



Project 24023

AD-CAPE

Automatic Differentiation for Computer Aided Process Engineering








Trial Application

December 1997 – August 1999

Budget 644 k€

The Partners : a Complementary Team

 SIMULOG	 ProSim			
AD Technology Supplier www.simulog.fr	CAPE Codes Supplier www.prosim.net	CAPE Research Laboratory www.univ-inpt.fr/~lgc/psa/pa1.html	End-User www.elf.fr	End-User www.bpamoco.com

Differentiation in CAPE Codes Development : a Necessity

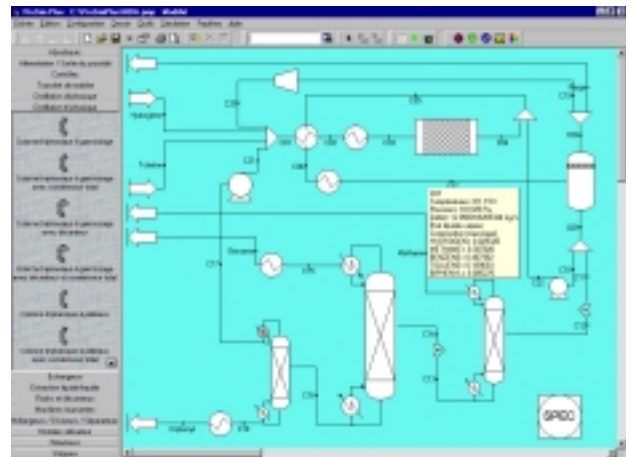
Numerical methods used in the solution of many CAPE problems require the computation of derivatives. Already useful in steady-state chemical process simulation, differentiation is now intensively required with the increasing use of **dynamic simulation** or **optimization**.

Various studies have shown the interest of using analytical derivatives in chemical process simulation packages. A 70-80% computing time saving, in comparison to derivatives computed by finite difference has been obtained using either Newton-Raphson-like methods for the resolution of a non-linear algebraic equation (NLAE) system (simulation) or a successive quadratic programming (SQP) method (optimization).

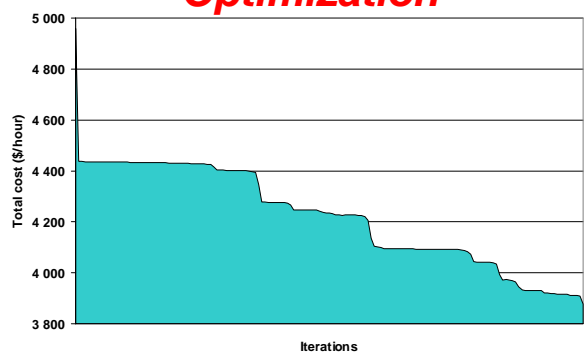
The advantages of **analytical derivatives** used in simulation routines are not only a matter of low cost. Much better accuracy is also achieved. This is a necessary condition to ensure **convergence**.

Besides process simulation and optimization, numerous applications could advantageously benefit from the availability of analytical derivatives. That includes in particular operating parameters **sensitivity analysis**, **MINLP** for optimal process synthesis, **parameter estimation** and data reconciliation, flexibility study, process control design.

Flowsheeting



Optimization



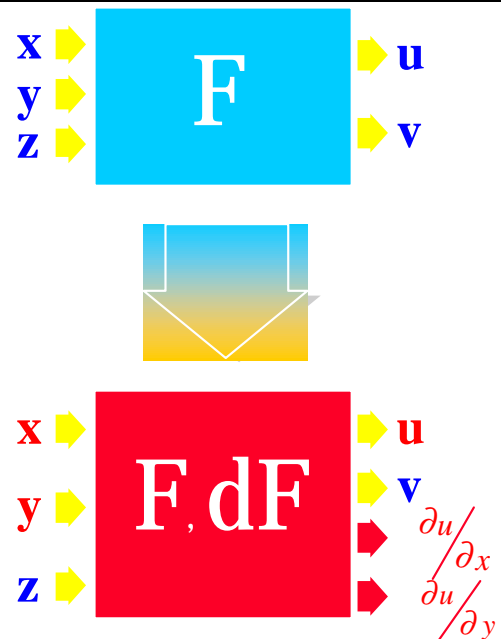
Automatic Differentiation : a Promising Technology

Both the accuracy and efficiency of the derivatives computation are of crucial importance for the convergence speed and robustness.

There are four approaches to compute derivatives currently used in CAPE codes development :

- Hand-made differentiation : time consuming and error-prone
- Finite differences : poor numerical precision and time consuming for Jacobian matrix computations
- Symbolic differentiation : not suited to handle branches or loops
- Automatic differentiation : from a source code computing a function, AD technology produces a new source code that computes its derivatives with respect to given input variables.

Consequently, AD technology appears as a promising technology that requires to be tested to find out its suitability to CAPE codes specificity.



Project Objectives : Trial of the Automatic Differentiation Software Odyssee[®] on CAPE Codes

The general objective of the project was the trial of the Automatic Differentiation software Odyssee[®] by industrial users on Sequential Modular Simulator codes.

