European Science Foundation

Outline Proposal for Scientific Programmes in Physical and Engineering Sciences 1999

Automated Analysis and Enhancement of Applications Code

(NESSy – Network Enabled Sensitivities System)

Principal Proposers

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Summary / Abstract

The primary goal of this joint R&D project in Scientific Computing and Engineering involving contributing institutions from several European countries is to provide fast and easy access to sensitivity information required in numerous areas within Engineering and Physical Sciences. The availability of this information in the form of accurate derivatives helps to save energy, improve manufacturing efficiency, reduce noise and chemical pollution to name only some areas of application. Spreading the principles behind Automatic Differentiation (AD) supported by robust and easy-to-use software tools (**NESSy-1** and **NESSy-2**) as well as the adaptation of the current research and development in this area to the user needs (strong links with industrial partners) will represent the main axes of the approach. Grants for young researchers interested in the application and/or development of AD techniques as well as workshops and summer schools for potential users and students will support this demanding project.

Today most mathematical models used for the simulation and optimization of, for example, physical, economic, chemical, financial, or engineering processes are implemented as computer programs written in some high-level imperative programming language. Due to the large variety of these languages desirable properties of these models such as portability or re-usability can be guaranteed only in some cases. This often hinders a faster and more transparent development of efficient methods for obtaining the desired results. Qualitative (e.g. sparsity patterns) as well as quantitative sensitivity information (e.g. derivatives and error estimates) are crucial for the systematic development and usage of computational models. In contrast to the well-known approach of using often very costly finite difference computations for approximating the derivatives AD provides efficient ways to calculate these values with machine precision by generating the appropriate derivative code. To support this claim reference solutions to large-scale commercial problems provided by the industrial partners will be generated using a selection of existing AD software tools. These tools will be combined into a joint library which can be accessed via the Internet (**NESSy-1**). We consider this to be a first step towards better applicability and, consequently, wider acceptance of AD.

Both AD developers and users agree about the fact that a standardized platform for the development of generic source code transformation algorithms that is able to handle virtually every programming language available would save research as well as industrial institutions relevant amounts of time and money. The **A**bstract **I**ntermediate **R**epresentation of computer programs within **NESSy-2** extended by a **G**eneric **D**ifferentiation **E**ngine will provide the desired functionality and thus allow a fast implementation of new AD algorithms. Currently, there is a wide range of theoretical results whose implementation, accessibility and applicability is hindered by the non-existence of a corresponding standard such as the here proposed programming environment. Therefore the implementation and development of algorithms building on **NESSy-2** will be an important part of the second half of this project. In co-operation with the industrial partners and other potential users this work will be accompanied by an extensive test phase and the generation of reference solutions of commercial codes using the new software tool.

One of the strengths of Scientific Computing are its strong links with people working in various fields of science and engineering who need and want to apply methods from state-of-the-art computational mathematics. Unfortunately one often observes a large gap between the developer on one side and the user on the other. Undoubtedly this project will not only contribute to narrowing this gap but additionally provide a standard that can be built on in the future.

R&D Keywords

Mathematical Modeling of Processes from Science and Engineering, Simulation and Optimization, Energy and Cost Minimization, Sensitivity Information, Derivatives, Automatic Differentiation

Status of Research / Programme Objectives

Status of Research : Recent years have seen many new developments in the area of AD (see [BBCG96] and [CoGr91]). They will be presented and discussed at the *3rd International Workshop on AD (AD2000)* which is going to be held from June 19th to 23rd 2000 in Nice, France (see http://www-sop.inria.fr/tropics/ad2000). However the theoretical results are only insufficiently supported by user-friendly software tools. Apart from providing access to only a small number of AD algorithms currently known the main draw-back of the existing European academic AD tool prototypes (e.g. Odyssee (INRIA), ADOL –C (Technical University Dresden), AD01 (Rutherford Appleton Laboratory)) is their limitation to processing only programs written in one programming language (mostly C or Fortran). These are the main arguments against AD formulated by potential users. On the other side there is a history of successful applications of AD to various problems from physical and engineering sciences and economy , e.g. weather models, integrated circuit simulation, optimum shape design, computational fluid dynamics, multi-body systems, and economic models. AD is about to become a major topic in the education of science and engineering students at several European universities. However it is often difficult to find appropriate teaching material.

AD should be regarded as a source code enhancement technique built on the rules for elemental partial differentiability and the chain rule. The resulting computer program is used to compute directional derivatives with machine precision. There are various methods of applying the chain rule leading to varying operations counts and memory requirements. Some directions of the current research in AD are the detection and exploitation of sparsity, cross-country pre-accumulation techniques for reducing operations counts, trajectory analysis for lowering memory requirements, checkpointing techniques as a trade-off between operations count and memory requirement, different program reversal strategies. The main application areas of AD are optimization and optimal control, differential and differential-algebraic equations, inverse and data identification problems, computational fluid dynamics. The implementation of the available theoretical knowledge will lead to a significant speed up of the process for solving these problems.

