Enzyme: High-Performance Automatic Differentiation

William S. Moses Valentin Churavy

Argonne NATIONAL LABORATORY

wmoses@mit.edu
CESMIX Group

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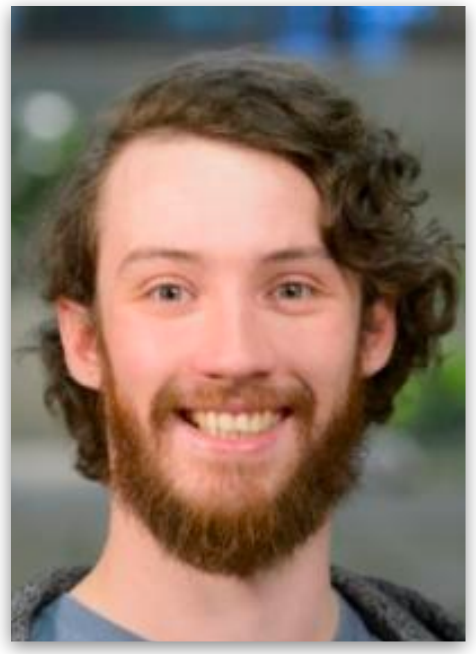
William S. Moses

Valentin Churavy

Ludger Paehler



Johannes Doerfert

Jan Hückelheim

Sri Hari Krishna Narayanan

Michel Schanen

Paul Hovland

Differentiation Is Key To Machine Learning And Science

- 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

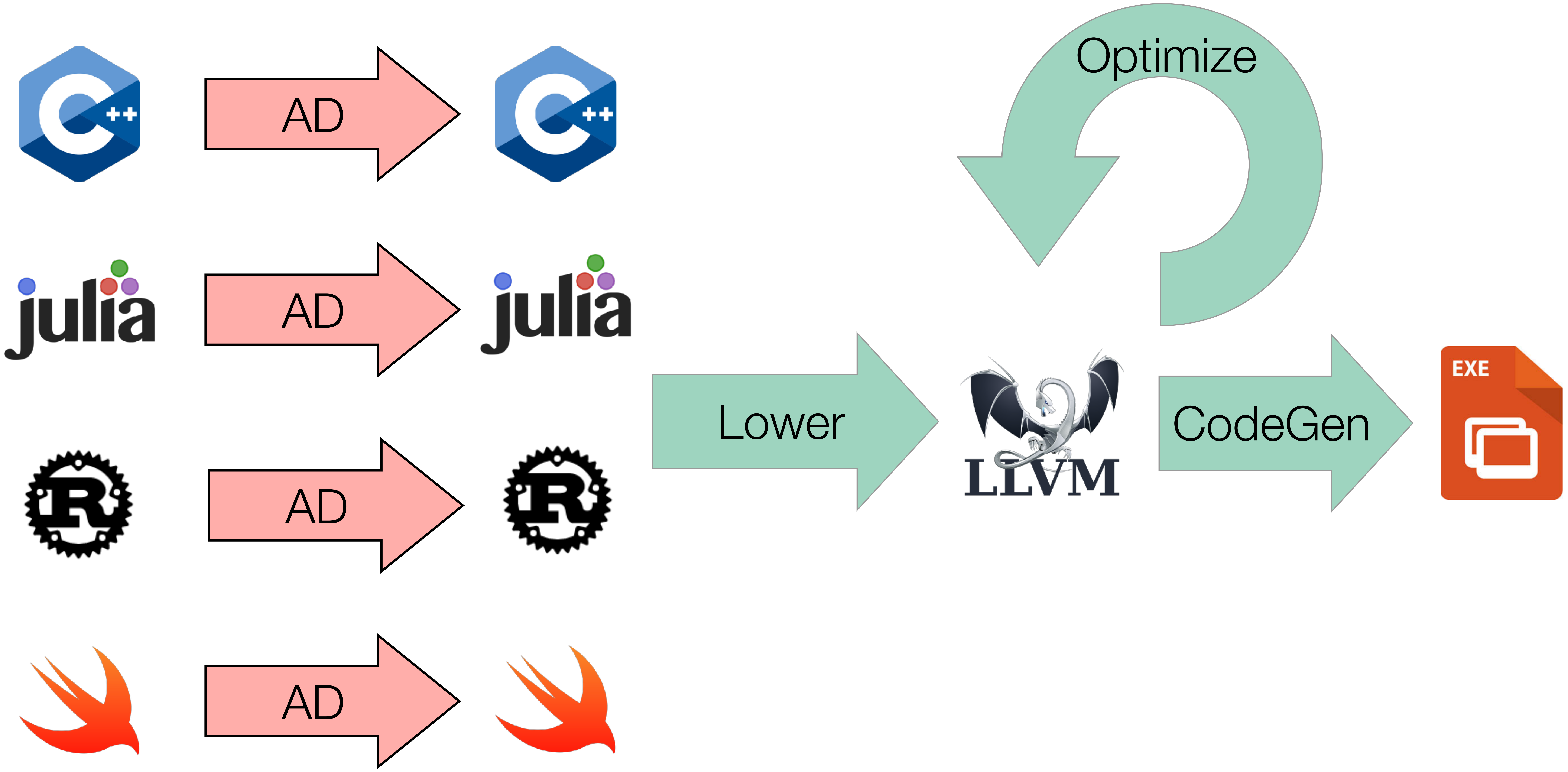
Existing AD Approaches

- Differentiable DSL (TensorFlow, PyTorch, DiffTaichi)
