Enzyme: High-Performance Automatic Differentiation of LLVM

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Differentiation Is Key To Machine Learning

- Computing derivatives is key to many algorithms
  - Machine learning (back-propagation, Bayesian inference, uncertainty quantification)
  - Scientific computing (modeling, simulation)
- When working with large codebases or dynamically-generated programs, manually writing derivative functions becomes intractable
- Community has developed tools to create derivatives automatically

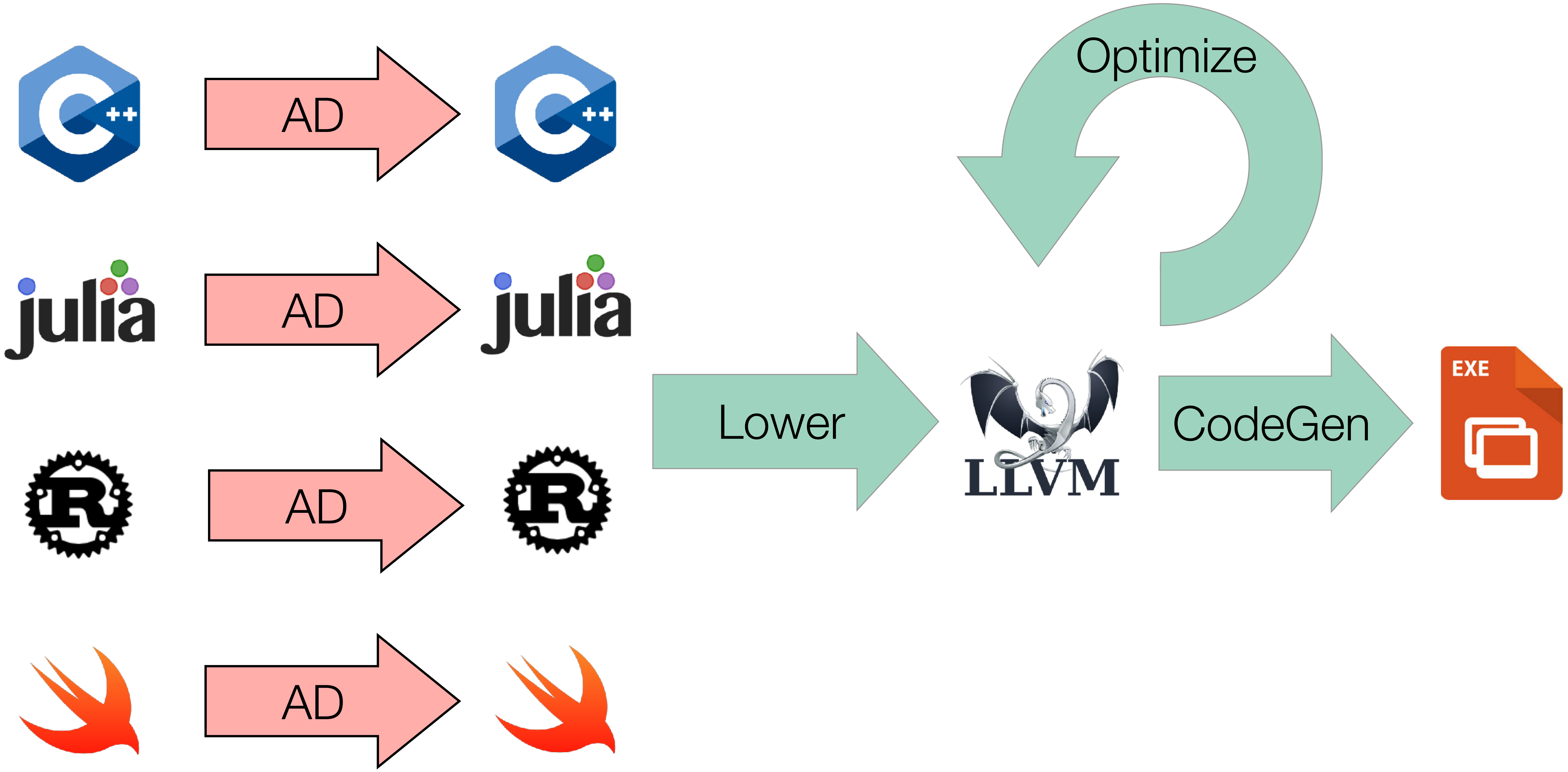
Existing AD Approaches

- Differentiable DSL (TensorFlow, PyTorch, DiffTaichi)
  - Provide a new language where all functions are differentiable
  - Requires rewriting everything in the DSL and the DSL must support all operations in original code
  - Fast if DSL matches original code well
- Operator overloading (Adept, JAX)
  - Provide 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

Existing AD Approaches

- 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
  - Difficult to use with external libraries

