Enzyme: Fast, Language Agnostic, Differentiation of Parallel Programs in LLVM

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Overview

• Extending the compiler to synthesize new code (derivatives) from specifications in existing code

• Performance and correctness challenges when synthesizing GPU code

• Novel optimizations enable efficient GPU execution

• Come to our full presentation on **Weds 3:30-4 CT (Room 220-221)!**
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, precision reduction)
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(epsilon)] / 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 Automatic Differentiation Pipelines
Enzyme Approach

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

Enzyme is **4.2x faster** than existing approaches!
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;
}
```
# GPU Memory Hierarchy

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

Slower, larger amount of memory
Correct and Efficient Derivative Accumulation

<table>
<thead>
<tr>
<th>Thread-local memory</th>
<th>Same memory location across all threads (some shared mem)</th>
<th>Others [always legal fallback]</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Non-atomic load/store</td>
<td>• Parallel Reduction</td>
<td>• Atomic increment</td>
</tr>
</tbody>
</table>

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

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

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

```cuda
__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

```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;
    dx[threadIdx.x] += dx_tmp;
    float da_tmp = x[threadIdx.x] * dy;
    reduce_accumulate(&da[0], da_tmp);
}
```
Efficient GPU Code

- Without optimization, GPU gradients must cache a large number of values
  - Complexity memory hierarchy => large caches slow down the program by several orders of magnitude, if it even fits at all
- Like the CPU, existing LLVM optimizations can reduce the overhead
- Unlike the CPU, existing LLVM optimizations aren’t sufficient
Novel AD + GPU Optimizations

- Come to our SC talk (Weds 3:30-4 CT, Room 220-221) for more

- [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

- ...
Allocation Merging

• Allocations (and any calls) on the GPU are expensive

• Given two allocations in the same scope, replace uses with a single allocation

```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;
```
## GPU Gradient Overhead

<table>
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<tr>
<th>No Optimization Before AD</th>
<th>1/6</th>
<th>~3000x</th>
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GPU AD is **intractable** without optimization!
Enzyme

- 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
- First general purpose reverse-mode GPU AD
- Novel GPU and AD-specific optimizations improve runtime by orders of magnitude
- Open source (enzyme.mit.edu & join our mailing list)!
- Ongoing work to support CPU parallelism (OpenMP, MPI) + Forward/Mixed Mode
Acknowledgements

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Tool for performing reverse-mode AD of statically analyzable LLVM IR

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

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

Ongoing work to support CPU parallelism (OpenMP, MPI) + Forward/Mixed Mode
Enzyme
Cache Reduction Example

- Some forward values need to be preserved to compute the reverse.
- By considering the dataflow graph, we can perform a min-cut to approximate smaller cache sizes.

Overwritten: $X$, $Y$

Required for Reverse: Sum

```
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

- Some forward values need to be preserved to compute the reverse.
- By considering the dataflow graph we can perform a min-cut to approximate smaller cache sizes.

```cpp
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);
}

delete[] x_cache;
delete[] y_cache;
```
Cache Reduction Example

- Some forward values need to be preserved to compute the reverse.
- 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]);
}
delete[] sum_cache;
```
Ablation Analysis of Optimizations

Unrolling

MallocCoalescing

PreOptimization

Unrolling

MallocCoalescing

PreOptimization

SpecPHI

PreOptimization

CacheLICM

Inlining

PreOptimization

Templating

PHI

LoopBound

PreOptimization

Forward (1x)

10x

100x

1000x

Overhead above Forward Pass

DG (ROCm)

5.4x

DG (CUDA)

17.8x 116.6x 1378.3x

LBM

6.4x 8.7x 19.87x

LULESH

2.0x 2.4x

RSBench

4.7x 9.5x

XSbench

3.2x 9.5x 16.3x 25.9x

OOM

Allocator

Recompute

InlineCacheABI

SpecPHI

PreOptimization

CacheLICM

Inlining

PreOptimization

Templating

PHI

LoopBound

PreOptimization

PreOpt
Ablation Analysis of Optimizations

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

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

- LBM Optimizations:
  - Allocator: 6.4x
  - Recompute: 8.7x
  - InlineCacheABI: 19.87x

- LULESH Optimizations:
  - SpecPHI: 2.0x
  - PreOptimization: 2.4x
  - PreOpt: 2979.1x

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

- XSbench Optimizations:
  - Templating: 3.2x
  - PHI: 9.5x
  - LoopBound: 16.3x
  - PreOptimization: 25.9x

- Overhead above Forward Pass:

  - Forward (1x)
  - 10x
  - 100x
  - 1000x
  - OOM
Ablation Analysis of Optimizations

- **DG (ROCm)**: Unrolling (5.4x), Allocator (2.0x), SpecPHI (2.4x)
- **DG (CUDA)**: Unrolling (17.8x), Allocator (6.4x), Inlining (8.7x), SpecPHI (9.5x), PreOptimization (9.87x)
- **LBM**: Unrolling (116.6x), Allocator (19.87x), SpecPHI (8.7x), PreOptimization (17.8x)
- **LULESH**: Inlining (2979.1x), CacheLICM (4.7x), PreOptimization (6372.2x)
- **RSBench**: Inlining (25.9x), CacheLICM (9.5x), PreOptimization (2.0x)
- **XSbench**: Unrolling (2.4x), Allocator (19.87x), SpecPHI (9.5x), PreOptimization (116.6x)

Overhead above Forward Pass

- Forward (1x) to 10x
- 10x to 100x
- 100x to OOM
GPU AD is Intractable Without Optimization!

