Chair of Aerodynamics and Fluid Mechanics
Department of Mechanical Engineering
Technical University of Munich

Differentiable Programming: Automatic Differentiation for State-of-the-Art CFD Solvers

M.Sc. Thesis, or IDP Project

Josef Winter & Ludger Pähler
josef.winter@tum.de & ludger.paehler@tum.de

Introduction

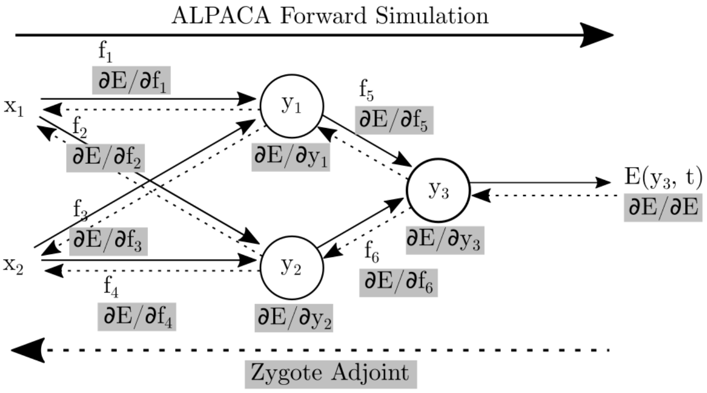
Differentiable programming is seen by many as the coming unifying paradigm of scientific computing and machine learning, which will enable better surrogate modeling, faster sensitivity analysis, the solving of more complex inverse problems and a new level of inference on large-scale scientific simulations by utilizing automatic differentiation. A first generation of differentiable solvers is pursuing this by building on limited machine learning DSLs, such as Tensorflow, which are unfit for such purpose as they are too constrained for complex scientific models and require the rewrite of existing software. We hence seek to enable a new generation of differentiable programming by building on the absolute state-of-the-art in computational fluid dynamics solvers for HPC with our in-house solver *ALPACA* and introducing a new breed of communication protocol to interface state-of-the-art automatic differentiation engines with HPC solvers.

Objectives

In this project we will build on the next generation of automatic differentiation [1] frameworks by using *Zygote.jl* [2] in formulating a new communication protocol built on top of the LLVM IR to interact with our CFD solver *ALPACA* to calculate gradients over program executions. For this we will build a first prototype taking cues from the architecture of *PPX*, an execution protocol for probabilistic programming, and formulate optimized adjoint calulations using *Zygote's* pullback functionality. This will then be validated and optimized for successively more complex testcases.

Requirements

- Knowledge of Julia
- C++ 17 familiarity
- Familiarity with the concept of adjoints
- Familiarity with LLVM
  - LLVM-based compilers
  - LLVM intermediate representations



[1] Baydin AG, Pearlmutter BA, Radul AA, Siskind JM. Automatic differentiation in machine learning: a survey. The Journal of Machine Learning Research. 2017 Jan 1;18(1):5595-637.

[2] Innes M, Edelman A, Fischer K, Rackauckas C, Saba E, Shah VB, Tebbutt W. A differentiable programming system to bridge machine learning and scientific computing. ArXiv abs/1907.07587. 2019 Jul.