An Introduction to Enzyme & Some Fun Recent Results

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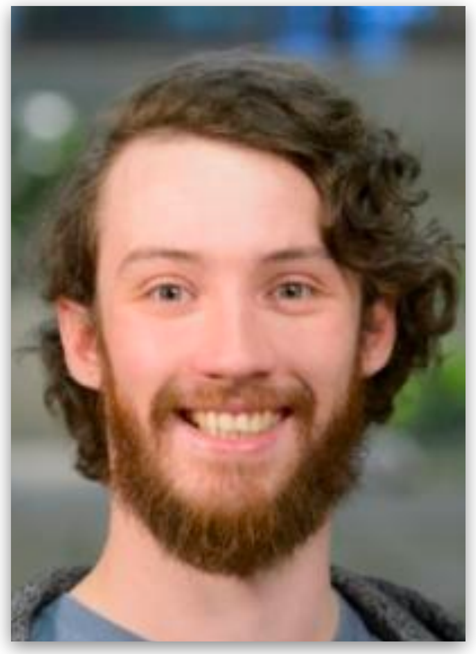
Johannes Doerfert


Jan Hückelheim


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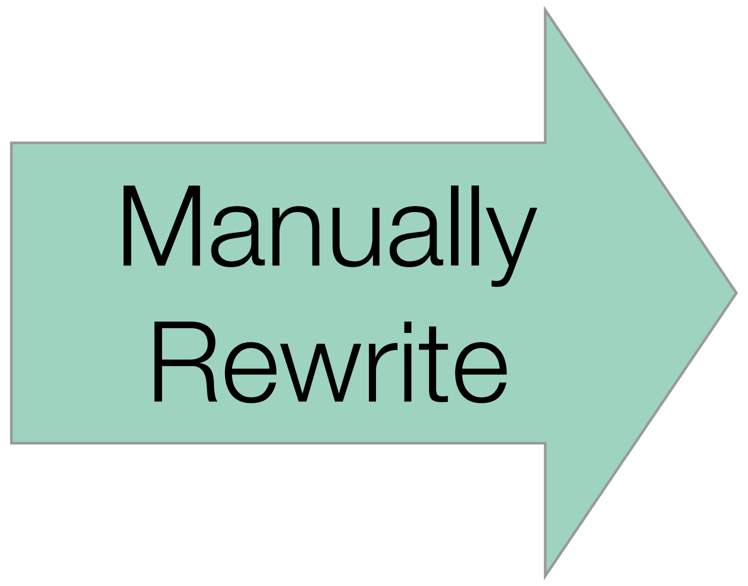
& more

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;
}
```

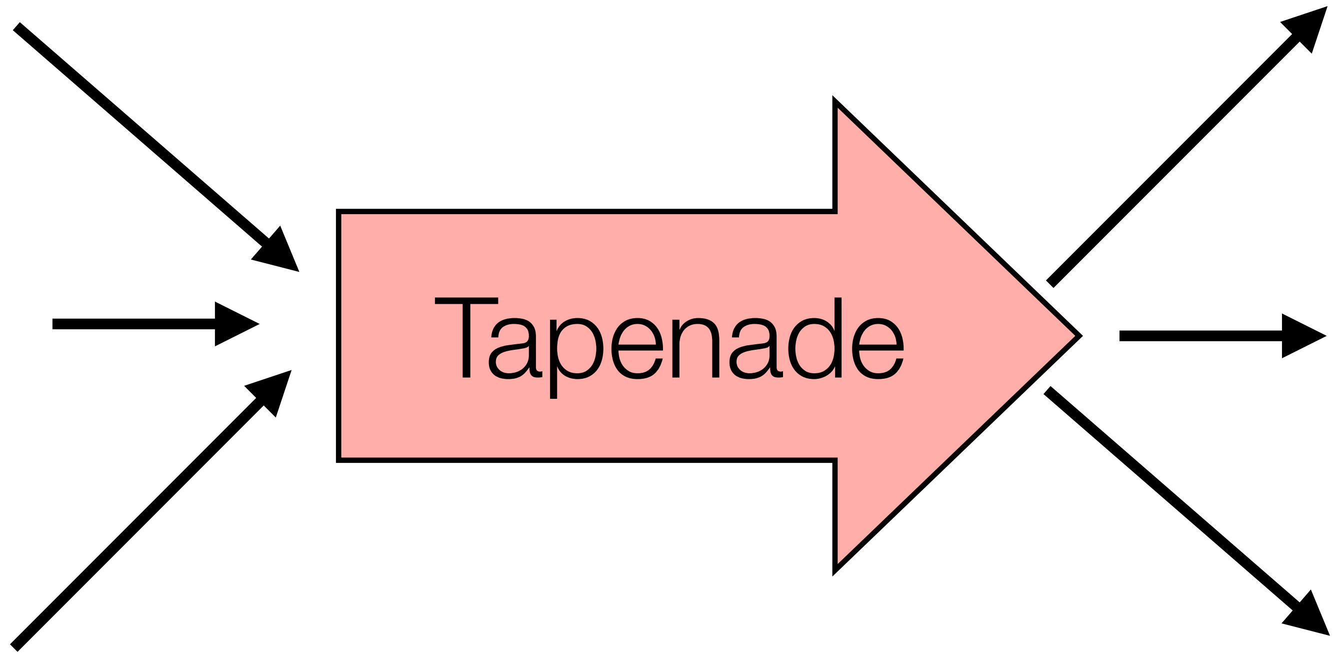
```
adept::Stack stack;
adept::adouble inp = 3.14;

// 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

```c
// myfile.h
```

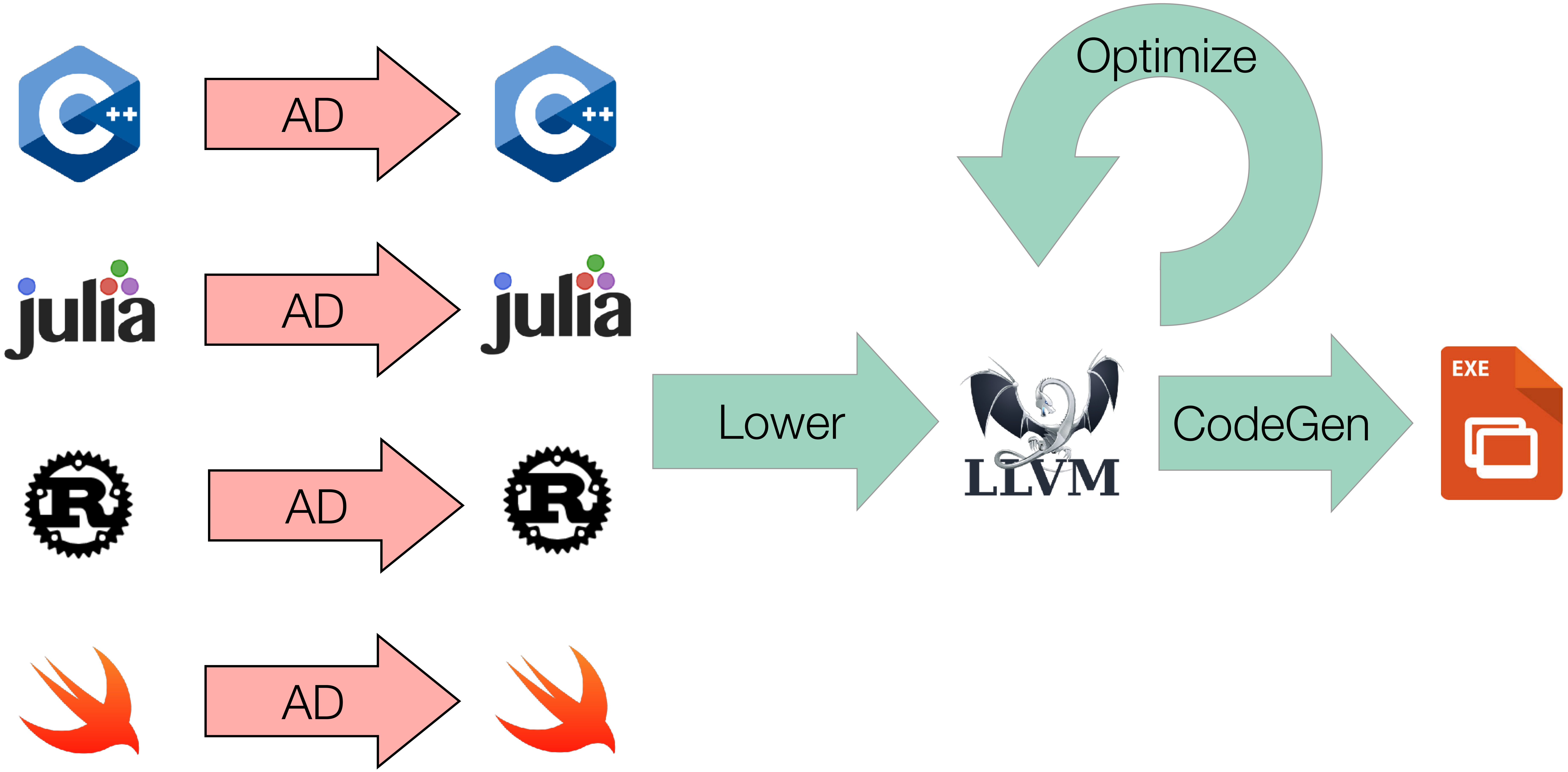
```c
// myfile.c
double relu3(double x) {
  if (x > 0)
    return pow(x,3)
  else
    return 0;
}
```




```c
// 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

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

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

Optimize

$O\left(n\right)$

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res = mag(in)
for i=0..n {
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AD

$O\left(n\right)$

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

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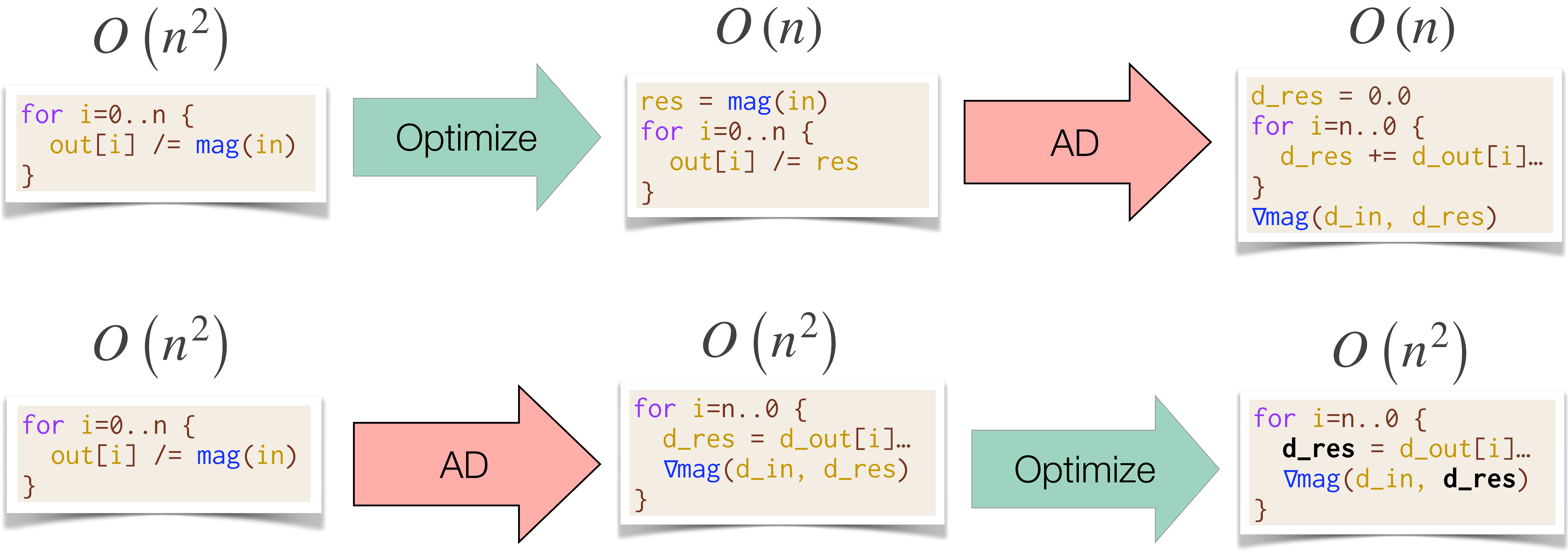
AD

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

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

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)
}
```

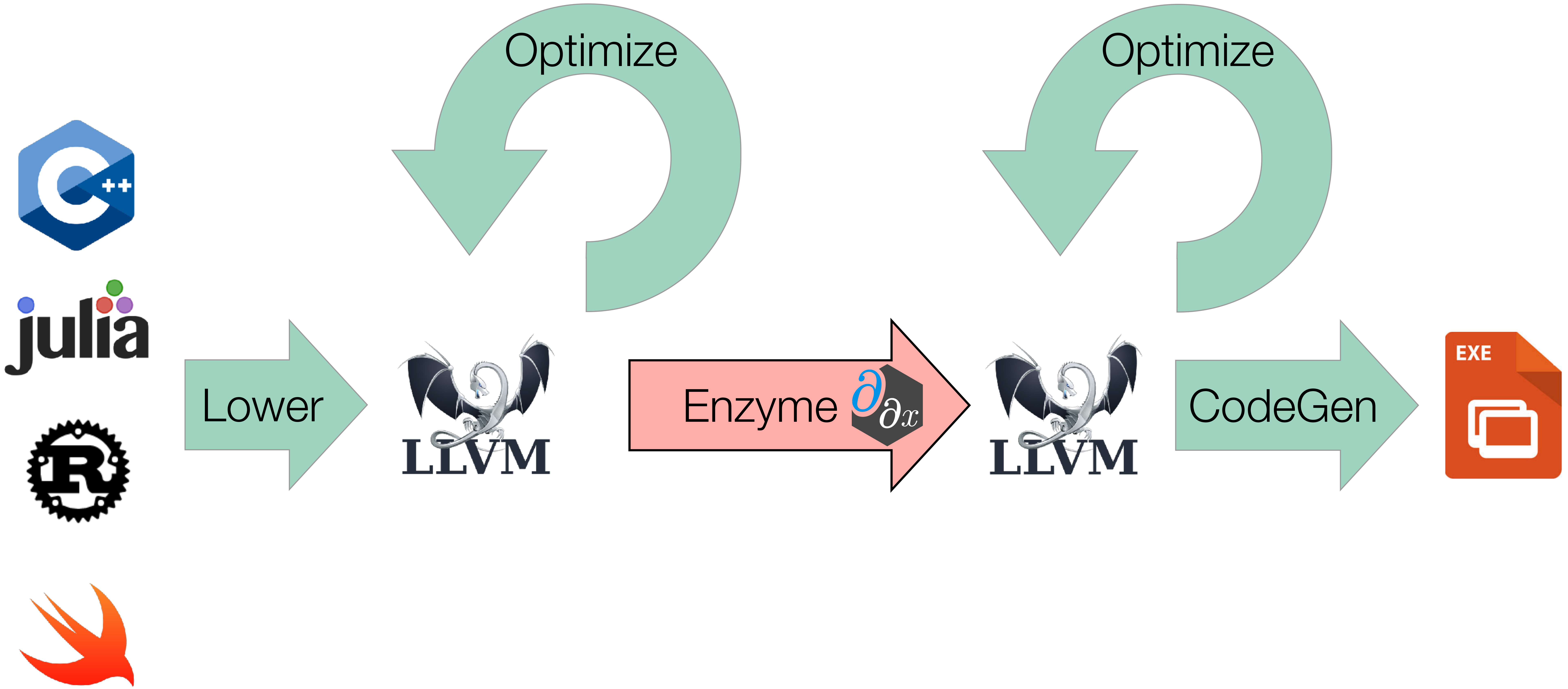
Optimize

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

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

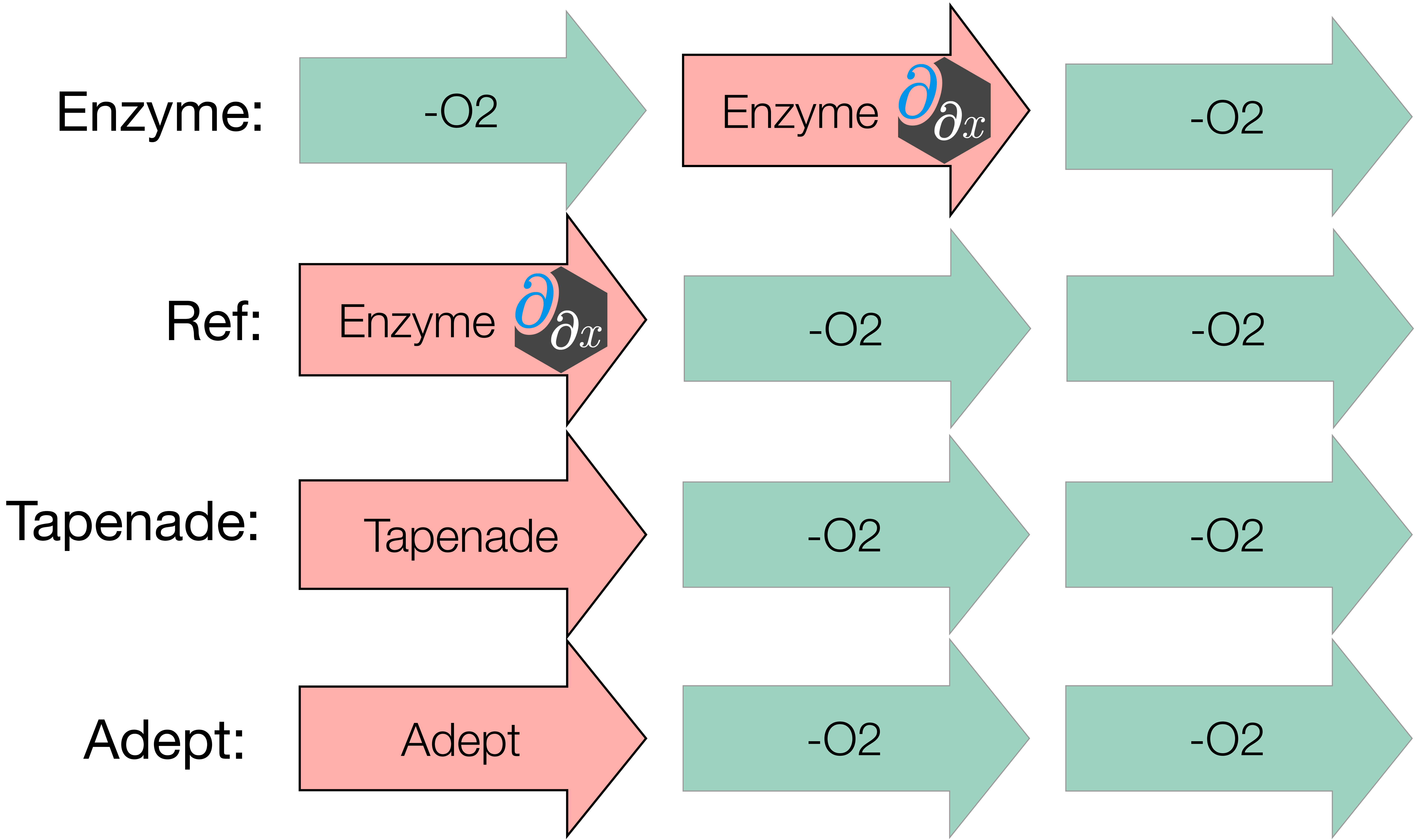
Enzyme Approach

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

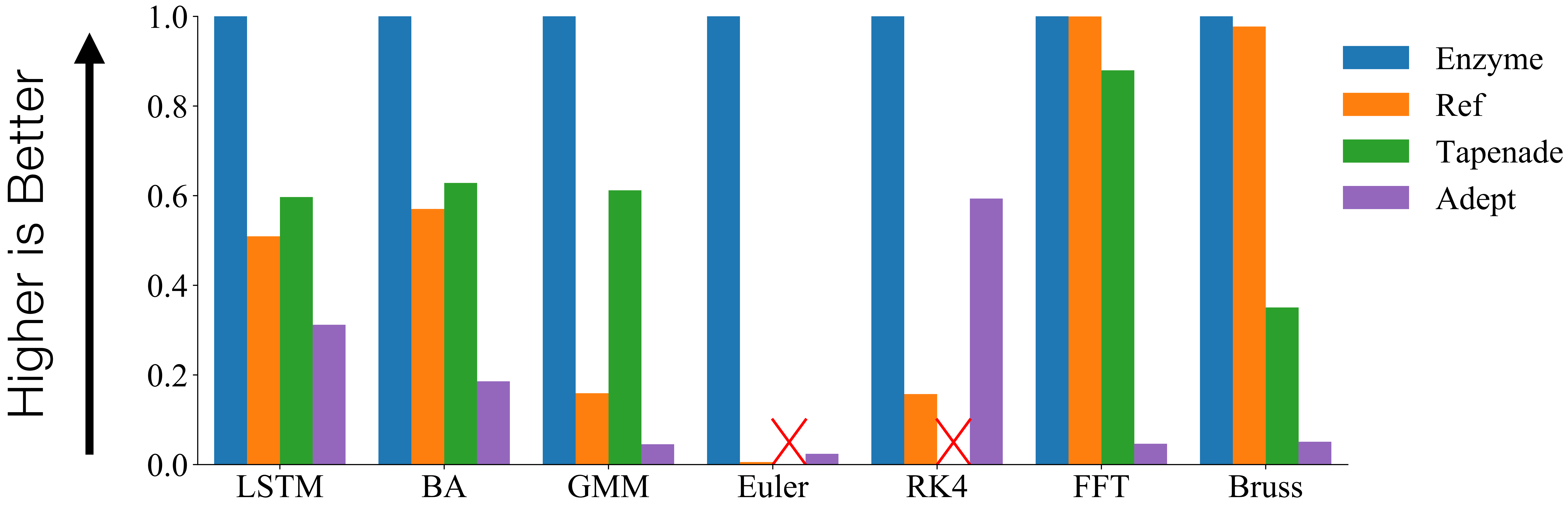


Experimental Setup

- 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];
...

