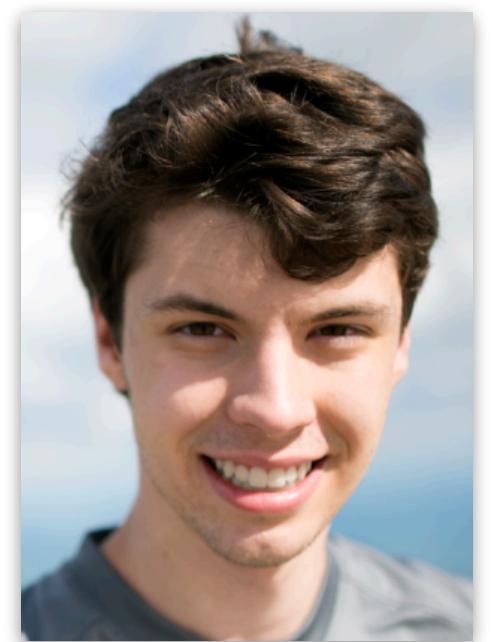


# AD-aware Compiler Optimizations in Enzyme MLIR



**Vimarsh Sathia**<sup>1</sup> Siyuan Brant Qian<sup>1</sup> Jan Hückelheim<sup>2</sup> Paul Hovland<sup>2</sup> William S. Moses<sup>1</sup>

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Sanchez-Ramirez<sup>◊</sup>, Simone Silvestri, Nora Loose<sup>♣</sup>, Ivan Ho, Vimarsh Sathia<sup>†</sup>, Jan Hueckelheim<sup>♣</sup>,  
Johannes De Fine Licht, Kevin Gleason<sup>§</sup>, Ludovic Rass, Gabriel Baraldi, Dhruv Apte<sup>#</sup>, Lorenzo  
Chelini<sup>◆</sup>, Jacques Pienaar<sup>§</sup>, Gaetan Lounes, Valentin Churavy, Sri Hari Krishna Narayanan<sup>♣</sup>, Navid  
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Narang, Tobias Grosser, Keno Fischer<sup>¶</sup>, Robert Hundt<sup>§</sup>, Albert Cohen<sup>§</sup>, Oleksandr Zinenko<sup>§ \*</sup>  
UIUC<sup>†</sup>, Google<sup>§</sup>, UCL<sup>★</sup>, MIT<sup>‡</sup>, NVIDIA<sup>◆</sup>, UT Austin<sup>#</sup>, [C]Worthy<sup>♣</sup>, BSC<sup>◊</sup>, Argonne National Laboratory<sup>♣</sup>,  
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# Outline

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- Compiler-Based Differentiation (Enzyme-LLVM)
- What is Enzyme-MLIR?
- Case Study: Tensor Algebra Optimization
- Case Study: Higher Order Derivatives
- AD-Specific Optimizations





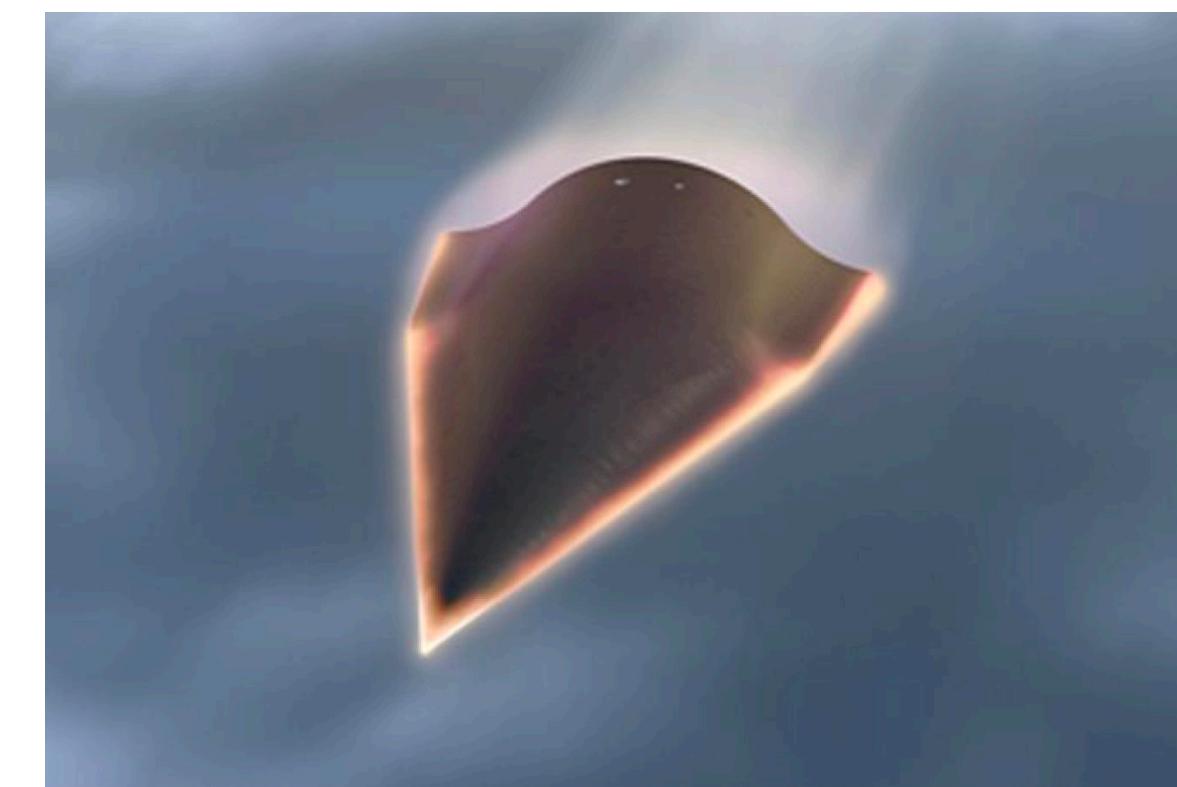
# Differentiation: Connecting Science and AI