The strategic goals of this project are the following :

- to collect results measurements based on the use of Automatic Differentiation in CAPE codes that are representatives of general simulation code using derivatives;
- to study and set-up a methodology based on the use of differentiation in CAPE code development process;
- to assess how much can be gained from using Automatic Differentiation technology in CAPE codes development process;
- to understand how to apply this new technology to the users specific needs and internal developments.

ProSim's targeted objectives are :

- to gain experience in AD technology and in the use of Odyssee[®] in maintenance (ProSim codes) and development of new codes (BP Amoco codes);
- to assess if AD technology is more efficient than hand-made differentiation currently used in CAPE code development and to measure if automatically generated codes reduce development time and improve maintainability;
- to identify if this technology can be used on legacy codes of our clients (low use of derivatives due to old numerical methods) in order to re-use them in another environment;
- to gain a competitive advantage by providing more efficient codes for process modeling and optimization, thanks to AD;
- to develop a new expertise in AD technology;
- to verify if the market needs AD service.

Two main components of the simulator were identified to be representative of CAPE codes and numerical methods used : thermodynamic models and unit operation modules.

Thermodynamic Models

Thermodynamic models for calculating physical and thermodynamic properties or fluid phase equilibria are intensively used in process modeling and simulation.

4 models tested from ProSim® library¹ and ELF² legacy codes:

- Activity coefficient model: 6-parameters¹ NRTL
- Explicit cubic equation of state: SRK¹
- Implicit cubic equations of state: SRK¹ and LKP¹
- Specific model: association in vapor phase AVP²

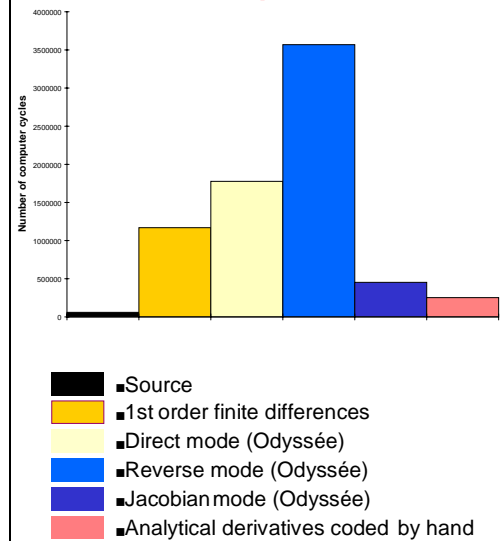
Several differentiation methods compared :

- Hand-coded analytical derivatives
- Order 1 and 2 finite differences
- Odyssee® differentiated code (3 modes)

The main results are the following:

- **Successful differentiation process**
- **Accuracy (Odyssee®) > accuracy (finite differences)**
- **Memory requirements (Odyssee®) ≅ Memory requirements (finite differences)**
- **CPU time (order 1 finite differences) < CPU time (Odyssee®) < 2 * CPU time (order 1 finite differences)**

CPU performances for NRTL model 20 components



Unit Operations

4 models tested from ProSim® library¹ and BP-AMOCO² legacy code:

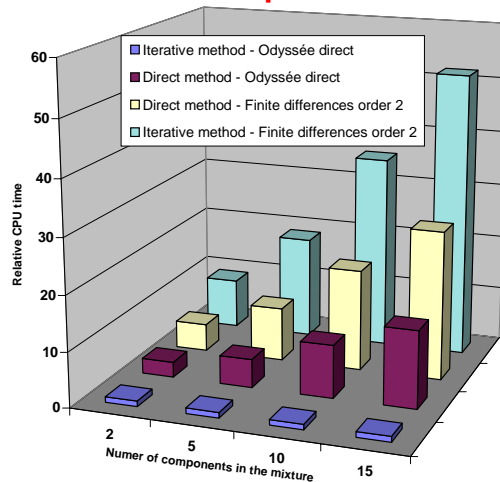
- Stream splitter¹
- Two phase liquid-vapor flash¹
- Heat exchanger¹
- Compressor²

Definition of an Automatic Differentiation strategy to apply efficiently Odyssee® to software architecture (centered around routines containing model equations) and sensitivity analysis

The main results are the following:

- **Successful differentiation process**
- **CPU time (Odyssee®) < CPU time (order 2 finite differences)**

Heat Exchanger Newton step calculation



AD-CAPE : Advantages for ProSim Users

A recognized advantage of ProSim solutions in process simulation and optimization is the efficiency of the numerical methods used. During this project ProSim has gained experience in AD technology. The main results are promising (accurate and rather efficient derivatives) and this technology is clearly useful for validation of hand-coded derivatives and for optimization. ProSim will take advantage of this expertise to be more active on new segments of the market where differentiation is intensively used : optimization, advanced process control, training simulation and control system validation.

ProSim users will take full advantage of the project results through the improvement of performance of ProSim codes. Furthermore, thanks to a partnership with Simulog, ProSim is now able to provide a new service to its customers : to improve end-users legacy codes (thermodynamic models, modules for specific processes, etc...) in order to re-use them.