Automated Batching and Differentiation of Scalar Code in Enzyme

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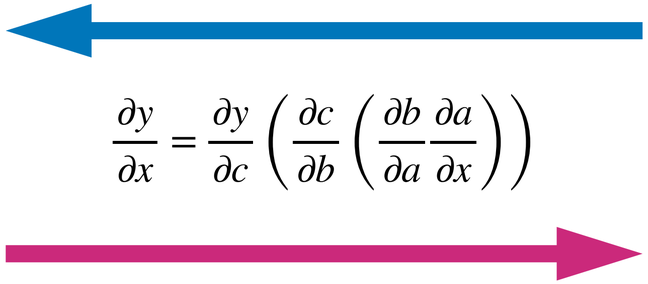
Overview

1. Compiler-based Automatic Differentiation
2. Design of Vector-Mode / Batching
3. Usage Examples
4. Benchmarks
5. Future Work

Compiler-based Automatic Differentiation

Forward- and Reverse-Mode

- Forward-Mode
  - Evaluation performed right to left
  - Information flow in same direction as computation, no caching required
  - Efficient for functions $f : \mathbb{R}^n \to \mathbb{R}^m$ where $m \gg n$
- Reverse-Mode
  - Evaluation performed left to right
  - Information flow in opposite direction as computation, elaborate caching required
  - Efficient for functions $f : \mathbb{R}^n \to \mathbb{R}^m$ where $m \ll n$



$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial c}\left(\frac{\partial c}{\partial b}\left(\frac{\partial b}{\partial a}\frac{\partial a}{\partial x}\right)\right)$$

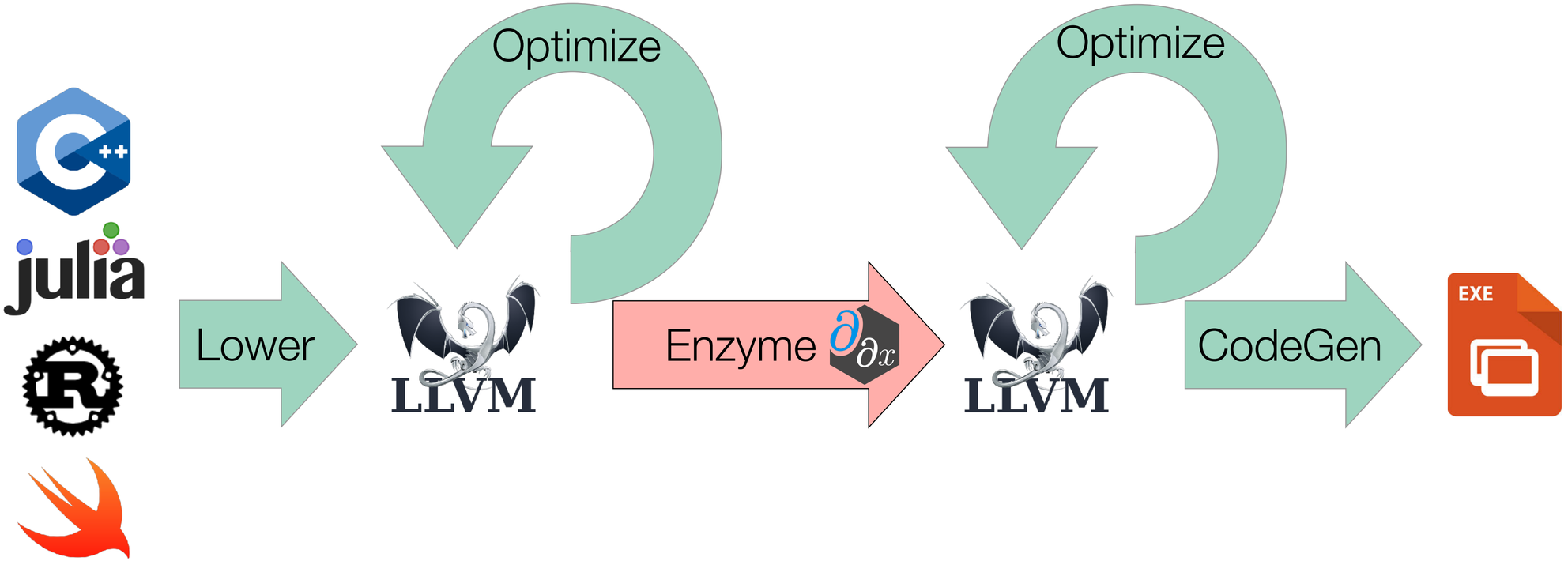
Compiler-based Automatic Differentiation

