Third MODE Workshop on
Differentiable Programming for Experiment Design

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COMPILER C | R RESEARCH

Efficient C++ Derivatives Through Source Transformation AD With Clad

Vassil Vassilev, Princeton
compiler-research.org

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Motivation

Provide automatic differentiation for C/C++ that works with~~out~~ little code modification (including legacy code)

AD. Chain Rule

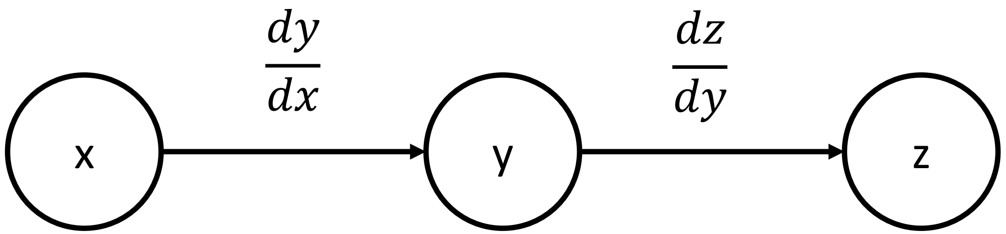
$$\frac{dz}{dx} = \frac{dz}{dy} . \frac{dy}{dx}$$

Intuitively, the chain rule states that knowing the instantaneous rate of change of *z* relative to *y* and that of *y* relative to *x* allows one to calculate the instantaneous rate of change of *z* relative to *x* as the product of the two rates of change.

"if a car travels twice as fast as a bicycle and the bicycle is four times as fast as a walking man, then the car travels 2 × 4 = 8 times as fast as the man." G. Simmons

AD. Algorithm Decomposition

```
y = f(x)
z = g(y)

dydx = dfdx(x)
dzdy = dgdy(y)
dzdx = dzdy * dydx
```

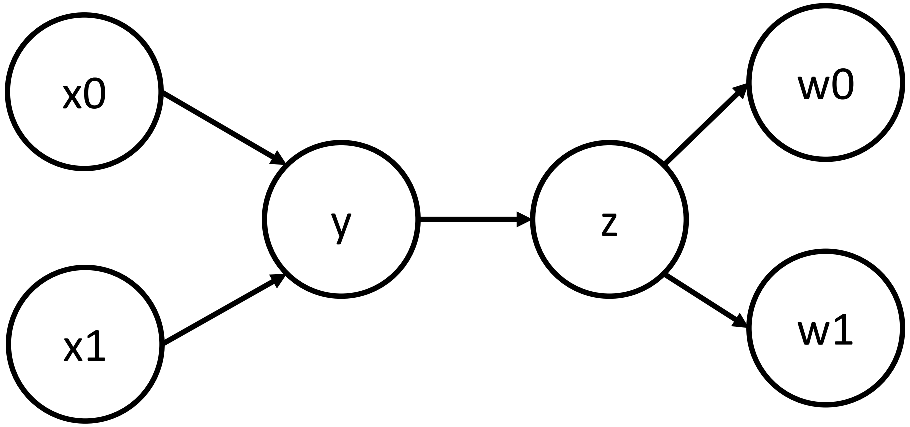


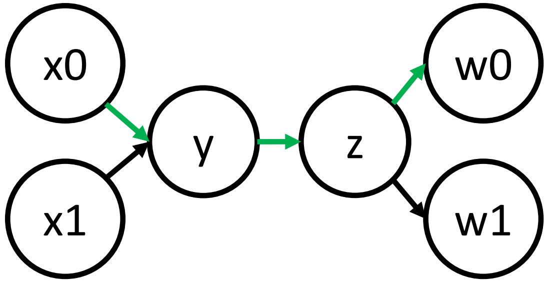
In the computational graph each node is a variable and each edge is derivatives between adjacent edges

We recursively apply the rules until we encounter an elementary function such as addition, substraction, multiplication, division, sin, cos or exp.

