EnzymeMLIR:
Combining Differentiation with High-Level Optimization

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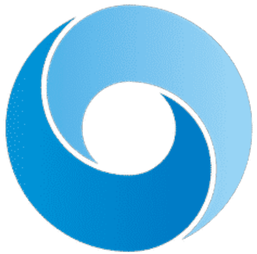
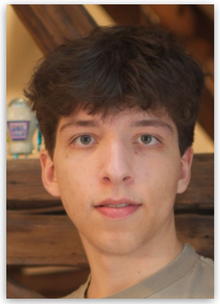


Paul Berg

Avik Pal



Jules Merckx

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Martin Eppert

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Alex Zinenko

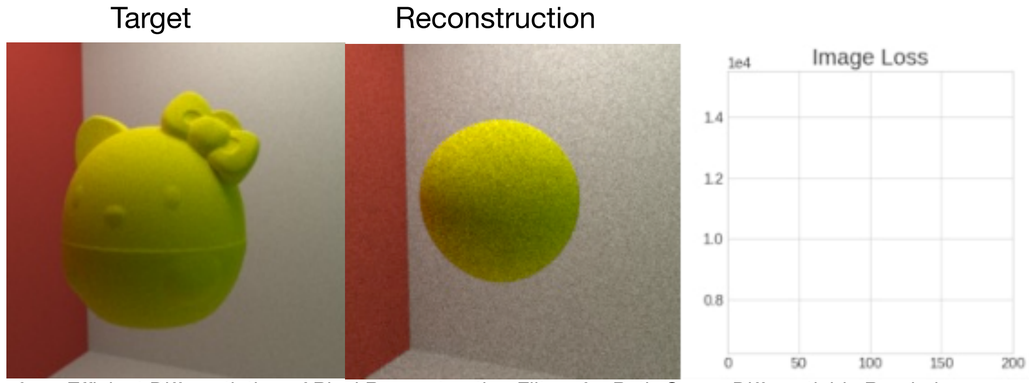
Outline

- Compiler-Based Differentiation (Enzyme-LLVM)  
- What is MLIR? 
- Compiler-Based Differentiation With High-Level Operations (EnzymeMLIR)  
- Some Fun Results

Differentiation: Connecting Science and AI

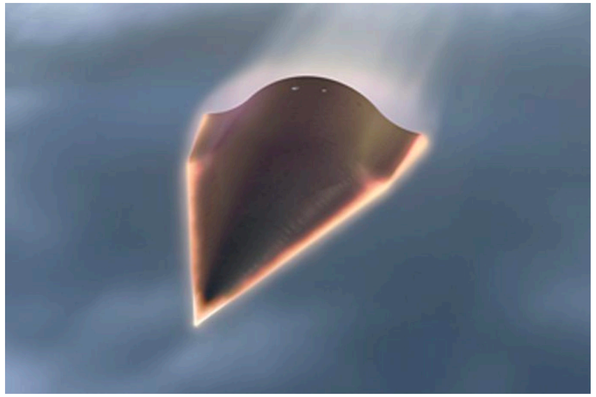
Derivatives are key to science + ML

- *Scientific Computing*: UQ, Differential Equation, Error Analysis
- *Machine Learning*: Back-Propagation, Bayesian Inference

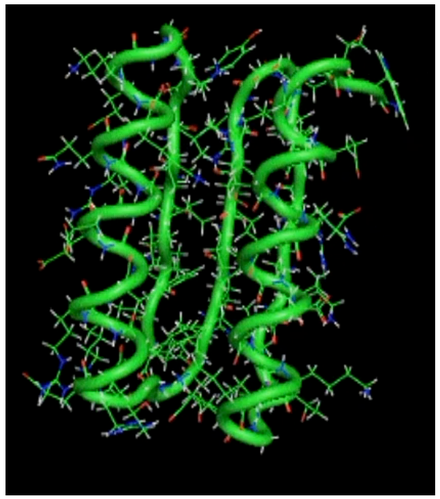


from Efficient Differentiation of Pixel Reconstruction Filters for Path-Space Differentiable Rendering, SIGGRAPH Asia 2022, Zihan Yu et al

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



from Center for the Exascale Simulation of Materials in Extreme Environments

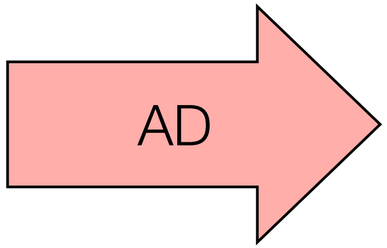


from Differential Molecular Simulation with Molly.jl, EnzymeCon 2023, Joe Greener (Cambridge)

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)
```

Differentiation is Expensive

Derivatives are the most costly and difficult to use algorithms

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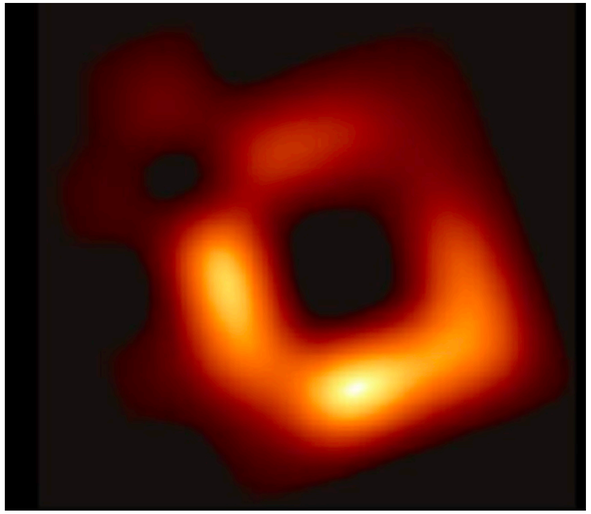
Derivatives are the most costly and difficult to use algorithms

Reconstructed image of M87
~1 week on cluster
Majority runtime is derivative



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Derivatives are the most costly and difficult to use algorithms

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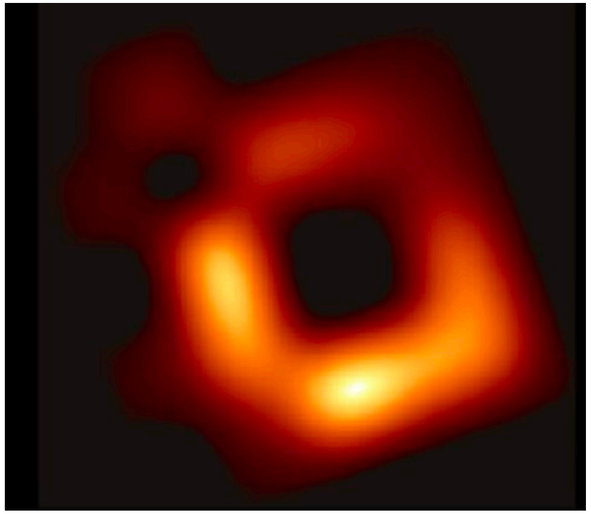

With Enzyme differentiation:
1 hour on 1 thread

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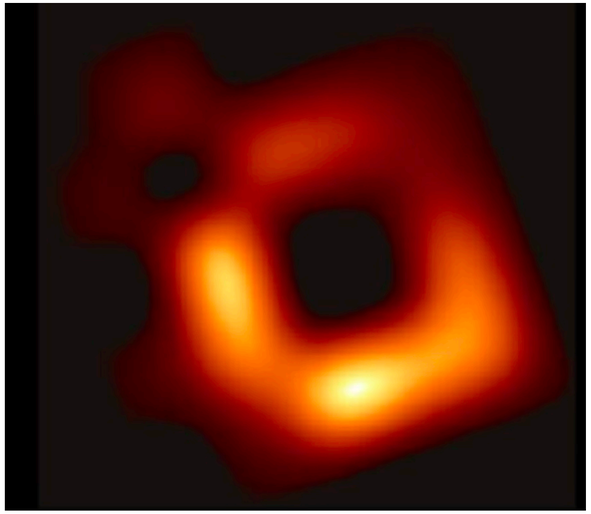
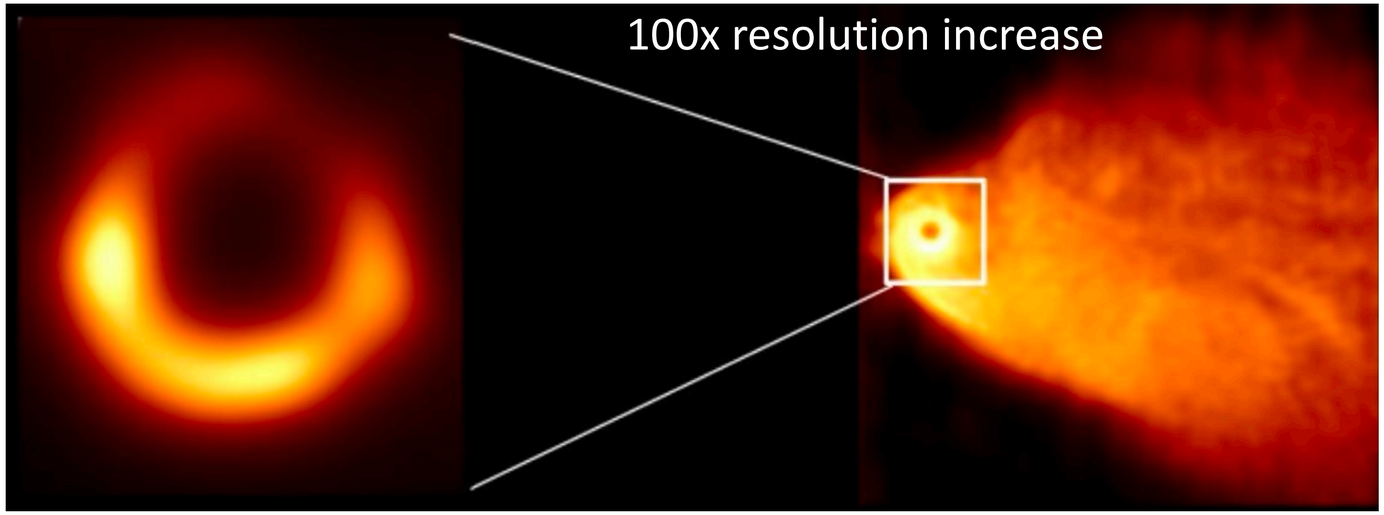


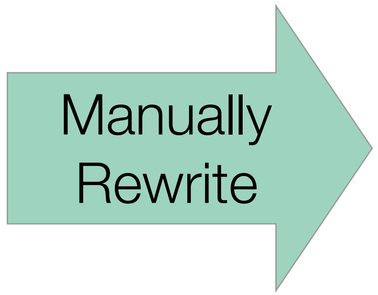
With Enzyme differentiation:
1 hour on 1 thread



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;
}
```




```
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

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

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

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

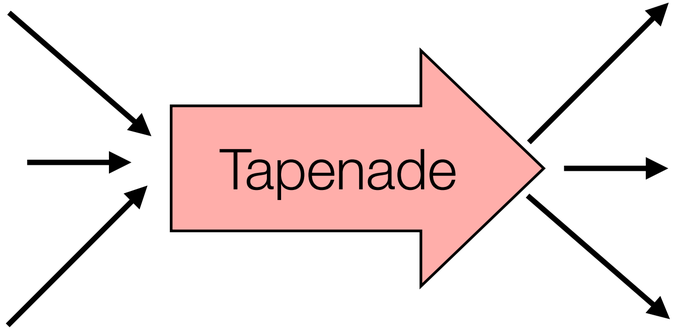
// Interpret all stack instructions
double res = inp.get_gradient(3.14);
```

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
```

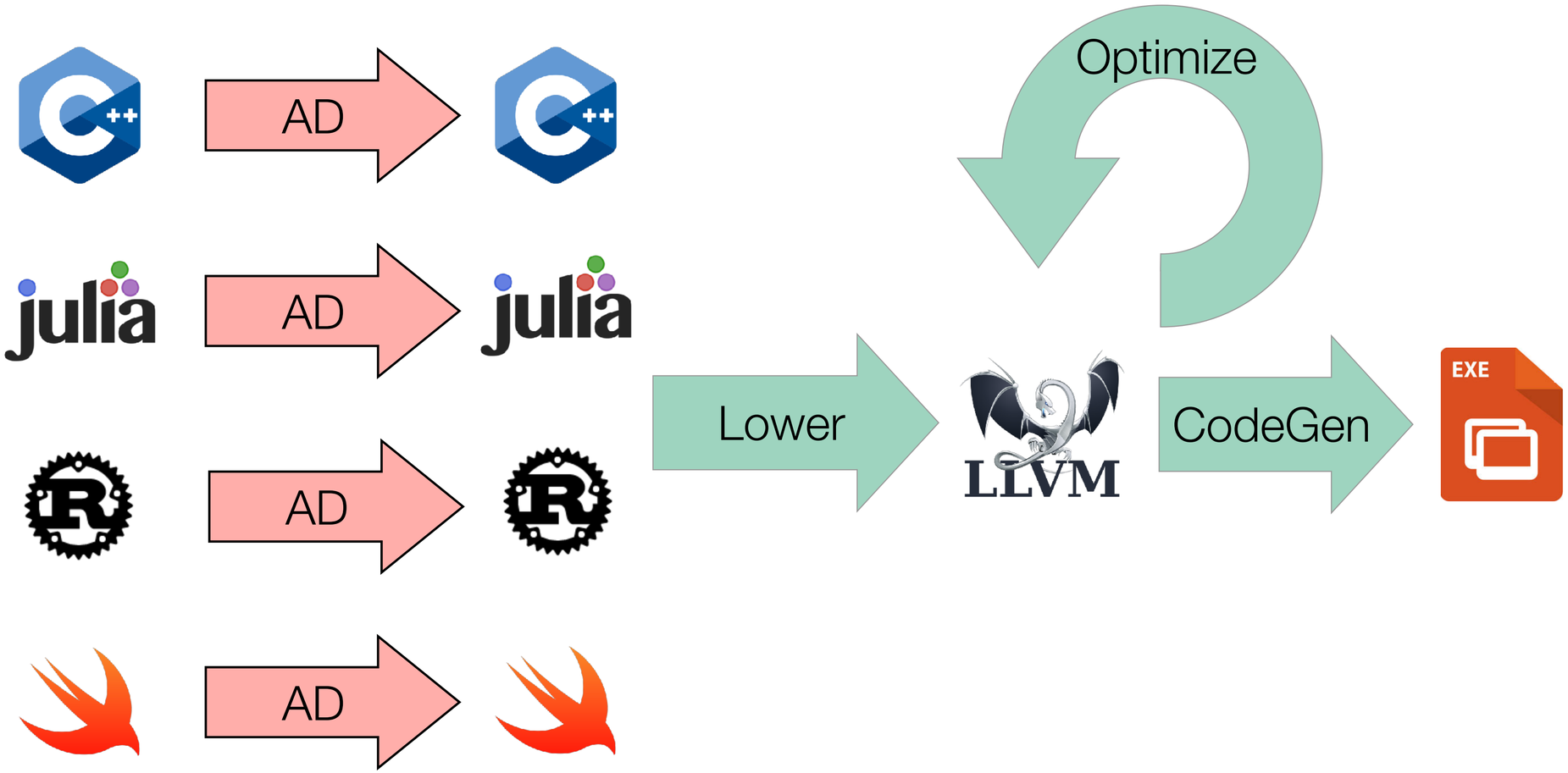
```
// myfile.c
double relu3(double x) {
  if (x > 0)
    return pow(x,3)
  else
    return 0;
}
```