  - Provide a new language 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
- 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

```
//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

$O(n)$

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

AD

$O(n)$

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

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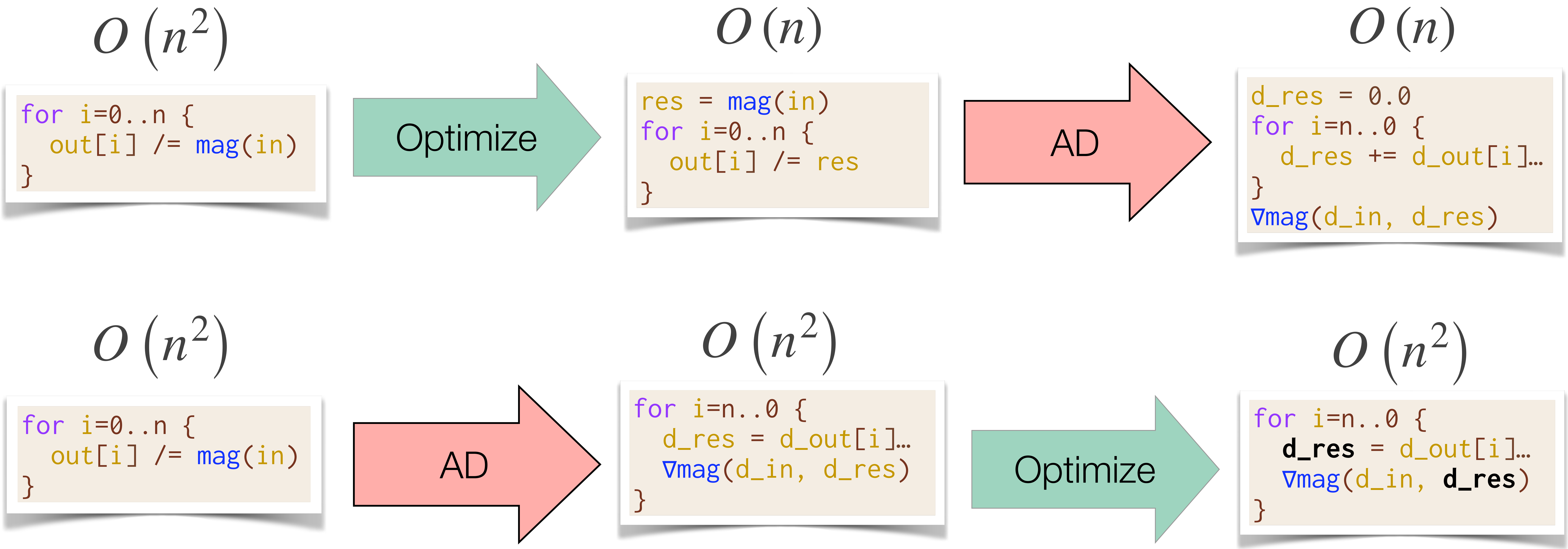
```
for i=n..0 {
  d_res = d_out[i]…
  ∇mag(d_in, d_res)
}
```

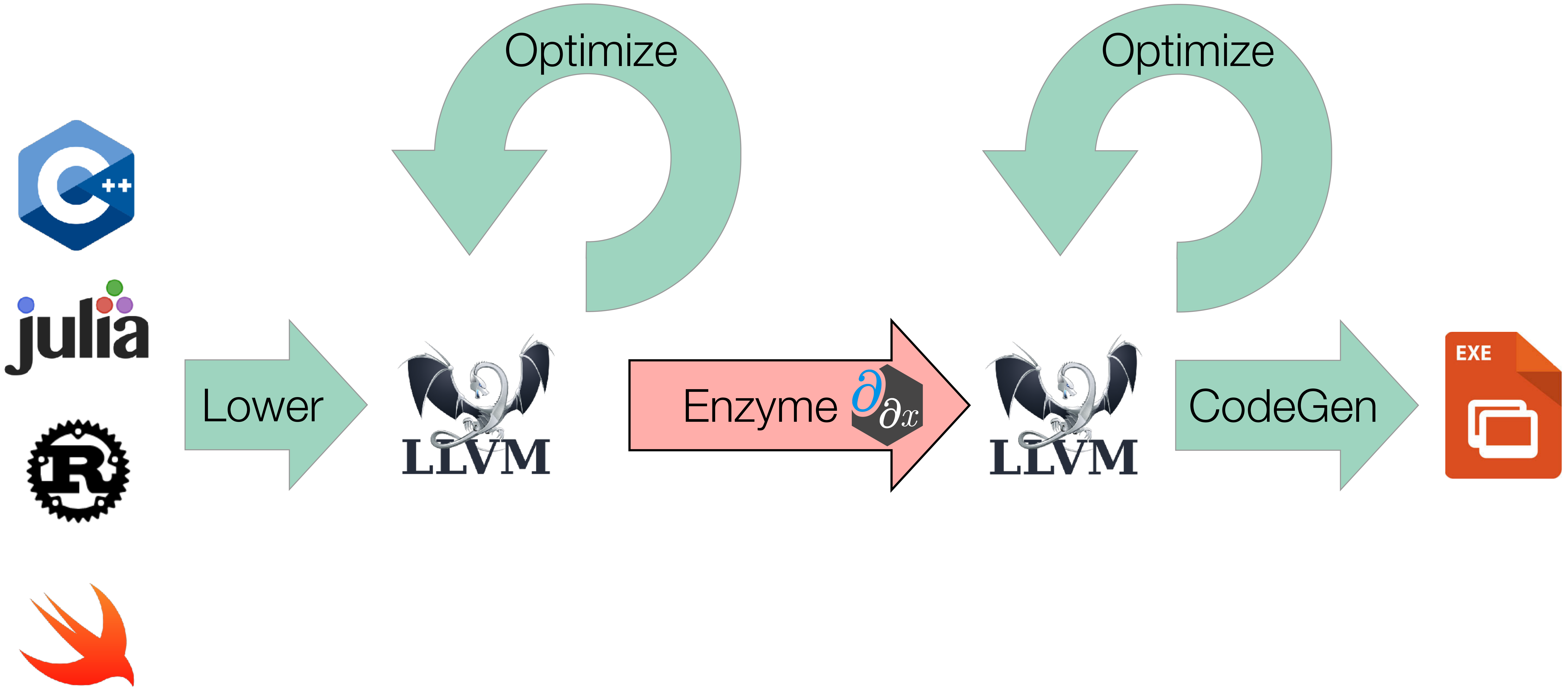
Optimization & Automatic Differentiation

