Automatic Differentiation for Adjoint Stencil Loops

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Outline

- Automatic Differentiation (AD)
- AD for parallel programs
- Stencil loops
- Our work: AD for stencil loops

Automatic differentiation (AD)

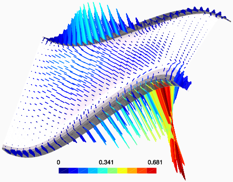
- Given a program ("primal") that implements some function

$$J = F(\alpha),$$

- AD generates a new program that implements its derivative.

Why would we want AD?

- Example: A fluid dynamics code that computes pressure loss in a pipe, subject to pipe geometry.
- AD computes derivative of pressure loss wrt. design parameters.



- We can automatically modify shape to minimise pressure loss
- Applications: Engineering optimisation, Imaging, Machine learning, ...

AD approaches

There are many ways of implementing AD:

Source-to-source transformation

- Creates code that computes partial derivative of each operation, and assembles them with chain-rule.
- Fast, efficient, but hard to get right. Mainly Fortran/C

Operator overloading

- Trace the computation at runtime, compute adjoints based on trace. Slow, huge memory footprint, easy to implement. Works for most high-level languages.

High level, manual or automated

- Start with problem definition, derive adjoint problem, implement the adjoint code separately.

Algorithmic differentiation (AD)

There are two fundamentally different modes:

Tangent mode, Forward mode

- Computes the Jacobian-vector product

$$\dot{J} = (\nabla F(x)) \cdot \dot{\alpha}.$$

- Derivatives are propagated along with the original computation.

Adjoint mode, Reverse mode, backpropagation

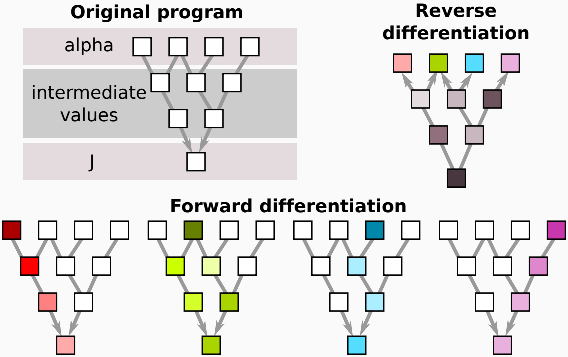
- Computes the transpose Jacobian-vector product

$$\bar{\alpha} = (\nabla F(x))^T \cdot \bar{J}.$$

- Path through original computation is traced, derivatives are propagated in reverse order.

Forward vs. reverse

- Tangent mode is simple to understand and implement, but: Need to re-run for every input.
- Adjoint mode is cheaper for many inputs and few outputs (run once, get all directional derivatives).



Challenge: derivative parallelisation in reverse mode

- If a shared memory region is read concurrently in original program, then the corresponding derivative will be updated concurrently.
- We can only easily parallelise adjoint if primal had *exclusive read access*[*]
- How can we detect this?
- What can we do otherwise?

[*] Förster (2014): Algorithmic Differentiation of Pragma-Defined Parallel Regions: Differentiating Computer Programs Containing OpenMP

Exclusive read access examples

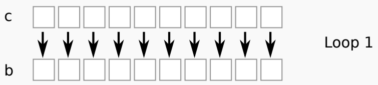
- Do these loops have exclusive read access?

```
! Example loop 1

real, dimension(10) :: b,c

!$omp parallel do
do i=1,10
  b(i) = sin(c(i))
end do
```

- Answer: Yes



Exclusive read access examples

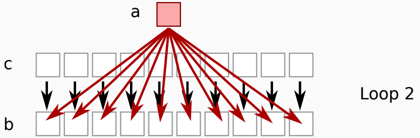
- Do these loops have exclusive read access?

```
! Example loop 2:

real :: a
real, dimension(10) :: b,c

!$omp parallel do
do i=1,10
  b(i) = a+c(i)
end do
```

- Answer: No



Exclusive read access examples

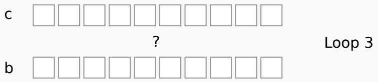
- Do these loops have exclusive read access?

```
! Example loop 3:

real, dimension(10) :: b,c
integer, dimension(10) :: neigh
call read_from_file(neigh)

!$omp parallel do
do i=1,10
  b(i) = c(neigh(i))
end do
```

- Answer: Depends on file contents



Solutions?

- Detecting exclusive read access is impossible in general
- Without exclusive read access, we must pay a price:
    - Use reductions (extra memory)
    - Use atomics (extra time)
    - Some combination
- Can we do better in special cases?