```
// grad_myfile.h
```

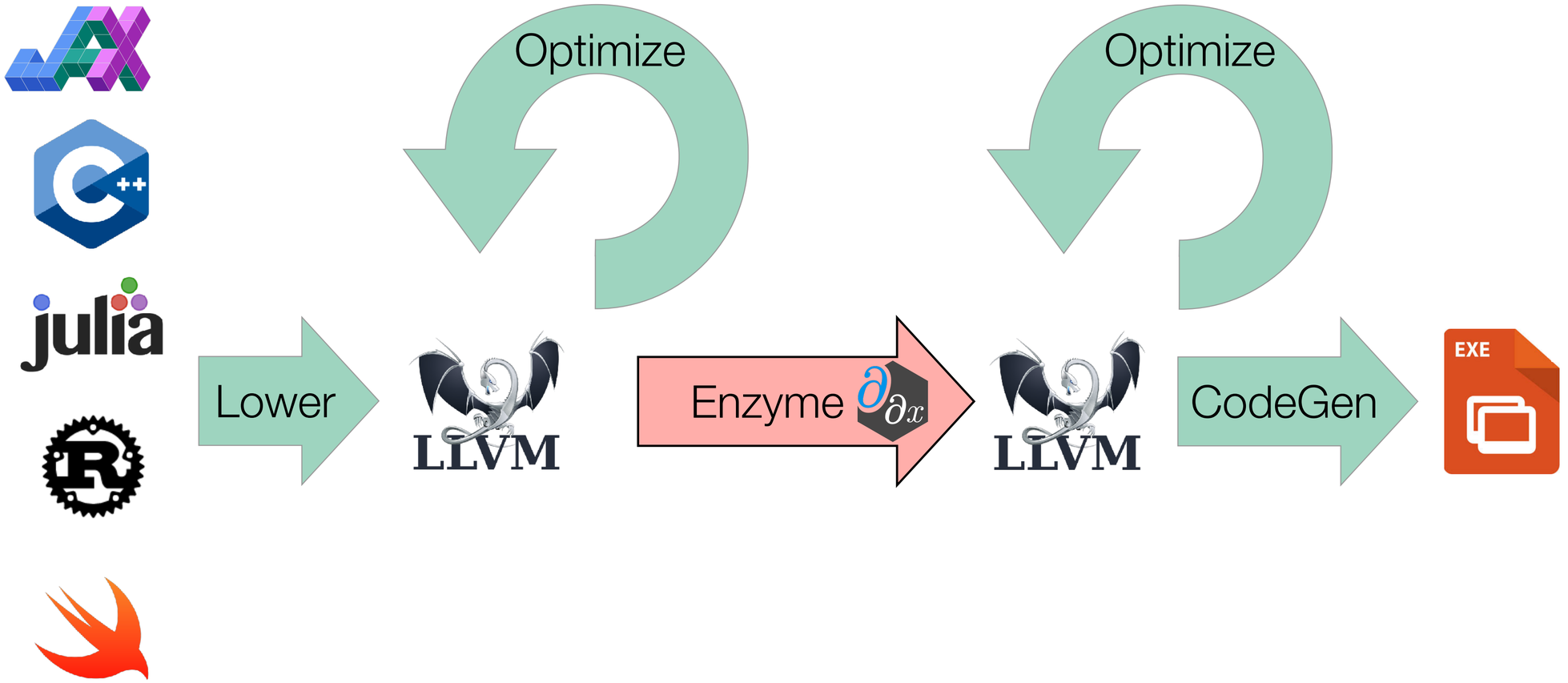
```
// grad_myfile.c
double grad_relu3(double x) {
  if (x > 0)
    return 3 * pow(x,2)
  else
    return 0;
}
```

Existing Automatic Differentiation Pipelines



Enzyme Approach

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



Case Study: Vector Normalization

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

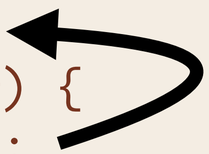
//Compute norm in O(n^2)
void norm(double[] out, double[] in) {

  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

$O(n^2)$

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

$O(n)$

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for i=0..n {
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for i=0..n {
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$O\left(n^2\right)$

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for i=0..n {
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$O\left(n^2\right)$

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for i=n..0 {
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Optimize

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

```
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!

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

```
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)
}
```

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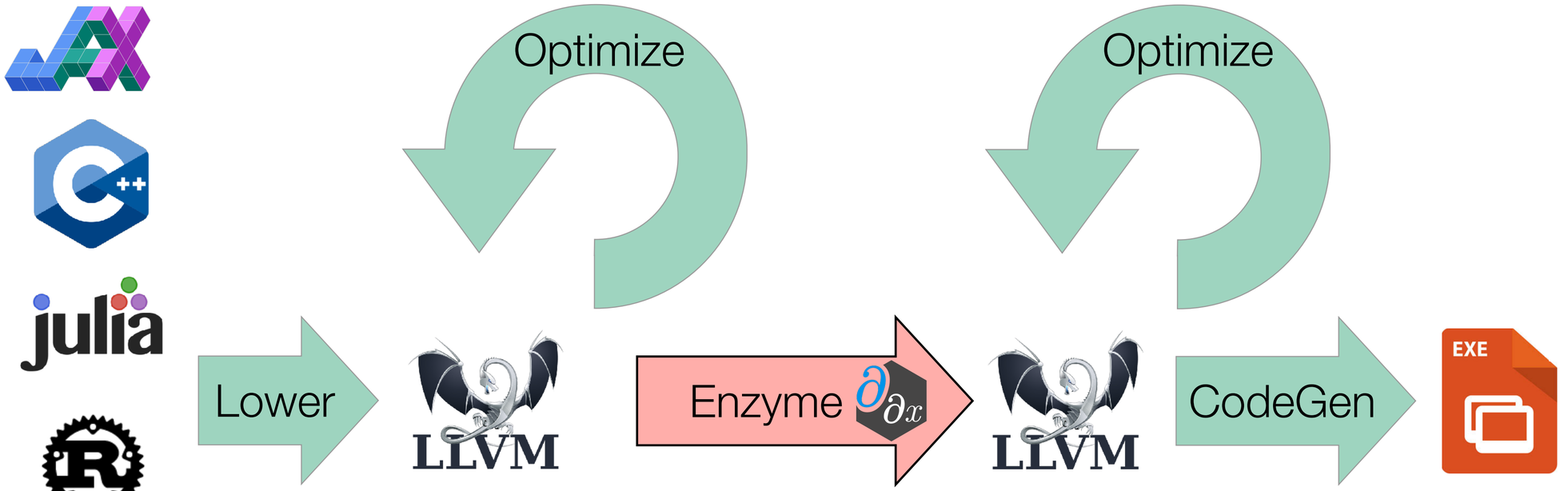
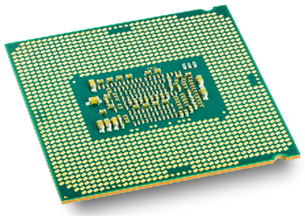
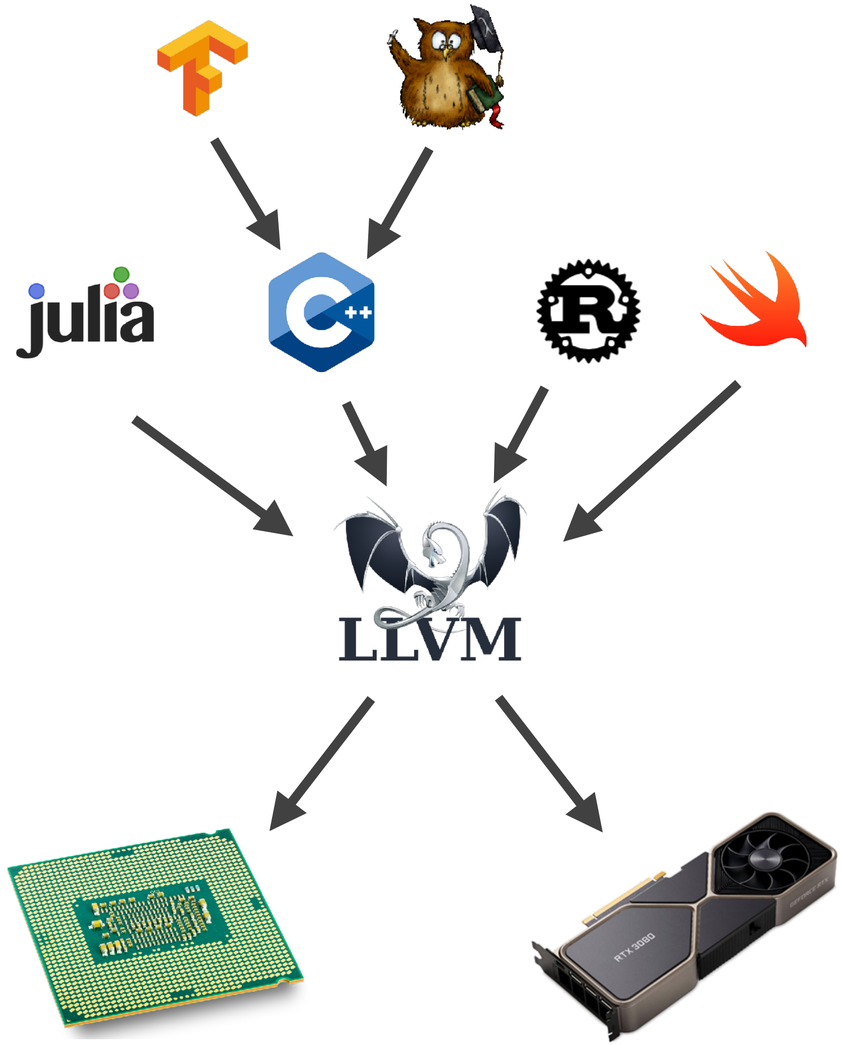




Why Does Enzyme Use LLVM?

- 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

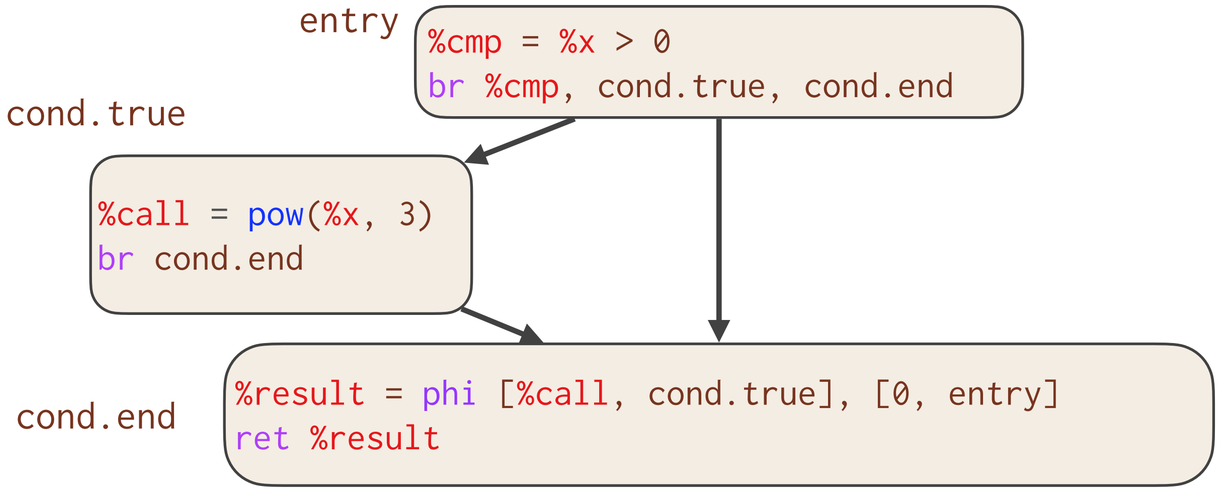
```c
double relu3(double x) {
  double result;
  if (x > 0)
    result = pow(x, 3);
  else
    result = 0;
  return result;
}
```

Enzyme Usage

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

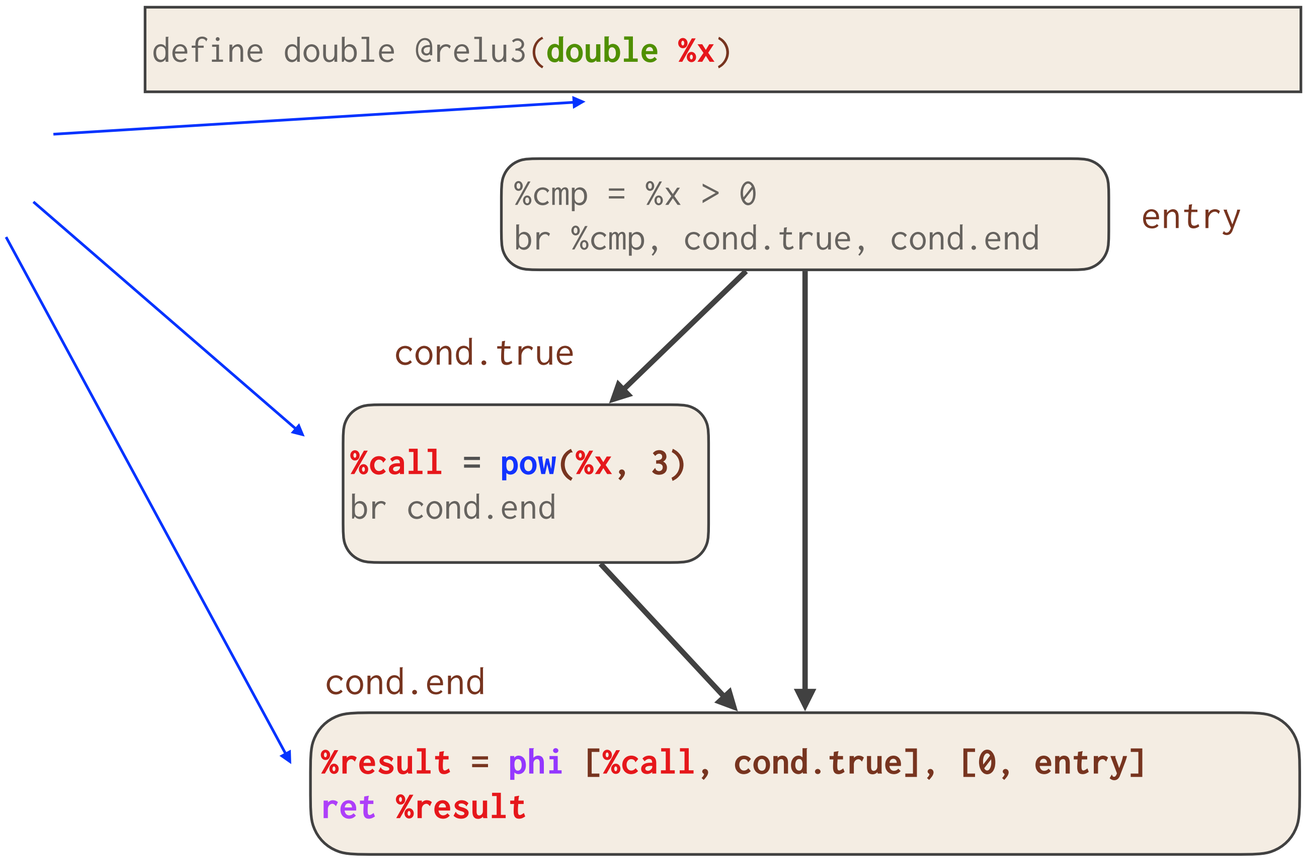
LLVM

```
define double @relu3(double %x)
```

