

A mixed approach to adjoint computation with algorithmic differentiation

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Abstract: Despite intensive research in the last decades the efficient provision of adjoints still forms a major bottleneck for many optimization applications based on large scale simulations of physical phenomena, including PDE solvers, linear and non-linear system solvers etc. Various algorithmic differentiation tools have been developed and applied to the simulation software. Up to now, there are two strictly disconnected approaches to implement algorithmic differentiation (AD), namely, source transformation and operator overloading. This separation was motivated by different features of the programming languages like Fortran and C++. In this joint work with S.H.K. Narayanan of Argonne National Laboratory we have for the first time combined the two approaches to implement AD for C++ codes. We use the source transformation tool ADIC and the operator overloading tool ADOL-C in a coherent way to propagate derivatives and obtain speedup. Source transformation is used for core routines that are repetitive where the transformed source can be optimized much better by modern compilers, and operator overloading to interconnect at the upper level, where source transformation isn't possible due to complex language constructs of C++. We present the first results of the mixed approach in this presentation.