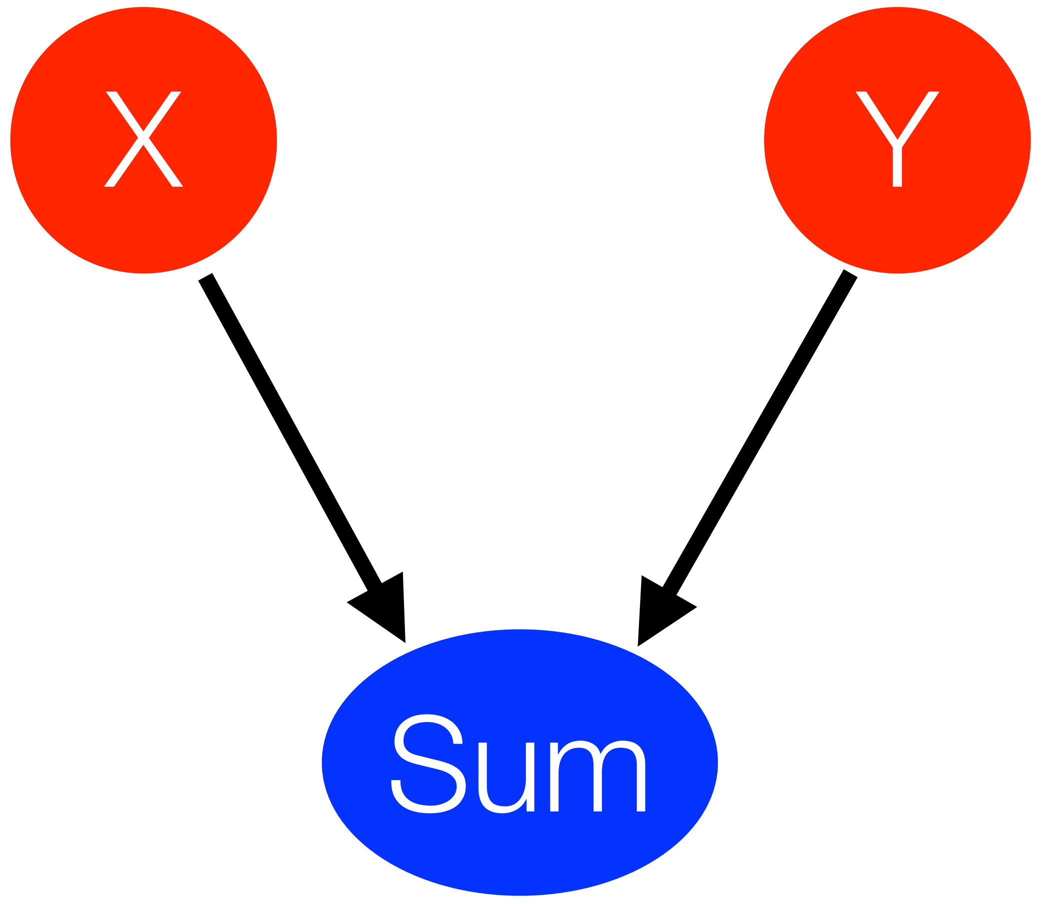
delete[] x_cache;
```

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];

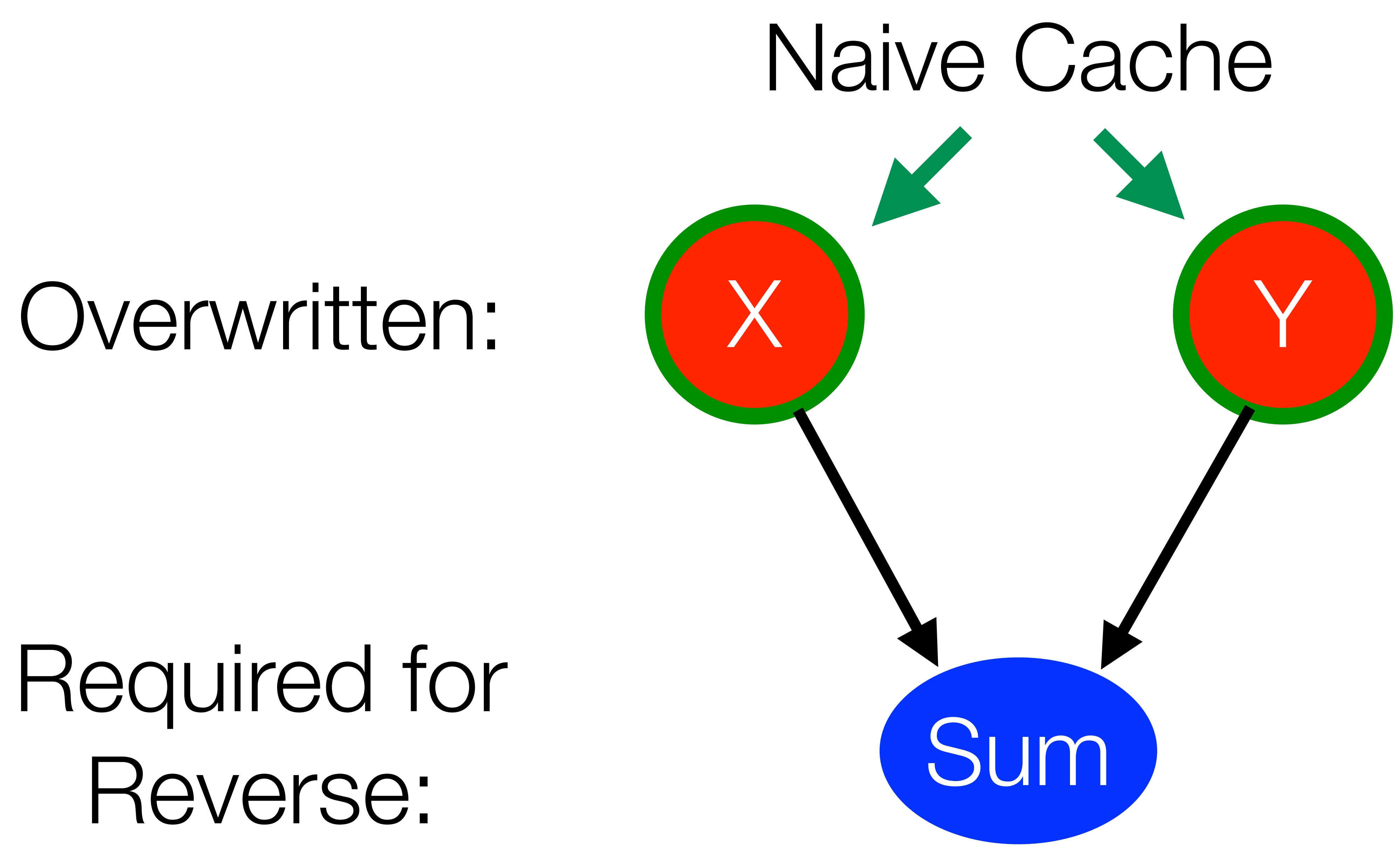

  use(sum);
}

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];

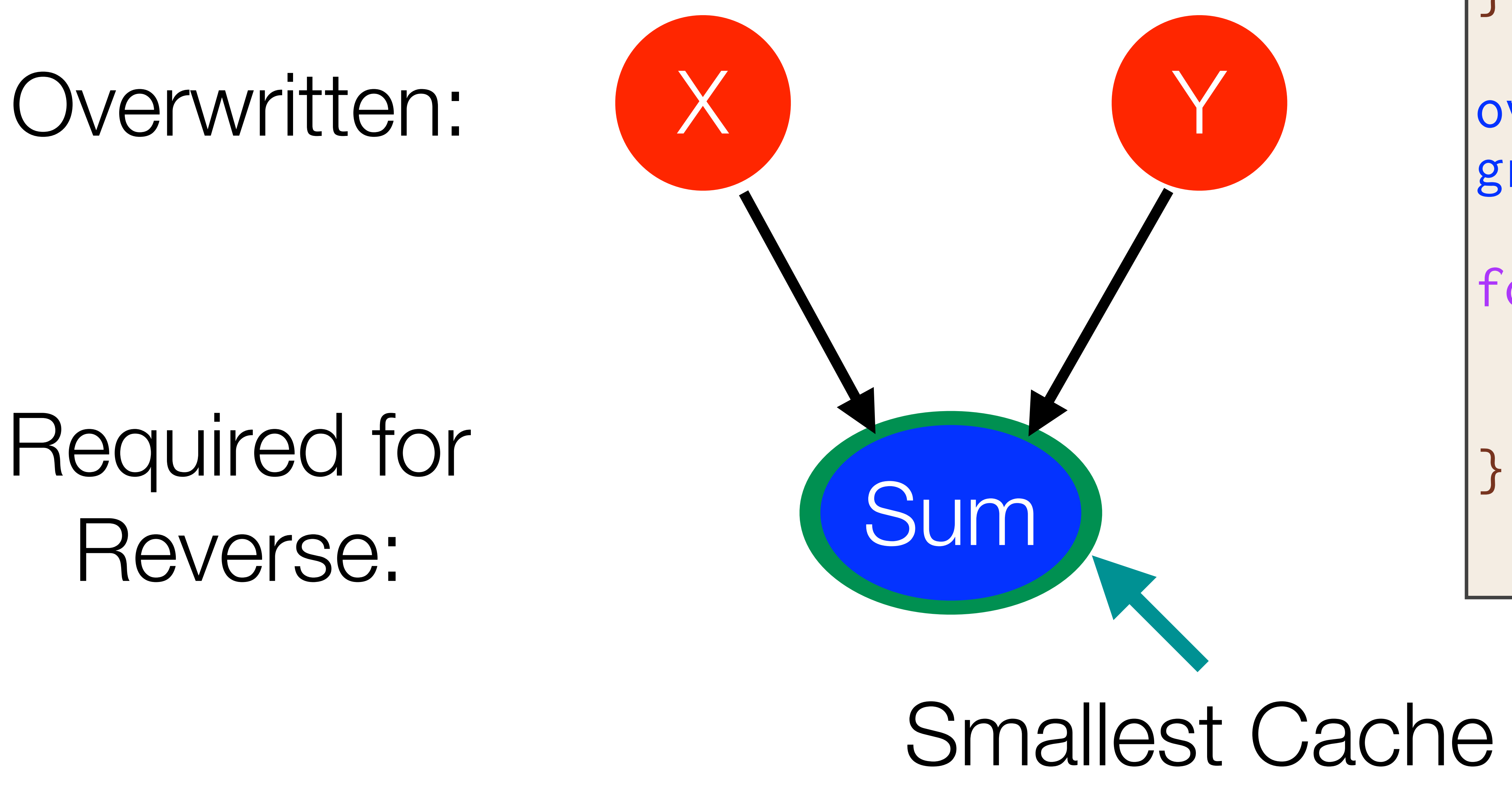
for(int i=0; i<10; i++) {
  double sum = x[i] + y[i];
  sum_cache[i] = sum;

  use(sum);
}

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

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

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

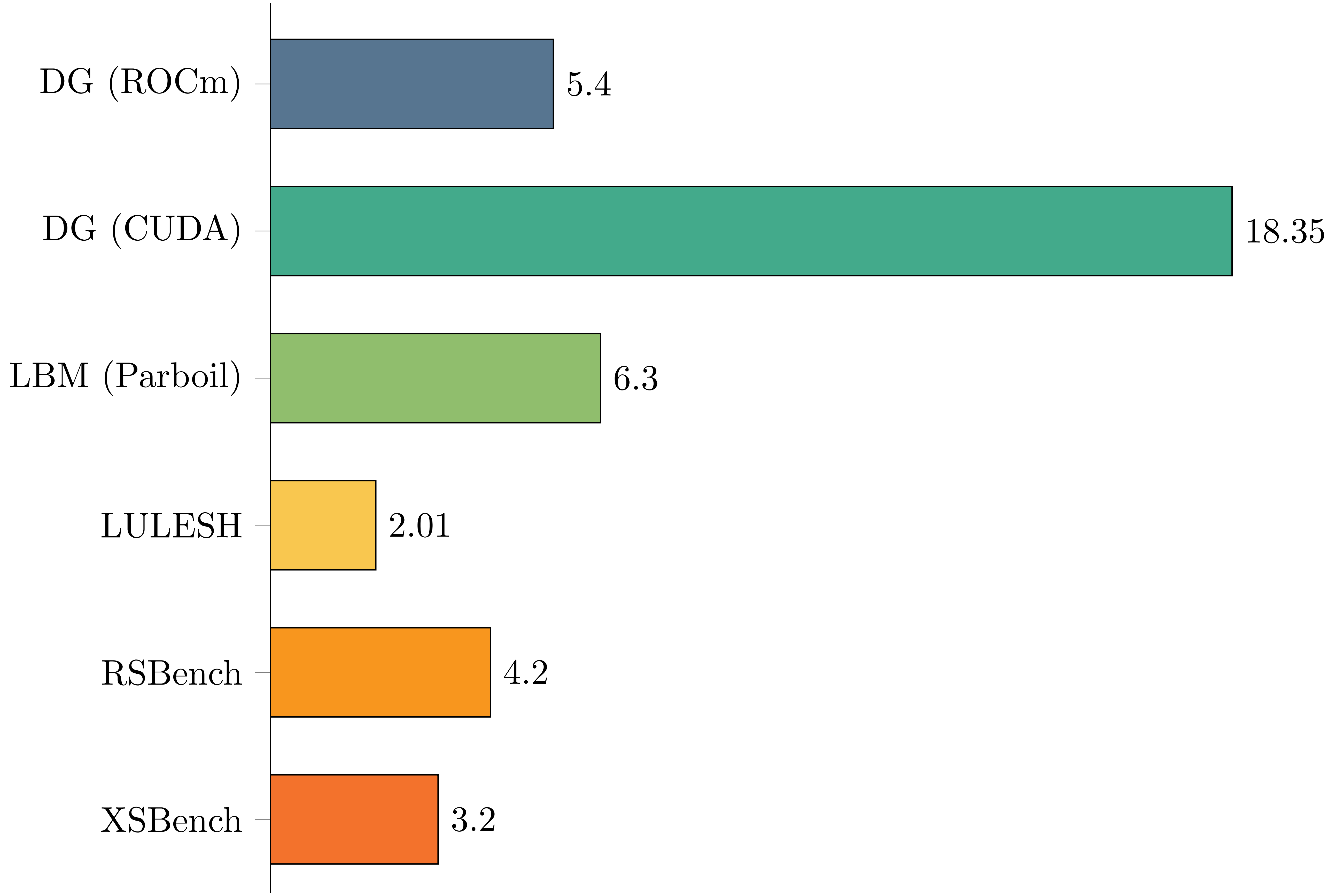


Novel AD + GPU Optimizations

- 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)



GPU Gradient Overhead

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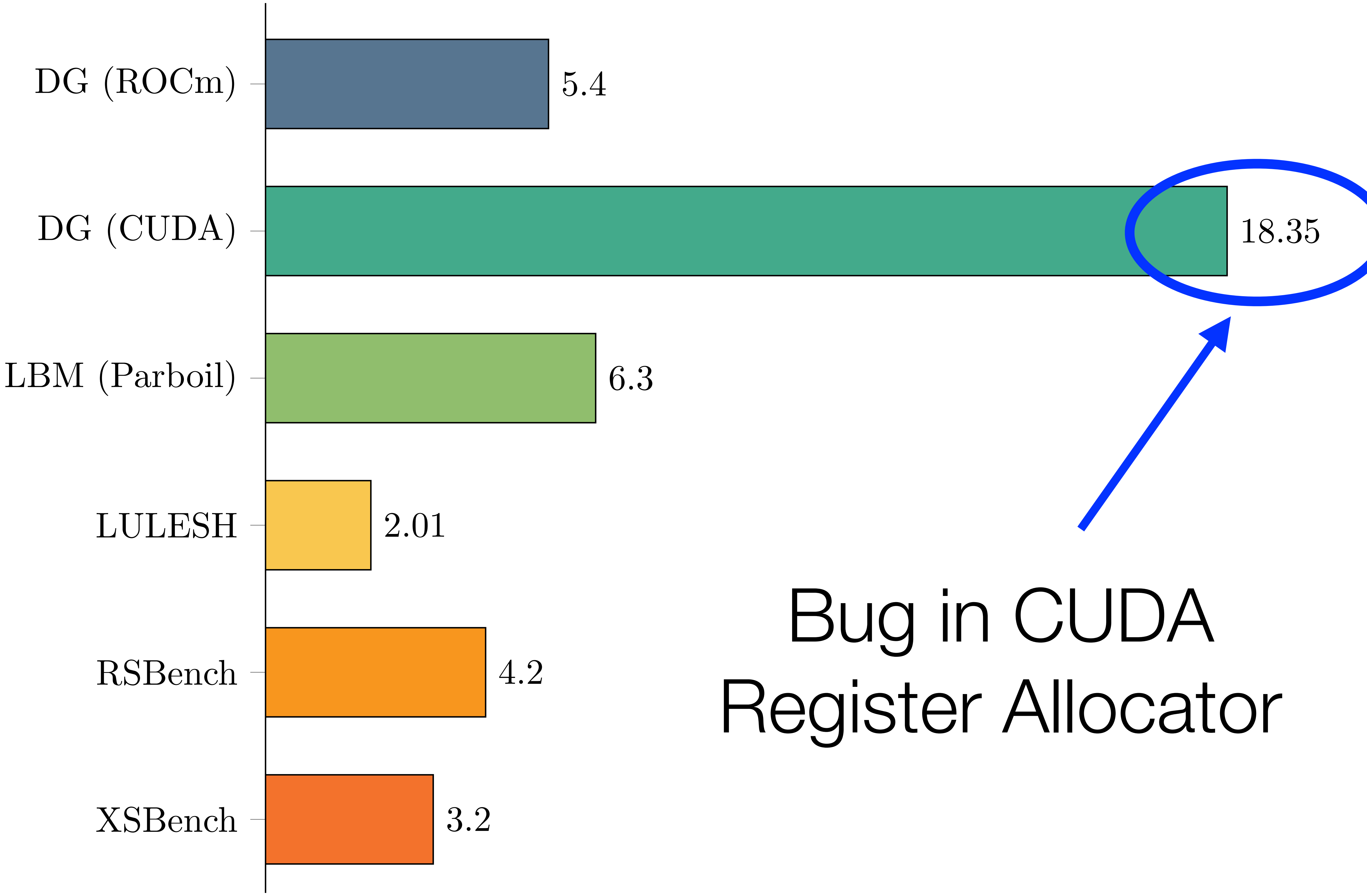


Ablation Analysis of Optimizations

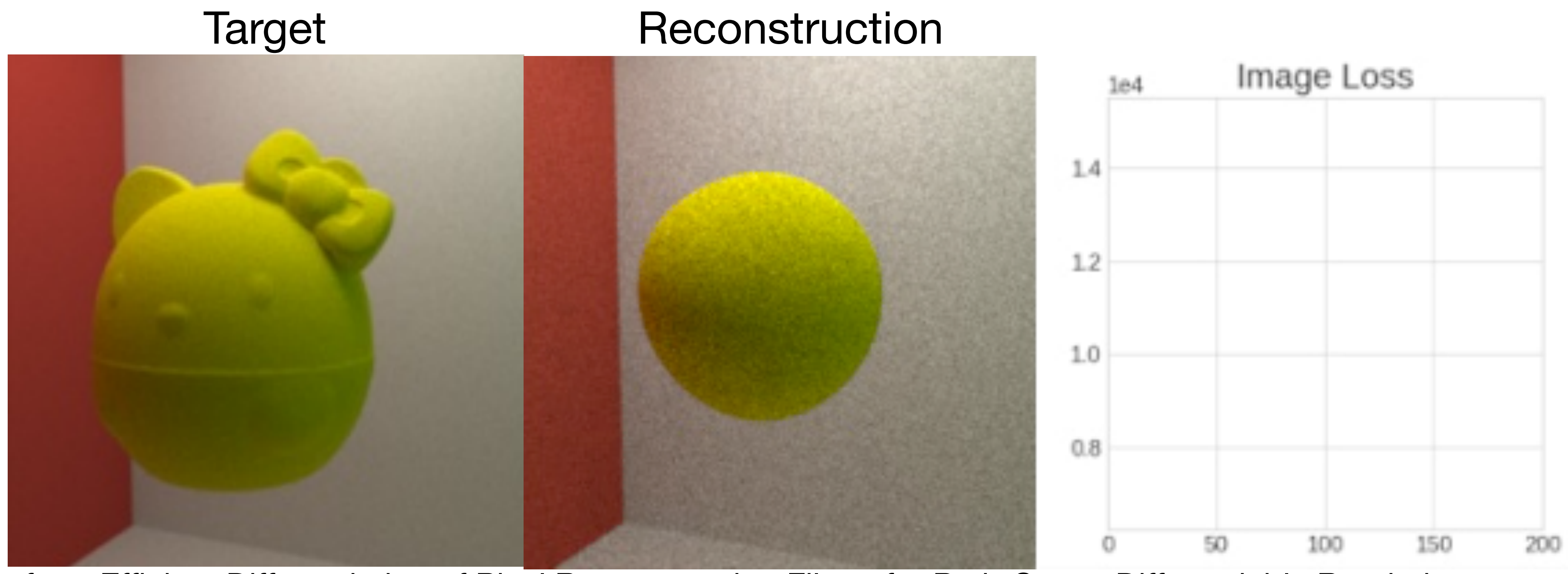
Ablation Analysis of Optimizations

Ablation Analysis of Optimizations

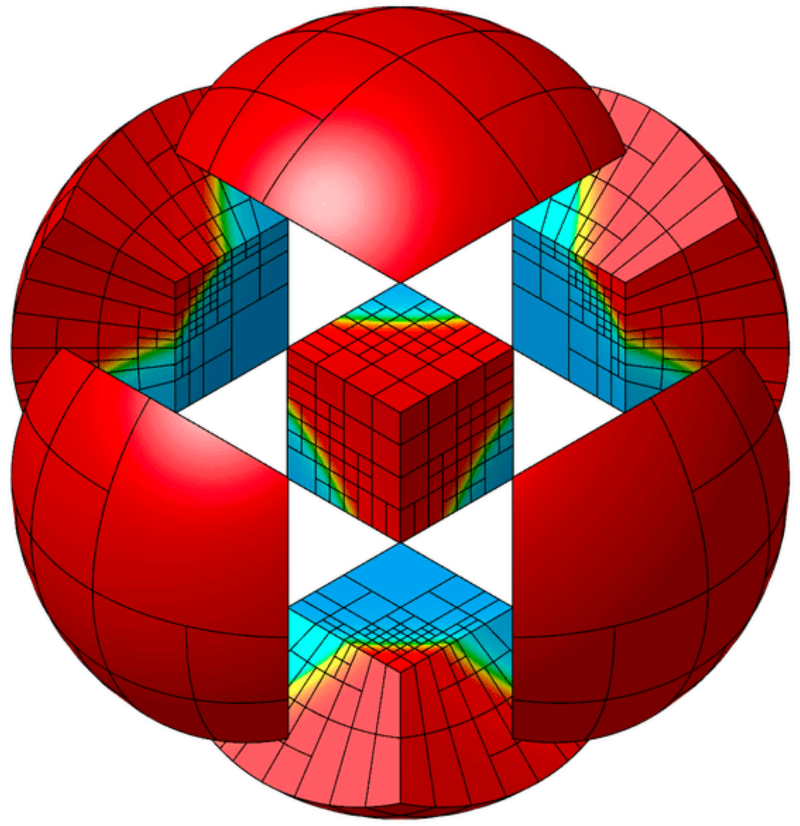
Ablation Analysis of Optimizations

GPU AD is Intractable Without Optimization!

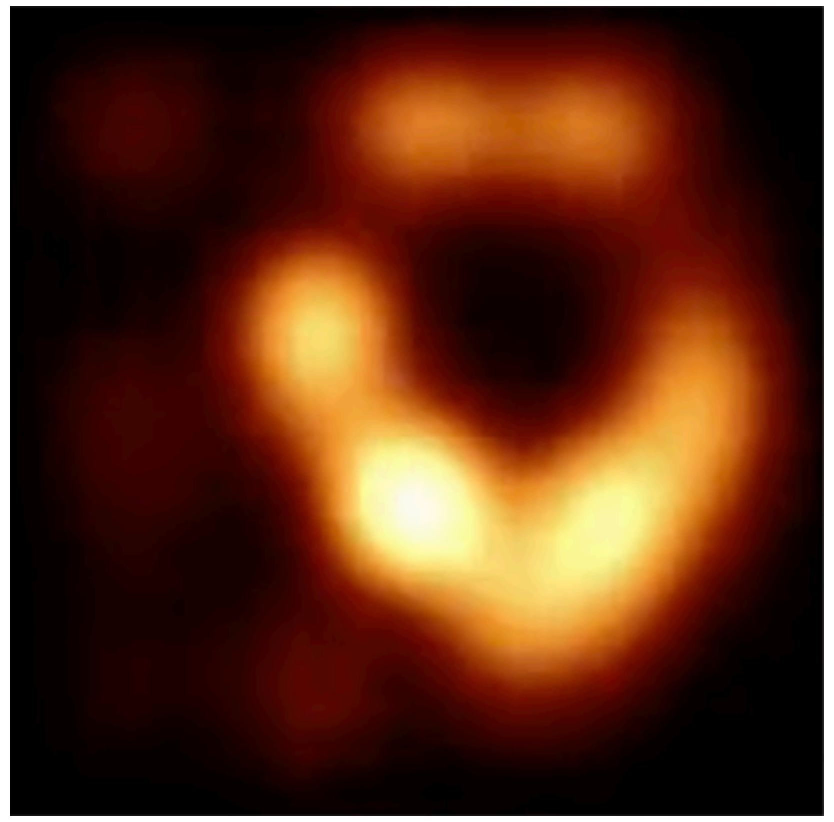
Enzyme-Powered Applications



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



from MFEM Team at LLNL



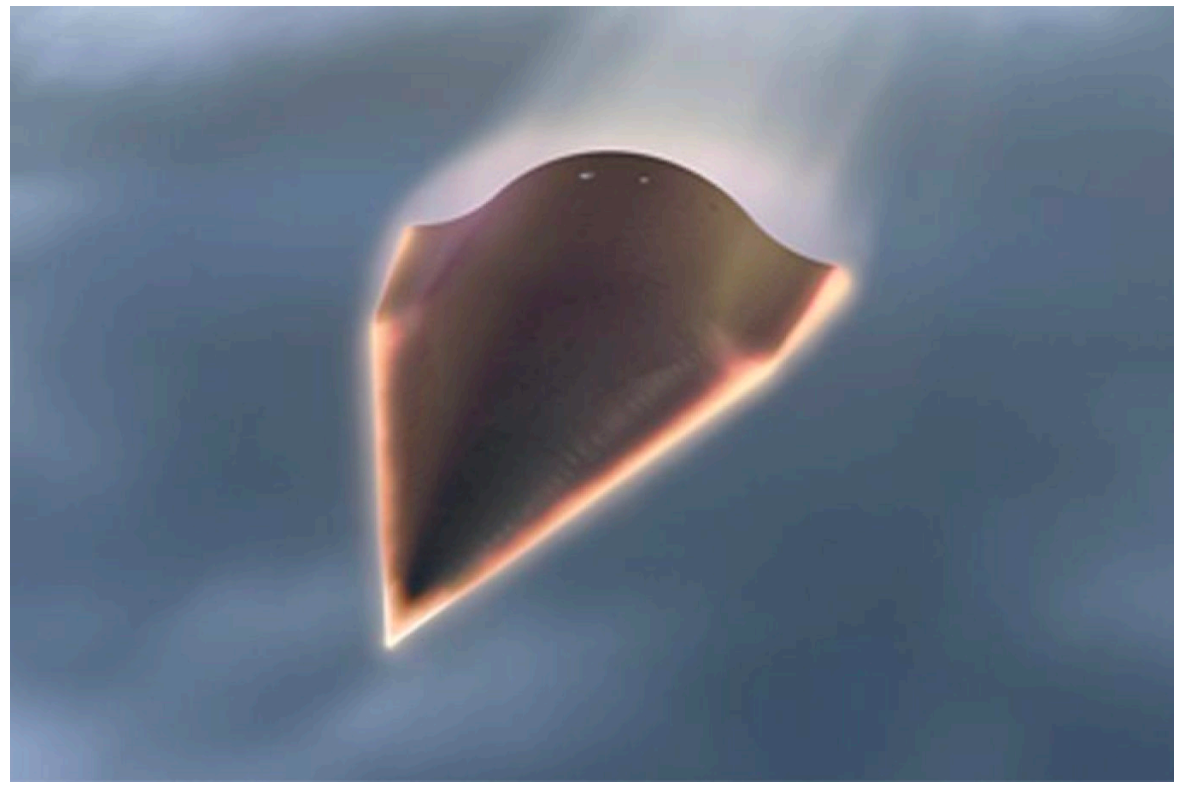
>100x speedup!

Prior:
5 days (cluster)

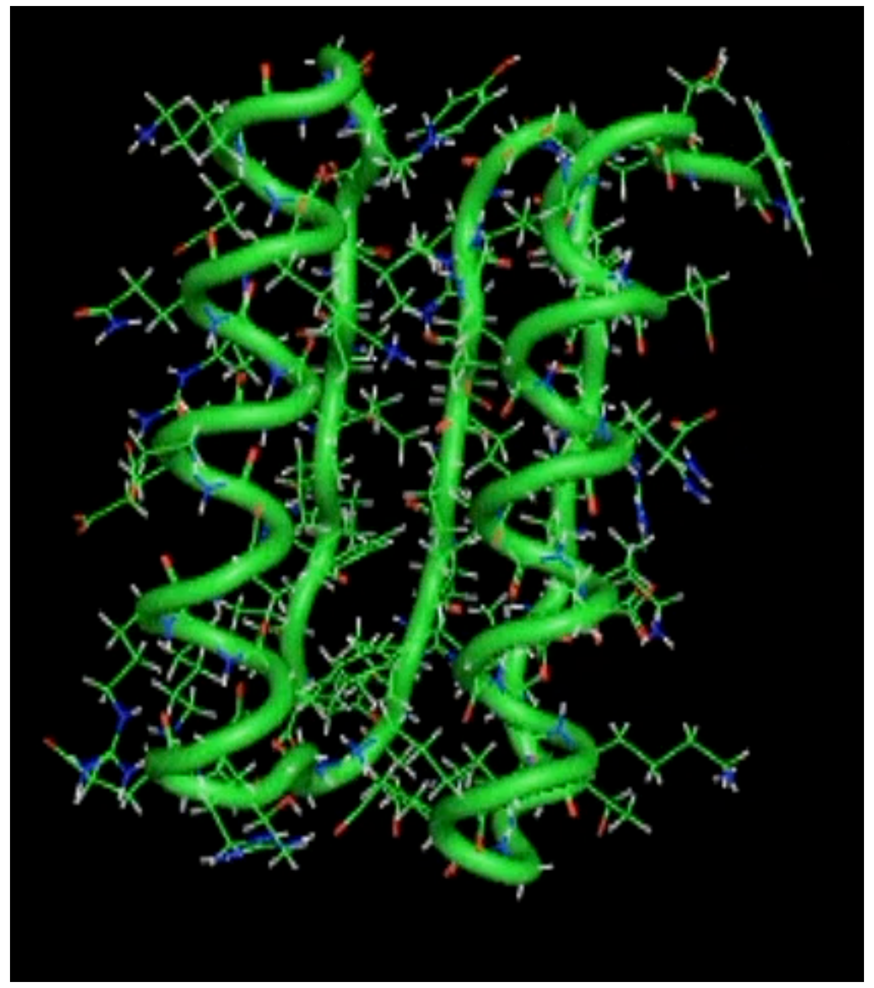
Enzyme-Based:
1 hour (laptop)

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)



from Center for the Exascale Simulation of Materials in Extreme Environments



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

SC22 Dallas, TX | hpc accelerates.

Scalable Automatic Differentiation of Multiple Parallel Paradigms through Compiler Augmentation


William S. Moses

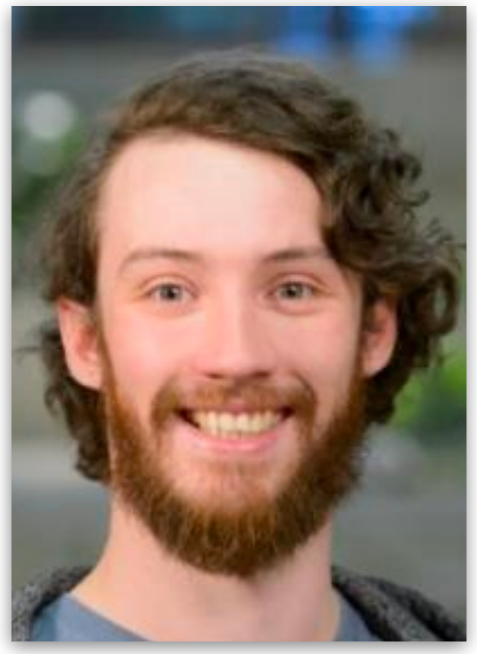

Sri Hari Krishna Narayanan


Ludger Paehler


Valentin Churavy


Jan Hückelheim

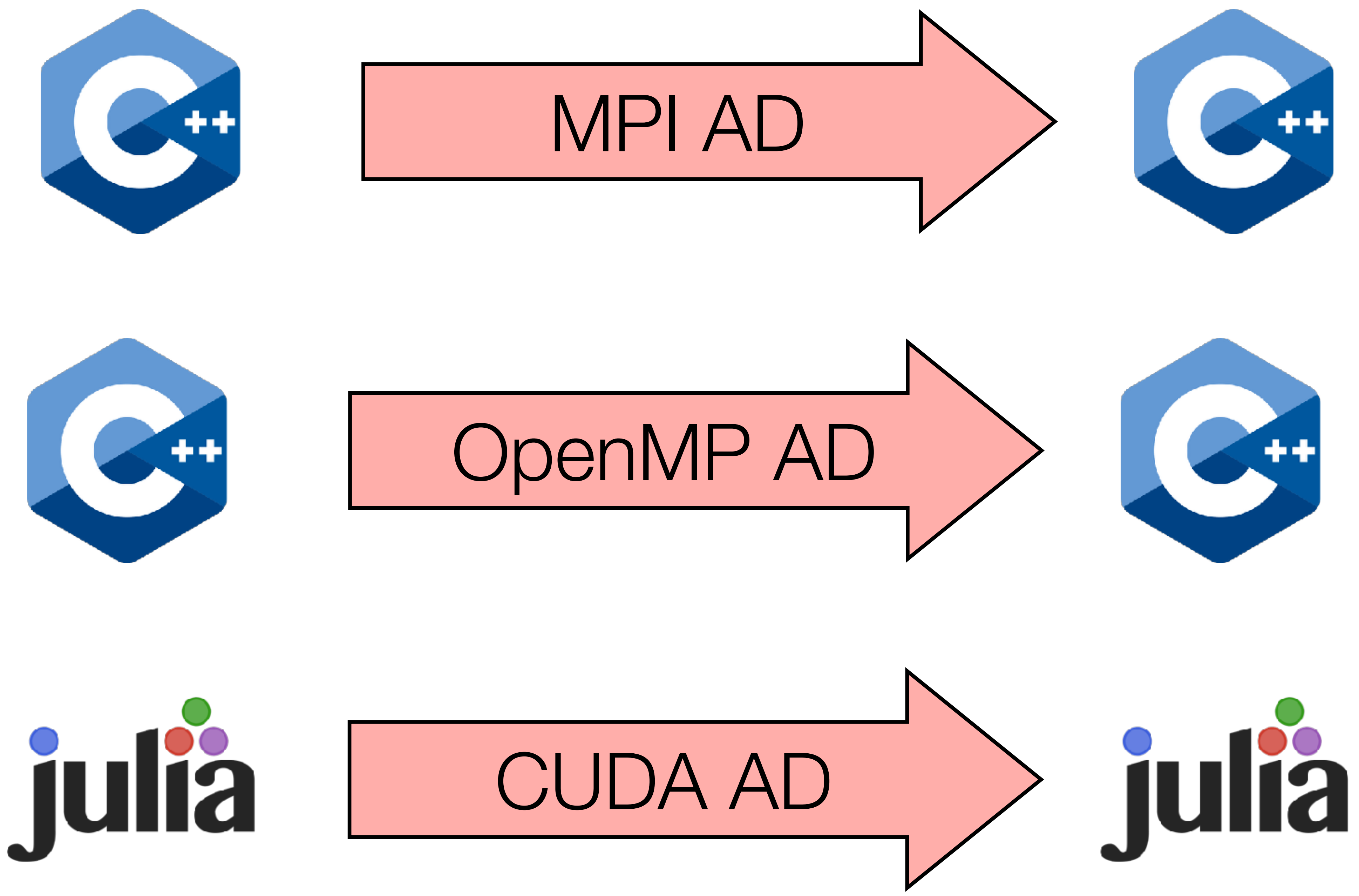

Michel Schanen


Johannes Doerfert


Paul Hovland

History of Parallel AD

- Prior AD tools are often built with a single language and parallel framework in mind
  - Differentiating code using multiple parallel frameworks may be difficult or impossible
- Require AD-specific rewriting to specify extra information
- Run at a source-level, preventing optimizations from being applied