The Advantages

- Ability to access and modify the program at any point during the compilation process
  - Ability to run optimizations before, and after differentiation
  - Identify source-line information from metadata
  - Rewrite & modify library calls
- Ability to run a JIT-compiler

Enzyme's Approach

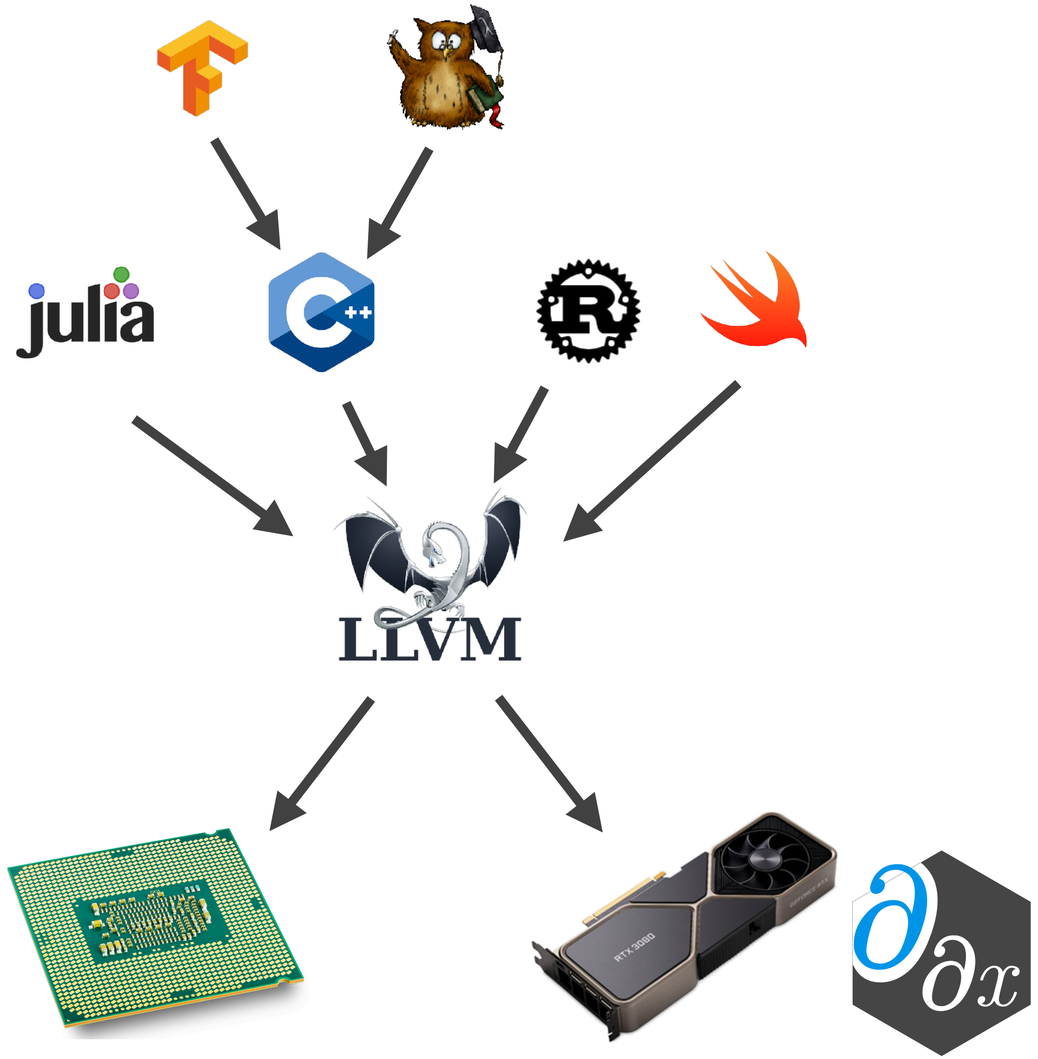
Optimize then Differentiate



Enzyme Frontends

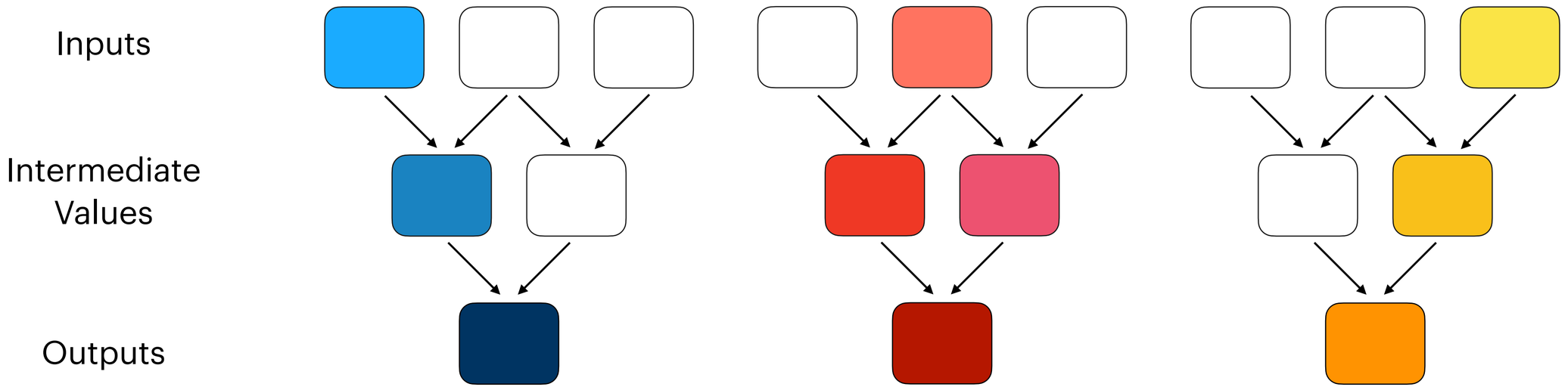
Deeply Rooted in the LLVM Ecosystem

- Generic low-level compiler infrastructure with many frontends
  - “Cross-platform assembly”
  - Many Backends (CPU, CUDA, AMDGPU, ..)
- Well-defined semantics
- Large collection of optimizations and analyses which can be utilised within the automatic differentiation



Vector Mode AD

Forward Mode



- **Forward Mode** computes the derivative of f with respect to one input
- **Reverse Mode** computes the gradients of f for all inputs

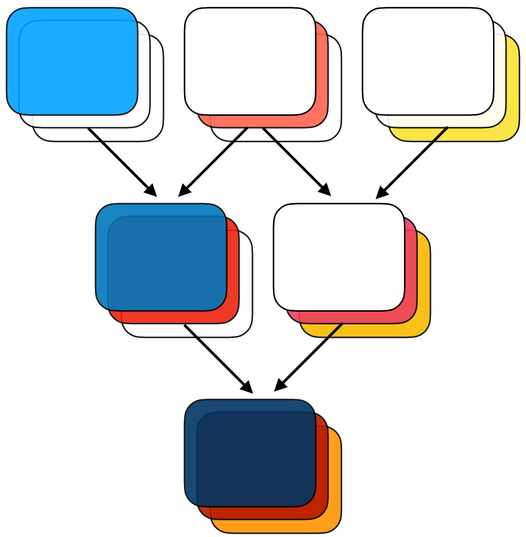
Vector Mode AD

Forward Mode

Inputs

Intermediate Values

Outputs



- Vector Mode maps perfectly to SIMD

Vector Mode AD

Use cases

- Make optimal use of available hardware
- Forward-mode AD, compute derivatives for all inputs
- Reverse-mode AD, compute gradients with respect to multiple outputs

Vector Mode AD

Benefits

- Avoid re-evaluation of the original function
- Cache values from the original function only once

