Enzyme: Fast and Effective Automatic Differentiation for Academia and Industry

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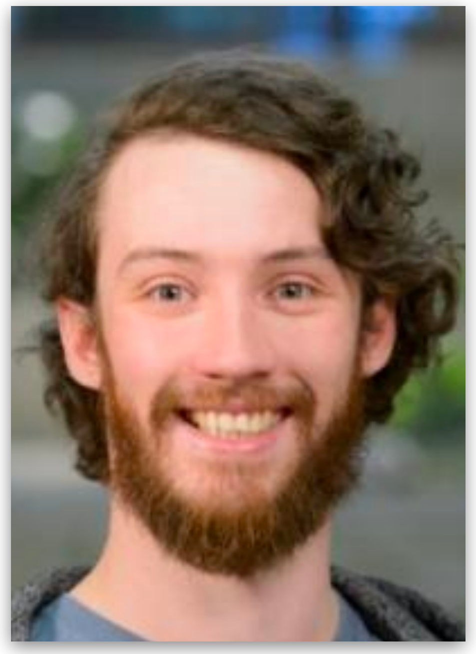

Johannes Doerfert

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Sri Hari Krishna Narayanan

Michel Schanen

Paul Hovland

Leila Ghaffari

Praytush Das

Tim Gymnich

Manuel Drehwald

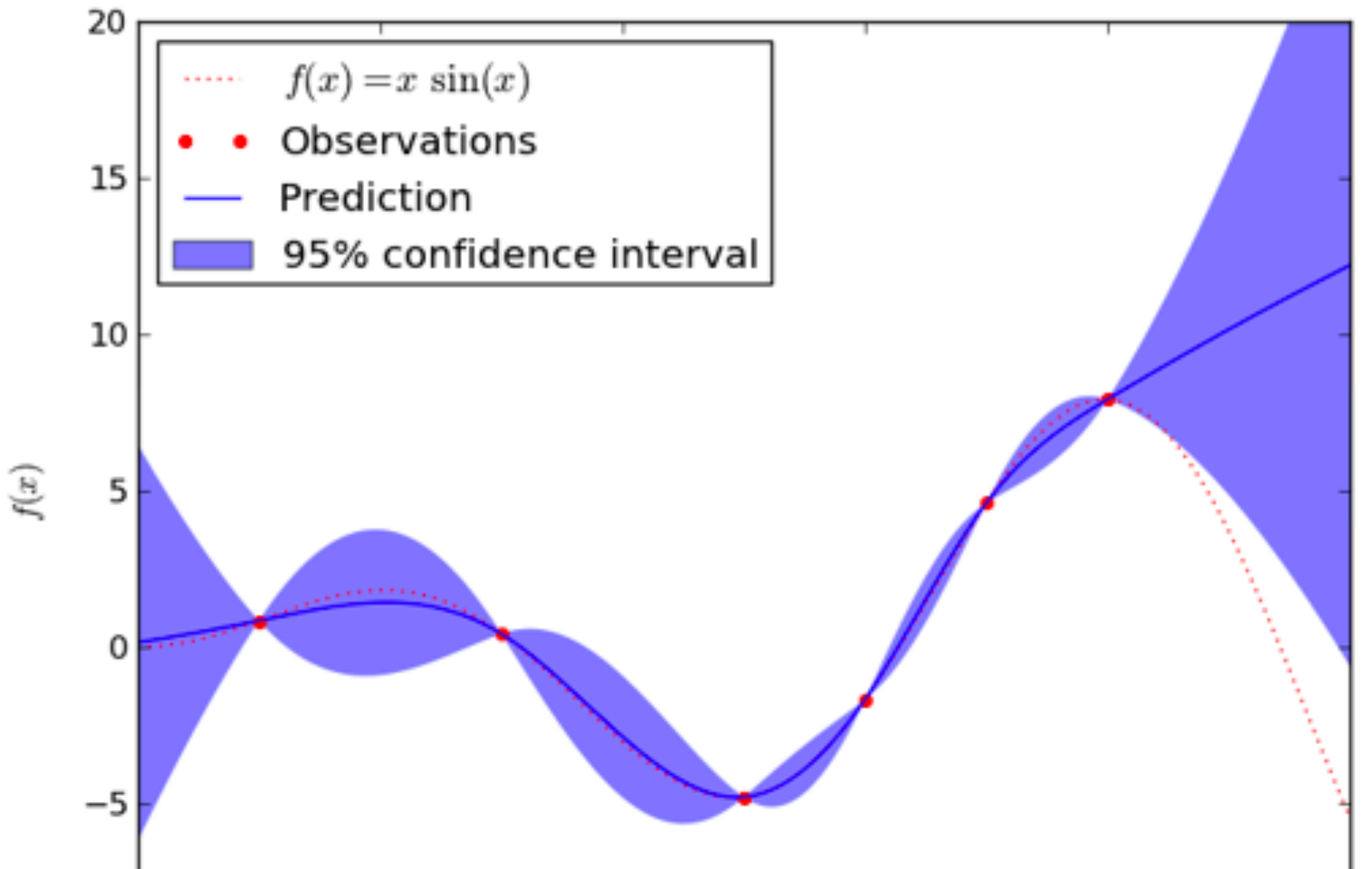
& more

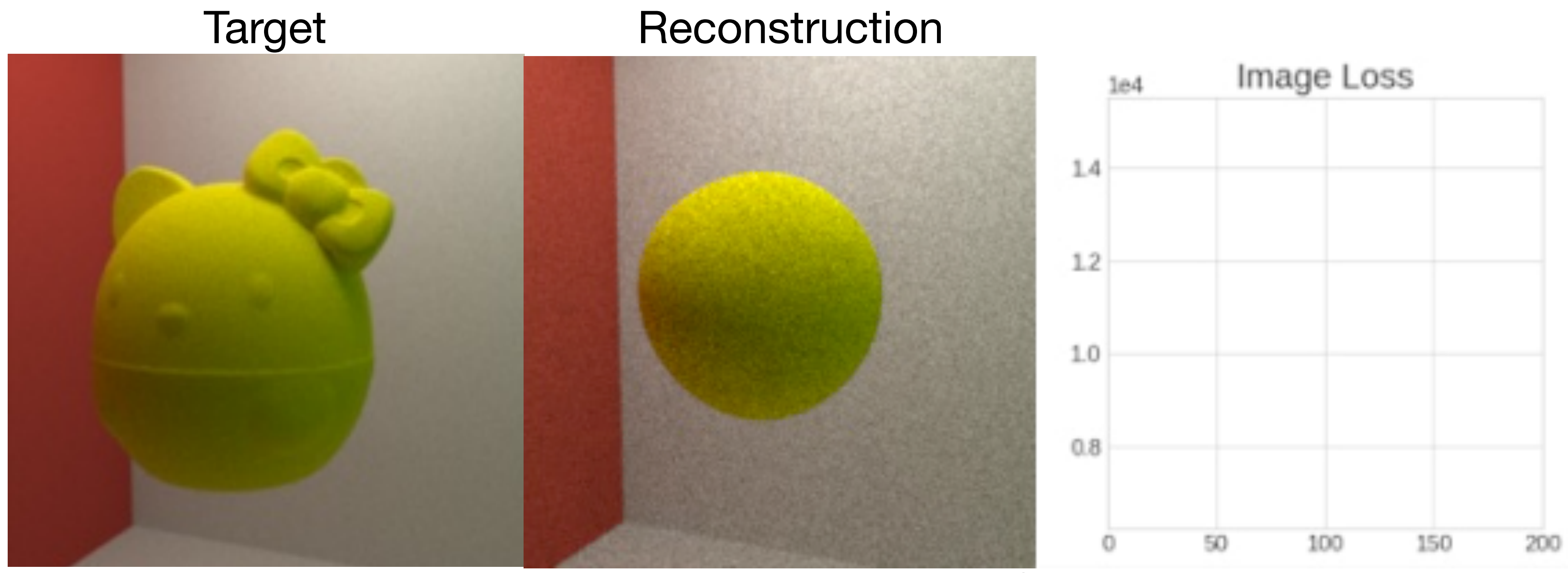
AP Calculus: Revisited

- Derivatives compute the rate of change of a function's output with respect to input(s)

$$f'(x) = \lim_{h \to 0} \frac{f(a+h) - f(a)}{h}$$

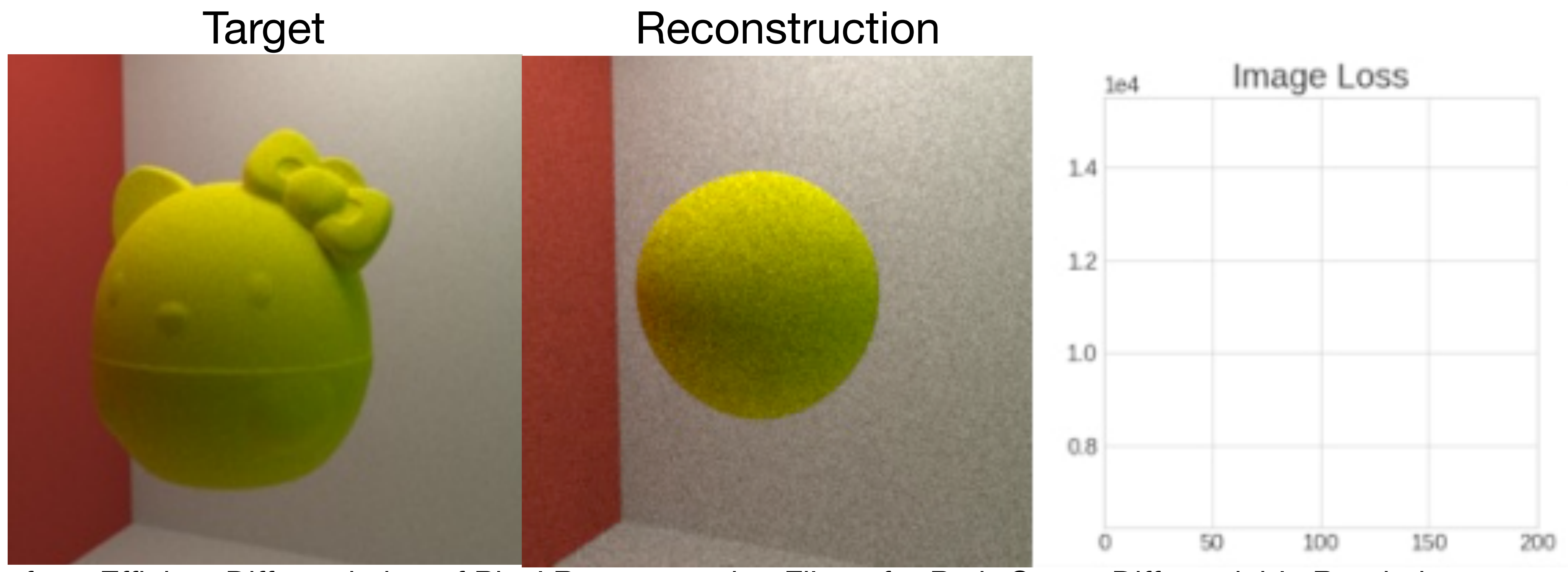
- Derivatives are used widely across science
  - Machine learning (back-propagation, Bayesian inference)
  - Scientific computing (modeling, simulation, uncertainty quantification)





from Efficient Differentiation of Pixel Reconstruction Filters for Path-Space Differentiable Rendering, SIGGRAPH Asia 2022, Zihan Yu et al