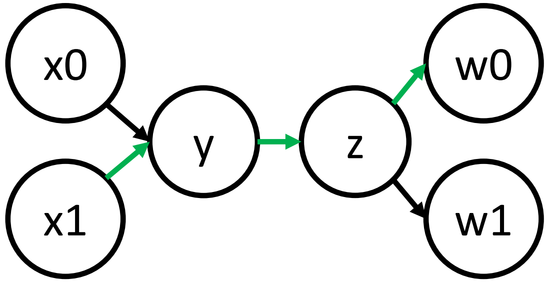
AD. Chain Rule

```
y = f(x0, x1)
z = g(y)
w0, w1 = l(z)
```

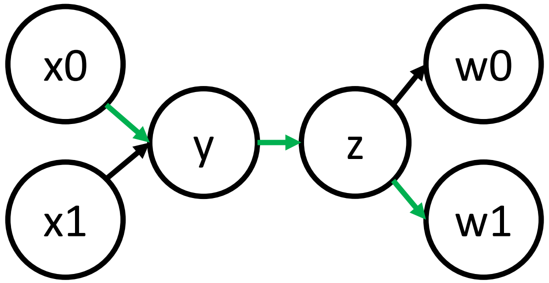




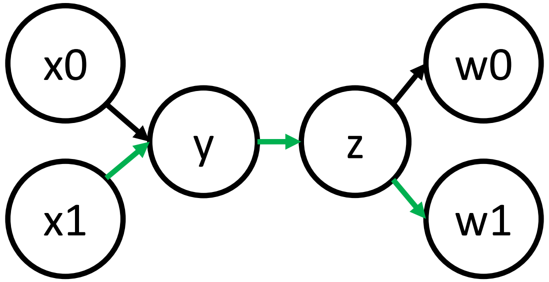
$$\frac{\partial w0}{\partial x0} = \frac{\partial w0}{\partial z}\frac{\partial z}{\partial y}\frac{\partial y}{\partial x0}$$



$$\frac{\partial w0}{\partial x1} = \frac{\partial w0}{\partial z}\frac{\partial z}{\partial y}\frac{\partial y}{\partial x1}$$



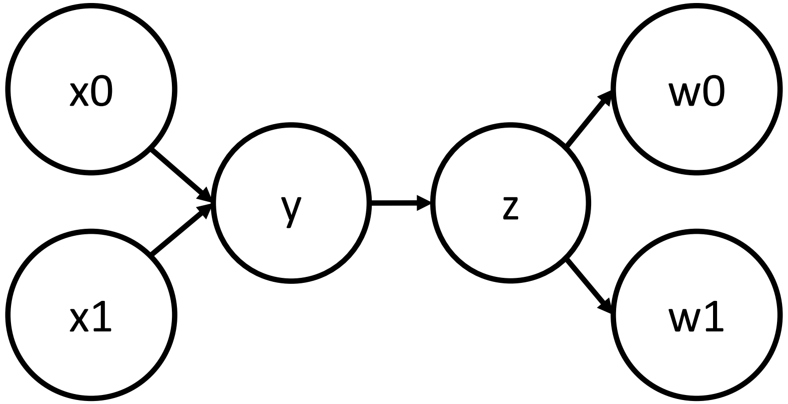
$$\frac{\partial w1}{\partial x0} = \frac{\partial w1}{\partial z}\frac{\partial z}{\partial y}\frac{\partial y}{\partial x0}$$



$$\frac{\partial w1}{\partial x1} = \frac{\partial w1}{\partial z}\frac{\partial z}{\partial y}\frac{\partial y}{\partial x1}$$

