Clad — Automatic Differentiation for C++ Using Clang

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Motivation

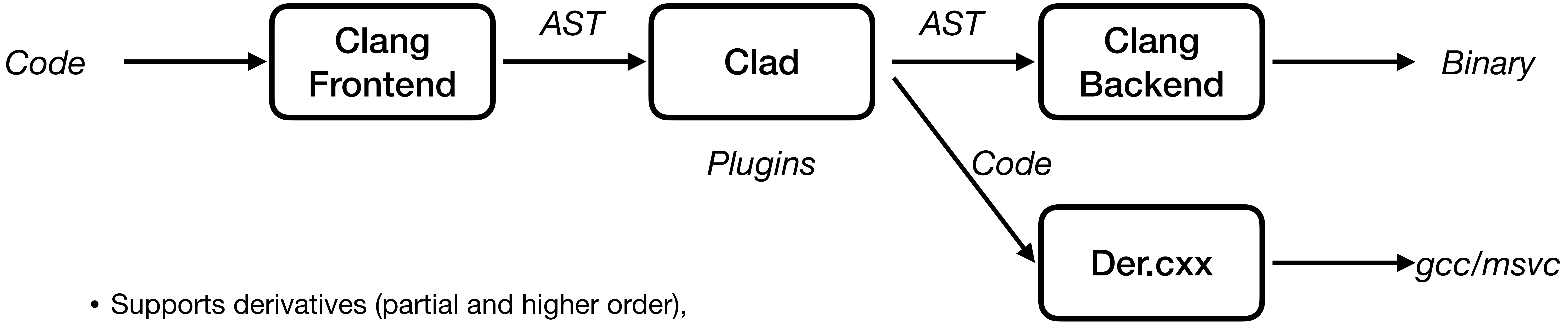
Provide automatic differentiation for C/C++ that works without code modification (including legacy code)

Clang Compilation Pipeline. Clad

```
double f(double x) {
    return x * x;
}
```

```
FunctionDecl f 'double (double)'
|-ParmVarDecl x 'double'
`-CompoundStmt
  `-ReturnStmt
    `-BinaryOperator 'double' '*'
      |-ImplicitCastExpr 'double' <LValueToRValue>
      | `-DeclRefExpr 'double' lvalue ParmVar 'x' 'double'
      `-ImplicitCastExpr 'double' <LValueToRValue>
        `-DeclRefExpr 'double' lvalue ParmVar 'x' 'double'
```

```
FunctionDecl 0x7f7f801dbff8 <<invalid sloc>> <invalid sloc> f_darg0 'double (double)'
|-ParmVarDecl 0x7f7f801dc090 <<invalid sloc>> <invalid sloc> used x 'double'
`-CompoundStmt 0x7f7f801dc3d0 <<invalid sloc>>
  |-DeclStmt 0x7f7f801dc190 <<invalid sloc>>
  | `-VarDecl 0x7f7f801dc118 <<invalid sloc>> <invalid sloc> used _d_x 'double' cinit
  |   `-ImplicitCastExpr 0x7f7f801dc178 <<invalid sloc>> 'double' <IntegralToFloating>
  |     `-IntegerLiteral 0x7f7f801dc0f8 <<invalid sloc>> 'int' 1
  `-ReturnStmt 0x7f7f801dc398 <<invalid sloc>>
    `-BinaryOperator 0x7f7f801dc318 <<invalid sloc>> 'double' '+'
      |-BinaryOperator 0x7f7f801dc298 <<invalid sloc>, T.cpp:3:32> 'double' '*'
      | |-ImplicitCastExpr 0x7f7f801dc268 <<invalid sloc>> 'double' <LValueToRValue>
      | | `-DeclRefExpr 0x7f7f801dc1a8 <<invalid sloc>> 'double' lvalue Var 0x7f7f801dc118 '_d_x' 'double'
      | `-ImplicitCastExpr 0x7f7f801dc280 <col:32> 'double' <LValueToRValue>
      |   `-DeclRefExpr 0x7f7f801dc208 <col:32> 'double' lvalue ParmVar 0x7f7f801dc090 'x' 'double'
      `-BinaryOperator 0x7f7f801dc2f0 <col:30, <invalid sloc>> 'double' '*'
        |-ImplicitCastExpr 0x7f7f801dc2c0 <col:30> 'double' <LValueToRValue>
        | `-DeclRefExpr 0x7f7f801dc1d0 <col:30> 'double' lvalue ParmVar 0x7f7f801dc090 'x' 'double'
        `-ImplicitCastExpr 0x7f7f801dc2d8 <<invalid sloc>> 'double' <LValueToRValue>
          `-DeclRefExpr 0x7f7f801dc1a8 <<invalid sloc>> 'double' lvalue Var 0x7f7f801dc118 '_d_x' 'double'
```



- Supports derivatives (partial and higher order), gradients, hessians and jacobians.
- Provides low-level derivative access primitives
- Allows embedding in frameworks

```
double f_darg0(double x) {
    double _d_x = 1;
    return _d_x * x + x * _d_x;
}
```

Clad. Usage

```
// clang -Xclang -add-plugin -Xclang clad -Xclang -load
//       -Xclang libclad.so …
// 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 declaration.
  res = pow2_darg0(3);
  return 0;
}
```

The body will be generated by clad.

