

Introduction to Algorithmic Differentiation

aka: Computational Differentiation / Rechnergestütztes Differenzieren

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Informatik 12:
Software and Tools for Computational Engineering (STCE)

RWTH Aachen

Warm-Up

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1 | $y = \sin(x)$

1 | $y = \exp(\sin(x))$

1 | $y = x * p$

1 | $y * = x$

```
1 | float f(float x) {  
2 |     return cos(x);  
3 | }
```

```
1 | double f(float x) {  
2 |     return 42.;  
3 | }
```

???

Who knows how to differentiate ...

```

1  ...
2
3  template<typename T, typename PT>
4  void paths(size_t ncs, size_t from, size_t to, T& x, const std::vector<T>& p, const std::
   vector<std::vector<PT>>& dW, T& s) {
5    using namespace std;
6    size_t n=p.size()-2;
7    T x0=x;
8    for (size_t j=from;j<to;j++) {
9      for (size_t i=0;i<n;i+=ncs) steps(j,i,i+ncs,x,p,dW);
10     T sig=1/(1+exp(-(x-p[n])/p[n+1])); s+=(x-p[n])*sig; x=x0;
11   }
12 }
13 ...

```

??? ... YOU WILL!

This course introduces **Algorithmic Differentiation (AD)** as the method of choice for computing first and higher derivatives of numerical simulation programs.

Warm-Up

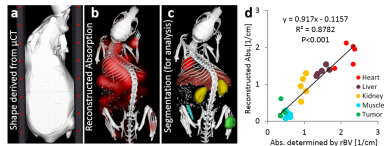
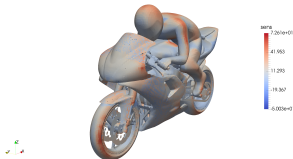
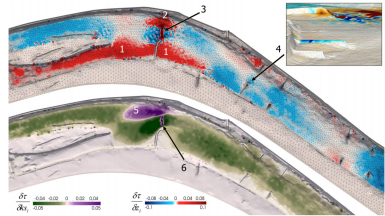
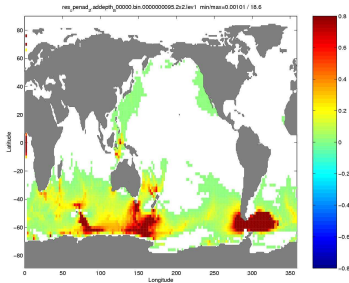
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Need for Cheap Gradients ...



... as well as aerospace, machine learning, finance, ...

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- ▶ AD by overloading
 - ▶ maths
 - ▶ sample code
 - ▶ dco/c++

- ▶ AD by hand
 - ▶ manual generation of derivative code

- ▶ AD by compiler
 - ▶ lexical analysis with flex
 - ▶ syntax analysis with bison
 - ▶ syntax-directed generation of derivative code

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- ▶ Lecture (U. Naumann on Tuesdays at 2:30pm in AH III)
- ▶ Tutorial (M. Towara on Wednesdays at 12:30pm in AH III)
 - ▶ VirtualBox Linux image for tutorial exercises contains dco/c++ and other software required
- ▶ Exams (90min written exams on Feb 24 / Mar 30, 2022)
- ▶ SiSc Lab → separate set of slides following this presentation

Questions?