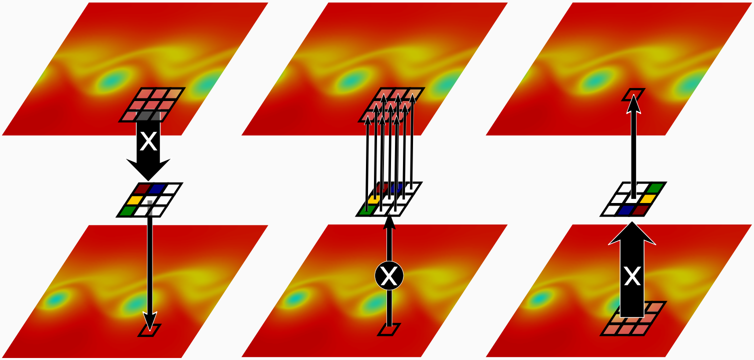
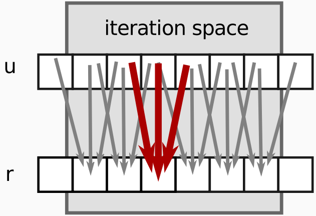


Figure 1: AD on a gather produces a scatter

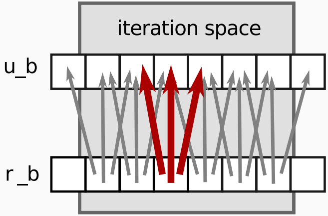
1D Stencil Example



The Stencil is originally a gather operation

```
#pragma omp parallel for private(i)
for ( i=1; i<=n - 1; i++ ) {
  r[i] = c[i]*(2.0*u[i-1]-3.0*u[i]+4*u[i+1]);
}
```

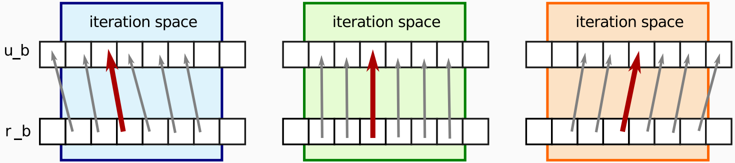
1D Stencil Example



AD converts it to a scatter

```
for ( i=1; i<=n-1; i++ ) {
  ub[i-1] += 2.0 * c[i] * rb[i];
  ub[i] -= 3.0 * c[i] * rb[i];
  ub[i+1] += 4.0 * c[i] * rb[i];
}
```

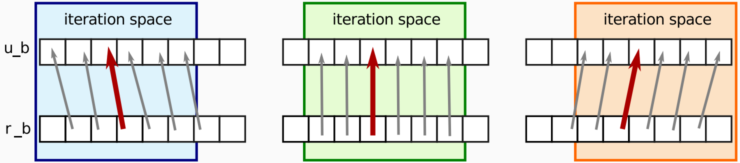
1D Stencil Example



The scatter can be split into individual updates

```
for ( i=1; i<=n-1; i++ ) {
  ub[i-1] += 2.0 * c[i] * rb[i];
}
for ( i=1; i<=n-1; i++ ) {
  ub[i] -= 3.0 * c[i] * rb[i];
}
for ( i=1; i<=n-1; i++ ) {
  ub[i+1] += 4.0* c[i] * rb[i];
}
```

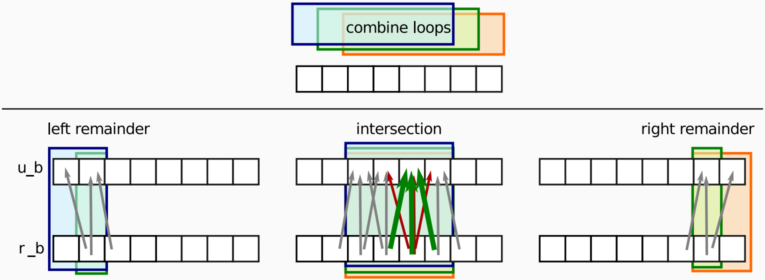
1D Stencil Example



Shift indices to write to loop counter element

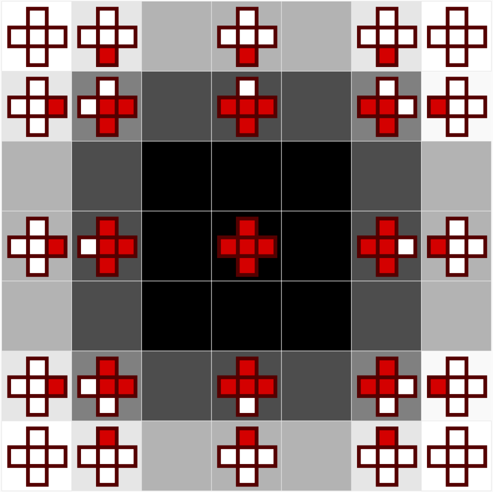
```
for ( j=0; j<=n-2; j++ ) {
  ub[j] += 2.0 * c[j+1] * rb[j+1];
}
for ( j=1; j<=n-1; j++ ) {
  ub[j] -= 3.0 * c[j] * rb[j];
}
for ( j=2; j<=n; j++ ) {
  ub[j] += 4.0 * c[j-1] * rb[j-1];
}
```

