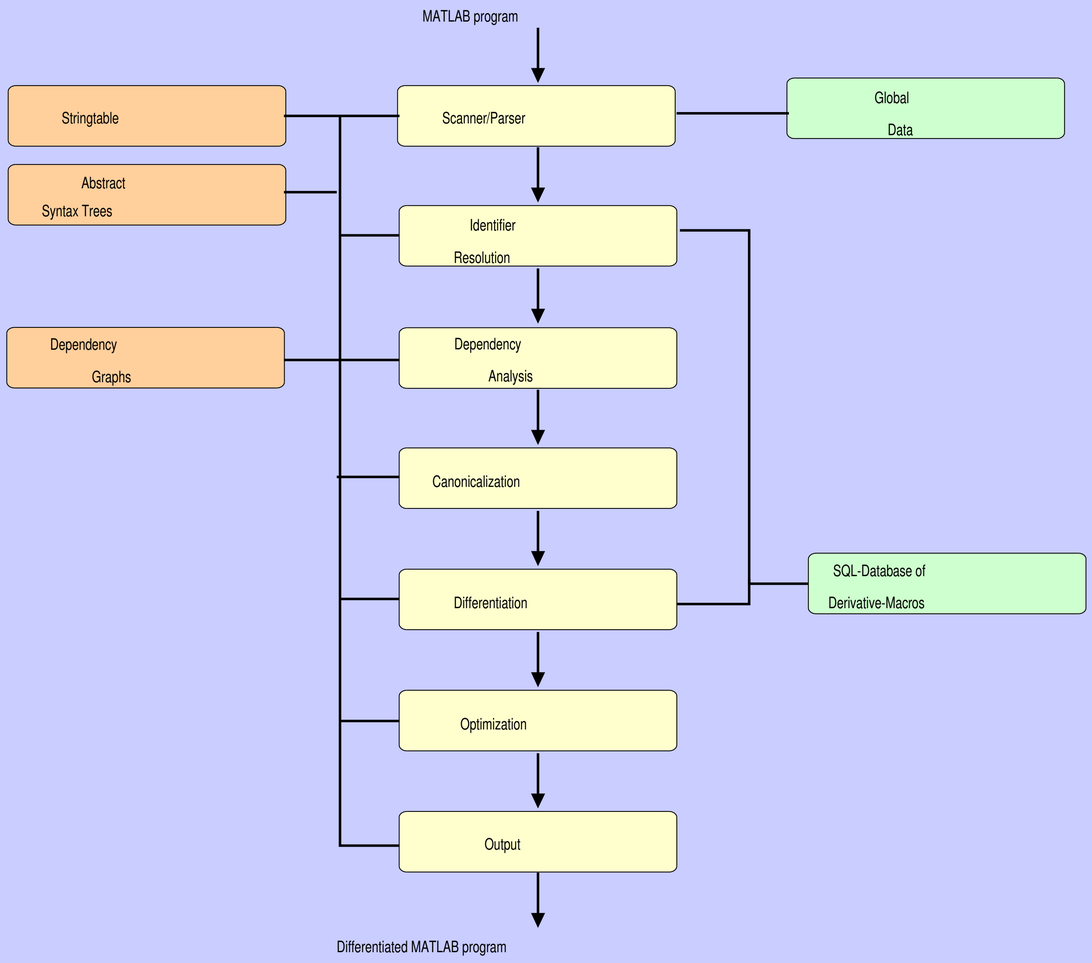
RHEINISCH-
WESTFÄLISCHE
TECHNISCHE
HOCHSCHULE
AACHEN

Aachen Institute for Advanced Study in Computational Engineering Science

Automatic Differentiation (AD)

The term AD comprises a set of techniques for the automatic generation of computer programs, evaluating the derivatives of some mathematical function that is given in the form of a computer program. AD-generated derivatives are free from truncation and cancellation errors.

ADiMat: AD for MATLAB



Features:

- Supports 95% of the MATLAB syntax
- Derivatives are specified in a macro language
- Successfully applied to large MATLAB codes
- OO-design, SQL database, interfaces to ADIFOR and ADIC

ADiCape: XSLT based tool for AD transformations of CapeML

CapeML: XML equation interchange format used in process engineering

AD Transformation:

