Electron deposition in semi-infinite media / Electron backscatter

Geant4 Validation

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1. Geant4 Validation
2. Geant4 Physics
3. Experimental setup and Geant4 simulation application
4. Simulation Results
   - General aspects
   - Part I: Energy deposition in semi-infinite media
   - Part II: Backscatter
1. Geant4 Validation

2. Geant4 Physics

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   - General aspects
   - Part I: Energy deposition in semi-infinite media
   - Part II: Backscatter
Large-scale validation study of Geant4 EM physics was performed:

* Low-energy domain (< 1 MeV) examined
  * Significant physics observables systematically investigated (energy deposition, backscattering)

* First results available
  * Important impact on future Geant4 developments
  * Significant guidance for users
Validation of Geant4 physics models

**Major goals**
- Guidance for users
  - Providing hints for optimal configuration of simulation parameters
  - Highlighting the abilities of physics models
- Feedback for developers
  - Improvement of models based on findings

**Systematic studies**
- Investigation of systematic conditions (Many materials, beam energies, ...)
- Can enormously facilitate the interpretation of the overall behaviour of models
Validation of Geant4 physics models (cont.)

- **Strategy and methods**
  - Modeling physics scenarios
  - Building simulation applications
  - Computation of relevant physical quantities
  - Comparison against experim. data
  - Comparison against reference data
    - e.g. NIST

- **Experimental validation approach**
  - Not trivial, since experimental conditions must be reproduced
  - Precise geometry setup required in simulation application
  - Physical quantities computed according to experimental measurement
Physics observables in the current validation process

Low-energy electron beams (<1MeV) incident on diff. materials:

1. Electron energy deposition in semi-infinite media
   - Spatial energy delivery as a function of depth

2. Backscattered particles
   - Backscattered fractions of primary electrons and electron energy

Quantitative Geant4 Validation

- Validation of low-energy electromagnetic physics models
- Comparison against experimental data
  (Sandia reports SAND79-0410.UC-34a and SAND80-1968.UC-34a)
Sandia validation data

- Measured for Monte Carlo validation purposes (TIGER code)
- Electron energy deposition values are **absolute**
  - Important issue in a physics validation process
  - Hardly found in literature
  - Measured with a high spatial resolution
  - Uncertainty claimed to be < 2.2%
  - Potential drawback: Systematic errors fully considered?
- Many different materials covered
  - From beryllium to uranium
- Varying beam energies and incident angles considered
  - 300keV - 1MeV (Energy deposition measurements), 28keV - 1MeV (Backscatter measurements)
  - 0° and 60° (Energy deposition measurements), 0°, 15°, 30°, 45°, 60°, 85° (Backscatter measurements)
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**Low-energy EM physics in Geant4**

- **Selectable physics models**
  - Process implementations based on different principles available
  - *Parametrized* and *analytical* models offered
  - Combining models adequately is the user’s responsibility
    - Makes toolkit more versatile but requires certain experience by the user
    - Guidelines given in examples and in “Geant4 User’s Guide for Application Developers”
    - Pre-prepared physics lists available

- **EM processes for $e^-$ and $\gamma$ in the low-energy domain**
  - Two packages: *Low-Energy* and *Standard*
  - Low-energy package: Two different approaches available
    - Library-based *(Livermore)* models
    - Penelope-like models
## Low-energy EM physics in Geant4 (cont.)

### Overview of EM processes

#### Focus on Liverm. models
- Library-based (Livermore)

#### Low-energy package
- **Electrons**
  - Ionisation
    - G4LowEnergyIonisation
    - G4PenelopeIonisation
    - G4eIonisation
  - Bremsstrahlung
    - G4LowEnergyBremsstrahlung
    - G4PenelopeBremsstrahlung
    - G4eBremsstrahlung
  - Multiple-Scattering
    - G4MultipleScattering

#### Standard package

#### Library-based (Livermore)

#### Penelope-like

#### Electrons

<table>
<thead>
<tr>
<th>Process</th>
<th>G4LowEnergyIonisation</th>
<th>G4PenelopeIonisation</th>
<th>G4eIonisation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ionisation</td>
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<tr>
<td>Bremsstrahlung</td>
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</tr>
<tr>
<td>Multiple-Scattering</td>
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</tbody>
</table>