```
void send(double* data, int size) {
  MPI_ISend(data, val);
}
```

```
void send(ADdouble* data, int size, void* buffer) {
  AD_MPI_ISend(data, val, buffer);
}
```

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;
}
```

Optimizations on Parallel AD

- Prior work on AD for GPU's demonstrated importance of combining optimizations with AD for performance

  "Reverse-Mode Automatic Differentiation and Optimization of GPU Kernels via Enzyme" @ SC'21

- E.g. determining memory to be thread-local lets us use a faster non-atomic add

Thread-local memory

- Non-atomic load/store

```
__device__
void f(…) {

  // Thread-local var
  double y;

  …

  d_y += val;
}
```

Others [always legal fallback]

- Atomic increment

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

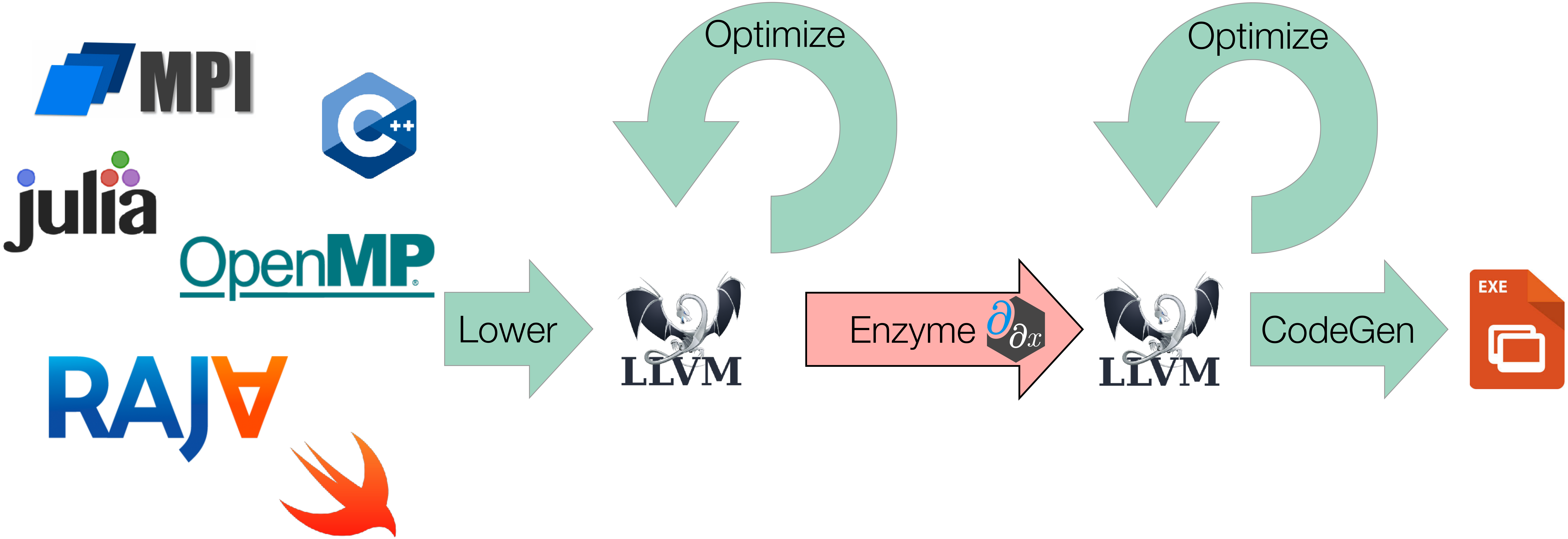
  …

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

Slower

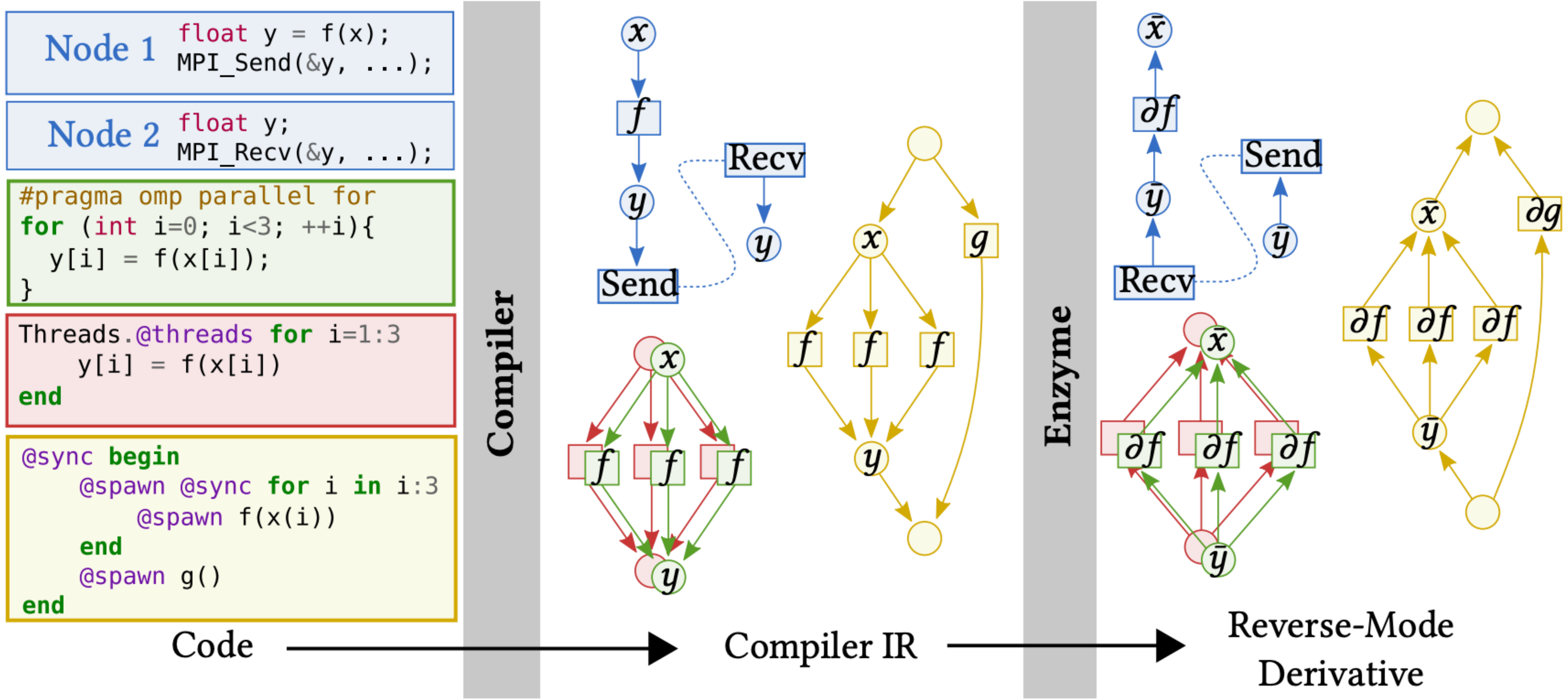
Enzyme Approach

Performing AD in the compiler lets us build a common tool to differentiate & optimize multiple parallel frameworks simultaneously!