Result via the clad function-like wrapper object

Result via function pointer call

Result via a forward declaration

Clad. Usage. CUDA

Work in progress by Ioana Ifrim

```
// clang -Xclang -load -Xclang libclad.so -Xclang -add-plugin -Xclang clad -lstdc++ -lcudart_static -ldl -lrt -pthread —cuda-path=... -lcuda ...
```

```
#include "clad/Differentiator/Differentiator.h"

typedef double(*func) (double);

__device__ __host__
double pow2(double x) {
  return x * x;
}

__device__ __host__
double pow2_darg0(double x);
```

Clad will provide a definition

```
__device__ func p_pow2 = pow2_darg0;
```

Static pointer to the device function

```
__global__
void compute(func op, double * d_x,
                double * result) {
    *result = (*op)(*d_x);
}
```

```
int main(void) {
  double x= 5.0;
  func h_pow2;
  double * d_x;

  cudaMalloc(&d_x, sizeof(double));
  cudaMemcpy(d_x, &x, sizeof(double), cudaMemcpyHostToDevice);

  double result;
  double * d_result, * h_result;
  cudaMalloc(&d_result, sizeof(double));
  h_result = &result;

  clad::differentiate(pow2,”x");

  cudaMemcpyFromSymbol(&h_pow2, p_pow2, sizeof(func));
  compute<<<1,1>>>(h_pow2, d_x, d_result);
  cudaDeviceSynchronize();
  cudaMemcpy(h_result, d_result, sizeof(double),
             cudaMemcpyDeviceToHost);

  printf("Result: %f\n", result);
}
```

Memory allocation

Copy device function pointer of differentiated function to host

Device Sync

People

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Initial prototype,
Forward Mode
GSoC

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Conception,
Mentoring, Bugs,
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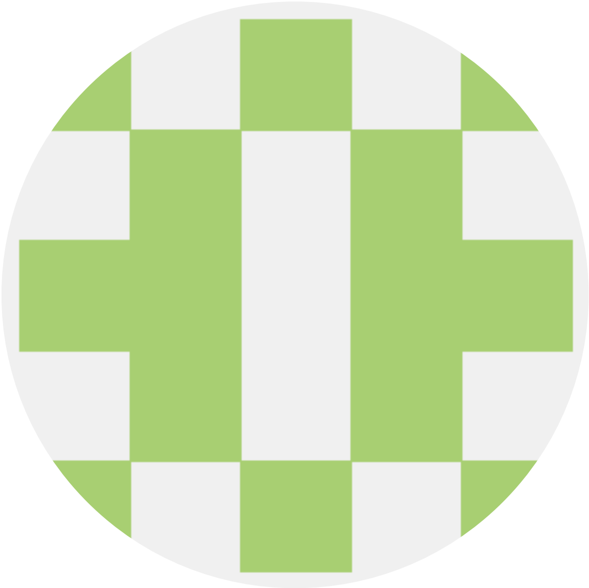

