Supercharging Programming Through Compiler Technology





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The Programmer's Burden

- The decline of Moore's law and an increasing reliance on computation => explosion of specialized software packages and hardware architectures.
- Domain-experts must customize programs and learn platform-specific API's, instead of working on their intended problem.
- Rather than each user bearing this burden, compilers can automatically generate fast, portable, and composable programs!







Extending the Boundaries of Compilers



Enzyme: fast, parallel, and rewrite-free *derivative generation*;



Tapir: understand and optimize *parallel programs*



Polygeist: *run GPU code on CPUs*, 2.7x faster than expert-written code, preserve program structure to leverage device parameters perform HLS

Tensor Comprehensions (TC): automatically generate fast tensor arithmetic



AutoPhase: ML-based optimization of programs/circuits

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 $A\vec{x}$

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AP Calculus: Revisited

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

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

- Derivatives are used widely across science ●
 - Machine learning (back-propagation, Bayesian inference) •
 - Scientific computing (modeling, simulation, uncertainty quantification) •





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



Automatic Derivative Generation

Derivatives can be generated automatically from definitions within programs •

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



• inputs (or outputs) at once, without approximation error!

```
// Numeric differentiation
// f'(x) approx [f(x+epsilon) - f(x)] / epsi
double grad_input[100];
for (int i=0; i<100; i++) {</pre>
  double input2[100] = input;
  input2[i] += 0.01;
  grad_input[i] = (f(input2) - f(input))/0.0
```

Unlike numerical approaches, automatic differentiation (AD) can compute the derivative of ALL

lon	<pre>// Automatic differentiation double grad_input[100];</pre>		
	<pre>grad_f(input, grad_input)</pre>		
0.1			
01;			

Existing AD Approaches (1/3)

- Differentiable DSL (TensorFlow, PyTorch, DiffTaichi) •
 - Provide a new language designed to be differentiated •
 - ٠ code
 - Fast if DSL matches original code well •

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

Manually Rewrite

Requires rewriting everything in the DSL and the DSL must support all operations in original

```
import tensorflow as tf
x = tf.Variable(3.14)
with tf.GradientTape() as tape:
  out = tf.cond(x > 0),
           lambda: tf.math.pow(x,3),
           lambda: 0
print(tape.gradient(out, x).numpy())
```



Existing AD Approaches (2/3)

- Operator overloading (Adept, JAX) •
 - •
 - May require writing to use non-standard utilities •
 - Often dynamic: storing instructions/values to later be interpreted •

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

Differentiable versions of existing language constructs (double = adouble, np.sum = jax.sum)

```
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





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++) {</pre>
    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++) {</pre> out[i] = in[i] / res;





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



ıt[i]... d_res)



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





Differentiating after optimization can create *asymptotically faster* gradients!

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







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





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 @<mark>relu3(</mark>double %x)





Case Study: ReLU3



define double @diffe_relu3(double %x, doub



ble %differet)				
nd	Allocate & zero adow memory for active values			
[%call, cond.true]	, [0, entry] cond.end			
ond.end				







Essentially the optimal hand-written gradient!

```
double diffe_relu3(double x) {
 double result;
 if (x > 0)
    result = 3 * pow(x, 2);
  else
    result = 0;
  return result;
```

Experimental Setup

ullet



Speedup of Enzyme



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

Automatic Differentiation & GPUs

- Prior work has not explored reverse mode AD of existing GPU kernels
 - 1. Reversing parallel control flow can lead to incorrect results
 - 2. Complex performance characteristics make it difficult to synthesize efficient code
 - 3. Resource limitations can prevent kernels from running at all



Efficient GPU Code

- For correctness, Enzyme may need to cache values in • order to compute the gradient
 - The complexity of GPU memory means large caches • slow down the program by several orders of magnitude, if it even fits at all
- Like the CPU, existing optimizations reduce the overhead •
- Unlike the CPU, existing optimizations aren't sufficient •
- Novel GPU and AD-specific optimizations can speedup by ٠ several orders of magnitude

```
// Forward Pass
out[i] = x[i] * x[i];
x[i] = 0.0f;
// Reverse (gradient) Pass
grad_x[i] += 2 * x[i] * grad_out[i];
• • •
```



Efficient Correct GPU Code

- For correctness, Enzyme may need to cache values in • order to compute the gradient
 - The complexity of GPU memory means large caches • slow down the program by several orders of magnitude, if it even fits at all
- Like the CPU, existing optimizations reduce the overhead •
- Unlike the CPU, existing optimizations aren't sufficient •
- Novel GPU and AD-specific optimizations can speedup by • several orders of magnitude

```
double* x_cache = new double[...];
// Forward Pass
out[i] = x[i] * x[i];
x_cache[i] = x[i];
x[i] = 0.0f;
// Reverse (gradient) Pass
grad_x[i] += 2 * x_cache[i]
               * grad_out[i];
• • •
delete[] x_cache;
```



Cache Reduction Example

 By considering the dataflow graph we can perform a min-cut to approximate smaller cache sizes.





Required for Reverse:

```
for(int i=0; i<10; i++) {</pre>
  double sum = x[i] + y[i];
  use(sum);
overwrite(x, y);
grad_overwrite(x, y);
for(int i=9; i>=0; i--) {
  • • •
  grad_use(sum);
```

Cache Reduction Example

 By considering the dataflow graph we can perform a min-cut to approximate smaller cache sizes.