Objectives : We aim for a bi-directional knowledge transfer between applied mathematics and engineering sciences in Europe with the goal to provide easy access for engineers to both qualitative and quantitative sensitivity information required for the simulation and optimization of computational models. To do so, it is necessary to synchronize research in the field of AD with the potential users needs. From the AD developers point of view we will work on a European concept for the systematic application of AD to the computation of derivatives. The formulation of an open standard for source code transformation based AD will improve the applicability, user-friendliness, robustness and portability of the tools to be developed significantly. We plan the implementation of a Network Enabled Sensitivities System in two steps : **NESSy-1** will provide fast interactive access to existing AD tools via the Internet. **NESSy-2** is planned to become a standardized differentiation engine providing access (by local installation or via the Internet) to state-of-the-art AD technology while being able to process virtually all high-level imperative programming languages. At least two reference solutions of large-scale engineering projects (e.g. commercial FE-based code for shape and topology optimization (CAD-FEM GmbH - Germany), commercial optimization code provided by ENGEL GmbH - Austria) will be generated using both **NESSy-1** and **NESSy-2**, respectively. **NESSy-2** will involve the development of an open standard for Abstract Intermediate Representation (AIR) of computer programs with respect to source code enhancement techniques; a Generic Differentiation Engine (GDE) representing an environment for the efficient development of AD algorithms building on AIR and providing a set of basic functionalities that allow the fast implementation of robust and complex AD algorithms; a network interface the conventions of which have to be discussed with both AD developers and users. The GDE of **NESSy-2** will be ideal for teaching AD to both students and potential users during two user workshops / summer schools. The majority of the participants of this project is directly involved in the mathematical education of students of Physical and Engineering Sciences. Clear AD teaching materials will be one of the key results of preparing these events.

It is planned to publish an "AD Newsletter" every April and October starting in 2002. Initially, it will be used to inform academic and industrial institutions within the participating countries about the latest developments in the field of AD. Later it should be extended to become a separate scientific journal containing articles written by both researchers and users. The existence of such a journal will not only contribute to widening the acceptance of AD but it will also represent a basis of communication between scientists and engineers.

As a "commercial off the shelf" technology it is foreseen to implement AD in European industry in collaboration with numerous industrial partners (see appendix). This should lead to the integration of AD as the technique of choice for computing derivatives into education in Physical and Engineering sciences. Many participants of this project are directly linked with both commercial and academic applications represented by the corresponding computer codes. They are all interested in enhancing these codes with accurate and efficient sensitivity information. This rich basis of applications and the fact that we will be able to exploit the entire knowledge in the field of AD currently available in Europe makes us very optimistic with respect to reaching our demanding objectives.

European Added Value

To compete in the world market it is necessary for European companies to shorten the product development cycle. An essential step towards this goal is virtual prototyping on the basis of advanced computer models. The convenient and efficient provision of a standard for source code transformation extended by up-to-date AD technology facilitates the systematic improvement of models and design thus allowing the transition from simulation to production. The main competitors of European AD tools are TAMC, ADIFOR / ADIC (USA) and Padre2 (Japan). Thanks to its features and its robustness ADIFOR has already reached a remarkable degree of acceptance. This AD tool is being developed at the Argonne National Laboratory. The same institution hosts NEOS - the Network Enabled Optimization Server providing access to a wide range of optimization algorithms that use AD to compute the required derivatives.

Bringing AD together with potential users in Europe will enable engineers to solve their problems more efficiently. Undoubtedly, the proposed project will put Europe at the leading edge of what we believe to be one of the most fundamental techniques in science and engineering, underpinning advances in many application areas.

European Context

The participants of this project are involved in both European and national projects related to simulation and optimization of physical and engineering processes, e.g. Esprit - **DECISON** (INRIA), ESF - **AMIF** (University of Paris), ISIS – **EUROMED** (University of Calabria), Esprit - **DANHIT** (University of Lyngby), DFG - **Forschergruppe** (Technical University Dresden), SFB F013 **Numerical and Symbolic Scientific Computing** (University of Linz), and SFB401 **Modulation of Flow and Fluid-Structure Interaction at Airplane Wings** (RWTH Aachen).