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IRIS-HEP Fellow

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US NSF

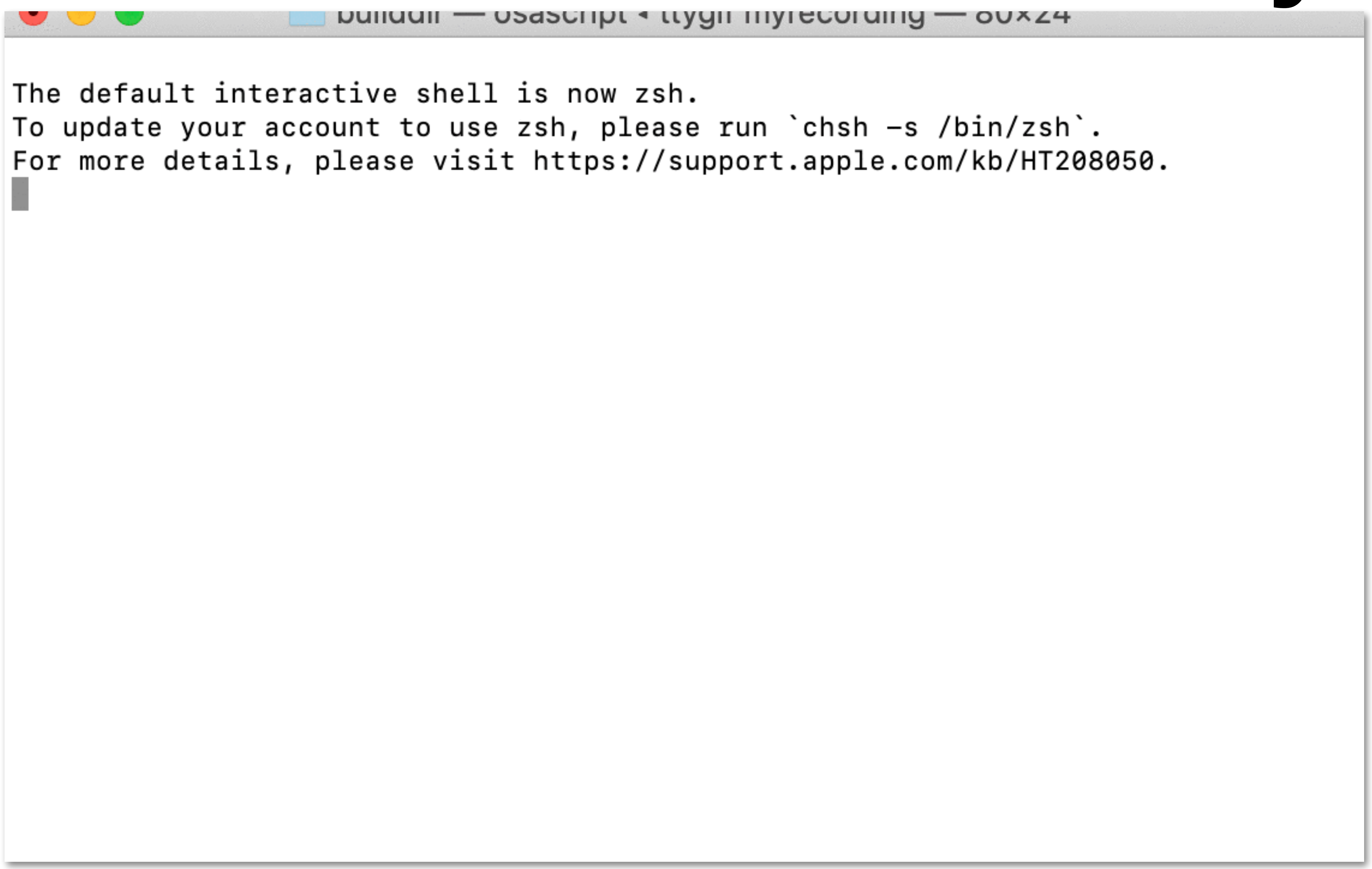
Integration of Clad in Cling and ROOT

Some domains benefit from supporting derivatives of user code. Interpretative languages such as python can provide that easily.

C++ has cling — an interactive, llvm-based C++ interpreter.

ROOT is a data analysis software package used to process data in the field of high-energy physics

Use of Clad on the fly



```
The default interactive shell is now zsh.
To update your account to use zsh, please run `chsh -s /bin/zsh`.
For more details, please visit https://support.apple.com/kb/HT208050.
█
```

The demo shows cling use clad as a plugin to produce a derivative on the fly

Clad as a Service

- A service capable of running AD on a given code at program’s runtime
- Runs embedded in your framework code with your favorite compiler

Clad as a Service

Declare the code to the interpreter

Move the interpreter result to the compile world

Cast and execute

```
#include <cling/Interpreter/Interpreter.h>
#include <cling/Interpreter/Value.h>

// Derivatives as a service.

void gimme_pow2dx(cling::Interpreter &interp) {
  // Definitions of declarations injected also into cling.
  interp.declare("double pow2(double x) { return x*x; }");
  interp.declare("#include <clad/Differentiator/Differentiator.h>");
  interp.declare("auto dfdx = clad::differentiate(pow2, 0);");

  cling::Value res; // Will hold the evaluation result.
  interp.process("dfdx.getFunctionPtr();", &res);

  using func_t = double(double);
  func_t* pFunc = res.getAs<func_t*>();
  printf("dfdx at 1 = %f\n", pFunc(1));
}

int main(int argc, const char* const* argv) {
 std::vector<const char*> argvExt(argv, argv+argc);
  argvEx.push_back("-fplugin=etc/cling/plugins/lib/clad.dylib");
  // Create cling. LLVMDIR is provided as -D during compilation.
  cling::Interpreter interp(argvExt.size(), &argvExt[0], LLVMDIR);
  gimme_pow2dx(interp);
  return 0;
}
```

```
./clad-demo
dfdx at 1 = 2.000000
```