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

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//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)
```

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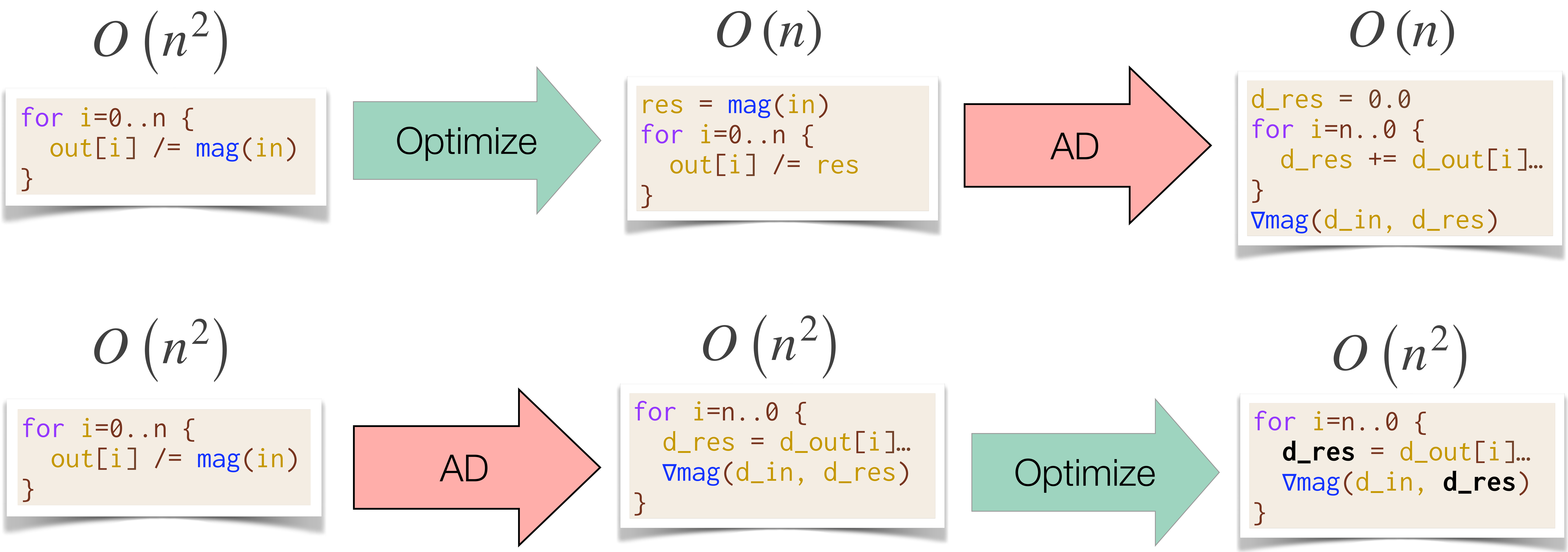
Optimization & Automatic Differentiation



Optimization & Automatic Differentiation

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

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