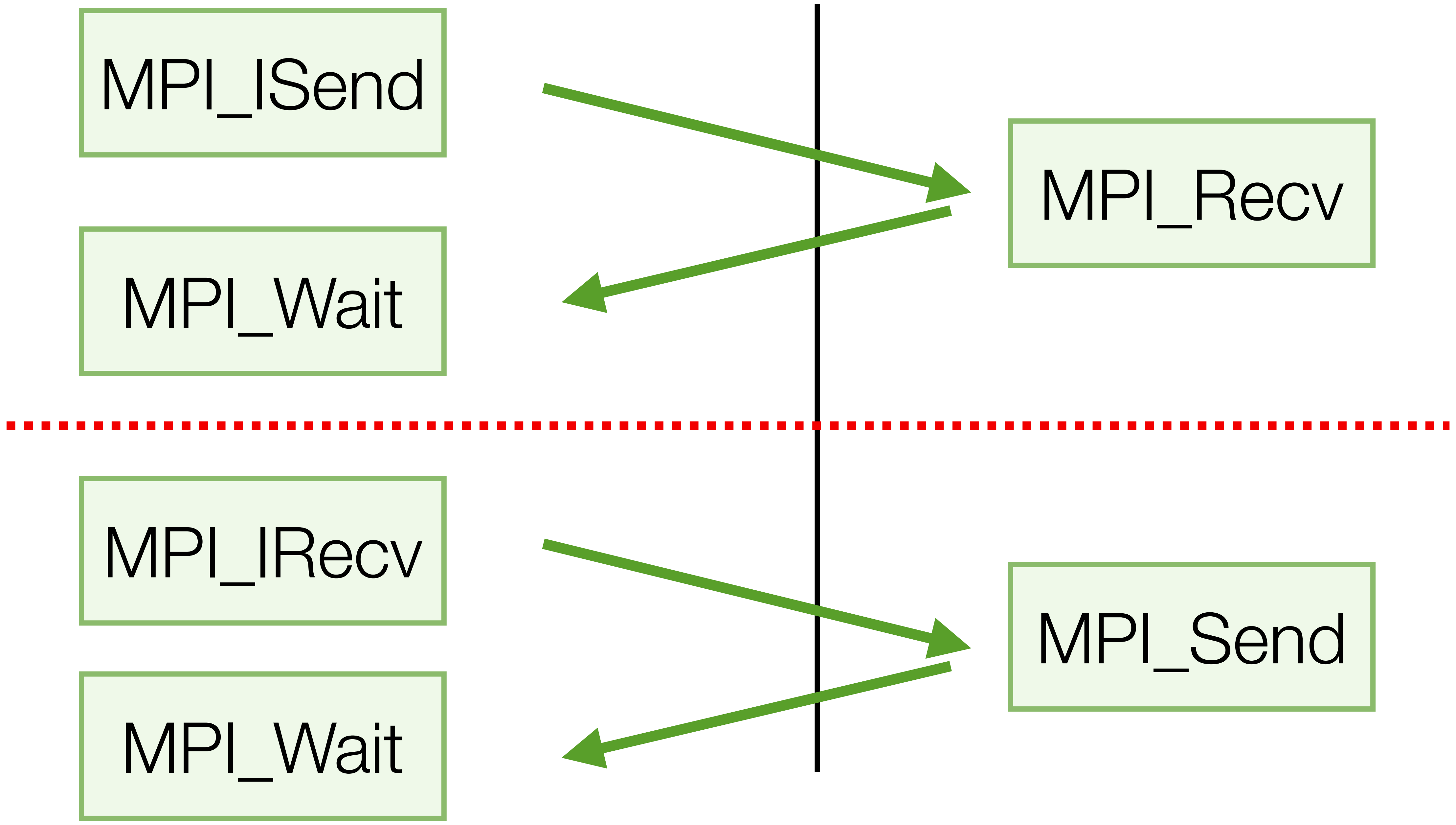
General Parallel Differentiation Framework

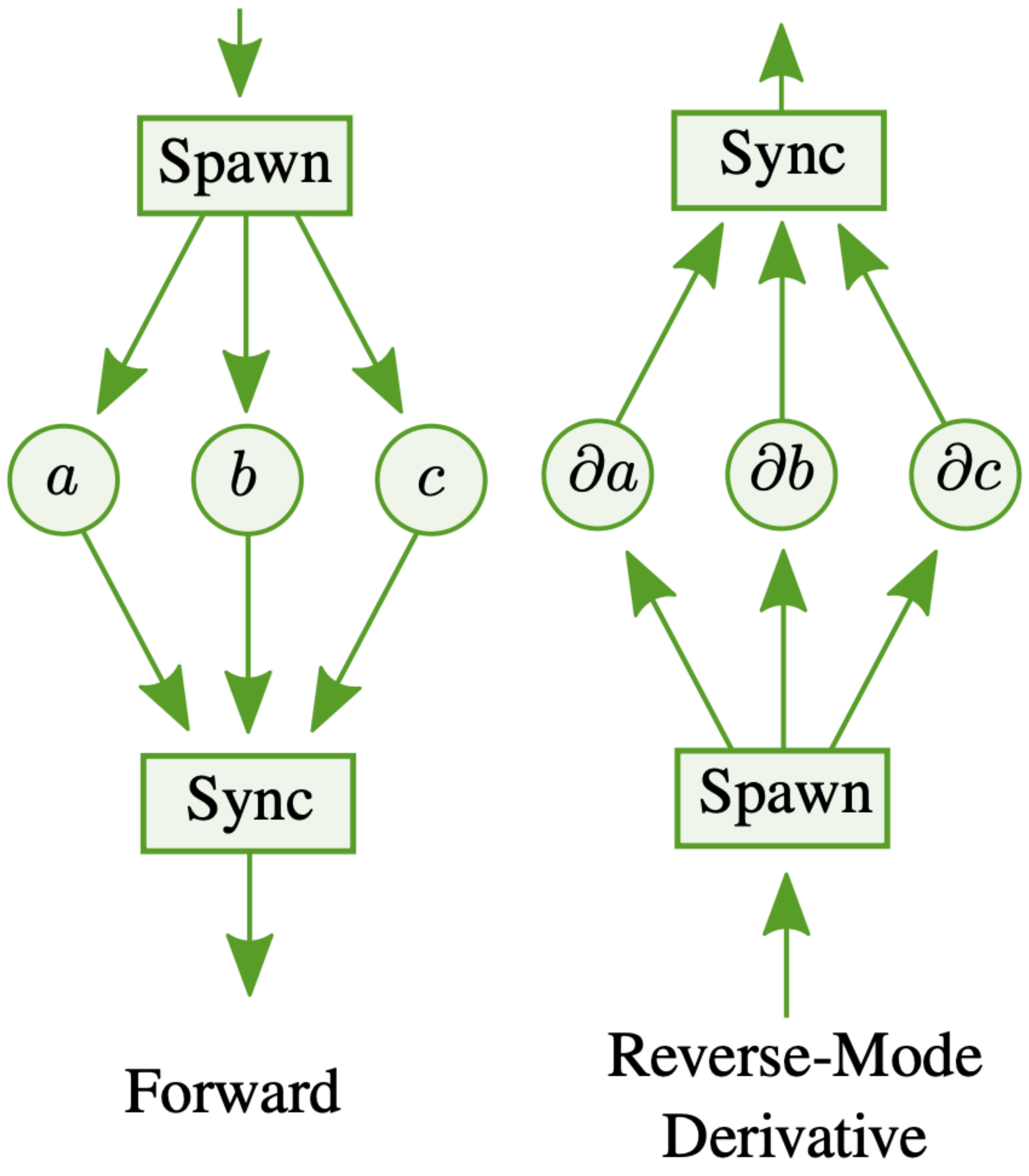
- Algorithm for fast and efficient AD of arbitrary DAG-style parallelism
- Interface for detecting and using parallel constructs in arbitrary frameworks
- General parallel-specific optimizations that improve the performance



Parallelism-Preserving Differentiation

- Computing the adjoint of an instruction in the reverse pass updates the derivative of the operands it used.
- Reversing the parallel dependency structure ensures that for a given value all derivative updates are performed before its definition





Framework Generality

- Implemented hooks for several parallel frameworks:
  - OpenMP
  - MPI
  - Julia Tasks
  - GPU (ROCM, CUDA)
  - GraphCore IPU
- Supports any higher-level framework built off these primitives
  - RAJA
  - MPI.jl
  - Julia @parallel
  - …

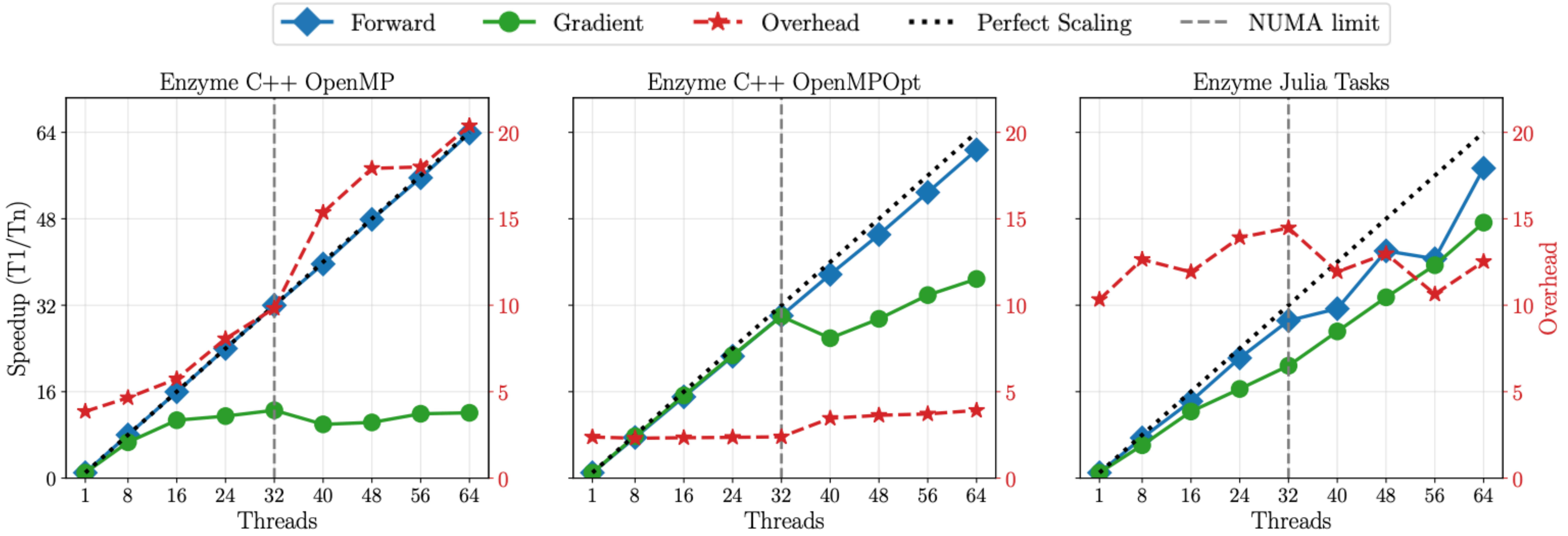
Construct Generality

- Higher-level parallel utilities are automatically handled by existing support for parallelism
  - Both source-level or manually written utilities are lowered to common form.
- If optimizations exist for higher-level utilities, Enzyme supports overriding
  - E.g. faster OpenMP *parallel for*, rather than differentiating via separate support for OpenMP parallel and work sharing loop

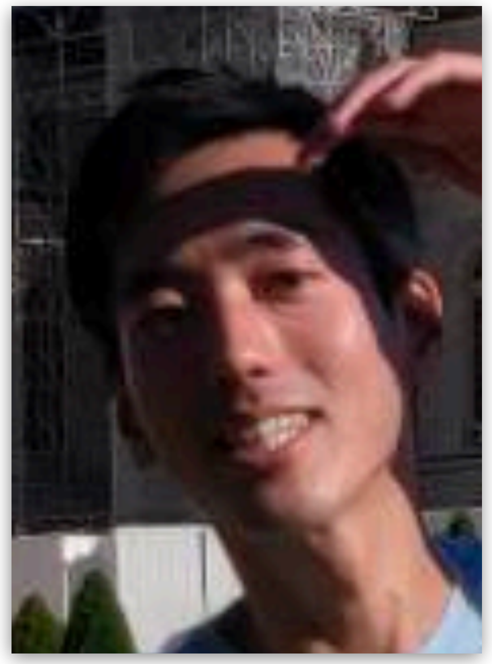
```
double min_per_thread[num_threads()];
#pragma omp parallel
{
  double min_value = 0;
  #pragma omp for
  for(int i = 0; i < N; i++)
    min_value = min(data[i], min_value);
  min_per_thread[omp_get_thread_num()] = min_value;
}
double final_val = 0;
for(int i = 1; i < omp_get_num_threads(); i++)
  final_val = min(final_val, min_per_thread[i]);
```

Evaluation Highlights: Strong Scaling (BUDE)

- Parallel optimizations enable Enzyme to keep the same scalability as the original program



Compiler Optimizations for Sparsity (in progress)



Kevin Mu

Jessie Michel

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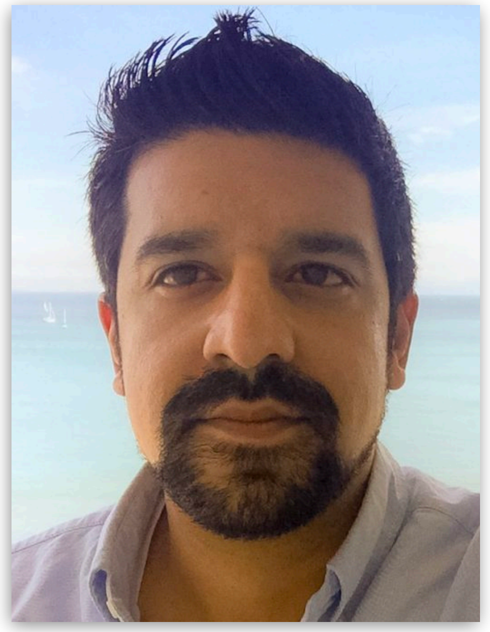
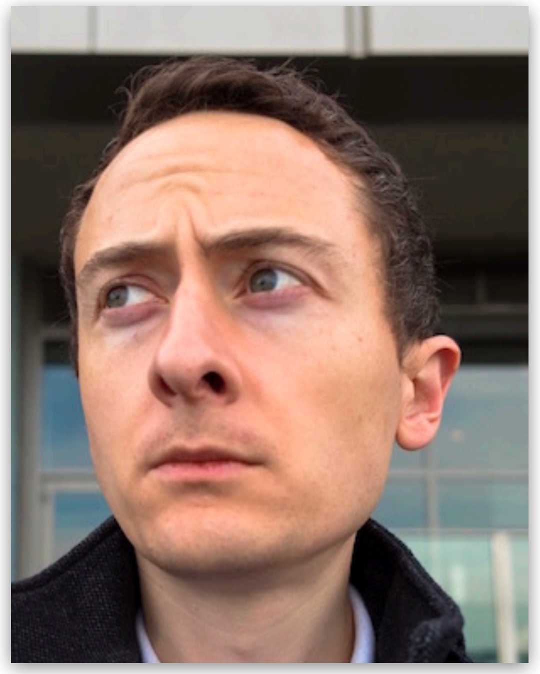


Shoaib Kamil

Zachary Tatlock

Alec Jacobson

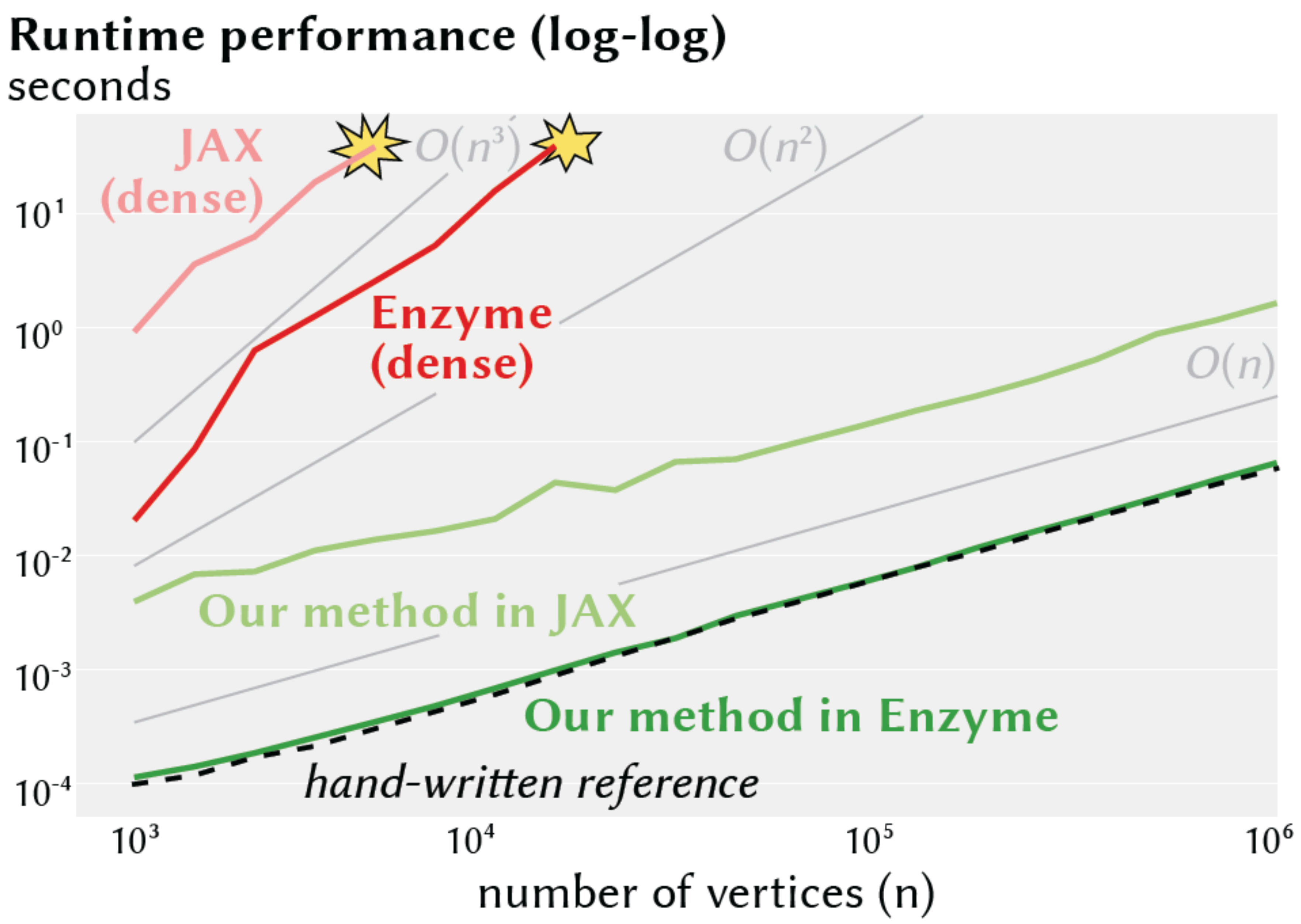


Jonathan Ragan-Kelley

Spadina-{Enzyme, JaX}

- Given a function of n inputs -> 1 output, nesting AD twice gives you a function to densely compute each element of a hessian.

- Compiler techniques (e.g. dead code elimination) interspersed within differentiation enables automatically reduction of computing and storage of the full dense matrix to just the non-zero elements.