#### Photons

<table>
<thead>
<tr>
<th>Process</th>
<th>G4LowEnergyPhotoelectric</th>
<th>G4PenelopePhotoelectric</th>
<th>G4PhotoElectricEffect</th>
</tr>
</thead>
<tbody>
<tr>
<td>Photoelectric effect</td>
<td>G4LowEnergyPhotoelectric</td>
<td>G4PenelopePhotoelectric</td>
<td>G4PhotoElectricEffect</td>
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<td>Compton scattering</td>
<td>G4LowEnergyCompton</td>
<td>G4PenelopeCompton</td>
<td>G4ComptonScattering</td>
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<tr>
<td>Rayleigh scattering</td>
<td>G4LowEnergyRayleigh</td>
<td>G4PenelopeRayleigh</td>
<td>G4GammaConversion</td>
</tr>
<tr>
<td>Conversion</td>
<td>G4LowEnergyGammaConversion</td>
<td>G4PenelopeGammaConversion</td>
<td>G4GammaConversion</td>
</tr>
</tbody>
</table>

* Standard G4MultipleScattering used for simulations involving processes of the Low-energy package
Simulation configuration

- **Parameters (optionally handled by the user)**
  - **Maximum step size of particle**
    - Determines accuracy of spatial resolution
    - Recommended: Size of the order of the scoring bins
  - **Production threshold** for generating secondaries
    - Lower limits: Liverm. 250eV, Penelope \(\sim100\)eV, Standard 1keV
    - Handled through a range cut parameter
    - \(\delta\)-ray production can significantly alter energy deposition

- **Multiple-scattering step limitation**
  - More Multiple-scattering parameters exists (not further considered)

- **Tracking**
  - **No tracking cut** exists in Geant4
    - All (produced and accepted) particles tracked to zero range
    - Secondary *production* can be controlled through (prod. threshold)
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Calorimetric measurements

- **Spatial energy delivery pattern**
  - Calorimeter foil placed between front layer and “infinite” layer
  - Calorimeter consists of same material as target
  - Energy deposition measured for different front layer thicknesses
  - Measurement depth = Front layer thickness + half the calorimeter thickness

- **Backscattered energy**
  - Energy deposition determined in target (bulk calorimeter)
  - Backscattered energy calculated as complement of measurement
  - (Theoretical) Bremsstrahlung-correction applied
**Geometry**

- **Semi-infinite target medium**
  - Lateral dimensions and thickness > maximum $e^-$-range

- **Primary particle vertex**
  - Direction determined by angle $\alpha$ between surface normal and beam axis
  - Beam impinges at target surface center

**Simulation code**

- **Geant4 application**
  - Simulation application was developed according to the experimental setup
Target/Detector modeling

Elaborate software design for describing target/detector geometry:

* Decorator design pattern applied (see figure)
  - Add-on layer can be placed dynamically in front of semi-infinite slab
  - Multi-slab geometry by nesting decorator (AddOnTargetLayer) recursively

* Facilitates future work involving multi-layer configurations

* Geometry parameters controlled through macro commands
  - Layer thickness, materials,...
  - Easy simulation control
  - No recompiling necessary to update geometry

```
TargetComponent

SemiInfiniteTarget
  G4Tubs* solid
  G4LogicalVolume* log
  G4VPhysicalVolume* phy

AddOnTargetLayer
  G4Tubs* solid
  G4LogicalVolume* log
  G4VPhysicalVolume* phy
```
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Simulation results

- **Systematic validation approach against Sandia data**
  - Various experimental configurations were investigated
    - Different target materials
    - Varying beam energies and incident angles
  - Several simulation configurations evaluated
  - Small subparts covered earlier by other authors (but no comprehensive collection)
    - E.g. O. Kadri *et al.*, “Geant4 simulation of electron energy deposition in extended media”, NIM B 258 (2007) 381-87

- **Due to lack of time only a subset of results can be presented**
  - Focus is on certain aspects
  - Paper with a complete collection of results in preparation with
Simulation results (cont.)

- **Setups and configurations considered in the presentation**
  - Systematic results presented for a few materials
  - Few beam energies considered
  - Geant4 versions 8.1-p02 and 9.0-p01 compared (for energy deposition results only)
    - Differences due to Multiple-Scattering model (Standard package)
    - Low-Energy package (Livermore, Penelope models) remains the same in both versions
  - Secondary particle production threshold evaluated

- **Further settings**
  - Maximum step size always set to 0.001 mm (lower recommended value)
  - Default value taken for Multiple-Scattering step limitation
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Geant4 Physics

Experimental setup and Geant4 simulation application

Simulation Results

Part I: Energy deposition in semi-infinite media

Part II: Backscatter

Z

Aluminium
Iron
Copper
Molybdenum
Tantalum

8.1-p02 vs 9.0-p01

Multiple Scattering

Aluminium
0.314 MeV, 0°

Experiment

Geant4 9.0-p01 Liverm. (Cut = 250 eV)
Geant4 8.1-p02 Liverm. (Cut = 250 eV)