Derivatives are key to science + ML

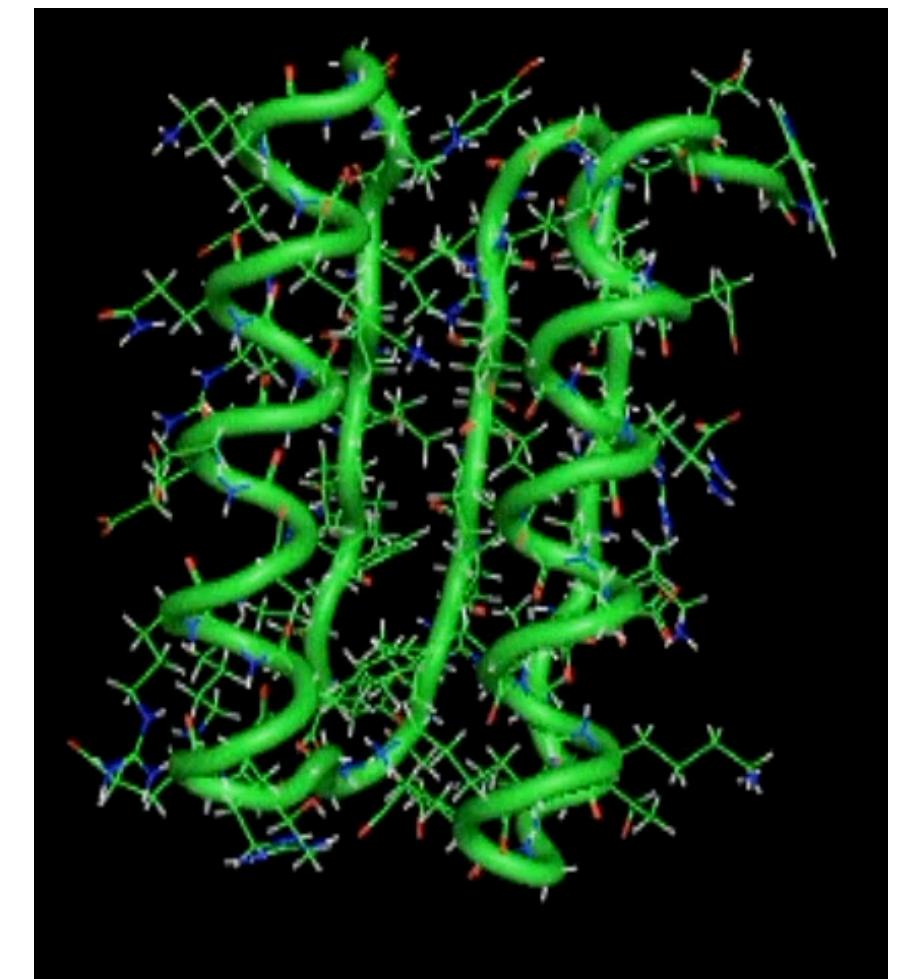
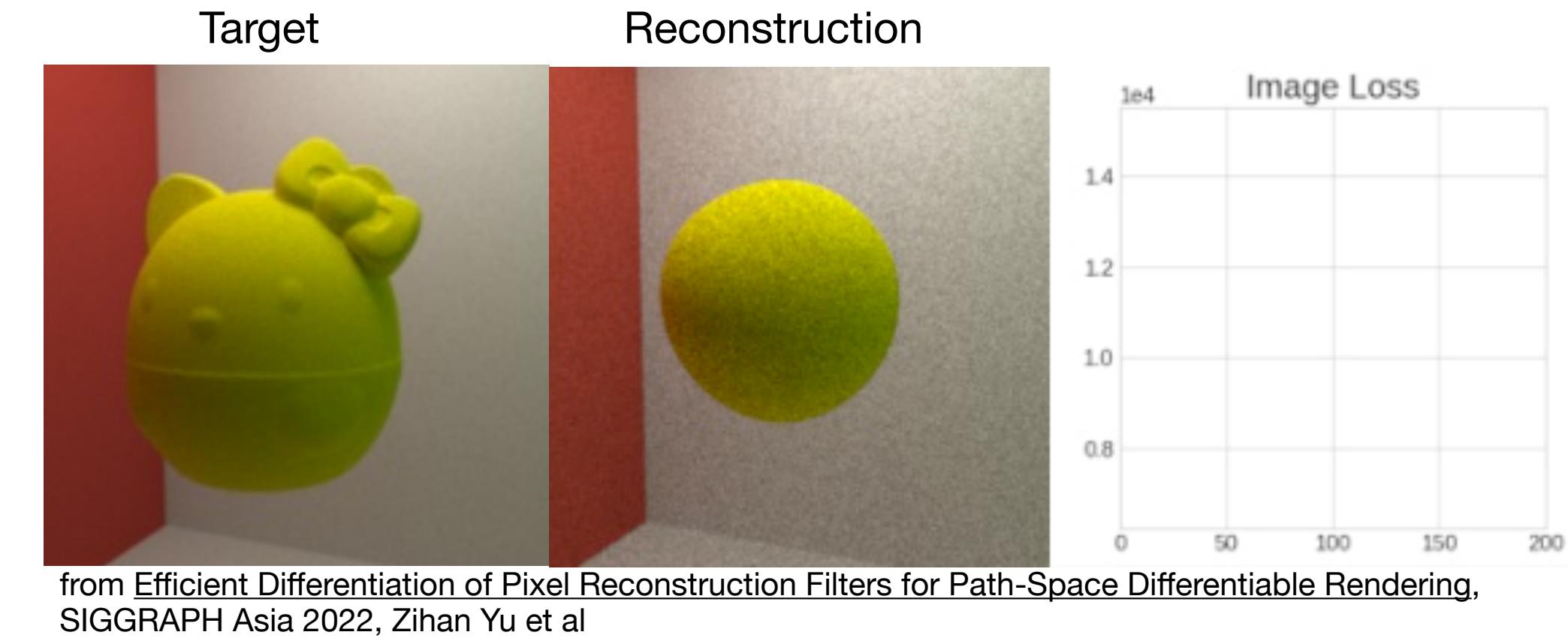
- Scientific Computing: UQ, Differential Equation, Error Analysis
- Machine Learning: Back-Propagation, Bayesian Inference



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



from [Center for the Exascale Simulation of Materials in Extreme Environments](#)

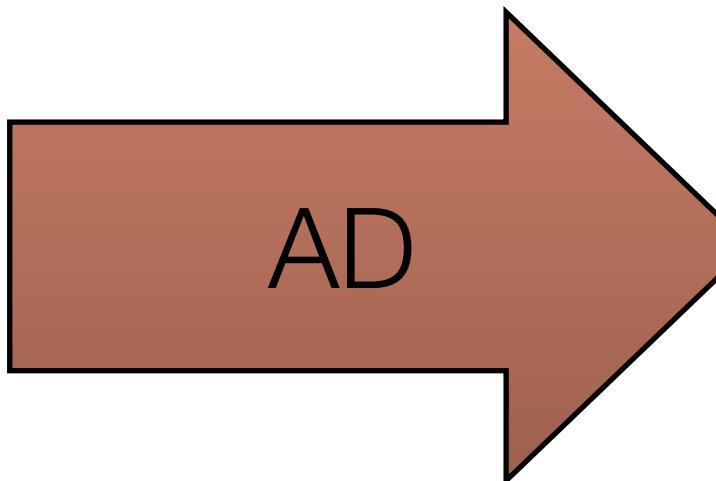


from [Differential Molecular Simulation with Molly.jl, EnzymeCon 2023, Joe Greener \(Cambridge\)](#)

# 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;  
}
```



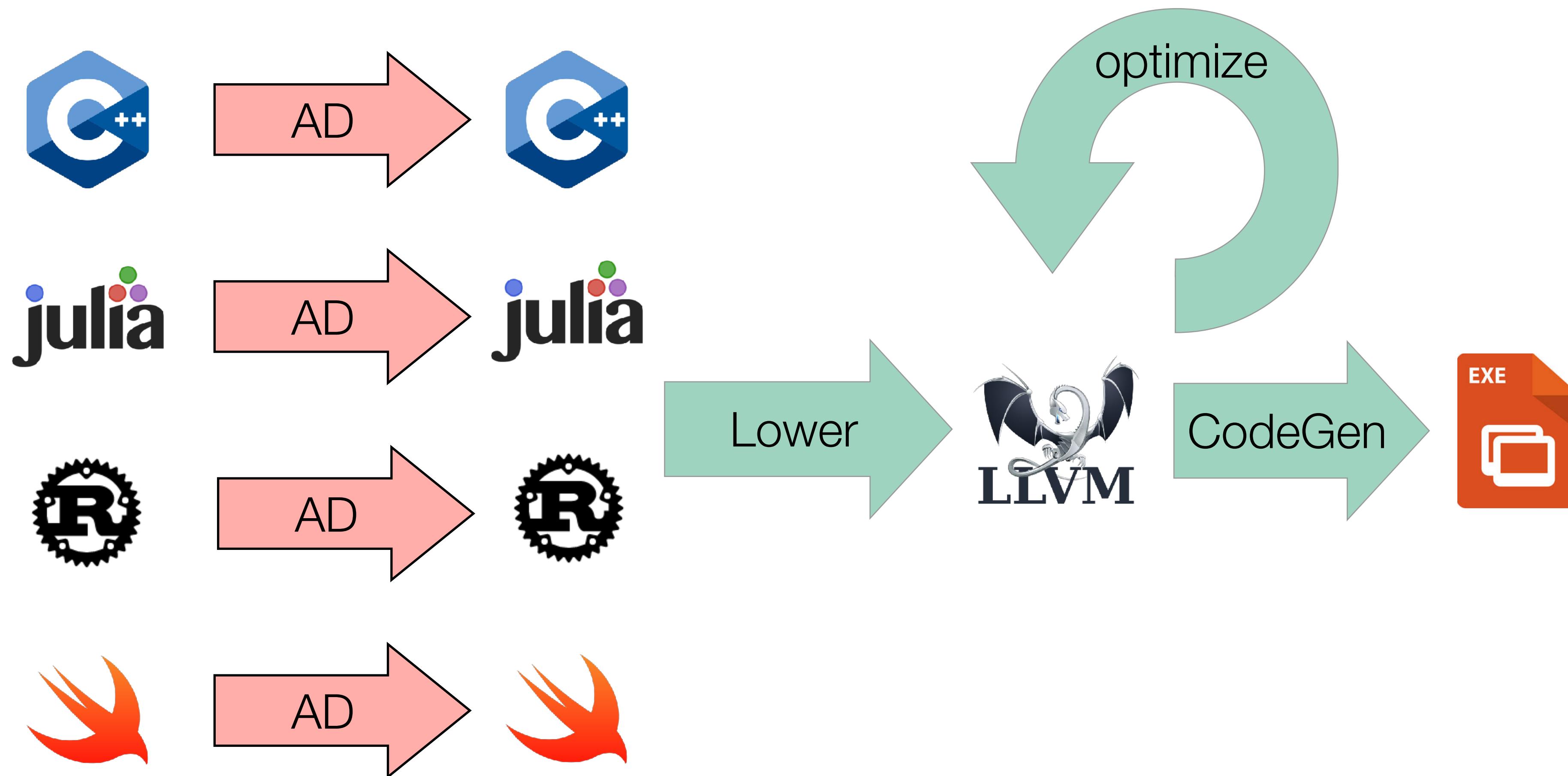
```
double grad_relu3(double x) {  
    if (x > 0)  
        return 3 * pow(x, 2)  
    else  
        return 0;  
}
```

- 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[i] = input[i];  
    input2[i] += 0.001;  
    grad_input[i] = (f(input2) - f(input))/0.001;  
}
```

```
// Automatic differentiation  
double grad_input[100];  
  
grad_f(input, grad_input)
```

