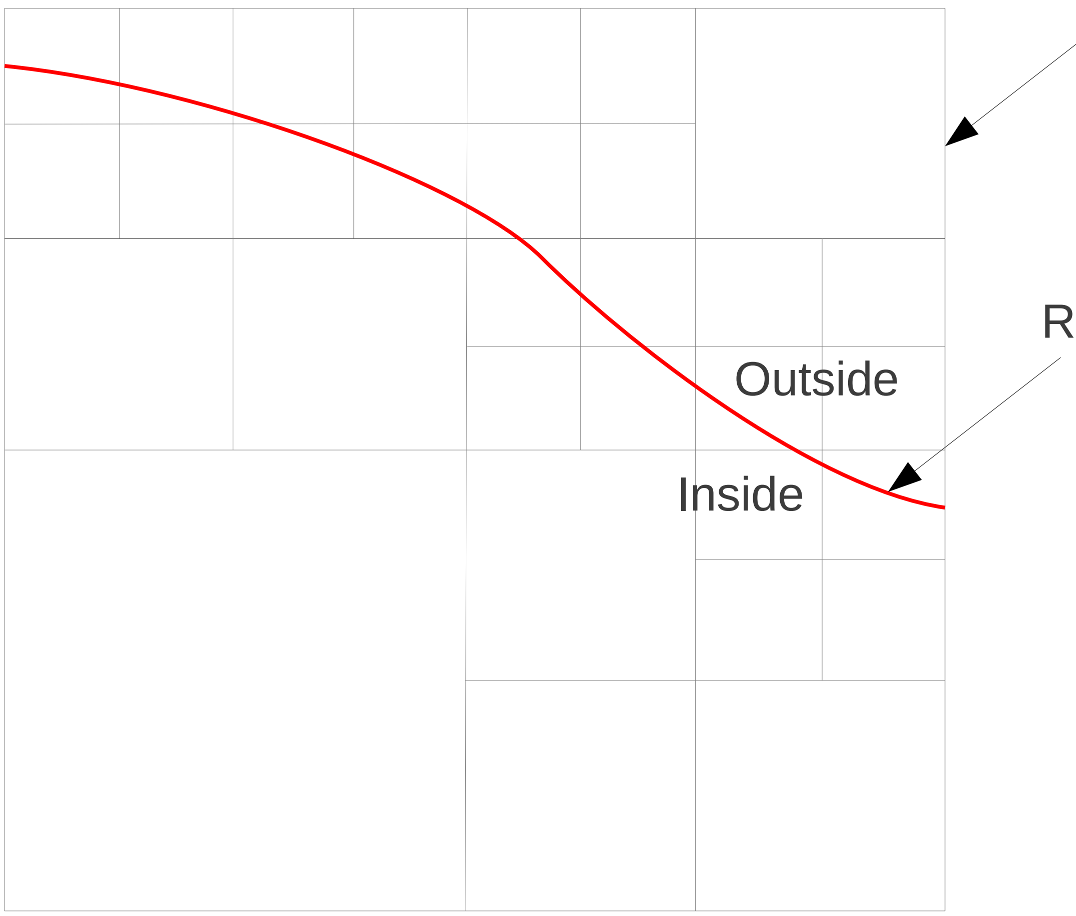
Closed-curve in 2D.