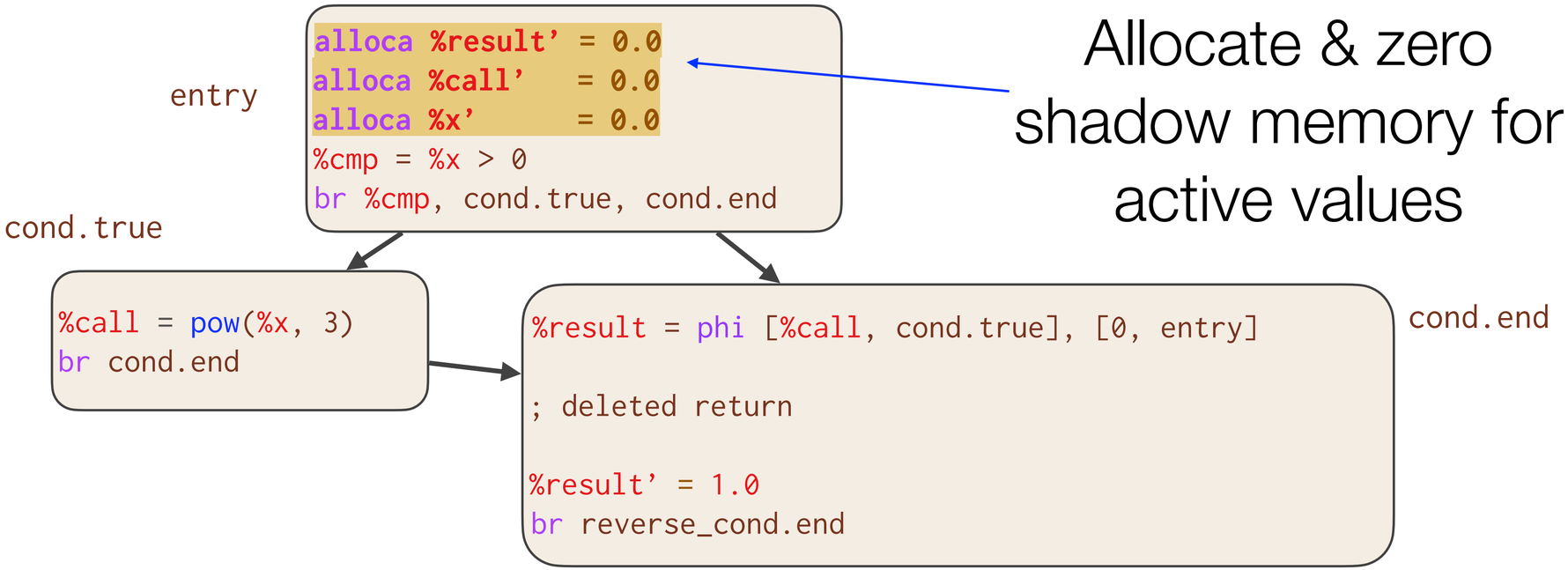


Case Study: ReLU3

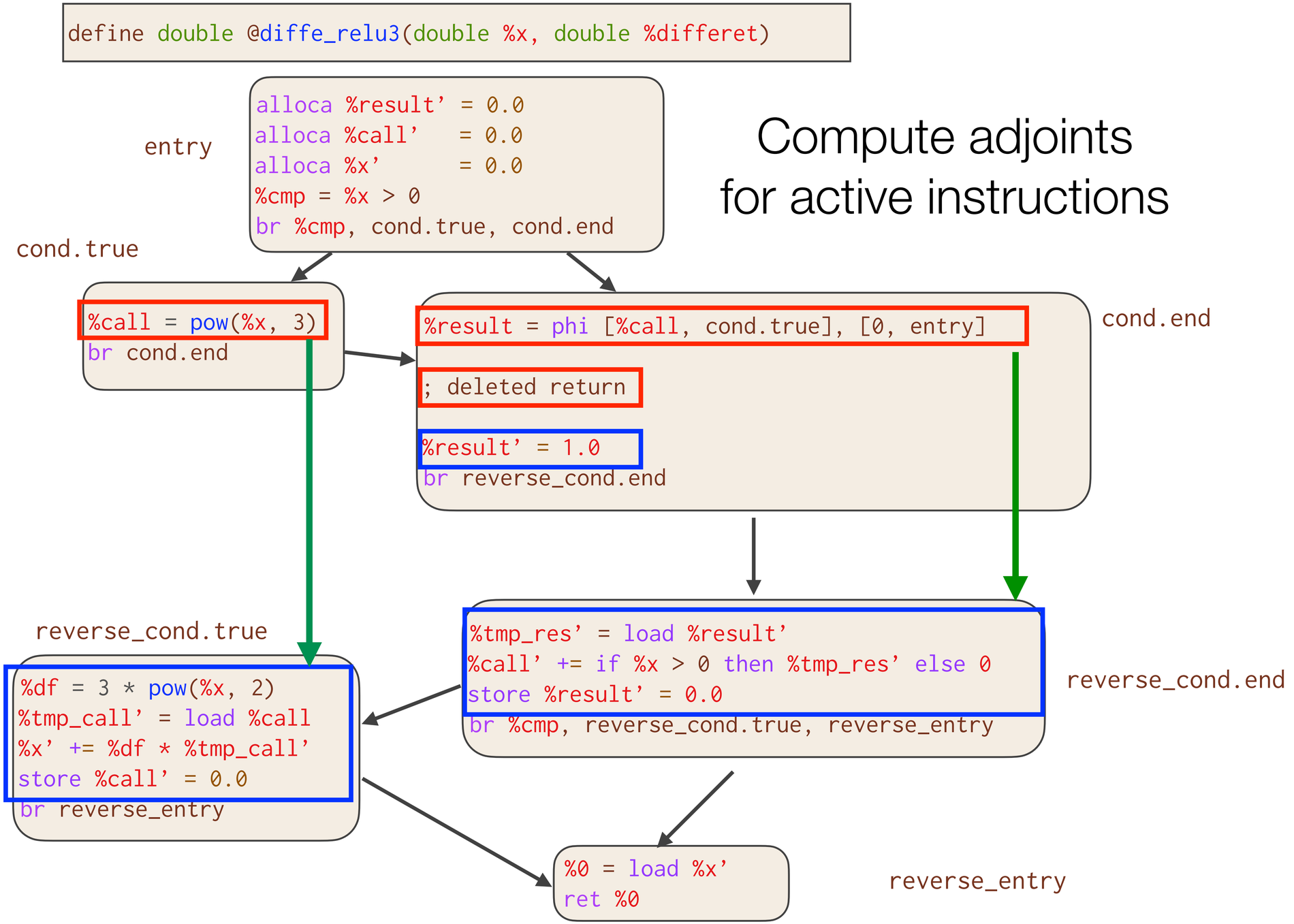
Active Instructions



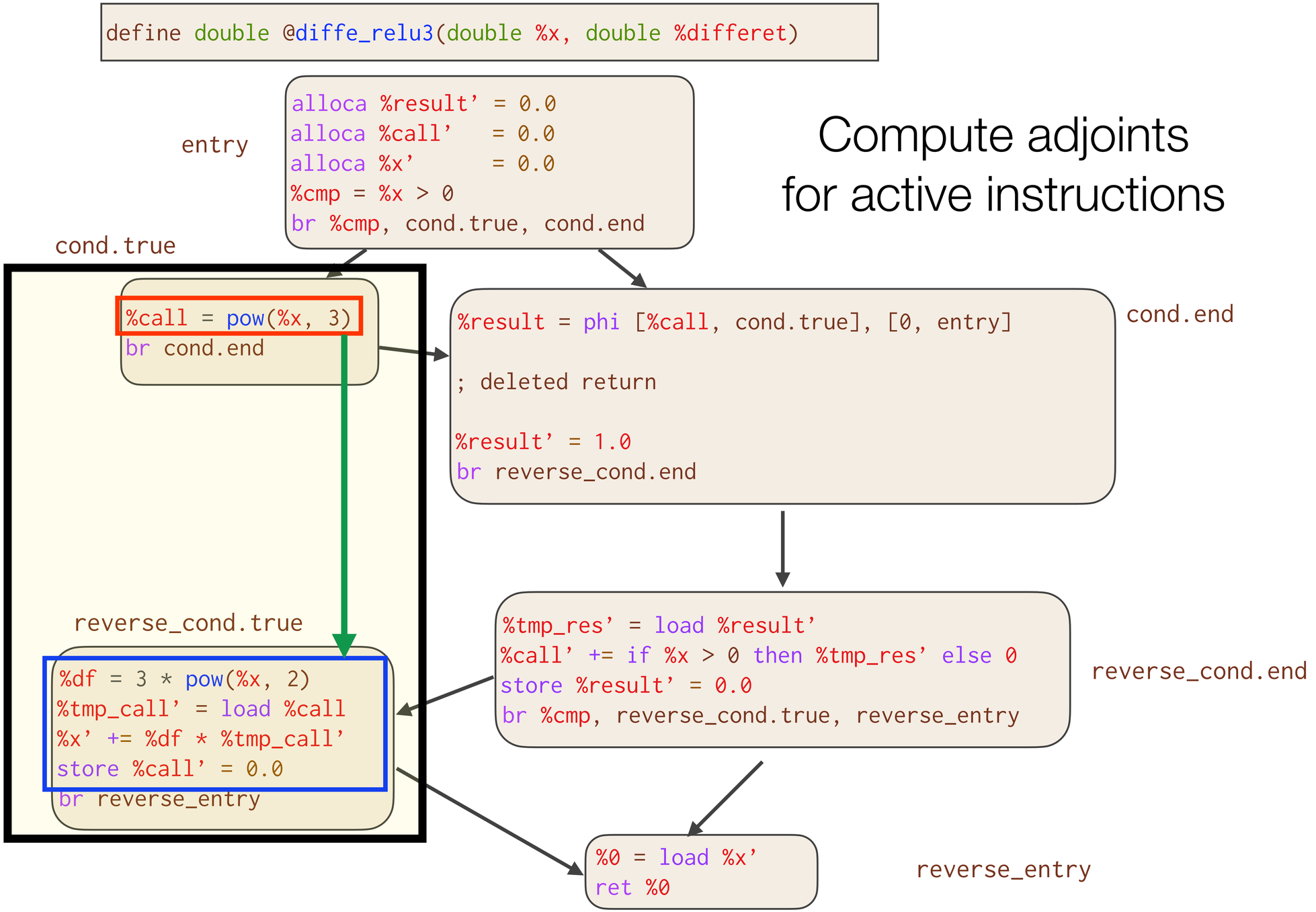
```
define double @diffe_relu3(double %x, double %differet)
```



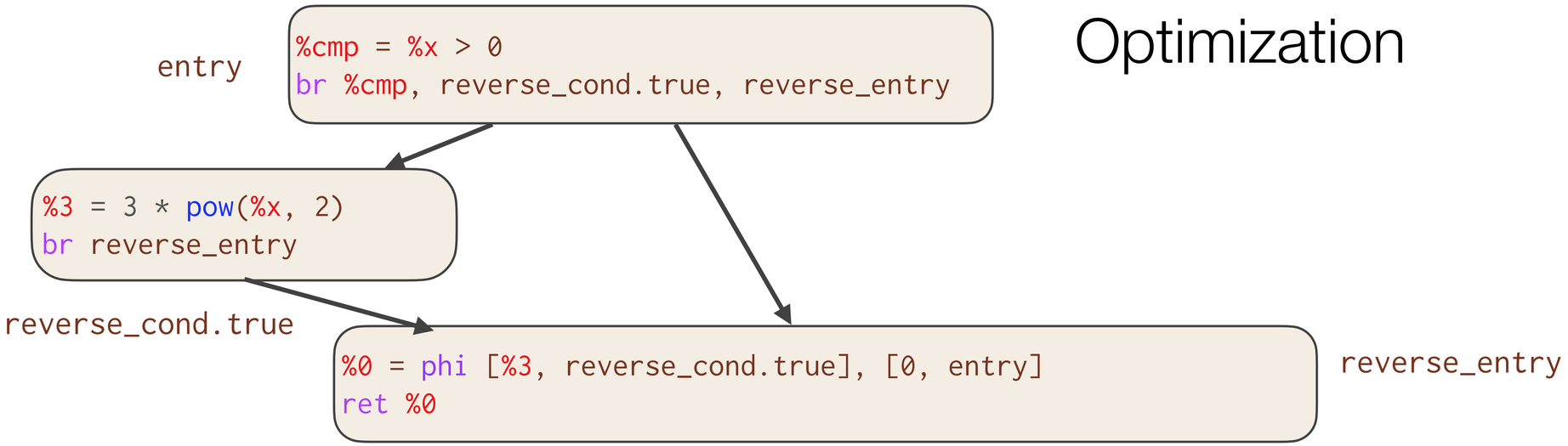
Allocate & zero shadow memory for active values



Compute adjoints for 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
%result = phi [%call, cond.true], [0, entry]
; deleted return
%result' = 1.0
br reverse_cond.end
cond.end
reverse_cond.true
%df = 3 * pow(%x, 2)
%tmp_call' = load %call
%x' += %df * %tmp_call'
store %call' = 0.0
br reverse_entry
%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.end
%0 = load %x'
ret %0
reverse_entry
Compute adjoints
for active instructions

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

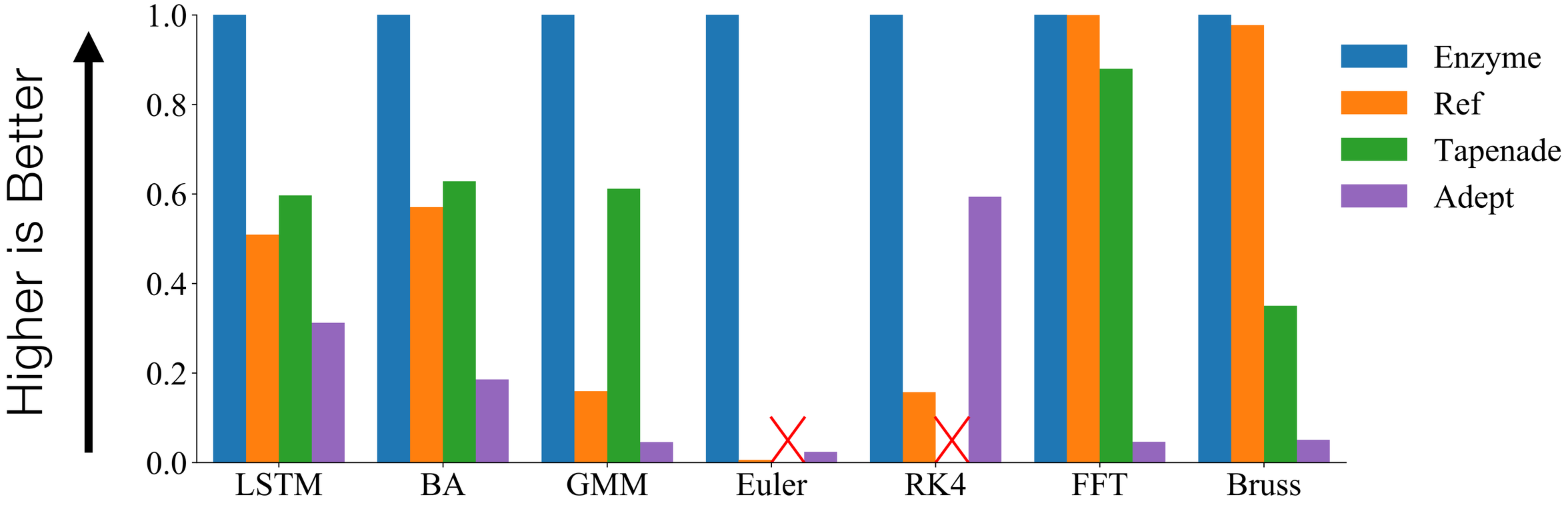


Post Optimization

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;
}
```

Enzyme CPU Speedups [NeurIPS'20]



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

Automatic Differentiation & GPUs [MCPHNSD @ SC'21]

- 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

Challenges of Parallel AD

- The adjoint of an instruction increments the derivative of its input
- 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* d_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;
}
```

GPU Memory Hierarchy

Per Thread	Per Block	Per GPU
Register	Shared Memory	Global Memory
~Bytes	~KBs	~GBs
Use Limits Parallelism	Use Limits Parallelism	

Slower, larger amount of memory

Correct and Efficient Derivative Accumulation

Thread-local memory

- Non-atomic load/store

```
__device__
void f(…) {

  // Thread-local var
  double y;

  …

  d_y += val;
}
```

Same memory location across all threads (some shared mem)

- 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; }
}
```

Slower

Synchronization Primitives

- Synchronization (`sync_threads`) ensures all threads finish executing codeA before executing codeB
- Sync is only necessary if A and B may access to the same memory
- Assuming the original program is race-free, performing a sync at the corresponding location in the reverse ensures correctness
- Prove correctness of algorithm by cases