Vector Mode AD

Case study: Expensive call

- Runtime of **f** mostly bound by call to slow
- Value of slow() takes place in derivative computation but does not propagate derivatives

```
float f(float x[2]) {
  float sum = x[0] + x[1];
  float val = slow();
  sum *= val;
  return sum;
}
```

Forward Mode AD

```
float df(float x[2], float d_x[2]) {
  float d_sum = d_x[0] + d_x[1];
  float val = slow();
  d_sum *= val;
  return d_sum;
}
```

Vector Mode AD

Case study: Expensive call

```
float f(float x[2]) {
  float sum = x[0] + x[1];
  float val = slow();
  sum *= val;
  return sum;
}
```

Forward Vector Mode AD

```
float[2] df_batch(float x[2],
                  float d_x[2][2]) {
  float d_sum[2];
  d_sum[0] += d_x[0][0] + d_x[0][1];
  d_sum[1] += d_x[1][0] + d_x[1][1];

  float val = slow();

  d_sum[0] *= val;
  d_sum[1] *= val;

  return d_sum;
}
```

Vector Mode AD

Simulating reverse mode

- Compute gradient with respect to
  - **x1** by setting **dx** to (1,0)
  - **x2** by setting **dx** to (0,1)

```
float[2] grad_f_batch(float x[2]) {
   float d_x[2][2] = {
     {1, 0},
     {0, 1}
   };
   return df_batch(x, d_x);
}
```

```
float[2] df_batch(float x[2],
                  float d_x[2][2]) {
  float d_sum[2];
  d_sum[0] += d_x[0][0] + d_x[0][1];
  d_sum[1] += d_x[1][0] + d_x[1][1];

  float val = slow();

  d_sum[0] *= val;
  d_sum[1] *= val;

  return d_sum;
}
```

Vector Mode
Design

1. Perform **Activity Analysis,** determine which instructions are required to compute the derivatives
2. Perform **Type Analysis**

4. **Synthesis**: Propagate with each active value a vector of derivatives
5. For each pointer store a vector of shadow pointers
6. Create shadow allocations for each heap data structure

8. Emit instructions for the application of the chain rules n-times according to vector width
9. Let the LLVM vectoriser do the rest

Usage
LLVM IR

```
declare [2 x double] @__enzyme_fwddiff(...)

define double @square(double %x) {
  %mul = fmul double %x, %x
  ret double %mul
}

define [2 x double] @dsquare(double %x, double %dx1, double %dx2) {
  %call = call [2 x double] (...) @__enzyme_fwddiff(double (double)* @square,
                                                    metadata !"enzyme_width", i64 2,
                                                    double %x, double %dx1, double %dx2)
  ret [2 x double] %call
}


define [2 x double] @dsquare(double %x, double %dx1, double %dx2) {
  %factor.i = fmul double %x, 2.0
  %1 = fmul double %factor.i, %dx1
  %2 = insertvalue [2 x double] undef, double %1, 0
  %3 = fmul double %factor.i, %dx2
  %4 = insertvalue [2 x double] %2, double %3, 1
  ret [2 x double] %4
}
```

