

IPCC ROOT



Princeton/Intel Parallel Computing Center

Progress Report

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Status 29.03-2017 — 18.04.2017

- ❖ Enable vectorization for ROOT through VecCore
 - ❖ PR#393 (+116 -29  30); PR#497 (+158 -31  2);
- ❖ Enables contributors to submit code employing the vectorization capabilities of the CPUs.
- ❖ Misc
 - ❖ more...

clad: Automatic Differentiation Library in ROOT

- ❖ Foreseen piece of work for Q3 of this year
- ❖ clad already got some interest by Intel people

clad: Integration plan

- ❖ Enable the use of the library within ROOT, connecting it to the cling interpreter (also Clang / LLVM based), etc.
- ❖ Update to the latest compiler versions, debug, etc.
- ❖ Integrate AD into specific non-trivial examples in Minuit (used for numerical minimization in ROOT) and TMVA (multivariate analysis) in ROOT.
- ❖ Benchmark those applications

clad: Integration plan. Scope

- ❖ In this first step we are not dealing with OpenCL or parallelization. The latter still has to come from the end user applications.
- ❖ After Q3 (Y1) we would likely use this infrastructure in RooFit in Y2. RooFit is ROOT's the data modeling and fitting package which is being reengineered.

clad: In a Nutshell

clad neither employs the slow symbolic nor inaccurate numerical differentiation. It uses the fact that every computer program can be divided into a set of elementary operations ($-$, $+$, $*$, $/$) and functions (sin, cos, log, etc). By applying the chain rule repeatedly to these operation, derivatives of arbitrary order can be computed.

C/C++ to C/C++ language transformer implementing the chain rule from differential calculus. For example:

```
constexpr double MyPow(double x) { return x*x; }
```



```
constexpr double MyPow_darg0(double x) { return (1. * x + x * 1.); }
```

clad: Advantages over Numerical Differentiation

```
#include <cmath>

double MyCos(double x) { return std::cos(x); }
double MySin(double x) { return std::sin(x); }
constexpr double MyPow(double x) { return x*x; }

typedef double (*SigF)(double);

// Simple finite differences numerical differentiator.
double derive(SigF f, double a, double h=0.01, double epsilon = 1e-7){
    double f1 = (f(a+h)-f(a))/h;
    double f2 = 0.;
    while (1) {
        h /= 2.;
        f2 = (f(a+h)-f(a))/h;
        double diff = std::abs(f2-f1);
        f1 = f2;
        if (diff < epsilon)
            break;
    }
    return f2;
}
```

clad: Advantages over Numerical Differentiation

```
#include <cmath>
```

```
double MyCos(double x) { return std::cos(x); }  
double MySin(double x) { return std::sin(x); }  
constexpr double MyPow(double x) { return x*x; }
```

```
// The derivatives are provided by clad but hardcoded here for simplicity, i.e.  
// you can run this example without installing clad.
```

```
double MyCos_darg0(double x) { return -std::sin(x) * (1.); }  
double MySin_darg0(double x) { return std::cos(x) * (1.); }  
constexpr double MyPow_darg0(double x) { return (1. * x + x * 1.); }
```


clad: Advantages over Numerical Differentiation

```
// No clad, using the simple numerical differentiator
int main () {
    printf("MyCos' at 30 is %f\n", derive(MyCos, 30));
    // For every point we need to iterate :( This causes
    // not only slow execution but precision loss!
    printf("MyCos' at 31 is %f\n", derive(MyCos, 31));
    printf("MySin' at 30 is %f\n", derive(MySin, 30));

    // Even if MyPow is a compile-time foldable we still loop!
    printf("MyPow' at 2 is %f\n", derive(MyPow, 2));
```

```
// From math we know that  $\sin x' = \cos x$ 
// Let's check if this was true.
if (derive(MySin, 30) == MyCos(30))
    printf("No precision loss!\n");
else
    printf("Precision loss!\n");
```

```
// Output:
// MyCos' at 30 is 0.988032
// MyCos' at 31 is 0.404038
// MySin' at 30 is 0.154252
// MyPow' at 2 is 4.000000
// Precision loss!
return 0;
```

Lines of assembly code

	-O0	-O3
gcc 6.1	150	63
clang 4	154	65
icc 17	181	129

Lines of assembly code

	-O0	-O3
gcc 6.1	223	141
clang 4	206	226
icc 17	279	283

```
// Using clad, employing automatic differentiation techniques
int main () {
    printf("MyCos' at 30 is %f\n", MyCos_darg0(30));
    // For every point we just need to call a function pointer!
    printf("MyCos' at 31 is %f\n", MyCos_darg0(31));
    printf("MySin' at 30 is %f\n", MySin_darg0(30));

    // The compile-time foldable MyPow folds away!
    printf("MyPow' at 2 is %f\n", MyPow_darg0(2));
```

```
// From math we know that  $\sin x' = \cos x$ 
// Let's check if this was true.
if (MySin_darg0(30) == MyCos(30))
    printf("No precision loss!\n");
else
    printf("Precision loss!\n");
```

```
// Output:
// MyCos' at 30 is 0.988032
// MyCos' at 31 is 0.404038
// MySin' at 30 is 0.154251
// MyPow' at 2 is 4.000000
// No precision loss!
```

```
return 0;
```

Thank you!

References:

- [1] clad — Automatic Differentiation with Clang, <http://llvm.org/devmtg/2013-11/slides/Vassilev-Poster.pdf>
- [2] clad Official GitHub Repository <https://github.com/vgvassilev/clad>
- [3] clad demos <https://github.com/vgvassilev/clad/tree/master/demos>
- [4] clad showcases <https://github.com/vgvassilev/clad/tree/master/test>
- [5] More automatic differentiation tools <http://www.autodiff.org/>