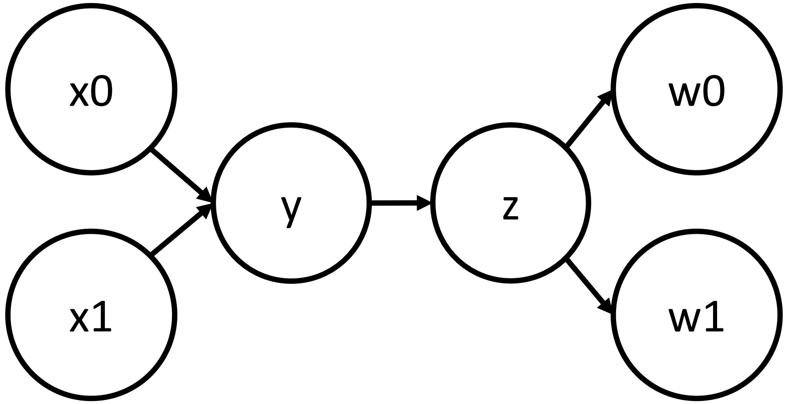
AD step-by-step. Forward Mode

```
dx0dx = {1, 0}
dx1dx = {0, 1}
y = f(x0, x1)

dydx = df(x0, dx0dx, x1, dx1dx)

z = g(y)

dzdx = dg(y, dydx)

w0, w1 = l(z)

dw0dx, dw1dx = dl(z, dzdx)
```



AD step-by-step. Reverse Mode

```
y = f(x0, x1)
z = g(y)
w0, w1 = l(z)

dwdw0 = {1, 0}
dwdw1 = {0, 1}

dwdz = dl(dwdw0, dwdw1)

dwdy = dg(y, dwdz)

dwx0, dwx1 = df(x0, x1, dwdy)
```



AD. Cheap Gradient Principle

- The computational graph has **common subpaths** which can be precomputed
- If a function has a single input parameter, no mater how many output parameters, **forward mode** AD generates a **derivative** that has the **same time complexity** as the original function
- More importantly, if a function has a **single output** parameter, **no matter how many input** parameters, reverse mode AD generates **derivative** with the **same time complexity** as the original function.

AD. Implementation Approaches

AD tools can be categorized by how much work is done before program execution

- *Tracing/Operator Overloading/Dynamic Graphs/Taping* -- Records the linear sequence of computation operations at runtime into a tape
- *Source Transformation* -- Constructs the computation graph and produces a derivative at compile time

Automatic vs Symbolic Differentiation

$$f(x) = e^{e^{e^{e^{e^x}}}}$$

Symbolic via Wolfram Alpha →

$$\frac{d}{dx}\left(e^{e^{e^{e^{e^x}}}}\right) = e^{x+e^{e^{e^{e^x}}}+e^{e^{e^x}}+e^{e^x}+e^x}$$

↑ *Figure out the analytical fn* ↓ *Handcode*

```cpp
// f(x)=e^(e^(e^(e^(e^x))))
#include <cmath>
double f (double x) {
  double result = x;
  for (unsigned i = 0; i < 5; i++)
    result = std::exp(result);
  return result;
}
```

AD →

↓ *Handcode*

```cpp
double f_dx(double x) {
  double result = x;
  double d_result = 1;
  for (unsigned i = 0; i < 5; i++) {
    result = std::exp(result);
    d_result *= result;
  }
  return d_result;
}
```

