Differentiating GATE/Geant4 with Derivgrind

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Background

Goal: Optimize the design of particle physics instruments with e. g. gradient-based optimization methods.

Objective Function: $J(\text{design parameters } x) = (\text{physics performance}) - \mu \cdot (\text{cost})$

Gradient descent to minimize J: $x_{\text{better}} = x_{\text{old}} - \alpha \cdot \nabla J(x_{\text{old}})$

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[1] Set of techniques to evaluate derivatives of computer-implemented functions.

[2] Monte-Carlo simulator of the passage of particles through matter. 850k lines of C++. Toolkits like GATE might add substantial amounts of code in C++ or other languages.

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  - ⊖ many discontinuities
  - ⊕ most general approach

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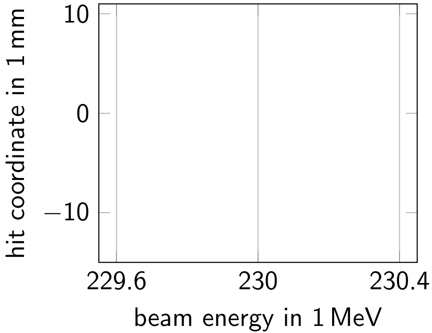
GATE/Geant4 Setup

- GATE is a medical imaging toolkit built on top of Geant4.
- In our setup, a single energetic proton passes through a human head and a digital tracking calorimeter (DTC) of the Bergen pCT collaboration.



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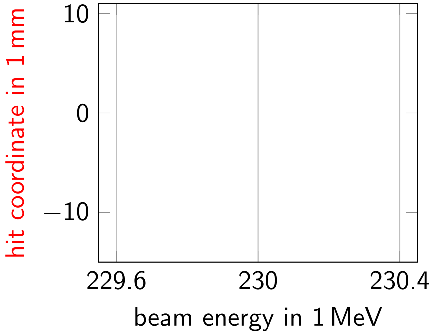

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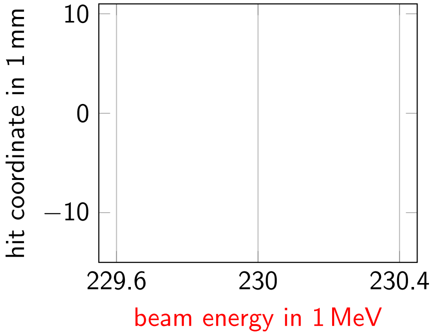

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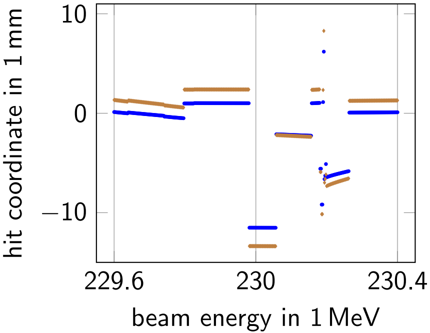
- The seed of the random number generator was fixed.



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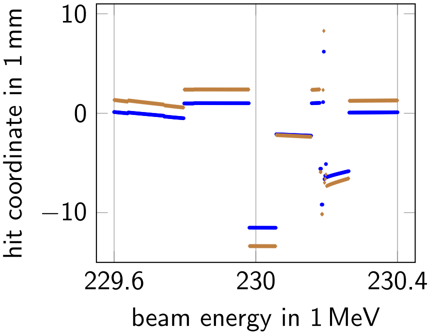
Why are there jumps?
At some point, a different physics process is selected. It consumes a different amount of random numbers, so the subsequent execution receives a shifted (i. e. entirely different) sequence of random numbers.

Is the function differentiable between the jumps?
It looks so, let's check at

$$x_0 = 230\,\text{MeV}$$

by evaluating difference quotients.