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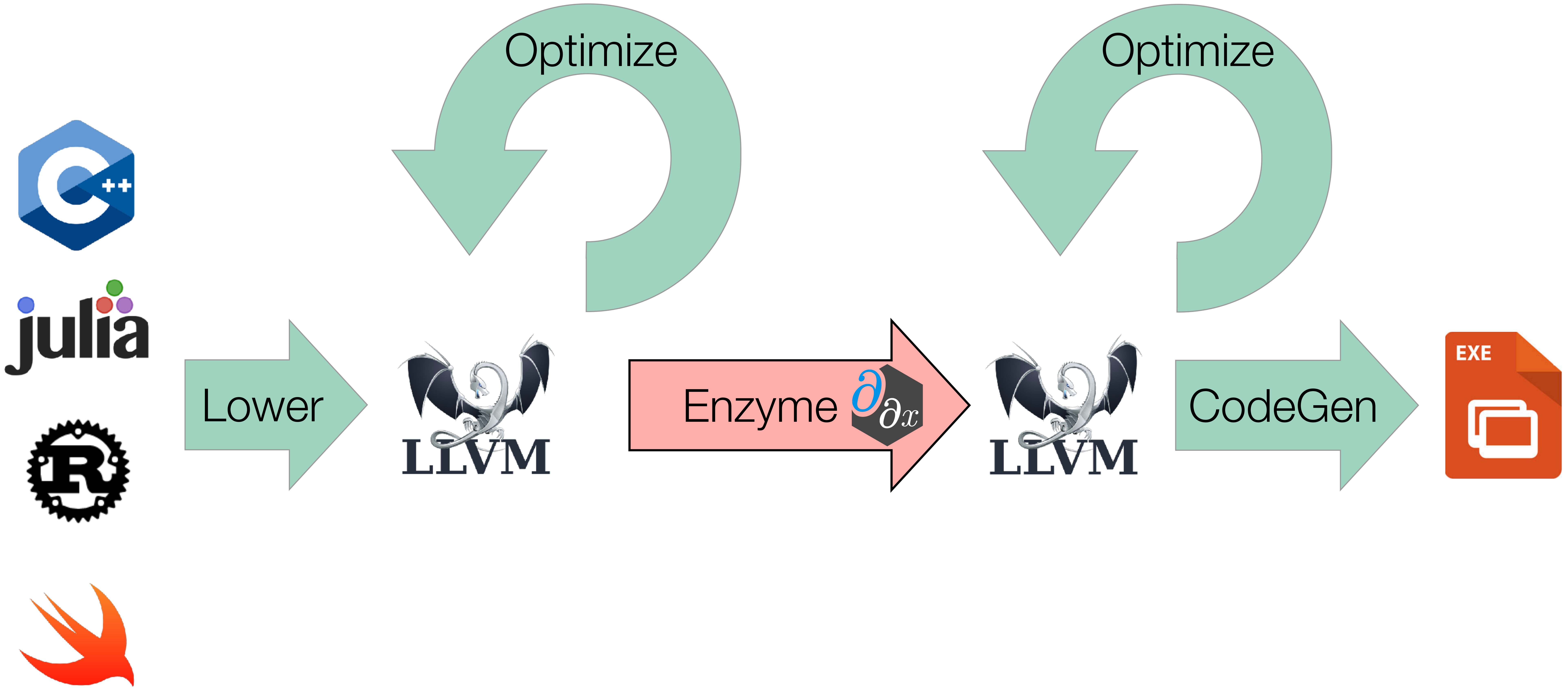
Optimize

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

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

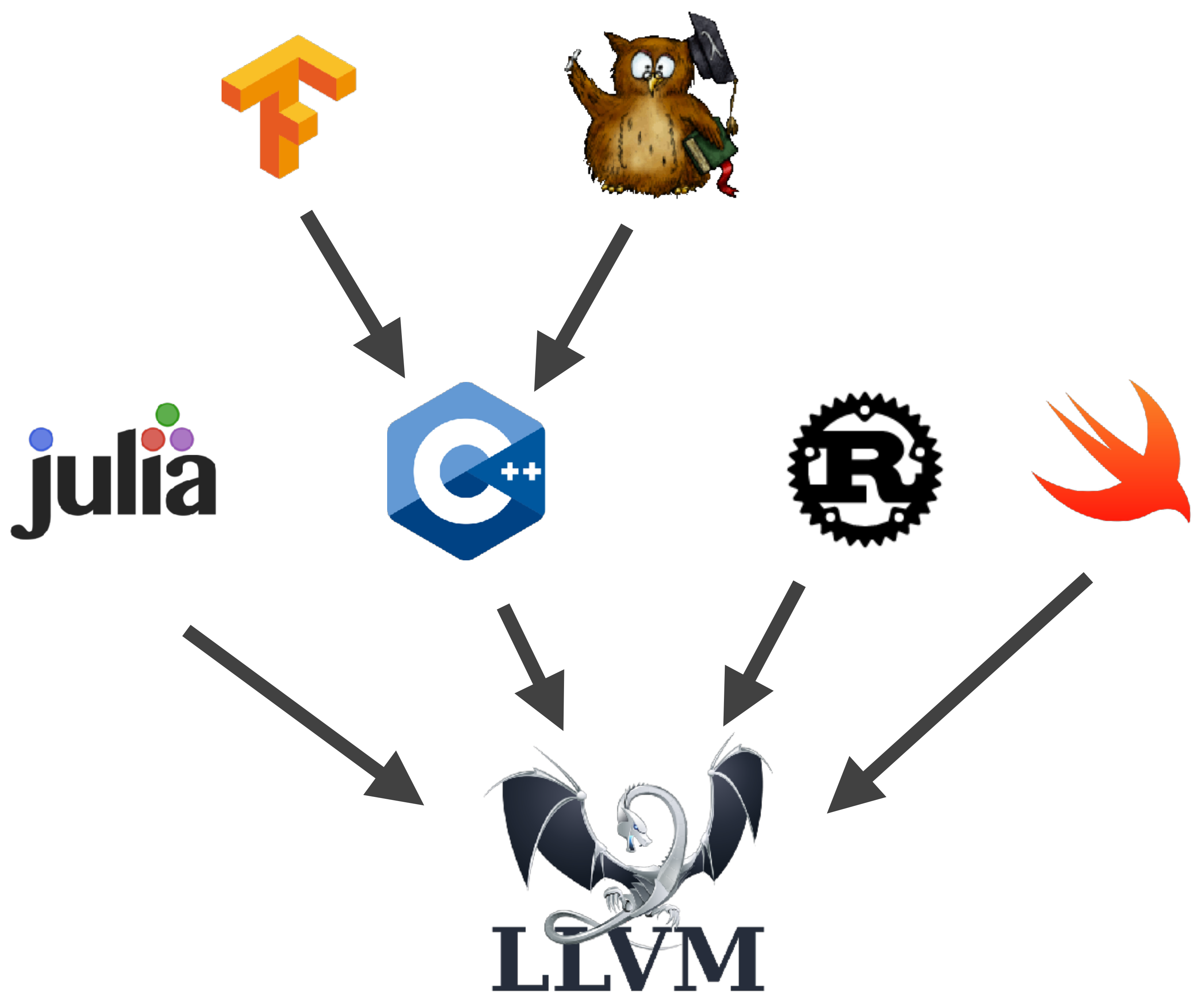
Enzyme Approach

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



Why Does Enzyme Use LLVM?

- Generic low-level compiler infrastructure with many frontends