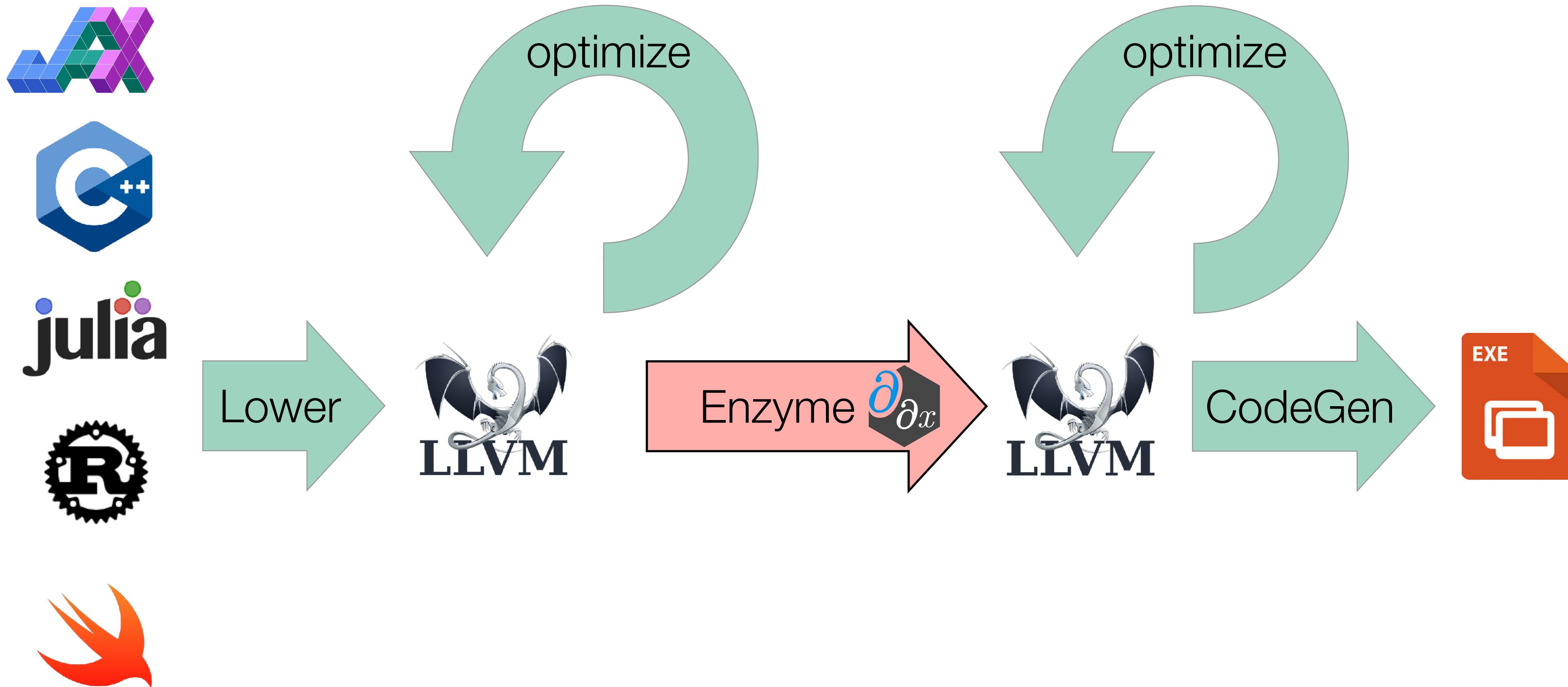
# Existing Automatic Differentiation Pipelines





# Enzyme Approach - Compiler Based Differentiation

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



# What is MLIR?



# Multi-Level Intermediate Representation (MLIR)

---

- New Compiler IR with user-defined dialects, instructions, optimizations
  - Arithmetic(arith), Linear Algebra(linalg), Complex Numbers(complex)
  - GPU Programming(gpu), Control Flow(scf)
  - Automatic Differentiation(EnzymeMLIR)

```
func @set(%arr: memref<?xf32>, %val: f32) -> f32 {  
    scf.for %ii = 0 to 10 {  
        memref.store %val, %arr [2 * %ii] : memref<?xf32>  
    }  
    %out = arith.mulf %val, %val : f32  
    return %out  
}
```

# Multi-Level Intermediate Representation (MLIR)

- New Compiler IR with user-defined dialects, instructions, optimizations
  - Arithmetic(arith), Linear Algebra(linalg), Complex Numbers(complex)
  - GPU Programming(gpu), Control Flow(scf)
  - Automatic Differentiation(EnzymeMLIR)
- **Mix and match operations and operands across multiple dialects** ★
- Core infrastructure of modern ML frameworks (JaX, PyTorch, TensorFlow)

```
func @set(%arr: memref<?xf32>, %val: f32) -> f32 {  
    scf.for %ii = 0 to 10 {  
        memref.store %val, %arr [2 * %ii] : memref<?xf32>  
    }  
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}
```

# Multi-Level Intermediate Representation (MLIR)

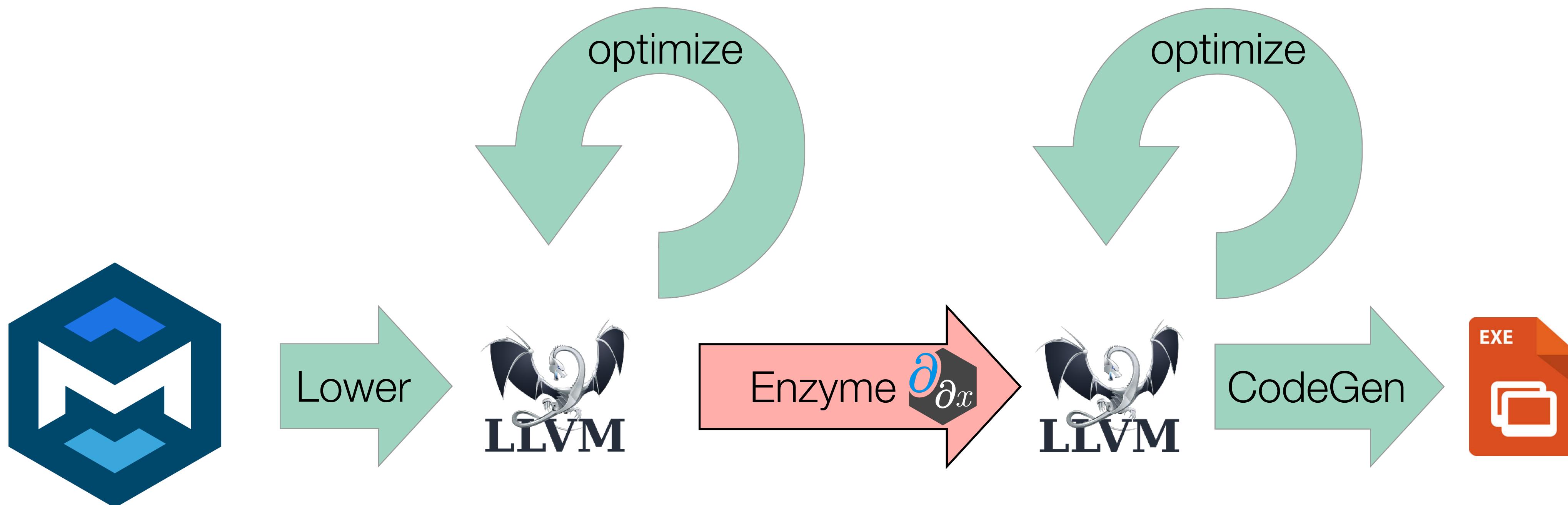
- New Compiler IR with user-defined dialects, instructions, optimizations
  - Arithmetic(arith), Linear Algebra(linalg), Complex Numbers(complex)
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  - Automatic Differentiation(EnzymeMLIR)
- Mix and match dialects and optimizations from multiple dialects
- Core infrastructure of modern ML frameworks (JaX, PyTorch, TensorFlow)

```
func @set(%arr: memref<?xf32>, %val: f32) -> f32 {  
    scf.for %ii = 0 to 10 {  
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    }  
    %out = arith.mulf %val, %val : f32  
    return %out  
}
```