Result from running the clad-demo binary

Benchmarks

General Benchmarks

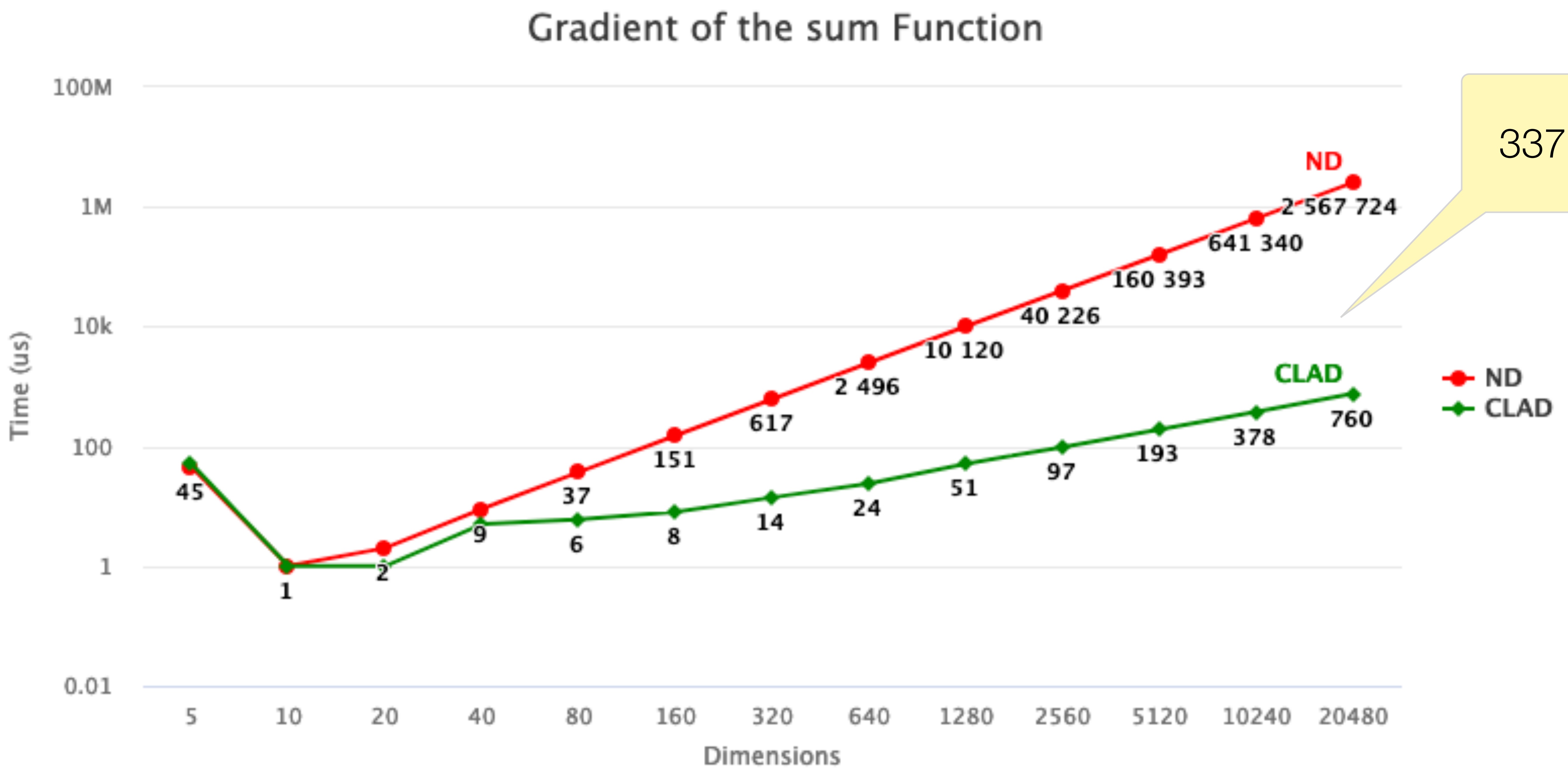
```
double* Numerical(double* p, int dim, double eps = 1e-8) {
  double* result = new double[dim]{};
  for (int i = 0; i < dim; i++) {
    double pi = p[i];
    p[i] = pi + eps;
    double v1 = sum(p, dim);
    p[i] = pi - eps;
    double v2 = sum(p, dim);
    result[i] = (v1 - v1)/(2 * eps);
     p[i] = pi;
  }
  return result;
}
```

Numerical differentiation based on the central differences

```
double* Clad(double* p, int dim) {
  auto result = new double[dim]{};
  auto sum_grad = clad::gradient(sum, "p");
  sum_grad.execute(p, dim, result);
  return result;
}
```

AD using Clad

```
double sum(double* p, int dim) {
  double r = 0.0;
  for (int i = 0; i < dim; i++)
    r += p[i];
  return r;
}
```



3378x speedup

Efremov, Clad: the automatic differentiation plugin for Clang, verified by Ioana Ifrim in 2021!

