Comparison between different composite material implementations in Merlin

Collimation Upgrade Specification Meeting #71

Monday, 23 May 2016
Outline

- Material implementation in Merlin
- Modeling of composite materials
- Comparison between Sixtrack and Merlin
- Cleaning performance with advanced collimator materials
Material implementation in Merlin

Improved model of composite materials used for LHC collimators:

- **Materials currently available in Merlin**

<table>
<thead>
<tr>
<th>Material</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon (graphite)</td>
<td>C</td>
</tr>
<tr>
<td>Beryllium</td>
<td>Be</td>
</tr>
<tr>
<td>Copper</td>
<td>Z</td>
</tr>
<tr>
<td>Aluminium</td>
<td>Al</td>
</tr>
<tr>
<td>Lead</td>
<td>Pb</td>
</tr>
<tr>
<td>Boron</td>
<td>B</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O</td>
</tr>
<tr>
<td>Tungsten</td>
<td>W</td>
</tr>
<tr>
<td>Carbon Diamond</td>
<td>CD</td>
</tr>
<tr>
<td>Copper Carbon Diamond</td>
<td>CuCD</td>
</tr>
<tr>
<td>CFC AC150K</td>
<td>AC150K</td>
</tr>
<tr>
<td>Inermet 180</td>
<td>IT180</td>
</tr>
<tr>
<td>Glidcop</td>
<td>GCOP</td>
</tr>
<tr>
<td>Molybdenum Carbide</td>
<td>Mo2C</td>
</tr>
<tr>
<td>Molybdenum Carbide Graphite</td>
<td>MoGr</td>
</tr>
</tbody>
</table>

- **Pure elements**

- **Recently added/updated Composite materials**
Material implementation in Merlin

A new CompositeMaterials class has been created and can be handled in two different ways.

The **MERLIN-SIXTRACK METHOD**

Composite materials treated as single chemical elements, i.e. by calculating off-line “effective” nuclear and atomic parameters based on material composition.

Calculated “effective” values used as inputs for scattering process.

Created for direct comparison with SixTrack.

The **MERLIN METHOD**

Rigorous treatment of nuclear point-like interactions with single compound components.

Selection of the material for the current interaction based on material compositions and cross-sections.

Current interaction based on nuclear and atomic parameters of the selected component.
Outline

- Material implementation in Merlin
- **Modeling of composite materials**
- Comparison between Sixtrack and Merlin
- Cleaning performance with advanced collimator materials
How to model composite materials in Merlin?

**Density** $\rho$ and **electrical conductivity** $\sigma_{\text{el}}$ (measured from available specimens)

<table>
<thead>
<tr>
<th></th>
<th>$Z$</th>
<th>$A$  [g/mol]</th>
<th>$\rho$ [g/cm$^3$]</th>
<th>$\sigma_{\text{el}}$ [MS/m]</th>
<th>at. content [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>CFC</td>
<td>6</td>
<td>12.01</td>
<td>1.67</td>
<td>0.14</td>
<td>100 C</td>
</tr>
<tr>
<td>MoGR</td>
<td>6.653</td>
<td>13.532</td>
<td>2.5</td>
<td>1</td>
<td>2.7 Mo$_2$C, 97.3 C</td>
</tr>
<tr>
<td>CuCD</td>
<td>11.898</td>
<td>25.238</td>
<td>5.4</td>
<td>12.6</td>
<td>25.7 Cu, 73.3 CD, 1 B</td>
</tr>
<tr>
<td>Glidcop</td>
<td>28.823</td>
<td>63.149</td>
<td>8.93</td>
<td>53.8</td>
<td>99.1 Cu, 0.9 Al$_2$O$_3$</td>
</tr>
<tr>
<td>Inermet180</td>
<td>67.657</td>
<td>166.68</td>
<td>18</td>
<td>8.6</td>
<td>86.1 W, 9.9 Ni, 4 Cu</td>
</tr>
</tbody>
</table>

**Atomic content** (calculated after production process of materials)

**Atomic number** $Z$ and **atomic weight** $A$ as average weighted on the atomic fraction of the components

**Mean excitation energy** $\bar{I}$, **radiation length** $\chi_0$, **electron density** $n_e$ are calculated as average weighted on the mass fraction of the components

The **nuclear reference cross section** is calculated as

$$\sigma_{pN} = \sum_i n_i \sigma_{pN\ i}$$

and the **mean free path** $\lambda_{\text{tot}}$ is given from the total cross section
How to model composite materials in Merlin?

```cpp
CompositeMaterial* CuCD = new CompositeMaterial();
CuCD->SetName("CopperCarbonDiamond");
CuCD->SetSymbol("CuCD");

CuCD->AddMaterialByMassFraction(CD, 0.3489);
CuCD->AddMaterialByMassFraction(Cu, 0.6467);
CuCD->AddMaterialByMassFraction(B, 0.0044);

CuCD->SetDensity(5400);
CuCD->SetConductivity(12.6E6);
CuCD->Assemble();
CuCD->VerifyMaterial();
```