Programme Work Plan

When			What	Who	Deliverables
2001	**A**	**Feb**	**Planning Meeting**	**PP, PSC, IP**	Work plan, specific objectives, technical details, web page
	B	**Mar – Feb (2002)**	**Grant for implementation of NESSy-1**	**1 YR**	**NESSy-1**
	C	**Mar – Sep (2003)**	**Implementation of NESSy-2**	**PP**	**NESSy-2** + AD-Algorithms
	D	**May**	**Workshop : State of the art in transition from Simulation to Optimization**	**PP, PSC, PU, IP**	Introduction of project to potential users, collection of application codes
	E	**Jul – Jun (2002)**	**2 Grants**	**2 YR**	2 reference solutions using **NESSy-1**
	T	**Jan – Dec**	**Human mobility and coordination**	**PP, PSC**	
2002	**F**	**Jun**	**Summer school : Automatic Differentiation**	**SC, SO, PU**	AD teaching materials
	G	**Sep**	**Co-ordination meeting**	**PP, PSC, IP**	Intermediate results, further actions
	T	**Jan – Dec**	**Human mobility and co-ordination**	**PP, PSC**	
	N	**Apr and Oct**	**AD – Newsletter**	**PP, PSC**	
2003	**H**	**Mar – Sep**	**NESSy-2 tests with industrial partners, Grants for implementation of NESSy-2**	**PP, IP, SC YR, SC**	Experience reports
	I	**Jul – Jun (2004)**	**2 Grants**	**2 YR**	2 large-scale reference solutions using **NESSy-2**
	J	**Oct**	**Co-ordination meeting**	**PP, PSC, IP**	Intermediate results, further actions
	K	**Oct – Jun (2005)**	**Development and Implementation of new AD-algorithms building on NESSy-2**	**PP**	Collection of AD-algorithms including common interface
	T	**Jan – Dec**	**Human mobility and co-ordination**	**PP, PSC**	
	N	**Apr and Oct**	**AD – Newsletter**	**PP, PSC**	
2004	**L**	**Jul**	**NESSy-2 users workshop / summer school**	**NU, PU, PP, PSC**	Documented applications of AD, improved teaching materials
	T	**Jan – Dec**	**Human mobility and co-ordination**	**PP, PSC**	
	N		**AD – Newsletter**	**PP, PSC**	
2005	**M**	**Jun**	**AD conference : AD 2005**	**PP, PSC, IP, NU, PU, ...**	Resume, latest research results, proceedings (project summary)
	N		**AD – Newsletter**	**PP, PSC**	

[PP = Project Participants ; PSC = Programme Steering Committee ; IP = Industrial Partners ; YR = Young Researcher ; PU = Potential Users of AD ; SC = Students from PP; SO = Students from other Organizations ; NU = Users of NESSy-2]

Duration / Budget : 5 years / 520 kEuro

Year	**Budget** (in kEuro)	Breakdown (in kEuro)
2001	**150**	**A** = 10, **B** = 50, **D** = 20, **E** = 50, **T** = 20
2002	**120**	**E** = 50, **F** = 30, **G** = 10, **T** = 20, **N** = 10
2003	**90**	**I** = 50, **J** = 10, **T** = 20, **N** = 10
2004	**110**	**I** = 50, **L** = 30, **T** = 20, **N** = 10
2005	**50**	**M** = 40, **N** = 10

[Actions that do not occur in the table above will be financed by participants, e.g. C]

Annex

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Prof. K. Schittkowski :	Prof. in Applied Computer Science University of Bayreuth, Germany
Prof. Y. Evtushenko (guest) :	Director of Computing Center Russian Academy of Science, Russia

Programme Collaboration (19 Contributing Institutions from 11 European Countries)

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Czech Rep.: Czech Academy of Science
Dr. R. Neruda – Scientific Secretary, Institute of Computer Science
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UK: University of Hertfordshire
Prof. B. Christianson – Full Prof., Faculty of Engineering and Information Science
Royal Military College of Science
Dr. S. Forth – Lecturer, Dept. of Informatics and Simulation
Russia (guest): Russian Academy of Science
Prof. Y. Evtushenko – Director of Computing Center

(Industrial) Partners (11 Companies/Institutes from 6 European Countries)

Austria: **ENGEL Maschinenbau GmbH**, Schwertberg
Danemark: **Danish National Environmental Research Institute**, Kobenhavn
France: **Dassault Aviation** Vaucresson, **Meteo France**
Germany: **Siemens** Munich, **CAD-FEM GmbH** Grafing, **GRS** Garching
UK: **DERA – British Aerospace** Defford, **Sierra Training Services** London, **ECMWF** Reading
Italy: **Alenia Aerospazio** Torino

5 Publications of the Principal Proposers

Prof. Bruce Christianson : [Chr99], [Chr00]
Prof. Andreas Griewank : [GrWa97], [Gri00]
Dr. Uwe Naumann : [Nau99]

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