  - “Cross platform assembly”
- Well-defined semantics
- Large collection of optimizations and analyses



Case Study: ReLU3

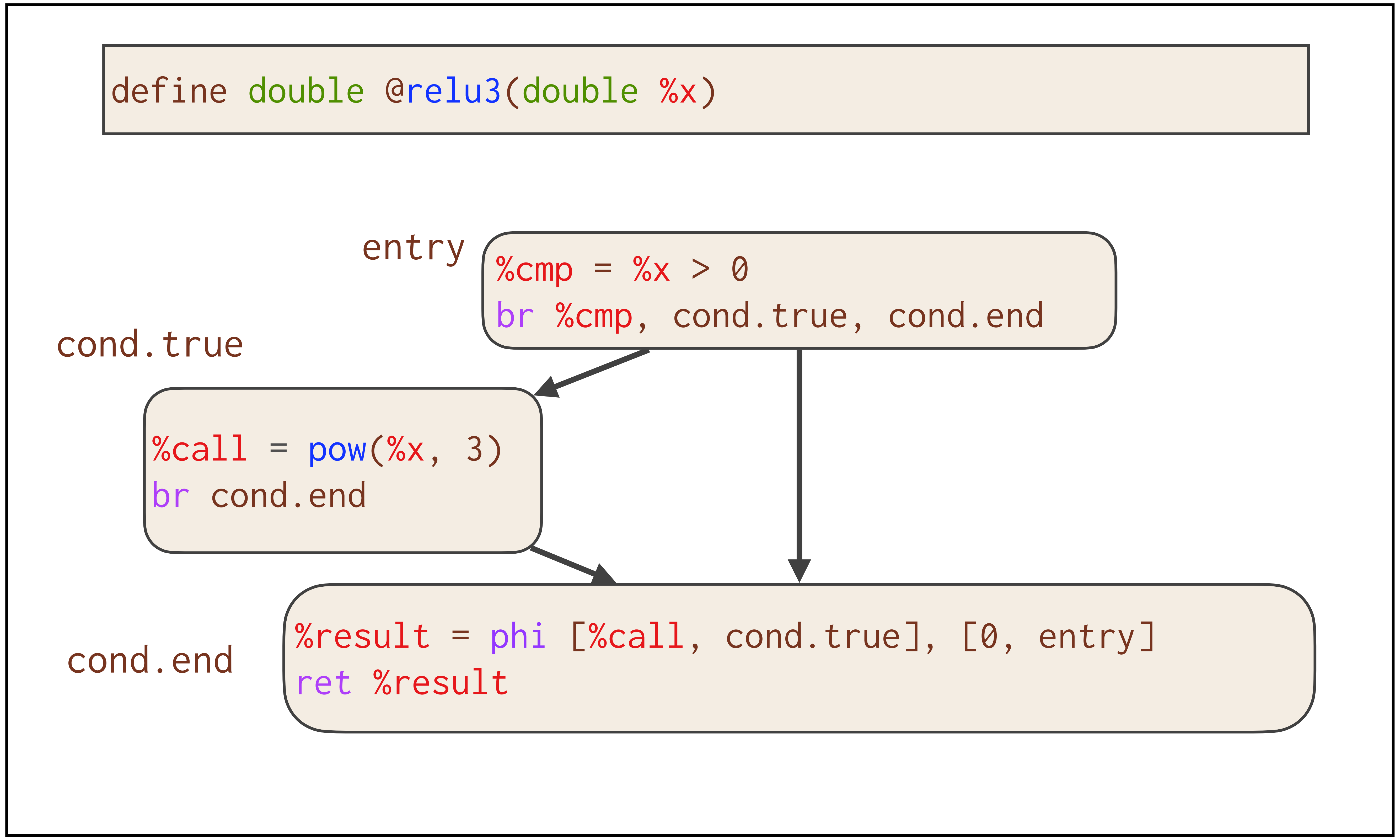
C Source

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

Enzyme Usage

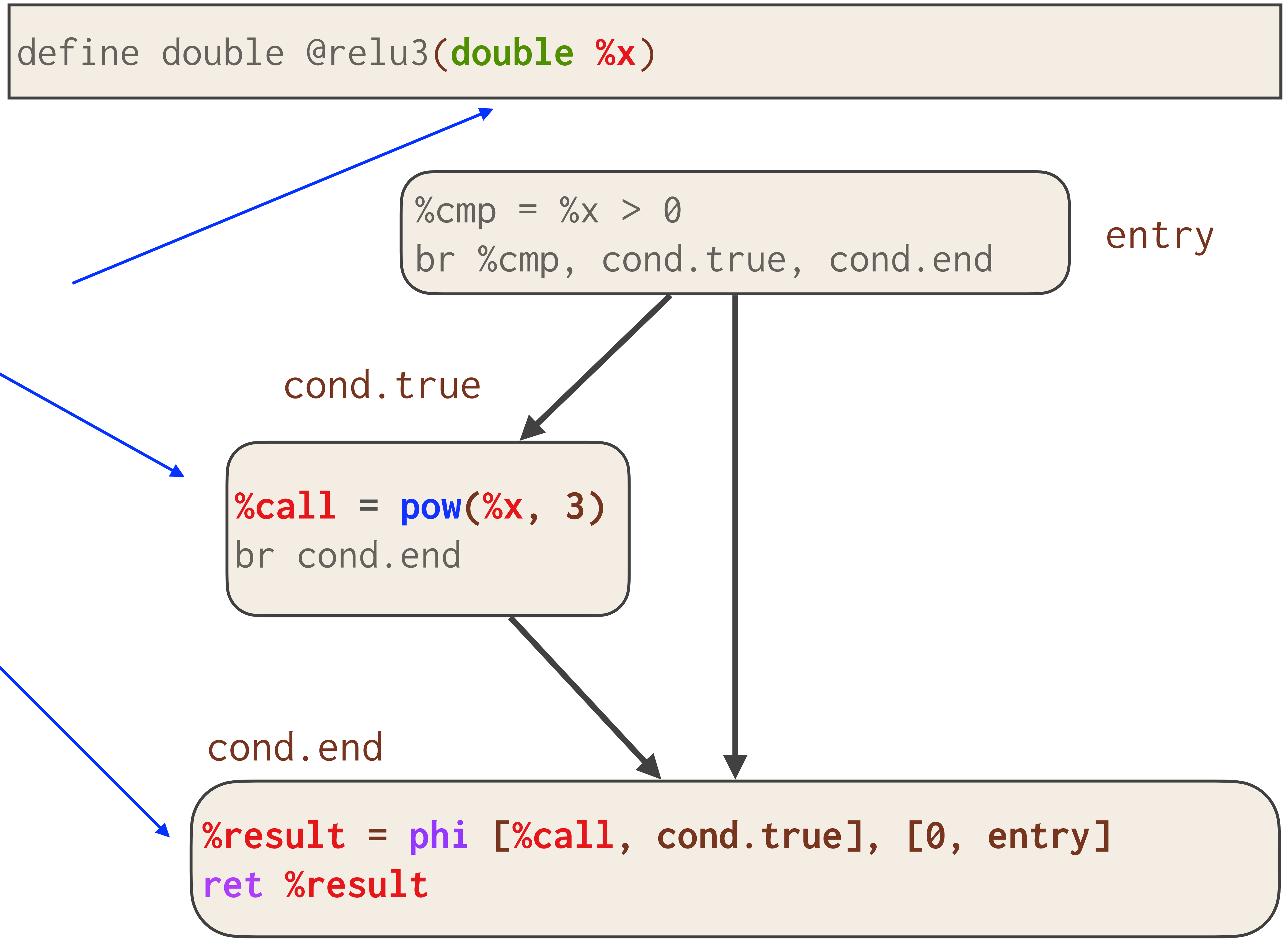
```c
double diffe_relu3(double x) {
  return __enzyme_autodiff(relu3, x);
}
```

LLVM



Case Study: ReLU3

Active Instructions