General Benchmarks

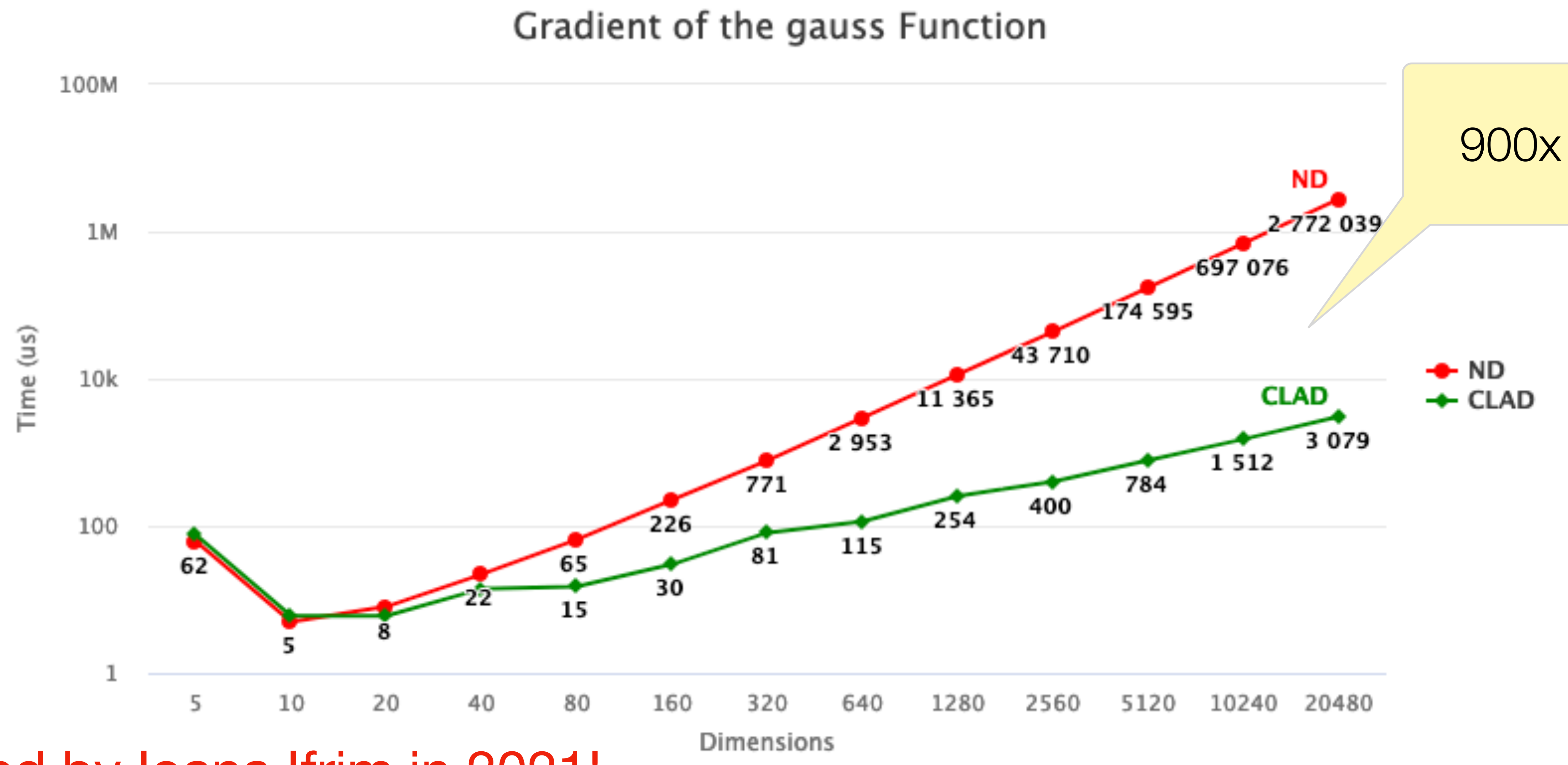
```
double* Numerical(double* p, int dim, double eps = 1e-8) {
  double* result = new double[dim]{};
  for (int i = 0; i < dim; i++) {
    double pi = p[i];
    p[i] = pi + eps;
    double v1 = sum(p, dim);
    p[i] = pi - eps;
    double v2 = sum(p, dim);
    result[i] = (v1 - v1)/(2 * eps);
     p[i] = pi;
  }
  return result;
}
```

Numerical differentiation based on the central differences

AD using Clad

```
double* Clad(double* p, int dim) {
  auto result = new double[dim]{};
  auto sum_grad = clad::gradient(sum, "p");
  sum_grad.execute(p, dim, result);
  return result;
}
```

```
double gaus(double* x, double* p, double sigma, int dim) {
  double t = 0;
  for (int i = 0; i< dim; i++)
    t += (x[i] - p[i]) * (x[i] - p[i]);
  t = -t / (2*sigma*sigma);
  return std::pow(2*M_PI, -dim/2.0) *
         std::pow(sigma, -0.5) * std::exp(t);
};
```



900x speedup

Efremov, Clad: the automatic differentiation plugin for Clang, verified by Ioana Ifrim in 2021!

