

Minutes of
AD2CompEng: Automatic Differentiation and Adjoints
Applied to Computational Engineering
Final Meeting
Stephenson Room
DCMT Shrivenham

Shaun Forth

6th March 2006

Present

- Cranfield University: Shaun Forth
- Southampton University: Andy Keane, Alex Forrester
- Sheffield University: Ning Qin, Alan Le Moigne
- Oxford University: Mike Giles
- Airbus UK: Murray Cross
- BAE Systems: Iain Barton
- Rolls-Royce: Leigh Lapworth

Matters Arising

From May 2004

- 2: SAF - draft guidelines for application programmers - NOT STARTED.

From June 2005

- 2: SAF/EMT: DGRINS2D - Discrepancies in optima found by AD and FD - coding error (incorrect sign) in use of AD constraint gradient resolves problem. COMPLETE
- 2: SAF/EMT: DGRINS2D - CPU ratios for differentiated solver to non-differentiated solver are inconsistent after original solver modified so array arguments passed and not indices to global arrays. Modifying the original code in this way was found to appreciably improve its performance as well as being advantageous to AD.
- 3: SAF: Complex-valued arithmetic used in S'ton MATLAB simulations - extend MAD to handle - not started though S'ton not ready to use it yet. ONGOING
- 4: SAF, EMT, NQ: liaison on 2D geometric optimisation problems. Proof of concept optimisations attempted. ONGOING
- 5: SAF, NQ: Investigate suitability of MERLIN adjoint differentiation. NOT ATTEMPTED.

Minutes

1. Shaun Forth reviewed progress (see slides) on the AD2CompEng project.
2. Andy Keane said that the final report should be made as impressive as possible since it would influence future EPSRC funding - the relevant Chapter in his recent book should be cited as a project outcome.
3. With regard to the differentiation of Sheffield's DGrins2D code (see slides), and since the last meeting in June 2005, Emmanuel Tadjouddine had produced and presented a conference paper for the International Conference on Numerical Analysis and Applied Mathematics [TFQ05b], with an extended version submitted to the Journal Applied Numerical Analysis and Computational Mathematics [TFQ05a]. Derivatives of objective (kinetic energy at a point above the jet) and constraint (average work performed by the membrane on the fluid) had been successfully obtained by forward mode AD. Reverse mode differentiation of the code had been performed using Tapenade, however there was an error in the code produced that had to be fixed by hand and the adjoint code had not been validated as yet. Optimisation using the forward mode had not been successful to date and, given Emmanuel Tadjouddine's recent departure to Aberdeen, Shaun Forth would complete this.
4. There then followed some discussion on the use of AD/adjoints in engineering design prompted by Andy Keane's observations that CAD tools do not support differentiation, that interconnecting various modelling, gridding and design tools to support differentiation would be difficult, and that assessing design robustness might be a more appropriate use of AD via control of the mean and variance of measures of the design. On behalf of Airbus, Murray Cross said that he believed error estimation and adaptivity via adjoint was also important and that a gradient descent design capability was required. Andy Keane asked whether Rolls-Royce had tried finite-differencing their CAD package Padran and Leigh Lapworth replied that this had not been attempted. Mike Giles noted that flutter and forced response in the frequency domain via differentiation was also a requirement. Murray Cross also remarked on the increasingly multi-disciplinary nature of design to which CAD was central.
5. Alex Forrester presented Southampton's work on "Gradient Enhanced Vibration Control" (see slides). The work on geometry repair utilised the adjoint version of BEAM3D developed earlier in the project. Minor changes to the code appeared to produce a scaling of the derivatives by a factor of 100. Andy Keane pointed out the difficulties in updating the differentiated code and Shaun Forth offered to debug. For larger problems the adjoint code was seen to be more efficient than finite-differencing.
6. Mike Giles's presentation focussed on the use of the AD tool Tapenade within a proof-of-concept CFD solver. Tapenade was used to calculate forward and adjoint sensitivity code for individual flux and boundary condition subroutines that were then used within a hand-coded forward or adjoint sensitivity "harness". The whole process could be automated and had been presented at a recent conference [GGD05]. Tapenade was now being used routinely in Oxford's work with Rolls-Royce on the HYDRA solver. The codes Oxford and Rolls-Royce use are still Fortran 77 based and suited to differentiation by Tapenade.
7. Ning Qin (see slides) presented Sheffield's work on blended wing-body and shock control via bumps. He highlighted the need for AD in unsteady CFD simulations.
8. Leigh Lapworth highlighted Rolls-Royce's requirement for AD to maintain forward and adjoint sensitivity versions of their HYDRA solver for design, sensitivities and error analysis.
9. There was some discussion on future projects and funding opportunities.

References

- [GGD05] M.B. Giles, D. Ghate, and M.C. Duta. Using automatic differentiation for adjoint cfd code development. *International Journal of Computational Fluid Dynamics*, submitted, 2005. Presented at the Post-SAROD Indo-French Workshop on "Recent Developments in Tools for Aerodynamics & Multidisciplinary Optimization", Bangalore, 12th - 13th December, 2005. See <http://web.comlab.ox.ac.uk/oucl/work/mike.giles/airfoil/>.
- [TFQ05a] Emanuel M. Tadjouddine, Shaun A. Forth, and Ning Qin. Automatic differentiation of a time-dependent CFD solver for optimisation of a synthetic jet. *Applied Numerical Analysis and Computational Mathematics*, Submitted, 2005.
- [TFQ05b] M. Tadjouddine, S.A. Forth, and N. Qin. Automatic differentiation of a time-dependent CFD solver for optimisation of a synthetic jet. In T.E. Simos, G. Psihoyios, and Ch. Tsitouras, editors, *ICNAAM International Conference on Numerical Analysis and Applied Mathematics 2005*, pages 514–517. WILEY-VCH Verlag GmbH & Co. KGaA, Sept. 2005.