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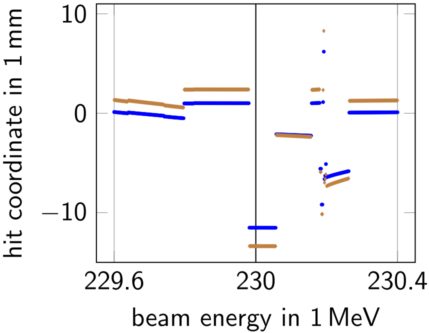

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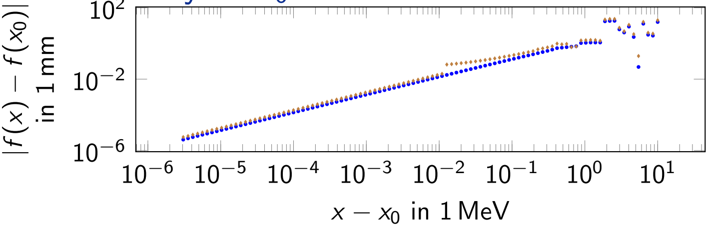

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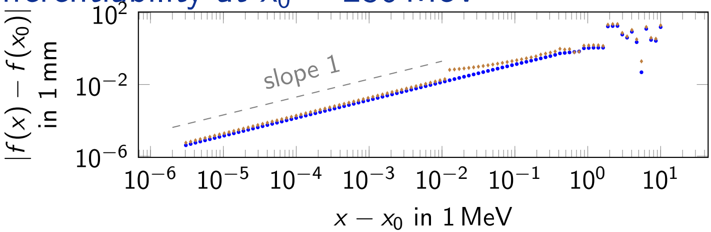

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Algorithmic Differentiation with Derivgrind

- AD tools allow to compute the derivatives of computer-implemented functions ("primal programs").
- To this end, they need to find out about the real-arithmetic computations performed by the primal program.
- Most AD tools do this in the source code or as part of the compiler.
- Derivgrind operates on machine code just before it runs on the CPU, achieving an unprecedented degree of independence from the source code of the primal program.

Derivgrind is available at `https://github.com/SciCompKL/derivgrind`

Declaring Inputs and Outputs to Derivgrind

```
+ #include "/somepath/include/valgrind/derivgrind.h"
```

“Seeding” dot values of the input variable (beam energy):

```
   if (command == pIonCmd) {
     pSourcePencilBeam->SetIonParameter(newValue);
   }
   if (command == pEnergyCmd) {
     double energy = pEnergyCmd->GetNewDoubleValue(newValue);
+    double one = 1.0;
+    DG_SET_DOTVALUE(&energy,&one,sizeof(double));
     pSourcePencilBeam->SetEnergy(energy);
   }
```

Obtaining dot values of output variables (hit position):

```
   if (m_rootHitFlag) m_treeHit->Fill();
+  float pos = *(float*)(m_treeHit->GetBranch("posX")->GetAddress());
+  float pos_d;
+  DG_GET_DOTVALUE(&pos,&pos_d,sizeof(float));
+  std::cout << "pos_d=" << pos_d << "\n";
```

Running GATE/Geant4 under Derivgrind

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valgrind --tool=derivgrind Gate ⟨args⟩
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  - When there is a real-arithmetic operation like $c = b \cdot a$, use differentiation rule like $\dot{c} = \dot{a} \cdot b + a \cdot \dot{b}$.

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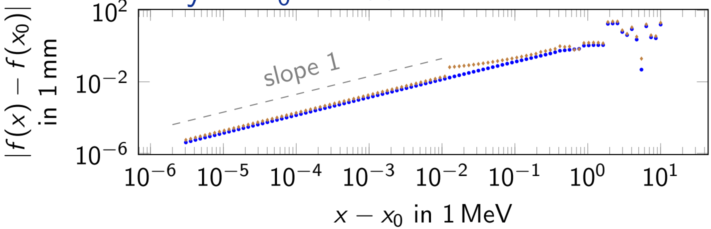
$\rightsquigarrow$ We see the original output, plus some Valgrind/Derivgrind messages, plus the dot values of the output variables.

Differentiability at $x_0 = 230\,\mathrm{MeV}$



$\rightsquigarrow$ The hit coordinate $f(x)$ is differentiable in the beam energy x at x_0.

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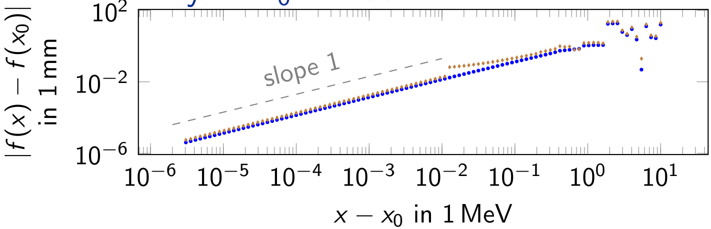

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Bit-Tricks in Geant4

- Geant4 defines and uses a function `G4Log` adapted from the VDT math library.
- `G4Log` first performs a “range reduction”, scaling its argument by power of 2 to map it into $[0.5, 1)$.
- This is done by setting the exponent bits to `0b01111111110` via bitwise operations.