## EnzymeMLIR autodiff

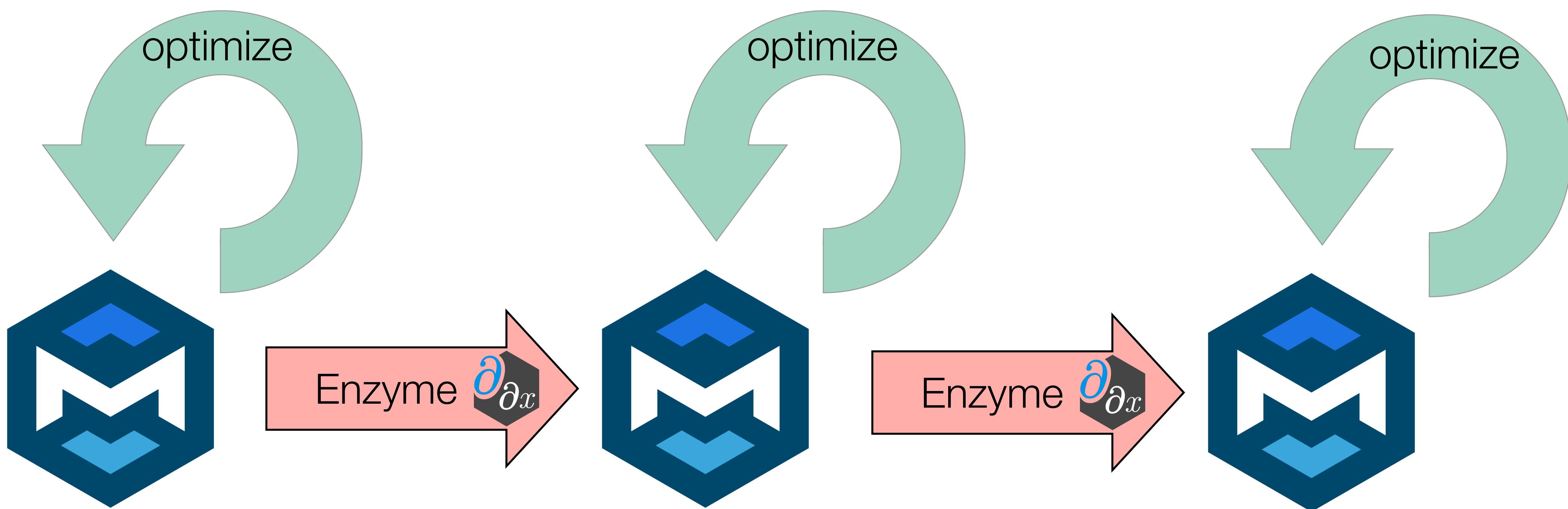
```
func @grad_set(%X: memref<?xf32>, %v: f32, %dout: f32) {  
    %out, %dv = enzyme.autodiff @set(%X,%v,%dout) {  
        activity = [enzyme_const, enzyme_active]  
        ret_activity = [enzyme_active]  
    } : (f32, f32)  
    return  
}
```

# Why Enzyme-MLIR?



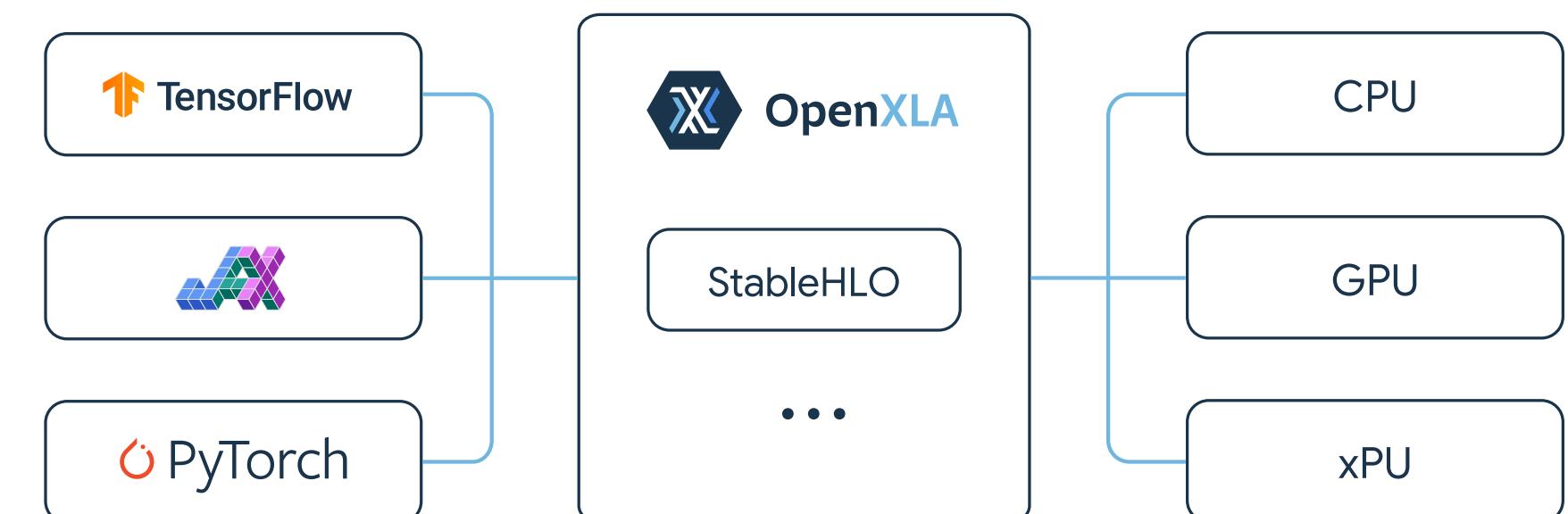
# Why Enzyme-MLIR?

**“Multi-level” coordination of AD and Optimization!**



# Case Study: Tensor Algebra Optimization

- **stablehlo** is a MLIR dialect which represents tensor algebra operations
- Implemented 200+ tensor rewrite rules to optimize code!
- **Hypothesis:** Optimizations on primal => ***outsized impact for derivatives***



Mon 3 Mar  
Displayed time zone: Pacific Time (US & Canada) [change](#)

17:40 20m ★ **The MLIR Transform Dialect - Your compiler is more powerful than you think**

Talk Martin Lücke University of Edinburgh, Michel Steuwer Technische Universität Berlin, Albert Cohen Google DeepMind, William S. Moses University of Illinois Urbana-Champaign, Alex Zinenko Google DeepMind

CGO 2025  
paper



# Tensor Algebra Optimization: example

- **stablehlo** is a MLIR dialect which represents tensor algebra operations
- Implemented 200+ tensor rewrite rules to optimize code!
- **Hypothesis:** Optimizations on primal => ***outsized impact for derivatives***

```
// Some example rules
x + 0 -> x
transpose(transpose(x)) -> x

// push slices up(reduce work)
slice(add(a,b)) -> add(slice(a),slice(b))

// push pads down(reduce work)
mul(pad(x,0),y) -> pad(mul(x,slice(y)),0)
```

```
x,y = tensor<10000xf32>
a = dot(x,y)
b = mul(a,z)
c = dot(b[0:10],4)
return c;
```