AD. Gradient Generation

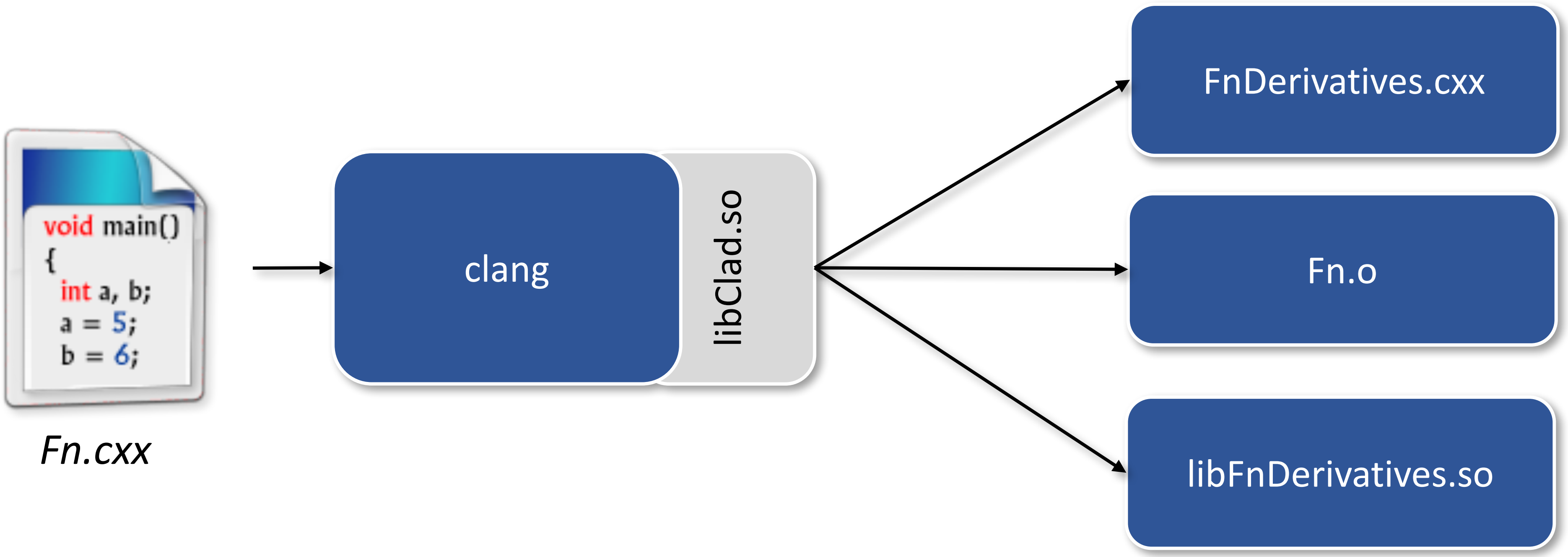
- Control Flow and Recursion fall naturally in forward mode.
- Extra work is required for reverse mode in reverting the loop and storing the intermediaries **in general**.

```
double f_reverse (double x) {
  double result = x;
  std::stack<double> results;
  for (unsigned i = 0; i < 5; i++) {
    results.push(result);
    result = std::exp(result);
  }
  double d_result = 1;
  for (unsigned i = 5; i; i--) {
    d_result *= std::exp(results.top());
    results.pop();
  }
  return d_result;
}
```

Clad. Design Principles

- ~~Look Ma' I can make a compiler generate a derivative!~~
- Make AD a first-class citizen to a high-performance language such as C++
- Support idiomatic C++ (compile-time programming such as constexpr, consteval)
- Infrastructure reuse – employ our compiler engineering skills
- Lower contribution entry barrier
- **Diagnostics**

High-Level Data Flow



- Compiler module, very similar to the template instantiator by idea and design.
- Generates f' of any given f using source transformation at compile time.

Programming Model

```
// clang++ -fplugin libclad.so —Iclad/include ...

// Necessary for clad to work include
#include "clad/Differentiator/Differentiator.h"
double pow2(double x) { return x * x; }
double pow2_darg0(double);

int main() {
  auto dfdx = clad::differentiate(pow2, 0);

  // Function execution can happen in 3 ways:
  // 1) Using CladFunction::execute method.
  double res = cladPow2.execute(1);

  // 2) Using the function pointer.
  auto dfdxFnPtr = cladPow2.getFunctionPtr();
  res = cladPow2FnPtr(2);

  // 3) Using direct function access through fwd declaratic
  res = pow2_darg0(3);
  return 0;
}
```

The body will be generated by Clad

Result via Clad's function-like wrapper

Result via function pointer call

Result via function forward declaration

Programming Model. Differential Operators

User-defined substituti

```
// MyCode.h
float custom_fn(float x);

namespace custom_derivatives {
  float custom_fn_dx(float x) {
    return x * x;
  }
}

float do_smth(float x) {
  return x * x + custom_fn(x);
}

int main() {
  clad::differentiate(do_smth, 0).execute(2); // will return 6
  return 0;
}
```

