Differentiating a Time-dependent CFD Solver

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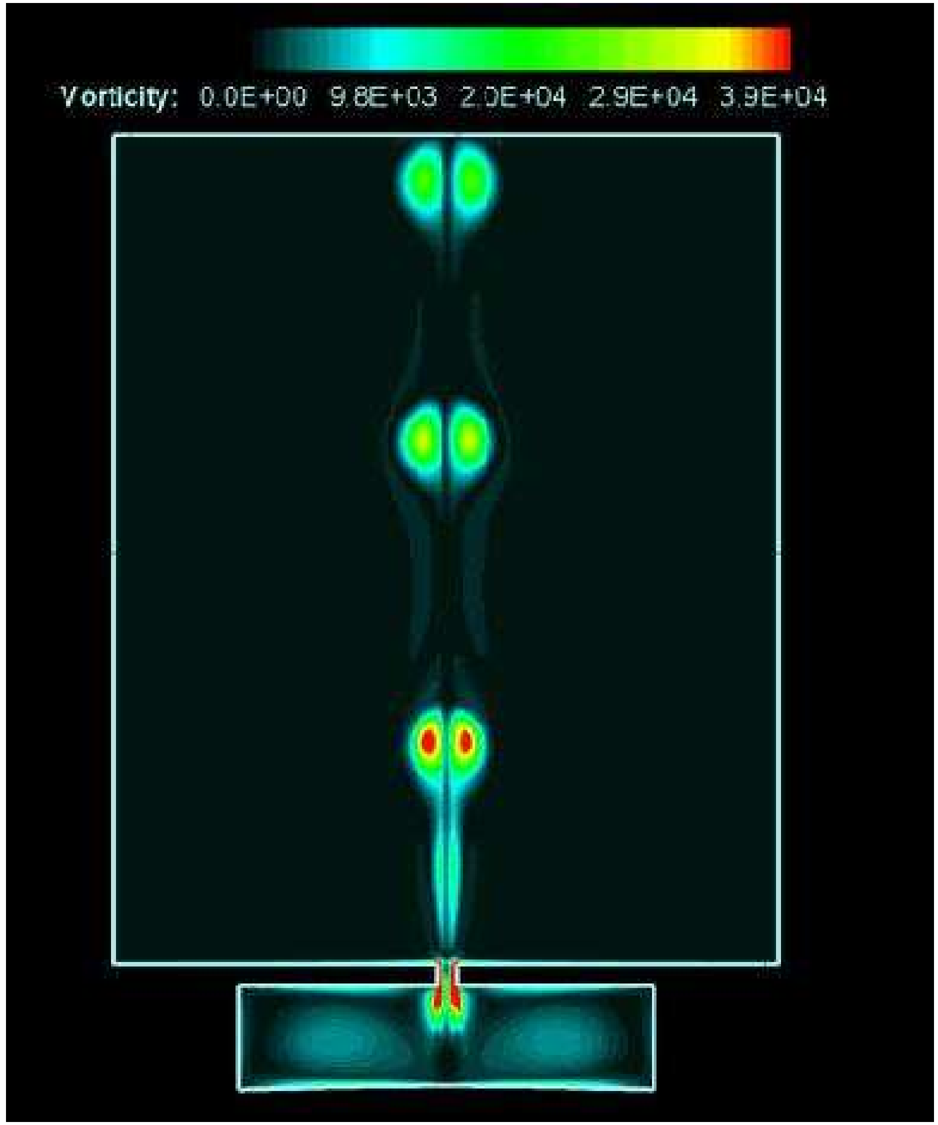
Introduction

- Aim: Tangent and Adjoint of a numerical code simulating a $2D$ model of a synthetic jet actuator.

- *Synthetic jet actuators* [GWP$^+$03]
  Synthetic jet actuators are small scale devices generating a jet-like motion by oscillating fluid in a chamber connected to the air flow via an orifice.