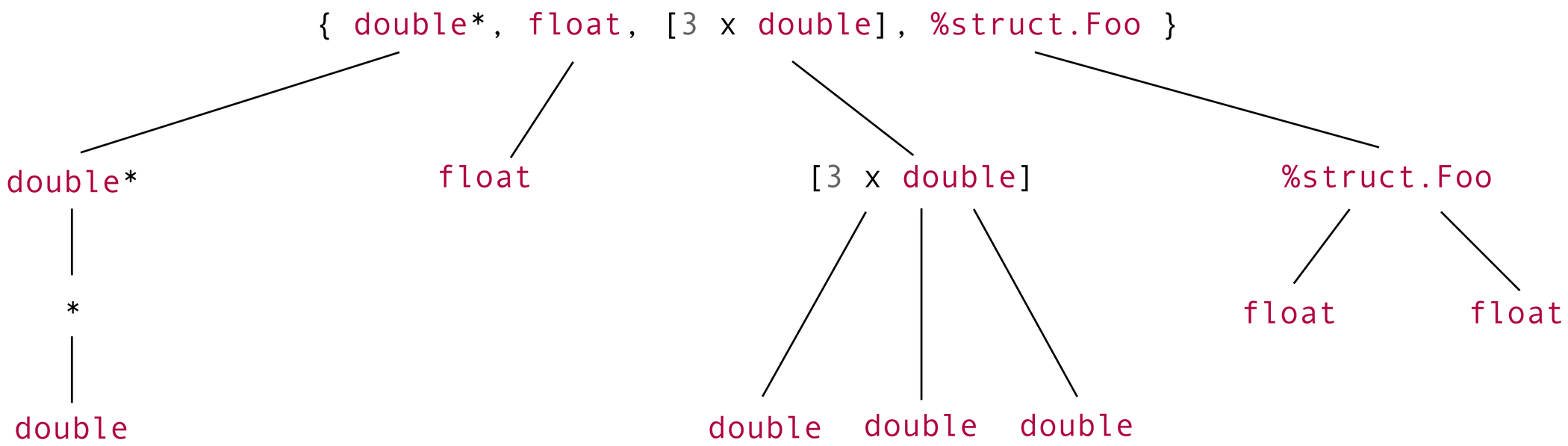
Optimizations

- Activity analysis, doesn’t propagate derivatives for inactive values
- Combine calls to allocation / free functions

```
float f(float x[2]) {
  float sum = x[0] + x[1];
  float val = slow(); // inactive
  sum *= val;
  return sum;
}
```

Vectorizing LLVM types

Type Trees



Vectorized at the root node `[2 x { double*, float, [3 x double], %struct.Foo }]`

Vectorized at the leaf nodes `{ [2 x double]*, [2 x float], [3 x [ 2 x double]], %struct.Foo2 }`

Vectorizing LLVM types
Discussion

- Vectorisation of the root node
  - Better compatibility, no modification of existing structs necessary
- Vectorisation of leaf nodes
  - Better memory locality, vectorized loads and stores