AD-Powered Applications



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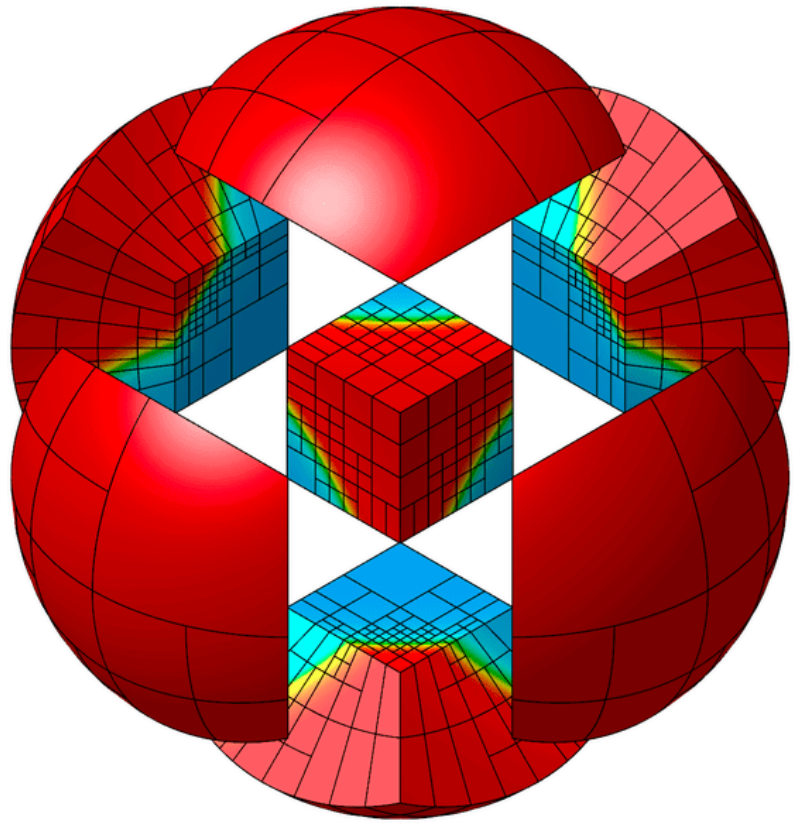
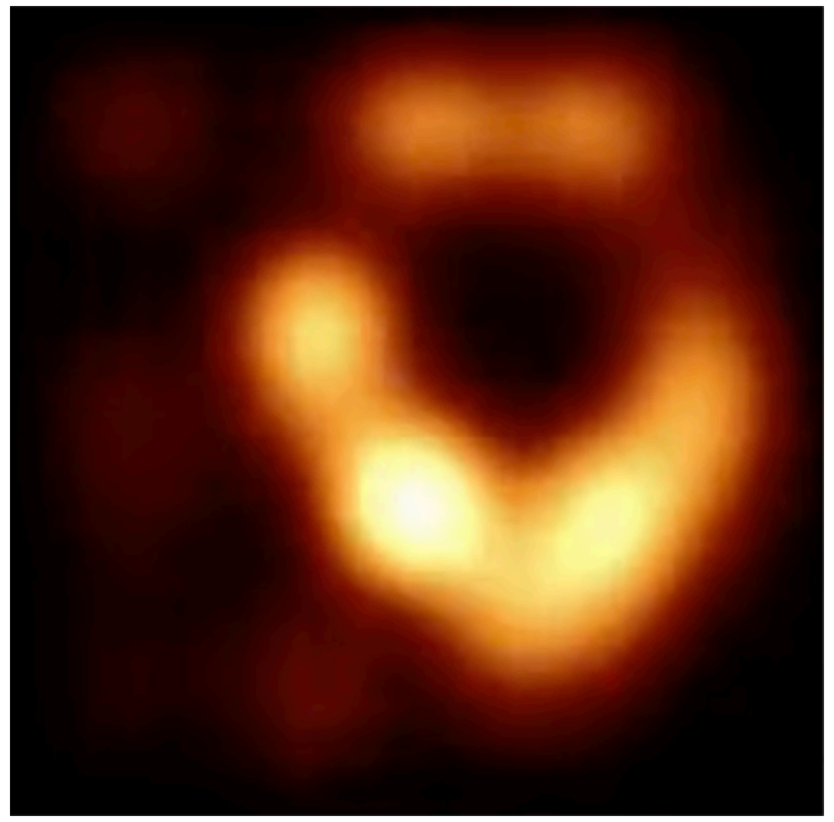
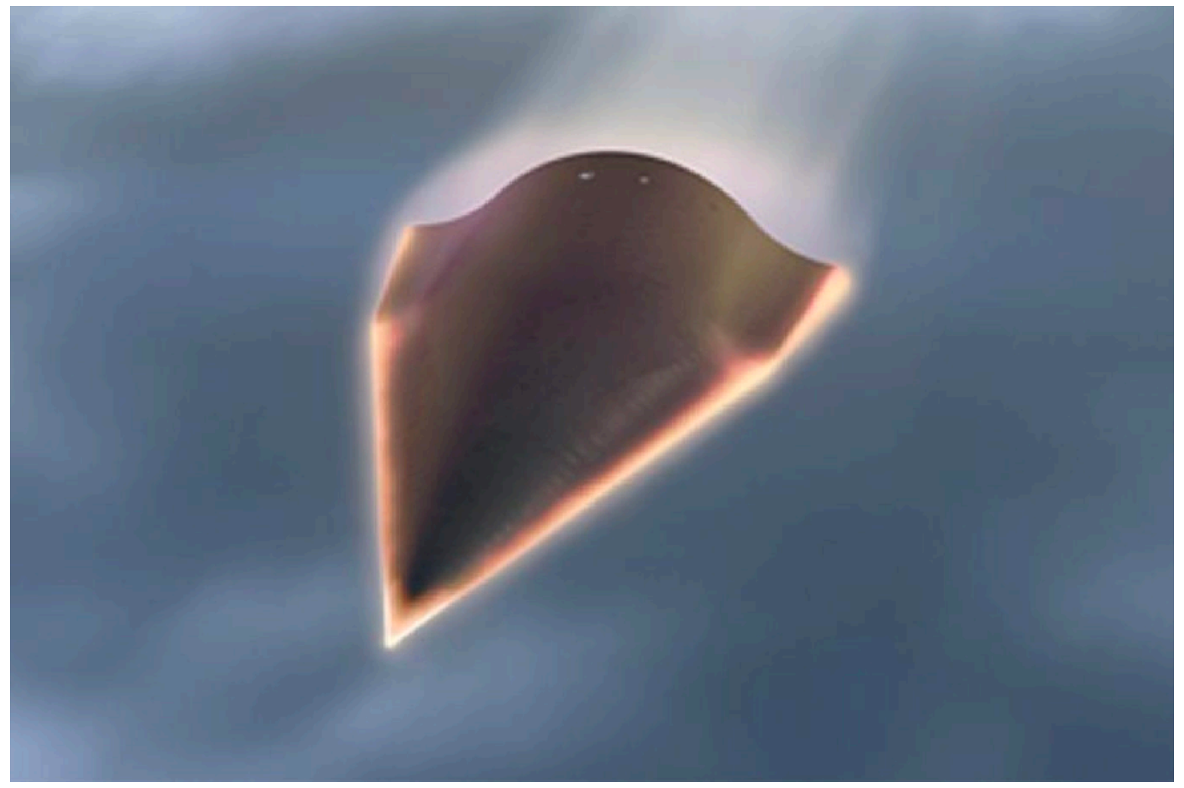


from MFEM Team at LLNL

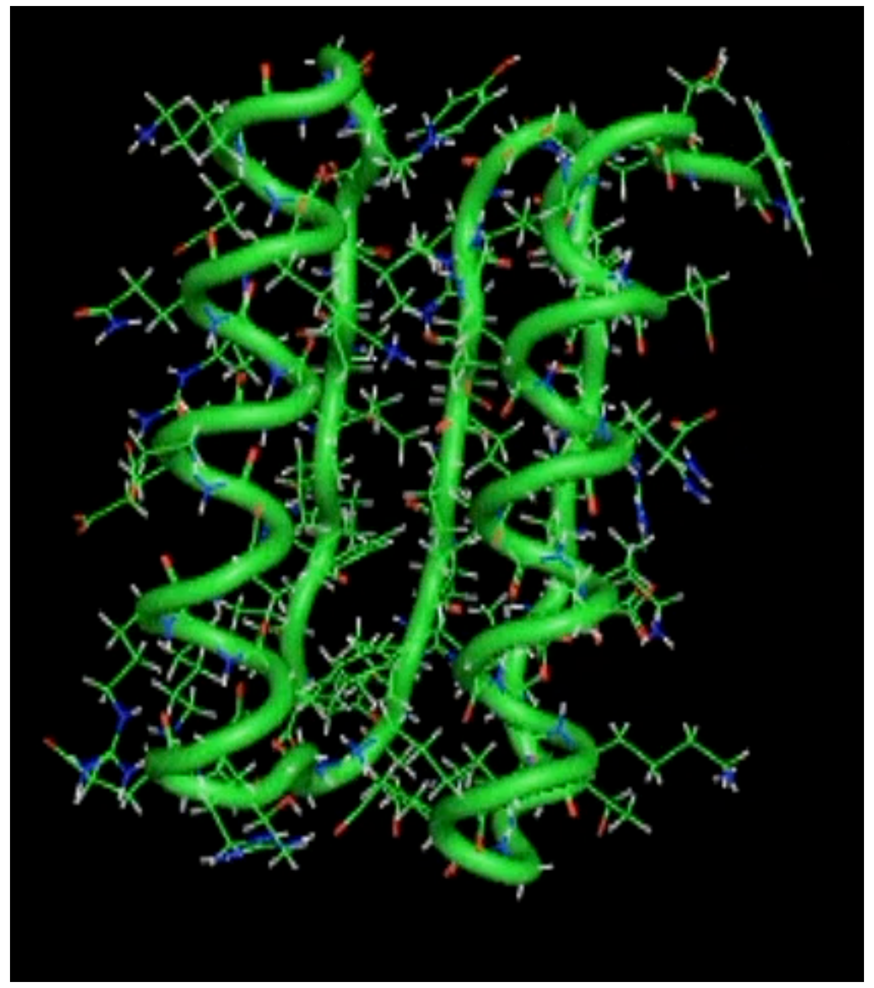


from Comrade: High Performance Black-Hole Imaging JuliaCon 2022, Paul Tiede (Harvard)

from CLIMA & NSF CSSI: Differentiable programming in Julia for Earth system modeling (DJ4Earth)



from Center for the Exascale Simulation of Materials in Extreme Environments

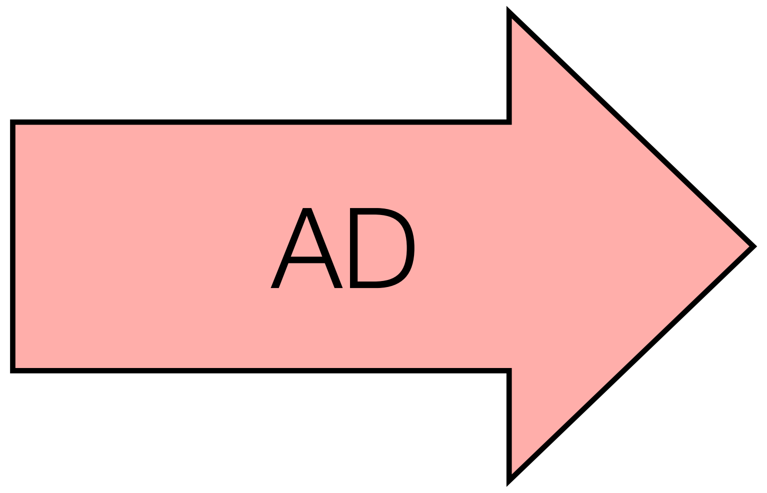


from Differential Molecular Simulation with Molly.jl, EnzymeCon 2023, Joe Greener (Cambridge)

Automatic Derivative Generation

- Derivatives can be generated automatically from definitions within programs

```
double relu3(double x) {
  if (x > 0)
    return pow(x,3)
  else
    return 0;
}
```




```
double grad_relu3(double x) {
  if (x > 0)
    return 3 * pow(x,2)
  else
    return 0;
}
```