- *Possible Applications*
  - Embed into aircraft wing to control flow separation
  - Propulsion system for microfluid systems

Synthetic Jet



Mesh Movement Algorithm

- Time-dependent Navier-Stokes eqn.s on a moving mesh.
- Mesh movement for interior point $\mathbf{x}_i^{new} = \mathbf{x}_i + \Delta\mathbf{x}_i$ governed by forced boundary motion smoothed into interior mesh,

$$\Delta\mathbf{x}_i = \frac{1}{D_i} \sum_{j \in \text{Nbr}(i)} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} \Delta\mathbf{x}_j, \text{ with } D_i = \sum_{j \in \text{Nbr}(i)} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|},$$

repeated 50 times - Gauss-Seidel smoothing/linear solve.

The Time-Dependent CFD Solver

- Finite-volume semi-discretisation of N-S equations for cell i,

$$\frac{\partial V_i \mathbf{q}_i}{\partial t} = \mathbf{R}_i(\mathbf{q}, \mathbf{x}).$$

- Backward Euler gives nonlinear system for $\mathbf{q}^{n+1}$.

$$\begin{aligned} \frac{V_i^{n+1}\mathbf{q}_i^{n+1} - V_i^n \mathbf{q}_i^n}{\Delta t} &= \mathbf{R}_i(\mathbf{q}_i^{n+1}, \mathbf{x}^n) \\ 0 &= \mathbf{R}_i(\mathbf{q}_i^{n+1}, \mathbf{x}^n) - \frac{V_i^{n+1}\mathbf{q}_i^{n+1} - V_i^n \mathbf{q}_i^n}{\Delta t} \end{aligned}$$

- Introduce pseudo-timestepping with pseudo-time τ,

$$V_i^{n+1}\frac{\partial \mathbf{q}_i^{n+1}}{\partial \tau} = \mathbf{R}_i(\mathbf{q}_i^{n+1}, \mathbf{x}^n) - \frac{V_i^{n+1}\mathbf{q}_i^{n+1} - V_i^n \mathbf{q}_i^n}{\Delta t}.$$

- Iterate to convergence using low-storage 4-stage Runge-Kutta scheme.

Schema of the Numerical Code

```
Read in mesh geometry X (nodes, cells, faces)
Initialise flow variables and boundary conditions
Read in design variables designvars : a, p
Read in number of time-steps N and celopt
Set F = 0
For i from 0 to N
 Move the mesh boundary using a sin scheme a sin(pX + φ)
 Update interior mesh then cell and face information
 While (not converged) !  FIXPOINT
  Converge the flow variables using a RK4 solve:
   Compute residual R = r(Q, j) for each cell j
   Update the flow variables Q using R
 End While
 Update F = F + Σ_{i=2,3} Q(i, celopt)^2
EndDo
```

Fortran 95 Features of the code

- The input code (4500 loc) uses dynamic allocation, modules, derived types and array operations
- A derived type example

```
type bound_type !define the boundary structure
 integer(2)::uns !unsteady flag
 integer(2)::dim !dimensional or not(1=Yes)
 integer(2)::var !
 real(8), allocatable::bQ(:,:)!primitive Q
 character::TP*80 !type,
 character*32::extra(2)!store extra information.
end type bound_type
```

Fortran 95 Features of the code

- A Module Example

```
module mesh_info
 use prop
 ...
 integer(4)::nodenum !  number of nodes
 integer(4)::cellnum !  number of cells
 integer(4)::facenum !  number of faces
 integer(2)::nthread !  number of threads
 type(node_type), allocatable::node(:)  !node set
 type(cell_type), allocatable::cell(:)  !cell set
 type(face_type), allocatable::face(:)  !face set
 type(thre_type), allocatable::thre(:)  !thread set
end module mesh_info
```

- To differentiate this CFD solver, we used the AD tools TAF and TAPENADE.

Code Preparation

- TAF forward worked and gave consistent results with FD.
- TAF generated adjoint used to blow up at runtime (?)
- To further investigate the adjoint, we cleaned up the original code by using a *sed* script:
  - real(8) $\longrightarrow$ double precision (Portability)
  - integer(4) $\longrightarrow$ integer
  - Dynamic Allocation $\longrightarrow$ Static Allocation
  - Module $\longrightarrow$ Common Block
  - Derived Type $\longrightarrow$ set of arrays

First Results

- Mesh size: 654 nodes, 582 cells, 1235 faces
- 2 independents (period & amplitude) and 1 dependent (kinetic energy per cell volume = 572.0564 for this run).