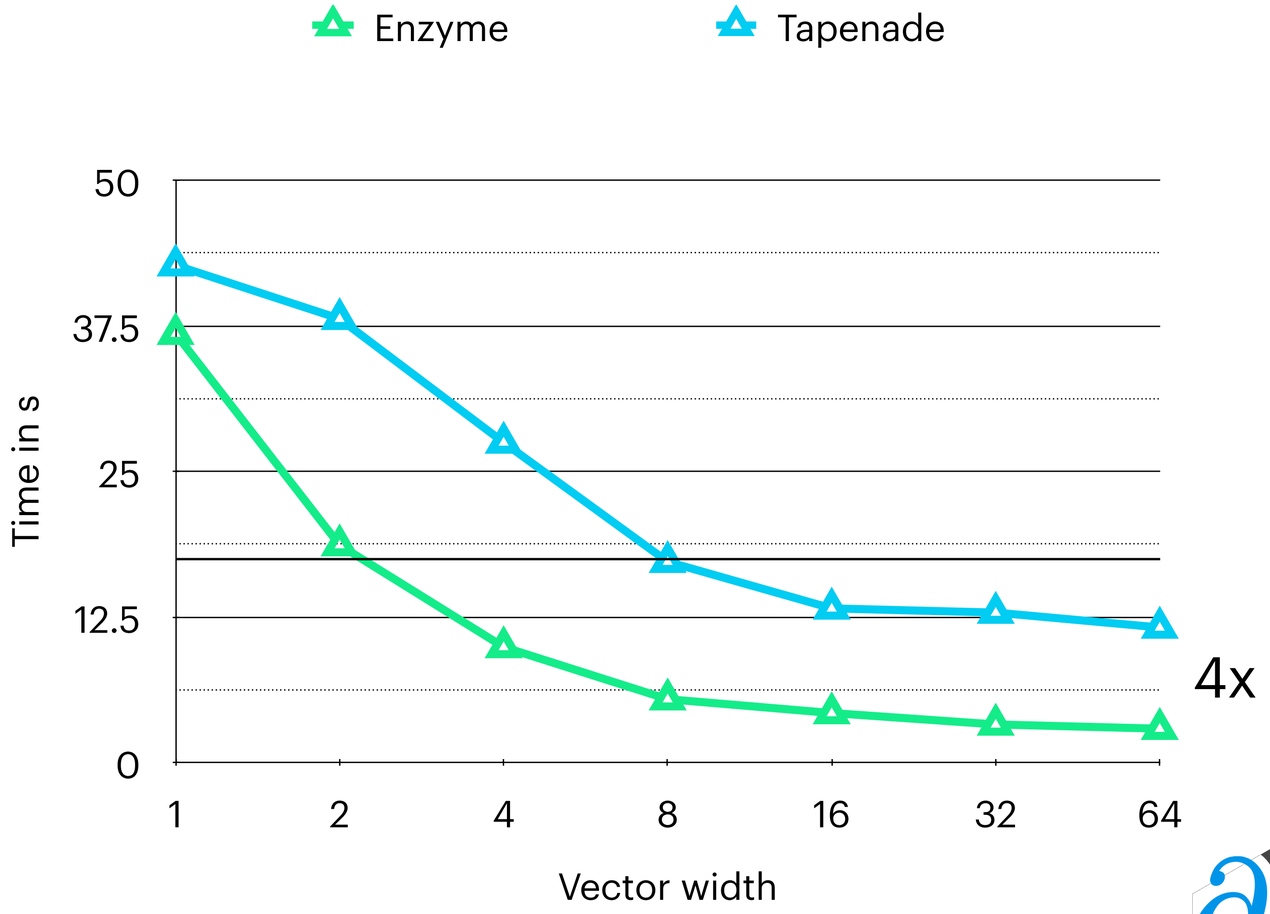
Benchmarks

A selection of AD Tools

	Forward Mode	Reverse Mode	Forward Vector Mode	Reverse Vector Mode
Enzyme	✅	✅	✅	✅
Tapenade	✅	✅	✅	✅
CoDiPack	✅	✅	✅	✅
Clad	✅	✅	❌	❌
