Source-transformation adjoints for an unstructured solver with OpenMP

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ABOUTflow

AD and OpenMP - didn't we have this already?

- OpenMP in ADOL-C for operator-overloading AD[1]
- Parallelisation of vector mode AD, parallel computation of Hessians, manual parallelisation of AD code[2]
- Toward source-transformation OpenMP[3]
- New here:
  1. **Automatic** OpenMP-parallelisation of source-transformed adjoint (i.e. it happens in the Makefile after code preparation)
  2. Hopefully **efficient** (i.e. adjoint as scalable as primal)
  3. Exploiting properties of a (very common) special case

[1] Bischof, Gürtler, Kowarz, Walther (2008): Parallel Reverse Mode Automatic Differentiation for OpenMP Programs with ADOL-C

[2] Martin Bücker et. al. (2001, 2002, 2004, 2008)

[3] Förster, Naumann, Utke (2011): Toward Adjoint OpenMP

The primal code

- MGopt: Queen Mary University of London in-house Finite Volume flow solver
- Runtime is important: some cases run for a week and more
- Much time spent in linear solver (not brute-force AD'ed)
- Other expensive part: Residual computation
  - OpenMP used for shared-memory parallelisation of primal
  - Tapenade used to create adjoint residual
  - We need a parallel adjoint residual

Primal structure

- Edge-based residual:

```
do edge=1...nEdges
  i,j = nodes(edge)
  res(i), res(j) += flux(u(i), u(j))
end do
```

Primal structure

- Edge-based residual:

```

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  i,j = nodes(edge)
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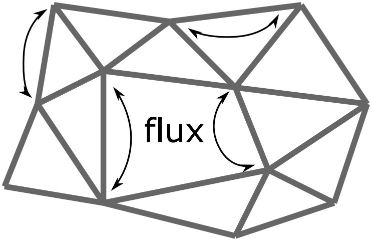
- Equivalent to iterating over edges in the graph:



How not to parallelise this: Part 1

- Can we do this?

```
!$OMP PARALLEL DO PRIVATE(edge,i,j)
do edge=1...nEdges
  i,j = nodes(edge)
  res(i), res(j) += flux(u(i), u(j))
end do
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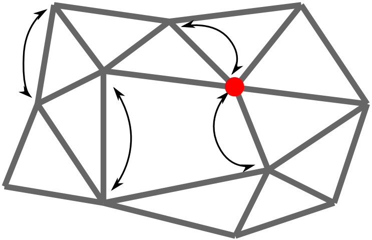
```

- No. There can be conflicting writes:



How not to parallelise this: Part 2

- Ok, but what about this?

```
!$OMP  PARALLEL DO PRIVATE(edge,i,j)
!$OMP& REDUCTION(+,res)
do edge=1,nEdges
  i,j = nodes(edge)
  res(i), res(j) += flux(u(i), u(j))
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```

- Segfault (not enough memory):
    - local copy of `res` for each thread
    - perfect for scalars, not so if `size(res) = meshsize`.

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- Segfault (not enough memory):
  - local copy of `res` for each thread
  - perfect for scalars, not so if `size(res) = meshsize`.
- Slow:
  - every thread writes only few values, local `res` copies are sparse
  - all elements on each thread are initialised with neutral element, then everything (here mostly zeroes) is reduced

Primal parallelisation

- Solution: edge colouring

```
do colour=1,nColours
  !$OMP PARALLEL DO PRIVATE(edge,i,j)
  do edge=firstEdge(colour),lastEdge(colour)
    i,j = nodes(edge)
    res(i), res(j) += flux(u(i), u(j))
  end do
end do
```

Primal parallelisation

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  !$OMP PARALLEL DO PRIVATE(edge,i,j)
  do edge=firstEdge(colour),lastEdge(colour)
    i,j = nodes(edge)
    res(i), res(j) += flux(u(i), u(j))
  end do
end do
```
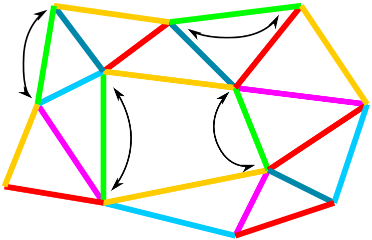

- All edges of one colour can be done in parallel



How not to adjoint this: Part 1

- Tapenade used to treat OpenMP pragmas as regular comments
- Comments are dumped in the adjoint code at (roughly) the same location as in the primal
- Unpredictable results, or does not compile

How not to adjoint this: Part 2

- Taf can do OpenMP, Tapenade could be extended
- How good can a general purpose AD tool do here?