Vassil Vassilev/ACAT14 1.09.14

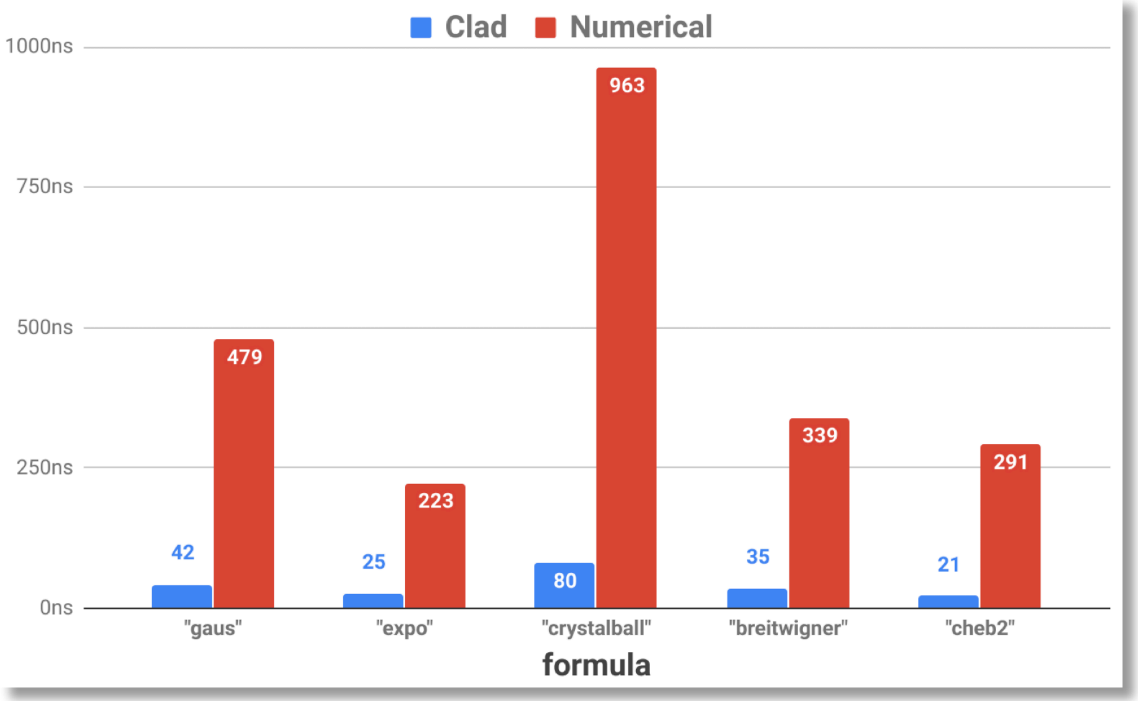
```
template <typename T1, typename T2>
CUDA_HOST_DEVICE ValueAndPushforward<decltype(::std::pow(T1(), T2())),
                                     decltype(::std::pow(T1(), T2()))>
pow_pushforward(T1 x, T2 exponent, T1 d_x, T2 d_exponent) {
  auto val = ::std::pow(x, exponent);
  auto derivative = (exponent * ::std::pow(x, exponent - 1)) * d_x;
  // Only add directional derivative of base^exp w.r.t exp if the directional
  // seed d_exponent is non-zero. This is required because if base is less than or
  // equal to 0, then log(base) is undefined, and therefore if user only requested
  // directional derivative of base^exp w.r.t base -- which is valid --, the result would
  // be undefined because as per C++ valid number + NaN * 0 = NaN.
  if (d_exponent)
    derivative += (::std::pow(x, exponent) * ::std::log(x)) * d_exponent;
  return {val, derivative};
}

```

Clad in High-Energy Physics

Clad is available in ROOT:

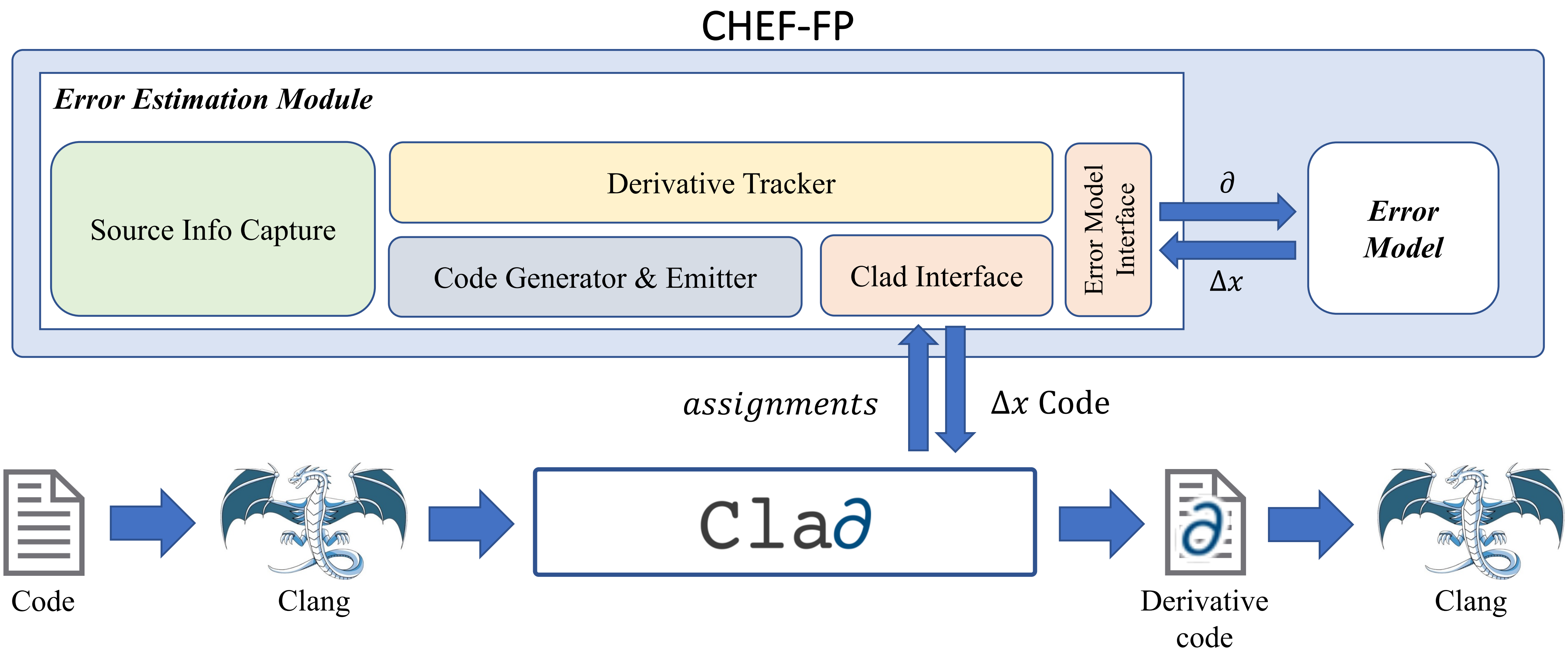
```
TF1* h1 = new TF1("f1", "formula");
TFormula* f1 = h1->GetFormula();
f1->GenerateGradientPar(); // clad
```

```
// clad
f1->GradientPar(x, result);
// numerical
h1->GradientPar(x, result);
```



gaus: Npar = 3,expo: Npar = 2, crystalball: Npar = 5, breitwigner: Npar = 5, cheb2: Npar = 4