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



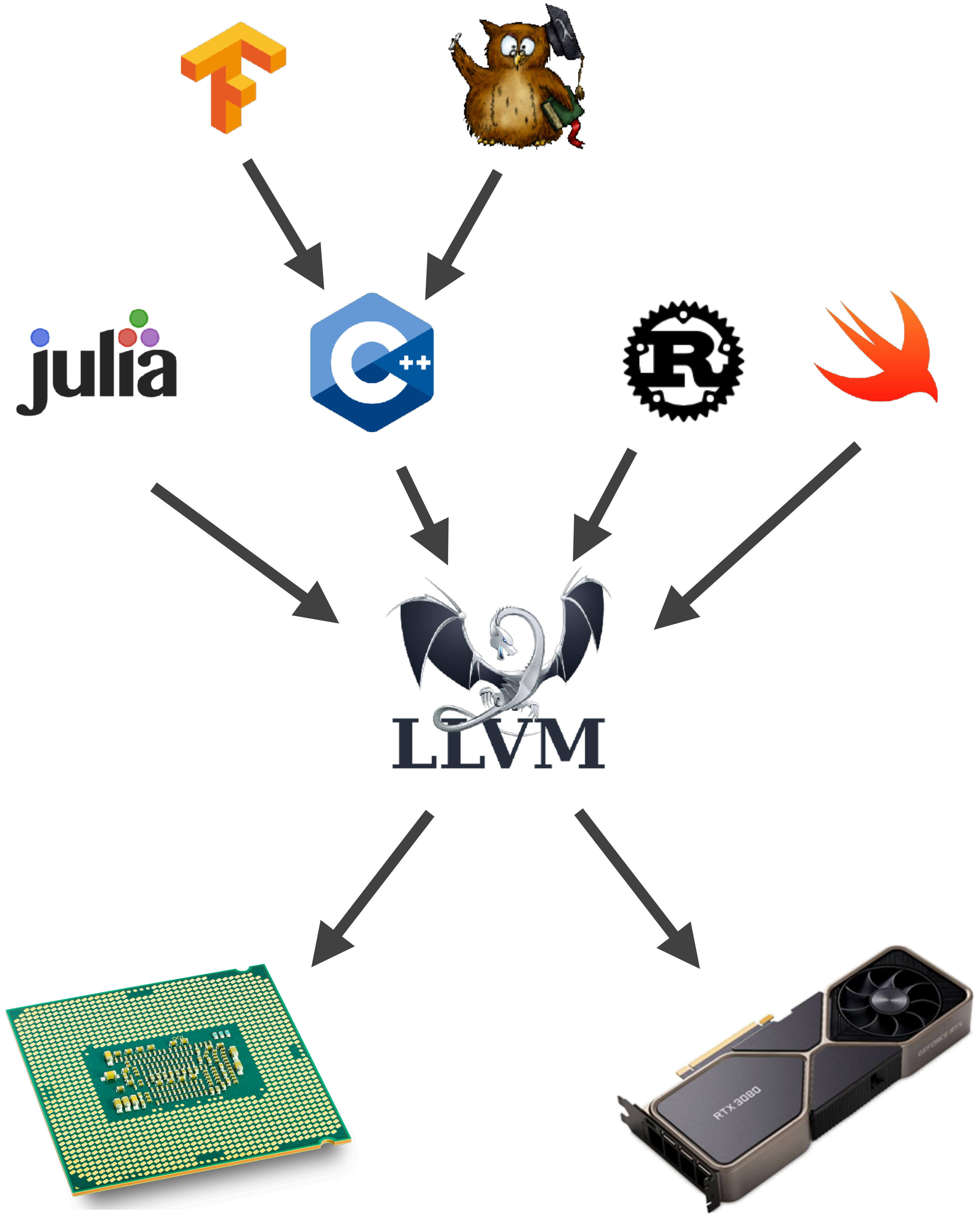
Enzyme Approach

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”
    - Many backends (CPU, CUDA, AMDGPU, etc)
- Well-defined semantics
- Large collection of optimizations and analyses

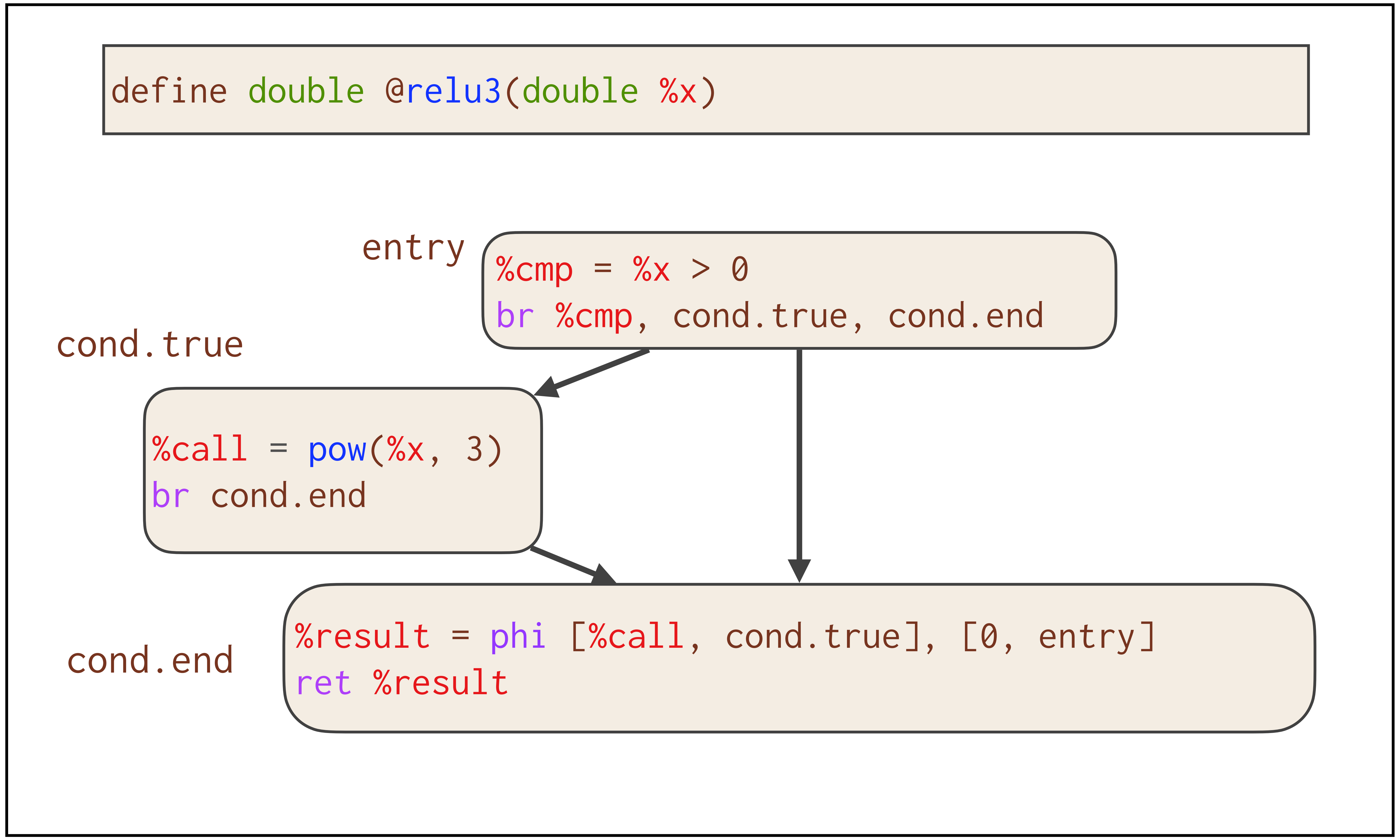


Case Study: ReLU3

C Source

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

LLVM

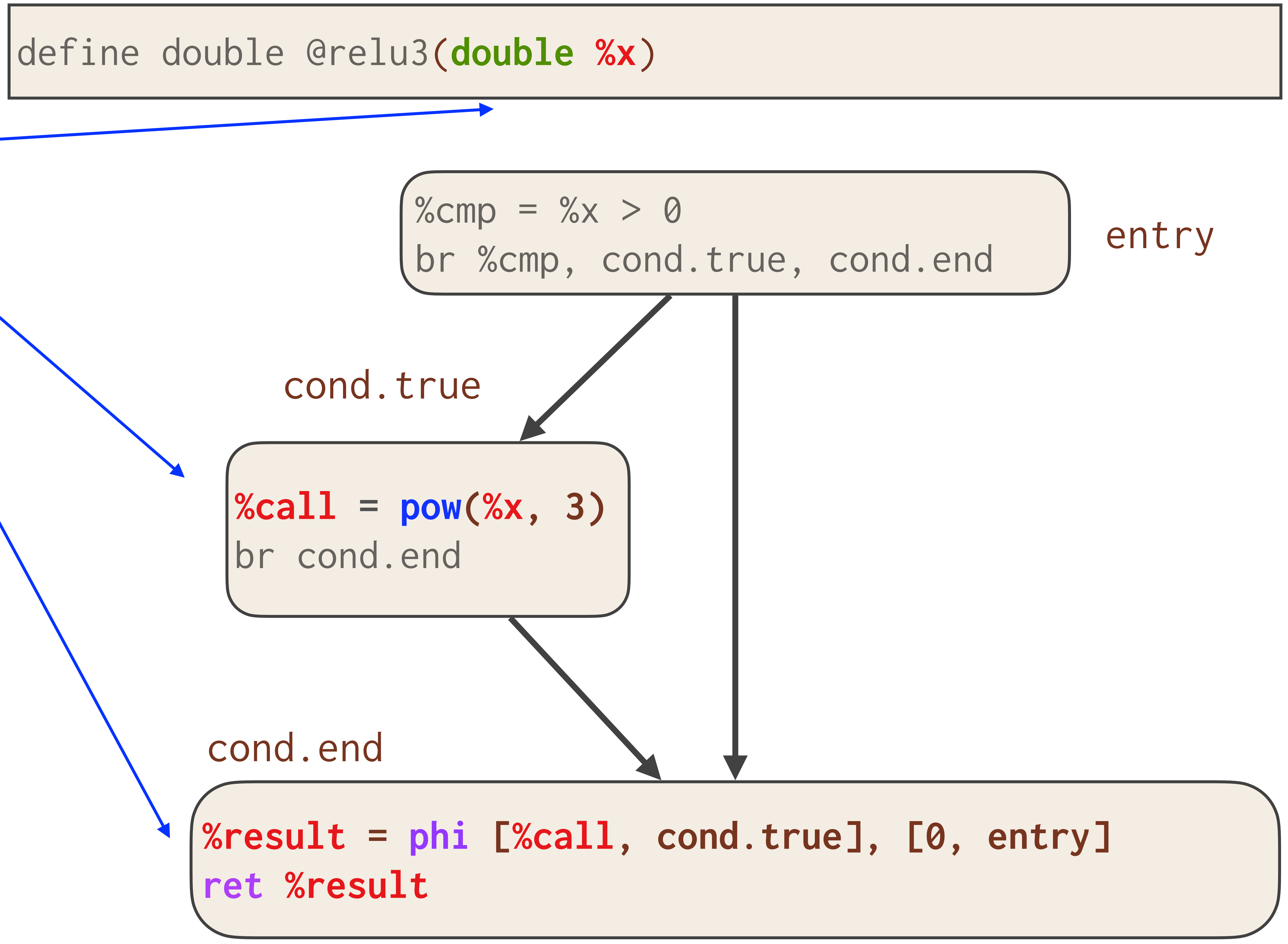


Enzyme Usage

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

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
```

