Automatic Differentiation for Parallel Programs

SIAM CSE 2021

Why do we need AD for parallel code?

- Most codes that care about performance exploit parallelism.
- **If the original program is parallel, can we recycle the parallelization for the derivative computation?**
- Short answer: Sometimes.
- The longer answer follows...

Forward Mode

- For distributed memory (e.g. MPI) in forward mode:
  - if a variable is sent, then its derivative must be sent.
  - if a variable is received, then its derivative must be received.

```
! Primal
call MPI_SEND( data, count, ... )
! Forward-mode AD
call TLS_MPI_SEND(data, datad, count, ... )
```

- For shared memory (e.g. OpenMP) in forward mode:
  - Derivative variables get the scope of primal counterparts.

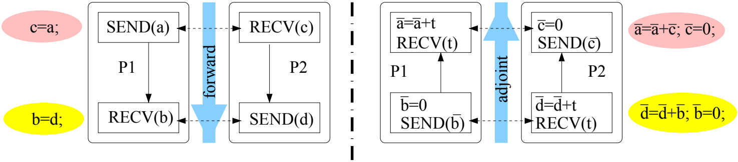
```
! Primal
!$omp parallel do private(c) shared(data)
! Forward-mode AD
!$omp parallel do private(c) shared(data, datad)
```

- Tapenade supports MPI and OpenMP.

Reverse-Mode AD for MPI

- Communication flow is reversed.
- If the original code sends, the adjoint code must receive.
- If the original code receives, the adjoint code must send.
- Challenges around non-blocking communication, one-sided communication, wildcards, and other subtleties.
- Adjoint MPI: libraries are available, and used e.g. by Tapenade

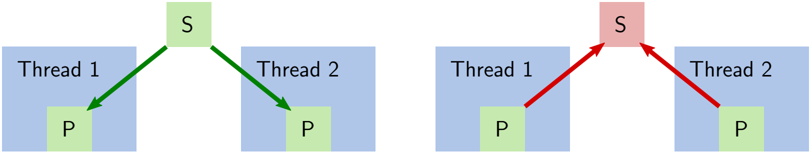
easy adjoints for blocking calls



Graphic: J. Utke, Adjoints of MPI programs, ECCO2 meeting slides, Argonne National Laboratory, 2008

Reverse-Mode AD for OpenMP

- Multiple threads run in parallel (e.g. on multi-core CPU)
- Memory visible to all threads, no explicit communication
- Parallel read-access is fine, parallel write access is a problem
- **Data-flow reversal potentially creates those problems!**



Breaking the parallelization barrier?

- Reverse AD for shared-memory parallel programs is hard, and will probably never work efficiently for *arbitrary* parallel input programs.
- For well-defined circumstances, much progress has been made, and there is promising ongoing research.
- Some tools (e.g. Tapenade) offer some support, new prototype tools and libraries are in development.
- In the meantime, if you need to differentiate a real-world parallel application *now* and can't wait for more research...

Going over the barrier instead?

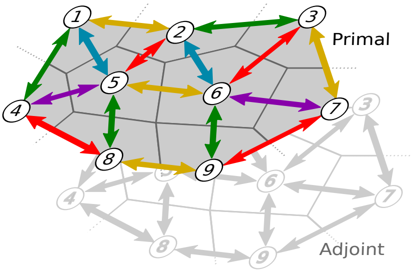
- There are (very successful) new high-level tools that operate on domain-specific languages, e.g. in PyTorch, TensorFlow, Halide, FireDrake
- Keep performance tweaks and parallelization "under the radar"
- Differentiate high-level code and express derivatives in terms of existing high-level building blocks.

```
! Primal
res = numpy.dot(a,b)
! Reverse-mode AD
ab = ab + numpy.multiply(b,resb)
bb = bb + numpy.multiply(a,resb)
```

- If the `dot` function is parallelized internally, we have parallel reverse-mode AD without doing any work.

Going under the barrier instead?

- Apply AD to individual iterations of parallel loops.
- Similarly: Apply AD to code blocks between MPI calls
- Manually take care of the communication reversal
- Sometimes, there are application properties that can be used to make life easier. Examples:
  - symmetry between read- and write-indices in parallel solvers means that parallelization can be safely re-used.
  - Halo / ghost cell exchange and domain decomposition often works similarly for the primal and reverse-AD code.



Parallel tool landscape

- Tapenade, ADOL-C, Adept support (all or some subset of) OpenMP and MPI in forward and reverse
- JAX, TensorFlow, PyTorch, Halide, ... go “over the barrier” and do high-level AD
- Many application-specific approaches exist for “under the barrier” parallel AD with hand-assembled parallelization
- Vector-forward and vector-reverse mode can be parallelized easily, even if the original program is sequential
- AD may *target* CUDA and parallel libraries for faster derivative computation, even if not fully supporting those languages as *input* programs
- Expect some potholes and road blocks when differentiating parallel programs.

Thank you

Questions?