Software for higher-order sensitivity analysis of parametric DAEs

Moritz Schmitz¹, Boris Gendler², Ralf Hannemann-Tamàs¹, Uwe Naumann², Wolfgang Marquardt¹

¹RWTH Aachen, Aachener Verfahrenstechnik - Prozesstechnik, Turmstrasse 46, 52062 Aachen ²RWTH Aachen, STCE, Süsterfeldstraße 65, 52072 Aachen

We introduce AC-SAMMM (The AaChen platform for Structured Automatic Manipulation of Mathematical Models), a new software infrastructure for efficient transformation and evaluation of expressions and their higher-order derivatives.

We describe the way this software can be used to perform automatically the translation of a model written in an equation-oriented environment such as Modelica into a subset of C/C++ and the generation of the model's higher-order derivative code by Algorithmic differentiation (AD) techniques. The generated C++ files are then automatically compiled into a highly optimized dynamic library. Together with the CAPE-OPEN based C++ interface ESO (an acronym for Equation Set Object) an easy to handle back end to any C++-based subroutine exists that provides very robust and efficient drivers and functions to access the model and its derivatives.

The derivatives are generated, using the derivative code compiler (dcc), an AD tool which provides source code transformation for a restricted but numerically relevant subset of C/C++. dcc can be applied repeatedly to its own output, to generate derivative codes of arbitrary order. It is possible to generate tangent-linear and adjoint code with dcc using for example features such as activity analysis, to-be-recorded analysis and vector mode.

Several case studies are presented and they show that our platform performs very well even for large-scale nonlinear systems (up to 2000 stiff DAE's) concerning generation-time of higher-order derivatives, compile- and evaluation-time. The AC-SAMMM infrastructure has been interfaced with the AVT.PT developed integrator NIXE with 2nd-order sensitivity capabilities, and can be used with state-of-the-art NLP solvers to solve a restricted class of multistage optimal control problems.