```
double* x_cache = new double[10];
double* y_cache = new double[10];
for(int i=0; i<10; i++) {</pre>
  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.

Overwritten:

Required for Reverse:



```
double* sum_cache = new double[10];
for(int i=0; i<10; i++) {</pre>
  double sum = x[i] + y[i];
  sum_cache[i] = sum;
  use(sum);
overwrite(x, y);
grad_overwrite(x, y);
for(int i=9; i>=0; i--) {
  grad_use(sum_cache[i]);
```

Novel AD + GPU Optimizations

- See our SC'21 paper for more (<u>https://c.wsmoses.com/papers/EnzymeGPU.pdf</u>) • 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

33

. . .

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)



18.35

GPU Gradient Overhead

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	Unrolling			
g	MallocCoalescing		PreOptimization	
116.6×		$1378.3 \times$		
	InlineCacheABI			
eOptimization				
			$2979.1 \times$	
	Inlining			Pre
				$6372.2 \times$
	PreOptimizatio	n		
100x	1()00x		

Overhead above Forward Pass





Overhead above Forward Pass



Overhead above Forward Pass



GPU AD is Intractable Without Optimization!





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



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





from MFEM Team at LLNL



Prior: 5 days (cluster)

Enzyme-Based: 1 hour (laptop)

from Comrade: High Performance Black-Hole Imaging JuliaCon 2022, Paul Tiede (Harvard)

from Center for the Exascale Simulation of Materials in Extreme Environments



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



The HPC Landscape Today

- - Multicore chips •
 - **Distributed clusters** •
 - Accelerators (e.g. GPUs, TPUs)



Cutting-edge scientific computing requires efficiently leveraging *parallelism*











```
//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);
  }
}</pre>
```

N = 64M

```
//Compute magnitude in O(n)
double mag(double[] x);
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void norm(double[] out, double[] in) {
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```

N = 64M

Serial Running time: 0.312 s





//Compute magnitude in O(n) double mag(double[] x); //Compute norm in O(n^2) work void norm(double[] out, double[] in) { parallel_for (int i=0; i<n; i++) {
 out[i] = in[i] / mag(in);</pre> parallel loop replaces the original serial loop

N = 64M

Serial Running time: 0.312 s





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Serial Running time: 0.312 s 18-core Running time: 180.657s



//Compute magnitude in O(n) double mag(double[] x); //Compute norm in O(n^2) work void norm(double[] out, double[] in) { parallel_for (int i=0; i<n; i++) {
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- N = 64M
 - Serial Running time: 0.312 s
- 18-core Running time: 180.657s
 - 1-core Running time: 2600.287s



Why the Parallel Slowdown?



Compiling Parallel Code



Parallel Lower

```
void norm(double[] out, double[] in)
{
    struct args_t args = { out, in };
    __cilkrts_pfor(body, args, 0, n);
}
```

```
void body(struct args_t args, int i)
```

```
double *out = args.out;
double *in = args.in;
out[i] = in[i] / mag(in);
```



Compiling Parallel Code





```
void norm(double[] out, double[] in)
{
    struct args_t args = { out, in };
    __cilkrts_pfor(body, args, 0, n);
}
void body(struct args_t args, int i)
{
    double *out = args.out;
    double *in = args.in;
    out[i] = in[i] / mag(in);
}
```

The compiler doesn't understand the parallel runtime and cannot move mag



Compiling Parallel Code (Realistic)

```
int fib(int n) {
  if (n < 2) return n;
  int x, y;
  x = spawn fib(n - 1);
  y = fib(n - 2);
  sync;
  return x + y;
```



Parallel Lower