1D Stencil Example




```
#pragma omp parallel for private(j)
for ( j=2; j<=n-2; j++ ) {
  ub[j] += 2.0 * c[j+1] * rb[j+1];
  ub[j] -= 3.0 * c[j] * rb[j];
  ub[j] += 4.0 * c[j-1] * rb[j-1];
}
ub[0] += 2.0 * c[1] * rb[1];
// ... other remainders: ub[1], ub[n-1], ub[n]
```

Higher dimensions



In higher dimensions, we need remainders for edges and corners

Performance Results - Scalability

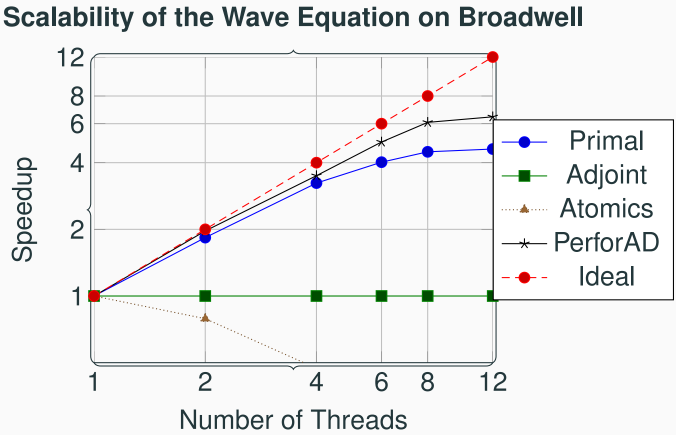


Figure 2: Speedups for the wave equation solver on a Broadwell processor, using up to 12 threads. The conventinal adjoint code with manual parallelisation does not scale at all. The primal and PerforAD-generated adjoint benefit from using all 12 cores.

Performance Results - Run times

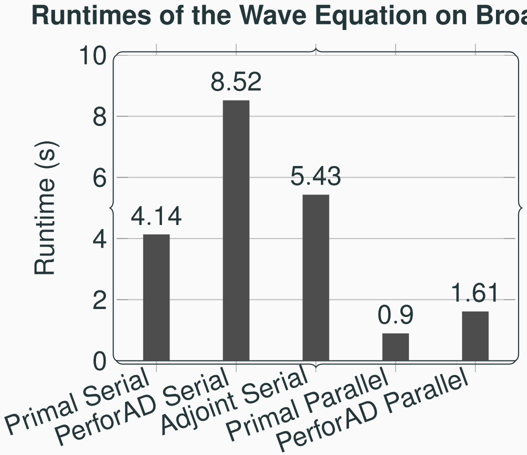


Figure 3: Absolute runtimes for wave equation primal and adjoint stencils and conventional adjoints in serial, as well as best observed primal and adjoint stencil run time in parallel. The best-observed performance of adjoint stencils was with 12 threads and is faster than the conventional adjoint by a factor of 3.4×.

PerforAD

- We release tool with this paper to generate these loop nests
- https://github.com/jhueckelheim/PerforAD

```
import sympy as sp; import perforad
# Define symbols
c = sp.Function("c")
u_1 = sp.Function("u_1"); u_1_b = sp.Function("u_1_b")
u_2 = sp.Function("u_2"); u_2_b = sp.Function("u_2_b")
i,j,k,D,n = sp.symbols("i,j,k,D,n")
# Build stencil expression
u_xx = u_1(i-1) - 2*u_1(i) + u_1(i+1)
expr = 2.0*u_1(i) - u_2(i) + c(i)*D*u_xx
lp = perforad.makeLoopNest(lhs=u(i), rhs=expr,
           counters = [i], bounds={i:[1,n-2]})
perforad.printfunction(name="wave1d_perf_b",
    loopnestlist=lp.diff({u:u_b, u_1:u_1_b, u_2: u_2_b}))
```

Conclusion, Future Work

- PerforAD-generated adjoint stencils preserve scalability of original program
- Paper discusses differentiation and code generation in more detail
- We also discuss reproducibility and floating point associativity
- See paper for full details, and runtimes on KNL
- Future work:
  - Explore other code generation strategies (e.g. fewer remainder loops, but with branches)
  - ML workloads
  - SIMD and GPU programs
  - Explore other polyhedral transformations in AD context

Thank you

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Questions?

References i