- Unlike numerical approaches, automatic differentiation (AD) can compute the derivative of ALL inputs (or outputs) at once, without approximation error!

```
// Numeric differentiation
// f'(x) approx [f(x+epsilon) - f(x)] / epsilon
double grad_input[100];

for (int i=0; i<100; i++) {
  double input2[100] = input;
  input2[i] += 0.01;
  grad_input[i] = (f(input2) - f(input))/0.001;
}
```

```
// Automatic differentiation
double grad_input[100];

grad_f(input, grad_input)
```

Existing AD Approaches (1/3)

- Differentiable DSL (TensorFlow, PyTorch, DiffTaichi)
  - Provide a new language designed to be differentiated
  - Requires rewriting everything in the DSL and the DSL must support all operations in original code
  - Fast if DSL matches original code well

```
double relu3(double val) {
  if (x > 0)
    return pow(x,3)
  else
    return 0;
}
```

Manually Rewrite

```
import tensorflow as tf

x = tf.Variable(3.14)

with tf.GradientTape() as tape:
  out = tf.cond(x > 0,
           lambda: tf.math.pow(x,3),
           lambda: 0
        )
print(tape.gradient(out, x).numpy())
```

Existing AD Approaches (2/3)

- Operator overloading (Adept, JAX)
  - Differentiable versions of existing language constructs (double => adouble, np.sum => jax.sum)
  - May require writing to use non-standard utilities
  - Often dynamic: storing instructions/values to later be interpreted

```cpp
// Rewrite to accept either
//    double or adouble
template<typename T>
T relu3(T val) {
  if (x > 0)
    return pow(x,3)
  else
    return 0;
}
```

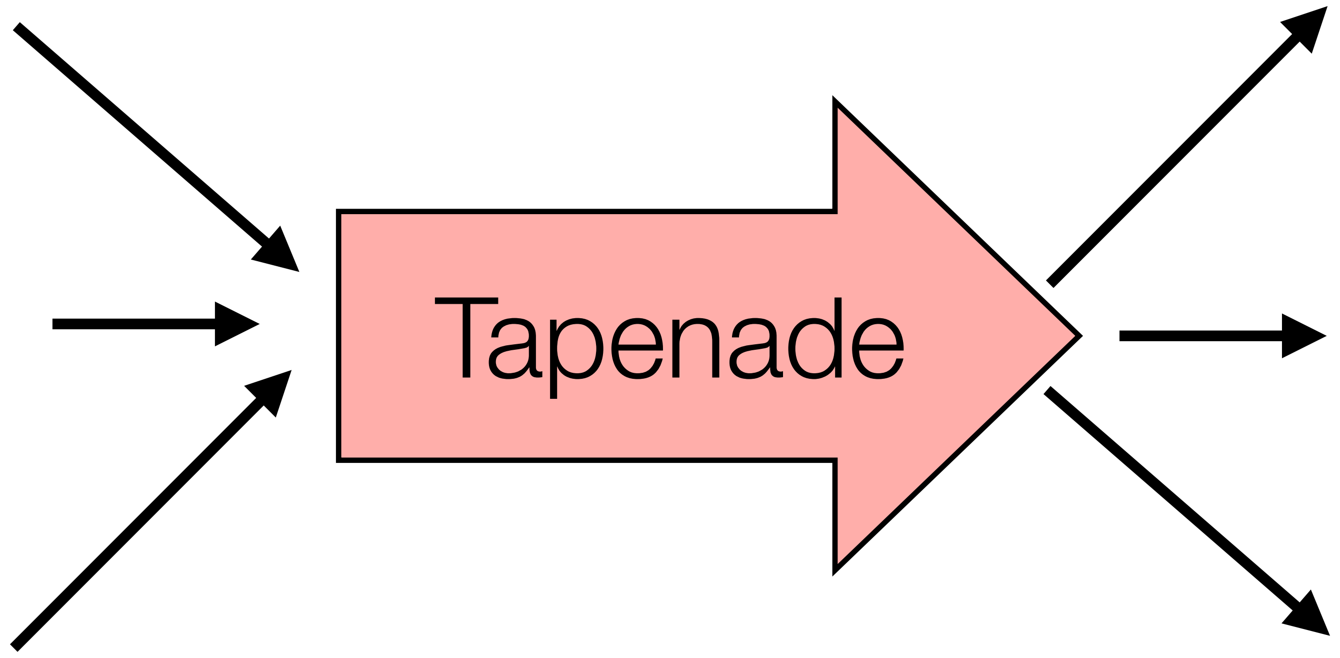
```cpp
adept::Stack stack;
adept::adouble inp = 3.14;

// Store all instructions into stack
adept::adouble out(relu3(inp));
out.set_gradient(1.00);

// Interpret all stack instructions
double res = inp.get_gradient(3.14);
```

Existing AD Approaches (3/3)

- Source rewriting
  - Statically analyze program to produce a new gradient function in the source language
  - Re-implement parsing and semantics of given language
  - Requires all code to be available ahead of time => hard to use with external libraries

```
// myfile.h
```

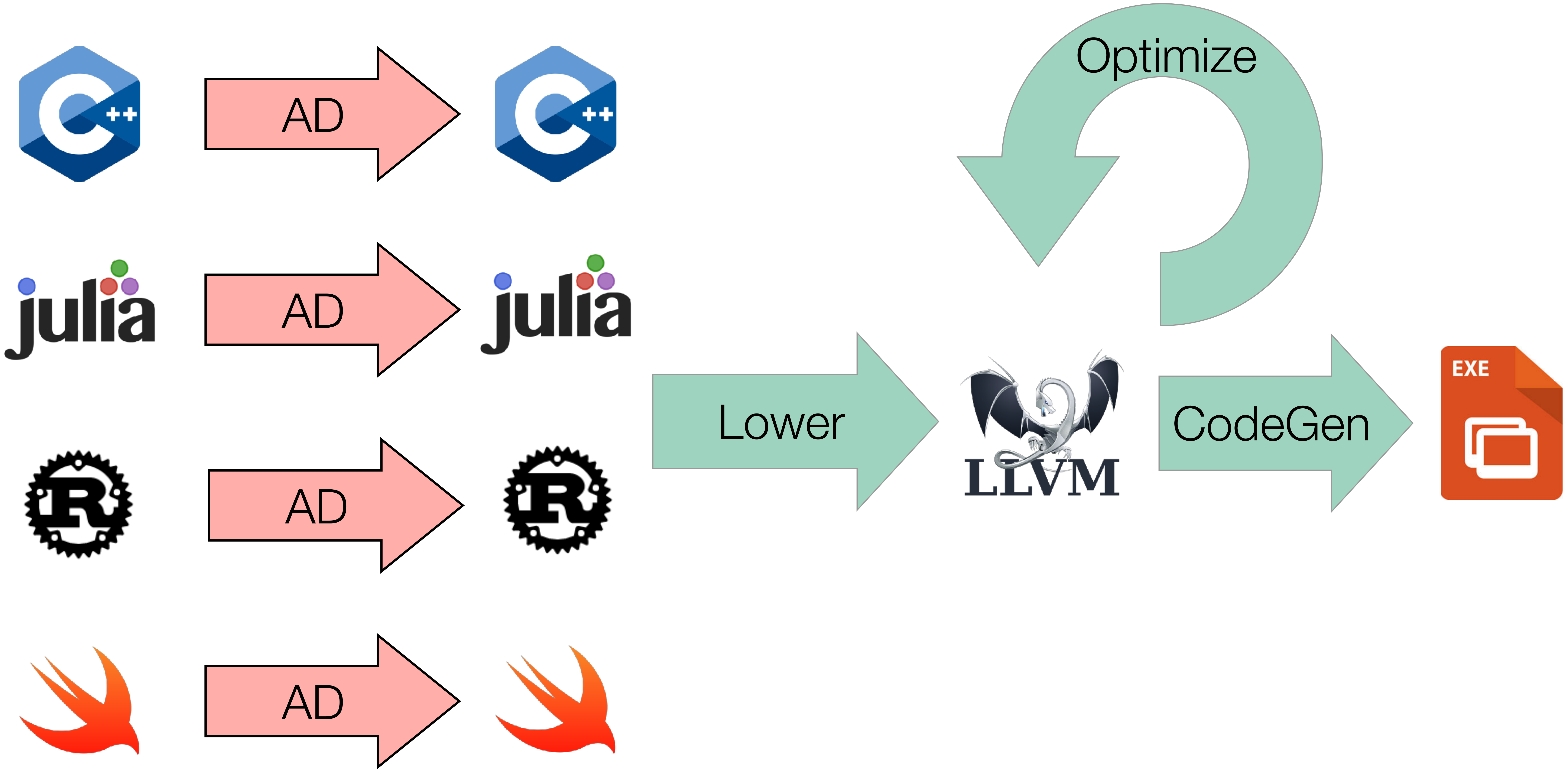
```c
// myfile.c
double relu3(double x) {
  if (x > 0)
    return pow(x,3)
  else
    return 0;
}
```




```
// grad_myfile.h
```

```c
// grad_myfile.c
double grad_relu3(double x) {
  if (x > 0)
    return 3 * pow(x,2)
  else
    return 0;
}
```

Existing Automatic Differentiation Pipelines



Case Study: Vector Normalization

```
//Compute magnitude in O(n)
double mag(double[] x);

//Compute norm in O(n^2)
void norm(double[] out, double[] in) {

  for (int i=0; i<n; i++) {
    out[i] = in[i] / mag(in);
  }
}
```

Case Study: Vector Normalization

```
//Compute magnitude in O(n)
double mag(double[] x);

//Compute norm in O(n)
void norm(double[] out, double[] in) {
  double res = mag(in);
  for (int i=0; i<n; i++) {
    out[i] = in[i] / res;
  }
}
```

Optimization & Automatic Differentiation

$O\left(n^2\right)$

```
for i=0..n {
  out[i] /= mag(in)
}
```

Optimize

$O\left(n\right)$

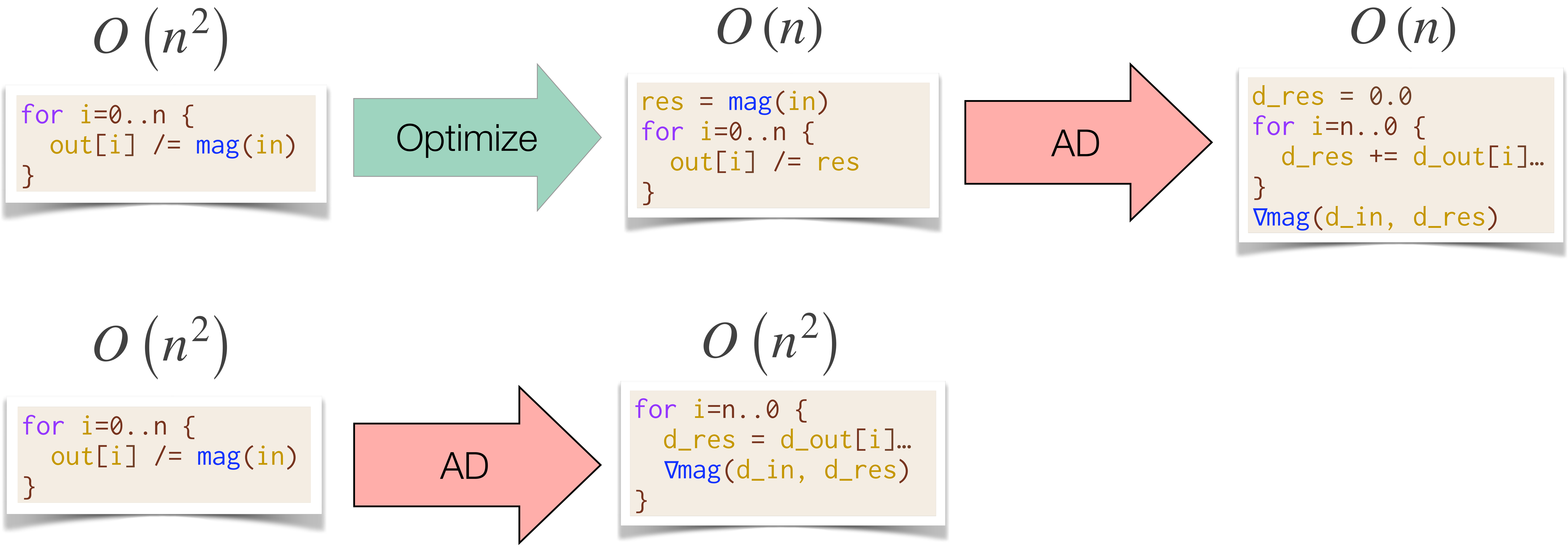
```
res = mag(in)
for i=0..n {
  out[i] /= res
}
```