```
int fib(int n) {
  __cilkrts_stack_frame_t sf;
  __cilkrts_enter_frame(&sf);
 if (n < 2) return n;
 int x, y;
 if (!setjmp(sf.ctx))
    spawn_fib(&x, n-1);
 y = fib(n-2);
 if (sf.flags & CILK_FRAME_UNSYNCHED)
   if (!setjmp(sf.ctx))
     __cilkrts_sync(&sf);
  int result = x + y;
  __cilkrts_pop_frame(&sf);
 if (sf.flags)
    __cilkrts_leave_frame(&sf);
 return result;
void spawn_fib(int *x, int n) {
  __cilkrts_stack_frame sf;
  __cilkrts_enter_frame_fast(&sf);
  __cilkrts_detach();
 *x = fib(n);
  __cilkrts_pop_frame(&sf);
  if (sf.flags)
    __cilkrts_leave_frame(&sf);
```

Idea: New Parallel Compilation Pipeline



Parallel IR: A Bad Idea?

From "[LLVMdev] LLVM Parallel IR," 2015:

- headaches."

Other communications, 2016–2017:

- "There are a lot of information needs to be represented in IR for [back end] transformations for OpenMP." [Private communication]
- "If you support all [parallel programming features] in the IR, a *lot* [of LOC]...would probably have to be modified in LLVM." [[RFC] IR-level Region Annotations]

"[I]ntroducing [parallelism] into a so far 'sequential' IR will cause severe breakage and

"[P]arallelism is invasive by nature and would have to influence most optimizations."

Example Previous Parallel IR

 Previous CFG-based parallel IR's represented tasks symmetrically.



Problem: The join block **breaks implicit assumptions** made by the compiler.

Example: Values from **all** predecessors of a join must be available at runtime [LMP97].



Tapir: Task-Based Asymmetric Parallel IR

- Tapir models parallel tasks asymmetrically via three new instructions: detach, reattach, and sync
- The successors of a detach may run in parallel.
- Code after a sync is guaranteed to have completed previously detached tasks.
- Tapir simultaneously represents the serial and parallel semantics of the program.



Tapir: Task-Based Asymmetric Parallel IR

• Reasoning about parallelism is a minor change to reasoning about the serial projection.



Maintaining Correctness

Problem: How does the compiler ensure that code motion does not introduce a determinacy race into otherwise race-free code?

- Consider moving memory operations around each new instruction.
- Moving code above a detach or below a sync serializes it and is always valid.
- Other potential races are handled by giving detach, reattach, and sync appropriate attributes and by slight modifications to mem2reg.



Maintaining Correctness

Problem: How does the compiler ensure that code motion does not introduce a determinacy race into otherwise race-free code?

- Consider moving memory operations around each new instruction.
- Moving code above a detach or below a sync serializes it and is always valid.
- Other potential races are handled by giving detach, reattach, and sync appropriate attributes and by slight modifications to mem2reg.

Serial optimization passes do not create bugs!





//Compute magnitude in O(n) double mag(double[] x); //Compute norm in O(n^2) work void norm(double[] out, double[] in) { parallel_for (int i=0; i<n; i++) {
 out[i] = in[i] / mag(in);</pre>

parallel loop replaces the original serial loop

- N = 64M
 - Serial Running time: 0.312 s
- 18-core Running time: 0.081 s
 - 1-core Running time: 0.321 s

Great work efficiency! $T_{\rm S}/T_1 = 97\%$







Decreasing difference between Tapir/LLVM and Reference



Polygeist: Extending Parallel IRs beyond Multicore

- Good IR representations are especially necessary for device-specific constructs, like GPU syncthreads
 - Necessary for good performance, but complexity means they're often used poorly
 - General abstracts can enable code written in one framework to be used *and highperformance* on many others without rewriting
 - Recompiled PyTorch's GPU backend to produce an efficient CPU backend that runs 2.7x faster than PyTorch's native CPU code!

global___ void bpnn_layerforward(...) { __shared___float node[HEIGHT]; __shared___float weights[HEIGHT][WIDTH]; **if** (tx == 0) node[ty] = input[index_in] ; // Unnecessary Barrier #1 // None of the read/writes below the sync (weights, hidden) // intersect with the read/writes above the sync // (node, input) ___syncthreads(); // Unnecessary Store #1 weights[ty][tx] = hidden[index]; ___syncthreads(); // Unnecessary Load #1 weights[ty][tx] = weights[ty][tx] * node[ty]; ...



Revisiting The Programmer's Burden





float y = f(x);Node 1 MPI_Send(&y, ...);

Node 2 float y; MPI_Recv(&y, ...);

#pragma omp parallel for for (int i=0; i<3; ++i){</pre> y[i] = f(x[i]);

Threads.@threads for i=1:3 y[i] = f(x[i])end

@sync **begin** @spawn @sync for i in i:3 @spawn f(x(i)) end @spawn g() end

Code





Revisiting The Programmer's Burden (published at SC22)



Conclusions

- problem.
- code.

Enzyme generates fast derivatives of programs needed for science and machine learning, without x user rewriting



Tapir understands the parallelism within programs, enabling existing optimizations to apply with minimal modification. Polygeist extends these ideas to GPU programs and enables write-once runanywhere.

climate science to physics to material science

Explosion of specialized software packages and hardware architectures -> scientists spending more time learning how to optimize programs and use platform-specific API's than working on their intended

• Rather than burdening the user, compilers can automatically generate fast, portable, and composable

• All these tools are open source and used in academia and industry and in disciplines that range from

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- their intended problem.
- Rather than burdening the user, compilers can automatically generate fast, portable, and composable code.



Enzyme generates fast derivatives of programs needed for science and machine learning, without user rewriting



Tapir understands the parallelism within programs, enabling existing optimizations to apply with minimal modification.

from climate science to physics to material science

Explosion of specialized software packages and hardware architectures -> scientists spending more time learning how to optimize programs and use platform-specific API's than working on

• All these tools are open source and used in academia and industry and in disciplines that range