Software and Tools for Computational Engineering
RWTH AACHEN UNIVERSITY
Software and Tools for Computational Engineering
Prof. Dr. rer. nat. Uwe Naumann

Master Thesis / Bachelor Thesis / Student Researcher Position

Computation of Higher Derivative Tensors

Description: Algorithmic Differentiation (AD) returns exact derivatives of numerical simulation programs with machine accuracy by exploiting elemental symbolic differentiation and the chain rule of differential calculus. The reverse mode of AD builds *adjoint codes* that are advantageous for problems with a small set of outputs, as it occurs frequently in many fields of computational science and engineering. For some methods second or even higher derivatives are required, e.g. in solving optimal control problems, solving inverse problems, or design and robust optimization.

Goal: In this thesis, different methods for the improvement of computing higher derivative tensors should be considered. For efficiency reasons, exploiting symmetry and sparsity of these tensors is indispensable and can be achieved by various techniques (e.g. special seedings, Taylor series propagation or graph coloring). Application and implementation of these techniques is part of the work.

Profile: You should have programming experience in C/C++. In addition, knowledge in the field of algorithmic differentiation and numerical simulation is desirable.

If you are interested in a bachelor or master thesis or a student researcher position (up to 19 hours a week) on this topic, please do not hesitate to contact us!

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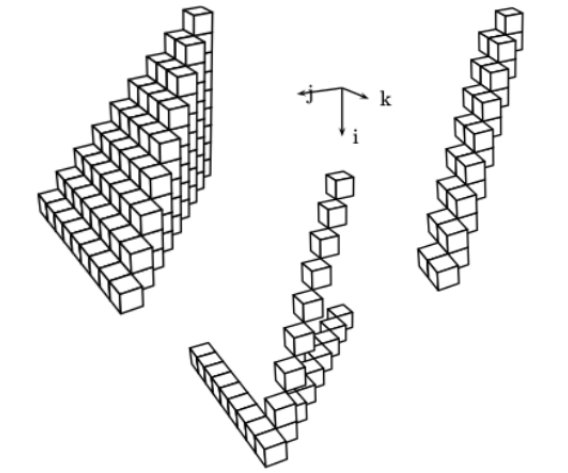

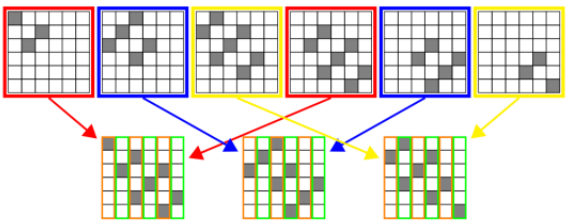

procedure SymmetricApproach($n, \mathbf{x}$)
  $lb, ub \leftarrow$ LoadBalancing(n)
  for $i_2 \leftarrow lb, ub$ **do**
    for $i_3 \leftarrow 1, i_2$ **do**
      for $i_4 \leftarrow 1, i_3$ **do**
        $\mathbf{x}^{(2)} \leftarrow \mathbf{e}_{i_2}, \quad \mathbf{x}^{(3)} \leftarrow \mathbf{e}_{i_3}, \quad \mathbf{x}^{(4)} \leftarrow \mathbf{e}_{i_4}, \quad y_{(1)} \leftarrow 1$
        $\mathbf{x}_{(1)}^{(2,3,4)} \leftarrow \mathrm{F}_{(1)}^{(2,3,4)}(\mathbf{x}, \mathbf{x}^{(2)}, \mathbf{x}^{(3)}, \mathbf{x}^{(4)}, y_{(1)})$
        for $i_1 \leftarrow i_2, n$ **do**
          $\left[D^4 F\right]_{i_1,i_2,i_3,i_4} \leftarrow \left[x_{(1)}^{(2,3,4)}\right]_{i_1}$
        end for
      end for
    end for
  end for
  return $D^4 F$
end procedure