Method	Gradient		# Sig. F
TAF(fwd)	-3230806.74033	54833.2739837	11
TAF(rev)	-2990768.62366	51687.4932185	1
TAPENADE(fwd)	-3230806.74031	54833.2739834	11
TAPENADE(rev)	-3230806.74033	54833.2739835	11

- DEBUG: Can AD tools adopt *optimisation options* as compilers do?

Potential Debug Problem

- Consider an array partially overwritten [Ralf Giering]

```
subroutine incompletarray(bval,ff,nx,ny)
double precision::ff(nx,ny), ...  !declarations
ff = 2.d0
call boundary(bval,ff,nx,ny)!partially overwrites ff
end subroutine incompletarray
```

- By default, TAF adjoint code will look as follows:

```
subroutine adincompletarray(bval,adbval,ff,adff,nx,ny
!  declarations
call boundary (bval,ff,nx,ny)
!Recomputation of ff is wrong
call adboundary(adbval,adff,nx,ny)
end subroutine adincompletarray
```

- TAF assumes `boundary` completely overwrites `ff` so recomputation algorithm omits `ff=2.d0` line and `ff` has incorrect value.

Some Observations

- TAF adjoint, by default uses a recomputation strategy but provides a fair tradeoff off between storage/recomputation via directives.
- TAPENADE adjoint provides a recursive checkpointing strategy performed at subroutine levels to tradeoff off between storage and recomputation.
- TAPENADE's Stack may be insufficient in terms of memory requirement.
- We have coded Fortran 95 taping routines with RAM buffer (module array) and local disk files using direct access.

Exploiting Code Insights

- Fixed Point Iteration (Rule 22 of [Gri00, p. 299]): Fixed point iterations can and should be adjoined by recording only single steps.

Method	CPU(∇F) (s)	Tape_size	$\frac{\text{CPU}(\nabla F)}{\text{CPU}(F)}$
TAPENADE(fwd)	69	—	3.8
TAPENADE(rev)	7755	1.585 GB	484.6
TAPENADE(rev,FP)	5751	0.182 GB	319.5
TAPENADE(rev,FP,Par.)	5715	0.180 GB	317.5

- The gradient $\nabla F = \left[\begin{array}{cc} -3230835.9523 & 54833.2466 \end{array} \right]$ (using the same number of iterations as for the forward pass) is up to 6 significant digits as compared to the gradient using the mechanical adjoining used by TAPENADE.