Calculates all composite material properties
Outline

- Material implementation in Merlin
- Modeling of composite materials
- **Comparison between Sixtrack and Merlin**
- Cleaning performance with advanced collimator materials
Comparison of different methods

TEST CASE

Pencil beam 6.4*10^6 particles

1 cm long block of different materials

CuCD
MoGr
CFC for reference

Simulations have been done with:

1. Merlin using the **MERLIN METHOD**
2. Merlin using SixTrack approximation (**MERLIN SIXTRACK METHOD**)  
3. SixTrack
Single diffractive scattering

Not evident differences are evident comparing the MERLIN METHOD and the MERLIN SIXTRACK METHOD.
Multiple Coulomb scattering
Polar angle distribution

MERLIN and SixTrack provide very similar results, which is expected since MCS is a type of interaction based on bulk material properties.
Multiple Coulomb scattering _ Energy loss

Merlin includes energy loss fluctuation as from Landau-Vavilov
SixTrack mainly relies on the mean energy loss as from Bethe-Bloch
Multiple Coulomb scattering _ Energy loss

**MoGr**

**CuCD**
Total elastic scattering

Polar angle distribution

MoGr

CuCD

CERN
Outline

- Material implementation in Merlin
- Simulation model of composite materials
- Comparison between Sixtrack and Merlin
- Cleaning performance with advanced collimator materials
Cleaning simulations with advanced collimators

- What is the impact of using new materials on the cleaning efficiency?
- Does it worsen/improve the collimation performance?

Two cases simulated with Merlin for the nominal LHC (7 TeV) scenario, where replaced

1. All TCSGs in IR7 with MoGr/CuCD*

1. All TCPs in IR7 with MoGr/CuCD**

** E. Quaranta et al., ”Collimation cleaning at the LHC with advanced secondary collimator materials”, IPAC15, Richmond, Virginia, USA
Replacement of IR7 TCSGs with novel materials
Merlin simulations

- Losses on first two TCSG: +11-18% than CFC
- Differences in losses on TCSGs further downstream less apparent

Results are consistent with those previously obtained with SixTrack
Replacement of IR7 TCSGs with novel materials

**SIXTRACK**

**MERLIN**

![Graphs showing loss ratio over CFC collimator losses for SIXTRACK and MERLIN](image)

- **SIXTRACK**
  - MoGr
  - CuCD
  - Inermet

- **MERLIN**
  - MoGr
  - CuCD

CERN
Replacement of IR7 TCPs with novel materials
Merlin simulations

TCPs in **CuCD** $\rightarrow$ \(~10\%\) more losses in TCP.C6L7
TCPs in **MoGr** $\rightarrow$ \(~5\%\) more losses in TCP.C6L7
Replacement of IR7 TCPs with novel materials_MERLIN

TCPs in **CuCD** $\rightarrow$ ~ 10% more losses in TCP.C6L7
~ 5-60% loss reduction on TCSGs

TCPs in **MoGr** $\rightarrow$ ~ 5% more losses in TCP.C6L7
~ 10-40% loss reduction on TCSGs

![Graph showing normalized losses and loss ratios over CFC collimator losses for different TCP configurations in CuCD and MoGr.](chart)
Cleaning inefficiency in the DS region

TCPs/TCSGs in CFC

Integrated Cleaning inefficiency in DS1
1.66×10^{-4}

Integrated Cleaning inefficiency in DS2
1.06×10^{-4}

TCPs in MoGr

TCPs in CuCD

Integrated Cleaning inefficiency in DS1
5.67×10^{-4}

Integrated Cleaning inefficiency in DS2
6.65×10^{-5}
Cleaning inefficiency in the DS region

TCPs/TCSGs in CFC

1.66 \times 10^{-4} \quad 1.06 \times 10^{-4}

TCSGs in MoGr

1.77 \times 10^{-4} \quad 8.93 \times 10^{-5}

TCSGs in CuCD

1.44 \times 10^{-4} \quad 9.39 \times 10^{-5}
Conclusions

- Composite materials have been successfully implemented in MERLIN and are available for simulations of collimation cleaning at the LHC.

- From a first comparison between MERLIN and SixTrack no relevant differences between the different approaches of the two codes in treating composite materials are evident.