```
codeA();

sync_threads;

codeB();
```

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

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) {
  // Forward Pass

  y[threadIdx.x] = a[0] * x[threadIdx.x];

  // Reverse Pass

  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 Example

```
__device__
void inner(float* a, float* x, float* y) {

  y[threadIdx.x] = a[0] * x[threadIdx.x];

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__device__
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}
```

```
__device__
void diffe_inner(float* a, float* da,
                 float* x, float* dx,
                 float* y, float* dy) {
  // Forward Pass

  y[threadIdx.x] = a[0] * x[threadIdx.x];

  // Reverse Pass

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

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

  float da_tmp = x[threadIdx.x] * dy;
  reduce_accumulate(&da[0], da_tmp);
}
```

CUDA.jl / AMDGPU.jl Example

```
function compute!(inp, out)
    s_D = @cuStaticSharedMem eltype(inp) (10, 10)
    ...
end

function grad_compute!(inp, out)
    Enzyme.autodiff_deferred(compute!, inp, out)
    return nothing
end

@cuda grad_compute!(Duplicated(inp, d_inp),
                    Duplicated(out, d_out))
```

```
function compute!(inp, out)
    s_D = AMDGPU.alloc_special(…)
    ...
end

function grad_compute!(inp, out)
    Enzyme.autodiff_deferred(compute!, inp, out)
    return nothing
end

@rocm grad_compute!(Duplicated(inp, d_inp),
                    Duplicated(out, d_out))
```

See Below For Full Code Examples

https://github.com/wsmoses/Enzyme-GPU-Tests/blob/main/DG/

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];
...

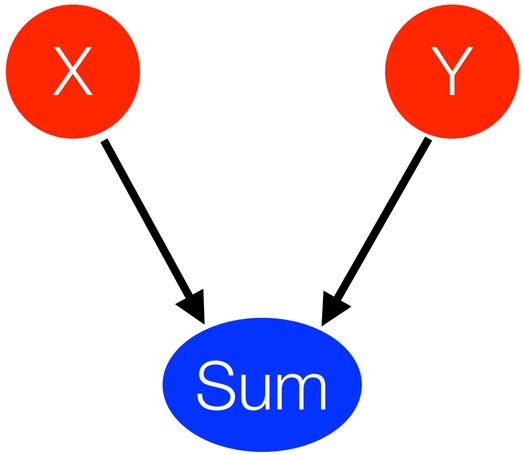
delete[] x_cache;
```

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);

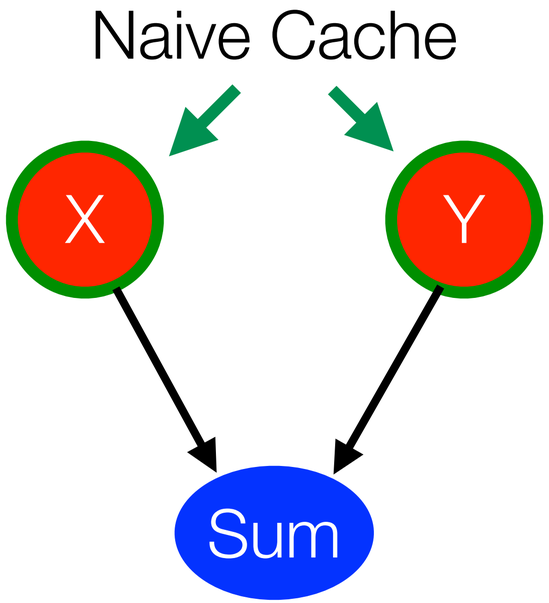
for(int i=9; i>=0; i--) {
  ...
  grad_use(sum);
}
```

Cache Reduction Example

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

Overwritten:

Required for Reverse:




```
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);
}

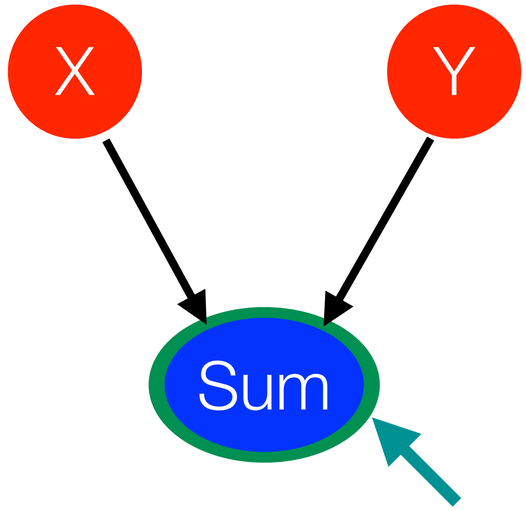
overwrite(x, y);
grad_overwrite(x, y);

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

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

Overwritten:

Required for Reverse:



Smallest Cache

Allocation Merging

- Allocations (and any calls) on the GPU are expensive
- Given two allocations in the same scope, replace uses with a single allocation
- Beneficial for not just AD, but any GPU programs!

```
double* var1 = new double[N];
double* var2 = new double[M];

use(var1, var2);

delete[] var1;
delete[] var2;
```

```
double* var1 = new double[N + M];
double* var2 = var1 + N;

use(var1, var2);

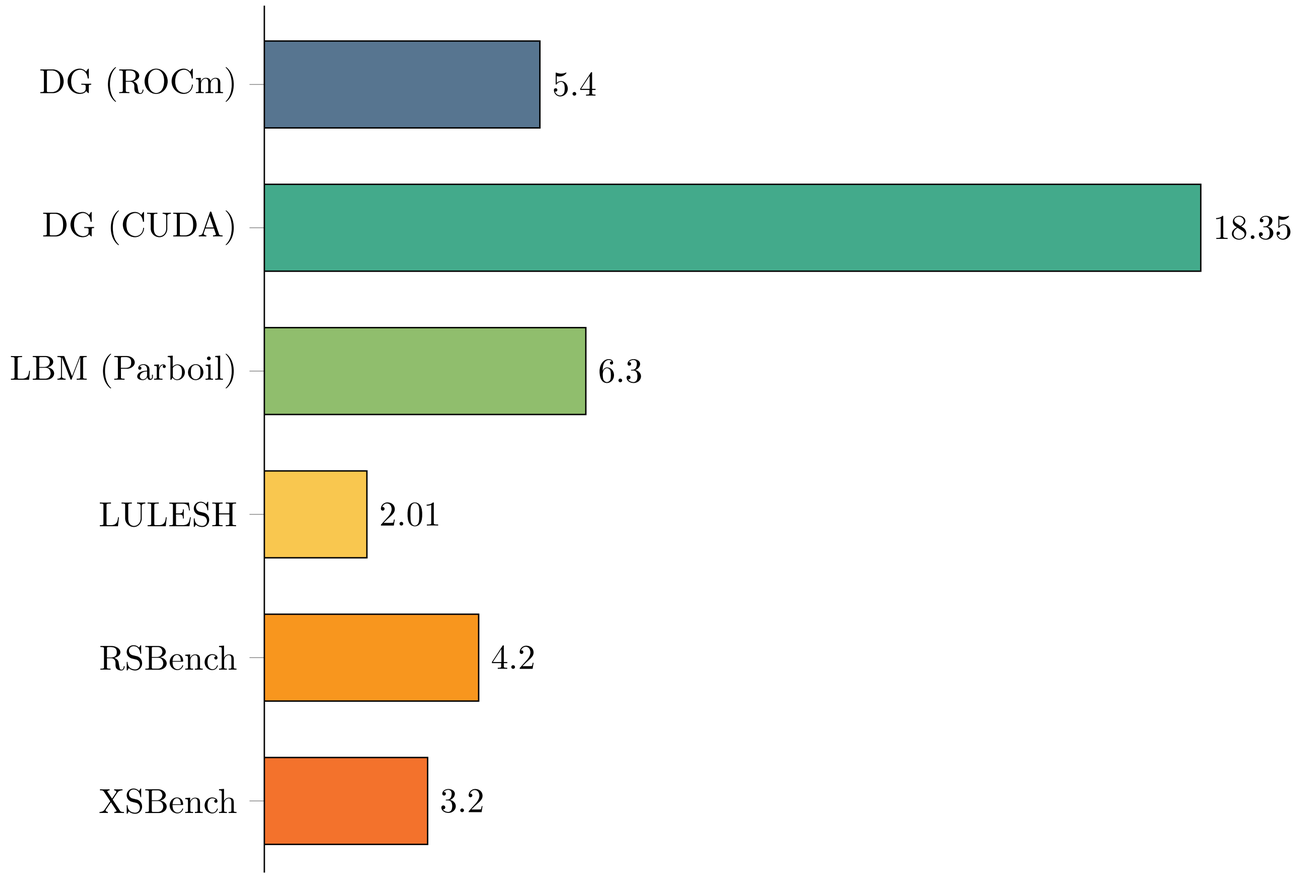
delete[] var1;
```

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 [MCPHNMJ'21]

- 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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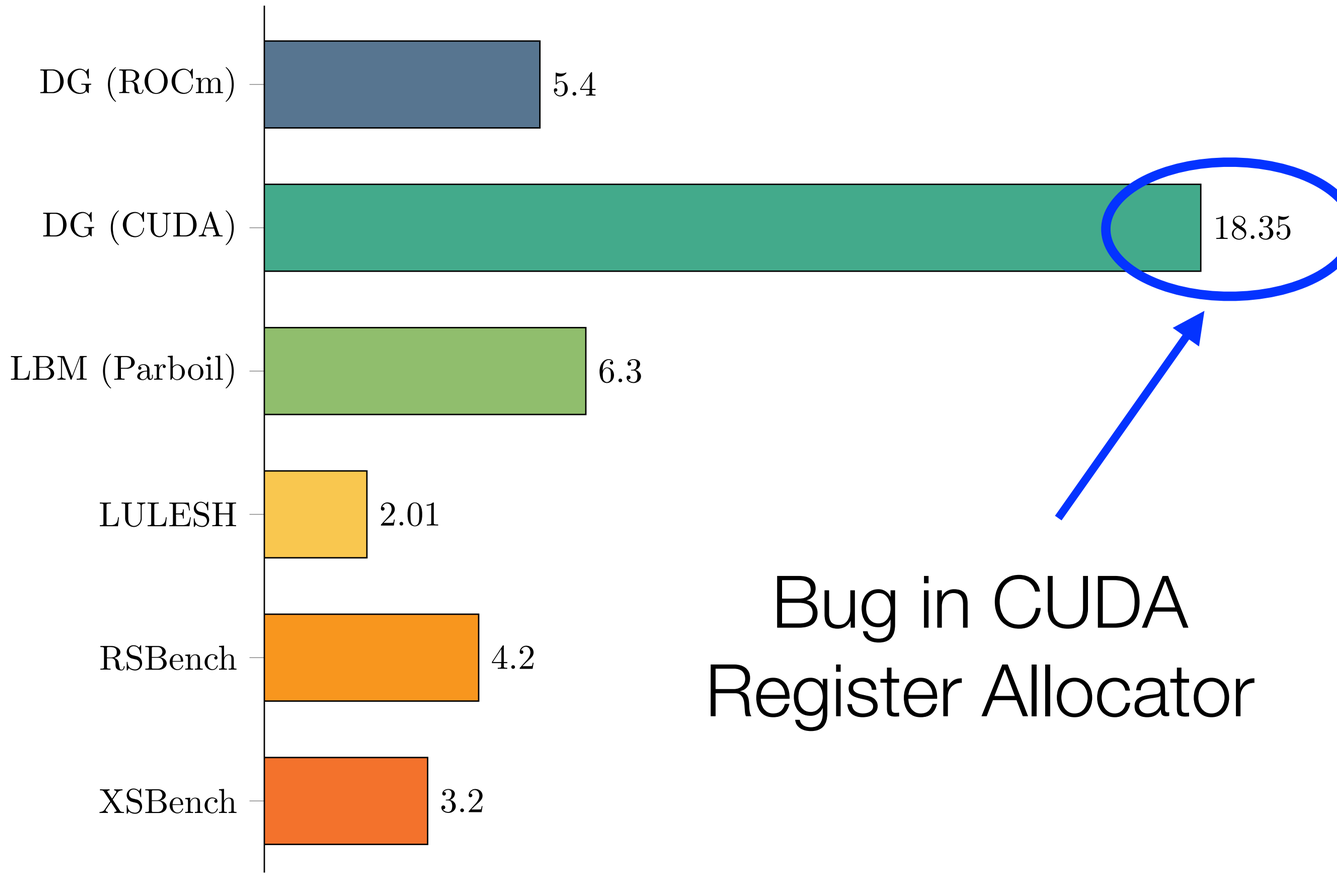
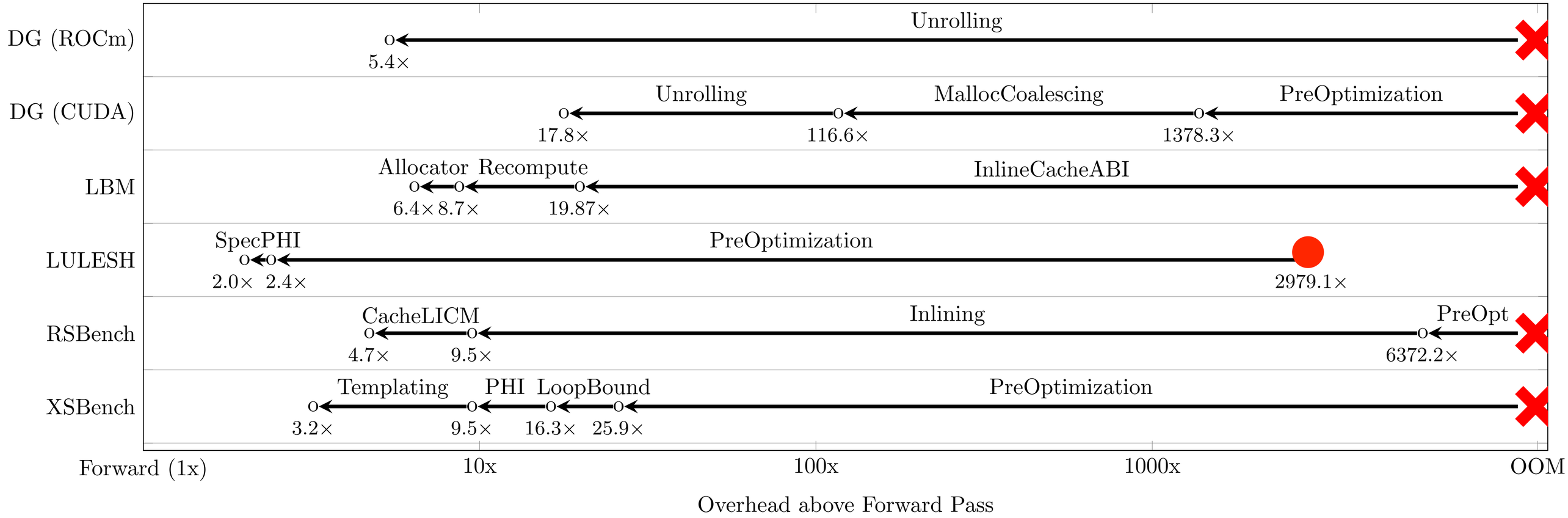
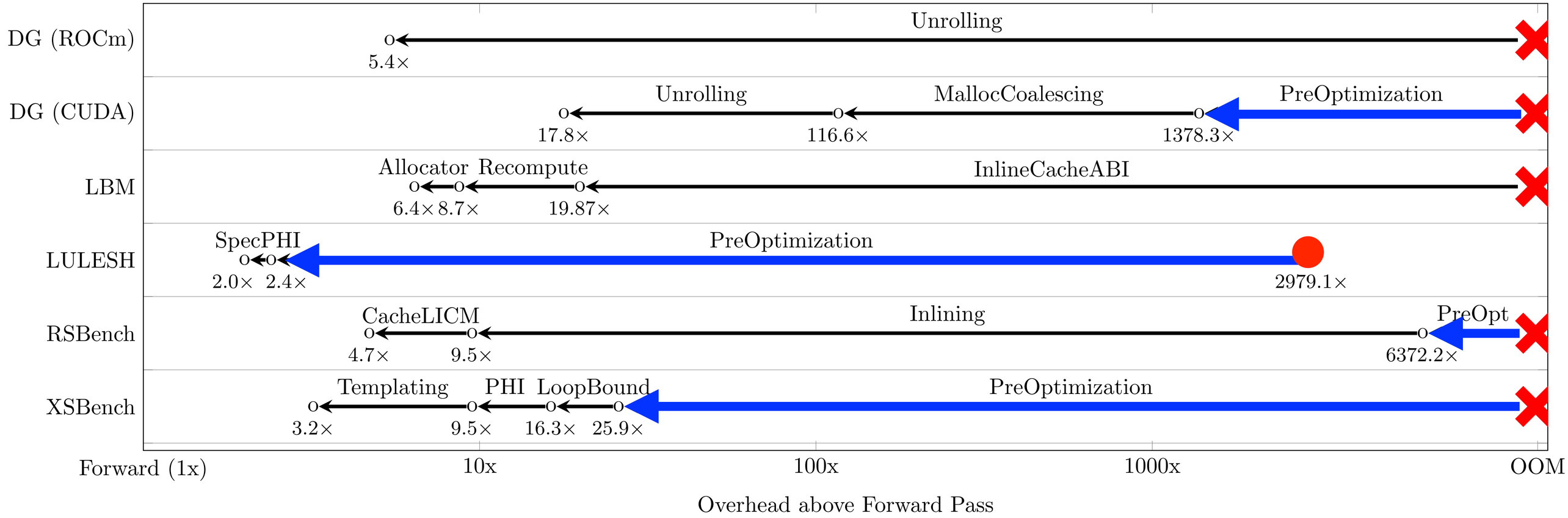