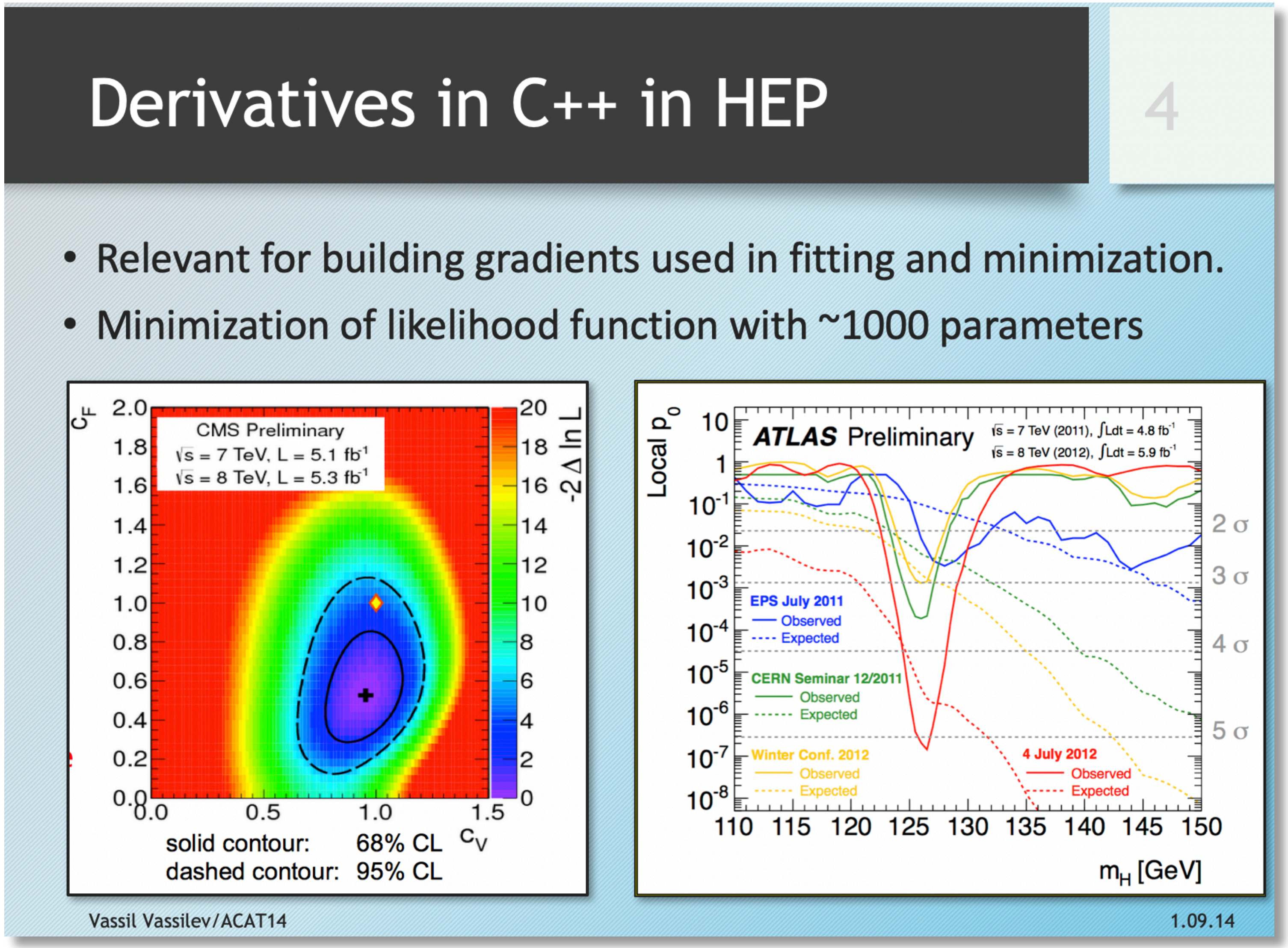
Clad in FP Error Analysis: CHEF-FP



There and Back Again

Social Engineering, Progress, Social Engineering…

In the meanwhile: Cling, ROOT6, C++ Modules, IPCC-ROOT, compiler-research.org, Clang-Repl …



Future Prospects

- Grey box AD
  - Enhance the pushforward/pullback mechanisms to avoid common AD pitfalls
- Further advancements and applications on floating point error estimation
  - Controlling the error limits helps the energy efficiency of algorithms
- Robust activity analysis
- A research platform AD in C/C++
  - Combines all power of Clang Static Analyzer, LLVM Optimization Passes, Control Flow Graphs

Violeta Ilieva
Initial prototype, Forward Mode

Vassil Vassilev
Conception, Mentoring, Bugs, Integration, Infrastructure

Martin Vassilev
Forward Mode, CodeGen

Alexander Penev
Conception, CMake, Demos, Jupyter

Aleksandr Efremov
Reverse Mode

Jack Qui
Hessians

Roman Shakhov
Jacobians

Oksana Shadura
Infrastructure, Co-mentoring

Pratyush Das
Infrastructure

Garima Singh
FP error estimation, RooFit, Bugs

Ioana Ifrim
CUDA AD

Parth Arora
Initial support classes, functors, pullbacks

Baidyanath Kundu
Array Support, ROOT integration

Vaibhav Thakkar
Forward Vector Mode

Thank you!