```
define double @diffe_relu3(double %x, double %differet)
```

entry

```
alloca %result' = 0.0
alloca %call'   = 0.0
alloca %x'      = 0.0
%cmp = %x > 0
br %cmp, cond.true, cond.end
```

Allocate & zero shadow memory for active values

cond.true

```
%call = pow(%x, 3)
br cond.end
```

cond.end

```
%result = phi [%call, cond.true], [0, entry]

; deleted return

%result' = 1.0
br reverse_cond.end
```

Compute adjoints for active instructions

```
define double @diffe_relu3(double %x, double %differet)
```

entry

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cond.end

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%result' = 1.0
br reverse_cond.end
```

reverse_cond.end

```
%tmp_res' = load %result'
%call' += if %x > 0 then %tmp_res' else 0
store %result' = 0.0
br %cmp, reverse_cond.true, reverse_entry
```

reverse_cond.true

```
%df = 3 * pow(%x, 2)
%tmp_call' = load %call
%x' += %df * %tmp_call'
store %call' = 0.0
br reverse_entry
```

reverse_entry

```
%0 = load %x'
ret %0
```

```
define double @diffe_relu3(double %x, double %differet)
```

Compute adjoints for active instructions

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cond.true
```
%call = pow(%x, 3)
br cond.end
```

cond.end
```
%result = phi [%call, cond.true], [0, entry]

; deleted return

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reverse_cond.end
```
%tmp_res' = load %result'
%call' += if %x > 0 then %tmp_res' else 0
store %result' = 0.0
br %cmp, reverse_cond.true, reverse_entry
```

reverse_cond.true
```
%df = 3 * pow(%x, 2)
%tmp_call' = load %call
%x' += %df * %tmp_call'
store %call' = 0.0
br reverse_entry
```

reverse_entry
```
%0 = load %x'
ret %0
```

Post Optimization

```
define double @diffe_relu3(double %x)
```

entry

```
%cmp = %x > 0
br %cmp, reverse_cond.true, reverse_entry
```

reverse_cond.true

```
%3 = 3 * pow(%x, 2)
br reverse_entry
```

reverse_entry

```
%0 = phi [%3, reverse_cond.true], [0, entry]
ret %0
```

Essentially the optimal hand-written gradient!