```
do colour=nColours,1
 !$OMP  PARALLEL DO PRIVATE(edge,i,j)
 !$OMP& REDUCTION(+,ub)
 do edge=lastEdge(colour),firstEdge(colour)
  i,j = nodes(edge)
  ub(i),ub(j) += flux_b(u(i), u(j), res(i), &
                      & res(j), resb(i), resb(j))
 end do
end do
```

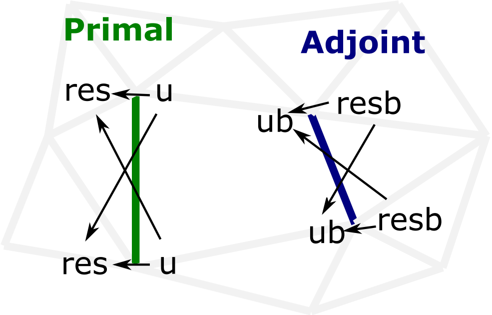
- No tool will understand our colouring on its own
- Tool has to be conservative, either use reduction (slow, memory) or atomic/critical sections (slow)

Adjoint parallelisation in principle

- Actually it is all easy: communication is symmetric!

Adjoint parallelisation in principle

- Actually it is all easy: communication is symmetric!
- Primal and adjoint read and write in the same way



Adjoint parallelisation with colouring

- The edges are still separated by colour after brute-force AD
- We can use the same OpenMP pragma as before

```
do colour=nColours,1
 !$OMP PARALLEL DO PRIVATE(edge,i,j)
 do edge=lastEdge(colour),firstEdge(colour)
  i,j = nodes(edge)
  ub(i),ub(j) += flux_b(u(i), u(j), res(i), &
                     & res(j), resb(i), resb(j))
 end do
end do
```

Adjoint parallelisation in practice

- How to we make this automatic? We know that:
  - if variable `foo` is private, `foob` is private
  - if variable `bar` is shared, `barb` is shared
  - **what happens to new variables that are created in adjoint code, e.g. temp1, temp2, arg1, arg2...?**
- Need some post-processing that will
  - Wipe all misplaced OpenMP statements from Tapenade output
  - Place new pragmas with correct scoping
  - **How to do this correctly without using a full Fortran parser?**

"Outlining" of parallel regions

- OpenMP compiler trick: place parallel region into new subroutine to take care of scoping[4]
- shared variables are arguments, passed call-by-reference
- private variables are local variables inside subroutine
- **idea: let's do this before passing code to AD tool**

[4] Liao et.al. (2007): OpenUH: An optimizing, portable OpenMP compiler

Source-transformed outlined code

- OpenMP defaults: everything shared by default, except loop counter (edge) and local subroutine variables (i,j)
- this is exactly what we need for the adjoint as well

```
do colour=1,nColours !forward
  !$OMP PARALLEL DO
  do edge=firstEdge(colour),lastEdge(colour)
    call flux_loopbody(edge,res,u)
  end do
end do
do colour=nColours,1 !reverse
 !$OMP PARALLEL DO
 do edge=lastEdge(colour),firstEdge(colour)
    call flux_loopbody_b(edge,res,resb,u,ub)
 end do
end do
```

Another small technicality

- Forward sweep pushes intermediate results to stack
- Reverse sweep pops them from stack
- Need to make sure that
  - each thread has its own stack
  - parallel regions are used in forward and reverse code consistently

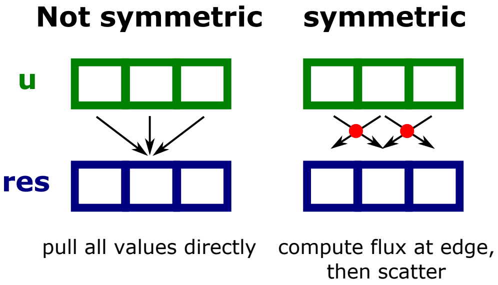
How it works, finally

- All bodies of parallel loops are placed in subroutine with special suffix (`_loopbody`)
- Python script removes all OpenMP pragmas from Tapenade output
- Before every loop that contains call to `*_loopbody` or `*_loopbody_b`, insert

  `!$OMP PARALLEL DO DEFAULT(SHARED)`
- Replace all calls to `PUSHINTEGER(n)` by `THREADPUSHINTEGER(n,numThread)`, likewise for all other push/pop routines.
- Link thread-safe stack instead of Tapenade stack

Conclusion: What works, what doesn't?

- if communication pattern is symmetric, we can automatically generate parallel AD code
- sometimes, code can be reorganised to become symmetric[5]



- some things are not symmetric. Boundaries are a problem.

[5] ask me for an example code if interested

Acknowledgments

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`http://aboutflow.sems.qmul.ac.uk`

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