cond.true

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

cond.end

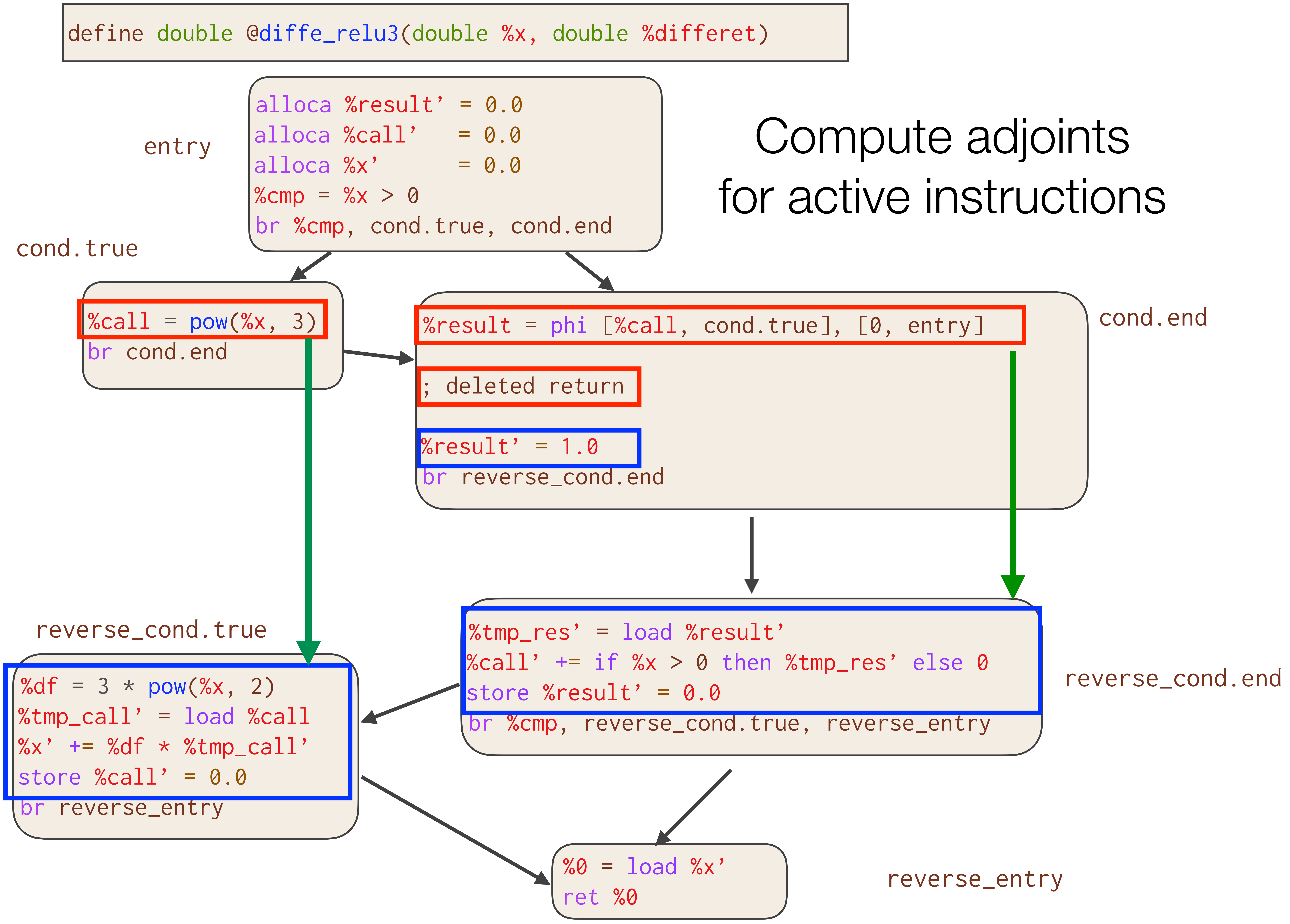
```
%result = phi [%call, cond.true], [0, entry]

; deleted return

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

Allocate & zero shadow memory for active values

Compute adjoints for active instructions



Compute adjoints for active instructions

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br %cmp, cond.true, cond.end
```