AD

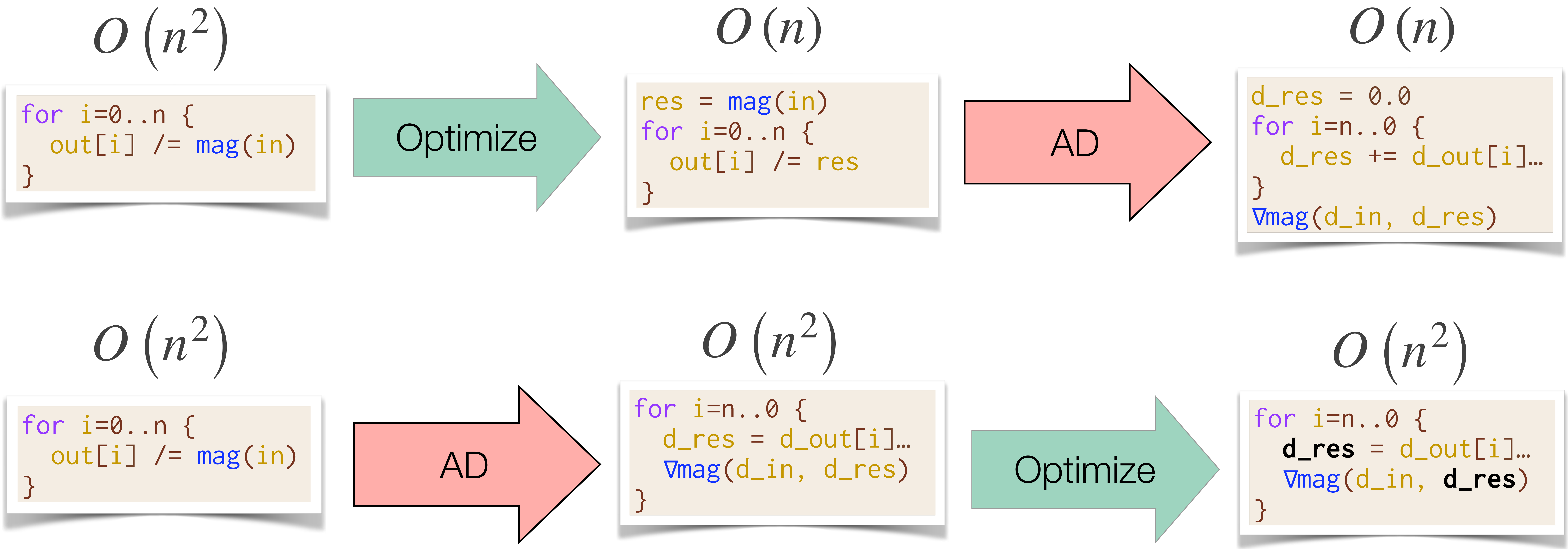
$O\left(n\right)$

```
d_res = 0.0
for i=n..0 {
  d_res += d_out[i]…
}
∇mag(d_in, d_res)
```

Optimization & Automatic Differentiation



Optimization & Automatic Differentiation



Optimization & Automatic Differentiation

Differentiating after optimization can create ***asymptotically faster*** gradients!

$O\left(n^2\right)$

```
for i=0..n {
  out[i] /= mag(in)
}
```

Optimize

$O\left(n\right)$

```
res = mag(in)
for i=0..n {
  out[i] /= res
}
```

AD

$O\left(n\right)$

```
d_res = 0.0
for i=n..0 {
  d_res += d_out[i]…
}
∇mag(d_in, d_res)
```

$O\left(n^2\right)$

```
for i=0..n {
  out[i] /= mag(in)
}
```

AD

$O\left(n^2\right)$

```
for i=n..0 {
  d_res = d_out[i]…
  ∇mag(d_in, d_res)
}
```

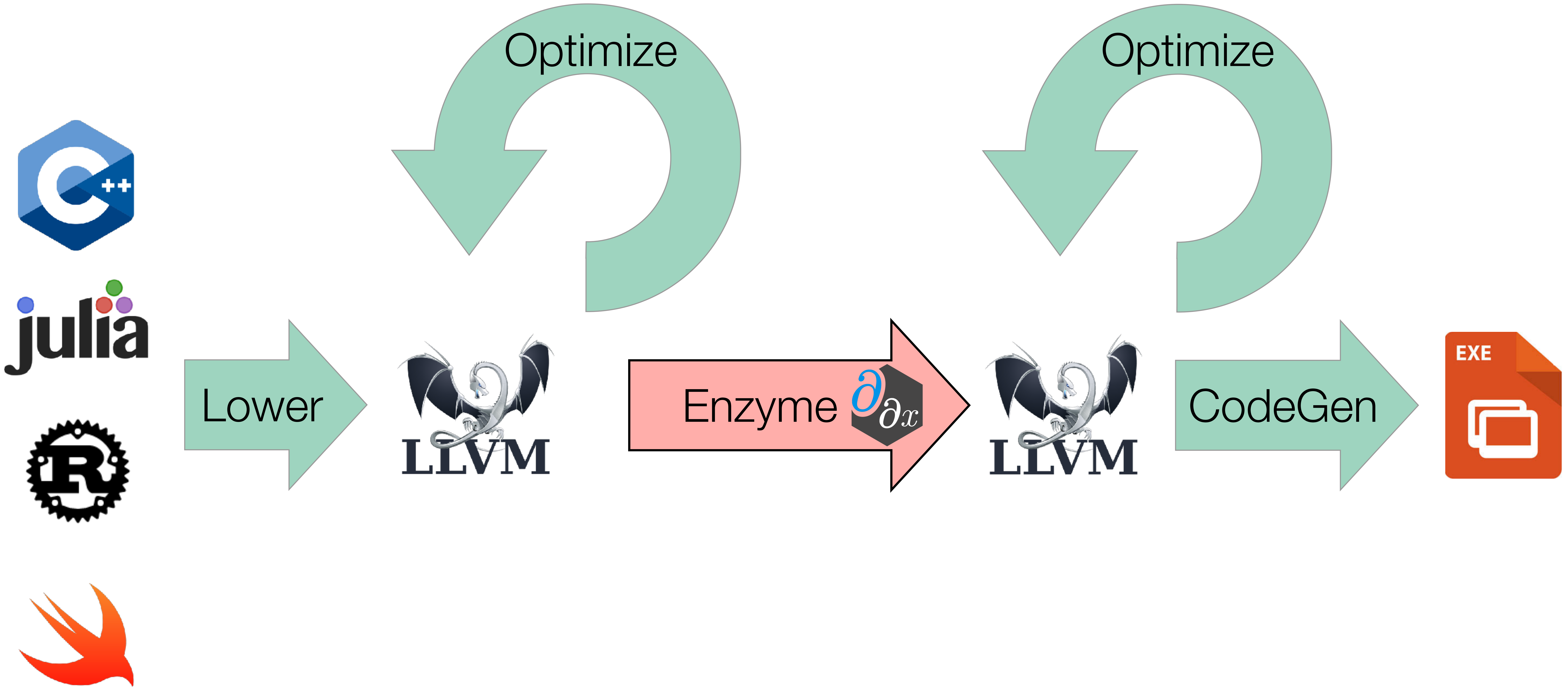
Optimize

$O\left(n^2\right)$

```
for i=n..0 {
  d_res = d_out[i]…
  ∇mag(d_in, d_res)
}
```

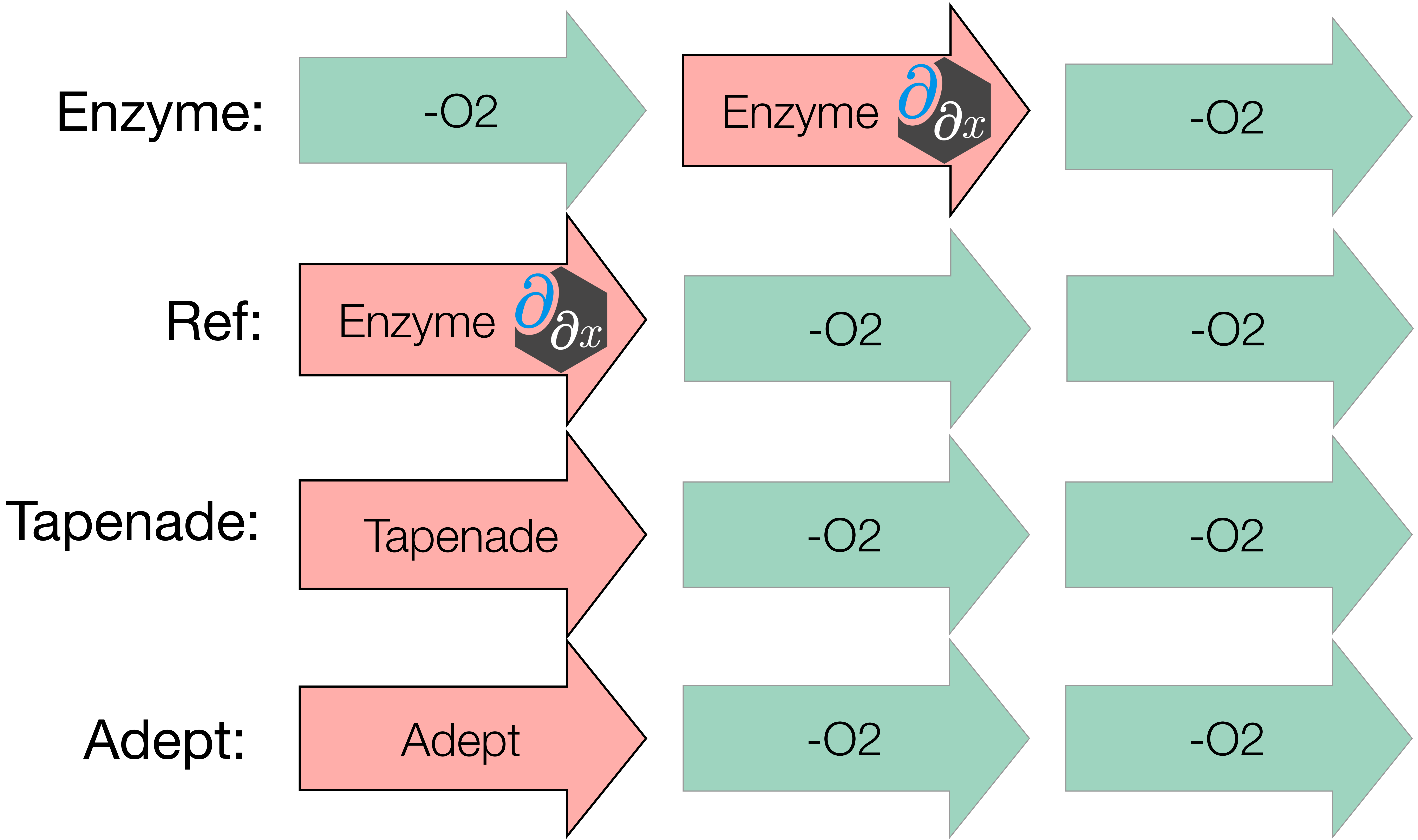
Enzyme Approach

Performing AD at low-level lets us work on ***optimized*** code!