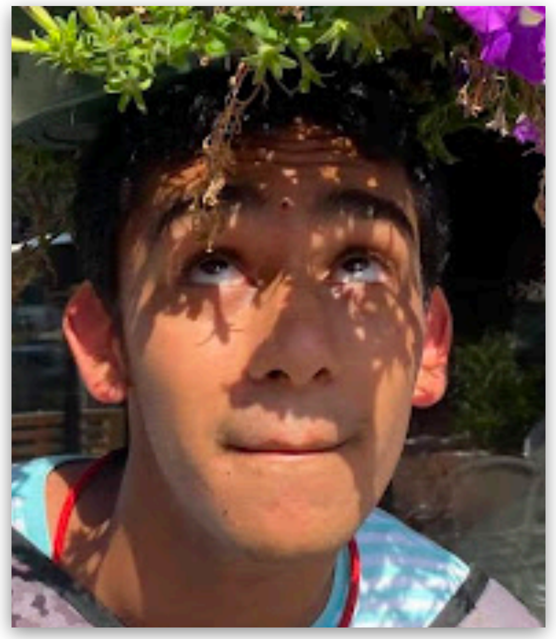

```
void hessian(double* in, double* outputs) {

  for(int i=0; i<n; i++)
   __enzyme_fwddiff(
      +[](double* in, double* out) {
        __enzyme_autodiff(f, in, out);
      },
      enzyme_dup, in, &identity[i * n],
      enzyme_dupnoneed, nullptr, &outputs[i * n]);
}
```

```
void hessian(double* in, double* outputs) {
  for(int i=0; i<n; i++)
   __enzyme_fwddiff(
      +[](double* in, double* out) {
        __enzyme_autodiff(f, in, out);
      },
      enzyme_dup, in, __enzyme_todense(ident_load, ident_store, n),
      enzyme_dupnoneed, nullptr,
         __enzyme_todense(csr_load, csr_store, n));
}
```

BLASphemy: Leveraging Compiler Information for Efficient Differentiable Linear Algebra (in progress)

Manuel Drehwald



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Valentin Churavy

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Compiling Linear Algebra

- Linear Algebra is some of the most common operations in science — it is natural to want to AD through it.
- Prior work has explored (e.g. differentiating BLAS calls with other BLAS calls), but operated on the source level
- Compilation has historically provided significant performance advantages for such computations by rewriting the code to improve spatial/temporal locality, parallelism, kernel launches, among others
  - Open question: combining scheduling with AD? See Enzyme-MLIR

```c
// x and y are double arrays
//  of length N
sum0 = dot(x, y);
sum1 = dot(x, z);
```

```c
// Sequential application
sum0 = 0;
for (int i = 0; i < N; i++) {
    sum0 += x[i] * y[i];
}
for (int i = 0; i < N; i++) {
    sum1 += x[i] * z[i];
}
```

```c
// Fused application
sum0 = 0;
sum1 = 0;
for (int i = 0; i < N; i++) {
    sum0 += x[i] * y[i];
    sum1 += x[i] * z[i];
}
```

Our Work

1. Differentiate high-level linear algebra (e.g. BLAS, LAPACK) functions directly.
   - Better scaling as can leverage parallelism/machine-specific tuning
2. Replace BLAS calls with corresponding serial execution, differentiate at an instruction level
   - Enables cross-kernel optimization and better integration with caching, but only sequential execution
3. Integrate BLAS deeply within AD framework compilation analyses to improve performance (alias analysis, activity analysis, to be recorded/differential use analysis, caching)
   - Enables performance optimizations before AD, e.g. hoisting code out of loops, getting rid of unnecessary computations, as well as avoiding caching if not needed for derivative or overwritten

Size	Enzyme LL(1)	Enzyme TG(64)	Zygote(64)
1	**0.001**	0.001	0.004
2	**0.001**	0.001	0.004
4	**0.001**	0.001	0.004
8	**0.001**	0.001	0.004
16	**0.002**	0.002	0.004
32	0.003	**0.003**	0.005
64	0.013	**0.011**	0.010
128	0.067	**0.066**	0.039
256	0.182	**0.106**	0.129
512	0.738	**0.319**	0.486
1024	2.826	**1.150**	2.225
2048	16.985	13.646	**9.925**
4096	70.837	**66.082**	92.268

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
- Efficient sparse differentiation with Spadina (also implemented in JaX)
- Efficient BLAS differentiation/optimization
- Open source (enzyme.mit.edu & join our mailing list)!
- Lots more ongoing work including scheduling, checkpointing, and more

Acknowledgements

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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.

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

Enzyme

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

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

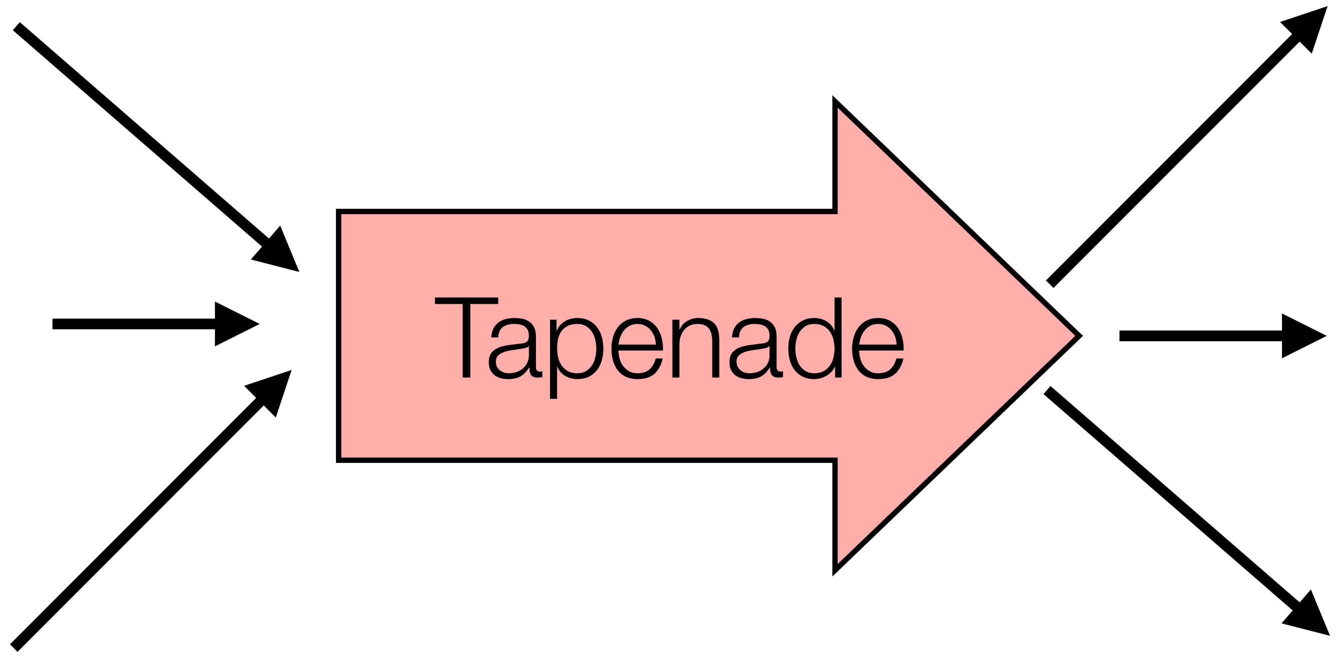
```
adept::Stack stack;
adept::adouble inp = 3.14;

// 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

```c
// myfile.h
```

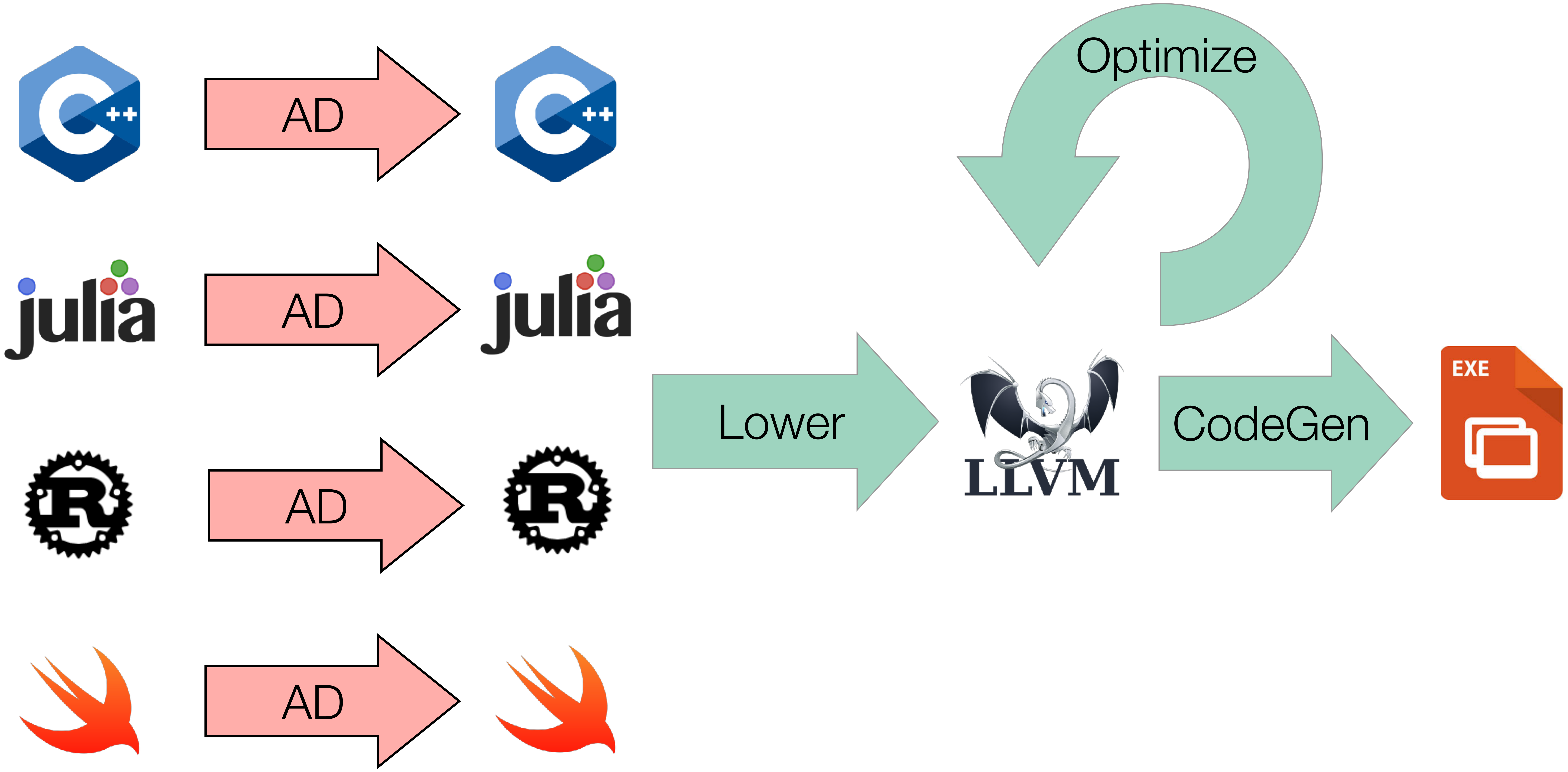
```c
// myfile.c
double relu3(double x) {
  if (x > 0)
    return pow(x,3)
  else
    return 0;
}
```




```c
// 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

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```
for i=0..n {
  out[i] /= mag(in)
}
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$O\left(n\right)$

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

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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)
}
```

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)
}
```

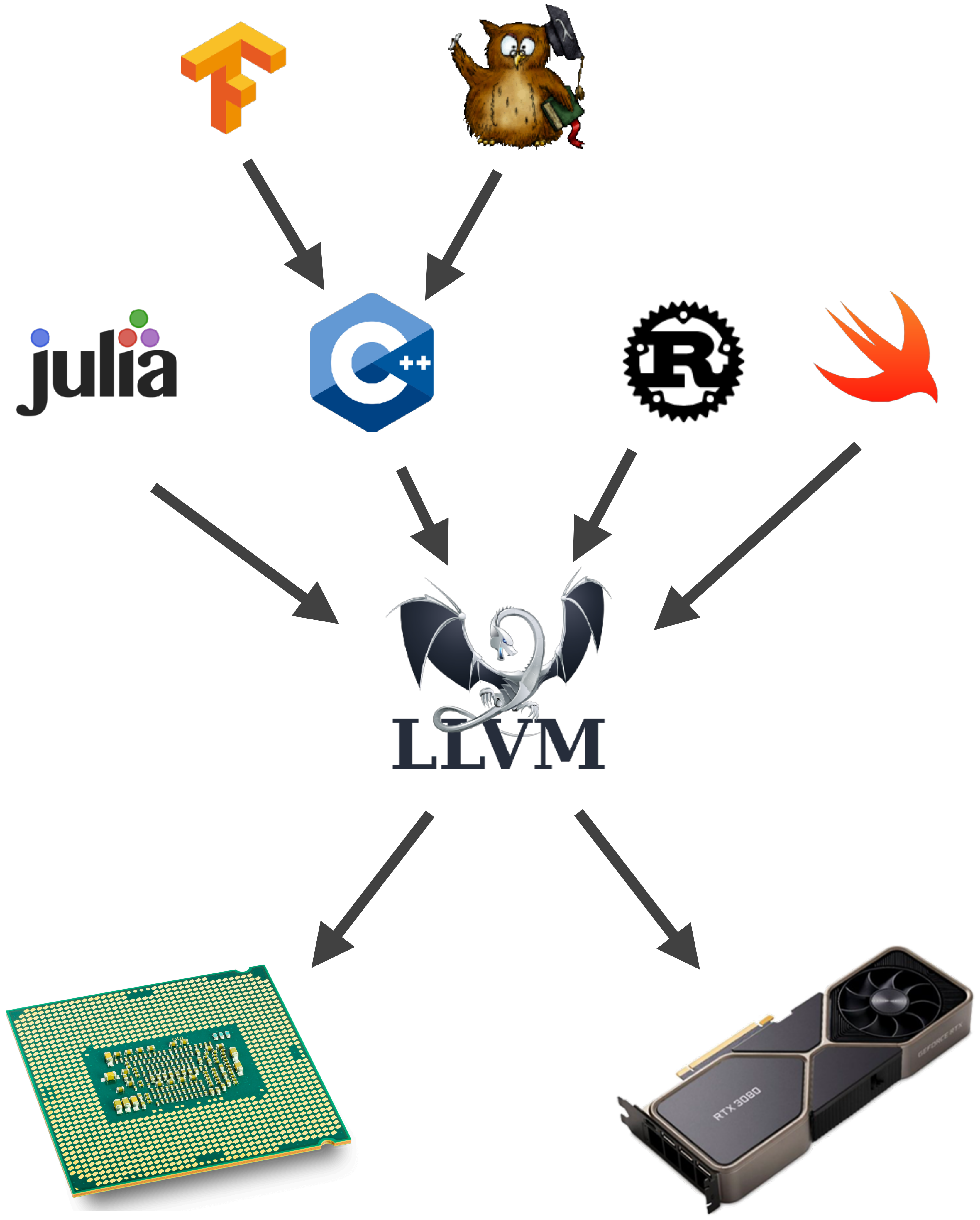
Optimize

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

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

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



Challenges of Low-Level AD

- Low-level code lacks information necessary to compute adjoints

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

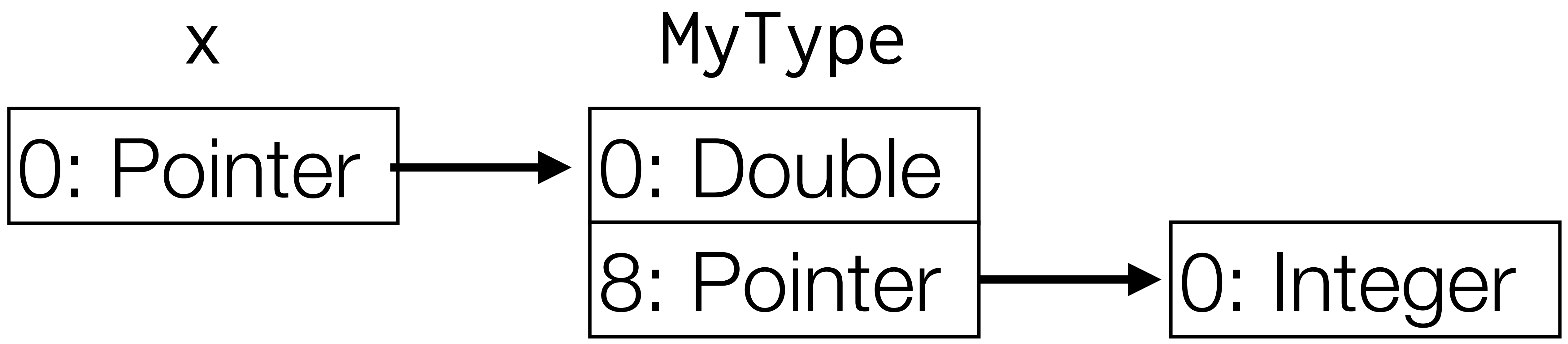
```
void grad_f(double* dst, double* dst',
            double* src, double* src') {
  // Forward Pass
  memcpy(dst, src, 8);

  // 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;
}
```

Type Analysis

- 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

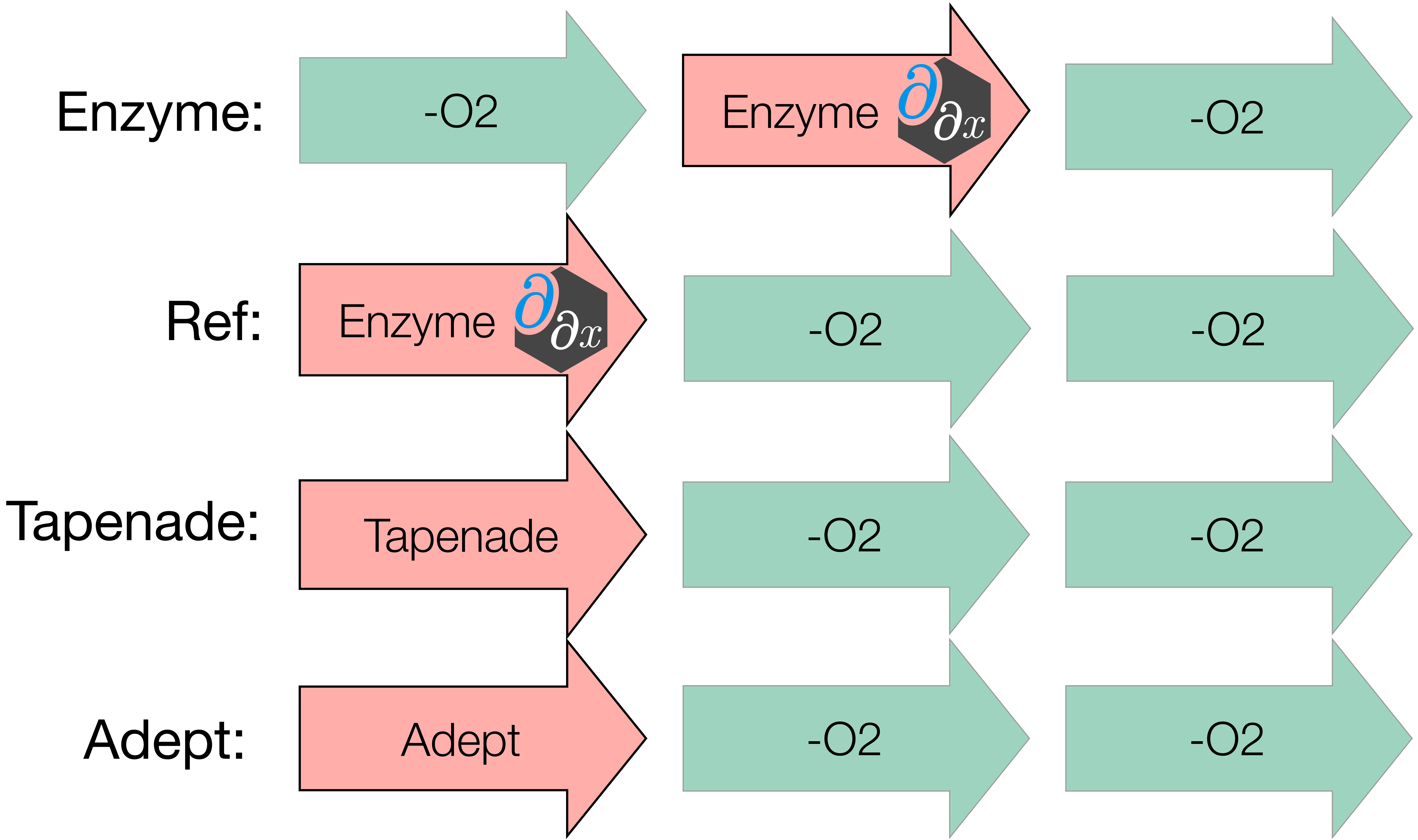
```
struct MyType {
  double;
  int*;
}

x = MyType*;
```



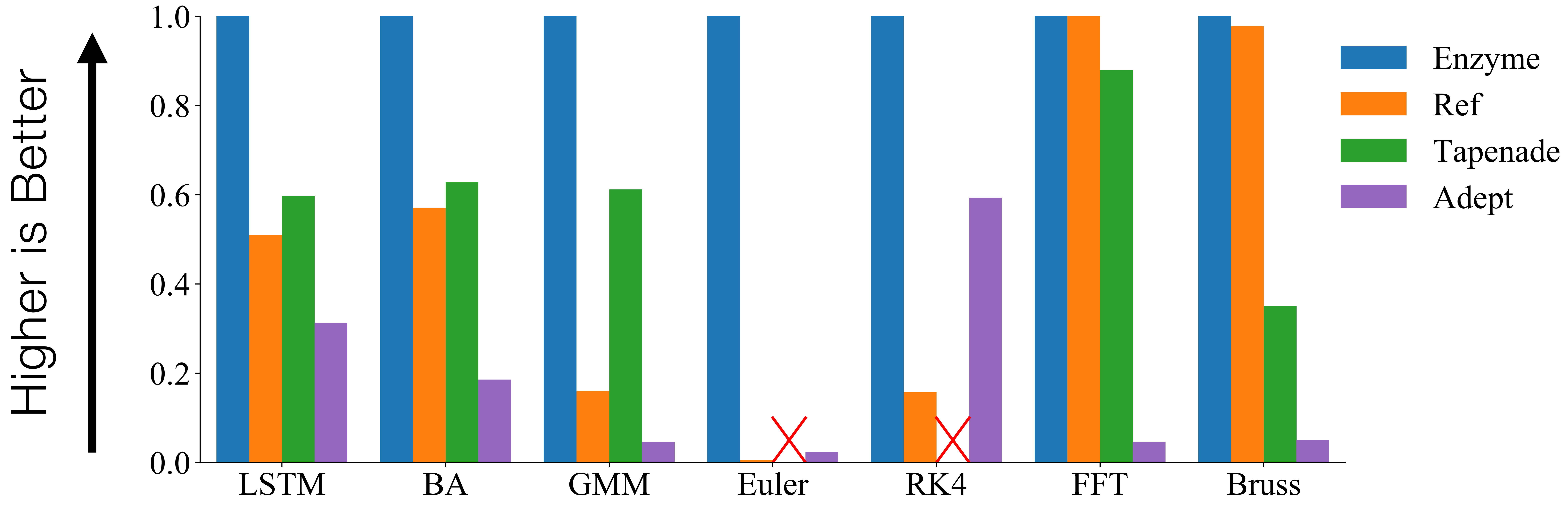

```
types(x) = {[0]:Pointer, [0,0]:Double, [0,8]:Pointer, [0,8,0]:Integer}
```

