Introduction to Algorithmic Differentiation

aka: Computational Differentiation

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

RWTH Aachen

Contents

Outline

Legal

Warm-Up

Motivation

Contents

Admin

See RWTHmoodle for document outlining the legal side of recording Zoom sessions.

▶ no issues if video and audio disabled

▶ if video and/or audio enabled, then you agree to the terms and conditions

Q&A sessions will (probably) not be recorded.

Outline

```
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 │ }
```

???

Warm-Up
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.
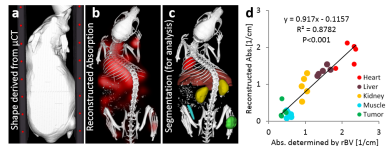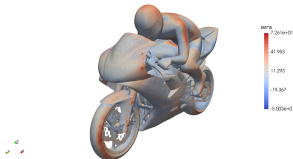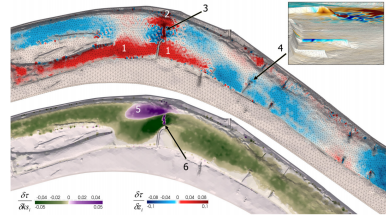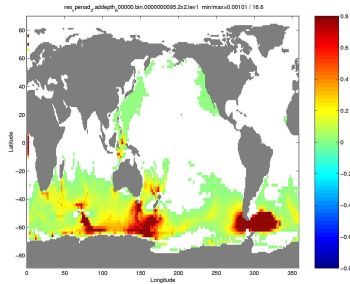
Outline

Need for Cheap Gradients ...

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

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Contents

Admin

Contents
Overview

- ▶ 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

Outline

- Lecture (videos, slides, code @ RWTHmoodle)

- Q&A (U. Naumann on Tuesdays at 10:30am live @ Zoom; invites @ RWTHmoodle)

- Tutorial (M. Towara on Thursdays at 12:30am live @ Zoom; invites @ RWTHmoodle)
  - VirtualBox Linux image for tutorial exercises contains dco/c++ and other software required

- Exams (90min written exams in Feb/Mar/Apr t.b.a.)

- SiSc Lab $\rightarrow$ separate set of slides following this presentation

Questions?