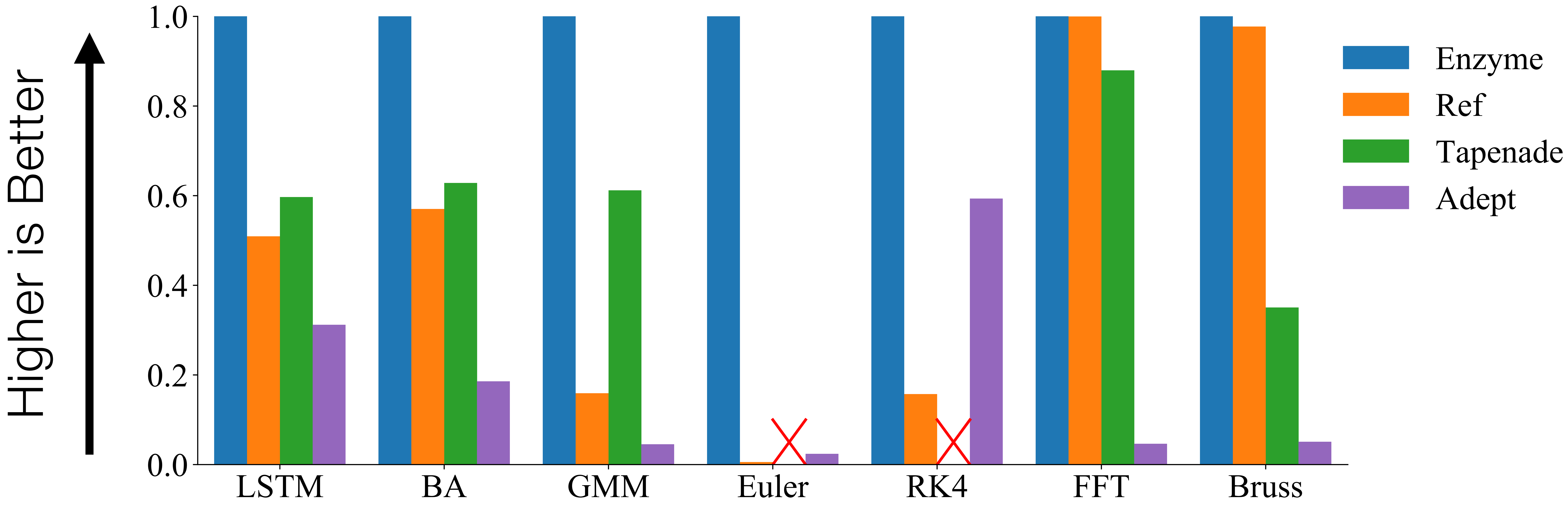


Experimental Setup

- Collection of benchmarks from Microsoft's ADBench suite and of technical interest



Speedup of Enzyme



Enzyme is ***4.2x faster*** than Reference!

Automatic Differentiation & GPUs

- Prior work has not explored reverse mode AD of existing GPU kernels

  1. Reversing parallel control flow can lead to incorrect results

  2. Complex performance characteristics make it difficult to synthesize efficient code

  3. Resource limitations can prevent kernels from running at all

Efficient GPU Code

- For correctness, Enzyme may need to cache values in order to compute the gradient
  - The complexity of GPU memory means large caches slow down the program by several orders of magnitude, if it even fits at all
- Like the CPU, existing optimizations reduce the overhead
- Unlike the CPU, existing optimizations aren't sufficient
- Novel GPU and AD-specific optimizations can speedup by several orders of magnitude

```
// Forward Pass

out[i] = x[i] * x[i];

x[i] = 0.0f;

// Reverse (gradient) Pass

...
grad_x[i] += 2 * x[i] * grad_out[i];
...
```

~~Efficient~~ Correct GPU Code

- For correctness, Enzyme may need to cache values in order to compute the gradient
  - The complexity of GPU memory means large caches slow down the program by several orders of magnitude, if it even fits at all
- Like the CPU, existing optimizations reduce the overhead
- Unlike the CPU, existing optimizations aren't sufficient
- Novel GPU and AD-specific optimizations can speedup by several orders of magnitude

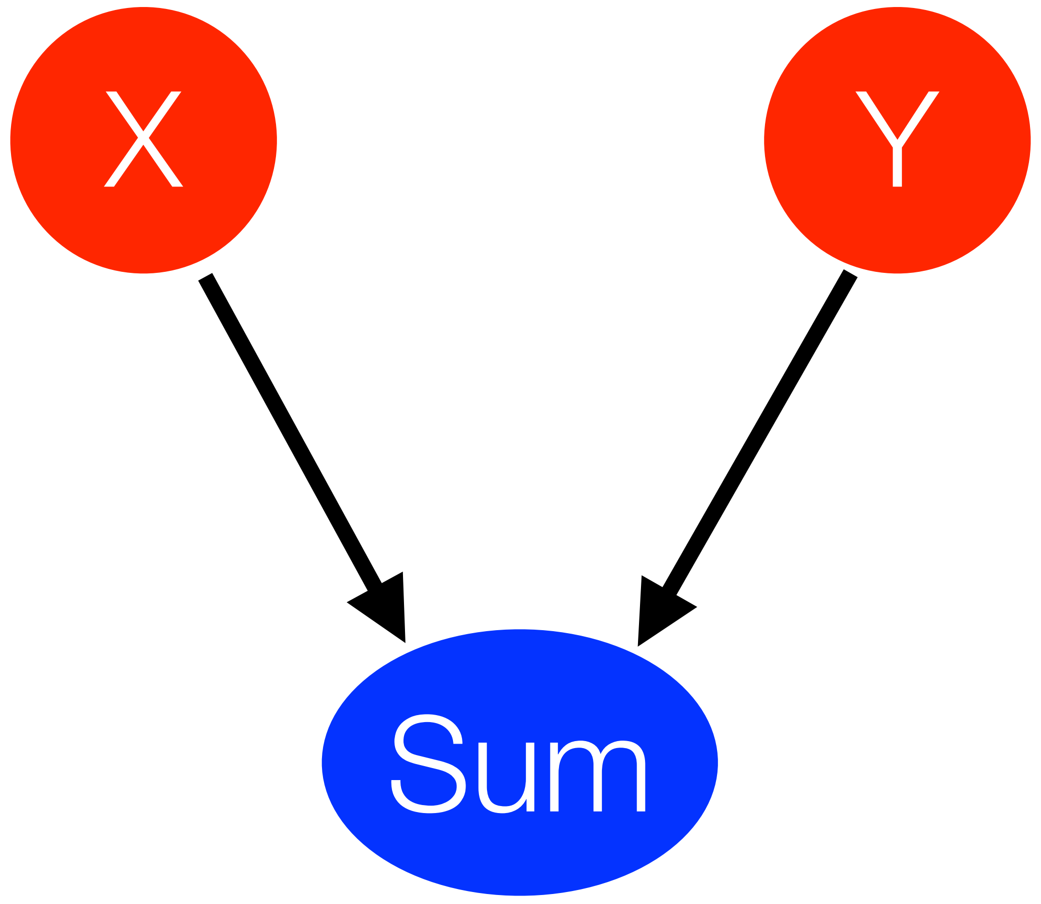
```
double* x_cache = new double[…];

// Forward Pass

out[i] = x[i] * x[i];
x_cache[i] = x[i];

x[i] = 0.0f;

// Reverse (gradient) Pass

...
grad_x[i] += 2 * x_cache[i]
               * grad_out[i];
...

delete[] x_cache;
```

Cache Reduction Example

- By considering the dataflow graph we can perform a min-cut to approximate smaller cache sizes.

Overwritten:

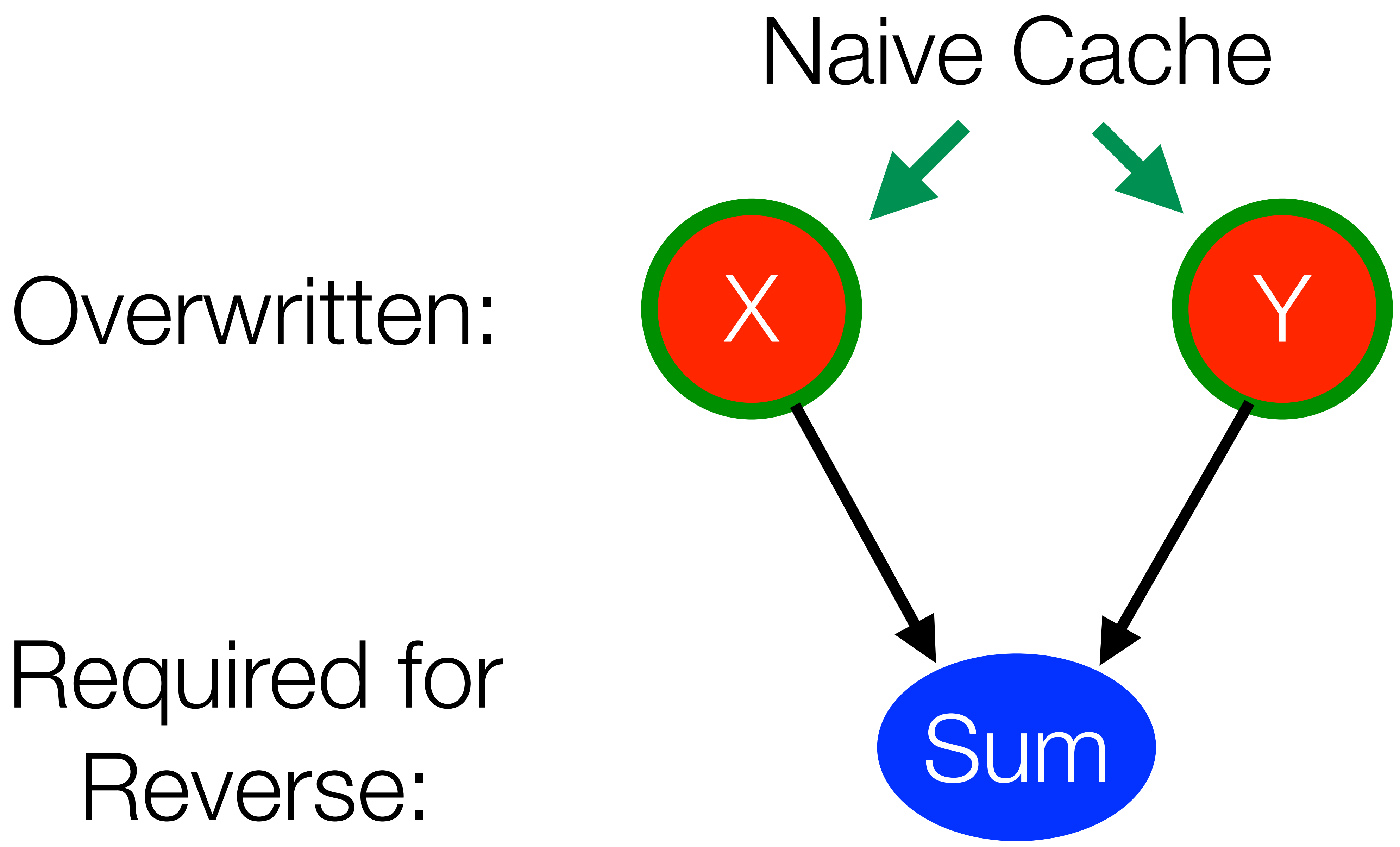
Required for Reverse:




```
for(int i=0; i<10; i++) {
  double sum = x[i] + y[i];


  use(sum);
}

overwrite(x, y);
grad_overwrite(x, y);

for(int i=9; i>=0; i--) {
  ...
  grad_use(sum);
}
```

