Enzyme: High-Performance, Cross-Language, and Parallel Automatic Differentiation

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AP Calculus: Revisited

• Derivatives compute the rate of change of a function’s output with respect to input(s)

\[ f'(x) = \lim_{h \to 0} \frac{f(a + h) - f(a)}{h} \]

• Derivatives (& generalizations like gradients) used widely across science

• Machine learning (back-propagation, Bayesian inference, uncertainty quantification)

• Scientific computing (modeling, simulation)
Automatic Derivative Generation

- Derivatives can be generated automatically from definitions within programs

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

```c
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!

```c
// Numeric differentiation
// f’(x) approx [f(x+epsilon) - f(x)] / epsilon
double grad_input[100];

for (int i=0; i<100; i++) {
    double input2[100] = input;
    input2[i] += 0.01;
    grad_input[i] = (f(input2) - f(input))/0.001;
}
```

```c
// Automatic differentiation
double grad_input[100];

grad_f(input, grad_input)
```
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

```python
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())
```

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

```cpp
// 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
#include "myfile.h"

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

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

// grad_myfile.h

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

```c
//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

\[ O(n^2) \]

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

Optimize

\[ O(n) \]

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

\[ O(n) \]

\[
\text{d_res} = 0.0 \\
\text{for } i=n..0 \{ \\
\text{d_res} += \text{d_out}[i]... \\
\}
\]

\[ \triangledown \text{mag}(\text{d_in}, \text{d_res}) \]
Optimization & Automatic Differentiation

$O(n^2)$

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

$O(n)$

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

for $i=n..0$ {
    d_res += d_out[$i$]...
}

$O(n)$

d_res = 0.0
for $i=n..0$ {
    d_res += d_out[$i$]...
}

$\nabla$ mag(d_in, d_res)

$O(n^2)$

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

$O(n^2)$

for $i=n..0$ {
    d_res = d_out[$i$]...

    $\nabla$ mag(d_in, d_res)
Optimization & Automatic Differentiation

\[ O(n^2) \]
\[
\text{for } i=0..n \{ \\
\quad \text{out}[i] /= \text{mag}(\text{in}) \\
\}
\]

Optimize

\[ O(n) \]
\[
\text{res} = \text{mag}(\text{in}) \\
\text{for } i=0..n \{ \\
\quad \text{out}[i] /= \text{res} \\
\}
\]

AD

\[ O(n) \]
\[
\text{d_res} = 0.0 \\
\text{for } i=n..0 \{ \\
\quad \text{d_res} += \text{d_out}[i] \\
\}
\]
\[
\nabla \text{mag}(\text{d_in}, \text{d_res})
\]

Optimize

\[ O(n^2) \]
\[
\text{for } i=n..0 \{ \\
\quad \text{d_res} = \text{d_out}[i] \\
\quad \nabla \text{mag}(\text{d_in}, \text{d_res})
\}
\]
Optimization & Automatic Differentiation

Differentiating after optimization can create \textit{asymptotically faster} gradients!

\[ O(n^2) \quad \text{Optimize} \quad O(n) \quad \text{AD} \quad O(n) \]

\begin{align*}
\text{for } i=0..n & \{ \\
\text{out}[i] /= \text{mag}(\text{in}) & \}
\end{align*}

\begin{align*}
\text{res} = \text{mag}(\text{in}) & \\
\text{for } i=0..n & \{ \\
\text{out}[i] /= \text{res} & \}
\end{align*}

\begin{align*}
\text{d_res} = 0.0 & \\
\text{for } i=n..0 & \{ \\
\text{d_res} += \text{d_out}[i] & \}
\end{align*}

\[ \nabla \text{mag}(\text{d_in}, \text{d_res}) \]

\begin{align*}
\text{for } i=0..n & \{ \\
\text{out}[i] /= \text{mag}(\text{in}) & \}
\end{align*}

\begin{align*}
\text{for } i=n..0 & \{ \\
\text{d_res} = \text{d_out}[i] & \\
\nabla \text{mag}(\text{d_in}, \text{d_res}) & \}
\end{align*}

\[ \nabla \text{mag}(\text{d_in}, \text{d_res}) \]

\[ \text{for } i=n..0 & \{ \\
\text{d_res} = \text{d_out}[i] & \\
\nabla \text{mag}(\text{d_in}, \text{d_res}) & \}
\end{align*}
Performing AD at low-level lets us work on **optimized** code!
Why Does Enzyme Use LLVM?

- Generic low-level compiler infrastructure with many frontends
  - “Cross platform assembly”
  - Many backends (CPU, CUDA, AMDGPU, etc)
- Well-defined semantics
- Large collection of optimizations and analyses
Case Study: ReLU3

C Source

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

Enzyme Usage

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

LLVM

define double @relu3(double %x)

double relu3(double %x)
{
    %cmp = %x > 0
    br %cmp, cond.true, cond.end
    %call = pow(%x, 3)
    br cond.end
    %result = phi [%call, cond.true], [0, entry]
    ret %result
}
Case Study: ReLU3

define double @relu3(double %x)

%cmp = %x > 0
br %cmp, cond.true, cond.end

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

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

Active Instructions

Entry:

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

cond.end
%result = phi [%call, cond.true], [0, entry]
ret %result
Allocate & zero shadow memory for active values
Compute adjoints for active instructions

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

entry

alloca %result' = 0.0
alloca %call' = 0.0
alloca %x' = 0.0
%cmp = %x > 0
br %cmp, cond.true, cond.end

cond.true

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

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

; deleted return
%result' = 1.0
br reverse_cond.end

reverse_cond.true

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

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_entry

%0 = load %x'
ret %0

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

cond.true
%result = phi [%call, cond.true], [0, entry]
; deleted return
%result' = 1.0
br reverse_cond.end

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

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_entry
%0 = load %x'
ret %0
```
Essentially the optimal hand-written gradient!