z=0 Contour of a 3D equation

http://en.wikipedia.org/wiki/File:Level_set_method.jpg

Level-Set Method: a Primer

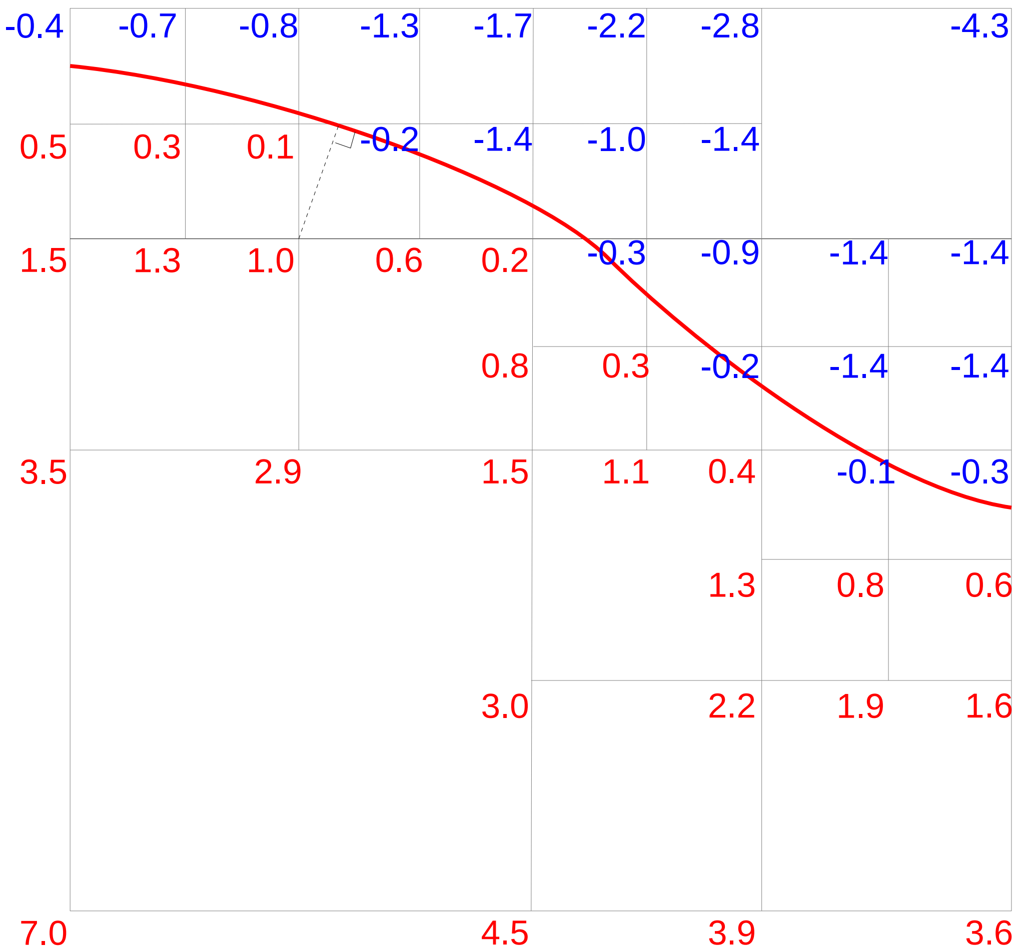
Background mesh



- Background mesh
  - Hierarchical
  - Narrow-band (Denser mesh near boundaries)