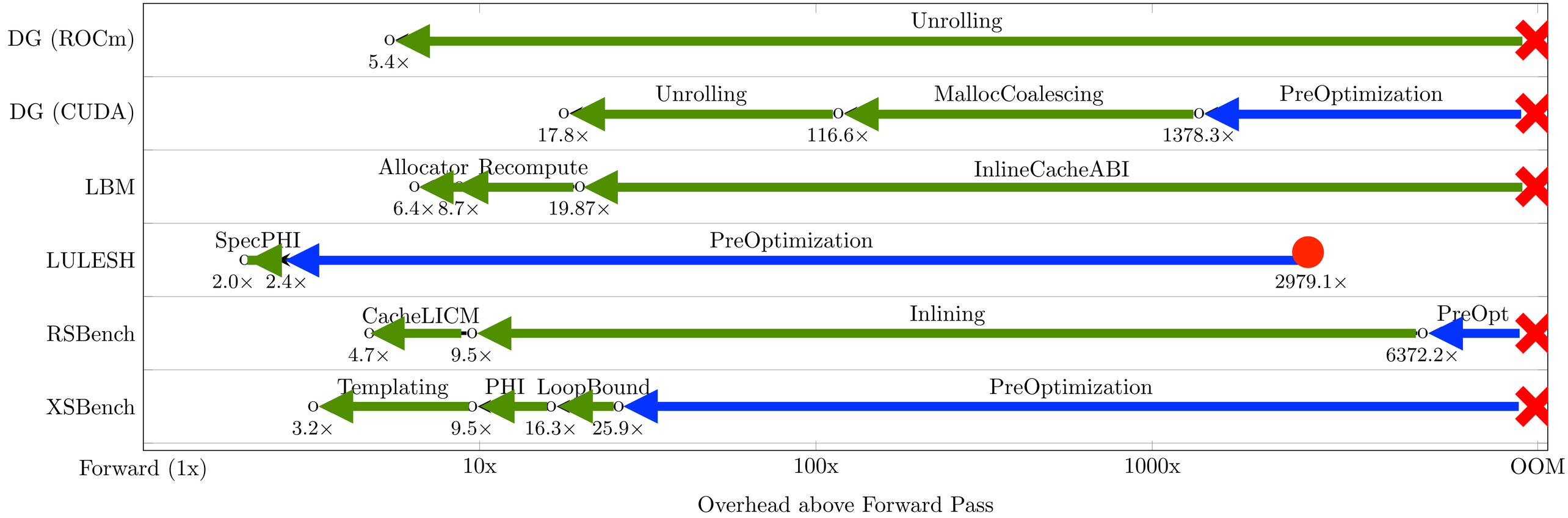
Ablation Analysis of Optimizations



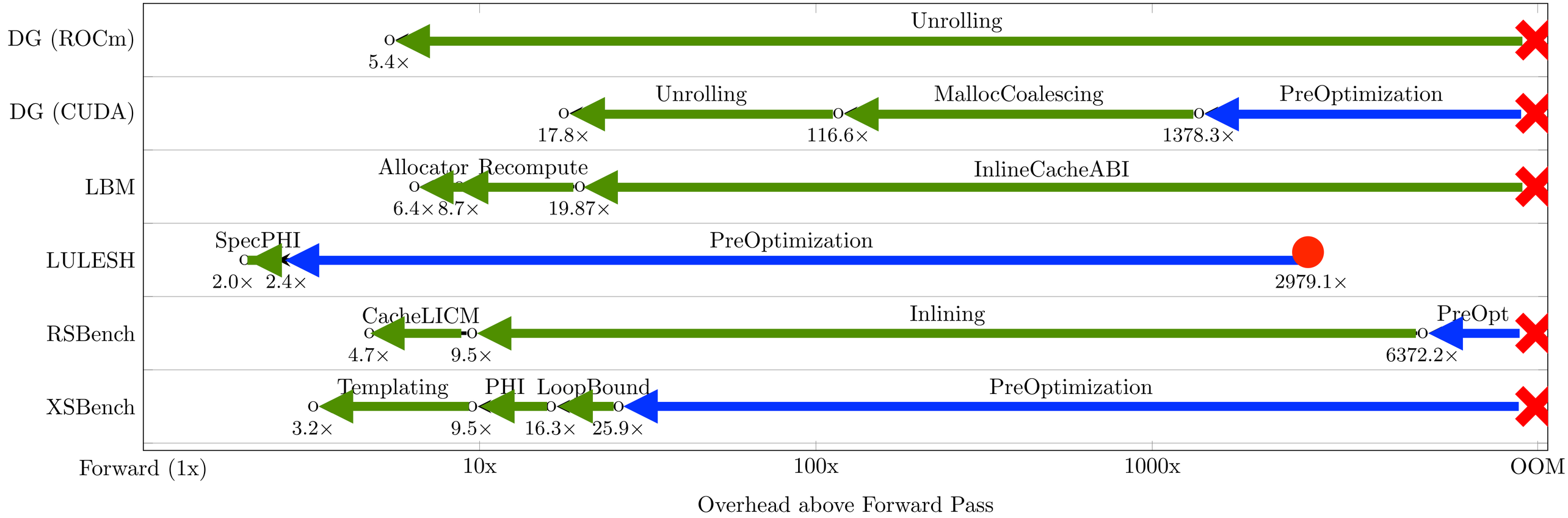
Ablation Analysis of Optimizations



Ablation Analysis of Optimizations



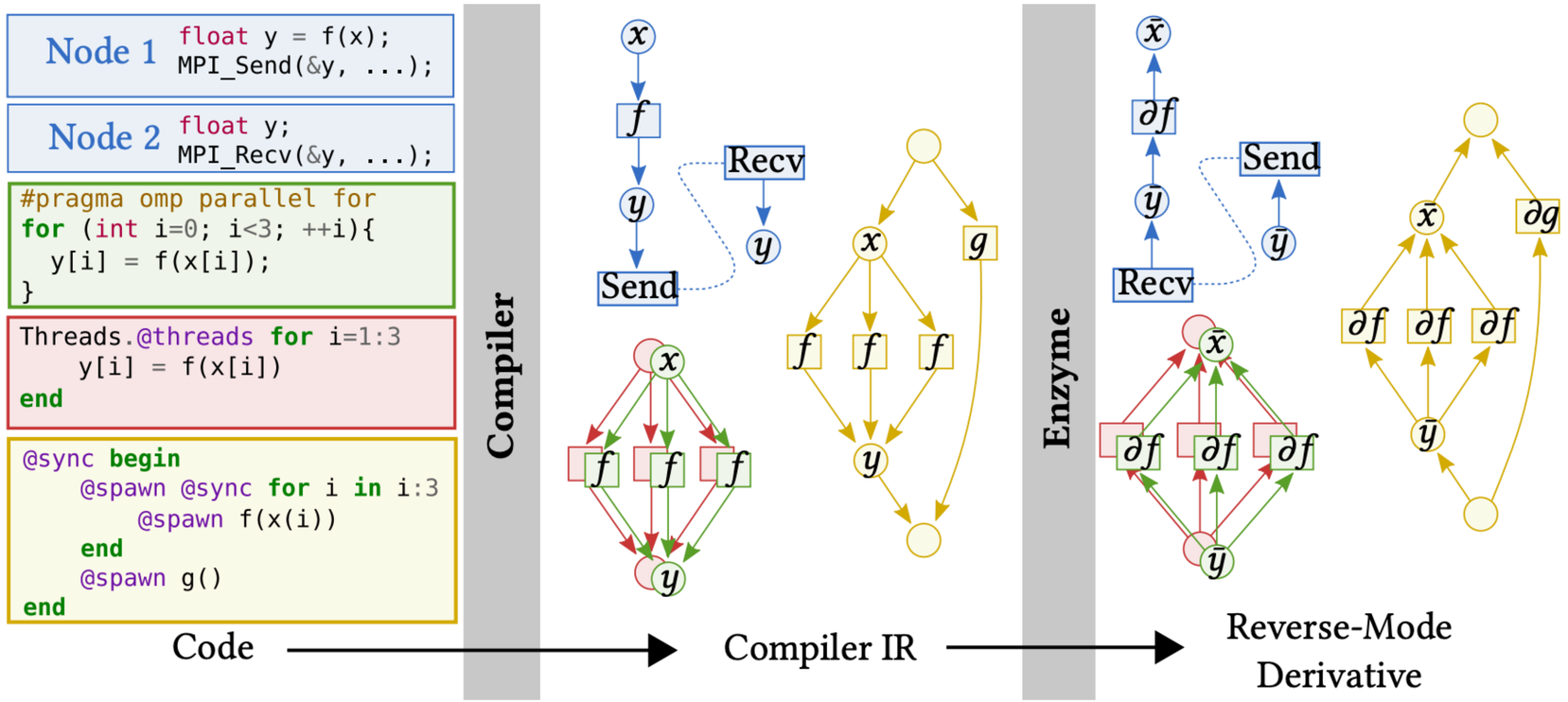
Ablation Analysis of Optimizations



GPU AD is Intractable Without Optimization!

Common Framework for Parallel AD [SC'22]

- Common infrastructure for supporting parallel AD (caching, race-resolution, gradient accumulation) enables parallel differentiation independent of framework or language.



- Enables differentiation of a combination of GPU (e.g. CUDA, ROCm), CPU (OpenMP, Julia Tasks, RAJA), Distributed (MPI, MPI.jl), and more

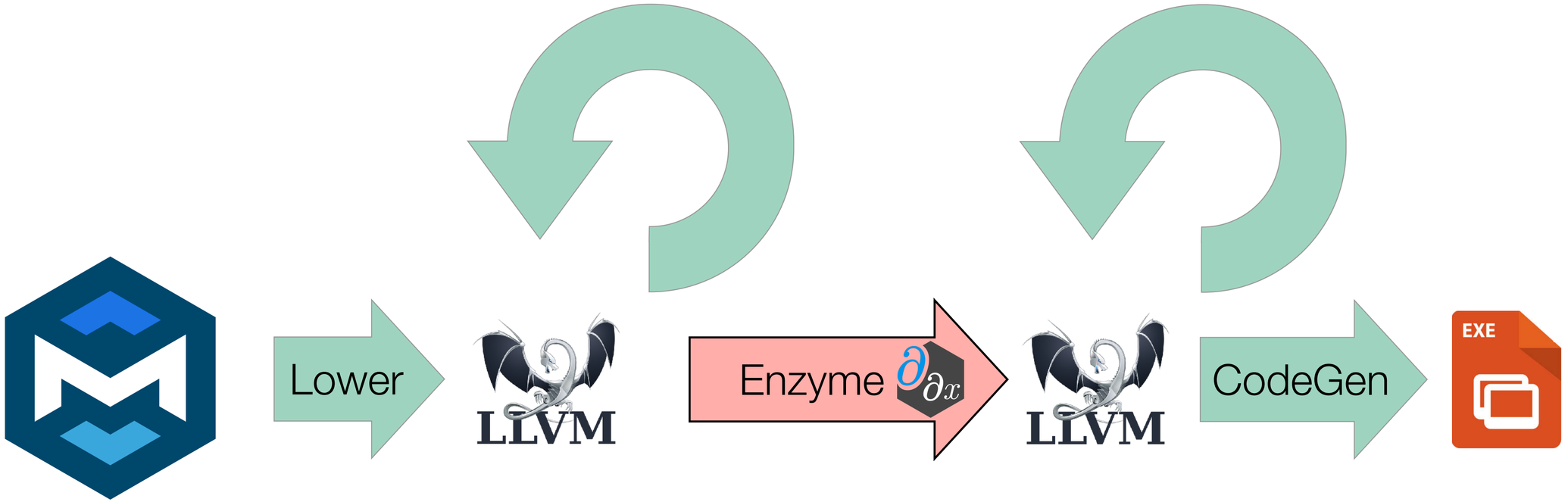
What is MLIR?

Multi-Level Intermediate Representation (MLIR)

- New Compiler IR with user-defined instructions, optimizations, analyses
  - Linear Algebra
  - GPU Programming
  - Fully Homomorphic Encryption
- Mix and match dialects and optimizations from multiple dialects
- Core infrastructure of modern ML frameworks (JaX, PyTorch, TensorFlow)
- Frontends for C++ (Polygeist), Julia (Reactant.jl)

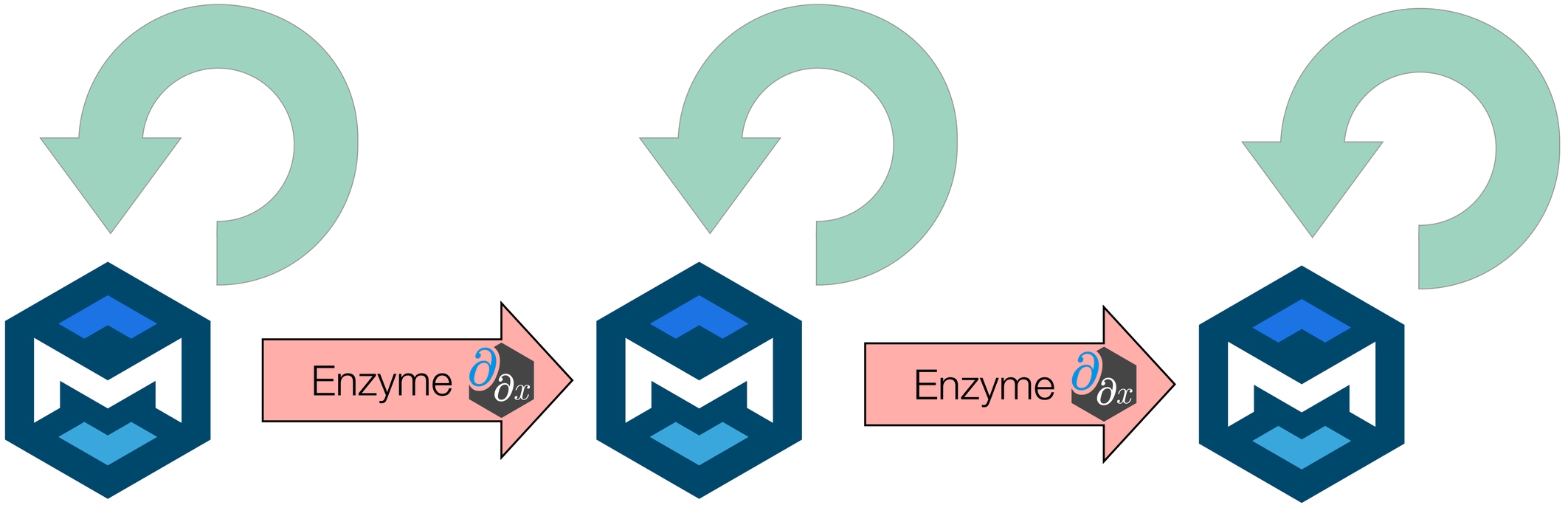
```
func @set(%arg0: memref<?xi32>, %arg1: i32) {
    affine.for %arg2 = 0 to 10 {
      affine.store %arg1, %arg0 [2 * %arg2] : memref<?xi32>
    }
    return
  }
}
```

Why MLIR?