# Tensor Algebra Optimization: reduce matmul size

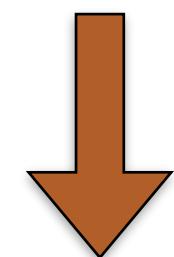
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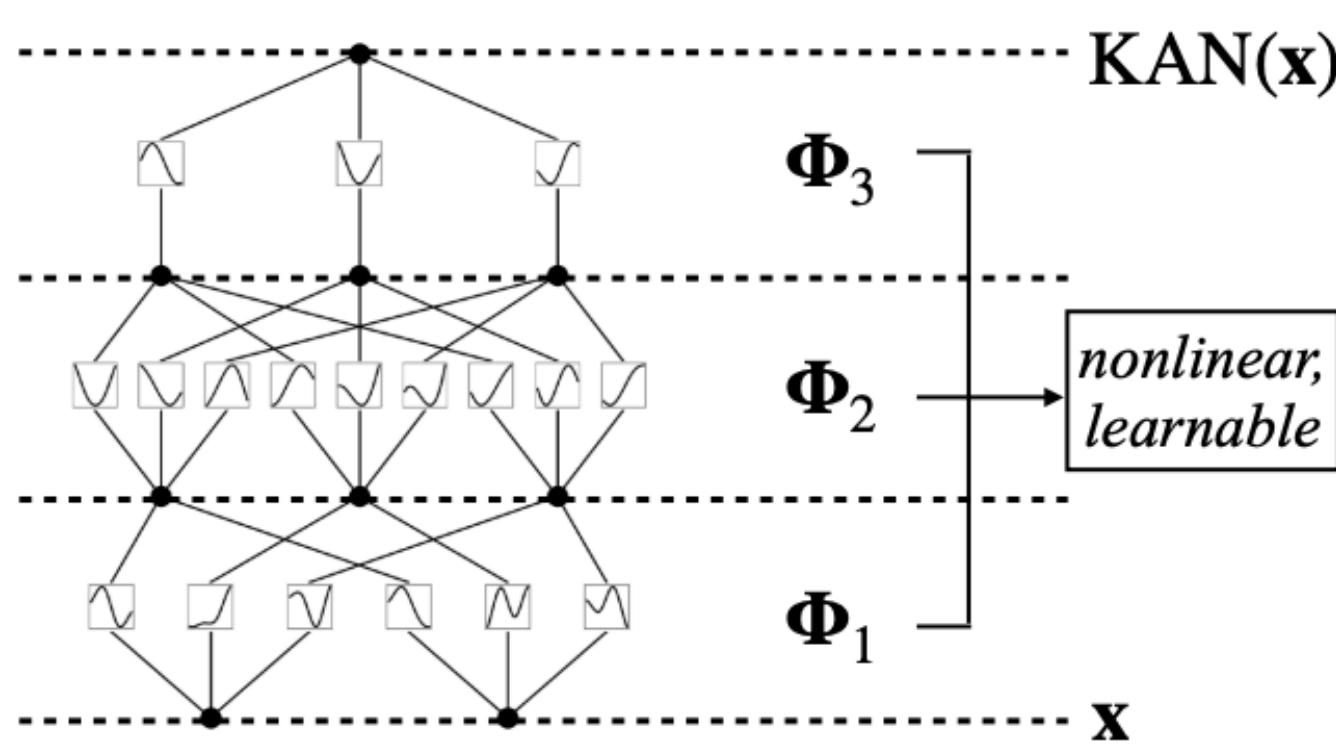


```
x,y = tensor<10000xf32>
a = dot(x,y)
b = mul(a[0:10],z[0:10])
c = dot(b,4)
return c;
```



# 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)

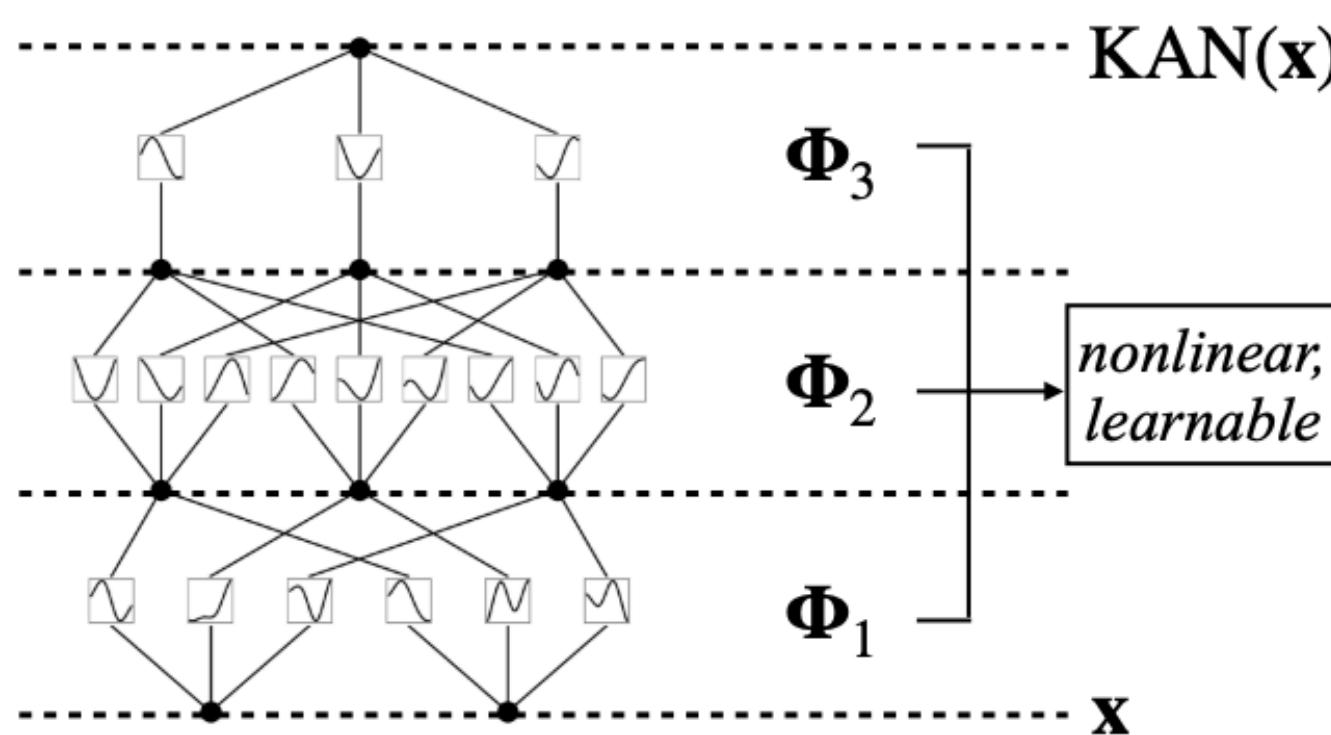
Backwards (Zygote + Julia)  
289.319 us ( 575 allocations)  
2099.000 us (1055 allocations)  
1772.000 us ( 877 allocations)

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

2.14x speedup  
(Primal)

# EnzymeMLIR in Julia (via Reactant.jl MLIR Frontend)

CUDA KAN network



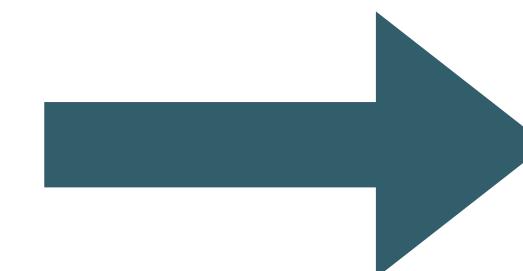
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2.14x speedup  
(Primal)



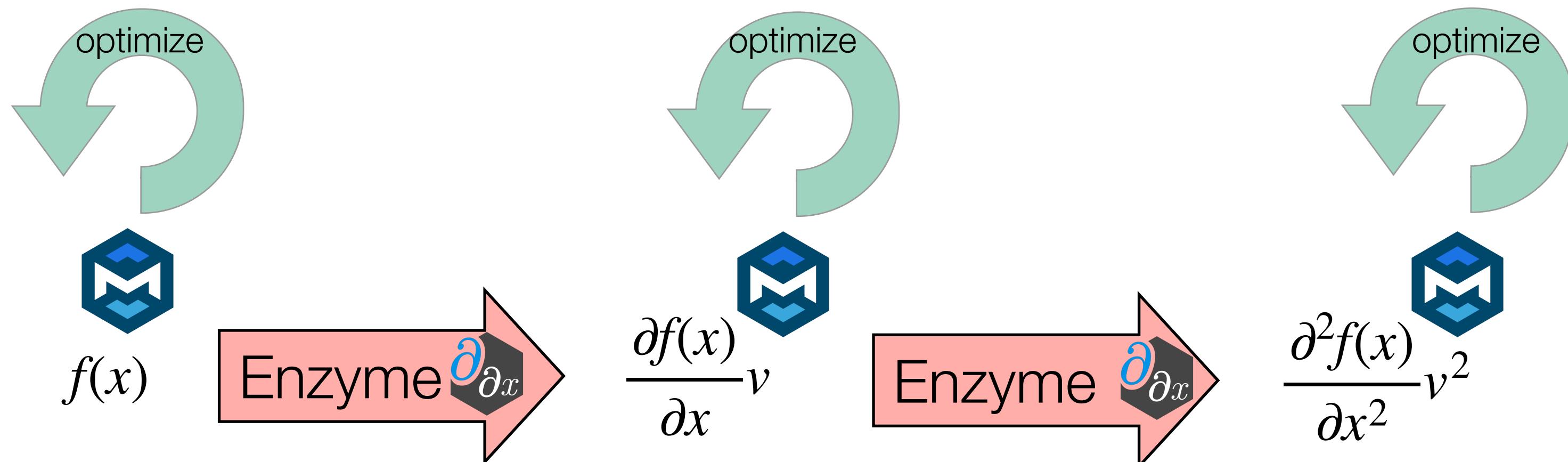
13.57x speedup  
(Derivative)

# Case Study: Higher Order Differentiation

- Mathematical structure in higher-order derivatives (like symmetry, sparsity) leaves significant room for perf engineering
- Progressively running optimizations *during AD* helps make computations tractable.