Level-Set Method: a Primer

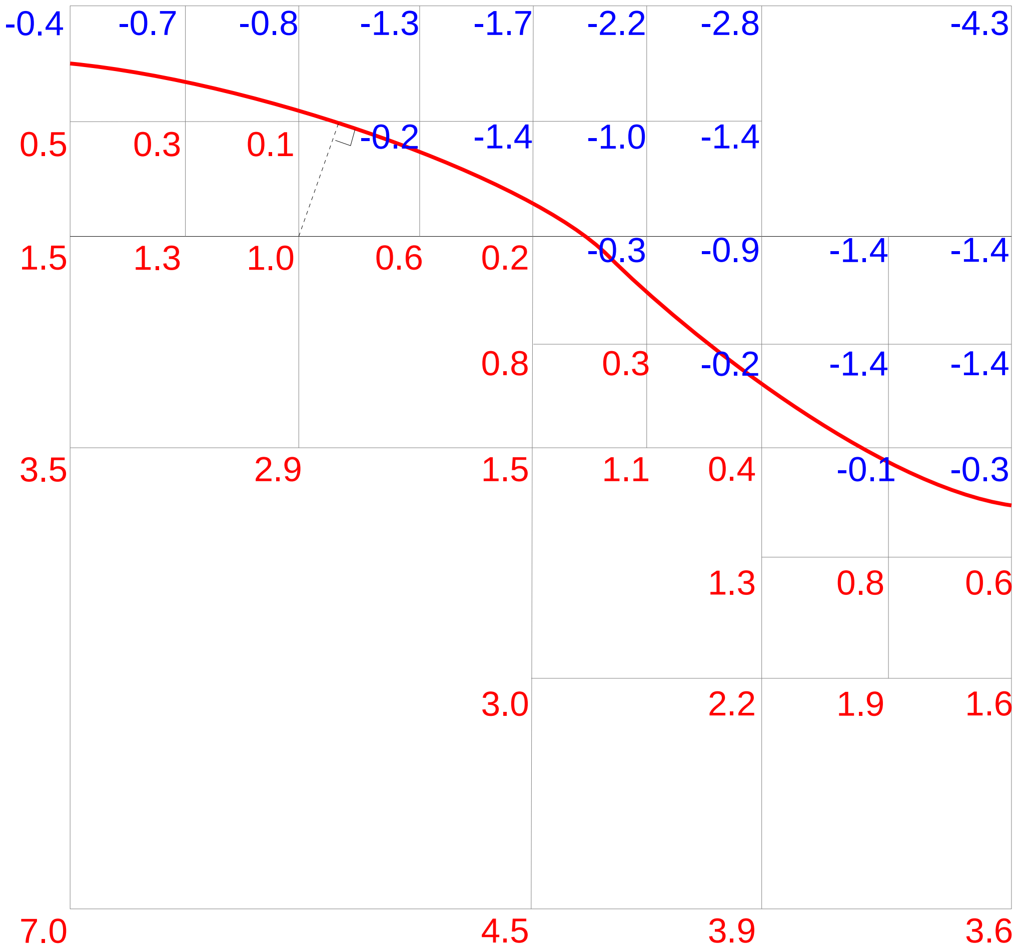
Initialization of Level Set



- Distance field
  - Inside region: >0
  - Outside region: <0
  - Value = Distance to nearest point on boundary
- Multiple Regions?
  - One distance field for each material
  - Special “tricks” to ensure
    - No overlapping
    - No holes

Level-Set Method: a Primer

Initialization of Level Set



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Level-Set Performance in G4 Context

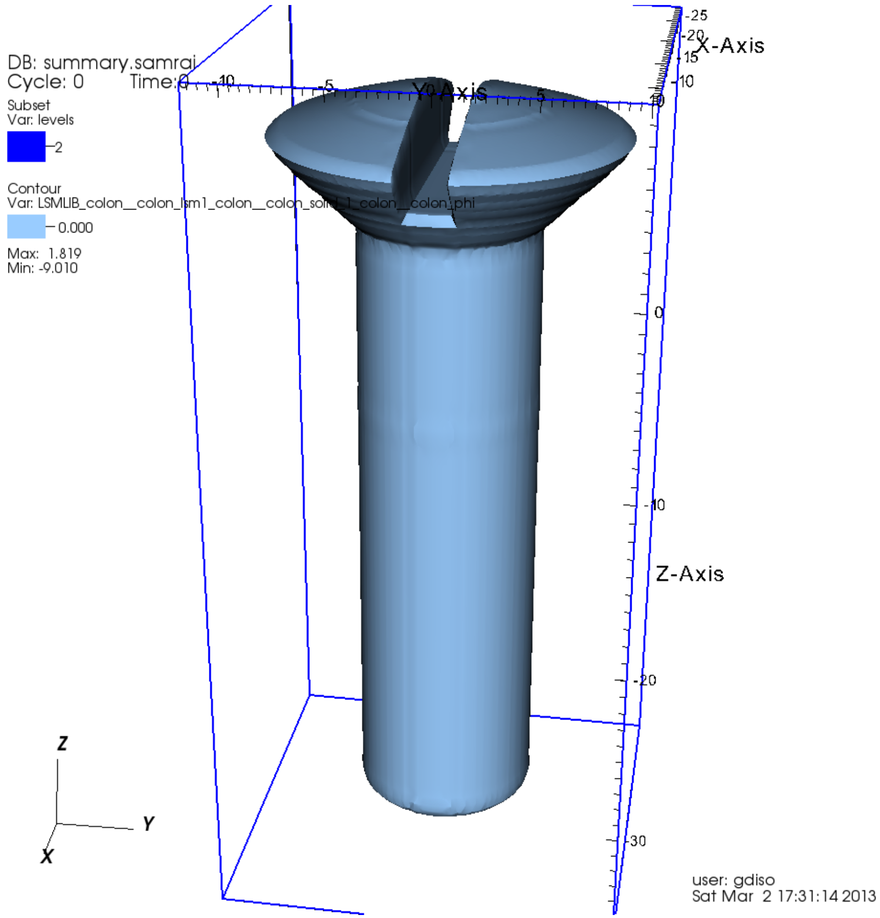
- K: number of regions
- N: level-of-details
  - Tessellated solids: number of mesh elements per surface area
  - Level-set: number of background mesh elements per surface area
- M: number of voxels