Why MLIR?

“Multi-level” coordination of AD and Optimization!



GPU Programming via LLVM

- Mainstream compilers do not have a high-level representation of parallelism, making optimization difficult or impossible
- This is accentuated for GPU programs where the kernel is kept in a separate module to allow emission of different assembly and synchronization is treated as a complete optimization barrier.

```
__global__ void normalize(int *out, int* in, int n) {
  int tid = blockIdx.x;
  if (tid < n)
    out[tid] = in[tid] / sum(in, n);
}

void launch(int *out, int* in, int n) {
  normalize<<<n>>>(d_out, d_in, n);
}
```

Host Code

```
target triple = "x86_64-unknown-linux-gnu”

define void @_Z6launchPiS_i(i32* %out,
                            i32* %in,
                            i32 %n) {
  call i32 @pushCallConfiguration(…)
  call i32 @cudaLaunch(@_device_stub, …)
  ret void
}
```

Device Code

```
target triple = ”nvptx”

define void @_Z9normalize(i32* %out,
                          i32* %in, i32 %n) {
  %4 = call i32 @llvm.tid.x()
  %5 = icmp slt i32 %4, %n
  br i1 %5, label %6, label %13

6:
  %8 = getelementptr i32, i32* %in, i32 %4
  %9 = load i32, i32* %8, align 4
  %10 = call i32 @_Z3sumPii(i32* %in, i32 %n)
  %11 = sdiv i32 %9, %10
  %12 = getelementptr i32, i32* %out, i32 %4
  store i32 %11, i32* %12, align 4
  br label %13

13:
  ret void
}
```

Preserving the GPU parallel structure [1]

- Polygeist/MLIR maintains GPU parallelism in a compiler-friendly form
- Enables optimization between caller and kernel
- Enable parallelism-specific optimization

```
__global__ void normalize(int *out, int *in, int n) {
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}

void launch(int *out, int* in, int n) {
  normalize<<<n>>>(d_out, d_in, n);
}
```

```
func @_Z6launch(%out: memref<?xi32>,
                %in: memref<?xi32>, %n: i32) {
  %c1 = constant 1 : index
  %c0 = constant 0 : index

  parallel (%tid) = (%c0) to (%n) step (%c1) {
    %2 = load %in[%tid]
    %sum = call @_Z3sumPii(%in, %n)
    %4 = divsi %2, %sum : i32
    store %4, %out[%tid]
    yield
  }
  return
}
```

[1] High-Performance GPU-to-CPU Transpilation and Optimization via High-Level Parallel Constructs, PPoPP'23

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    store %4, %out[%tid]
    yield
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  return
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```

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Preserving the GPU parallel structure [1]

- Polygeist/MLIR maintains GPU parallelism in a compiler-friendly form
- Enables optimization between caller and kernel
- Enable parallelism-specific optimization
- Optimizations on primal =>***outsized impact for derivatives***

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    yield
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  return
}
```

[1] High-Performance GPU-to-CPU Transpilation and Optimization via High-Level Parallel Constructs, PPoPP'23

Linear Algebra Optimizations

Wrote >200 different patterns!

Simplify code where possible

```
x + 0 -> x

transpose(transpose(x)) -> x

transpose(matmul(a,b)) ->
   matmul(b, a)
```

Often require program context

```
transpose(convert(reshape(x)))
 <-> reshape(convert(transpose(x))

slice(add(a, b)) ->
 add(slice(a), slice(b))


mul(pad(x, 0), y) ->
 pad(mul(x, slice(y)), 0)
```

```
x, y : tensor<100000xf32>

a = dot(x, y)

b = mul(a, z)

c = add(b, 4)

return c[0:10]
```

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```

```
x, y : tensor<100000xf32>

a = dot(x, y)

b = mul(a[0:10], z[0:10])

c = add(b, 4)

return c
```

Performance Engineering a Toy LLM

- Introduction of linear-algebra specific optimizations made a significant impact on training performance
  - 53% speedup of a run with 32x accelerators
  - 14-18.5% speedup for single accelerator

- Accessible now from github.com/EnzymeAD/Enzyme-JaX

```
Step: 2 loss: 12.880576133728027
Step: 3 loss: 12.785988807678223
Step: 4 loss: 12.652521133422852
Step: 5 loss: 12.482083320617676
…
Step: 19 loss: 9.190348625183105
Step: 20 loss: 8.928218841552734
Step: 21 loss: 8.660679817199707

Unopt: 0.479 samples/sec
```

```
Step: 2 loss: 12.88175106048584
Step: 3 loss: 12.786417007446289
Step: 4 loss: 12.652612686157227
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…
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Opt: 0.736 samples/sec
```

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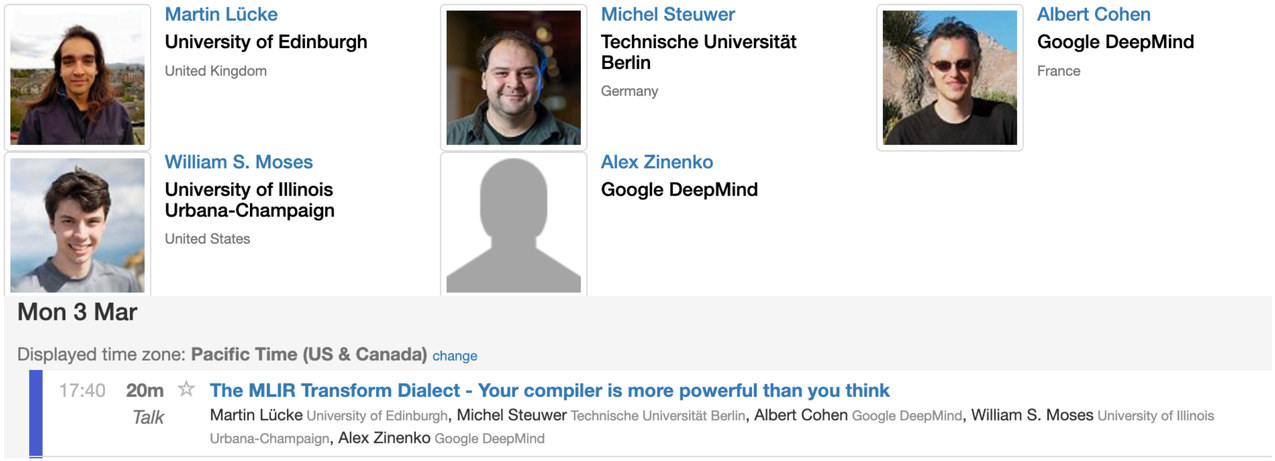


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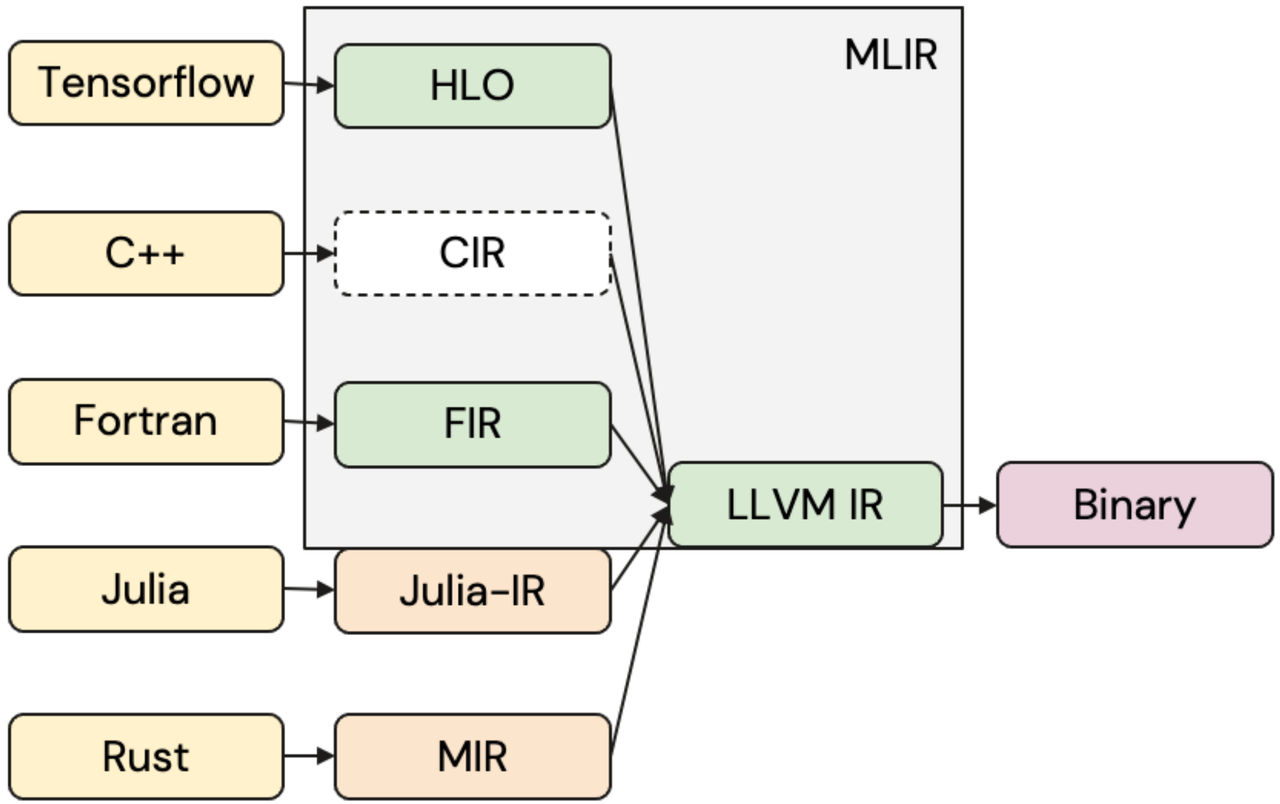
```

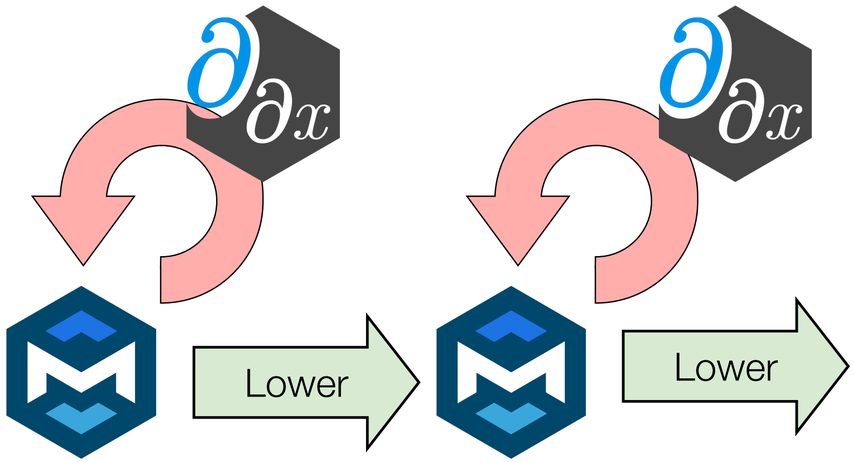
Multi-Level Differentiation

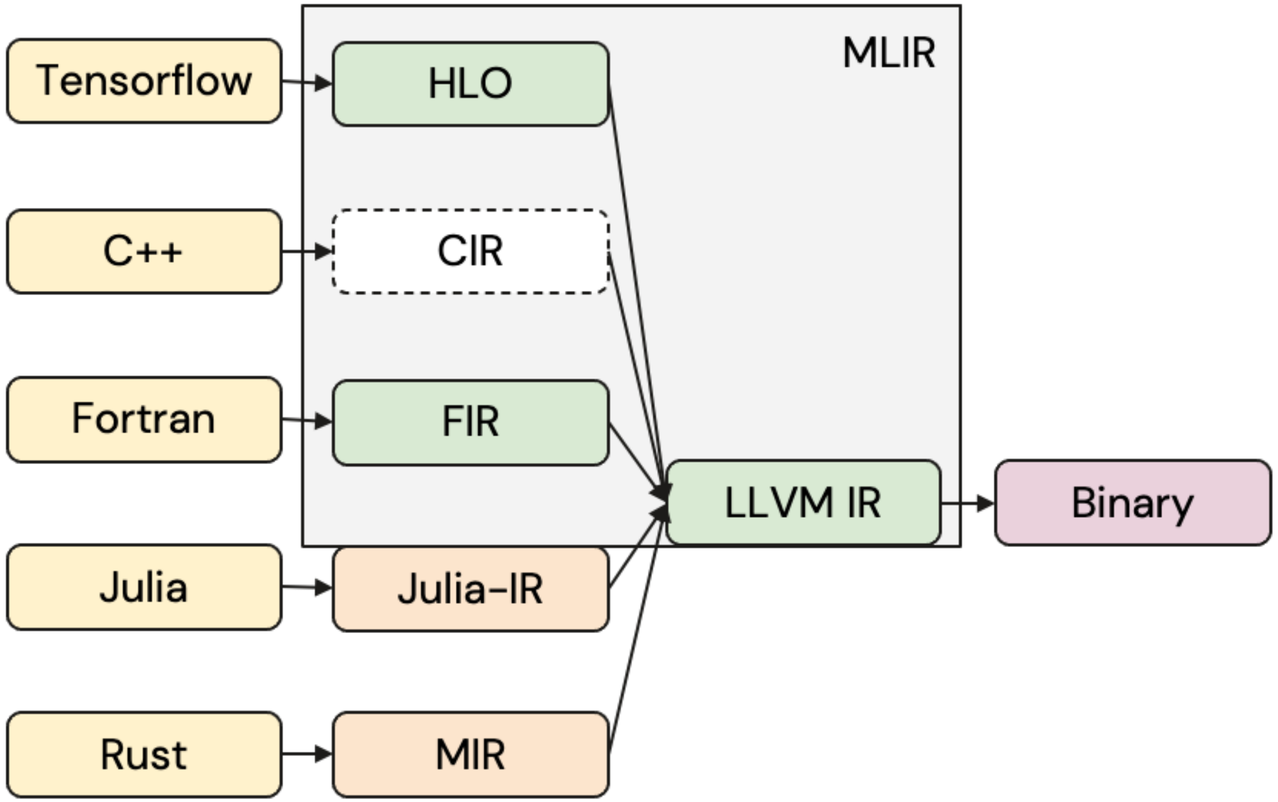
- Zoo of different MLIR dialects for various domains and optimizations
- Do we really have to write differentiation for each of the sub-abstractions again?