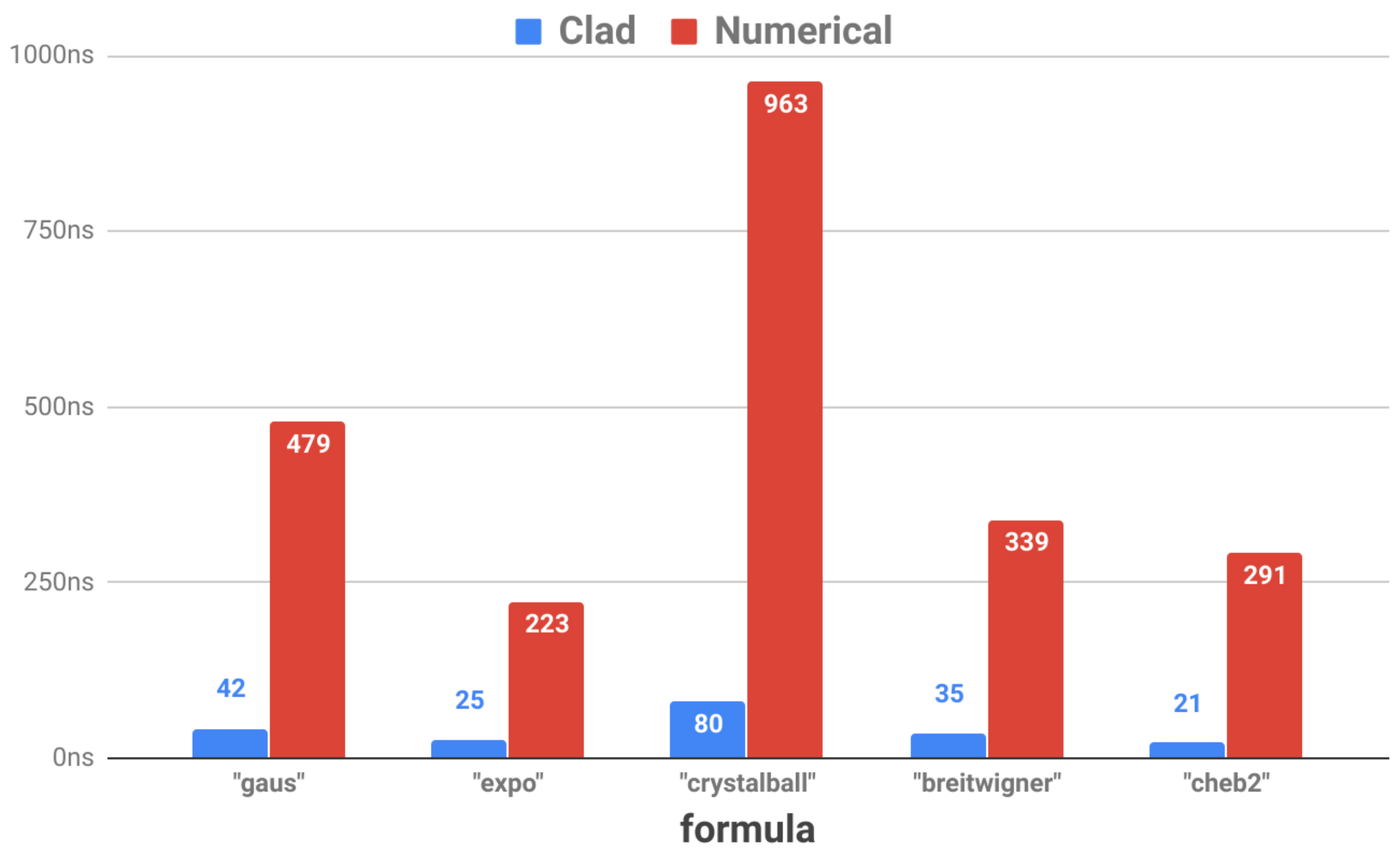
Integration in ROOT

Integration in ROOT TF1

- Use Clad to generate gradients for formula based functions

```
TF1* f1 = new TF1(“f1”, “[a]*x^2+[b]*x+[c]”);
// tell TFormula to generate gradient function
f1->GetFormula()->GenerateGradientPar();
// compute gradient using CLAD
std::vector<double> gradient(3);
f1->GradientPar(x.data(), gradient.data());
```