```
double diffe_relu3(double x) {
  double result;
  if (x > 0)
    result = 3 * pow(x, 2);
  else
    result = 0;
  return result;
}
```

Challenges of Low-Level AD

- Low-level code lacks information necessary to compute adjoints

```
void f(void* dst, void* src) {
  memcpy(dst, src, 8);
}
```

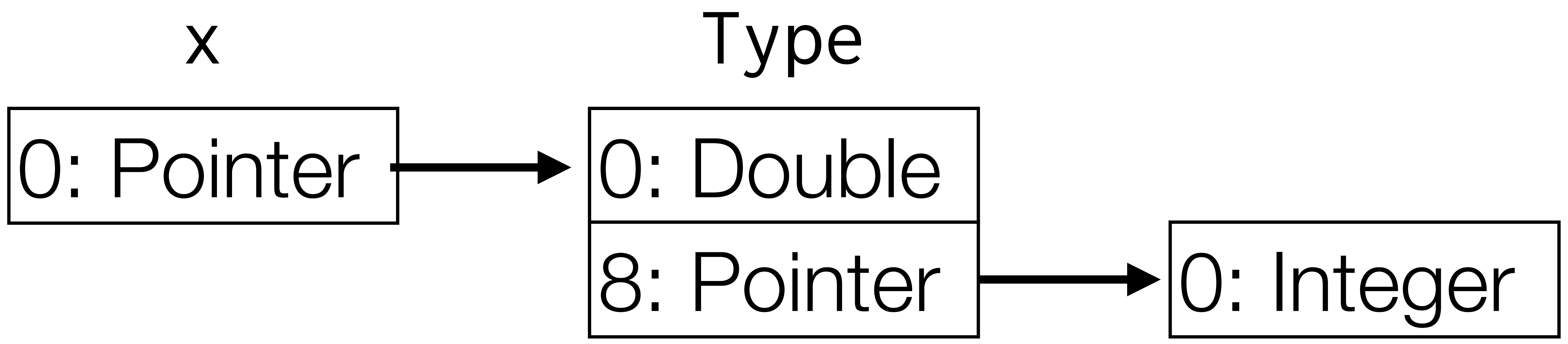
```
void grad_f(double* dst, double* dst',
            double* src, double* src') {
  // Forward Pass
  memcpy(dst, src, 8);

  // Reverse Pass
  src'[0] += dst'[0];
  dst'[0] = 0;
}
```

```
void grad_f(float* dst, float* dst',
            float* src, float* src') {
  // Forward Pass
  memcpy(dst, src, 8);

  // Reverse Pass
  src'[0] += dst'[0];
  dst'[0] = 0;
  src'[1] += dst'[1];
  dst'[1] = 0;
}
```

Challenges of Low-Level AD

- New interprocedural dataflow analysis that detects the underlying type of data
- Each value has a set of memory offsets : type
- Perform series of fixed-point updates through instructions