Experimental Setup

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



Speedup of Enzyme



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

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

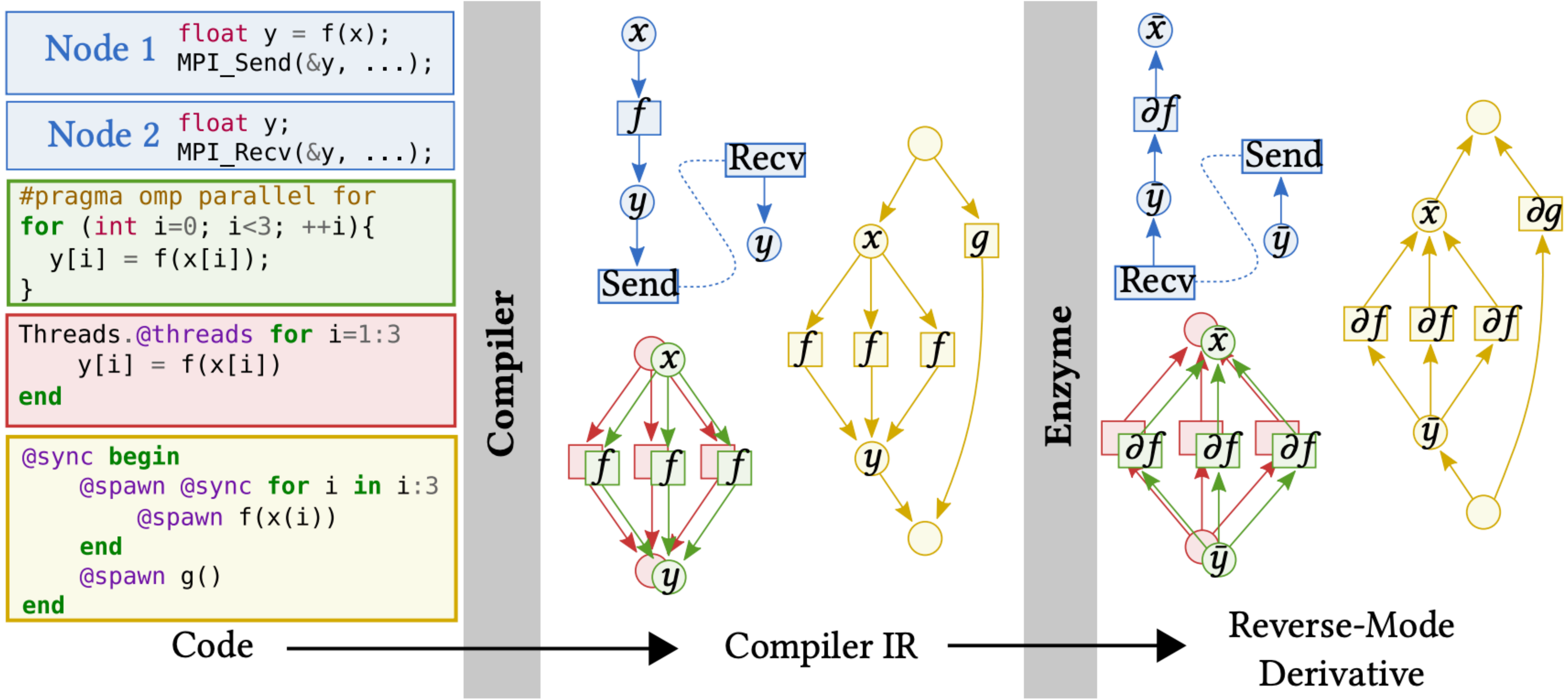
GPU Memory Hierarchy

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

Parallel Enzyme Design

- Algorithm for fast and efficient AD of arbitrary DAG-style parallelism
- Interface for detecting and using parallel constructs in arbitrary frameworks
- General parallel-specific optimizations that improve the performance
- Implemen… …asks, RAJA), Distribute…



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];

}

__device__
void __enzyme_autodiff(void*, …);

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void daxpy(float* a, float* da,
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```

```
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                 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

```julia
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))
```

```julia
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

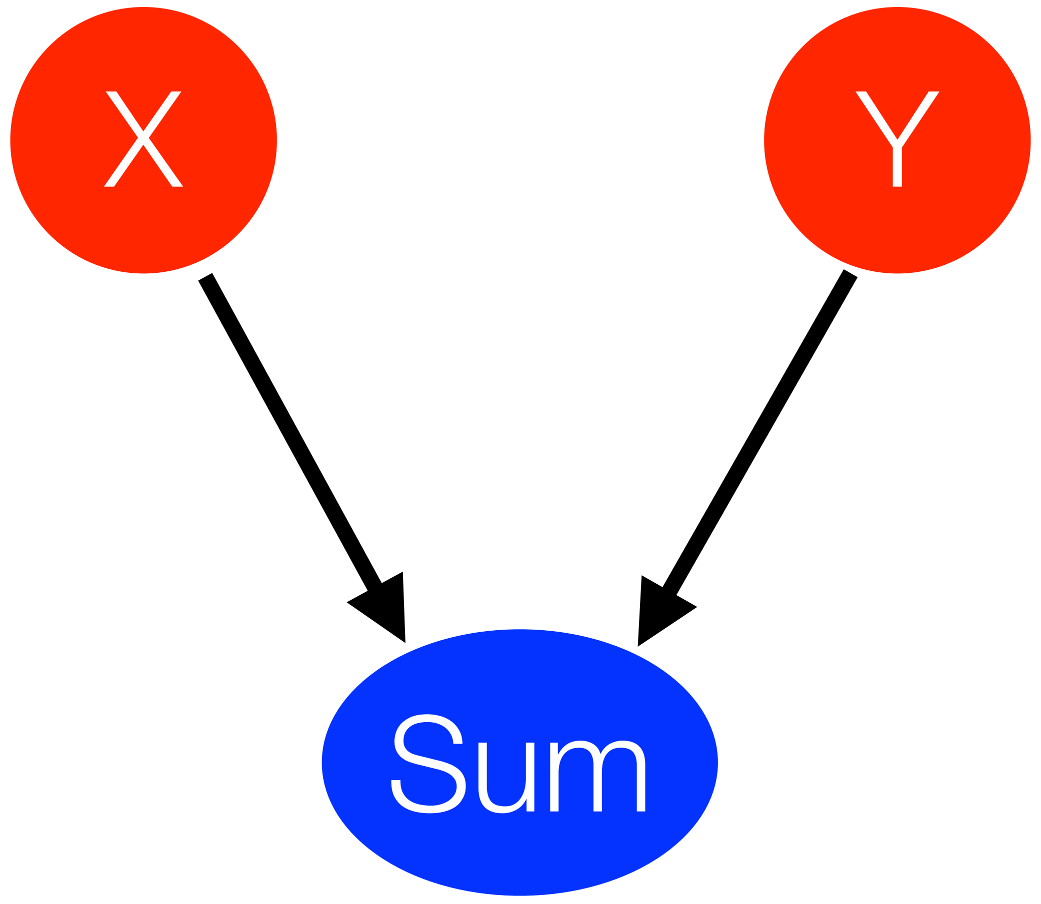
```
double* x_cache = new double[…];

// 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:

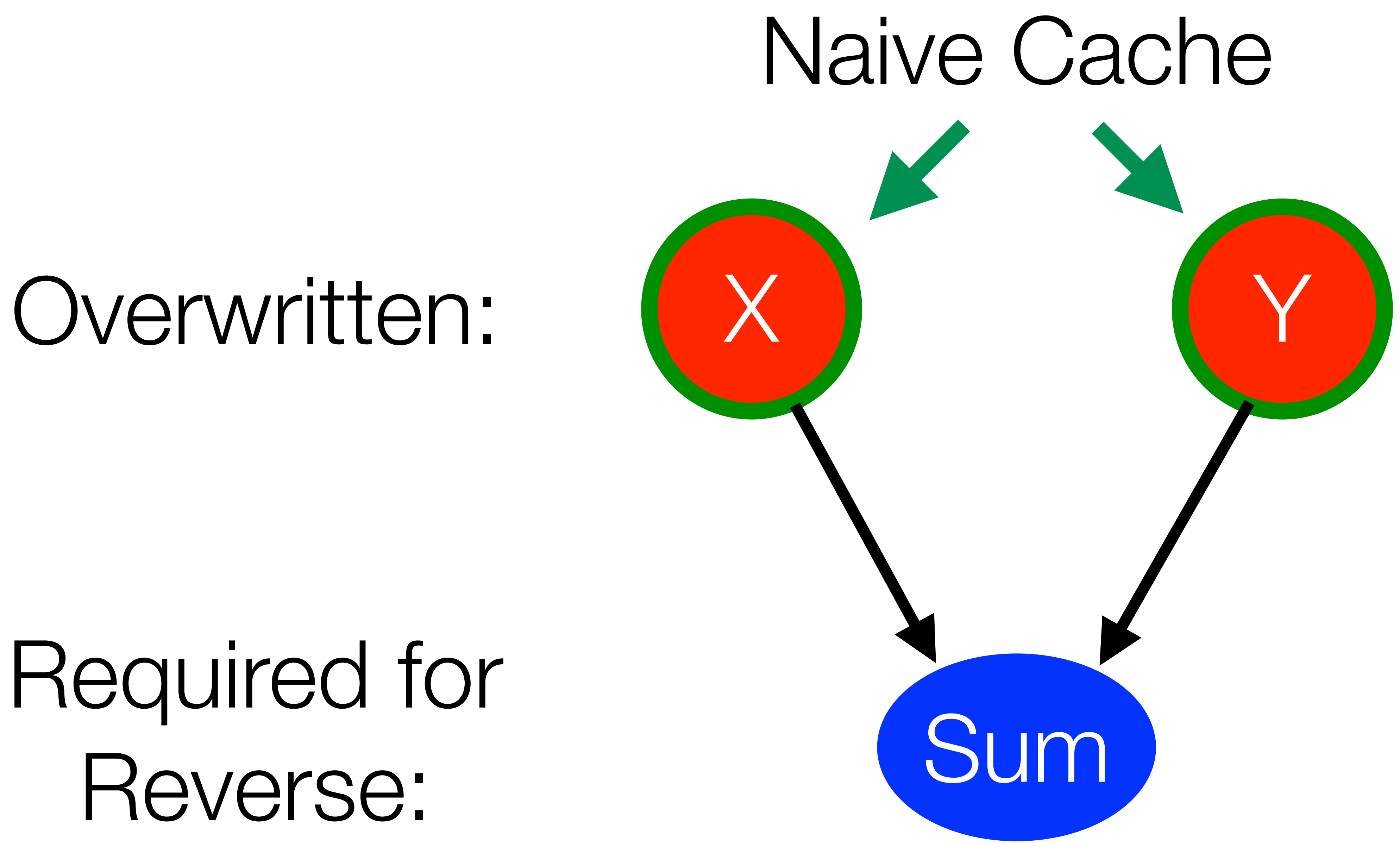
Required for Reverse:




```
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.

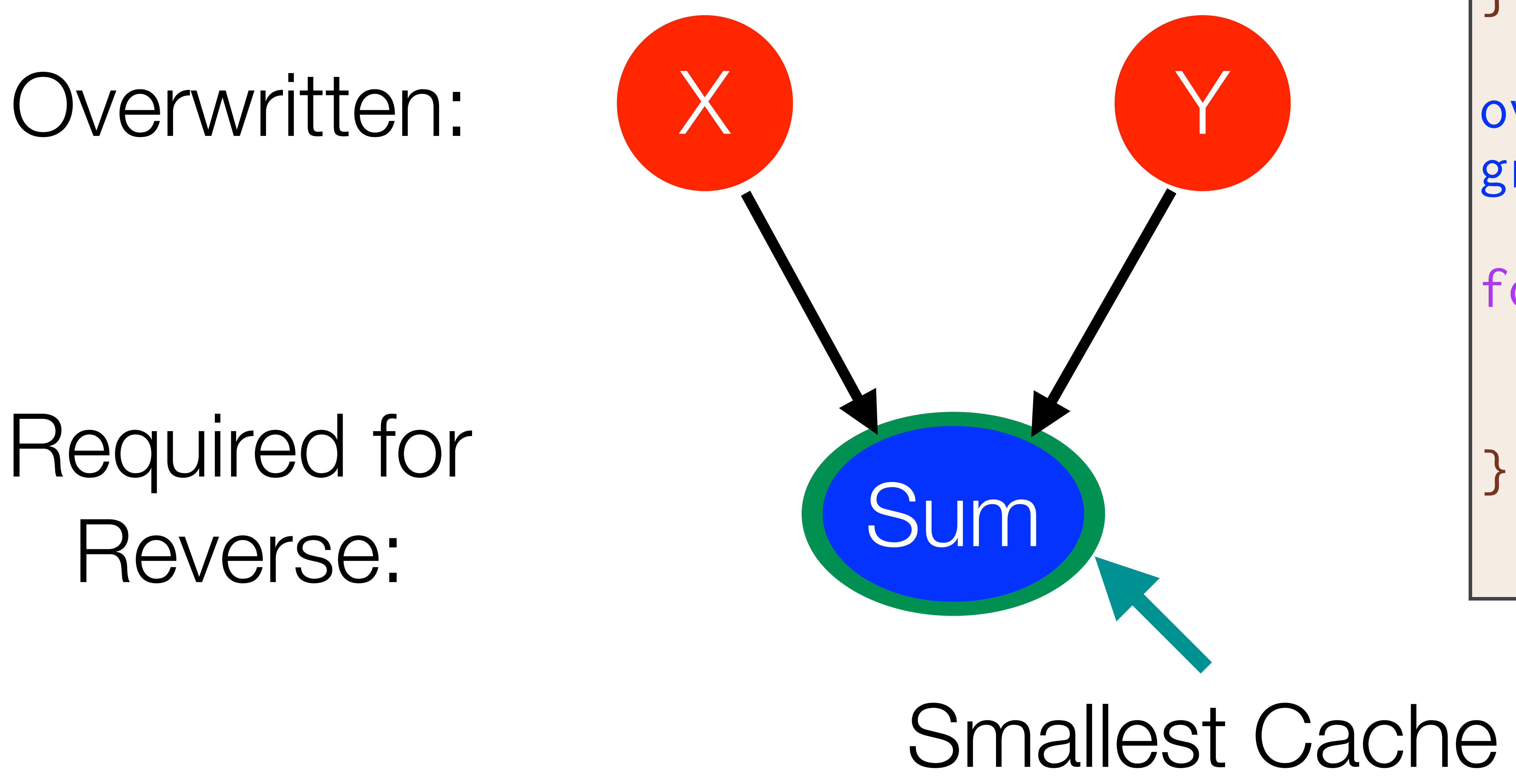



```
double* x_cache = new double[10];
double* y_cache = new double[10];

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]);
}
```



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;
```

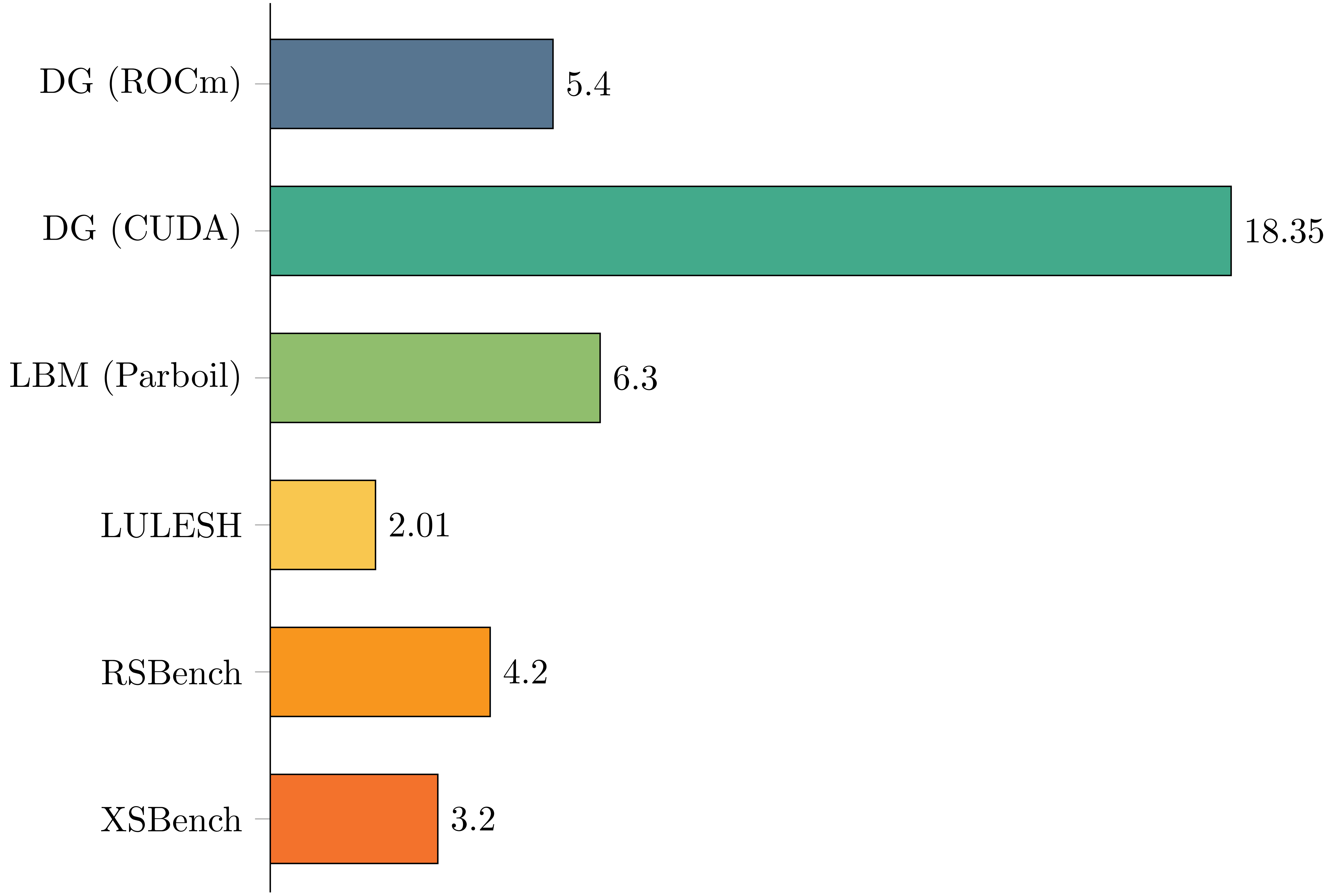
```
double* var1 = new double[N + M];
double* var2 = var1 + N;

use(var1, var2);