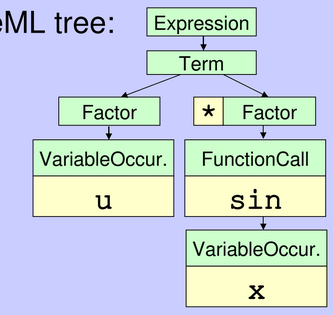
Original code: `u*sin(x)`

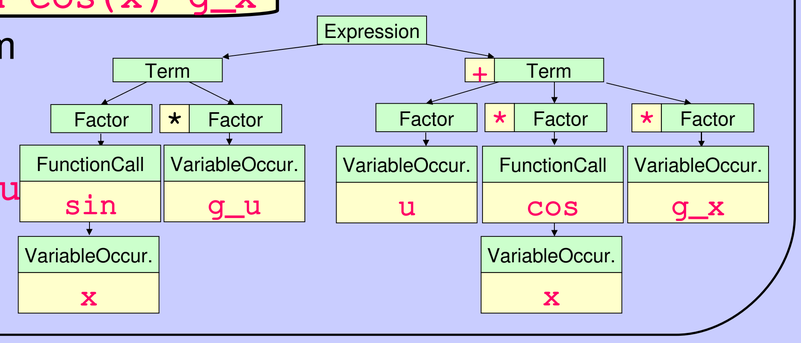
The original code is augmented by additional statements for the computation of derivatives.

Differentiated code: `sin(x)*g_u + u*cos(x)*g_x`

Each active program variable `u` is associated with a derivative object `g_u`

CapeML tree:





Dynamic optimization:

DAE: `M ∂x/∂t = F(x,u,t)`

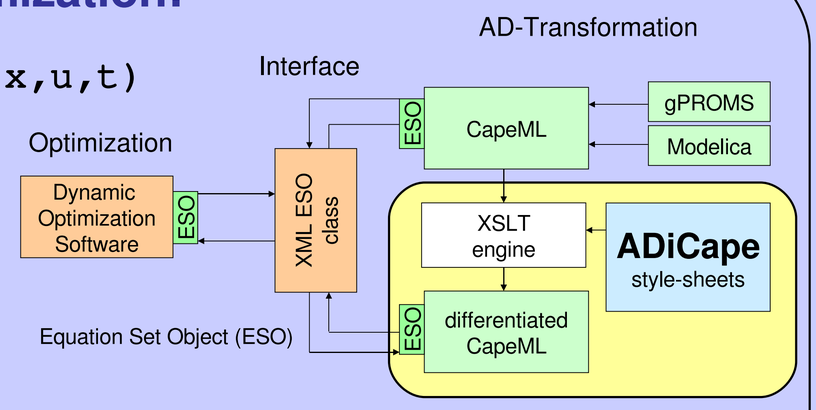
state: `x`

control `u`

time: `tϵ(t0,tf)`

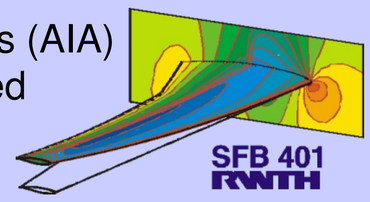
To obtain `∂F/∂x` and `∂F/∂u`, initialize

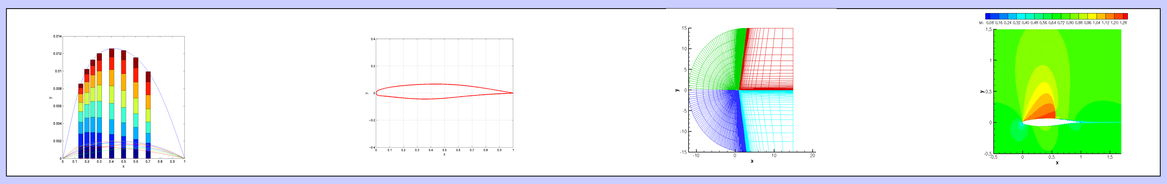
g_x(1:2)=(1.0,0.0) and **g_u(1:2)=(0.0,1.0)** ("seeding")