**symmetric derivatives**

$$\frac{\partial^2 f}{\partial x \ \partial y} = \frac{\partial^2 f}{\partial y \ \partial x}$$



**sparse Hessians**

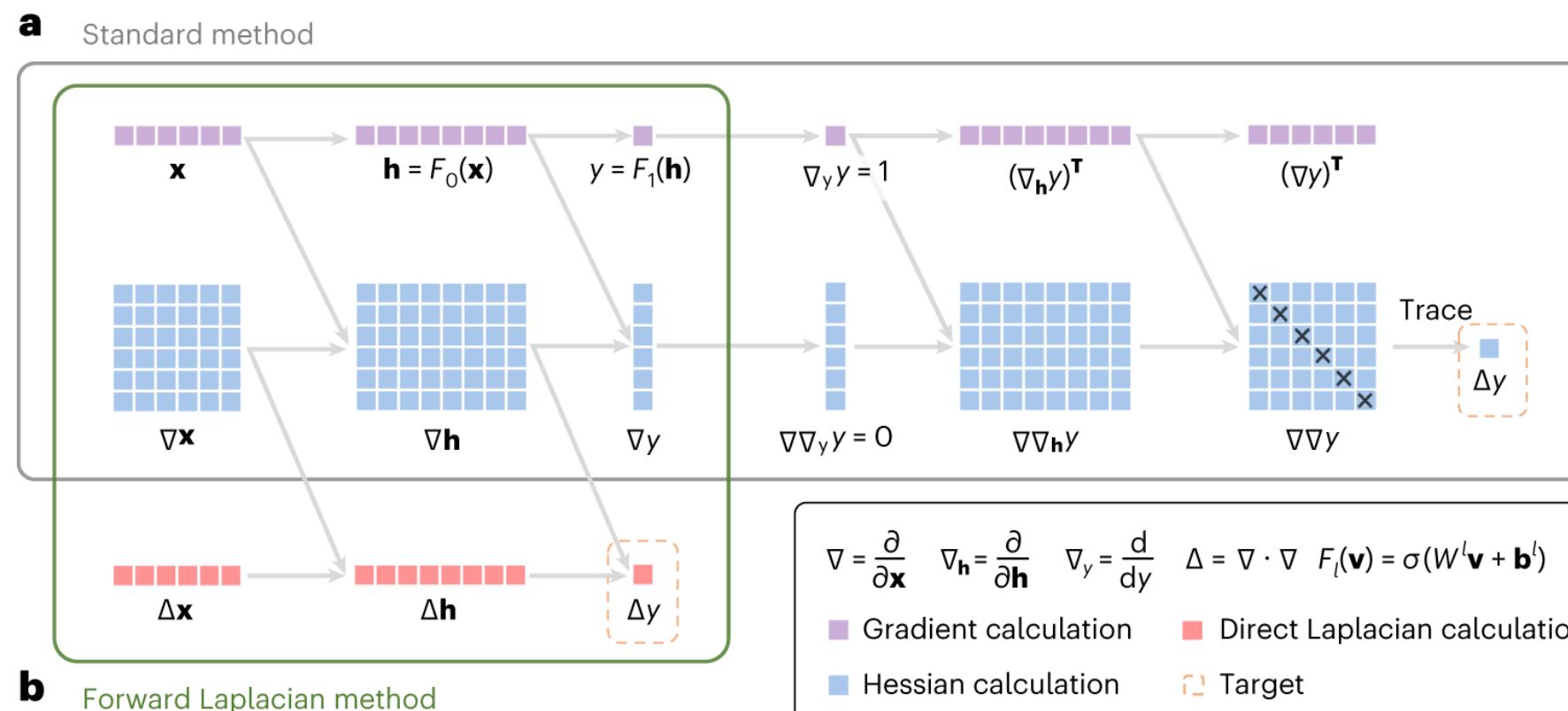
$$f(\vec{x}) = \sum_i a_i x_i^2$$

$$H(\vec{x}) = \begin{pmatrix} 2a_0 & 0 & 0 & \dots & 0 \\ 0 & 2a_1 & 0 & \dots & 0 \\ 0 & 0 & 2a_2 & \dots & 0 \\ 0 & 0 & 0 & \dots & 2a_n \end{pmatrix}$$



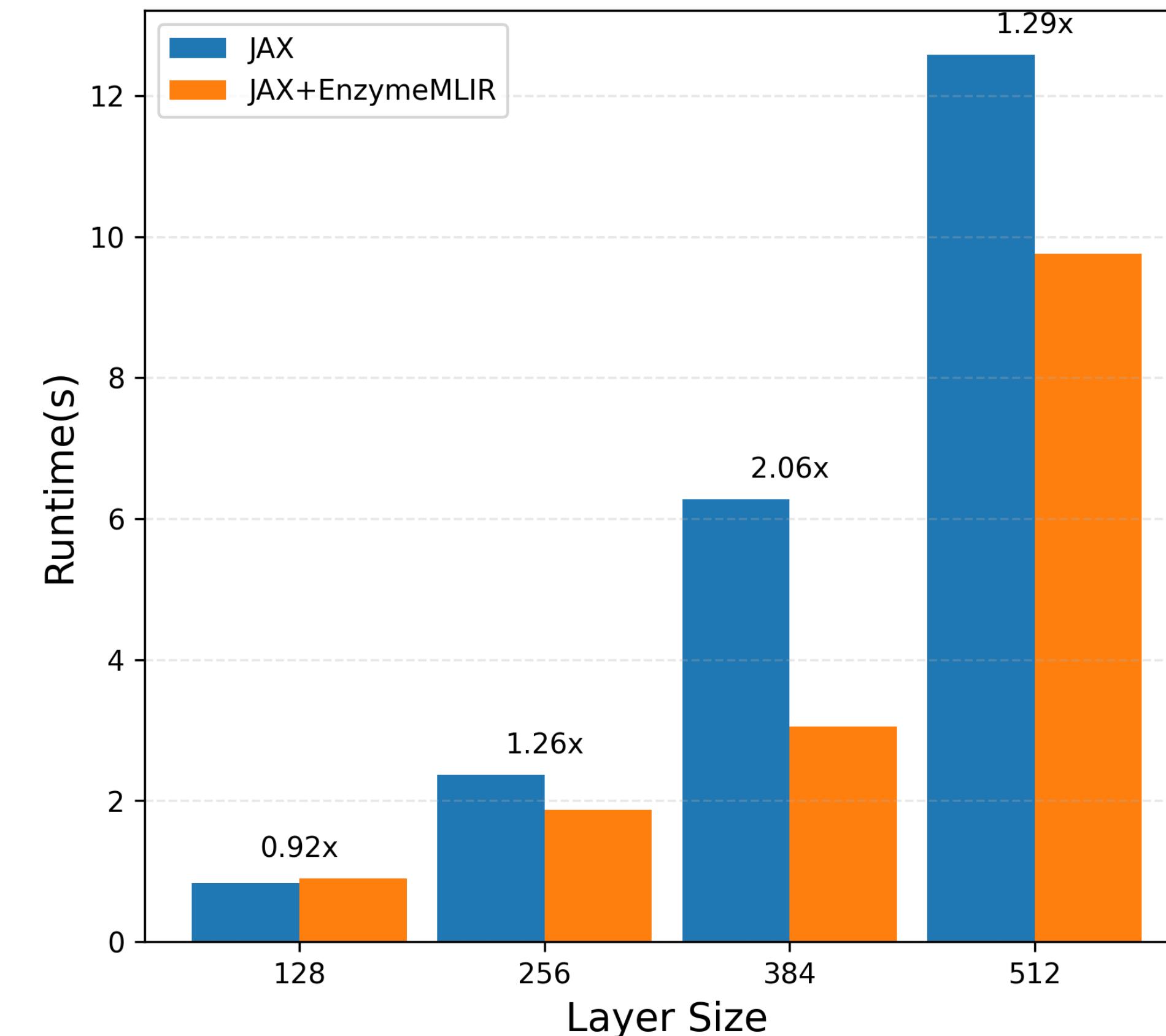
# EnzymeMLIR in Python (via JAX MLIR frontend)