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
```

reverse_cond.end

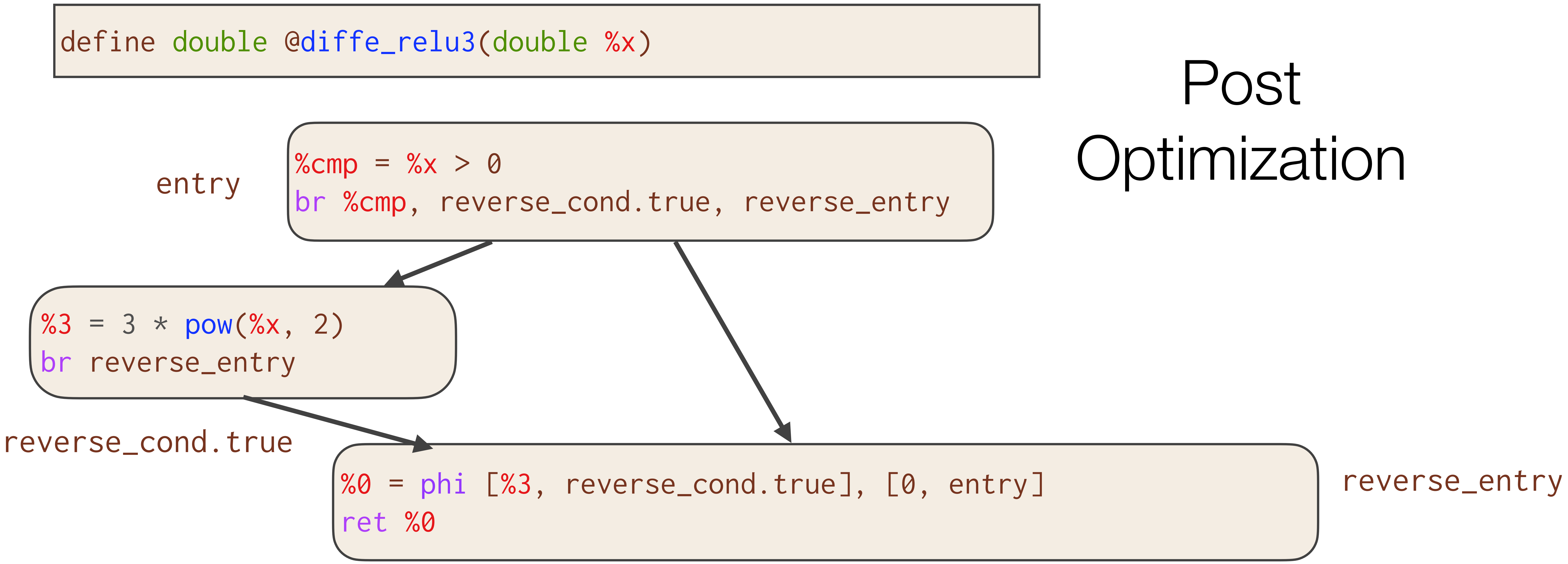
```
%tmp_res' = load %result'
%call' += if %x > 0 then %tmp_res' else 0
store %result' = 0.0
br %cmp, reverse_cond.true, reverse_entry
```

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

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);

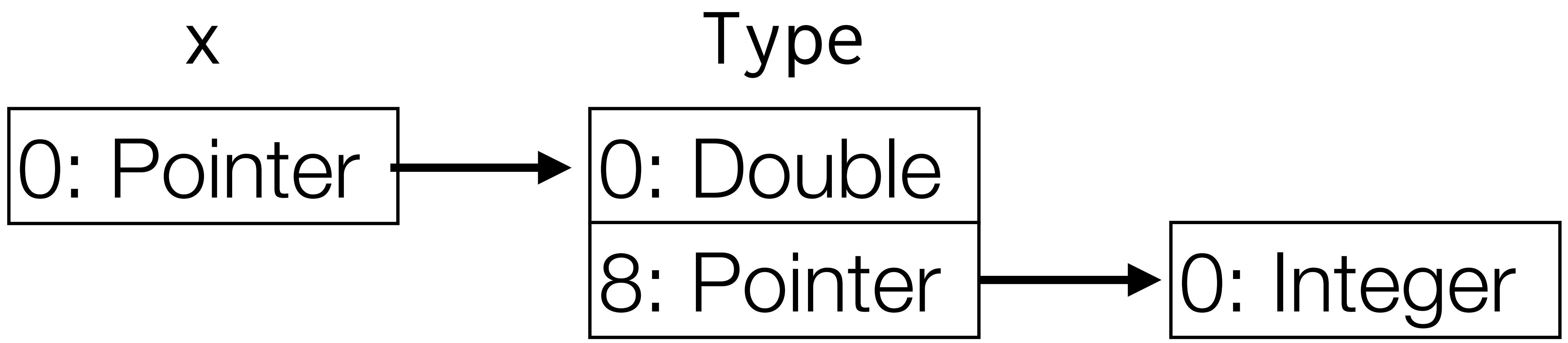
  // Reverse Pass
  src'[0] += dst'[0];
  dst'[0] = 0;
  src'[1] += dst'[1];
  dst'[1] = 0;
}
```