define double @diffe_relu3(double %x)

entry

%cmp = %x > 0
br %cmp, reverse_cond.true, reverse_entry

%3 = 3 * pow(%x, 2)
br reverse_entry

reverse_cond.true

%0 = phi [%3, reverse_cond.true], [0, entry]
ret %0

reverse_entry

Post Optimization
Challenges of Low-Level AD

- Low-level code lacks information necessary to compute adjoints

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

```c
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;
}
```

```c
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

```c
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

Enzyme: -O2

Ref: Enzyme -O2

Tapenade: Tapenade -O2

Adept: Adept -O2

Enzyme: -O2

Ref: Enzyme -O2

Tapenade: Tapenade -O2

Adept: Adept -O2
Speedup of Enzyme

Enzyme is 4.2x faster than Reference!
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)

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)

// Input tensor + size, and output tensor
void f(float* inp, size_t n, float* out);

// diffe_dupnoneed specifies not recomputing the output
void diffe(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);
}
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
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)

```c
void set(double* ar, double val) {
    parallel_for(int i=0; i<10; i++)
        ar[i] = val;
}

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;
}
```

Read Race

Write Race
<table>
<thead>
<tr>
<th>GPU Memory Hierarchy</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Per Thread</strong></td>
</tr>
<tr>
<td>Register</td>
</tr>
<tr>
<td>~Bytes</td>
</tr>
<tr>
<td>Use Limits Parallelism</td>
</tr>
<tr>
<td><strong>Per Block</strong></td>
</tr>
<tr>
<td>Shared Memory</td>
</tr>
<tr>
<td>~KBs</td>
</tr>
<tr>
<td>Use Limits Parallelism</td>
</tr>
<tr>
<td><strong>Per GPU</strong></td>
</tr>
<tr>
<td>Global Memory</td>
</tr>
<tr>
<td>~GBs</td>
</tr>
</tbody>
</table>

Slower, larger amount of memory

Use Limits Parallelism

~Bytes

~KBs

~GBs
Correct and Efficient Derivative Accumulation

Thread-local memory

- Non-atomic load/store

```c
__device__
void f(...) {
    // Thread-local var
double y;
    ...
d_y += val;
}
```

Same memory location across all threads (some shared mem)

- Parallel Reduction

```c
__device__
void f(...) {
    // Same var for all threads
double y;
    __device__
    void f(...) {
        ...
        reduce_add(&d_y, val);
    }
}
```

Others [always legal fallback]

- Atomic increment

```c
__device__
// Unknown thread-aliasing
void f(double* y) {
    ...
    atomic { d_y += val; }
}
```

Slower
Synchronization Primitives

- Synchronization (\texttt{sync\_threads}) ensures all threads finish executing \texttt{codeA} before executing \texttt{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
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

```c
__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);
}
```

```c
__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

```c
__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;
    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))

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

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

```c
// 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

```cpp
do 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.

```java
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.

