Sensitivity analysis based computational modeling

Jože Korelc

University of Ljubljana, Slovenia

Sensitivity analysis has become an indispensable part of modern computational algorithms. Nowadays, the automation of sensitivity analysis enables efficient evaluation of sensitivities that are exact except for the round of errors. For that purpose, the use of automatic differentiation tools and techniques gained much popularity and attention in recent years. However, big differences in the numerical efficiency of the resulting simulation codes between various implementations (dual number approach, code-to-code transformation approach, forward or direct approach, backward or adjoint approach, etc.) have been revealed. The background of those differences is explained as well as the limitations of various approaches. We propose a hybrid symbolic-automatic differentiation approach with code-to-code transformation and simultaneous stochastic expression optimization implemented in AceGen (www.fgg.uni-lj.si/symech/) as one of the most efficient approaches. Yet, the true advantages of automation become apparent only if the description of the problem, the notation, and the mathematical apparatus used is changed as well. It will be shown that the unification of the classical mathematical notation of computational models and the actual computer implementation can be achieved through an extended automatic differentiation technique combined with automatic code generation and sensitivity analysis. The automatic differentiation-based form (ADB form) of a classical mathematical notation of solid and contact mechanics, multi-scale analysis, stochastic analysis, optimization, and stability analysis will be presented. While the first order sensitivity analysis is already an established tool for the improvement of numerical algorithms, (e.g., optimization) is the second order sensitivity analysis still rarely used. This is mainly due to the high numerical cost, especially in the case of time-dependent problems. The benefits and drawbacks of the second-order forward and backward sensitivity approach when applied to multi-scale modeling and stochastic analysis will be compared. The talk introduces a fully consistently linearized two-level path-following algorithm as a solution algorithm for strongly nonlinear multi-scale problems. The approach also increases the concurrency of micro problems which can significantly improve the overall speed of the execution in multi-processor and multi-core systems.