

Fourth MODE Workshop on Differentiable Programming for Experiment Design



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Algorithmic Derivatives of Electromagnetic Shower Simulations

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Applying algorithmic differentiation to particle simulations like Geant4 would allow us to evaluate derivatives of simulation outputs with respect to inputs, e.g. of the mean energy depositions in calorimeter layers with respect to geometry parameters. Such derivatives could become instrumental for a number of application like detector optimization or parameter fitting in HEP. However, besides the technical challenge of applying AD to over one million lines of code, there is a number of mathematical/statistical challenges: Does the high density of discontinuities, induced for example by 'if' and 'while' statements in the code, cause problems in the derivative computation? Are we allowed to treat random numbers like constants with respect to AD? How large is the error when the mean pathwise derivative is evaluated as a proxy for the actual derivative of expectancies computed by Monte-Carlo algorithms?

To approach these questions, we have applied the operator-overloading AD tool CoDiPack to the compact G4HepEm/HepEmShow package for the simulation of electromagnetic showers in a simple sampling calorimeter. After disabling multiple scattering in the simulation, our pathwise gradient estimator approximates derivatives of energy depositions with only a small bias, which proved unproblematic in a simple optimization study. In this talk, we will report on our methodology and give an overview on our findings.

Authors: AEHLE, Max (Fachhochschule Worms (DE)); AEHLE, Max

Co-authors: LANGE, David; LANGE, David (Princeton University (US)); HEINRICH, Lukas Alexander (Technische Universität München (DE)); KAGAN, Michael (SLAC National Accelerator Laboratory (US)); NOVAK, Mihaly (CERN); GAUGER, Nicolas; VASILEV, Vassil (Princeton University (US))

Presenters: AEHLE, Max (Fachhochschule Worms (DE)); AEHLE, Max

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