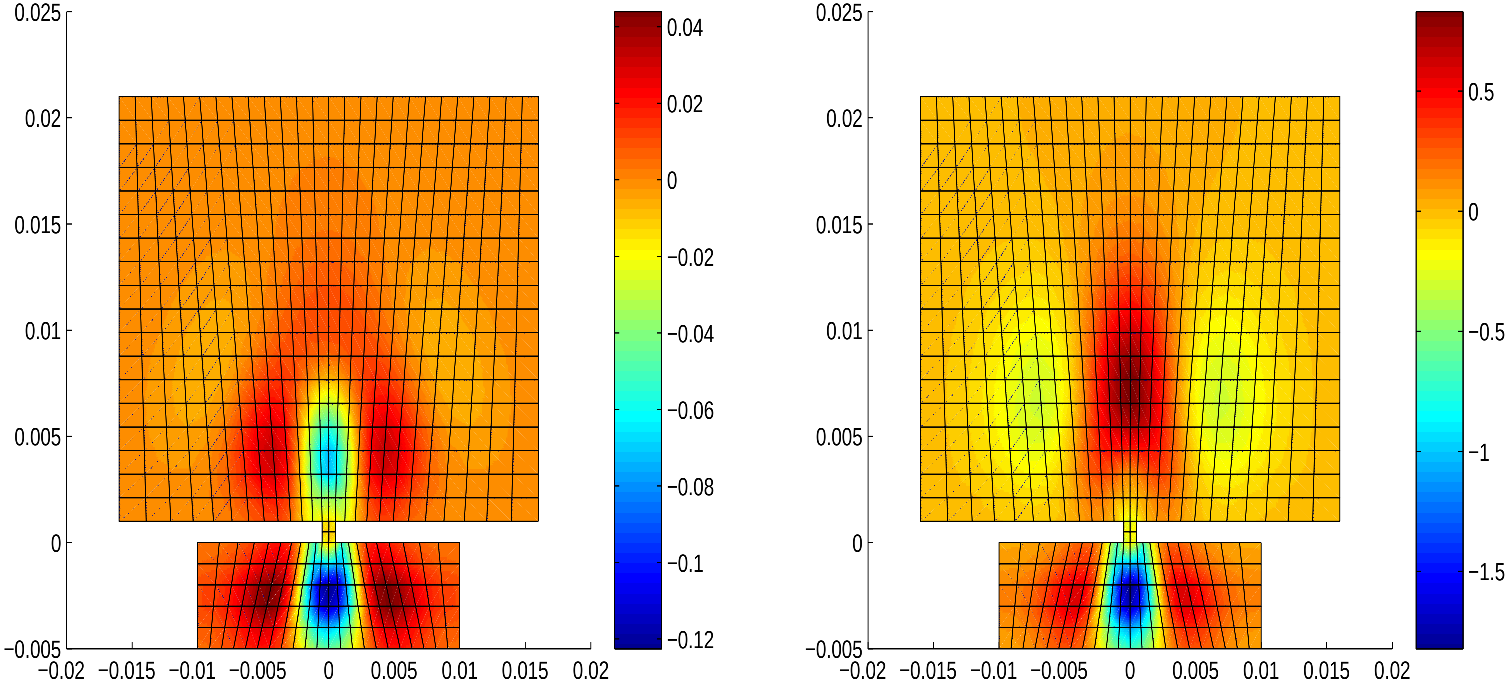
Optimisation

- Start Jet Animation
- Given a fixed amount of work $C(\mathbf{x})$ that the system cannot exceed, the objective is to maximise the kinetic energy $F(\mathbf{x})$ from a nominated cell in the upwards movement of the jet.

$$\max_{\mathbf{x}} F(\mathbf{x})$$
$$C(\mathbf{x}) \leq 1$$
$$10^{-3} \leq p \leq 10^{-1} \quad \texttt{!p is the period}$$
$$10^{-2} \leq a \leq 10^{-1} \quad \texttt{!a is the amplitude}$$

	Initial Guess		Optimun		
Method	Period	Ampl.	Period	Ampl.	Iter.
FMINCON	1.D-2	1.D-2	0.46D-2	0.45D-1	15
FMINCON(AD)	1.D-2	1.D-2	1.54D-2	1.05D-1	11

Velocity Profile at Convergence



On the Left [Right] is represented the upstream velocity profile of the jet before [after] the optimisation.

Concluding Remarks

- AD Adjoint mode performs better for applications with fairly large number of independents.
- For a given constraint, it is possible to choose the frequency and the amplitude of the fluid oscillation so as to maximise the kinetic energy of the jet's upwards movement.
- Improvements for the adjoint calculation (Fixpoint Iteration, Parallel Loops [HFH01]).
- Increase the number of the design variables in order to make the generated adjoint competitive.
- Run the adjoint for a finer mesh with (big number of nodes e.g., 20,000).
- It is safer to compile and run the original code on different platforms prior to differentiation!

References

References

[Gri00] Andreas Griewank. *Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation*. Number 19 in Frontiers in Appl. Math. SIAM, Philadelphia, Penn., 2000.

[GWP+03] Quentin Gallas, Guiquin Wang, Melih Papila, Mark Sheplak, and Louis Cattafesta. Optimization of synthetic jet actuators. *AIAA paper*, (0635), 2003.

[HFH01] Laurent Hascoët, Stefka Fidanova, and Christophe Held. Adjoining independent computations. In George Corliss, Christèle Faure, Andreas Griewank, Laurent Hascoët, and Uwe Naumann, editors, *Automatic Differentiation: From Simulation to Optimization*, Computer and Information Science, chapter 35, pages 285–290. Springer, New York, 2001.