```
struct Type {
  double;
  int*;
}

x = Type*;
```




```
types(x) = {[0]:Pointer, [0,0]:Double, [0,8]:Pointer, [0,8,0]:Integer}
```

Custom Derivatives & Multisource

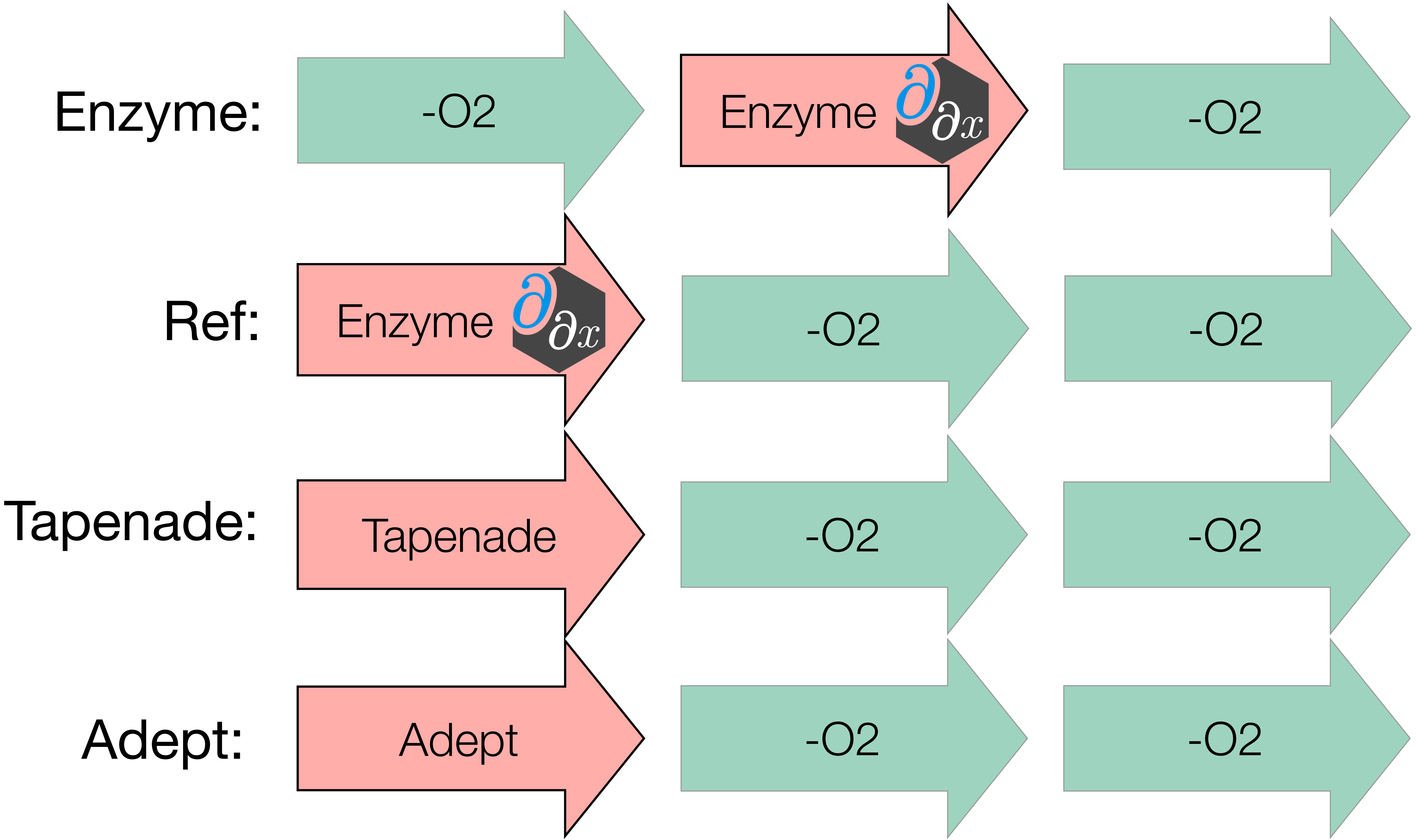
- One can specify custom forward/reverse passes of functions by attaching metadata

```
__attribute__((enzyme("augment", augment_func)))
__attribute__((enzyme("gradient", gradient_func)))
double func(double n);
```

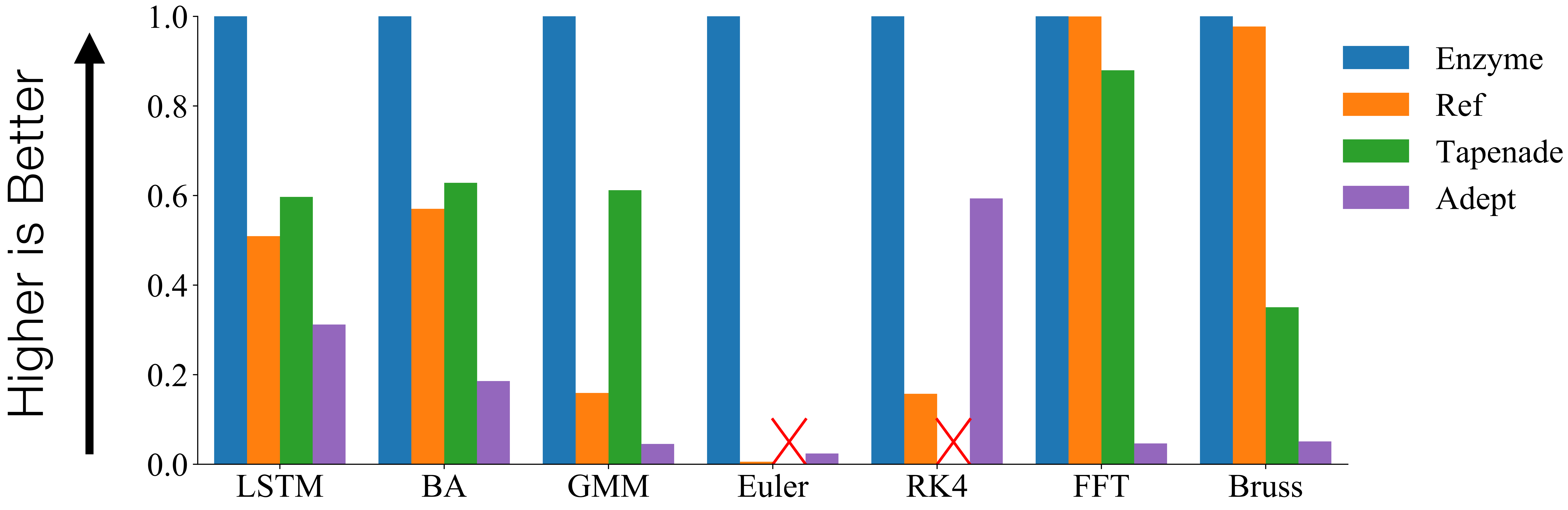
- Enzyme leverages LLVM's link-time optimization (LTO) & "fat libraries" to ensure that LLVM bitcode is available for all potential differentiated functions before AD

Experimental Setup

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



Speedup of Enzyme



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

Enzyme

- Tool for performing reverse-mode AD of statically analyzable LLVM IR
- Differentiates code in a variety of languages (C, C++, Fortran, Julia, Rust, Swift, etc)
- 4.2x speedup over AD before optimization
- State-of-the art performance with existing tools
- PyTorch-Enzyme & TensorFlow-Enzyme lets researchers use foreign code in ML workflow
- Open source (enzyme.mit.edu & join our mailing list)
- Current work: GPU AD, MPI AD

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END

PyTorch-Enzyme & TensorFlow-Enzyme

