

AD2CompEng - Automatic Differentiation and Adjoint Applied to Computational Engineering Progress Meeting 23rd June 2005

Shaun Forth

S.A.Forth@cranfield.ac.uk

Engineering Systems
Cranfield University (Shrivenham Campus)
RMCS Shrivenham
Swindon SN6 8LA

Agenda (times are approximate)

- 11:00 Arrival & Coffee
- 11:30 Project Overview & Progress Report - Shaun Forth
- 11:50 Adjoint Differentiation of a time-dependent CFD Solver - Mohamed Tadjouddine
- 12:40 Lunch
- 13:40 Gradient Enhanced Vibration Control - Alex Forrester
- 14:30 Computational Issues for Time-dependent CFD Solvers - Alan LeMoigne
- 15:20 Coffee
- 15:35 Review and agree actions
- 16:00 Close

Attendees (and Apologies)

Cranfield University : Shaun Forth, Mohamed Tadjouddine, John Pryce, Rahul Kharche.

Southampton University : Alex Forrester, (Andy Keane).

Oxford University : (Mike Giles).

Sheffield University : Ning Qin, Alan LeMoigne, H. Xia.

Cambridge University : David Radford.

ROLLS-ROYCE : (Leigh Lapworth).

AIRBUS UK : (Stefano Tursi, Murray Cross).

Minutes of Last Meeting & Matters Arising

2(a): MT - exploiting Hermitian property of BEAM3D matrix.

2: SAF - draft guidelines for application programmers.

3(b): ● MT/SAF makefile and instructions for BEAM3D differentiation.

● MT - strip out options in differentiated code.

● AJK - compare adjoint vs FD performance.

6: Obtain HYDRA license and meet Oxford/Cambridge team and review differentiation.

7: SAF,MT to visit NQ,AL to revise Phase 3 plan.

8: SAF,MT review introductory AD documents.

AD2CompEng Project

- Nov 2001 Proposal [FGQK01] & letters (RR, AUK) submitted.
- Mar 2002 Grant awarded - earliest start 1st Oct.
- Mar 2003 After recruitment difficulties Dia Zeidan appointed.
- Nov 2003 Dia Zeidan resigned.
- Dec 2003 Mohamed Tadjouddine starts on project.
- Mar 2004 Mohamed presents IMPNS Newton solver work at ICFD (Oxford) [TFQ04], paper published [TFQ04].
- Mar 2004 Shaun co-organises workshop on *AD in Large-Scale Optimisation* at EUCCO 2004 and presents initial differentiation of BEAM3D[FTK04].
- Jun 2004 First project meeting.
- Jul 2004 Mohamed presents BEAM3Dwork to AD2004 (Chicago) and paper accepted for publication [TFK04].

AD2CompEng Project

- **Sep 2004** Mohamed starts work on Sheffield's time-dependent `DGrins3D` CFD solver.
- **Apr 2004** Mohamed presents initial `DGrins3D` differentiation at 1st EuroAD Workshop.
- **Jun 2005** Second project meeting.

Phase 1: Eng. Design (Andy Keane)

- Structural optimisation problem.
- Adjoint (gradient) code for Meta-Lamarckian (hybrid gradient-descent/GA) optimisation.
- BEAM3D: complex valued arithmetic; large, dense linear solve (LAPACK); parallel loop over forcing frequencies.
- First adjoint solver developed by MT using ADIFOR 3.0 starting Jan 2004 and delivered May 2004 - in 5 months
- Only 1 month > plan, but 9 months behind schedule.
- ADIFOR work presented at European Conference on Computational Optimisation, Dresden, March 2004 [FTK04].
- Mohamed presents BEAM3Dwork to AD2004 (Chicago) and paper accepted for publication [TFK04].
- Unable to obtain consistent TAF generated gradients.
- Feb 2005 Alex starts using differentiated BEAM3D.

Phase 2: Aerospace Design (Mike Giles)

- Generate HYDRA adjoint via AD Tools (TapEnADe, TAF, ADIFOR 3) and compare performance (with hand-coding).
- Performance issues - flux adjoints via recomputation, parallel loops (residual accumulation), iterative-incremental techniques, suppressing differentiation in convergence acceleration techniques.
- Recently - Cusdin/Müller [CM03b, CM03a]: replace `abs` with branches, tape reduction by branch canonicalisation and interface contraction (flux into subroutine), inlining taping routines, local arrays for taping, eliminating common sub-expressions, unrolling small loops into single statements, pure differentiation, Runge-Kutta fixed-point solvers: AD adjoints **can** be as fast as hand-coding.
- At June 2004 project meeting it was agreed not to further pursue this phase.

Phase 3: Supersonic Adjoint (Ning Qin)

- Original proposal - use check-pointing (storage of intermediates) to reduce taping/recomputation in space-marched flow solver adjoint and apply to supersonic aircraft design.
- Now of less interest to Ning.
- At June 2004 project meeting it was agreed to differentiate time-dependent `DGrins3d` code.
- **Sep 2004** Mohamed starts work on Sheffield's time-dependent `textttDGrins3D` CFD solver.
- **Apr 2004** Mohamed presents initial `DGrins3D` differentiation at 1st EuroAD Workshop.
- Mohamed to report.

Phase 4: CFD Newton solvers (Ning Qin)

- Original proposal - use AD for large-scale Newton solvers in IMPNS space-marching solver.
- Now of less interest to Ning.
- Suggested looking at using AD to generate Newton solver from explicit unstructured mesh solver?

References

- [CM03a] P. Cusdin and J.-D. Müller. Deriving linear and adjoint codes for CFD using automatic differentiation. *Submitted to AIAA Journal, 2003.*
- [CM03b] P. Cusdin and J.-D. Müller. Improving the performance of code generated by automatic differentiation. School of Aeronautical Engineering Report QUB-SAE-03-04, Queen's University Belfast, School of Aeronautical Engineering, Faculty of Engineering, Queen's University, Belfast, Sep. 2003. Submitted to *Optimization Methods and Software.*
- [FGQK01] Shaun A. Forth, Michael B. Giles, Ning Qin, and Andrew J. Keane. AD2CompEng - automatic differentiation and adjoints applied to computational engineering. Case for Support in EPSRC Proposal, Oct. 2001.
- [FTK04] Shaun A. Forth, Mohamed Tadjouddine, and Andy Keane. Automatic differentiation for a structural optimization solver. Presented at EUCCO 2004 - European Conference on Computational Optimization, Minisymposia on Automatic Differentiation and

Large-Scale Optimization, Technical University of Dresden, Germany., March 29-31 2004.

- [TFK04] Mohamed Tadjouddine, Shaun A. Forth, and Andrew J. Keane. Adjoint differentiation of a structural dynamics solver. In Martin Bückner, George Corliss, Paul Hovland, Uwe Naumann, and Boyana Norris, editors, *AD2004: Proceedings of the 4th International Conference on Automatic Differentiation*, Lecture Notes in Computational Science and Engineering, page Accepted. Springer, 2004.
- [TFQ04] Mohamed Tadjouddine, Shaun A. Forth, and Ning Qin. Elimination AD applied to Jacobian assembly for an implicit compressible flow solver. In *Proceedings of the 8th Conference on Numerical Methods for Fluid Dynamics*. Institute for Computational Fluid Dynamics, Oxford University Computing Laboratory, Wolfson Building, Parks Road, Oxford, OX1 3QD, 29th Mar - 1st Apr 2004. CD-ROM, Submitted to International Journal for Numerical Methods in Fluids.