Mini_ker Project — FET–IST

December 2006

Overview

Whenever modelling is needed, either in industrial or research projects, simulation is not the end of the story; it is a beginning.

Simple models are thought as "model for understanding" because their structure and analytical aspects give fecund insight on real systems. However, in industrial problems and applied research fields, a model seldom exhibits obvious properties, and a numerical analysis is necessary to grab some understanding on reality.

The kernel of the present project[1] is to develop a simulation and modelling tool able to enrich the analysis of a problem using innovative numerical methods. Such a software will advance the state-of-the-art of modelling, offering facilities to give quantitative answers to qualitative questions.

Specifications and methods

An innovative modelling environment should be able to carry out, in addition to numerical simulation:

- sensitivity analyses in terms of initial conditions (stability, asymptotic stability), perturbation (contextual stability to canonical perturbations), uncertainty on parameters, mechanisms and experimental aspects, response to noise sources;
- and, in particular cases:
  - investigation of the propagation of uncertainties within a model;
  - optimal control of dynamic systems;
  - sensitivity of cost functions or summarising functions to changes in parameters;
  - stability to stochastic sources;
  - parametric studies (optimality in design analyses);
  - parametric identification (in experimental context);

The present project proposes a consistent and unique methodology to do so, based on the systematic use of the Tangent Linear System (and Circulating TLS) of the system. The present *Collaboration* has shown in various contexts how the *Transfer Evolution Formalism* (TEF), developed by the Collaboration, allows to conduct automatically all these functionalities.

A TEF model consists of a set of connected elementary objects (sub-models) that correspond to well-posed problems. As a consequence, the question of the inter-influence between objects is directly accessible. An additional benefit is that the systematic partitioning of systems under TEF gives immediate access to massive parallelisation of the code.

The TEF approach of modelling is now rich of 20 years of experience in various scientific fields, from theoretical research to industrial applications, among which engineering, fluid mechanics, chemistry, physics, economy, molecular biology, climatology, etc. This work has lead to numerous peer-reviewed publications in international journals (e.g., *Journal of Economic Behavior and Organization, Phys. Rev. Lett., J. Atmos. Sci., Electrophoresis*, etc.). For more information, see [Blanco *et al.*(1996), Platel *et al.*(2004), Hallegatte (2005), Hallegatte (2006), Lahellec *et al.*(2006), Hallegatte *et al.*(2006)], and numerous PhD theses.

The TEF *Collaboration*, and needs for further development

Twenty years of methodological development and numerical implementation have paralleled the development of the ZOOM code. More recently, a new simplified version, named Mini_ker— which is currently in its version **102**[2] — have been developed in three years, starting in August 2003;

[1] contact: A.Lahellec alain@lmd.jussieu.fr
[2] see http://www.lmd.jussieu.fr/doc/mini_ker_102.pdf

1D models). The basis of this software is a symbolic partial differential technique that gives access to all Jacobian matrices of the system at every point along the trajectory. In other words, the Tangent Linear System is computed together with the model trajectory, allowing a variety of analyses: systematic forward sensitivity analyses, calculation of the adjoint system and gradient computing, extended-Kalman filtering, linear and non-linear feedback studies, etc.

The proposed project consists in the development of a new version of the Mini_ker software in a renewed computering environment, allowing for a substantial improvement in dimension limitation, ready for massive parallelisation, and adapted to public diffusion for research and industrial applications.

In our knowledge, there is no other modelling tool gathering the analysing facilities of Mini_ker in its highly coherent approach based on: (i) TEF (partitioning and coupling); (ii) symbolic differentiation, and (iii) systematic exploitation of systems TLS.