Experiment

Geant4 9.0-p01 Liverm. (Cut = 250 eV)
Geant4 8.1-p02 Liverm. (Cut = 250 eV)

Aluminium
1.033 MeV, 0°
Geant4 Validation

Geant4 Physics

Experimental setup and Geant4 simulation application

Simulation Results

Part I: Energy deposition in semi-infinite media
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8.1-p02 vs 9.0-p01

Multiple Scattering

Iron

Energy deposition per unit length [MeV/g/cm²]

Fraction of a mean range

Experiment

Geant4 9.0-p01 Liverm. (Cut = 250 eV)
Geant4 8.1-p02 Liverm. (Cut = 250 MeV)

Experim. bin size

Iron

1.000 MeV, 0°

Experiment

Geant4 9.0-p01 Liverm. (Cut = 250 eV)
Geant4 8.1-p02 Liverm. (Cut = 250 eV)
Geant4 Validation
Geant4 Physics
Experimental setup and Geant4 simulation application
Simulation Results

Part I: Energy deposition in semi-infinite media
Part II: Backscatter

- Aluminium
- Iron
- Copper
- Molybdenum
- Tantalum

Energy deposition per unit length [MeV/g/cm²]

Fraction of a mean range

Copper
0.300MeV, 0°

Copper
0.500MeV, 0°

Experim. bin size

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Geant4 Validation

Experimental setup and Geant4 simulation application

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Part I: Energy deposition in semi-infinite media

Part II: Backscatter

Z

Energy deposition per unit length [MeV/g/cm²]

Fraction of a mean range

Molybdenum

Experim. bin size

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Part I: Energy deposition in semi-infinite media

- Aluminium
- Iron
- Copper
- Molybdenum
- Tantalum

Fraction of a mean range

Tantalum

0.300 MeV, 0°

0.6

Geant4 9.0-p01 Liverm. (Cut = 250 eV)
Geant4 8.1-p02 Liverm. (Cut = 250 eV)
Experiment

Tantalum

1.000 MeV, 0°

Energy deposition per unit length [MeV/g/cm²]

Fraction of a mean range

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Beam axis $\neq$ surface normal: Incident angle of $60^\circ$

**Graphs**

- **Aluminium**
  - Energy deposition per unit length [MeV/g/cm$^2$] vs. Fraction of a mean range
  - 0.314MeV, $60^\circ$
  - 1.033MeV, $0^\circ$

- **Molybdenum**
  - Energy deposition per unit length [MeV/g/cm$^2$] vs. Fraction of a mean range
  - 0.500MeV, $60^\circ$
  - 1.000MeV, $0^\circ$
Generation of secondaries: Influence of production threshold

Liverm. library based processes

Energy deposition
- Significant dependence on cut in range for Fe, Cu, Mo, Ta (for all considered beam energies)
- Peak: Differences up to 15% observed
- Effects due to angular distribution of secondary particles

Low prod. threshold (250eV)
- Underestimation of peak height for 1MeV beams
- Was rather stopping power measured? (Then higher cut would apply)
Summary (Part I)

- **Geant4 Livermore models**
  - Capable of reproducing experimentally measured spatial energy deposition for most materials with good precision
  - Some deficiencies in peak region observed (Experimental conditions correctly reproduced?)
  - Choice of production threshold for generating secondary particles significantly influences spatial energy deposition in high-Z materials

- **8.1-p02 vs 9.0-p01 (latest release)**
  - Considerable difference for low-Z materials
  - Effects due to Multiple-Scattering model
Low-Z material:

* Good agreement between simulation and experimental data for some angles

* Underestimation at low beam energies (109keV) and large angles

⇒ Playground for further investigation of Multiple-Scattering parameters
Aluminium:
* Good agreement for all considered and angles
Titanium:
* Good agreement observed for aluminium continues for titanium
Generation of secondaries: Influence of production threshold

- **Low production threshold (250eV)**
  - Can improve backscatter results (both, backscattered fraction of energy and charge)
  - See plots (Molybdenum, 109keV beam)
  - Systematics not discussed here (More information to be found in publication)
Summary (Part II)

- Geant4 Livermore models
  - Very good reproducibility of backscattered fractions of energy except for some deficiencies at beryllium
  - Multiple-Scattering parameters to be investigated in more detail for low-Z materials

Thank for your attention!