CPU Laplacian of Neural Net(NN)  
used in NN-based VMC



## Laplace operator

$$\nabla^2 f = \sum_{i=1}^n \frac{\partial^2 f}{\partial x_i^2}$$



1.324x speedup  
(Forward Laplacian)



# Ongoing Work



+



# Activity in EnzymeMLIR

- Enzyme attaches an activity attribute(**enzyme\_const**, **enzyme\_active**) to each input and output of function we want to differentiate
- Activities dictate how an **enzyme.autodiff** is lowered into gradient MLIR code.
- Optimizing activity assignment => ***optimizing generated derivative code***

```
func @square(%x: f32, %y: f32) -> (f32, f32) {  
    %o1 = arith.mulf %x, %x : f32  
    %o2 = arith.mulf %y, %y : f32  
    return %o1, %o2 : f32, f32  
}
```

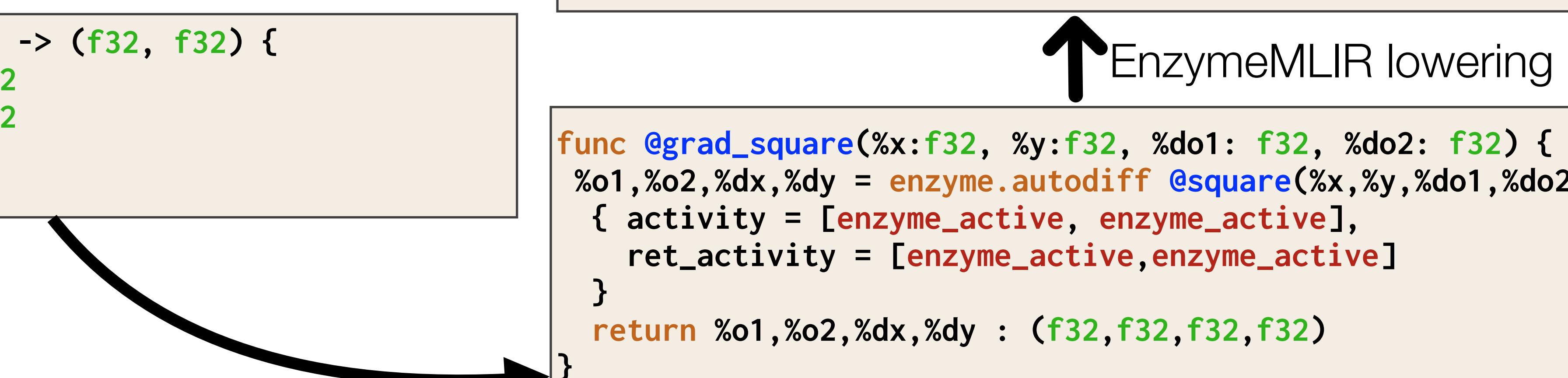
```
func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {  
    %o1,%o2,%dx,%dy = enzyme.autodiff @square(%x,%y,%do1,%do2)  
    { activity = [enzyme_active, enzyme_active],  
      ret_activity = [enzyme_active,enzyme_active]  
    }  
    return %o1,%o2,%dx,%dy : (f32,f32,f32,f32)  
}
```

# Activity in EnzymeMLIR

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func @square(%x: f32, %y: f32) -> (f32, f32) {  
    %o1 = arith.mulf %x, %x : f32  
    %o2 = arith.mulf %y, %y : f32  
    return %o1, %o2 : f32, f32  
}
```

```
func @grad_square(%arg0: f32, %arg1: f32, %arg2: f32, %arg3: f32) {  
    %0:4 = call @diffesquare(%arg0, %arg1, %arg2, %arg3)  
    return %0#0, %0#1, %0#2, %0#3 : f32, f32, f32, f32  
}  
  
func private @diffesquare(%arg0: f32, %arg1: f32, %arg2: f32, %arg3: f32) -> (f32, f32, f32, f32) {  
    %cst = arith.constant 0.000000e+00 : f32  
    %0 = arith.mulf %arg0, %arg0 : f32  
    %1 = arith.mulf %arg1, %arg1 : f32  
    %2 = arith.addf %arg2, %cst : f32  
    %3 = arith.addf %arg3, %cst : f32  
    %4 = arith.mulf %3, %arg1 : f32  
    %5 = arith.addf %4, %cst : f32  
    %6 = arith.mulf %3, %arg1 : f32  
    %7 = arith.addf %5, %6 : f32  
    %8 = arith.mulf %2, %arg0 : f32  
    %9 = arith.addf %8, %cst : f32  
    %10 = arith.mulf %2, %arg0 : f32  
    %11 = arith.addf %9, %10 : f32  
    return %0, %1, %11, %7 : f32, f32, f32, f32  
}
```



```
func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {  
    %o1,%o2,%dx,%dy = enzyme.autodiff @square(%x,%y,%do1,%do2)  
    { activity = [enzyme_active, enzyme_active],  
      ret_activity = [enzyme_active,enzyme_active]  
    }  
    return %o1,%o2,%dx,%dy : (f32,f32,f32,f32)  
}
```

# Reverse Mode Activity Canonicalization

- Depending on the program context, we can modify the activity assignment to **activity** and **ret\_activity**.
- **Idea:** Avoid unnecessary gradient computations, **before codegen**
- Before canonicalization, we **check variable uses** and **derivative values** (e.g. `dval = 0.0f`) to promote activity

Activity	Primal	Derivative
active	✓	✓
activenoneed	✗	✓
const	✓	✗
constnoneed	✗	✗



# Reverse Mode Activity Canonicalization - Example

```
func @square(%x: f32, %y: f32) -> (f32, f32) {  
    %o1 = arith.mulf %x, %x : f32  
    %o2 = arith.mulf %y, %y : f32  
    return %o1, %o2 : f32, f32  
}
```

```
func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {  
    %o1,%o2,%dx,%dy = enzyme.autodiff @square(%x,%y,%do1,%do2)  
    { activity = [enzyme_active,enzyme_active],  
        ret_activity = [enzyme_active,enzyme_active]  
    }  
    return %o2,%dx : (f32,f32)  
}
```

Activity	Primal	Derivative
active	✓	✓
activenoneed	✗	✓
const	✓	✗
constnoneed	✗	✗



# Reverse Mode Activity Canonicalization - Example

```
func @square(%x: f32, %y: f32) -> (f32, f32) {  
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func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {  
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    }  
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```

Activity	Primal	Derivative
active	✓	✓
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constnoneed	✗	✗

only need **o2** and **dx**



# Reverse Mode Activity Canonicalization - Example

```
func @square(%x: f32, %y: f32) -> (f32, f32) {  
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    return %o1, %o2 : f32, f32  
}
```

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func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {  
    %o1,%o2,%dx,%dy = enzyme.autodiff @square(%x,%y,%do1,%do2)  
    { activity = [enzyme_active,enzyme_active],  
        ret_activity = [enzyme_active,enzyme_active]  
    }  
    return %o2,%dx : (f32,f32)  
}
```

eliminate dy

```
func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {  
    %o1,%o2,%dx = enzyme.autodiff @square(%x,%y,%do1)  
    { activity = [enzyme_active, enzyme_const],  
        ret_activity = [enzyme_active, enzyme_const]  
    }  
    return %o2,%dx : (f32,f32)  
}
```

Activity	Primal	Derivative
active	✓	✓
activenoneed	✗	✓
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constnoneed	✗	✗



# Reverse Mode Activity Canonicalization - Example

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func @square(%x: f32, %y: f32) -> (f32, f32) {  
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    %o2 = arith.mulf %y, %y : f32  
    return %o1, %o2 : f32, f32  
}
```