Geometry predicates	Tessellated Solid	Voxelized TS G4.9.6	Level-set
Exact distance to region boundary along a given direction?	$O(N)$	$O(N\ M^{-1/3})$	$O(\log N)$
Conservative estimate of distance to region boundary?	$O(N)$	$O(M + N\ M^{-1/3})$	$O(1)$
Is the given point inside (outside) of the region?	$O(N)$	$O(N\ M^{-1/3})$	$O(1)$
In which region a given point is located?	$O(N \log K)$	$O(K\ N\ M^{-1/3})$	$O(\log K)$

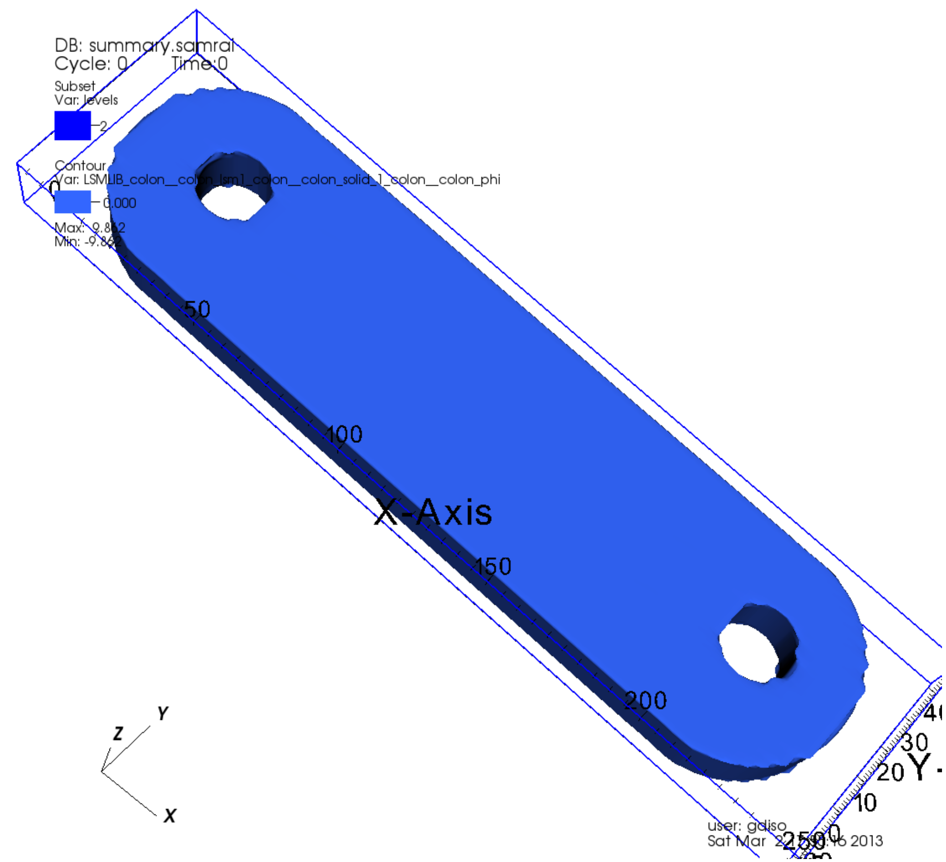
- Could be implemented as a Navigator, G4LevelSetNavigator
- We expect a 10x speedup tracking particles in complex geometries.