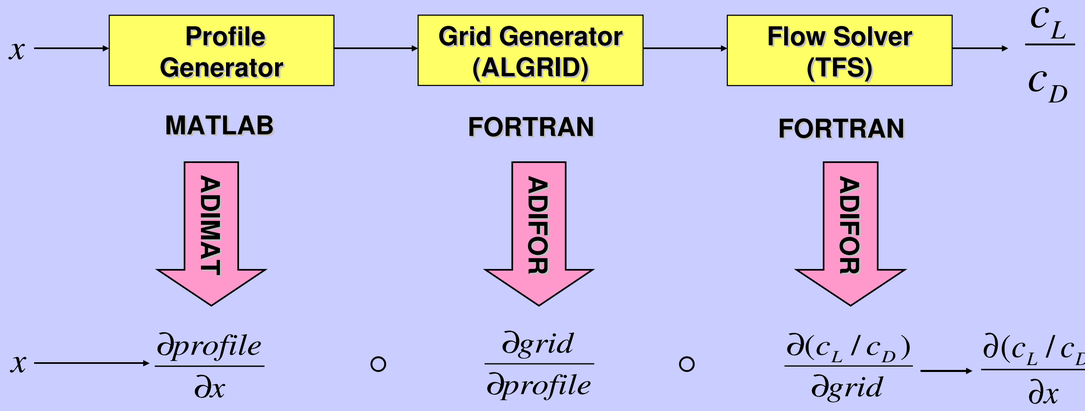


AD of a computational chain

- Collaboration with the Institute of Aerodynamics (AIA)
- For a given airfoil (profile) – here parameterized by x – lift and drag coefficients (C_L and C_D) are computed by a computational chain







AD Highlights @ RWTH Aachen

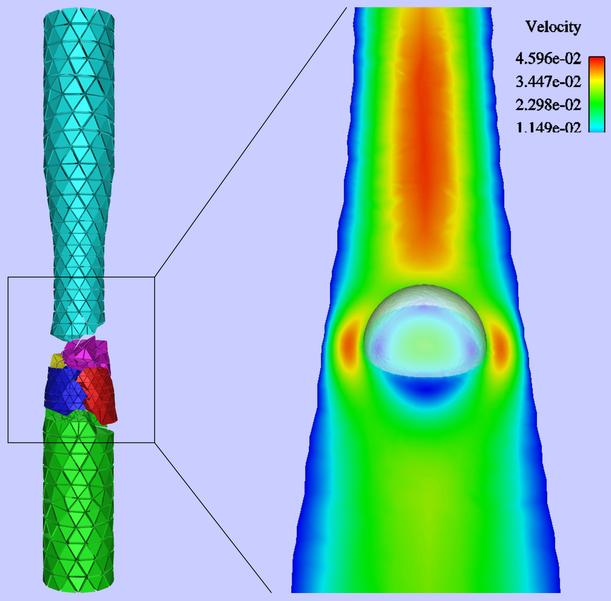
- TFS: The Flow Solver, developed at AIA
- QUADFLOW: adaptive flow solver, currently being developed by several RWTH institutes within SFB 401
- XNS: eXtended Navier-Stokes solver, developed by M. Behr et al.
- SEPRAN: general-purpose FEM package from TU Delft
- FLUENT: industrial general-purpose CFD code from Fluent Inc.,
  → **largest code processed by AD (≈ 1.6 million loc)**

Parallel FEM for a two phase flow problem

A levitated single droplet in a measurement cell can be modelled by the Navier-Stokes equations coupled with the level set equation.

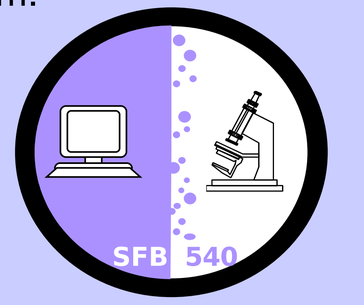
$$\begin{aligned} \rho(\phi)\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) &= -\nabla p + \rho(\phi)\mathbf{g} + \operatorname{div}(\mu(\phi)\mathbf{D}(\mathbf{u})) + \tau\kappa\delta_\Gamma\mathbf{n}_\Gamma \\ \operatorname{div}\mathbf{u} &= 0 \\ \phi_t + \mathbf{u}\nabla\phi &= 0 \end{aligned}$$

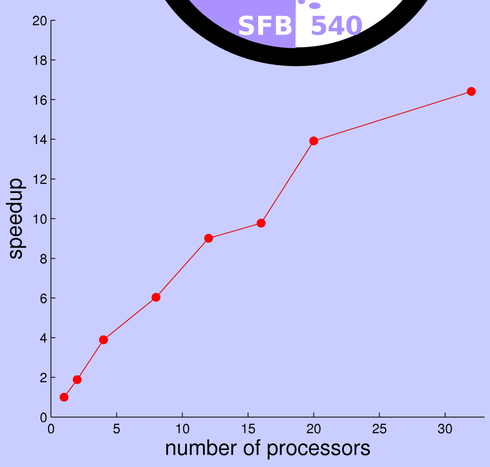
In collaboration with the Chair of Numerical Mathematics, the parallel CFD package DROPS, a finite element solver on unstructured multilevel grids, is developed to solve this problem.



Distribution of the tetrahedra among six processors

- 16k tetrahedra
- 72k unknowns





AMD Opteron 848 (2.2 GHz)
mpich2 / Gigabit-Ethernet
gcc compiler

Computer Science 12 (Scientific Computing) http://www.sc.rwth-aachen.de

Scientific Computing