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```

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eliminate dy

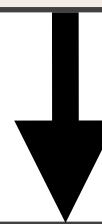
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    %o1, %o2, %dx = enzyme.autodiff @square(%x, %y, %do1)  
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    }  
    return %o2, %dx : (f32, f32)  
}
```



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```
func @square(%x: f32, %y: f32) -> (f32, f32) {
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    return %o1, %o2 : f32, f32
}
```

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func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {
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    { activity = [enzyme_active,enzyme_active],
      ret_activity = [enzyme_active,enzyme_active]
    }
    return %o2,%dx : (f32,f32)
}
```



don't return o1

```
func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {
    %o1,%o2,%dx = enzyme.autodiff @square(%x,%y,%do1)
    { activity = [enzyme_active, enzyme_const],
      ret_activity = [enzyme_active, enzyme_const]
    }
    return %o2,%dx : (f32,f32)
}
```

Activity	Primal	Derivative
active	✓	✓
activenoneed	✗	✓
const	✓	✗
constnoneed	✗	✗

```
func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {
    %o2,%dx = enzyme.autodiff @square(%x,%y,%do1)
    { activity = [enzyme_active, enzyme_const],
      ret_activity = [enzyme_activenoneed, enzyme_const]
    }
    return %o2,%dx : (f32,f32)
}
```



# Reverse Mode Activity Canonicalization - Example

```
func @square(%x: f32, %y: f32) -> (f32, f32) {
    %o1 = arith.mulf %x, %x : f32
    %o2 = arith.mulf %y, %y : f32
    return %o1, %o2 : f32, f32
}
```

```
func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {
    %o1,%o2,%dx,%dy = enzyme.autodiff @square(%x,%y,%do1,%do2)
    { activity = [enzyme_active,enzyme_active],
      ret_activity = [enzyme_active,enzyme_active]
    }
    return %o2,%dx : (f32,f32)
}
```

don't return o1

```
func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {
    %o1,%o2,%dx = enzyme.autodiff @square(%x,%y,%do1)
    { activity = [enzyme_active, enzyme_const],
      ret_activity = [enzyme_active, enzyme_const]
    }
    return %o2,%dx : (f32,f32)
}
```

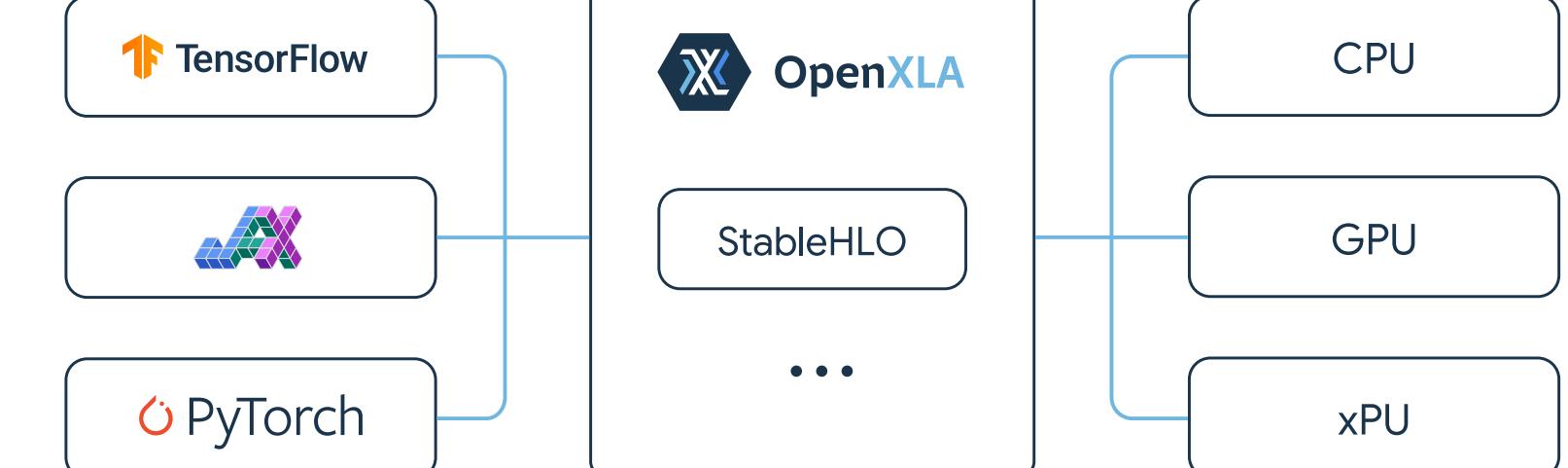
Activity	Primal	Derivative
active	✓	✓
activenoneed	✗	✓
const	✓	✗
constnoneed	✗	✗

```
func @grad_square(%x:f32, %y:f32, %do1: f32, %do2: f32) {
    %o2,%dx = enzyme.autodiff @square(%x,%y,%do1)
    { activity = [enzyme_active, enzyme_const],
      ret_activity = [enzyme_activenoneed, enzyme_const]
    }
    return %o2,%dx : (f32,f32)
}
```



# Summary

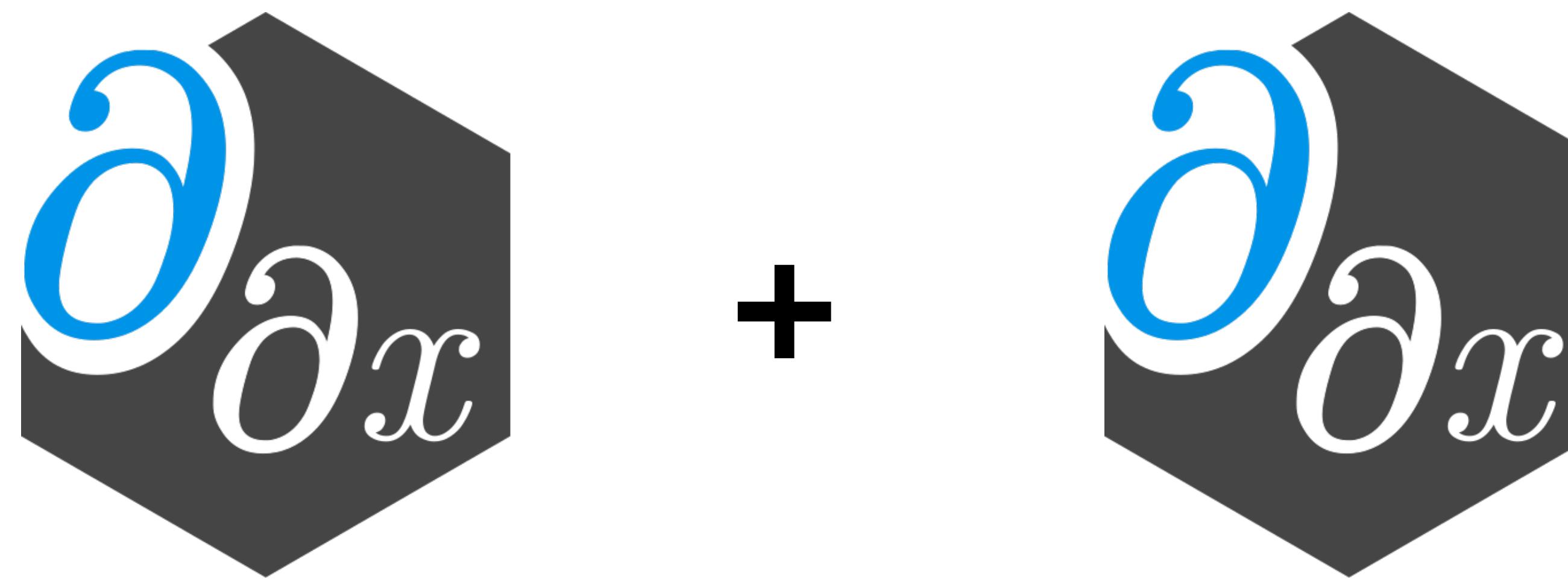
- Enzyme approach (AD + compiler)
- EnzymeMLIR dialect
- Tensor Algebra Optimization
- Higher Order Derivatives
- Return Activity Canonicalization



```
func @grad_set(%X: memref<?xf32>, %v: f32, %dout: f32) {  
    %out, %dv = enzyme.autodiff @set(%X, %v, %dout) {  
        activity = [enzyme_const, enzyme_active]  
        ret_activity = [enzyme_active]  
    } : (f32, f32)  
    return  
}
```



# Backup slides





# 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


$$O(n^2)$$

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

Optimize

$$O(n)$$

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

AD

$$O(n)$$

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

# 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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$$O(n^2)$$

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

Optimize

$$O(n^2)$$

```
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!