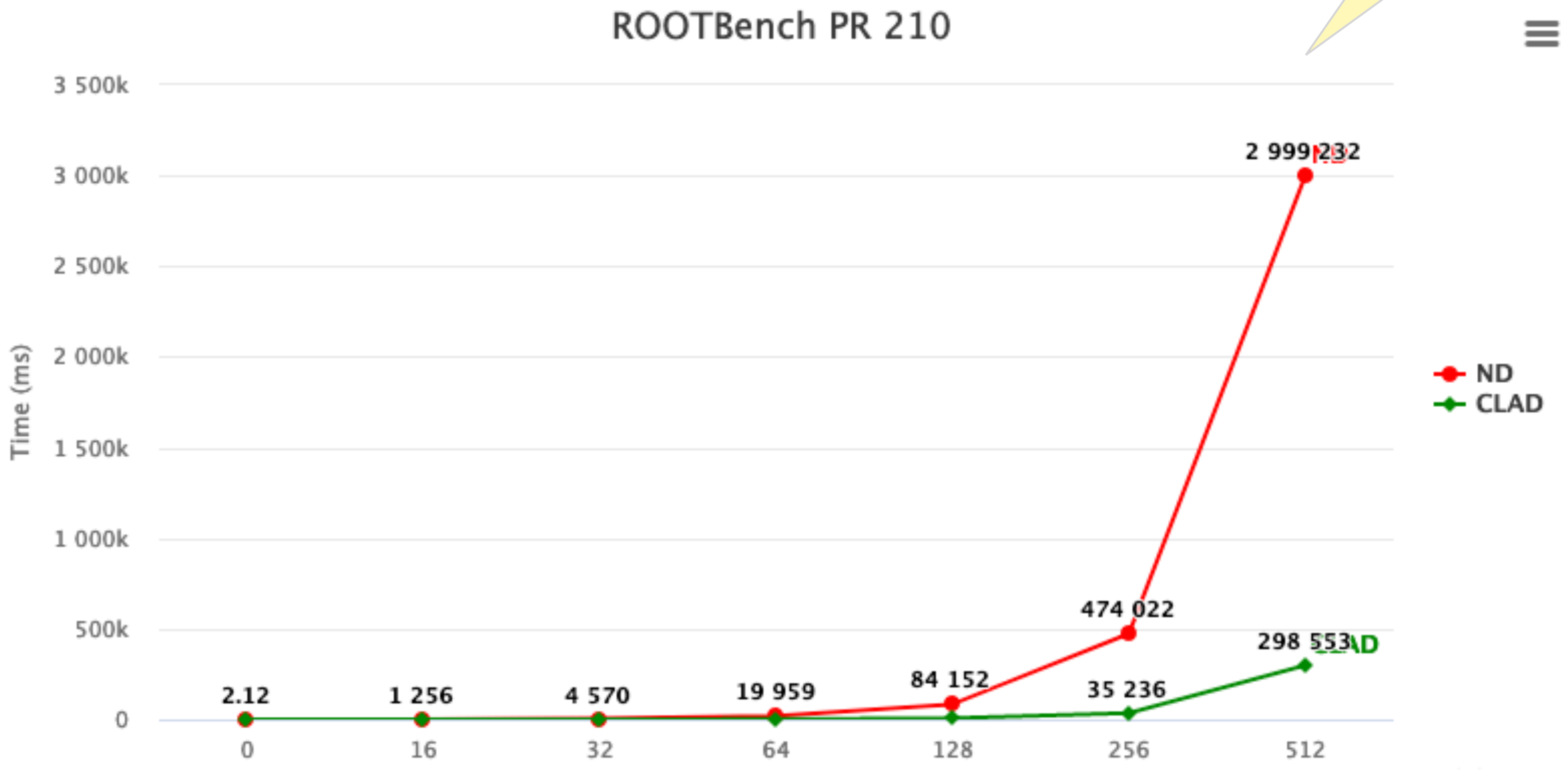
- When Clad is not available use numerical differentiation