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*;
}

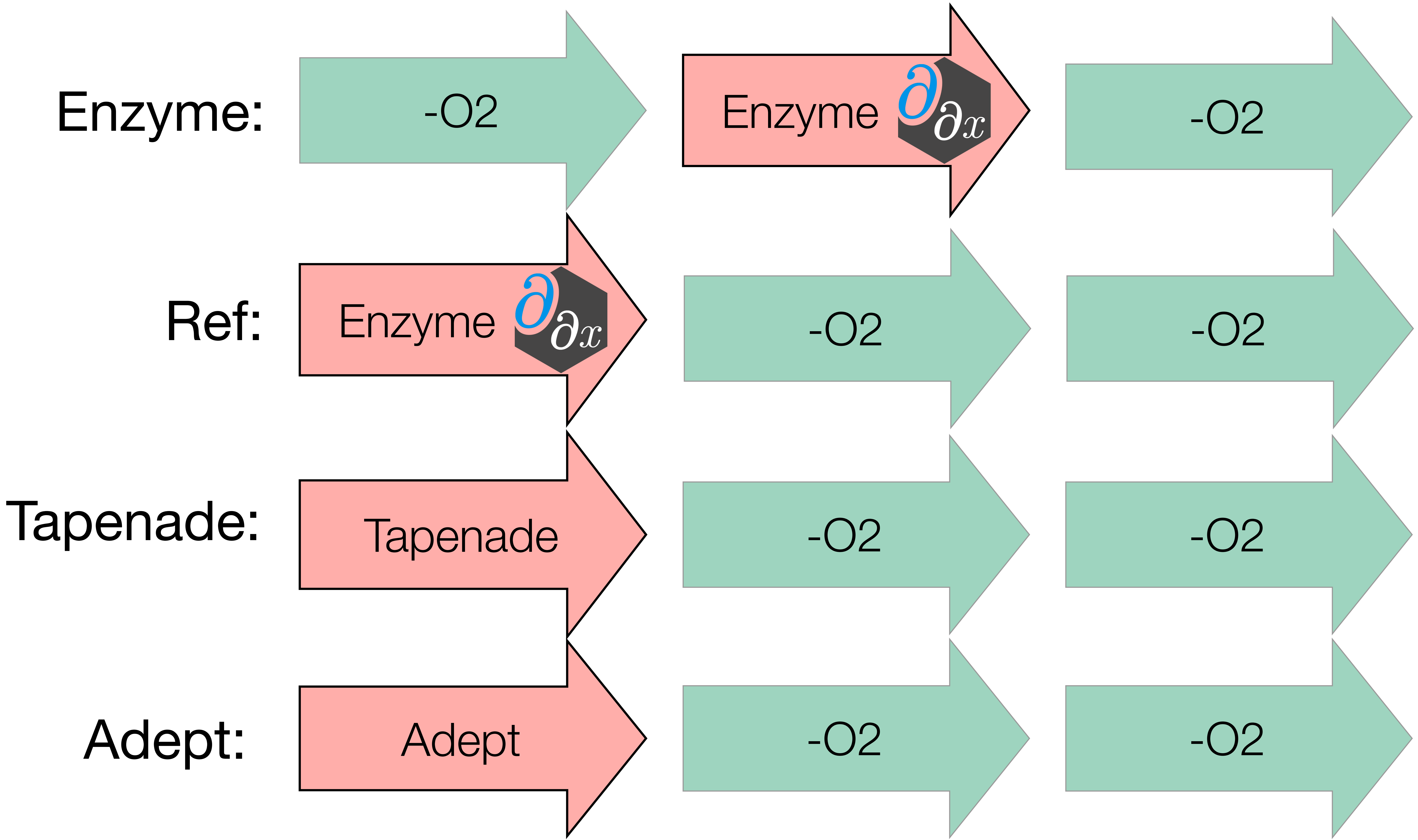
x = Type*;
```



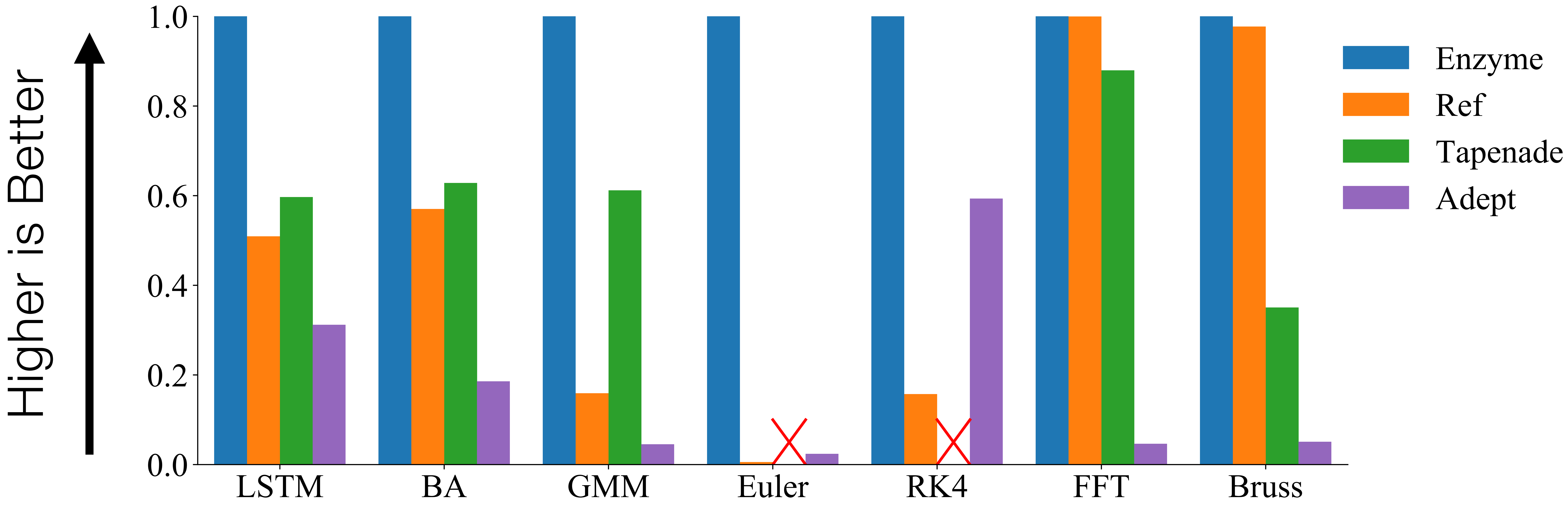

```
types(x) = {[0]:Pointer, [0,0]:Double, [0,8]:Pointer, [0,8,0]:Integer}
```

Experimental Setup

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



Speedup of Enzyme



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

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

# Create some initial tensor
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);
}
```

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 on CPU
- State-of-the art performance with existing tools
- First general purpose reverse-mode GPU AD
- Novel GPU and AD-specific optimizations improve runtime by several orders of magnitude
- PyTorch-Enzyme & TensorFlow-Enzyme lets researchers use foreign code in ML workflow

