Introduction to Algorithmic Differentiation
aka: Computational Differentiation

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

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Recording Live Zoom Sessions

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.
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Warm-Up
Who knows how to differentiate ...

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

1 | float $f(\text{float } x) \{$
2 | \hspace{1em} return $\cos(x)$;
3 | \}

1 | double $f(\text{float } x) \{$
2 | \hspace{1em} return 42.;
3 | \}

???
Warm-Up
Who knows how to differentiate ...

```cpp
... template<typename T, typename PT>
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) {
    using namespace std;
    size_t n=p.size()−2;
    T x0=x;
    for (size_t j=from;j<to;j++) {
        for (size_t i=0;i<n;i+=ncs) steps(j,i,i+ncs,x,p,dW);
        T sig=1/(1+exp(−(x−p[n])/p[n+1])); s+=(x−p[n])*sig; x=x0;
    }
}
... ???

???

... YOU WILL!

This course introduces Algorithmic Differentiation (AD) as the method of choice for computing first and higher derivatives of numerical simulation programs.
Motivation
Need for Cheap Gradients ... as well as aerospace, machine learning, finance, ...
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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
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What, When, Where, Who, How?

- 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 → separate set of slides following this presentation
Questions?