

Minutes of  
AD2CompEng: Automatic Differentiation and Adjoint  
Applied to Computational Engineering  
Progress Meeting 14th May 2004  
Whitworth Conference Centre  
RMCS Shrivenham

Shaun Forth

18th May 2004

**Present**

- Cranfield University: Shaun Forth, Mohamed Tadjouddine, John Pryce
- Southampton University: Andy Keane
- Oxford University: Mike Giles, Sergio Campobasso, Mihai Duta
- Cambridge University: David Radford
- Sheffield University: Alan LeMoigne
- Rolls-Royce: Leigh Lapworth
- AIRBUS UK: Stefano Tursi
- BAE SYSTEMS: Paul Dawson

**Apologies**

- Sheffield University: Ning Qin
- Cranfield University: Mark Savill
- University of Hertfordshire: Bruce Christianson
- AIRBUS UK: Murray Cross
- BAE SYSTEMS: David Standingford

**Minutes**

1. Shaun Forth presented an overview of the AD2CompEng project. In particular, he noted that progress under the research officer Dia Zeidan had been very slow. Dia Zeidan left the project towards the end of 2003 and Dr Mohamed Tadjouddine had taken up the work. Shaun also noted that since the project was submitted to EPSRC in November 2001 there had been developments in the field and changes to Co-Investigators requirements which may necessitate changing the details of the investigation but not the objectives.

2. Mohamed Tadjouddine gave a presentation regarding adjoint differentiation of Andy Keane's BEAM3D structural-response program. Several points were raised:
  - (a) Cranfield had changed the linear solver used from a NAG routine to an LAPACK routine. Andy Keane stated that the matrix involved was Hermitian and this should be exploited. **ACTION** Mohamed Tadjouddine - investigate whether routine options or an other LAPACK routine could be used to exploit Hermitian property.
  - (b) Andy Keane expressed general reservations regarding making changes to validated code to enable differentiation. Such changes in a commercial code would necessitate expensive revalidation. This issue was not as important in code under development.
  - (c) All agreed that clear guidelines were needed for application programmers to ensure they avoided constructs that hindered differentiation.

**ACTION** Shaun Forth - produce draft guidelines for application programmers.
3. Andy Keane described how the differentiation of BEAM3D was perceived from the perspective of the application programmer.
  - (a) The AD tool generated lots of different versions of the original Fortran routines, all of which were very long and difficult to understand.
  - (b) Andy had noticed a discrepancy between which variables he wanted derivatives of and which were calculated by the Cranfield supplied adjoint code. It was not possible to modify the adjoint code since both the forward and reverse pass of the adjoint had to be consistently modified to prevent failure of the calculation. Shaun said that the aim was to have things set up so that Andy could make changes to the differentiation. A makefile could be configured to automate most of the process and Paul Dawson (BAE) confirmed that this had satisfactorily been achieved with the Flite-3D code differentiated by Shaun. Andy congratulated Mohamed on the rapid progress achieved since he started manning the project.
 

**ACTION** Mohamed Tadjouddine/Shawn Forth - set up makefile and instructions so that Andy can perform adjoint differentiation and assist Andy in installing ADIFOR.

**ACTION** Mohamed Tadjouddine - strip out all options in differentiated code apart from adjoint calculation.

**ACTION** Andy Keane - compare performance of adjoint enabled optimisation with finite-difference calculations (currently consuming vast CPU hours on Andy's system).
  - (c) Andy noted that noise in calculation would affect PDE-constrained optimisation and would trap optimiser in local minimum. GA-type methods would circumvent this problem.
4. David Radford gave a presentation on use of Tapenade in generating adjoint code for HYDRA. Issues not fully addressed concerned: Tapenade zeroing adjoints in the differentiated routine requiring hand-editing the generated adjoint, Shaun remarked that this could be avoided by placing a "wrapper" routine around that being differentiated; Tapenade taping all iterates in local Newton iterations; excessive taping.
  - (a) Andy Keane noted the problems associated with getting sensitivities with respect to CAD inputs and how this might hinder long-term take-up of adjoint/AD methods. It was agreed that differentiating CAD packages was not part of the AD2CompEng project but that this issue should be noted in the final project report.
5. Mike Giles presented some ideas on quantifying uncertainty in CFD modelling and that necessitated use of second derivative information. Mike explained that the ideas were to be pursued in a separate research proposal.

6. Given recent work by Cusdin/Muller (Belfast), there was then discussion on how best to pursue the Cranfield-Oxford collaboration under the AD2CompEng project. In the first instance, given experience gained on Flite3D with Airbus/BAE, Cranfield would review Oxford's approach and advise on automating the differentiation process using makefiles and, where needed, sed scripts. It was noted that Cranfield now hold a license for HYDRA and secure communication would be set up with ROLLS to facilitate access.

**ACTION** Shaun Forth - Obtain copy of HYDRA and arrange to meet Oxford/Cambridge team to review progress, assist in automating, and assess whether it would be fruitful to apply other AD tools.

7. Shaun noted that since writing the proposal in 2001 Ning Qin had changed Universities and was pursuing research with new computer codes and would prefer not work on the IMPNS parabolized Navier-Stokes flow solver. To fit in with the aims of the AD2CompEng programme Shaun explained that a changed plan of work should involve generation of a CFD Newton solver and a time-dependent adjoint solver. Alan LeMoigne explained that Sheffield were developing a parallelized unstructured mesh CFD package with embedded Newton solve and, given his PhD work, felt that use of AD in this task would be very beneficial and worthwhile. Additionally he felt that a time-dependent adjoint capability would be of value. All present agreed that these would be suitable for study under the project.

**ACTION** Shaun Forth, Mohamed Tadjouddine, Alan LeMoigne, Ning Qin - to meet Thurs 27th May to assess suitability of Sheffield computer programs and revise plans.

8. General Discussion. All co-investigators and industrial representatives present agreed that they were unaware of a suitable, accessible (non-mathematical) explanation of adjoint methods.

**ACTION** Shaun Forth/Mohamed Tadjouddine - Review existing documents, including Tapenade's, and if suitable previous work not available then start to produce one.

#### **Date of next meeting**

It was agreed to meet in 6 months time.

**ACTION** Shaun Forth - find suitable dates for November.

**Close**