Level-Set Example: Build from B-Rep

Bolt: built from a STEP file

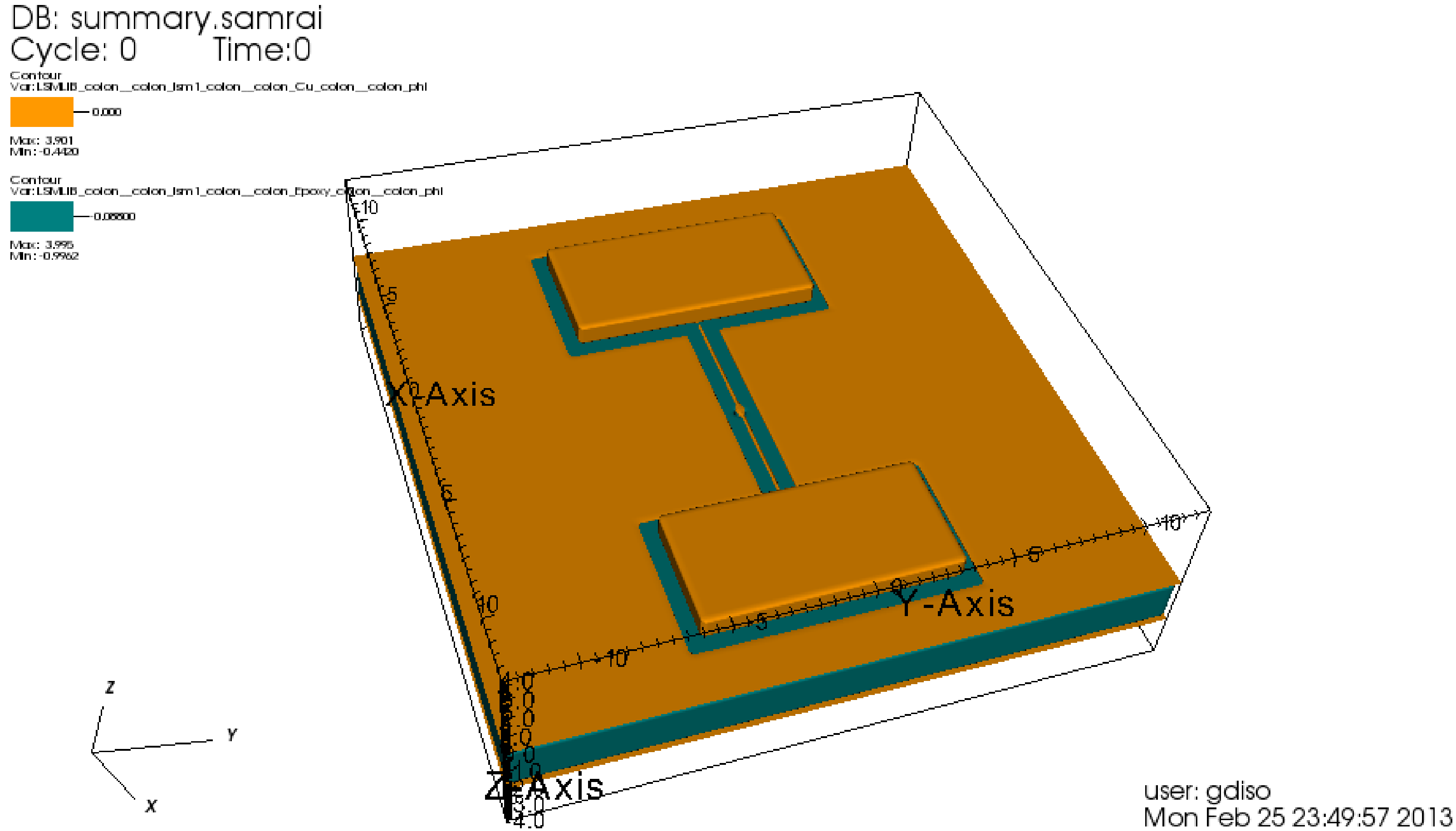


Spanner: built from a STEP file

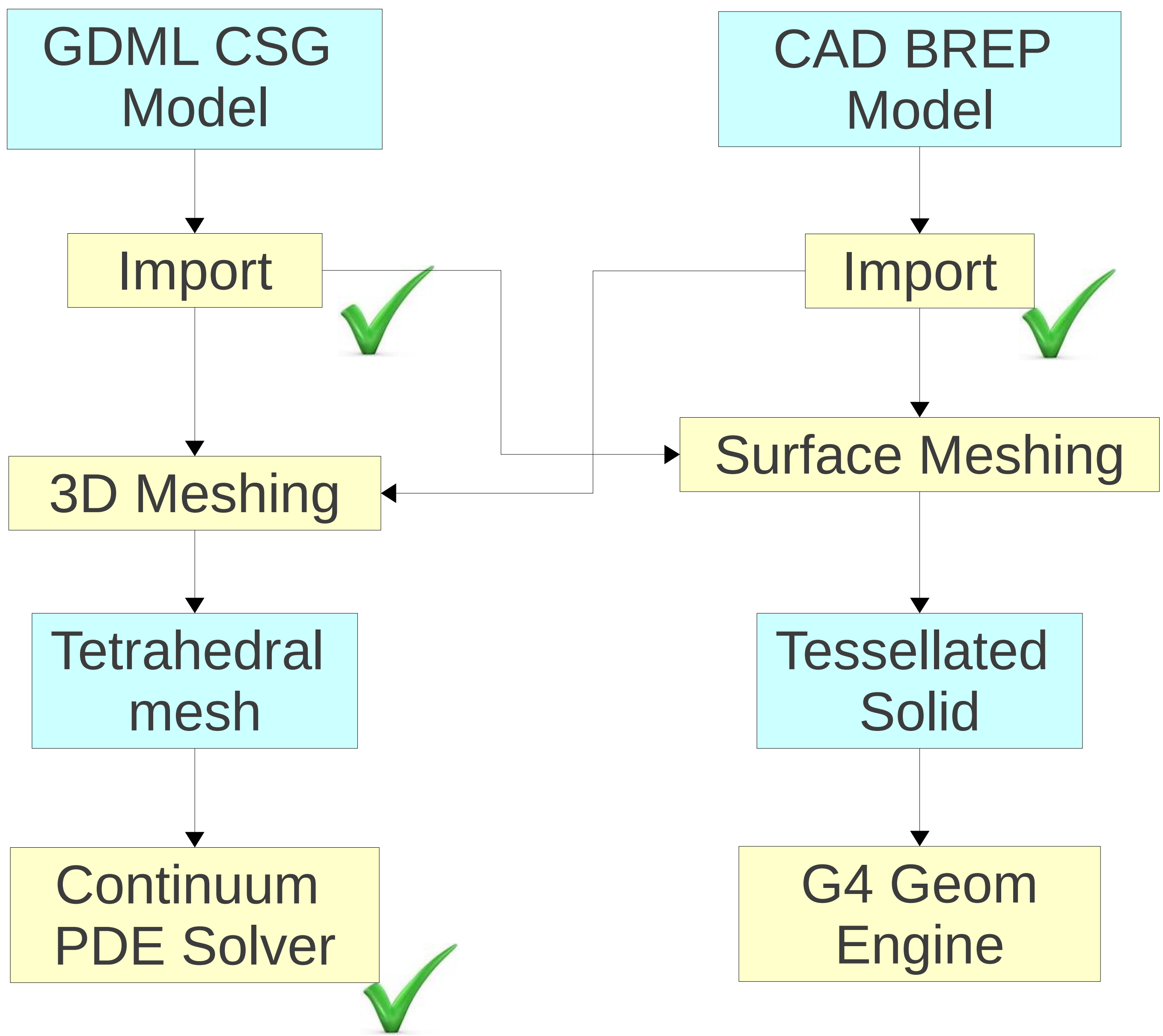


Level-Set Example: Build from CSG

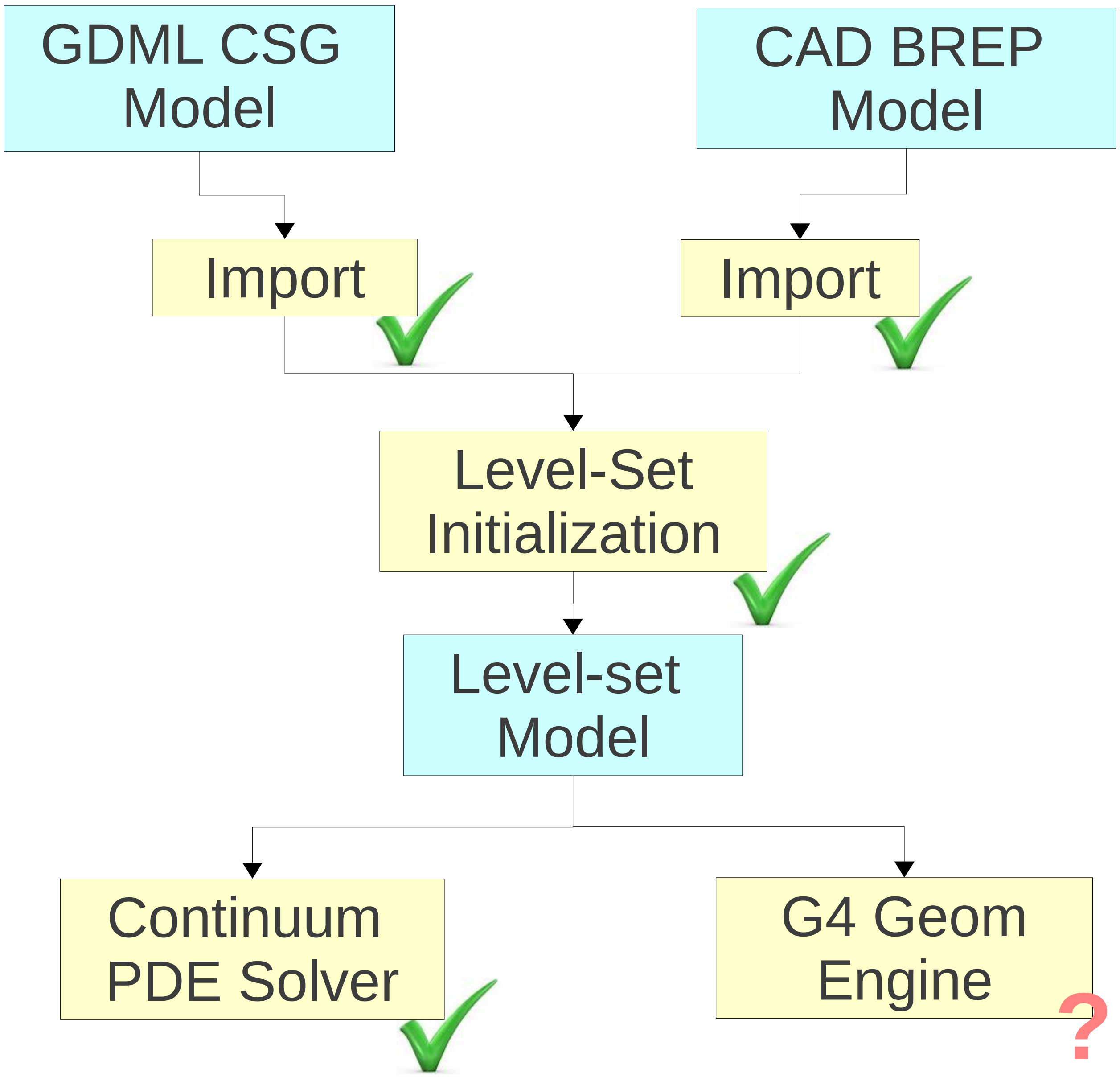
PCB, built from a GDML file



Current Geometry Modeling



Road Map on Level-Set Methods



Summary

- 3D Simulator of Internal Charging Effect
  - Geant4 for particle transport simulation
  - Continuum PDE solver for Poisson/continuity equations

- Computation bottleneck in particle tracking

- Proposal of Level-Set-based geometry engine in Geant4
  - Speedup particle tracking in complex geometries
  - Unified geometric description in G4 and Continuum PDE solver
  - Enough demand to justify G4LevelSetNavigator ?