delete[] var1;
```

Novel AD + GPU Optimizations

- See our SC paper (Nov 17) 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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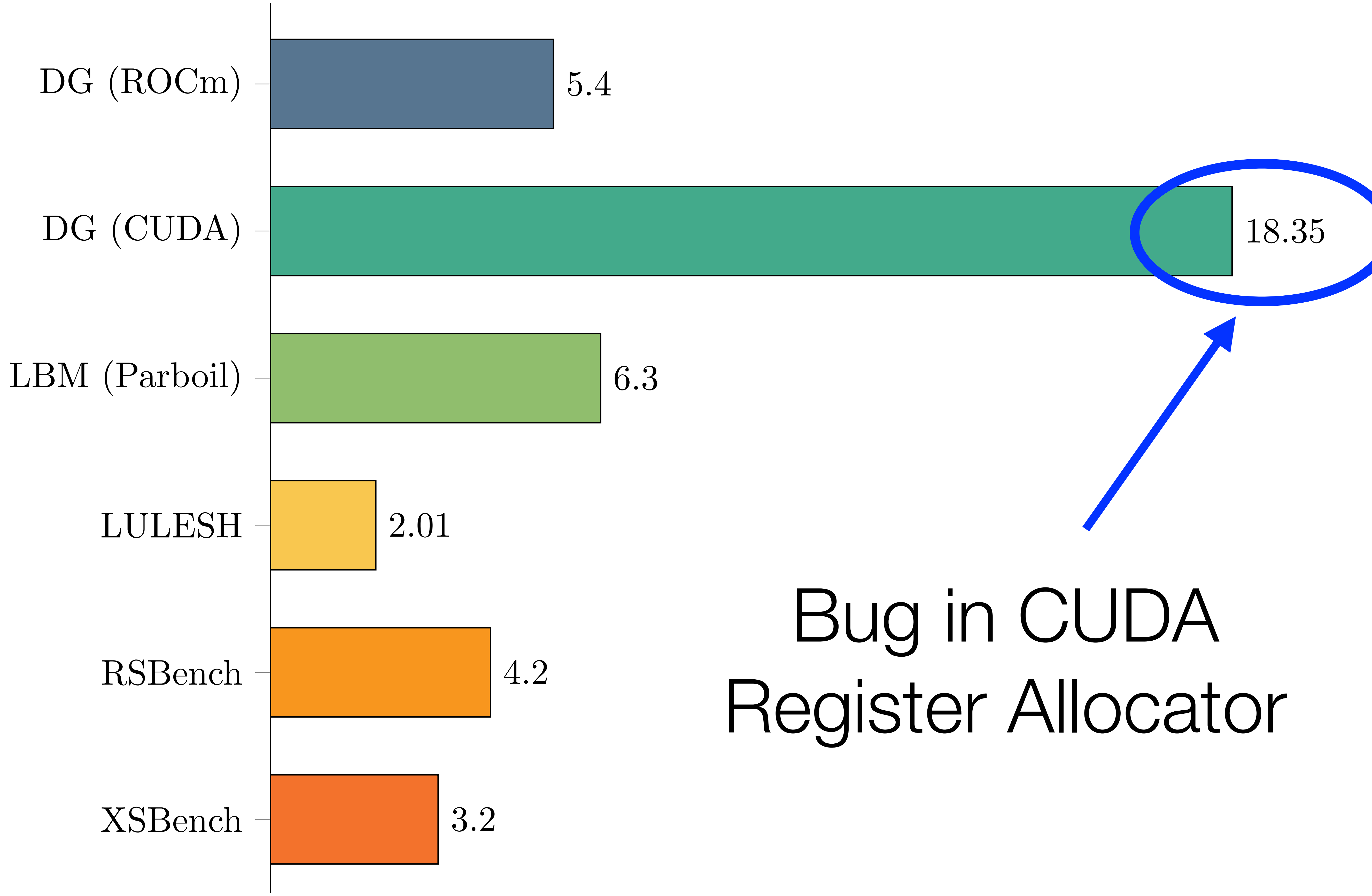


Ablation Analysis of Optimizations

Ablation Analysis of Optimizations

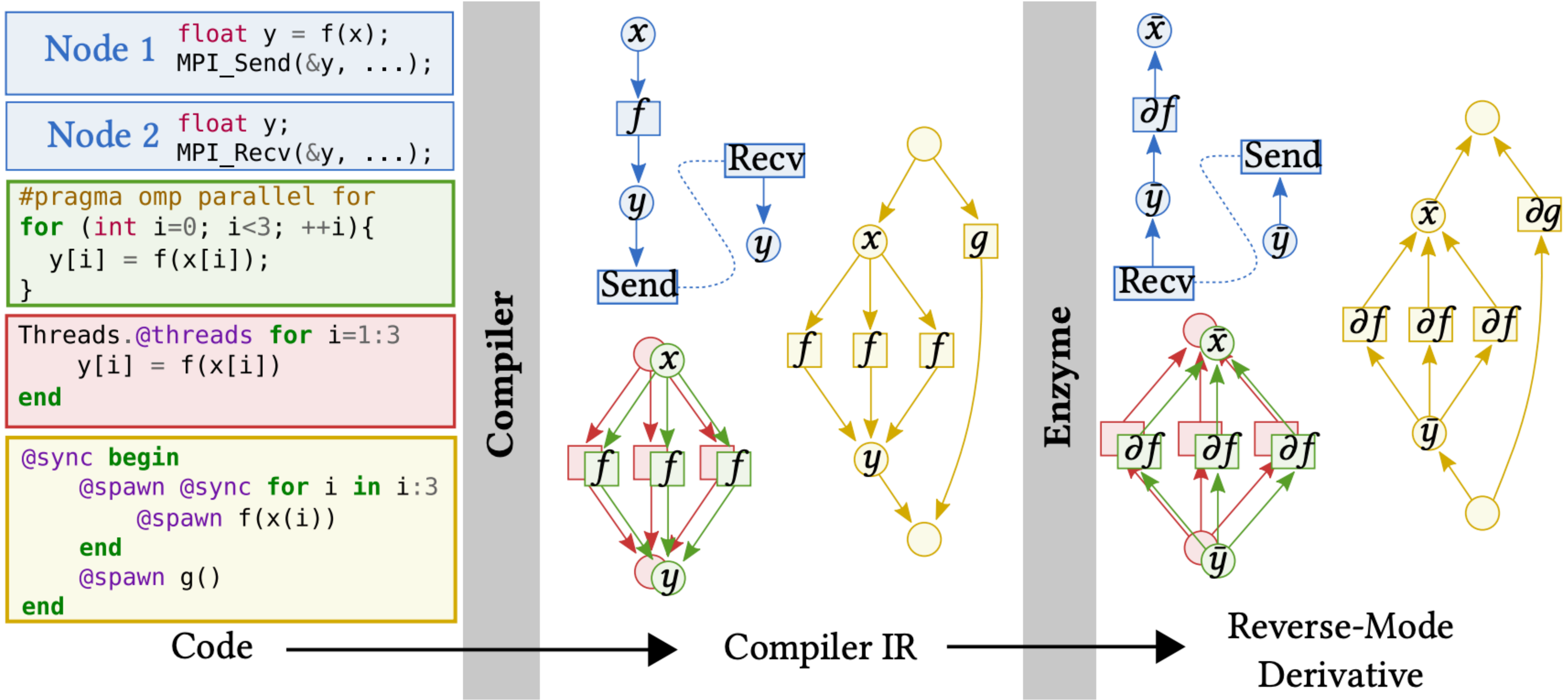
Ablation Analysis of Optimizations

Ablation Analysis of Optimizations

GPU AD is Intractable Without Optimization!

Common Framework for Parallel AD (Ongoing, To Be Published)

- 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

Enzyme

- Tool for performing forward and 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
- Open source (enzyme.mit.edu & join our mailing list)!
- Ongoing work to support Mixed Mode, Batching, Checkpointing

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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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- Open source (enzyme.mit.edu & join our mailing list)!
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Enzyme

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);
}
```

Cache

- Adjoint instructions may require values from the forward pass
  - e.g. ∇(x * y) => x dy + y dx
- For all values needed in the reverse, allocate memory in the forward pass to store the value
- Values computed inside loops are stored in an array indexed by the loop induction variable
  - Array allocated statically if possible; otherwise dynamically `realloc`’d

When LLVM Doesn’t Cut It

- Enzyme relies on optimizations such as LICM and CSE to eliminate redundant loads, and thus redundant caches.

- Since we instead need to preserve values for the reverse pass, these optimizations may not apply

```
for(int i=0; i<N; i++) {
  for(int j=0; j<M; j++) {

    use(array[j]);
  }
}

overwrite(array);
```

When LLVM Doesn't Cut It

- Enzyme relies on optimizations such as LICM and CSE to eliminate redundant loads, and thus redundant caches.
- Since we instead need to preserve values for the reverse pass, these optimizations may not apply
- This requires far more caching than necessary

```
double* cache = new double[N*M];

for(int i=0; i<N; i++) {
  for(int j=0; j<M; j++) {
    cache[i*M+j] = array[j];
    use(array[j]);
  }
}

overwrite(array);
grad_overwrite(array);

for(int i=0; i<N; i++) {
  for(int j=M-1; i<M; i++) {
    grad_use(cache[i*M+j], d_array[j]);
  }
}
```

When LLVM Doesn't Cut It

- Enzyme relies on optimizations such as LICM and CSE to eliminate redundant loads, and thus redundant caches.
- Since we instead need to preserve values for the reverse pass, these optimizations may not apply
- This requires far more caching than necessary
- By analyzing the read/write structure, we can hoist the cache.

```
double* cache = new double[M];
memcpy(cache, array, sizeof(double)*M);
for(int i=0; i<N; i++) {
  for(int j=0; j<M; j++) {

    use(array[j]);
  }
}

overwrite(array);
grad_overwrite(array);

for(int i=0; i<N; i++) {
  for(int j=M-1; i<M; i++) {
    grad_use(cache[j], d_array[j]);
  }
}
```

Cache

- Adjoint instructions may require values from the forward pass
  - e.g. ∇(x * y) => x dy + y dx
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- Values computed inside loops are stored in an array indexed by the loop induction variable
  - Array allocated statically if possible; otherwise dynamically `realloc`’d

Case Study: Read Sum

```
double sum(double* x) {
  double total = 0;

  for(int i=0; i<10; i++)
    total += read() * x[i];

  return total;
}
```

```
void diffe_sum(double* x, double* xp) {
  return __enzyme_autodiff(sum, x, xp);
}
```

```
define double @sum(double* %x)
```

entry

```
br for.body
```

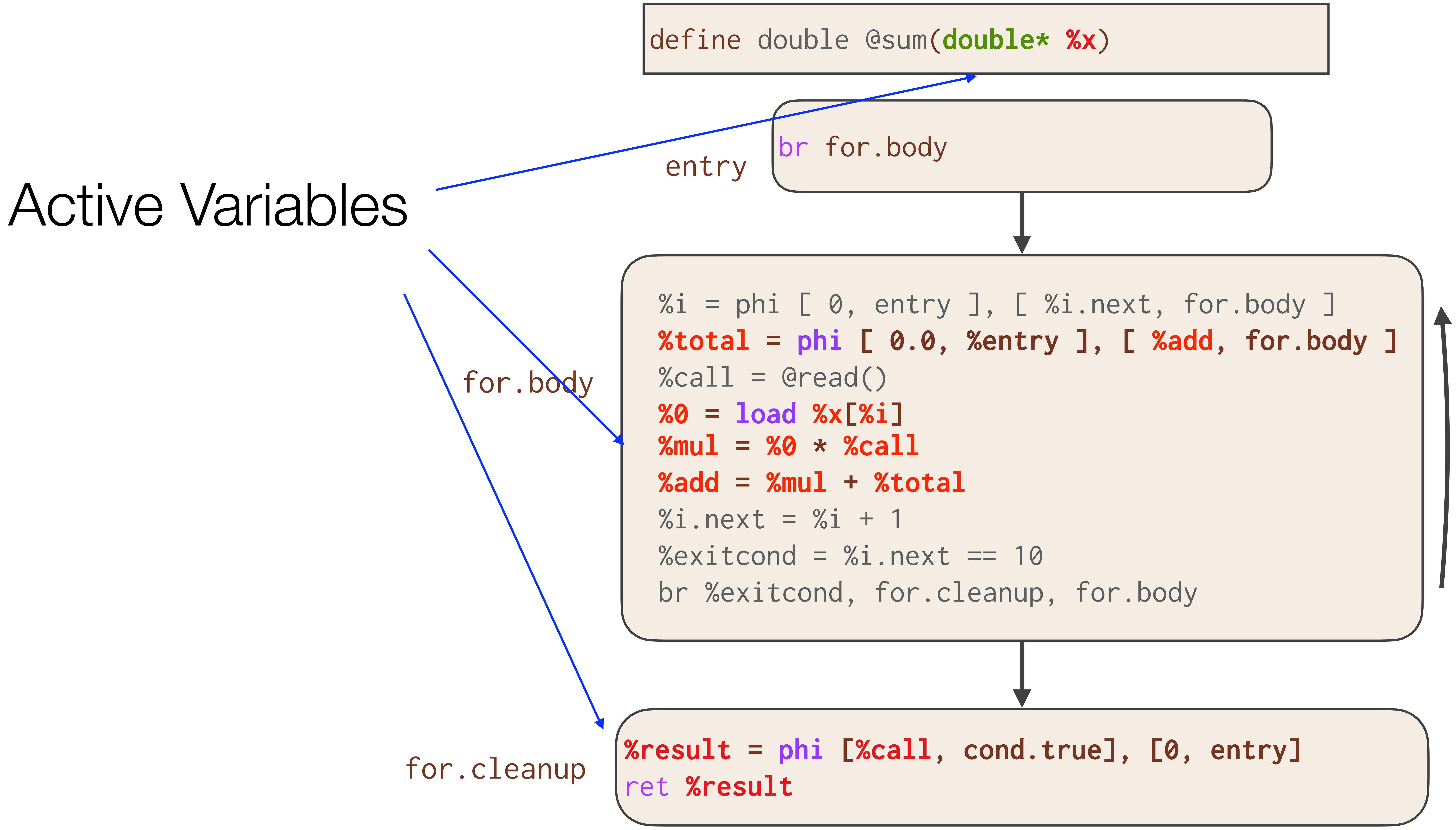
for.body

```
%i = phi [ 0, entry ], [ %i.next, for.body ]
%total = phi [ 0.0, %entry ], [ %add, for.body ]
%call = @read()
%0 = load %x[%i]
%mul = %0 * %call
%add = %mul + %total
%i.next = %i + 1
%exitcond = %i.next == 10
br %exitcond, for.cleanup, for.body
```

for.cleanup

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

Case Study: Read Sum



Case Study: Read Sum

Each register in the for loop represents a distinct active variable every iteration

```
define double @sum(double* %x)
```

entry

```
br for.body
```

for.body

```
%i = phi [ 0, entry ], [ %i.next, for.body ]
%total = phi [ 0.0, %entry ], [ %add, for.body ]
%call = @read()
%0 = load %x[%i]
%mul = %0 * %call
%add = %mul + %total
%i.next = %i + 1
%exitcond = %i.next == 10
br %exitcond, for.cleanup, for.body
```

for.cleanup

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

```
define double @diffe_sum(double* %x, double* %xp)
```

entry

```
alloca %x'      = 0.0
alloca %total'  = 0.0
alloca %0'      = 0.0
alloca %mul'    = 0.0
alloca %add'    = 0.0
alloca %result' = 0.0

br for.body
```

Allocate & zero shadow memory per active value

for.body

```
%i = phi [ 0, entry ], [ %i.next, for.body ]
%total = phi [ 0.0, %entry ], [ %add, for.body ]
%call = @read()
%0 = load %x[%i]
%mul = %0 * %call
%add = %mul + %total
%i.next = %i + 1
%exitcond = %i.next == 10
br %exitcond, for.cleanup, for.body
```

for.cleanup

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

```
define double @diffe_sum(double* %x, double* %xp)
```

Cache forward pass variables for use in reverse

entry

```
alloca %x'      = 0.0
alloca %total'  = 0.0
alloca %0'      = 0.0
alloca %mul'    = 0.0
alloca %add'    = 0.0
alloca %result' = 0.0
%call_cache = @malloc(10 x double)
br for.body
```

for.body

```
%i = phi [ 0, entry ], [ %i.next, for.body ]
%total = phi [ 0.0, %entry ], [ %add, for.body ]
%call = @read()
store %call_cache[%i] = %call
%0 = load %x[%i]
%mul = %0 * %call
%add = %mul + %total
%i.next = %i + 1
%exitcond = %i.next == 10
br %exitcond, for.cleanup, for.body
```

for.cleanup

```
%result = phi [ %call, cond.true], [0, entry]
@free(%cache)
ret %result
```

After lowering & some optimizations

```
define void @diffe_sum(double* %x, double* %xp)
```

entry

```
%call_cache = @malloc(10 x double)
br for.body
```

for.body

```
%i = phi [ 0, entry ], [ %i.next, for.body ]
%total = phi [ 0.0, %entry ], [ %add, for.body ]
%call = @read()
store %call_cache[%i] = %call
%i.next = %i + 1
%exitcond = %i.next == 10
br %exitcond, reversefor.body, for.body
```

reversefor.body

```
%i' = phi [ 9, for.body ], [ %i'.next, reversefor.body ]
%i'.next = %i' - 1
%cached_read = load %call_cache[%i']
store %xp[%i'] = %cached_read + %xp[%i']
%exit2 = %i = 0
br %exitcond, %exit2, reversefor.body
```

exit

```
@free(%cache)
ret
```

Case Study: Read Sum

```
define void @diffe_sum(double* %x, double* %xp)
```

entry

```
%call0 = @read()
store %xp[0] = %call0
%call1 = @read()
store %xp[1] = %call1
%call2 = @read()
store %xp[2] = %call2
%call3 = @read()
store %xp[3] = %call3
%call4 = @read()
store %xp[4] = %call4
%call5 = @read()
store %xp[5] = %call5
%call6 = @read()
store %xp[6] = %call6
%call7 = @read()
store %xp[7] = %call7
%call8 = @read()
store %xp[8] = %call8
%call9 = @read()
store %xp[9] = %call9
ret
```

After more optimizations

```
void diffe_sum(double* x, double* xp) {
   xp[0] = read();
   xp[1] = read();
   xp[2] = read();
   xp[3] = read();
   xp[4] = read();
   xp[5] = read();
   xp[6] = read();
   xp[7] = read();
   xp[8] = read();
   xp[9] = read();
}
```

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

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

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

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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

GPU Automatic Differentiation

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

- 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)
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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

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]

Enzyme Differentiation Algorithm

- Type Analysis
- Activity Analysis
- Synthesize derivatives
  - Forward pass that mirrors original code
  - Reverse pass inverts instructions in forward pass (adjoints) to compute derivatives
- Optimize

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

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

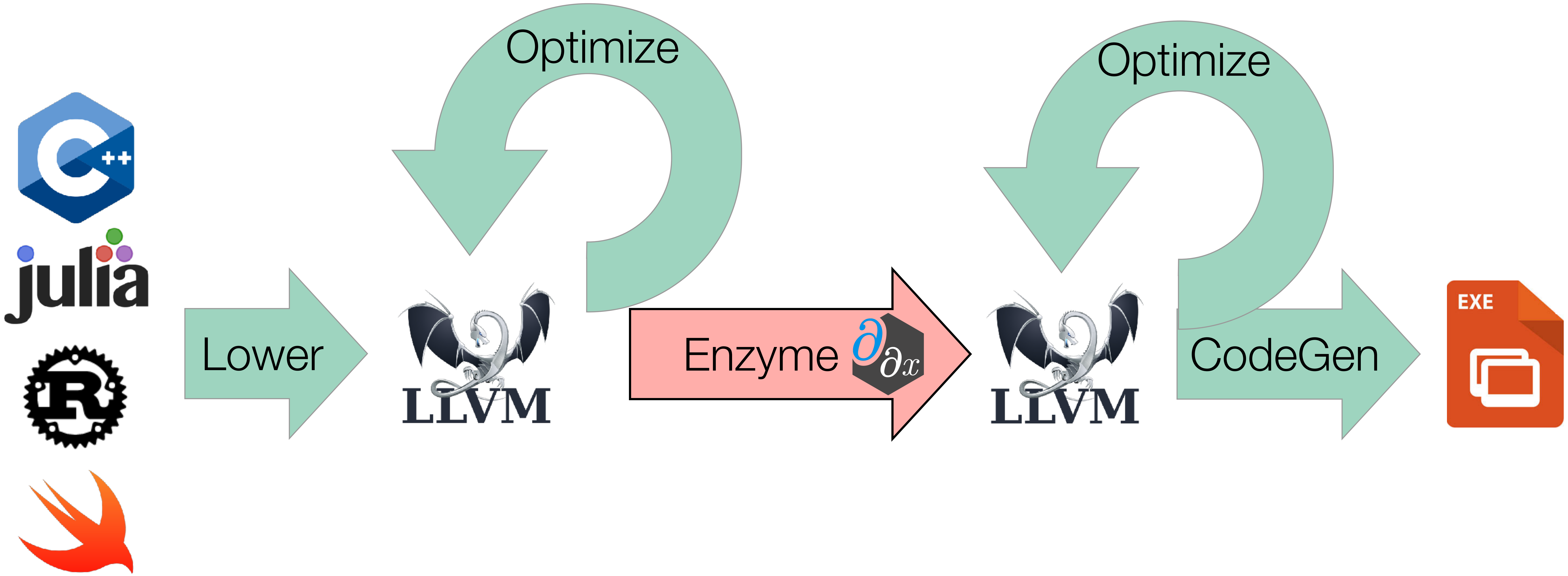
def step(bodies, dt):
  acc = []
  for i in range(len(bodies)):
    acc.push(torch.zeros([3]))
    for j in range(len(bodies)):
      if i == j: continue
      acc[i] += force(bodies[i], bodies[j]) /
                         bodies[i].mass

  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
```

AD-Specific Cache

- Some optimizations require domain-specific knowledge

- Not all values are needed for the reverse pass. By considering the dataflow graph we can perform a min-cut to approximate smaller cache sizes.

    - Not all (loop) sizes are known at compile-time, so this must be a heuristic

```
double xy_cache=x[0] + y[0];


use(x[0] + y[0]);

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

grad_use(xy_cache);
```

AD-Specific Cache

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```
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double y_cache=y[0];

use(x[0] + y[0]);

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

grad_use(x_cache + y_cache);
```

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double xy_cache=x[0] + y[0];


use(x[0] + y[0]);