- Simulation results of halo cleaning in the LHC with novel materials for the secondary and primary collimators have been presented and the results are consistent with those previously obtained with SixTrack.

- The study could be extended including tools like FLUKA.

*Thank you for your attention*
Backup slides
## Properties of composite materials in Merlin and SixTrack

<table>
<thead>
<tr>
<th>Property</th>
<th>MoGr</th>
<th>CuCD</th>
<th>Glidcop</th>
<th>Inermet180</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Z$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Merlin</td>
<td>6.611</td>
<td>11.896</td>
<td>28.824</td>
<td>67.66</td>
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<tr>
<td>SixTrack</td>
<td>6.653</td>
<td>11.898</td>
<td>28.823</td>
<td>67.657</td>
</tr>
<tr>
<td>$A$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Merlin</td>
<td>13.44</td>
<td>25.23</td>
<td>63.145</td>
<td>166.7</td>
</tr>
<tr>
<td>SixTrack</td>
<td>13.532</td>
<td>25.238</td>
<td>63.149</td>
<td>166.68</td>
</tr>
<tr>
<td>$\rho , [g/cm^3]$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Merlin</td>
<td>2.5</td>
<td>5.4</td>
<td>8.93</td>
<td>18</td>
</tr>
<tr>
<td>SixTrack</td>
<td>2.5</td>
<td>5.4</td>
<td>8.93</td>
<td>18</td>
</tr>
<tr>
<td>$\sigma_d , [M_S/m]$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Merlin</td>
<td>1</td>
<td>12.6</td>
<td>53.8</td>
<td>8.6</td>
</tr>
<tr>
<td>SixTrack</td>
<td>1</td>
<td>12.6</td>
<td>53.8</td>
<td>8.6</td>
</tr>
<tr>
<td>$\chi_0 , [m]$</td>
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<td></td>
<td></td>
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<tr>
<td>Merlin</td>
<td>0.1214</td>
<td>0.03164</td>
<td>0.01443</td>
<td>0.00385</td>
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<tr>
<td>SixTrack</td>
<td>0.11931</td>
<td>0.03162</td>
<td>0.01442</td>
<td>0.00385</td>
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<tr>
<td>$\frac{dE}{dx}$</td>
<td></td>
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<tr>
<td>Merlin</td>
<td>0.7188</td>
<td>1.981</td>
<td>2.685</td>
<td>5.576</td>
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<tr>
<td>SixTrack</td>
<td></td>
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<tr>
<td>$b_n , [GeV/c^2]$</td>
<td></td>
<td></td>
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<tr>
<td>Merlin</td>
<td>79.69</td>
<td>121.3</td>
<td>223.59</td>
<td>427</td>
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<tr>
<td>SixTrack</td>
<td>76.665</td>
<td>114.961</td>
<td>208.669</td>
<td>392.137</td>
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<tr>
<td>$\lambda_{tot} , [m]$</td>
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<tr>
<td>Merlin</td>
<td>0.2301</td>
<td>0.1259</td>
<td>0.0892</td>
<td>0.0577</td>
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<tr>
<td>SixTrack</td>
<td>0.2484</td>
<td>0.1356</td>
<td>0.0942</td>
<td>0.0603</td>
</tr>
<tr>
<td>Merlin Modified</td>
<td>0.2257</td>
<td>0.1259</td>
<td>0.0892</td>
<td>0.0577</td>
</tr>
</tbody>
</table>
Cleaning inefficiency in the DS region

<table>
<thead>
<tr>
<th>IR7 configuration</th>
<th>Integrated Cleaning inefficiency in DS1</th>
<th>Integrated Cleaning inefficiency in DS2</th>
</tr>
</thead>
<tbody>
<tr>
<td>TCPs/TCSGs in CFC</td>
<td>1.660×10^{-4}</td>
<td>1.061×10^{-4}</td>
</tr>
<tr>
<td>TCPs in MoGr TCSGs in CFC</td>
<td>1.184×10^{-4}</td>
<td>6.651×10^{-5}</td>
</tr>
<tr>
<td>TCPs in CuCD TCSGs in CFC</td>
<td>4.991×10^{-5}</td>
<td>3.69×10^{-5}</td>
</tr>
<tr>
<td>TCPs in CFC TCSGs in MoGr</td>
<td>1.77×10^{-4}</td>
<td>8.93×10^{-5}</td>
</tr>
<tr>
<td>TCPs in CFC TCSGs in CuCD</td>
<td>1.44×10^{-4}</td>
<td>9.39×10^{-5}</td>
</tr>
</tbody>
</table>
Total elastic scattering energy loss

Minor changes between MoGr and CFC
Total elastic scattering energy loss

Graphs showing elastic and ionization scattering for MoGr and CuCD.