Enzyme

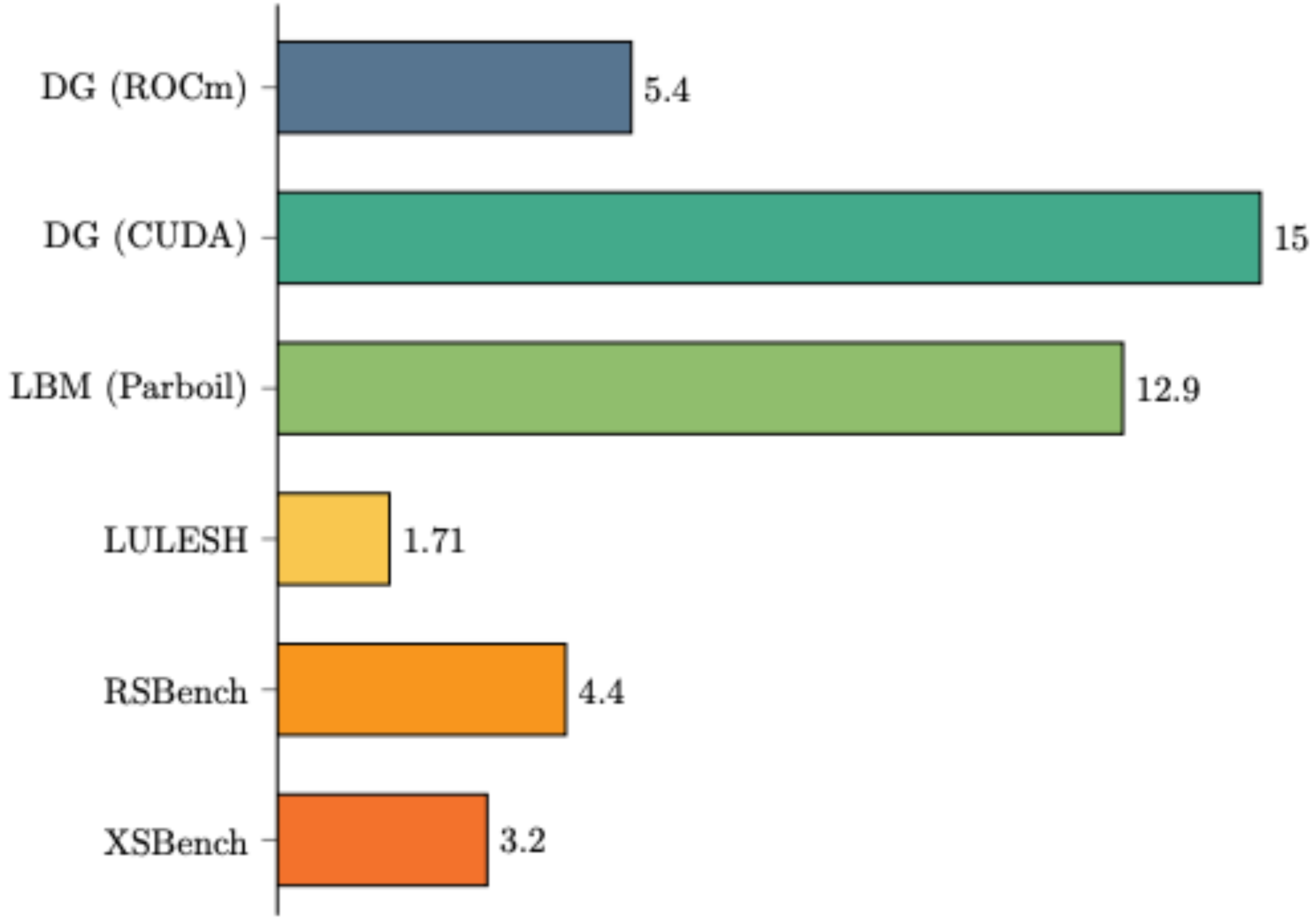
Enzyme on the GPU

- Care must be taken to both ensure correctness and maintain parallelism.
- GPU programs have much lower memory limits. Performance is highly dependent on the number of memory transfers.
- Without first running optimizations reverse-mode AD of large kernels is intractable (OOM).
- Novel GPU and AD-specific optimizations can make a difference of several orders of magnitude when computing gradients.

Test	Overhead
Forward	1
AD, Optimized	4.4
AD, No CacheLICM	343.7
AD, Bad Recompute Heuristic	1275.6
AD, No Inlining	6372.2
AD, No PreOptimization	OOM

GPU Gradient Overhead

- Evaluation of both original code and derivative of all inputs (forward or numeric differentiation requires 1 evaluation per input):
  - DG: discontinuous-galerkin (DG) volume 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)



CUDA Automatic Differentiation

- Enzyme enables differentiation of CPU programs without rewriting them in a DSL.
- Similarly, GPU programs cannot currently be differentiated without being rewritten in a differentiable language (e.g. PyTorch).
- Enzyme enables reverse-mode AD of general existing GPU programs by:
  - Resolving potential data race issues
  - Differentiating parallel control (syncthreads)
  - Differentiating CUDA intrinsics (e.g. threadIdx.x /llvm.nvvm.read.ptx.sreg.tid.x)
  - Handling shared memory

Challenges of Parallel AD

- Benign read race in forward pass => Write race in reverse pass (undefined behavior)

```
void set(double* ar, double val) {

  parallel_for(int i=0; i<10; i++)
    ar[i] = val;
}
```

Read Race

Write Race

```
double gradient_set(double* ar, double val) {
  double d_val = 0.0;

  parallel_for(int i=0; i<10; i++)
    ar[i] = val;

  parallel_for(int i=0; i<10; i++) {
    d_val += d_ar[i];
    d_ar[i] = 0.0;
  }

  return d_val;
}
```

Parallel Memory Detection

Thread-local memory

- Non-atomic load/store

```
__device__
void f(…) {

  // Thread-local var
  double y;

  …

  d_y += val;
}
```

Same memory location across all threads

- Parallel Reduction

```
// Same var for all threads
double y;

__device__
void f(…) {

  …

  reduce_add(&d_y, val);
}
```

Others [always legal fallback]

- Atomic increment

```
__device__
// Unknown thread-aliasing
void f(double* y) {

  …

  atomic { d_y += val; }
}
```

CUDA Automatic Differentiation

```
%res = load %ptr
```

```
%tmp = load %d_res
store %d_res = 0
atomic %d_ptr += %tmp
```

```
store %ptr = %val
```

```
%tmp = load %d_ptr
store %d_ptr = 0
load/store %d_val += %tmp
```

- Shadow Registers `%d_res` and `%d_val` are ***thread-local*** as they shadow thread-local registers.
  - No risk of races and no special handling required.
- Both `%ptr` and shadow `%d_ptr` might be raced upon and require analysis.

Differentiation of SyncThreads

- Sync is only necessary if A and B may write to the same memory
- Four cases for what sync could represent:

  1. All stores in A must complete prior to a load in B
  2. All loads in A must complete prior to a store in B
  3. All stores in A must complete prior to a stores in B [clobber]
  4. All load in A must complete prior to a load in B [unnecessary sync]

```
codeA();

sync_threads;

codeB();
```

CUDA Performance Improvements

- Enzyme may need to cache values from the forward pass for later use in a reverse pass computation
  - When a value needs caching, Enzyme allocates memory (via malloc inside kernel)
  - Potentially quite slow
  - May overwhelm the amount of GPU heap memory

```
void f(float* in, float* out) {
  float tmp;
  for (int i=0; i<N; i++) {
    tmp = compute(in, i);
    out[i] = tmp * tmp + …;
  }
}
```

Value `tmp` is overwritten every iteration and must be cached

```
void diffe_f(float* in, float* out) {
  float* tmp_cache = malloc(…);

  for (int i=0; i<N; i++) {
    …
    tmp_cache[i] = tmp;
  }

  for (int i=N-1; i>=0; i--) {
    …
    d_tmp[0] = 2 * tmp_cache[0] * d_out[i];
    d_compute(…);
  }

  free(tmp_cache);
}
```

Case 1: Store, Sync, Load

```
codeA(); // store %ptr

sync_threads;

codeB(); // load %ptr

…

diffe_codeB(); // atomicAdd %d_ptr

sync_threads;

diffe_codeA(); // load %d_ptr
               // store %d_ptr = 0
```

Correct

- Load of `d_ptr` must happen after all atomicAdds have completed

Case 2: Load, Sync, Store

```
codeA(); // load %ptr

sync_threads;

codeB(); // store %ptr

…

diffe_codeB(); // load %d_ptr
               // store %d_ptr = 0

sync_threads;

diffe_codeA(); // atomicAdd %d_ptr
```