Multi-Level Differentiation

- Zoo of different MLIR dialects for various domains and optimizations
- Do we really have to write differentiation for each of the sub-abstractions again?
- No! By leveraging deferred/“multi-level” differentiation

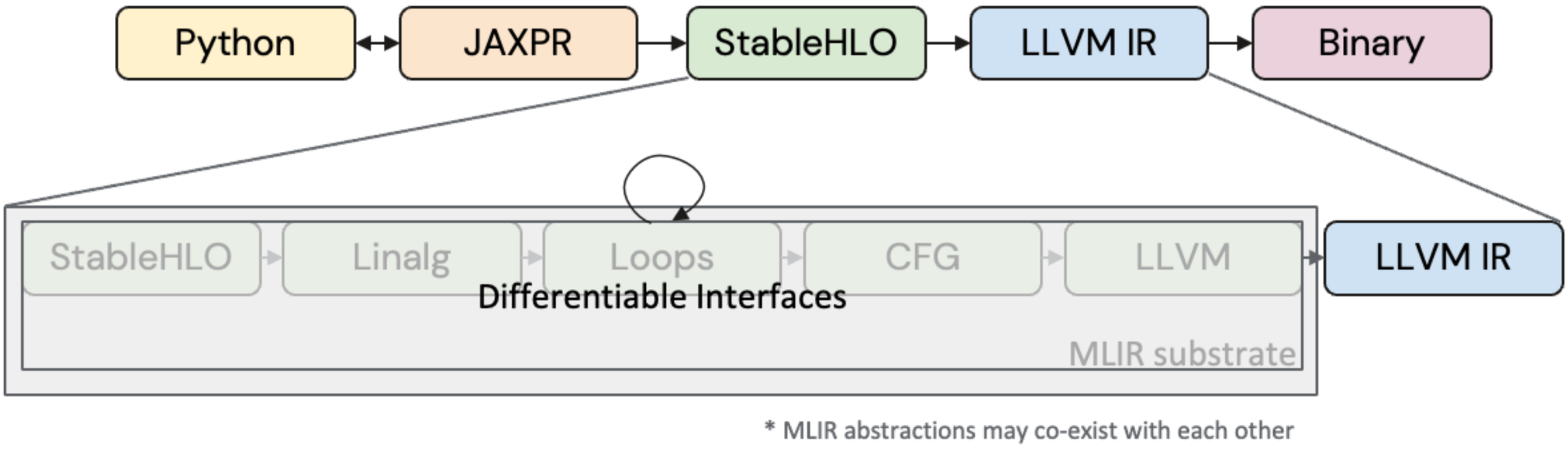




Integrating a Dialect with Enzyme

+

Differentiation Rules as Interfaces on Operations



Operation Interfaces

Interface Methods To Implement

- `createForwardModeTangent`
  generates the IR for forward tangent(s)

- `createReverseModeAdjoint`
  generates the IR for backward tangent(s)

- `cacheValues`
  generates the IR to store values from the primal computation needed for the tangent

- `createShadowValues`
  generates the IR to allocate and initialize shadow memory needed for the tangent

Example: Float Scalar/Vector Multiplication

```
d(res) = addf(mulf(LHS, d(RHS)),
              mulf(d(LHS), RHS));
```

```
d(LHS) += mulf(pop(cache[0]), d(res))
d(RHS) += mulf(pop(cache[1]), d(res))
```

```
push(cache[0], RHS)
push(cache[1], LHS)
```

```
Noop
```

Control Flow Interfaces

Interface Methods To Implement

- `createWithShadows`
  creates a copy of the operation with placeholders for shadow values in data flow

- `createReverseControlFlow`
  creates a copy of the operation with reverted control flow and placeholders for body

Example: “for” loop

```
-       scf.for i=0..N args(a, b)
    => scf.for i=0..N args(a, da, b, db)
```

```
-       scf.for i=0..N
    => scf.for ii=0..N {
         i=N-ii-1
       }
```

Type Interfaces

Interface Methods To Implement
[only needed for reverse mode]

- `getShadowType`
  returns mutable type suitable for storing in shadow memory. If mutable, can return self.

- `createNullValue`
  generates the IR initializing the a null shadow of this type

- `createAddToOp`
  generates the IR adding a value of this type to the shadow

Example: Float

```
memref<self>
```

```
%shadow = memref.alloca()
%shadow[] = constant(cast<..>(0.0))
```

```
%shadow[] += val
```

Concise AD Definitions in ODS/Tablegen

```
def : MLIRDerivative<"arith", "DivFOp", (Op $x, $y),
 // Reverse mode.
 [
   (DivF (DiffeRet), $y),
   (NegF (MulF (DivF (DiffeRet), $y), (DivF $x, $y)))
 ],
 // Forward mode (defaults to sum of reverse mode in absence).
```

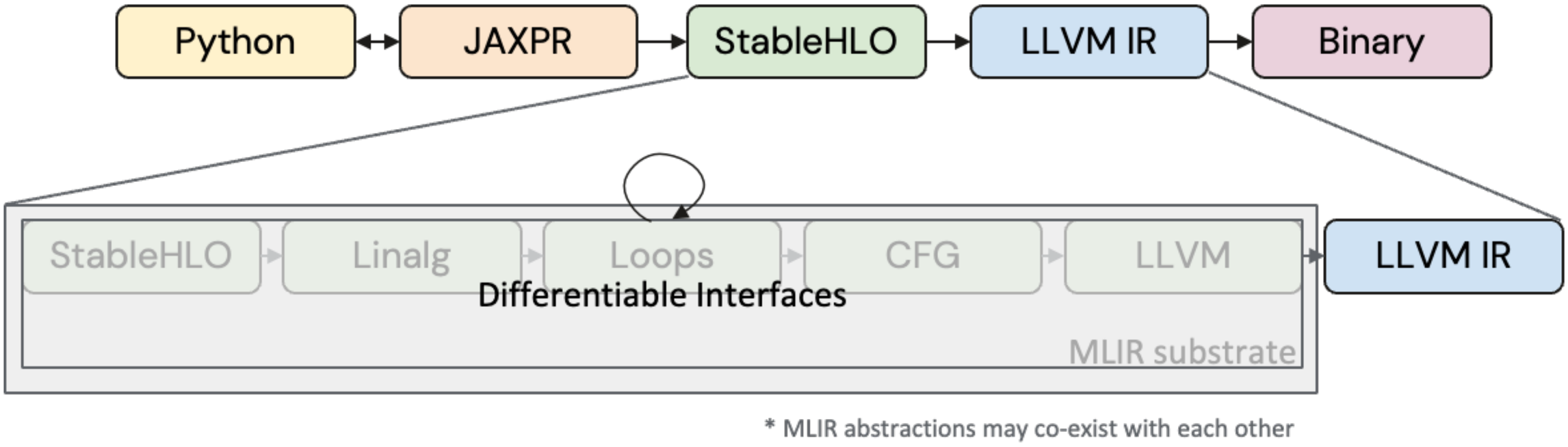
Concise AD Definitions in ODS/Tablegen

```
def : MLIRDerivative<"arith", "DivFOp", (Op $x, $y),
 // Reverse mode.
 [
   (DivF (DiffeRet), $y),
   (NegF (MulF (DivF (DiffeRet), $y), (DivF $x, $y)))
 ],
 // Forward mode (defaults to sum of reverse mode in absence).
 (DivF (SubF (SelectIfActive $x, (MulF (Shadow $x), $y),
                                 (ConstantFP<"0","arith","ConstantOp"> $x)),
             (SelectIfActive $y, (MulF (Shadow $y), $x),
                                 (ConstantFP<"0","arith","ConstantOp"> $y))),
       (MulF $y, $y)),
 // Activity flow between $x,$y and the result without storage.
 [($x DiffeRet "0"), ($y DiffeRet "0")],
>;
```

Ongoing Work

+

What is the Right Level of Abstraction for AD?

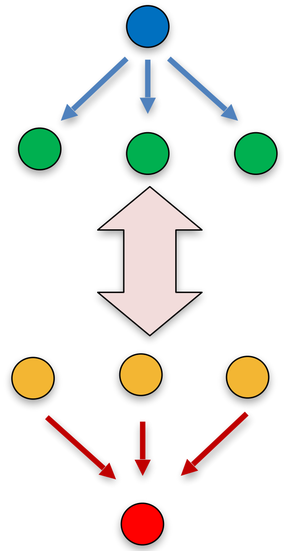


* MLIR abstractions may co-exist with each other

MLIR Enables Joint Optimization of Differentiation + Parallelism

Differentiation changes how we want to parallelize code

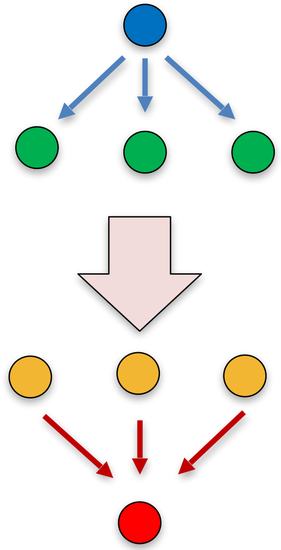
- Scatters <-> Gathers



MLIR Enables Joint Optimization of Differentiation + Parallelism

Differentiation changes how we want to parallelize code

- Scatters <-> Gathers
- Can create **race conditions**



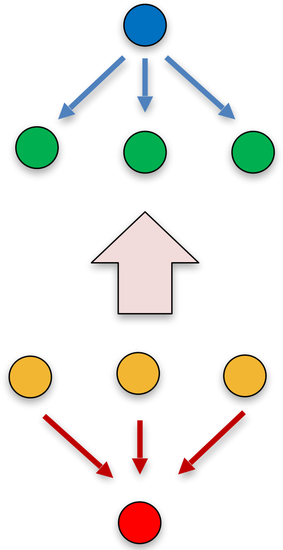
```
void set(double* ar, double val) {
  pfor(int i=0; i<n; i++) {
     ar[i] = val;
  }
  …
}
```

```
void grad_set(double* ar, double* d_ar) {
  double d_val = 0;
  pfor (int i=0; i<n; i++) {
     d_val += d_ar[i];
  }
  …
```

MLIR Enables Joint Optimization of Differentiation + Parallelism

Differentiation changes how we want to parallelize code

- Scatters <-> Gathers
- Can create **race conditions**
- Serial Primal => Parallel Derivative



```
double sum(double* x) {
  double S = 0.0;
  for (int i = 0; i < N; i++) {
    S += x[i] * x[i];
  }
  return S;
}
```

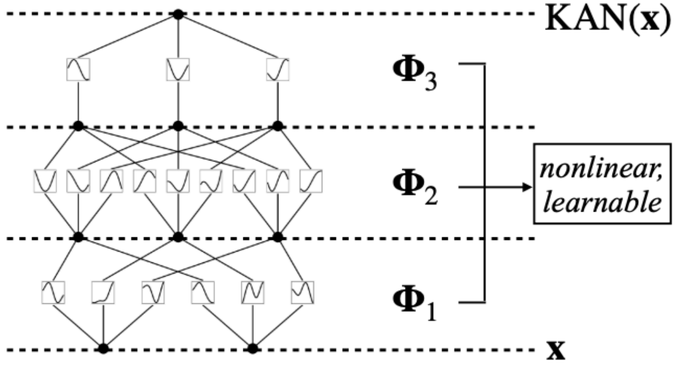
```
void grad_sum(double* x, double* d_x,
              double d_S) {
  pfor (int i = 0; i < N; i++) {
    d_x[i] += 2.0 * x[i] * d_S;
  }
}
```

Brief Results

+

EnzymeMLIR in Julia (via Reactant.jl MLIR Frontend)

CUDA KAN network




```
Forward (regular Julia)
 47.586 us ( 248 allocations)
234.233 us (1022 allocations)
134.028 us ( 668 allocations)

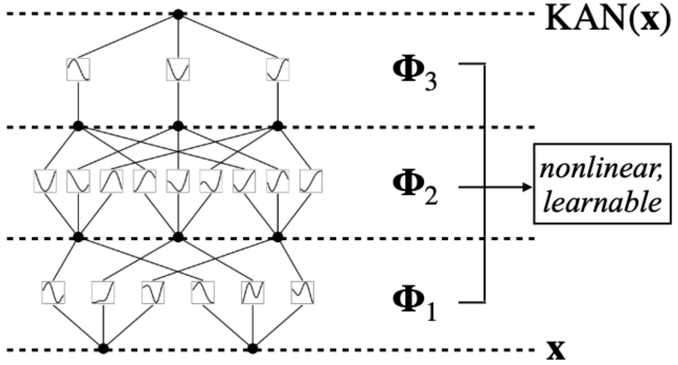
Forward (Reactant)
 39.873 us (  2 allocations)
 68.439 us (  6 allocations)
 55.889 us (  6 allocations)
```

```
Backwards (Zygote + Julia)
 289.319 us ( 575 allocations)
2099.000 us (1055 allocations)
1772.000 us ( 877 allocations)

Backwards (EnzymeMLIR + Reactant)
  51.691 us (  3 allocations)
 104.193 us (  3 allocations)
  80.020 us (  3 allocations)
```

EnzymeMLIR in Julia (via Reactant.jl MLIR Frontend)

CUDA KAN network

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  104.193 us (  3 allocations)
   80.020 us (  3 allocations)
```

2.14x speedup (Primal)

13.57x speedup (Derivative)

Takeaways

- Compilers Make Differentiation Fast and Easy to use
  - Key to this is interaction with Optimization
- MLIR enables preserving and optimizing high-level structure
- EnzymeMLIR enables differentiation to combine with high-level optimization
  - Extensible for use with any MLIR dialect
  - Enables significant performance gains when combined with linear algebra, parallel optimizations
- All open source (GitHub.com/EnzymeAD/Enzyme ; GitHub.com/EnzymeAD/Enzyme-JaX ; GitHub.com/EnzymeAD/Reactant.jl)

Case Study: ReLU3

C Source

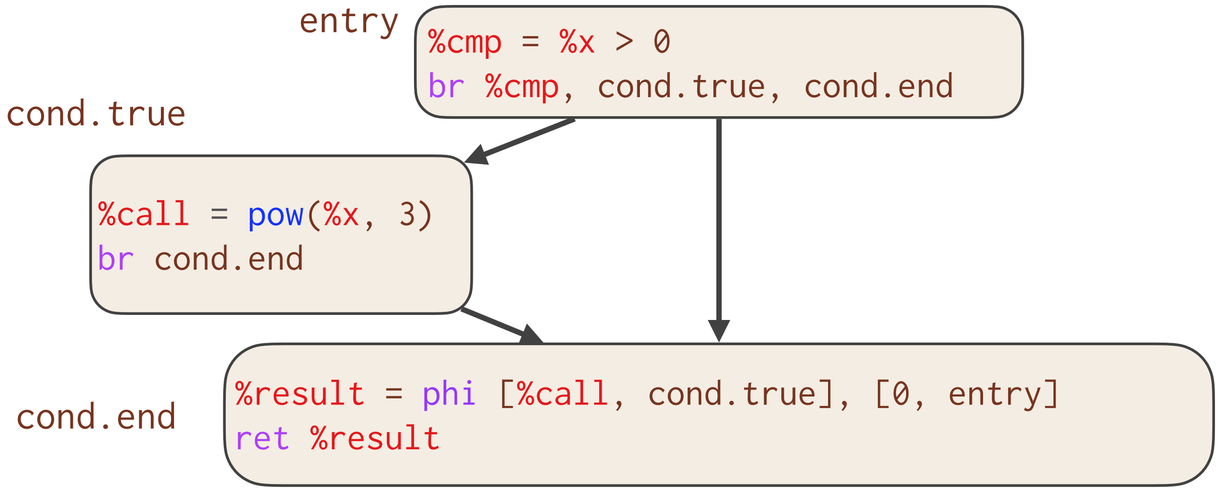
```
double relu3(double x) {
  double result;
  if (x > 0)
    result = pow(x, 3);
  else
    result = 0;
  return result;
}
```

Enzyme Usage

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

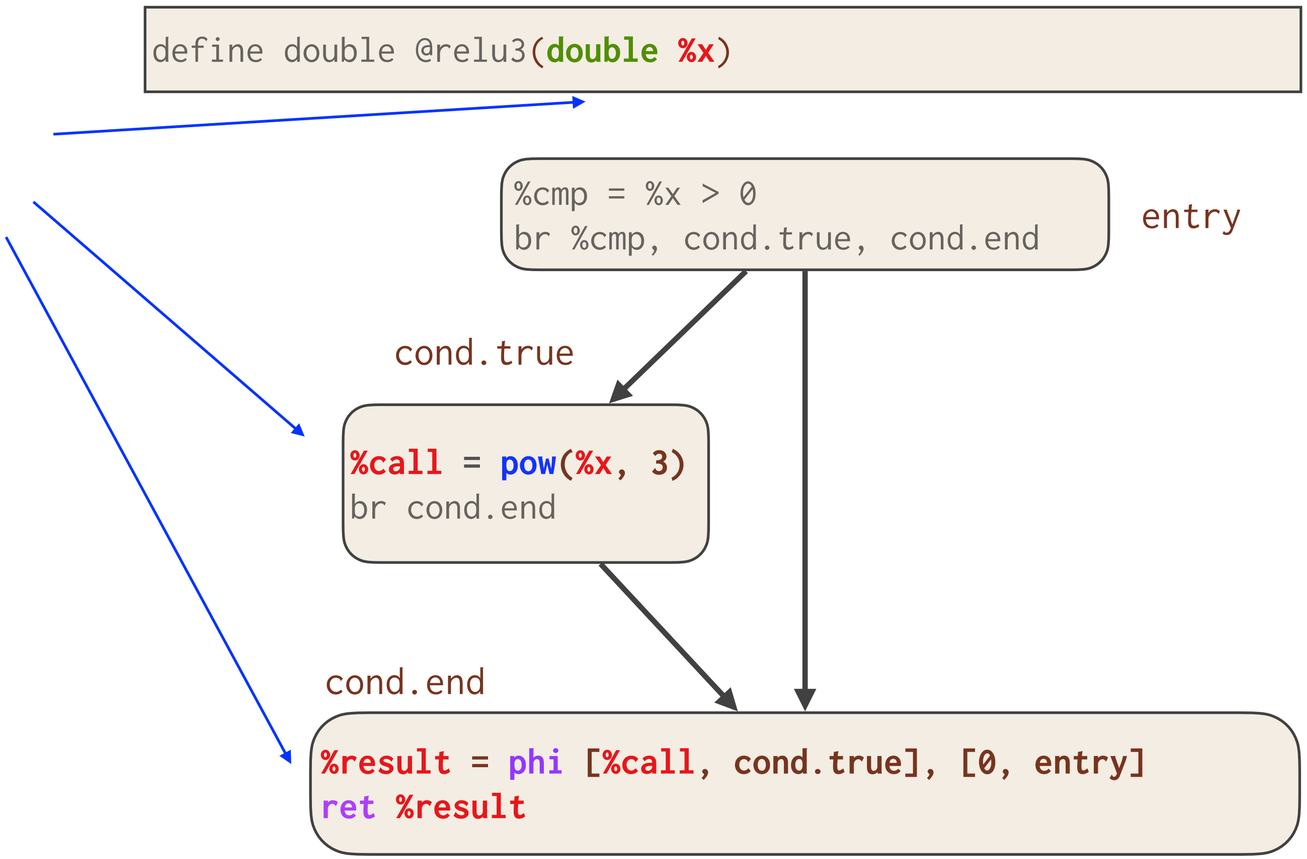
LLVM