```python
import torch
from torch_enzyme import enzyme

# Create some initial tensor
inp = …

# Apply foreign function to tensor
out = enzyme("test.c", “f").apply(inp)

# Derive gradient
out.backward()
print(inp.grad)
```

```python
import tensorflow as tf
from tf_enzyme import enzyme

inp = tf.Variable(…)
# Use external C code as a regular TF op

out = enzyme(inp, filename=“test.c",
             function=“f”)

# Results is a TF tensor
out = tf.sigmoid(out)
```

```c
// Input tensor + size, and output tensor
void f(float* inp, size_t n, float* out);

// diffe_dupnoneed specifies not recomputing the output
void diffef(float* inp, float* d_inp, size_t n, float* d_out) {
  __enzyme_autodiff(f, diffe_dup, inp, d_inp, n, diffe_dupnoneed, (float*)0, d_out);
}
```

Compiler Analyses Better Optimize AD

- Existing
- Alias analysis results that prove a function does not write to memory, we can prove that additional function calls do not need to be differentiated since they cannot impact the output
- Don’t cache equivalent values
- Statically allocate caches when a loop’s bounds can be determined in advance

Decomposing the “Tape”

- Performing AD on a function requires data structures to compute
  - All values necessary to compute adjoints are available [cache]
  - Place to store adjoints [shadow memory]
  - Record instructions [we are static]
- Creating these directly in LLVM allows us to explicitly specify their behavior for optimization, unlike approaches that call out to a library
- For more details look in paper

Conventional Wisdom: AD Only Feasible at High-Level

- Automatic Differentiation requires high level semantics to produce gradients
- Lack of high-level information can hinder performance of low-level AD
  - “AD is more effective in high-level compiled languages (e.g. Julia, Swift, Rust, Nim) than traditional ones such as C/C++, Fortran and LLVM IR […]” -Innes[1]

[1] Michael Innes. Don’t Unroll Adjoint: Differentiating SSA-Form Programs. arXiv preprint arXiv:1810.07951, 2018

Differentiation Is Key To Machine Learning

```cpp
// C++ nbody simulator

void step(std::array<Planet> bodies, double dt) {
  vec3 acc[bodies.size()];
  for (size_t i=0; i<bodies.size(); i++) {
    acc[i] = vec3(0, 0, 0);
    for (size_t j=0; j<bodies.size(); j++) {
      if (i == j) continue;
      acc[i] += force(bodies[i], bodies[j]) /
                         bodies[i].mass;
    }
  }
  for (size_t i=0; i<bodies.size(); i++) {
    bodies[i].vel += acc[i] * dt;
    bodies[i].pos += bodies[i].vel * dt;
  }
}
```

```python
// PyTorch rewrite of nbody simulator
import torch

def step(bodies, dt):
  acc = []
  for i in range(len(bodies)):
    acc.push(torch.zeros([3]))
    for j in range(len(bodies)):
      if i == j: continue
      acc[i] += force(bodies[i], bodies[j]) /
                         bodies[i].mass

  for i, body in enumerate(bodies):
    body.vel += acc[i] * dt
    body.pos += body.vel * dt
```

- Hinders application of ML to new domains
- Synthesizing gradients aims to close this gap

Activity Analysis

- Determines what instructions could impact derivative computation
- Avoids taking meaningless or unnecessary derivatives (e.g. d/dx cpuid)
- Instruction is active iff it can propagate a differential value to its return or memory
- Build off of alias analysis & type analysis
  - E.g. all read-only function that returns an integer are inactive since they cannot propagate adjoints through the return or to any memory location

Enzyme Overturns Conventional Wisdom

- As fast or faster than state-of-the-art tools
  - Running after optimization enables a ***4.2x speedup***
- Necessary semantics for AD derived at low-level (with potential cooperation of frontend)