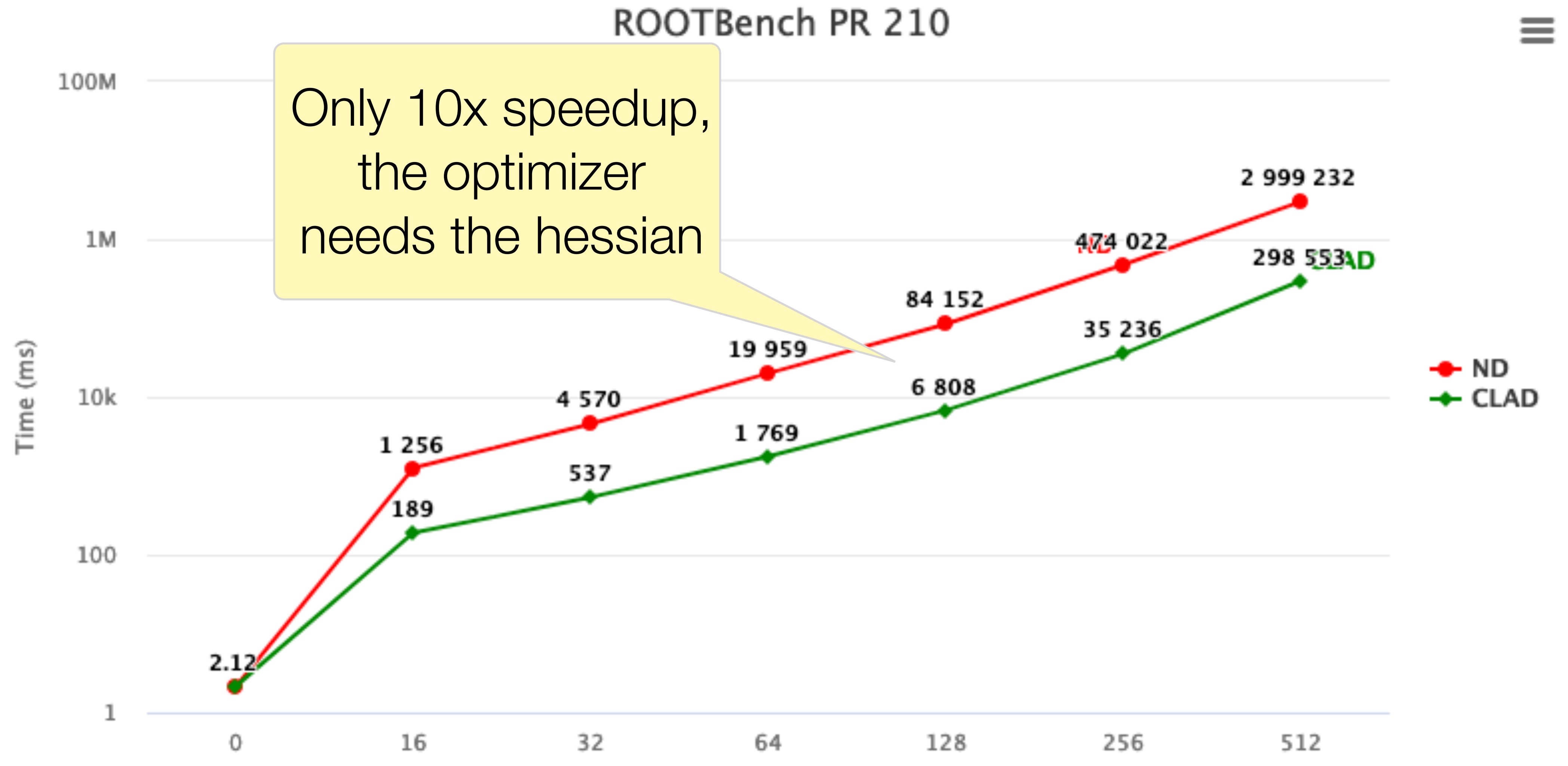


Clad in ROOT

TFormula is a ROOT class which bridges compiled and interpreted code.

Work by Lorenzo Moneta





Only 10x speedup, the optimizer needs the hessian

Future

- Clad works for the cases we tested, however, there are a lot of unexplored codes
- We need a gradual adoption to allow improving the implementation if necessary.
- Work on standardization of AD in C++ https://wg21.link/P2072
- Full support of arrays
- Develop error estimation framework — at compile time and at runtime
- Retarget code on GPGPU — OpenCL and/or CUDA
- Support functor objects
- Make the derivation process explicitly configurable
- Integration with Enzyme

Thank you.

https://github.com/vgvassilev/clad

```
void sum_grad_0(double *p, int dim, double *_result) {
    double _d_r = 0;
    unsigned long _t0;
    int _d_i = 0;
    clad::tape<int> _t1 = {};
    double r = 0.;
    _t0 = 0;
    for (int i = 0; i < dim; i++) {
        _t0++;
        r += p[clad::push(_t1, i)];
    }
    double sum_return = r;
    goto _label0;
  _label0:
    _d_r += 1;
    for (; _t0; _t0--) {
        double _r_d0 = _d_r;
        _d_r += _r_d0;
        _result[clad::pop(_t1)] += _r_d0;
        _d_r -= _r_d0;
    }
}
```