Adept	✅	✅	❌	❌

Benchmarks
AD Bench - LSTM

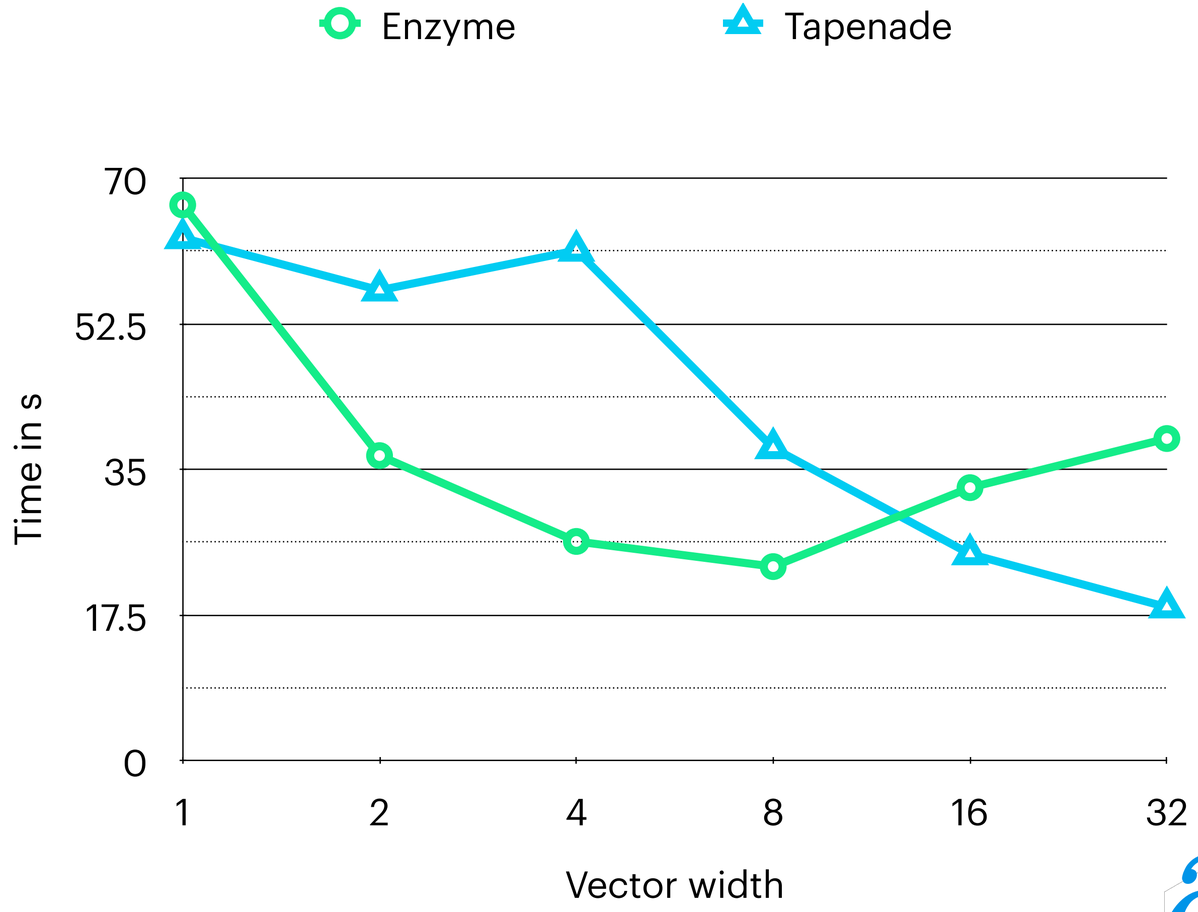
- Vector width of 1 to 64
- Problem too big to vectorize at once
- Up to 4x speedup, due to activity analysis