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

grad_use(xy_cache);
```

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

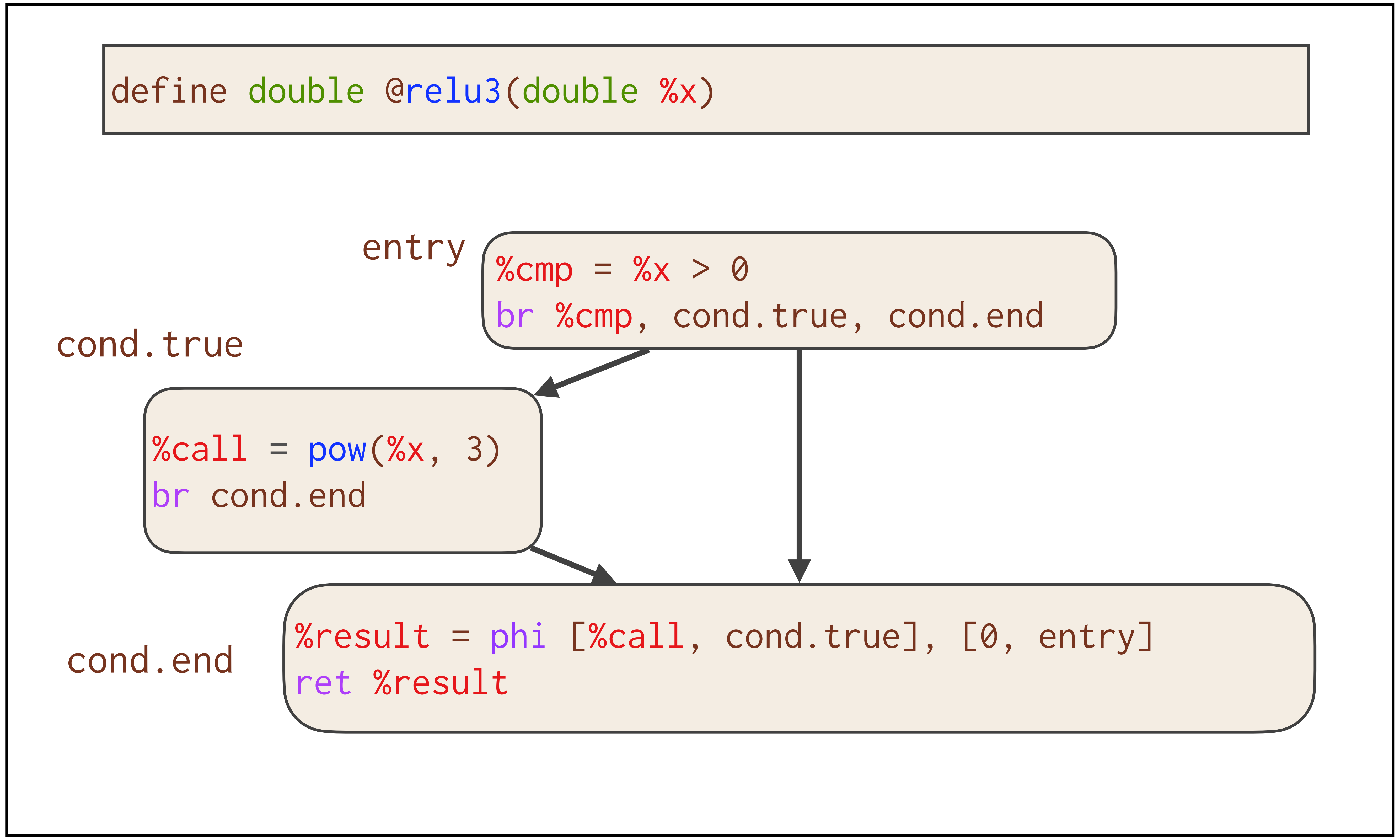
- Source rewriting
  - Statically analyze program to produce a new gradient function in the source language
  - Re-implement parsing and semantics of given language
  - Requires all code to be available ahead of time
  - Difficult to use with external libraries

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

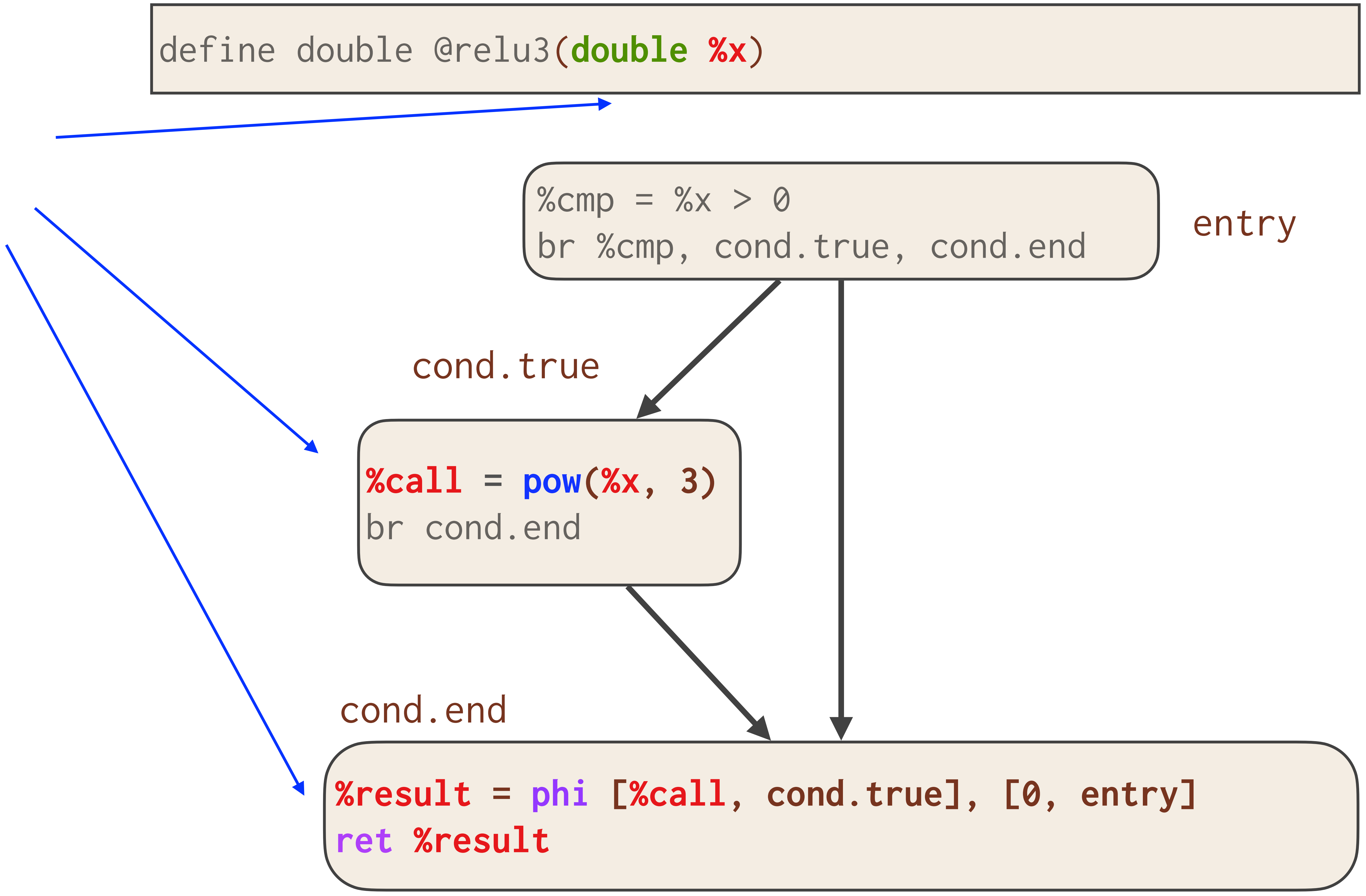


Enzyme Usage

```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

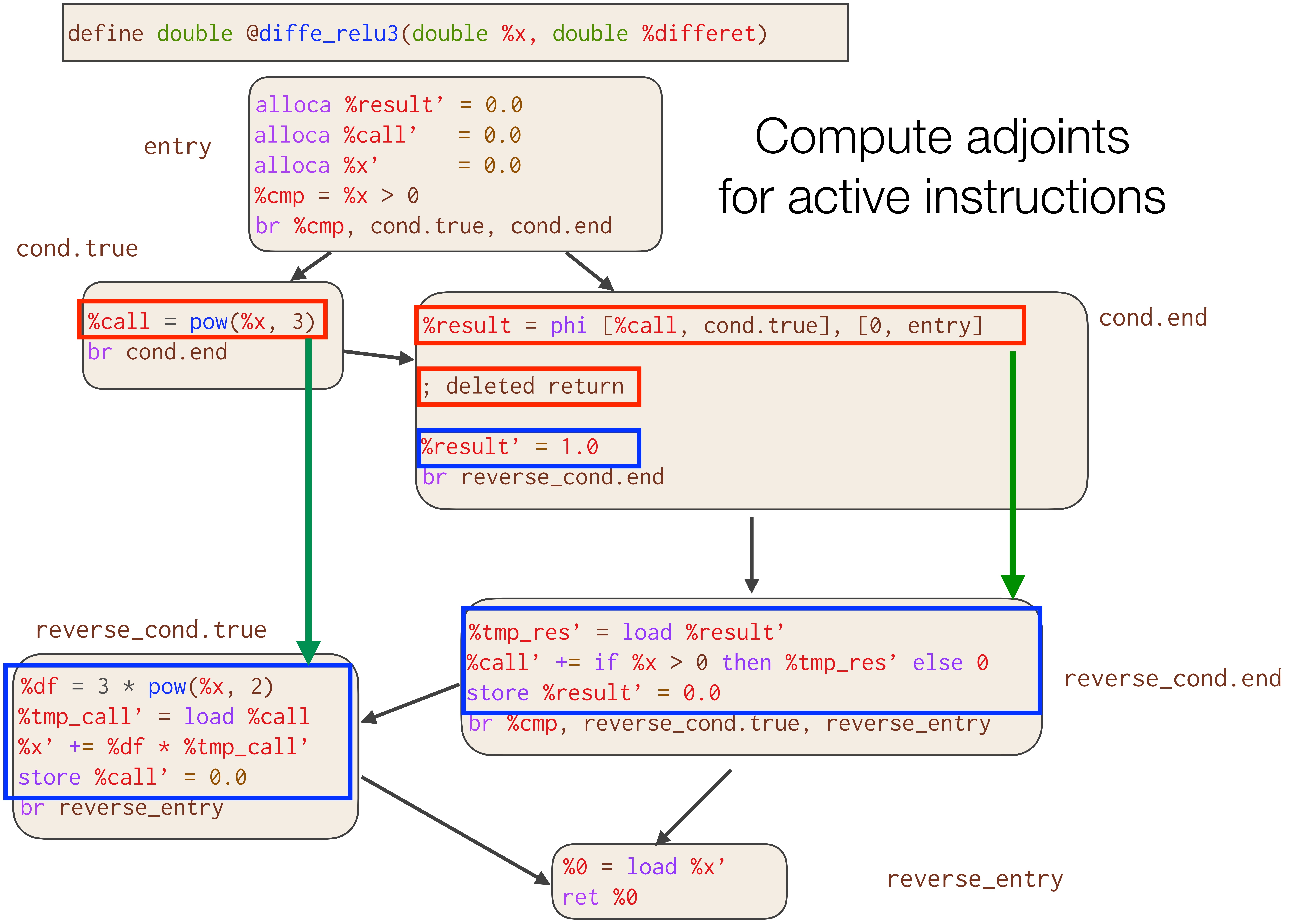
```
%call = pow(%x, 3)
br cond.end
```

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

```
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
```

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

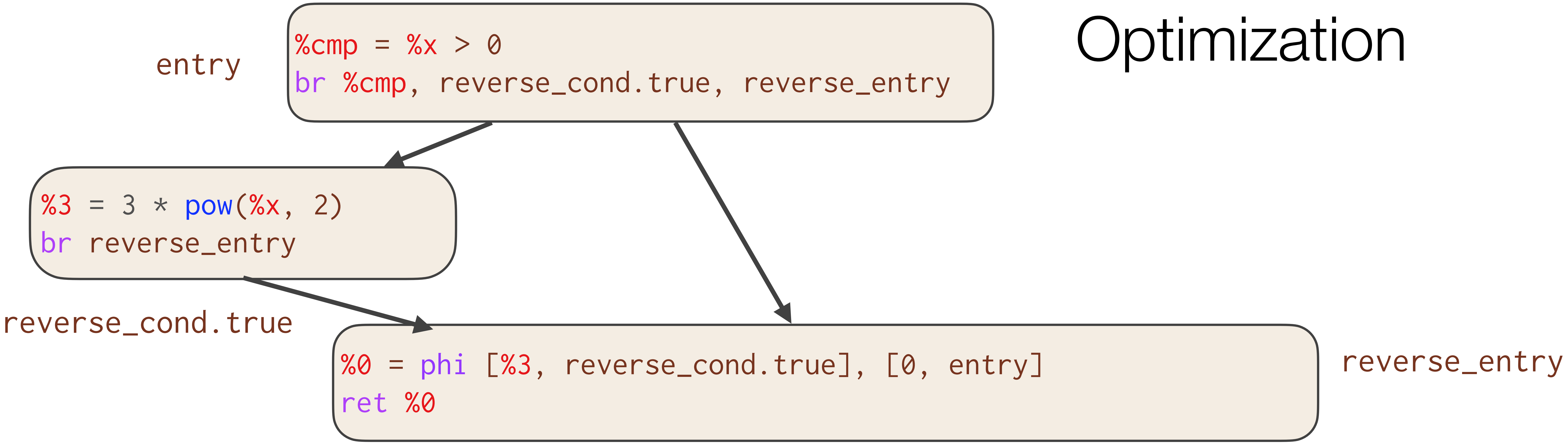
```
%df = 3 * pow(%x, 2)
%tmp_call' = load %call
%x' += %df * %tmp_call'
store %call' = 0.0
br reverse_entry
```

reverse_entry

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

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

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);
}
```

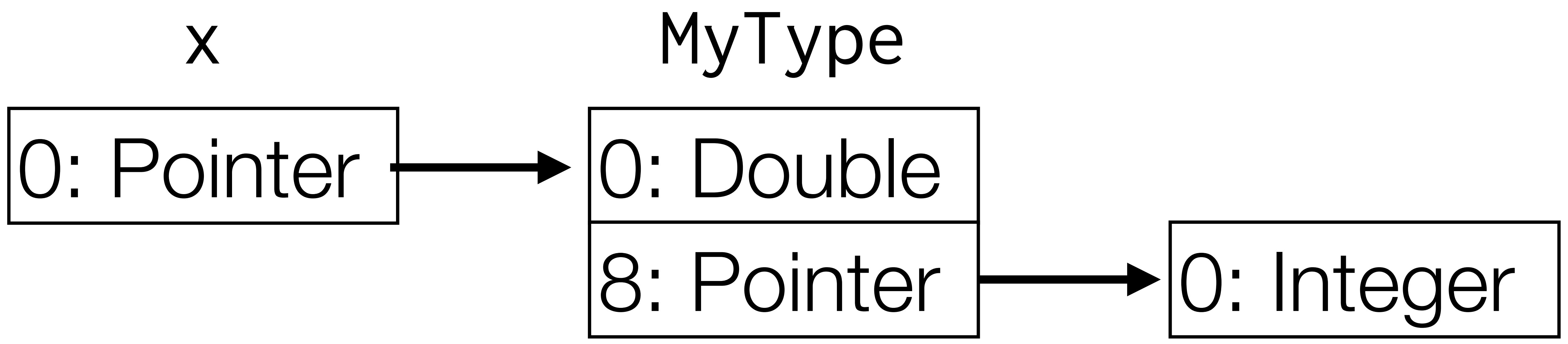
```
void grad_f(double* dst, double* dst',
            double* src, double* src') {
  // Forward Pass
  memcpy(dst, src, 8);

  // 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;
}
```

Type Analysis

- 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 MyType {
  double;
  int*;
}

x = MyType*;
```




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

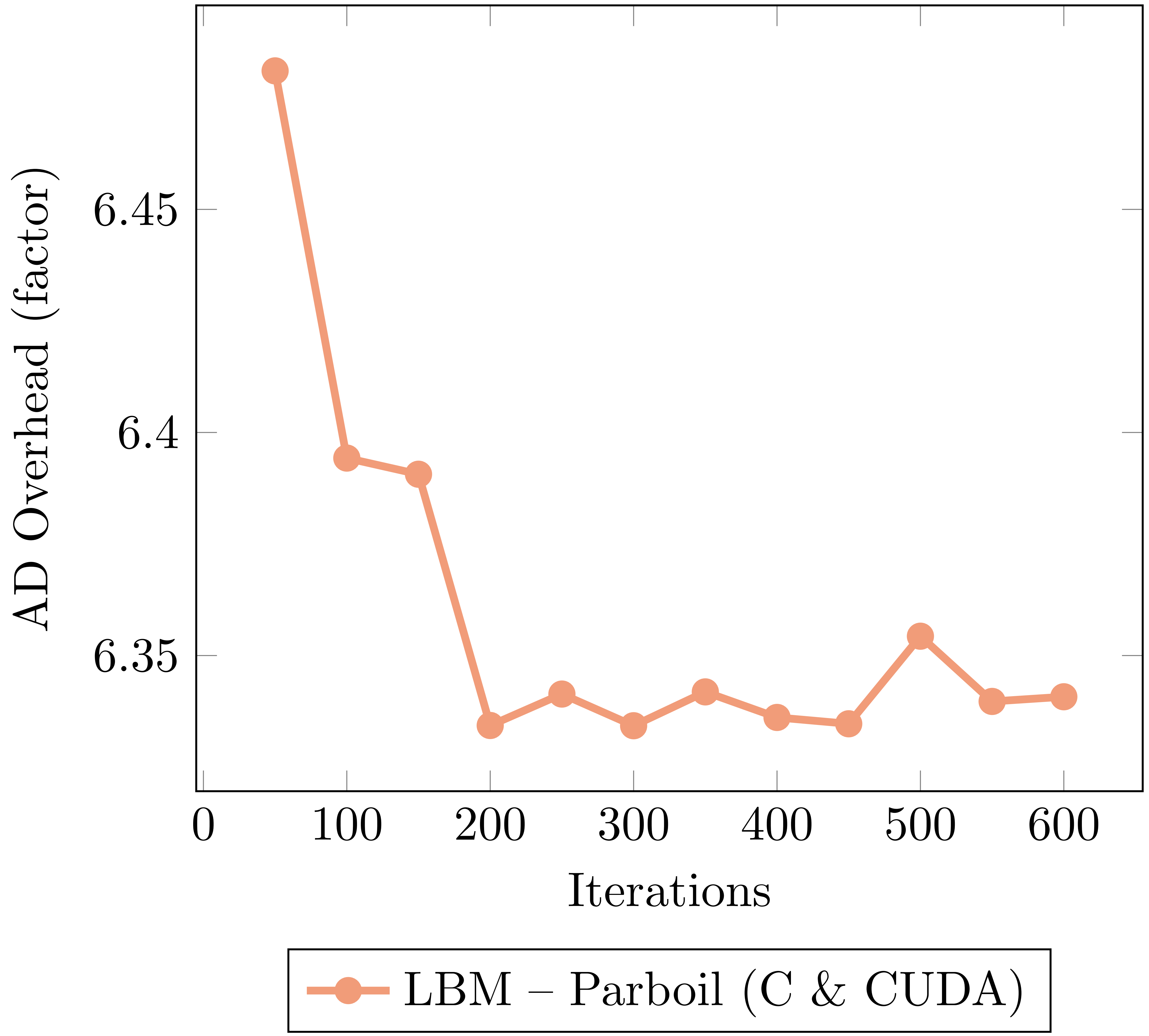
Case 3: Store, Sync, Store

```
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

Scalability Analysis (Fixed Thread Count)



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; }
}
```

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 square(double val) {
  return val * val;
}
```

Manually Rewrite

```
import tensorflow as tf

x = tf.Variable(3.14)

with tf.GradientTape() as tape:
  out = tf.math.square(x)

print(tape.gradient(out, x).numpy())
```

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

```
double square(double val) {
  return val * val;
}
```

Tool Rewrite

```
double grad_square(double val) {
  return 2 * val;
}
```

```
$ tapenade -b -o out.c -head “square(val)/(out)” square.c
```

Parallel Automatic Differentiation in LLVM

```
%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.

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

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
```

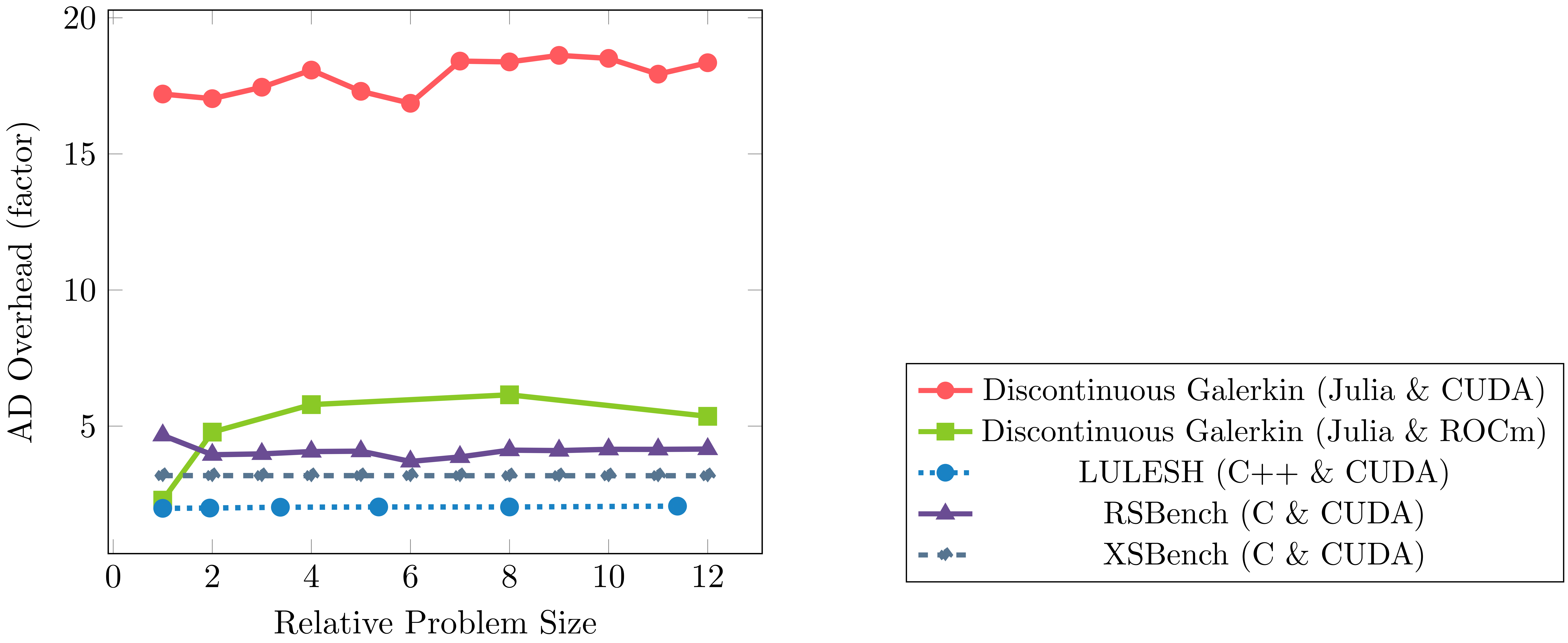
All uses of stores to d_ptr in diffe_B will correctly complete prior to diffe_A ✓

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 ✓

Scalability Analysis (Fixed Work Per Thread)



Parallel Optimization: Loop Indexing

- 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;
```

Evaluation

- Differentiated nine distinct versions of LULESH and miniBUDE applications, in a variety of parallel frameworks, and in both C++ and Julia
  - LULESH: unstructured hydrodynamics solver
  - miniBUDE: computational kernels of a molecular docking engine
- Compare performance and scalability against non-differentiated code, as well as a state of the art MPI AD tool (CoDiPack)
- Benchmarks available at: https://github.com/EnzymeAD/Enzyme-sc22

Evaluation Highlights: Runtime Overhead (LULESH)

- Overhead is stable and small, independent of number of MPI nodes, or language/ framework