Ablation Analysis of Optimizations
Synchronization Primitives

- Synchronization \((\text{sync\_threads})\) ensures all threads finish executing \text{codeA} before executing \text{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
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
CUDA.jl / AMDGPU.jl Example

See Below For Full Code Examples

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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<th>Code Name</th>
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<td>18.35</td>
</tr>
<tr>
<td>LBM (Parboil)</td>
<td>6.3</td>
</tr>
<tr>
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GPU Gradient Overhead

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![GPU Gradient Overhead Diagram]

Bug in CUDA Register Allocator
Case 1: Store, Sync, Load

```c
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
Case Study: Vector Normalization

```c
//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

$O(n^2)$

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

Optimize

$O(n)$

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

AD

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

\[ O(n^2) \]

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

\[ O(n) \]

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

\[
\nabla\text{mag}(d_{\text{in}}, d_{\text{res}})
\]

\[ O(n^2) \]

for \( i=n..0 \) {
    \text{d_res} = d_{\text{out}[i]}
\}

\[
\nabla\text{mag}(d_{\text{in}}, d_{\text{res}})
\]
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)

$O(n^2)$

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

AD

$O(n^2)$

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)
}

Optimize
Optimization & Automatic Differentiation

Differentiating after optimization can create *asymptotically faster* gradients!

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

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

\[
\begin{align*}
O(n^2) & \quad \text{AD} \\
\text{d_res} = 0.0 & \quad \text{for } i=n..0 \{ \\
& \quad \text{d_res} += \text{d_out}[i] \\
\} \\
\n\text{\nabla \text{mag}(\text{d_in, d_res})} & \quad \text{for } i=n..0 \{ \\
& \quad \text{d_res} = \text{d_out}[i] \\
& \quad \text{\nabla \text{mag}(\text{d_in, d_res})} \\
\}
\end{align*}
\]
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())
```

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

Manually Rewrite
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
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);
```
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.

```c
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)

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

%exitcond = %i.next == 10
br %exitcond, for.cleanup, for.body

%add = %mul + %total
%i.next = %i + 1
%exitcond = %i.next == 10
br %exitcond, for.cleanup, 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

double entry {
for.body
entry br for.body
for.body
for.body
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
define double @diffe_sum(double* %x, double* %xp)

Cache forward pass variables for use in reverse

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
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
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

- 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
- 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)
  • Handling shared memory
Enzyme

- 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
- 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
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[1]

Differentiation Is Key To Machine Learning

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

```python
import torch

# PyTorch rewrite of nbody simulator
def step(bodies, dt):
    acc = []
    for i in range(len(bodies)):
        acc[i] = 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
```

```c++
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

• 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 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

- 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);
grd_overwrite(x, y);
grd_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;
}
```

Enzyme Usage

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

LLVM

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

Entry

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

Cond.true

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

Cond.end

```llvm
%result = phi [%call, cond.true], [0, entry]
ret %result
```
Case Study: ReLU3

Active Instructions

```
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
```
Allocate & zero shadow memory for active values

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

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

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

%result' = 1.0
br reverse_cond.end
```
Compute adjoints for active instructions

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

entry

cond.true

 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

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

; deleted return

%result’ = 1.0
br reverse_cond.end

cond.end

reverse_cond.true

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

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

reverse_entry
Define `double @diffe_relu3(double %x, double %differet)`

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

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

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

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

Allocate %result' = 0.0
Allocate %call' = 0.0
Allocate %x' = 0.0
%cmp = %x > 0
br %cmp, reverse_cond.true, reverse_entry

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

%0 = load %x'
ret %0

Compute adjoints for active instructions

Reverse_cond.true

Reverse_cond.end

Reverse_entry
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);
}
```

```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}
```
Case 3: Store, Sync, Store

```c
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 AD Overhead (factor) vs. Iterations for LBM - Parboil (C & CUDA).]
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

```python
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())
```

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

Manually Rewrite
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 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

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)

![Graph showing scalability analysis](image)

- Discontinuous Galerkin (Julia & CUDA)
- Discontinuous Galerkin (Julia & ROCm)
- LULESH (C++ & CUDA)
- RSbench (C & CUDA)
- XSBench (C & CUDA)
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)

entry %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]
ret %result

cond.end

double etype_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);
}
Case Study: ReLU3

Active Instructions

```
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
```
Allocate & zero shadow memory for active values

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

entry
entry
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

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

; deleted return

%result' = 1.0
br reverse_cond.end
```

Define double @diffe_relu3(double %x, double %differet)
Compute adjoints for active instructions

```llvm
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.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
}
```
define double @diffe_relu3(double %x, double %differet)

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

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

alloca %temp_res’ = load %result’
%call’ = if %x > 0 then %temp_res’ else 0
store %result’ = 0.0
br %cmp, reverse_cond.true, reverse_entry

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

%0 = load %x’
ret %0

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

double differelu3(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);
}
```

```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

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

\[
types(x) = \{[0]:\text{Pointer}, [0,0]:\text{Double}, [0,8]:\text{Pointer}, [0,8,0]:\text{Integer}\}
\]
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 \texttt{realloc\textasciitilde}
Experimental Setup

- Collection of benchmarks from Microsoft’s ADBench suite and of technical interest
PyTorch-Enzyme & TensorFlow-Enzyme

```
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)
```

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

// diffe_dupnoneed specifies not recomputing the output
void diffe_dup(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);
}
```
Speedup of Enzyme

Enzyme is \textbf{4.2x faster} than Reference!