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Differentiating GATE/Geant4 with Derivgrind

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The computational assessment of a proposed detector design usually involves Monte-Carlo simulations of how particles interact with the detector. For example, the Bergen Proton CT (pCT) collaboration uses the program GATE based on Geant4 for the development of its digital tracking calorimeter. It would be interesting to see a differentiated simulation being used as part of a differentiable assessment pipeline in the context of MODE, instead of simplified simulators or surrogate models. One obstacle on the way to this goal is the technical complexity associated with differentiating big and complicated software projects like Geant4 with classical source-code-based AD tools.

To reduce this complexity, we have built Derivgrind, a novel AD tool applicable to compiled programs. Under a few assumptions on how a program performs real arithmetic, users of Derivgrind only need to edit a small number of lines in its source code, in order to indicate the input and output variables. In this talk, we showcase the application of Derivgrind to a downsized GATE/Geant4 setup adapted from the Bergen pCT collaboration, producing correct forward- and reverse-mode partial derivatives.

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