```java
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.

```cpp
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]);
}
• By considering the dataflow graph we can perform a min-cut to approximate smaller cache sizes.
```
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!

```c
double* var1 = new double[N];
double* var2 = new double[M];
use(var1, var2);
delete[] var1;
delete[] var2;
```

```c
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
- ...

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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

- 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)

![Diagram showing GPU Gradient Overhead]

Bug in CUDA Register Allocator
Ablation Analysis of Optimizations

DG (ROCm)
- DG (CUDA)
- LBM
- LULESH
- RSbench
- XSBench
- Forward (1x)

Unrolling
10x
100x
OOM

Overhead above Forward Pass

Unrolling
MalloCoalescing
PreOptimization

Allocator
Recompute
InlineCacheABI

SpecPHI
PreOptimization

CacheLICM
Inlining
PreOpt

Templating
PHI
LoopBound
PreOptimization

5.4x
17.8x
116.6x
1378.3x
6.4x
8.7x
19.87x
2.0x
2.4x
4.7x
9.5x
3.2x
9.5x
16.3x
25.9x
2979.1x
6372.2x
9x
1378.3x

PreOptimization

Allocator
Recompute
Ablation Analysis of Optimizations

Overhead above Forward Pass
Ablation Analysis of Optimizations

- **DG (ROCm)**
  - Unrolling: 5.4x
  - PreOptimization

- **DG (CUDA)**
  - Unrolling: 17.8x
  - MallocCoalescing: 116.6x
  - PreOptimization: 1378.3x

- **LBM**
  - Allocator: 6.4x
  - Recompute: 8.7x
  - InlineCacheABI

- **LULESH**
  - SpecPHI: 2.0x
  - PreOptimization: 2979.1x

- **RSBench**
  - CacheLICM: 4.7x
  - Inlining: 9.5x
  - PreOpt: 6372.2x

- **XSbench**
  - Templating: 3.2x
  - PHI: 9.5x
  - LoopBound: 16.3x
  - PreOptimization

Overhead above Forward Pass
Ablation Analysis of Optimizations

GPU AD is Intractable Without Optimization!
• Tool for performing reverse-mode AD of statically analyzable LLVM IR

• Differentiates code in a variety of languages (C, C++, Fortran, Julia, Rust, Swift, etc)

• 4.2x speedup over AD before optimization on CPU

• State-of-the art performance with existing tools

• First general purpose reverse-mode GPU AD

• Novel GPU and AD-specific optimizations improve runtime by several orders of magnitude

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

• Ongoing work to support CPU parallelism (OpenMP, MPI) + Forward/Mixed Mode
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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

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Cache

- Adjoint instructions may require values from the forward pass
  
  - e.g. $\nabla(x \ast y) \Rightarrow x \, dy + y \, dx$

- 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.

```c
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.

```cpp
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. $\nabla(x \times y) \Rightarrow x \ dy + y \ dx$
  
- 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
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)

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

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)
Case Study: Read Sum

Active Variables

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

%result = phi [%call, cond.true], [0, entry]
ret %result
```
Case Study: Read Sum

Each register in the for loop represents a distinct active variable every iteration.
Allocate & zero shadow memory per active value
Cache forward pass variables for use in reverse

```c
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
%call_cache = @malloc(10 x double)
br 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

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

After lowering & some optimizations
Case Study: Read Sum

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

<table>
<thead>
<tr>
<th>Test</th>
<th>Overhead</th>
</tr>
</thead>
<tbody>
<tr>
<td>Forward</td>
<td>1</td>
</tr>
<tr>
<td>AD, Optimized</td>
<td>4.4</td>
</tr>
<tr>
<td>AD, No CacheLICM</td>
<td>343.7</td>
</tr>
<tr>
<td>AD, Bad Recompute Heuristic</td>
<td>1275.6</td>
</tr>
<tr>
<td>AD, No Inlining</td>
<td>6372.2</td>
</tr>
<tr>
<td>AD, No PreOptimization</td>
<td>OOM</td>
</tr>
</tbody>
</table>
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.
Enzyme

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- 4.2x speedup over AD before optimization
- 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)
  - Differentiating CUDA intrinsics (e.g. threadIdx.x /llvm.nvvm.read.ptx.sreg.tid.x)
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Custom Derivatives & Multisource

- One can specify custom forward/reverse passes of functions by attaching metadata