Cache Reduction Example

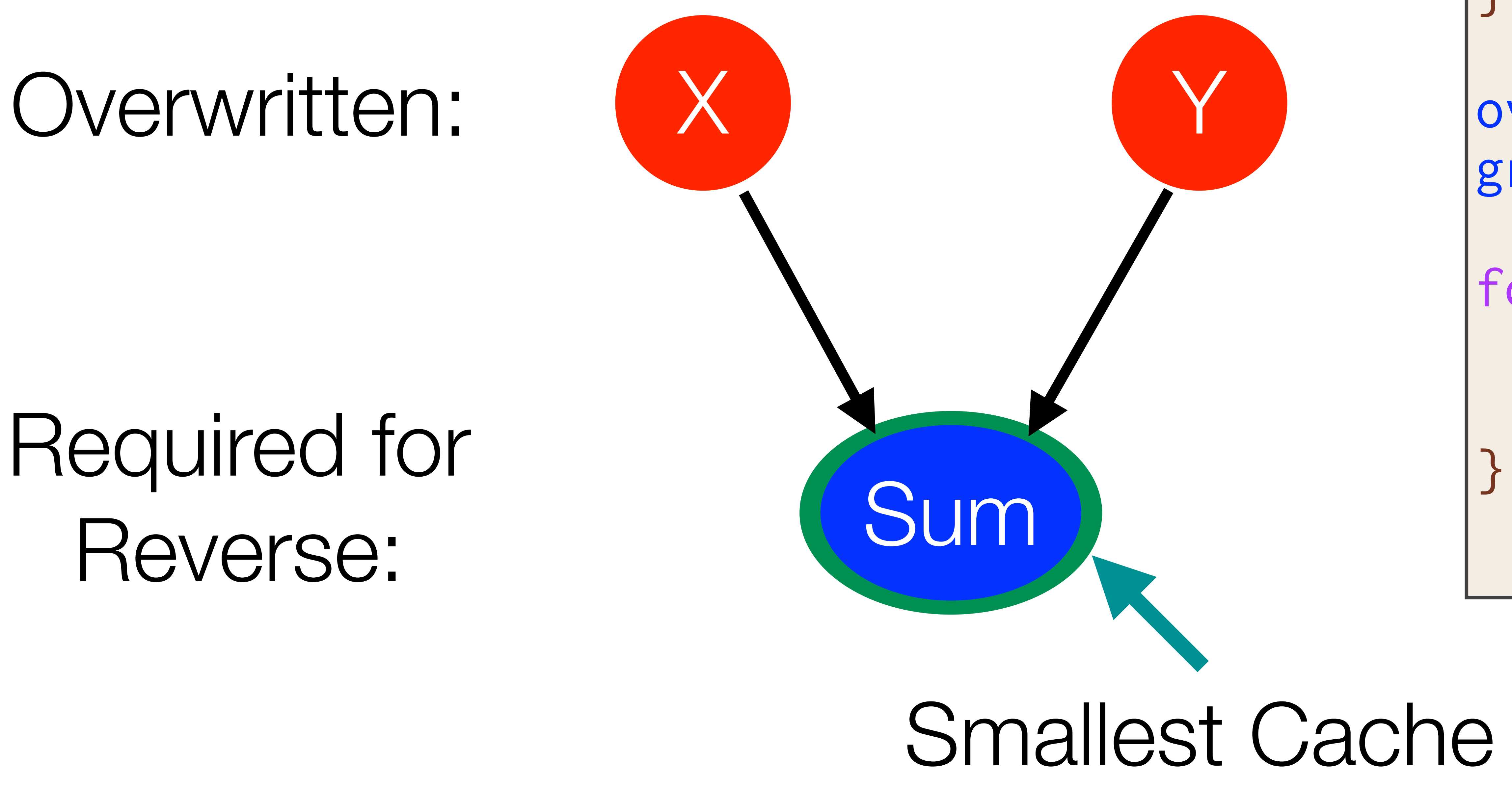
- By considering the dataflow graph we can perform a min-cut to approximate smaller cache sizes.




```
double* x_cache = new double[10];
double* y_cache = new double[10];

for(int i=0; i<10; i++) {
  double sum = x[i] + y[i];
  x_cache[i] = x[i];
  y_cache[i] = y[i];
  use(sum);
}

overwrite(x, y);
grad_overwrite(x, y);

for(int i=9; i>=0; i--) {
  double sum = x_cache[i] + y_cache[i];
  grad_use(sum);
}
```

Cache Reduction Example

- By considering the dataflow graph we can perform a min-cut to approximate smaller cache sizes.



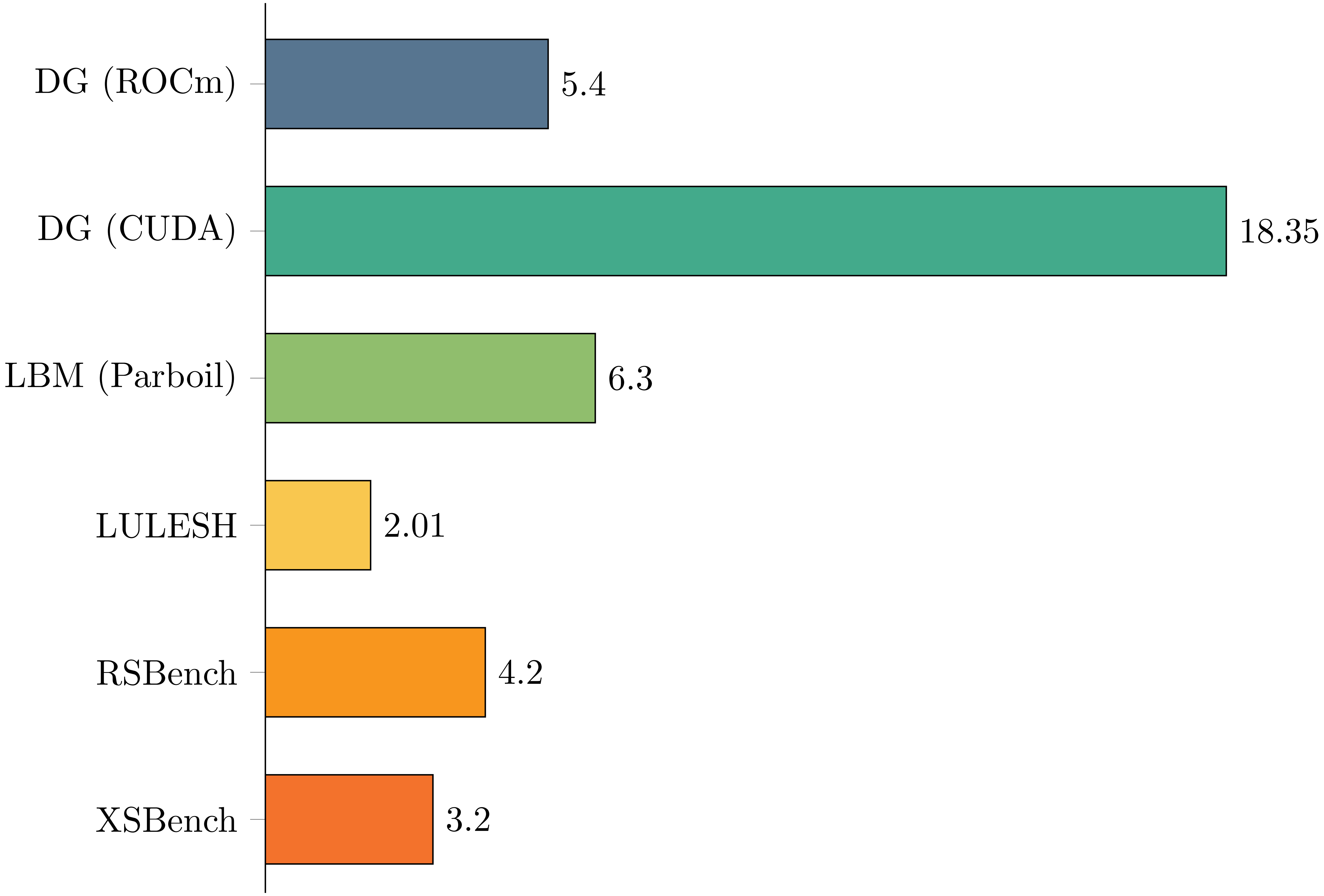

```
double* sum_cache = new double[10];

for(int i=0; i<10; i++) {
  double sum = x[i] + y[i];
  sum_cache[i] = sum;

  use(sum);
}

overwrite(x, y);
grad_overwrite(x, y);

for(int i=9; i>=0; i--) {

  grad_use(sum_cache[i]);
}
```

Novel AD + GPU Optimizations

- See our SC’21 paper for more (https://c.wsmoses.com/papers/EnzymeGPU.pdf)
  Reverse-Mode Automatic Differentiation and Optimization of GPU Kernels via Enzyme. SC, 2021
- [AD] Cache LICM/CSE
- [AD] Min-Cut Cache Reduction
- [AD] Cache Forwarding
- [GPU] Merge Allocations
- [GPU] Heap-to-stack (and register)
- [GPU] Alias Analysis Properties of SyncThreads
- …

GPU Gradient Overhead

- Evaluation of both original code and gradient
  - DG: Discontinuous-Galerkin integral (Julia)
  - LBM: particle-based fluid dynamics simulation
  - LULESH: unstructured explicit shock hydrodynamics solver
  - XSBench & RSBench: Monte Carlo simulations of particle transport algorithms (memory & compute bound, respectively)



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- Evaluation of both original code and gradient
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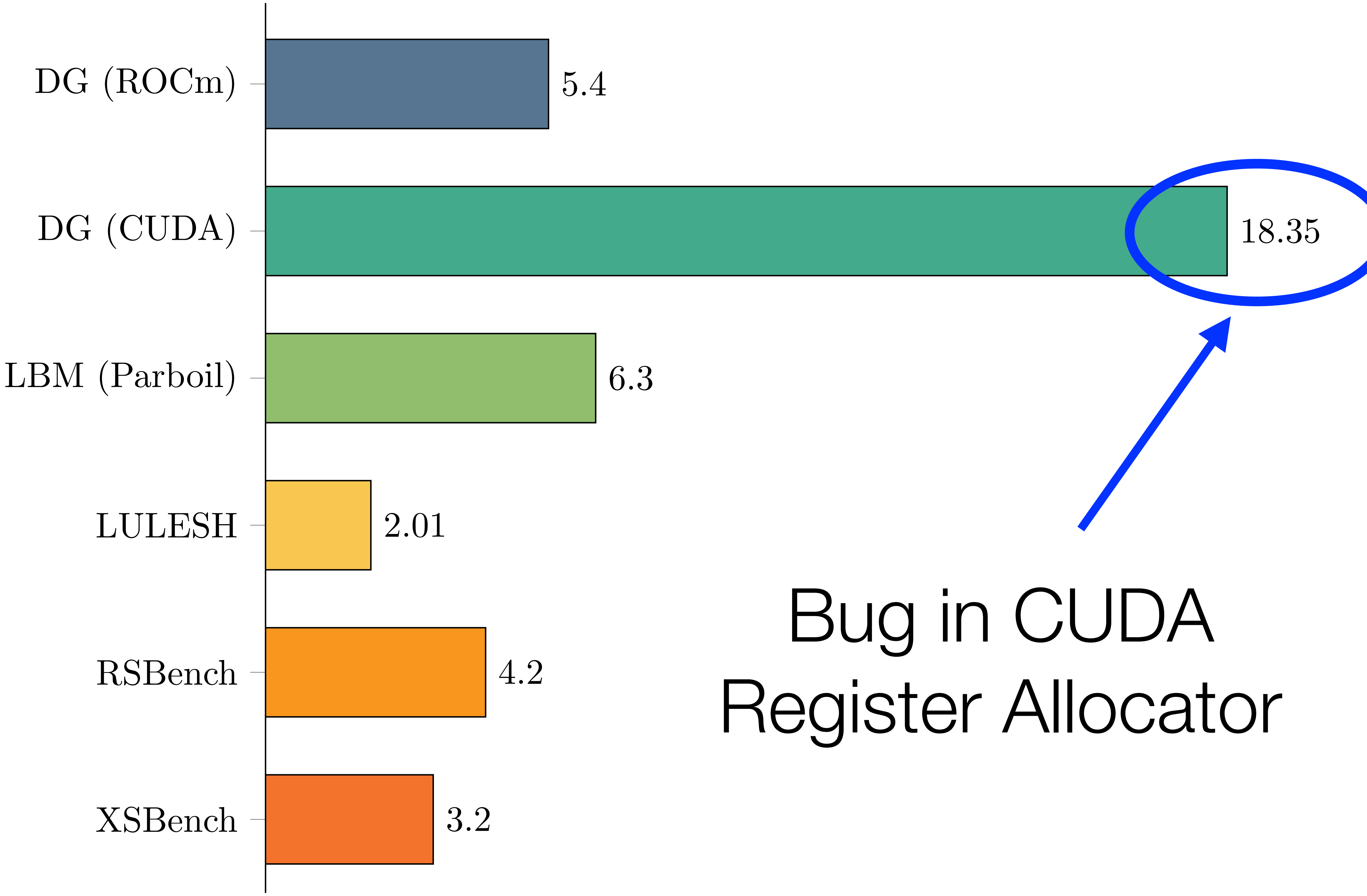