```
define double @relu3(double %x)
```

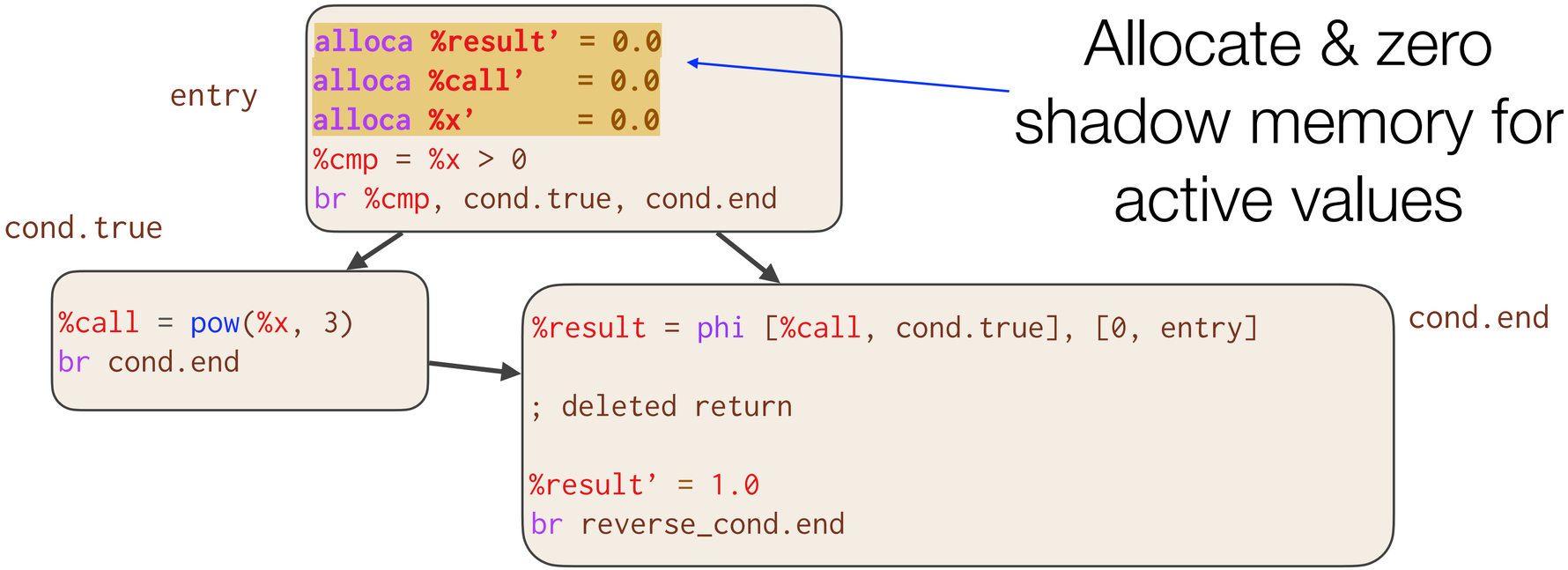


Case Study: ReLU3

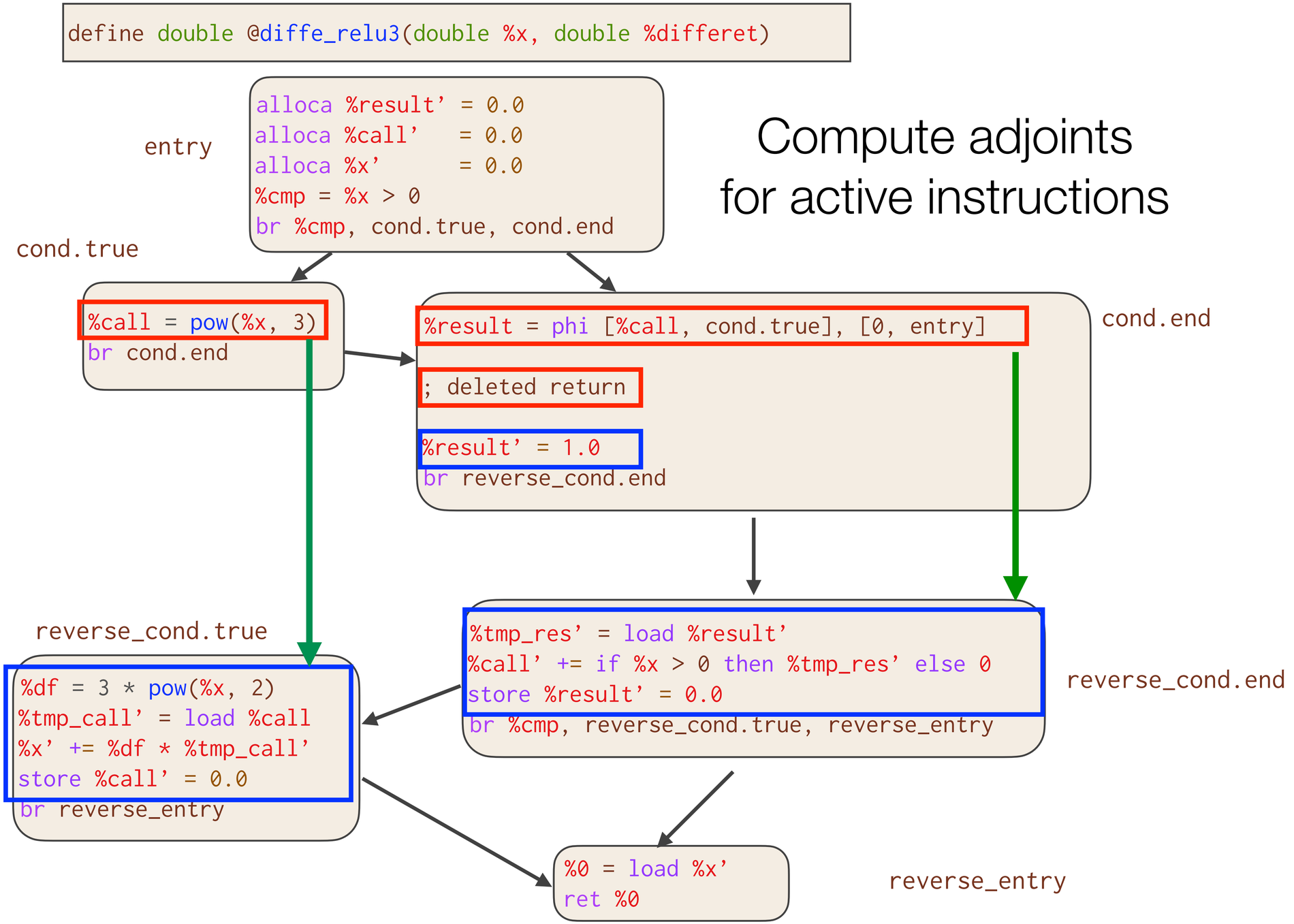
Active Instructions



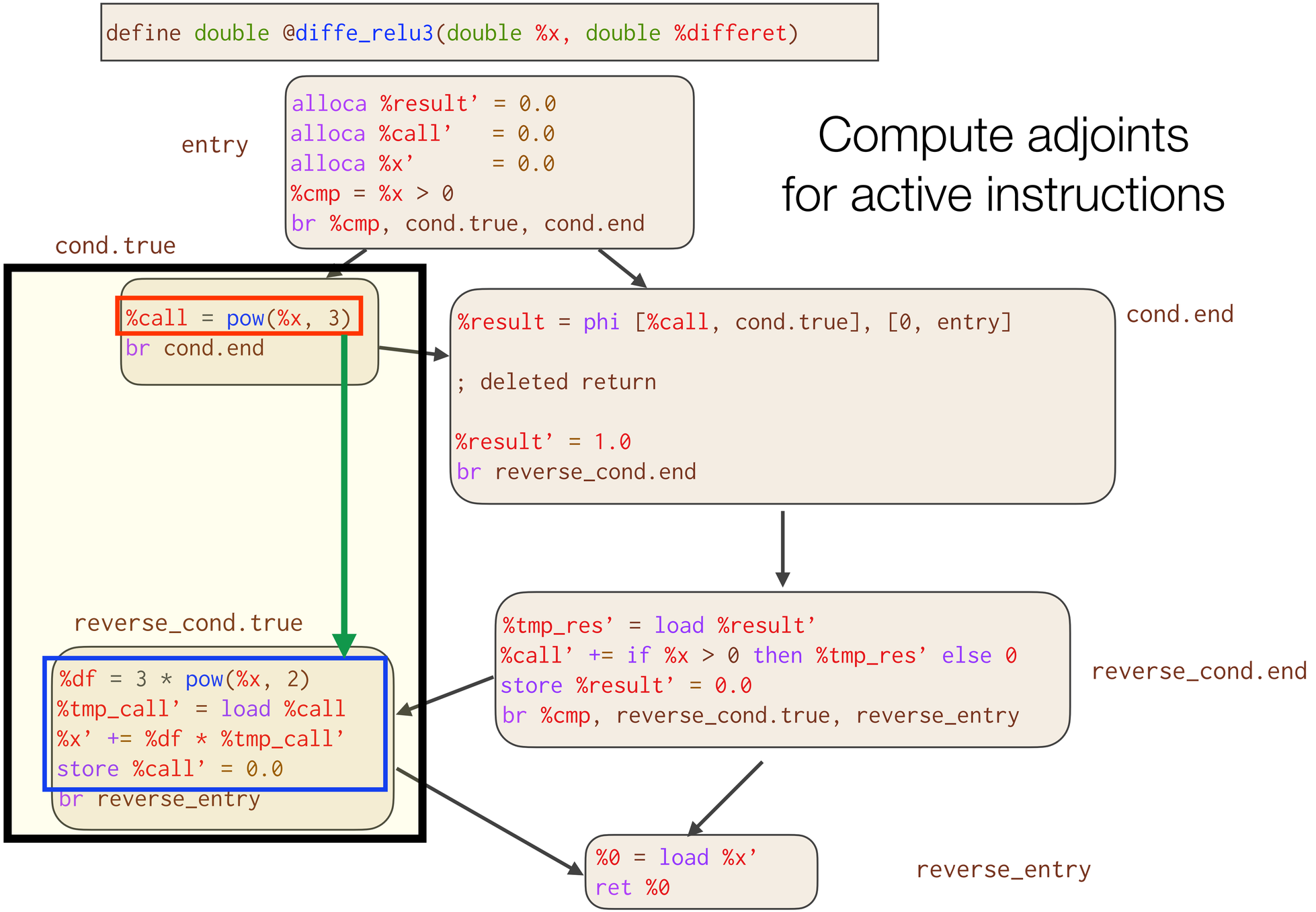
```
define double @diffe_relu3(double %x, double %differet)
```



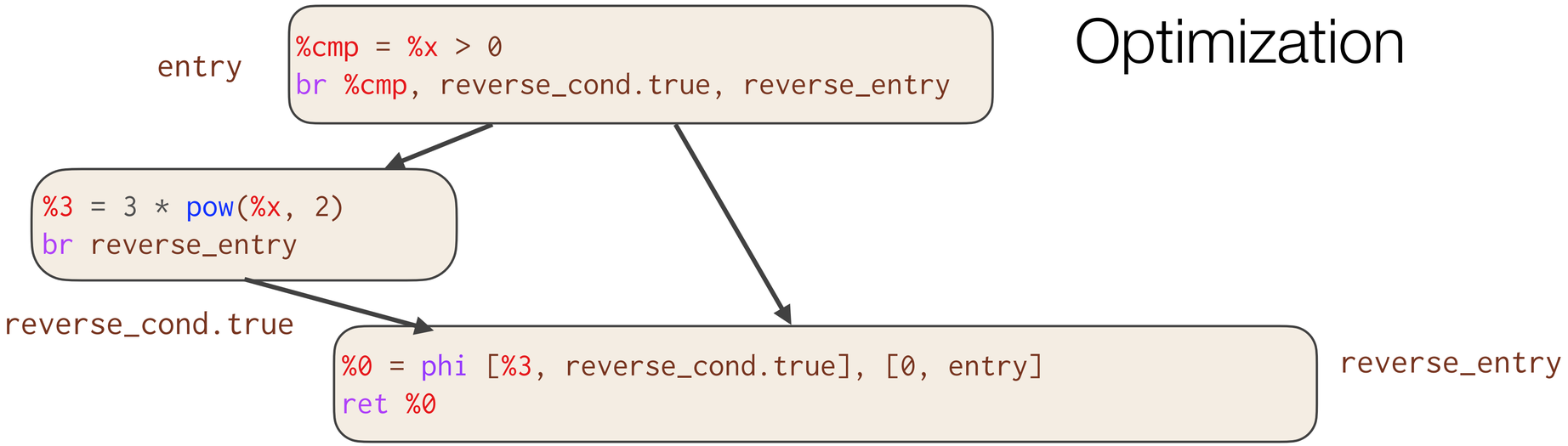
Allocate & zero shadow memory for active values



Compute adjoints for 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
%result = phi [%call, cond.true], [0, entry]
; deleted return
%result' = 1.0
br reverse_cond.end
cond.end
reverse_cond.true
%df = 3 * pow(%x, 2)
%tmp_call' = load %call
%x' += %df * %tmp_call'
store %call' = 0.0
br reverse_entry
%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.end
%0 = load %x'
ret %0
reverse_entry
Compute adjoints
for active instructions

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



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;
}
```