Companion research applications

The Mini_ker project will be the occasion of boosting modelling activities among the teams involved in the TEF-ZOOM collaboration. Our major projects are:

- The investigation of climate-economy interactions, a very active field where interaction dynamics is of primary importance to study and anticipate the impacts of global warming [Hallegatte (2006), Hallegatte (2005)] and to propose mitigation and adaptation actions.
- the modelling of non autonomous feedback dynamics in Climate Sciences, which is an important issue to understand and predict Global Climate Change. The CTLS methodology developed in the *Collaboration* allowed substantial progress in this domain [Lahellec *et al.*(2006), Hallegatte *et al.*(2006)].
- The use of models as accompanying tools for experimental studies. Emerging technology systems offer a very stimulating context, because models are intimate parts of the development of experimental facilities. Two main applications are scheduled: the modelling of compost-based bio-filters for air treatment and the development of high-technology heating loops for spacecraft.
- The development of modelling methodologies for architects and engineers. During pre-designing phases, indeed, important decisions are usually taken from expertise only. To provide guidance from models, new modelling approaches are required. To progress in this direction, our approach will be applied to racing-boat pre-designing.

List of participants

The project is based on the TEF-ZOOM collaboration, constituted of:

- the Laboratoire de Météorologie Dynamique (CNRS-UPMC-INSU-IPSL, Paris, France), with Alain Lahellec as principal investigator and leader of the Mini_ker project, Jean-Yves Grandpeix (former leader of the ZOOM project), and Robert Franchisseur, consultants;
- the Centre International de Recherche sur l'Environnement et le Développement (CIRED, UMR CNRS-EHESS-ENPC-ENGREF, Paris, France) with Stéphane Hallegatte, principal investigator and Fran cois Gusdorf, consultant;
- the Laboratoire d'Énergétique (UPS, Toulouse, France) with Stéphane Blanco, as principal investigator, and Sébastien Dufour, consultant;
- the I.U.T. Tarbes (France), with Vincent Platel, principal investigator;
- the ENSIMAC (Albi, France) with Mouna El Hafi and Olivier Fudym, consultants;
- the Plateforme Environnement (ENS, Paris, France) with Patrice Dumas, consultant;

and on our industrial partners (two sme's) and "referent firms" :

- HPC-sa, presided by Bernard Lécussan (PI), numerical and software methods (Toulouse, France);
- Actis, emerging industry of new isolating materials (Toulouse, France);
- Benjamin Muyl and Guillaume Verdier (naval architects currently working for the Areva challenge of the America's Cup) for testing methods in ship pre-designing (Valencia, Spain and Southampton University);

[Hallegatte (2006)] Hallegatte, S., 2006: Business cycles, bifurcation and chaos in a neoclassical model with investment dynamics, *Journal of Economic Behavior and Organization*, **in press**.

[Lahellec *et al.*(2006)] Lahellec, A., S. Hallegatte, J.-Y. Grandpeix, P. Dumas, and S. Blanco, 2006: Feedback gain in nonlinear dynamical systems, *Phys. Rev. Lett.*, **submitted**.

[Cadet et Lécussan (2006)] Cadet G. and B. Lécussan 2006: Simulation de propagation d'ondes par lancer de rayon sur de très grands modèles, *Revue Technique et Sciences Informatiques*.

[Hallegatte *et al.*(2006)] Hallegatte, S., A. Lahellec, and J.-Y. Grandpeix, 2006: An elicitation of the dynamic nature of water feedback in Climate Change using a 1D model, *J. Atmos. Sci.*, **63**, 1878–1894.

[Hallegatte (2005)] Hallegatte, S., 2005: The long timescales of the climate-economy feedback and the climatic cost of growth, *Environment Modeling and Assessment*, **10**, 277–289.

[Platel *et al.*(2004)] Pouzet E., J.L. Joly, V. Platel, J.Y. Grandpeix, C. Butto 2004: Dynamic response of a Capillary pumped loop subjected to various heat load transients, *Int. J. Heat Mass Tansfer*, **47**, 2293–2316.

[Torguet *et al.*(2003)] Torguet P., B. Bréholée, P. Siron, J.P. Jessel, B. Lécussan 2003: An HLA (DoD High Level Architecture) distributed Virtual Reality Application on a Linux cluster, *in:* 3rd IEEE/ACM Int. Symposium on Cluster Computing and the GRID, Tokyo, Japon.

[Blanco *et al.*(1996)] Blanco, S., J. Clifton, J. Joly, and G. Peltre, 1996: Protein separation by electrophoresis in a nonsieving amphoteric medium, *Electrophoresis*, **17**, 1126–1133.