```c
__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

Differentiation Is Key To Machine Learning

- Hinders application of ML to new domains
- Synthesizing gradients aims to close this gap

```python
import torch

def step(bodies, dt):
    acc = []
    for i in range(len(bodies)):
        acc[i] = vec3(0, 0, 0)
        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
```

```cpp
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;
    }
}
```
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

```c
%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

```c
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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- 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

```plaintext
double x_cache=x[0];
double y_cache=y[0];
use(x[0] + y[0]);
overwrite(x, y);
grad_overwrite(x, y);
grad_use(x_cache + y_cache);
```
AD-Specific Cache

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```plaintext
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

```llvm
define double @relu3(double %x)
{
entry
    %cmp = %x > 0
    br %cmp, cond.true, cond.end
cond.true
    %call = pow(%x, 3)
    br %call, cond.end
cond.end
    %result = phi [%call, cond.true], [0, entry]
    ret %result
}
```

Enzyme Usage

```c
double diffe_relu3(double x) {
    return __enzyme_autodiff(relu3, x);
}
```
Case Study: ReLU3

Active Instructions

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

%cmp = %x > 0
br %cmp, cond.true, cond.end

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

%result = phi [%call, cond.true], [0, entry]
ret %result
```
define double @diffe_relu3(double %x, double %differet)

Allocate & zero shadow memory for active values

entry

cond.true

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

%result' = 0.0
alloca %result' = 0.0
alloca %call' = 0.0
alloca %x' = 0.0
%cmp = %x > 0
br %cmp, cond.true, cond.end

%result = phi [%call, cond.true], [0, entry]
; deleted return
%result' = 1.0
br reverse_cond.end

cond.end
Compute adjoints for active instructions

```c
#define double @diffe_relu3(double %x, double %differ)

alloca %result' = 0.0
alloca %call' = 0.0
alloca %x' = 0.0
%cmp = %x > 0
br %cmp, cond.true, cond.end

%result = phi [%call, cond.true], [0, entry]
; deleted return
%result' = 1.0
br reverse_cond.end

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

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

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

Define double @diffe_relu3(double %x, double %differ)
Define double @diffe_relu3(double %x, double %differet)

entry

alloca %result’ = 0.0
alloca %call’ = 0.0
alloca %x’ = 0.0
%cmp = %x > 0
br %cmp, cond.true, cond.end

cond.true

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

%result = phi [%call, cond.true], [0, entry]
; deleted return
%result’ = 1.0
br reverse_cond.end

reverse_cond.true

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

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

%0 = load %x’
ret %0

Compute adjoints for active instructions
Essentially the optimal hand-written gradient!

define double @diffe_relu3(double %x)

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

```c
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

```c
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)

![Graph showing Scalability Analysis](image)

- **AD Overhead (factor)**
- **Iterations**
- **LBM – Parboil (C & CUDA)**
CUDA Example

```c
__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

Manually Rewrite

def double_square(double val):
    return val * val;

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

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

Tool Rewrite

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

$ tapenade -b -o out.c -head "square(val)/(out)" square.c
Parallel Automatic Differentiation in LLVM

- Shadow Registers \( %d\_res \) and \( %d\_val \) are \textit{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

```c
// codeA
CodeA(); // load %ptr
sync_threads;

// codeB
CodeB(); // store %ptr
...

// codeF
CodeF(); // load %d_ptr
// store %d_ptr = 0
sync_threads;

// codeG
CodeG(); // atomicAdd %d_ptr
```

- All of the stores of \( d\_ptr \) will complete prior to any atomicAdds

Correct

- 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)

[Graph showing AD Overhead (factor) vs. Relative Problem Size for different benchmarks: Discontinuous Galerkin (Julia & CUDA), Discontinuous Galerkin (Julia & ROCm), LULESH (C++ & CUDA), RSBench (C & CUDA), XSBench (C & CUDA).]