12th Gen Intel(R) Core(TM) i9-12900K

Benchmarks
AD Bench - GMM

- Vector width of 1 to 32
- Problem too big to vectorize at once
- Scaling issues beyond vector width of 8



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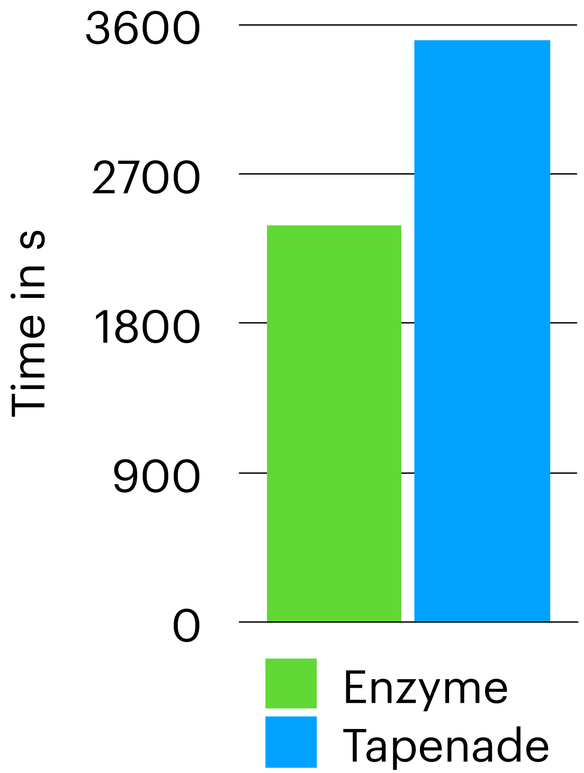
Benchmarks
LIBOR

- Vector width = problem size
- 46% speedup over Tapenade



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Future Work

- Dynamic vector width
- Type tree vectorized at the leaf nodes
- Support for OpenMP & MPI parallelism
- Support for GPUs (PTX, ROCm)

Summary

- Tool for performing reverse and forward-mode AD of statically analyzable LLVM IR
- Differentiates code in languages going to the LLVM IR (C, C++, Fortran, Julia, Rust, Swift, Haskell, etc) and parallel frameworks (OpenMP, MPI, CUDA, ROCm, Julia Threads)
- Work in progress
- Open source: https://github.com/EnzymeAD/Enzyme
- Compiler Explorer: https://enzyme.mit.edu/explorer

Questions