Ablation Analysis of Optimizations

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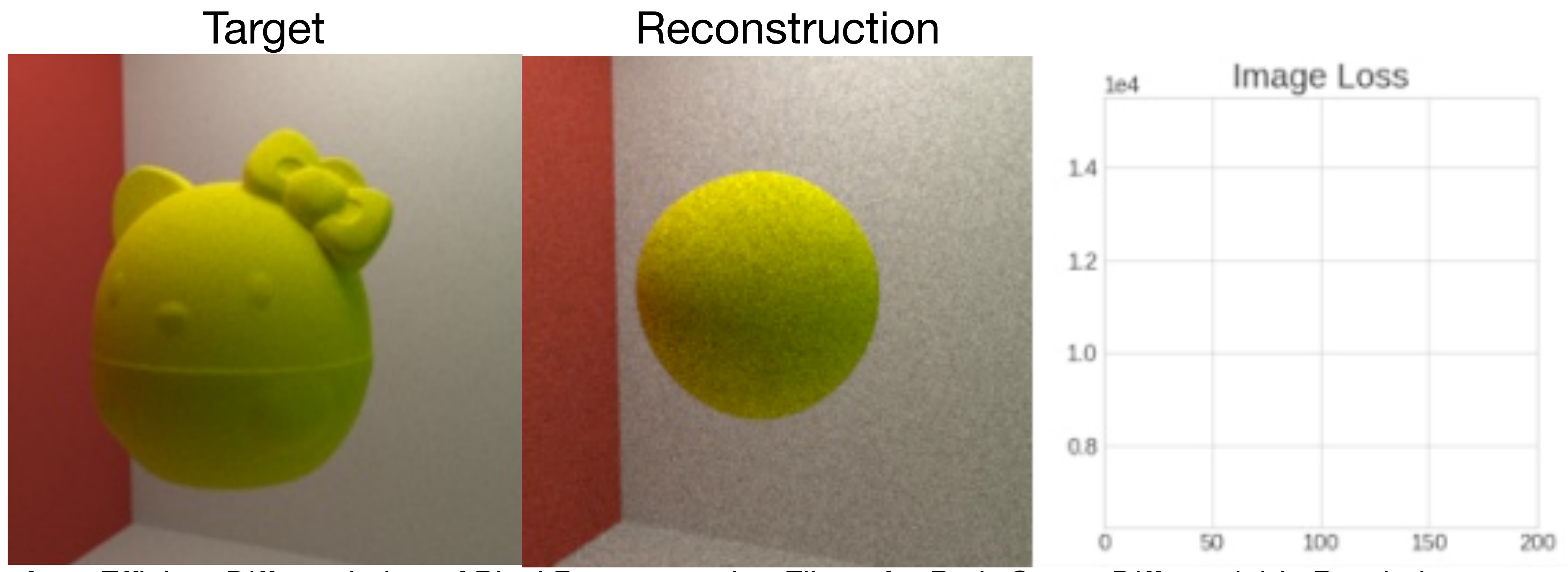
Ablation Analysis of Optimizations

Ablation Analysis of Optimizations

GPU AD is Intractable Without Optimization!

Enzyme-Powered Applications



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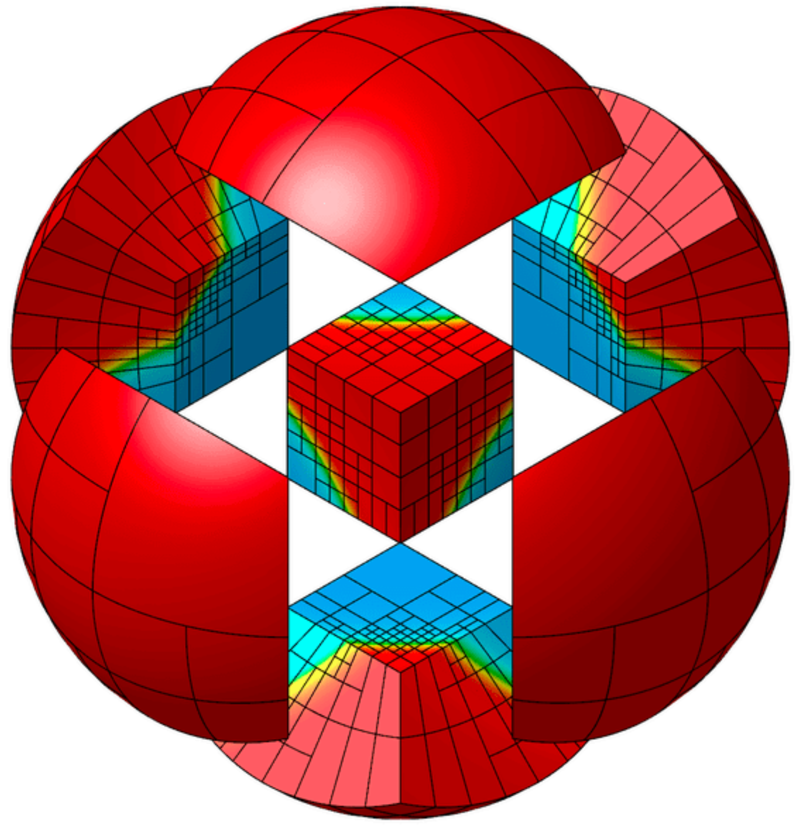
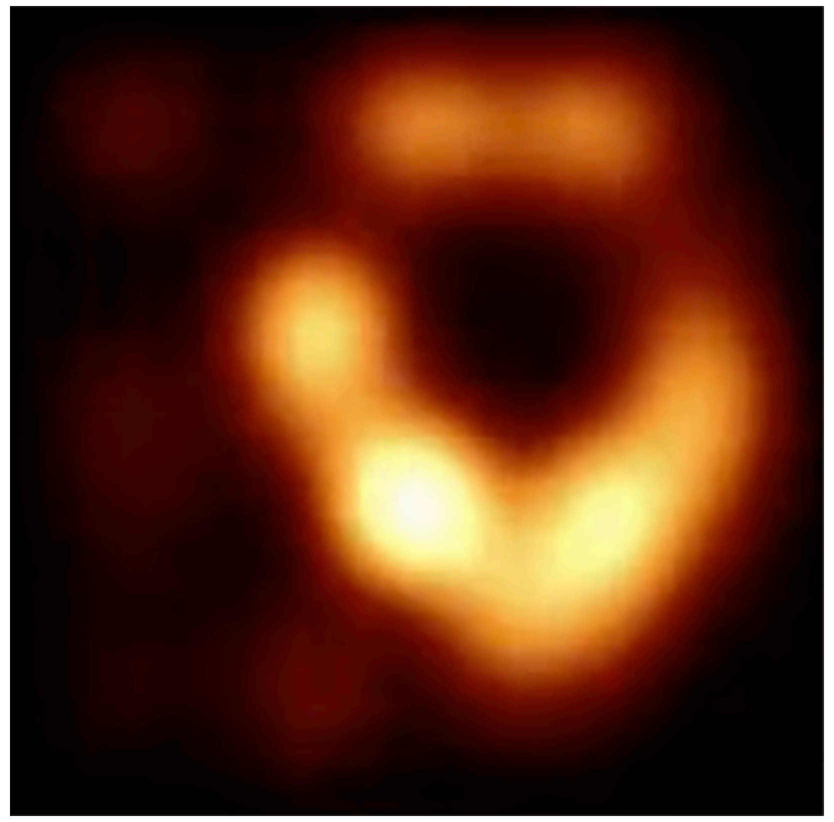


from MFEM Team at LLNL



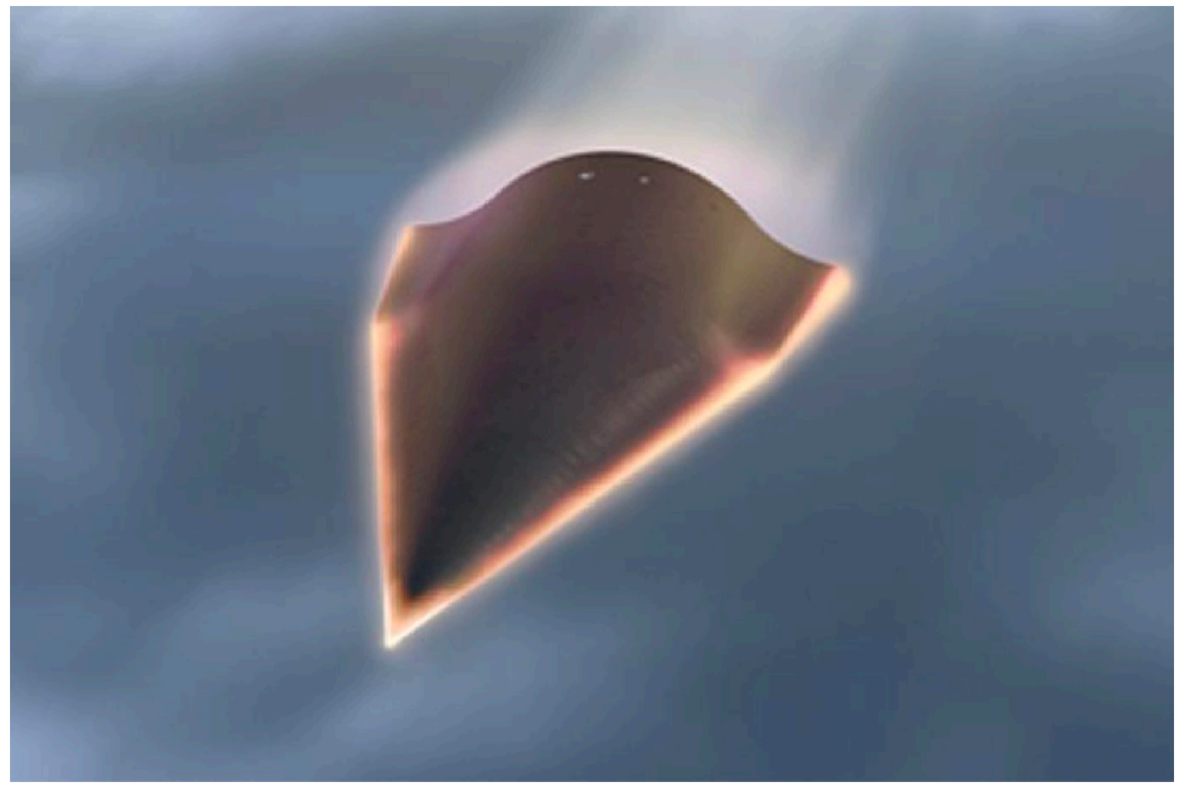
>100x speedup!