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- Derivgrind's dot value propagation does not recognize this as an arithmetic operation.
- Fix: Edit Geant4 source code, replacing body of `G4Log` by call to `log`.

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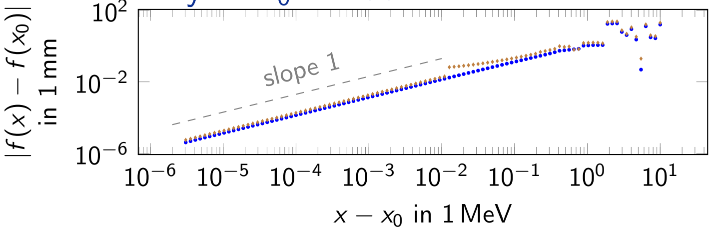

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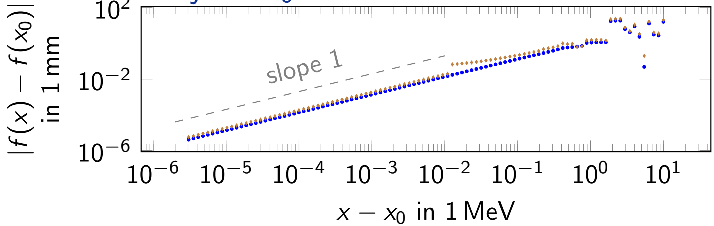

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Declaring Inputs and Outputs, Reverse Mode

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Declaring output variables (hit position):

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```
tape-evaluation $PWD
```

⇝ Computes the derivatives.

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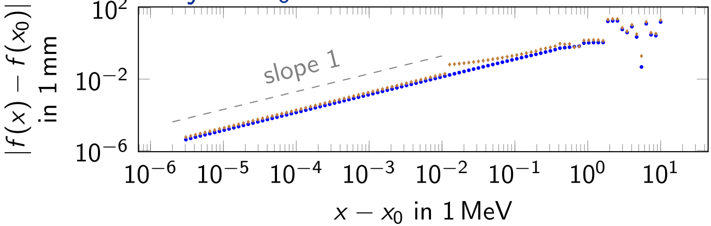

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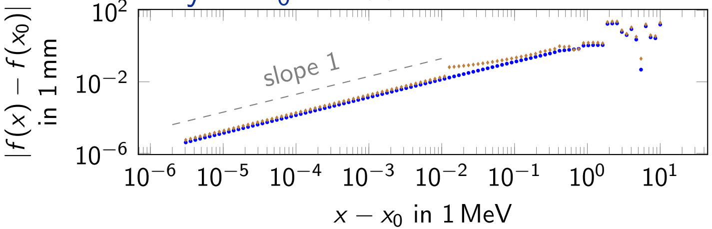

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Summary

- Derivgrind implements forward-mode AD and operator-overloading-style reverse-mode AD for compiled programs like GATE/Geant4.
- Very limited access to primal source code needed, only in order to identify input/output variables (and for debugging in case of failure).
- In the case of unsupported bit-tricks, Derivgrind might miss or misunderstand real-arithmetic dependencies.
- In our GATE/Geant4 setup, this happened but could be fixed (in debug mode).

Next Steps

- Create bit-trick-finding tool. Right now we can discover the `G4Log` bit-trick automatically, but we don't know yet why Derivgrind fails for the release-mode GATE/Geant4.
- Work on more difficult example and connect AD derivatives to optimizer.
  - Can anyone propose a simple yet meaningful Geant4 setup with some inputs, some outputs, and an objective function defined on them?
- Try out other AD tools, e. g.
  - CoDiPack – operator-overloading tool developed in Kaiserslautern.
  - Enzyme or CLAD – compiler-based; Geant4 libs can be built statically.

Contact Information

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Chair for Scientific Computing
University of Kaiserslautern-Landau (RPTU)

Derivgrind is available at https://github.com/SciCompKL/derivgrind

Project E-Mail Address: derivgrind@projects.rptu.de

Video (7 min) about Derivgrind+LibreOffice Calc:
https://t1p.de/tt4ne

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