Correct

- All of the stores of `d_ptr` will complete prior to any atomicAdds

No cross-thread race here since that's equivalent to a write race in B

Case 3: Store, Sync, Store

```
codeA(); // store %ptr

sync_threads;

codeB(); // store %ptr

…

diffe_codeB(); // load %d_ptr
               // store %d_ptr = 0

sync_threads;

diffe_codeA(); // load %d_ptr
               // store %d_ptr = 0
```

✔ Correct

- All stores to `d_ptr` in diffe_B will complete prior to diffe_A, ensuring only the clobbering store has its derivative incremented

CUDA Automatic Differentiation

- Most CUDA intrinsics [e.g. threadIdx.x] are inactive and recomputable and thus are incorporated into Enzyme without any special handling

- Derivative of syncthreads is a syncthreads at the corresponding place in reverse pass

- Shared memory is handled by making a second shared memory allocation to act as the shadow for any potentially active uses

CUDA Example

```
__device__ void inner(float* a, float* x, float* y) {
  y[threadIdx.x] = a[0] * x[threadIdx.x];
}
__device__ void __enzyme_autodiff(void*, …);

__global__ void daxpy(float* a, float* da, float* x, float* dx, float* y, float* dy) {
  __enzyme_autodiff((void*)inner, a, da, x, dx, y, dy);
}
```

```
__device__ void diffe_inner(float* a, float* da, float* x, float* dx, float* y, float* dy) {
  y[threadIdx.x] = a[0] * x[threadIdx.x];

  float dy = dy[threadIdx.x];
  dy[threadIdx.x] = 0.0f;

  float dx_tmp = a[0] * dy;
  atomic { dx[threadIdx.x] += dx_tmp; }

  float da_tmp = x[threadIdx.x] * dy;
  atomic { da[0] += da_tmp; }
}
```

CUDA Performance Improvements

- Introduce optimizations to reduce the use of memory
  - Alias Analysis to determine legality of recomputing an instruction
    - More aggressive alias analysis properties of syncthreads
  - Don’t cache unnecessary values
    - Move cache outside of loops when possible
  - Heap-to-stack [and to register]
  - Don’t cache memory itself acting as a cache [such as shared memory]

CUDA Evaluation

	Forward Pass	Gradient No Opt	+ Standard Opts	+ Cache Opts
XSBench-CUDA	1.0s	OOM	20.1s	5.0s
RSBench-CUDA	1.9s	OOM	>540s	7.8s

Evaluated on a 2080 Super FE

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- State-of-the art performance with existing tools
- Differentiate GPU kernels
- Open Source (enzyme.mit.edu / github.com/wsmoses/Enzyme)
- PyTorch-Enzyme & TensorFlow-Enzyme imports foreign code in ML workflow

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- The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the United States Air Force or the U.S. Government.

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END

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

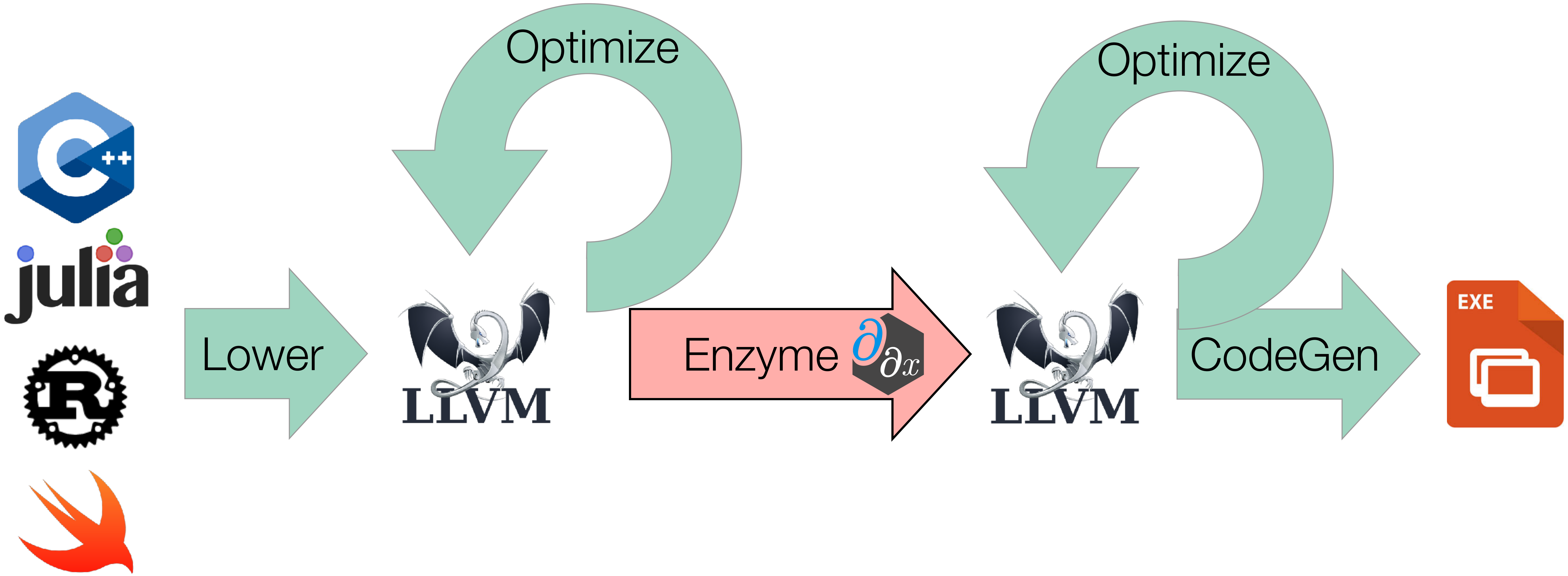
```
// C++ nbody simulator

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;
  }
}
```

```
// 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

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)



Parallel Memory Detection

- Thread-local memory
    - Non-atomic load/store
- Same memory location across all threads
    - Parallel Reduction
- Others [always legal fallback]
    - Atomic increment

```
%tmp = load %d_res
store %d_res = 0
atomic %d_ptr += %tmp
```

Differentiation of SyncThreads

Case 3 [write sync write]

```
codeA(); // store %ptr

sync_threads;

codeB(); // store %ptr

…

diffe_codeB(); // load %d_ptr
               // store %d_ptr = 0

sync_threads;

diffe_codeA(); // load %d_ptr
               // store %d_ptr = 0
```

All uses of stores to d_ptr in diffe_B will correctly complete prior to diffe_A

Case 4 [read sync read]

```
codeA(); // load %ptr

sync_threads;

codeB(); // load %ptr

…

diffe_codeB(); // atomicAdd %d_ptr

sync_threads;

diffe_codeA(); // atomicAdd %d_ptr
```

Original and differential sync unnecessary and legal to include

CUDA Performance Improvements

- Introduce optimizations to reduce the use of memory
  - Alias Analysis to determine legality of recomputing an instruction
    - More aggressive alias analysis properties of syncthreads
  - Don’t cache unnecessary values
    - Move cache outside of loops when possible
  - Heap-to-stack [and to register]
  - Don’t cache memory itself acting as a cache [such as shared memory]
  - PHI Node unwrapping

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