Prior:
5 days (cluster)

Enzyme-Based:
1 hour (laptop)

from Comrade: High Performance Black-Hole Imaging JuliaCon 2022, Paul Tiede (Harvard)

from CLIMA & NSF CSSI: Differentiable programming in Julia for Earth system modeling (DJ4Earth)



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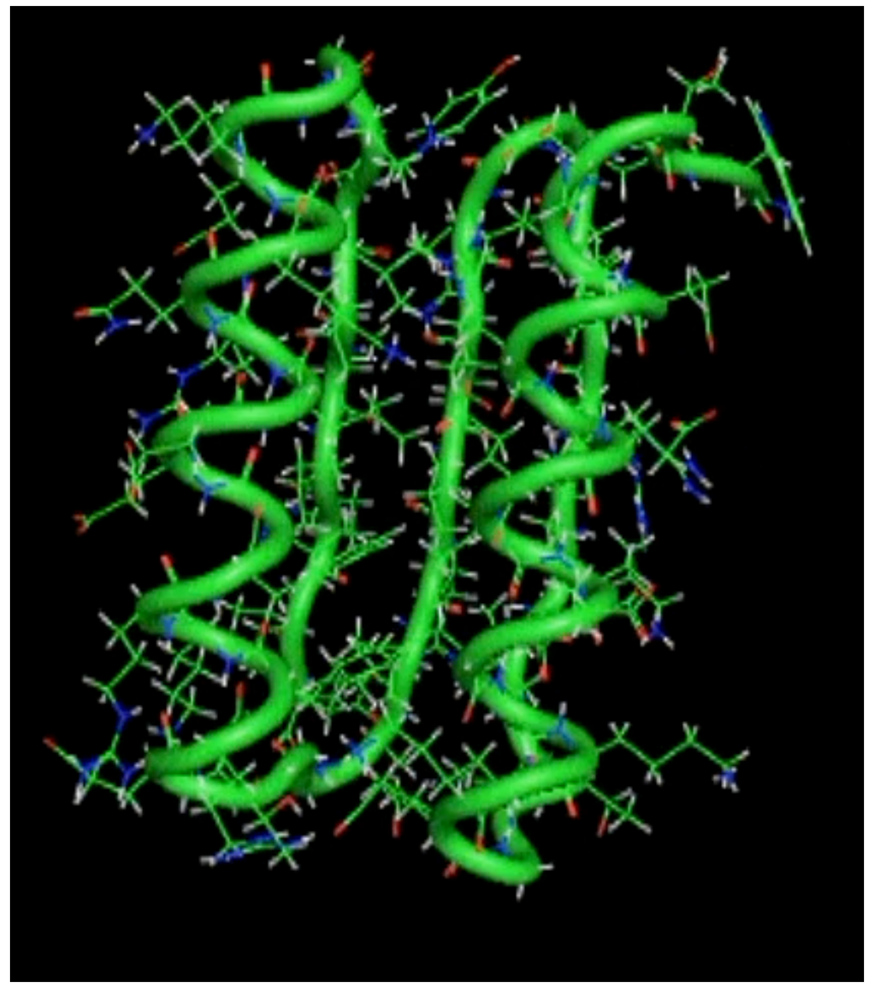
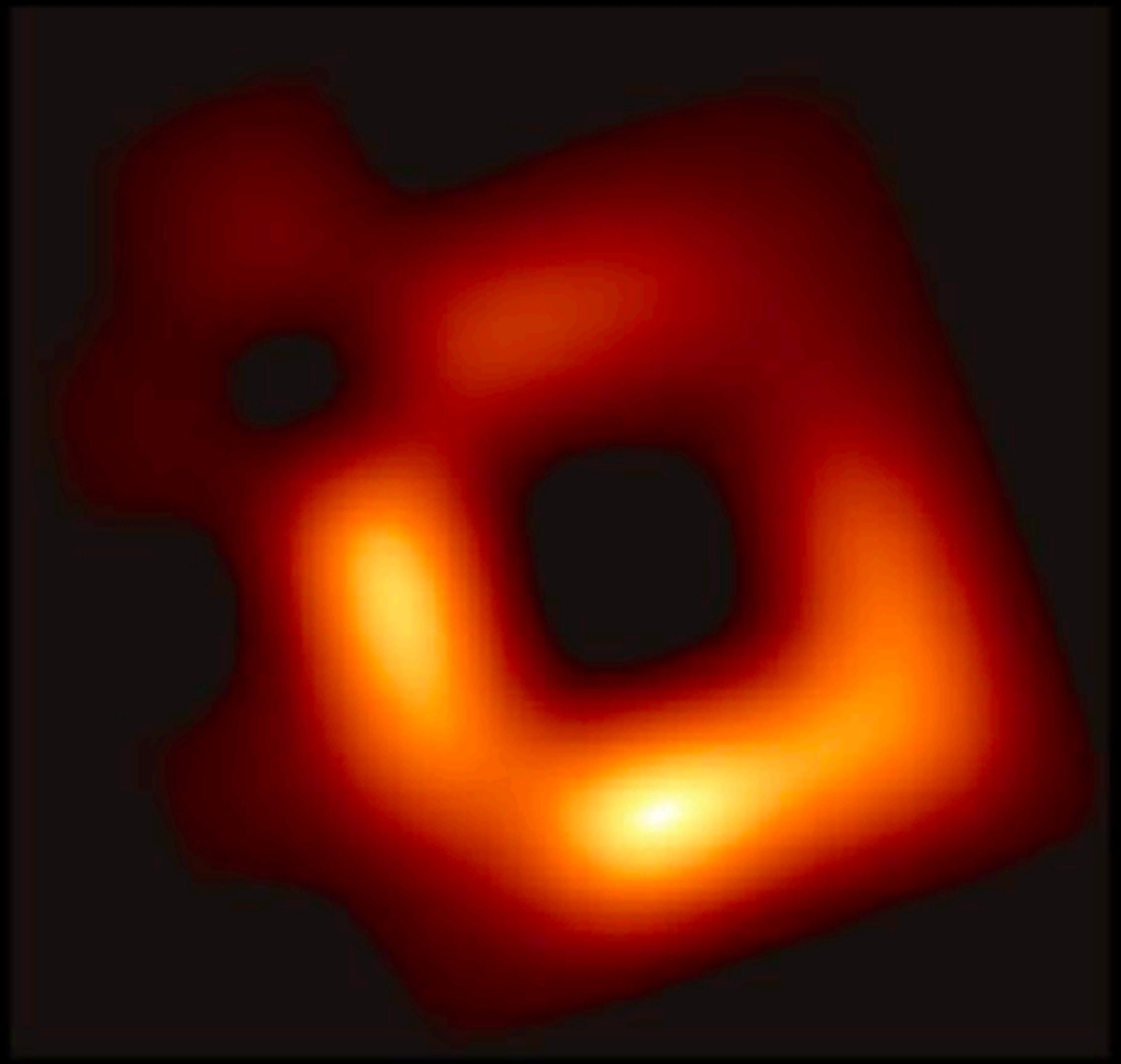


from Differential Molecular Simulation with Molly.jl, EnzymeCon 2023, Joe Greener (Cambridge)

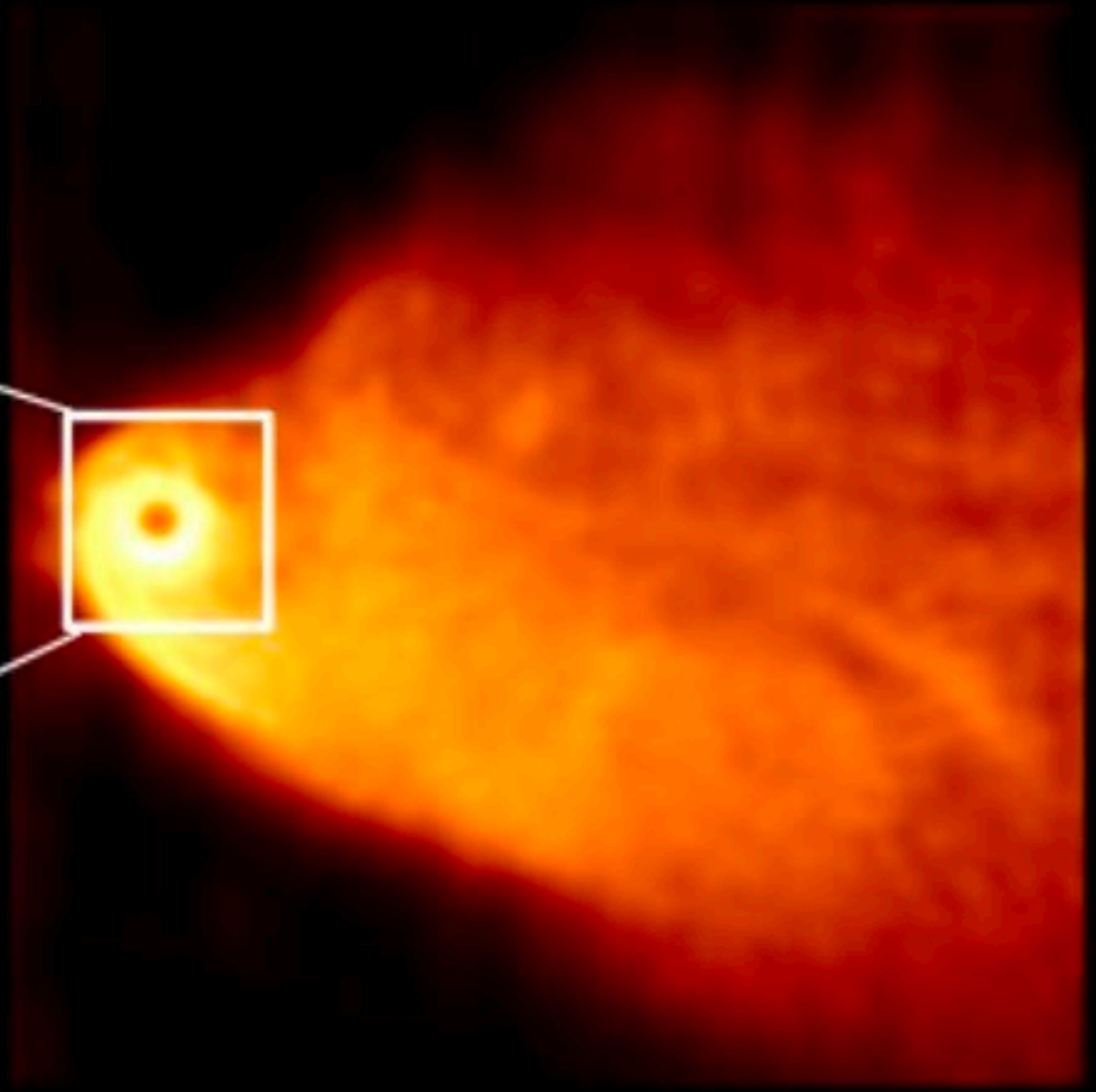
Accelerated Black Hole Imaging with Julia & Enzyme

EHT Tools M87 2017
Image Analysis: ~ **1 week** (cluster)



Julia+Enzyme M87 2017
Image Analysis: **1 hour** (1 thread)

Julia+Enzyme next-generation images
Image Analysis: **1-2 days (8 threads)**
(100x increase in computational complexity)



Simulation

Comrade.jl: Julia Bayesian Black Hole Imaging

Paul Tiede, Harvard & Smithonian | CfA

∂/∂x Enzyme

- Tool for performing reverse-mode (and forward mode) AD of statically analyzable LLVM IR
- Differentiates code in a variety of parallel frameworks (OpenMP, MPI, Julia Tasks, GPU), and languages (C, C++, Fortran, Julia, Rust, Swift, etc)
- Parallel and AD-specific optimizations crucial for performance
- Keep similar scalability as non-differentiated code
- Open source (enzyme.mit.edu & join our mailing list)!
- Ongoing work to support Mixed Mode, Batching, Checkpointing, and more

A Growing Enzyme Community (EnzymeCon 2023)

- 40 attendees spanning developers, users, and everywhere in between.

- 17 great talks from AD internals, to algorithms, to climate science, to physics, and beyond (https://enzyme.mit.edu/conference).

- Talks live streamed to YouTube (to be split individually soon):
    - Day 1 Link
    - Day 2 Link

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