Certification of errors in numerical simulations
Preservation of invariants by post-processing and adaptivity (mesh, scheme, solvers, model) for industrial needs

CEA/EDF/INRIA numerical analysis summer school

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1 Certification of errors in numerical simulations

Numerical simulation of partial differential equations (PDEs) has become an essential tool for finding approximate solutions to physical problems. It leads to several important questions:

- What is the **error** in the **numerical approximation**?
- Can we **certify the result**, give a safety margin?
- Can we estimate the error in **quantities of interest** identified by the user (point value of the solution, flow through a part of the boundary)?
- Can we have this information for an **affordable cost**, much smaller compared to the cost of the numerical simulation itself?

It is the theory of a posteriori error estimates [1, 10, 16, 6, 13] and in particular recent contributions [9, 5, 11, 2, 14] which make it possible to give affirmative answers to these questions. Exposing these latest advances, in detail for simple model problems, will be the central pillar of the proposed summer school.

2 Preservation of invariants by post-processing

The peculiarity of the approaches in [9, 5, 2, 14] is that they actually provide an **improvement of the numerical approximation**. These improvements make it possible to satisfy another highly desired property in numerical simulations: the **preservation of invariants**. More precisely, for example, it turns out that it is not completely essential to use a numerical scheme dedicated to local mass conservation. We can find a locally conservative field for a scheme non-conservative by construction via a **local postprocessing** which is already part of the a posteriori error evaluation. This applies similarly for primal quantities. One day in the school will be devoted to this subject.

3 Adaptivity of mesh, scheme, and solvers

The theory of posterior error estimates is also the basis of the concept of **adaptivity** of **mesh** [3, 15, 12], but also more broadly, including the **scheme** [11] or the **linear and nonlinear solvers** [4, 8, 7]. To give the participants an idea of the power of such an adaptivity, scientific seminars will discuss practical recipes to:

- give a **guaranteed bound** of the **total error** at each moment (time step, iteration of the solvers) in the numerical algorithm;

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- **estimate** the different **error components**, associated with the discretization in time, discretization in space, scheme, nonlinear solver, or linear solver;
- balance the different error components via **adaptive choice** of **time step** and **mesh**, **parameters** of the scheme, or **stopping criteria** of the linear and nonlinear solvers;
- design nested **adaptive solvers** to **significantly reduce** the **computational time**;
- get a better **robustness** of the **simulation codes**.

4 A posteriori control and adaptivity for industrial needs

The issue of automatic steering of scientific calculations impacts various applications of numerical simulations in engineering. Today, it is studied more broadly in connection with multiscale analysis, model reduction, optimal control, inverse problems, uncertainty quantification, the treatment of strongly nonlinear problems with instabilities... In all these subjects, the goal is to calculate just at the right cost, by finding the best compromise between efficiency and precision, according to the objective of the simulation, with a guaranteed margin of the error of simulation. Part of the presentations and discussions will therefore address these themes, focusing on industrial needs and current research challenges. We can list for example:

- the **adaptivity** of the **model** (choice of the PDE model such as the LES (large eddy simulation) model, choice of the components and parameters of the model) and choice of the **regularization** for stiff or degenerate problems (form, parameters);
- the **multiscale adaptivity**;
- the **quantification of uncertainties**;
- the contribution of new tools, such as those related to **machine learning**, for the control of numerical simulations.

Finally, to contribute to the **transfer** of research tools to the **industry**, the following applications will be considered:

- mechanics of viscous fluids;
- diffusion and simplified transport in neutronics;
- solid mechanics;
- complex flows in porous media (storage of dangerous waste, geological sequestration of CO_2).

Practical organization

- Monday–Thursday mornings: lectures dispensed by international experts, detailing the basic ideas from Sections 1–3.
- Monday–Thursday afternoons: tutorials supervised by assistants, computer implementation of the basic ideas from Sections 1–3.
- Monday–Thursday evenings: exhibition of the more advanced ideas in a form of short scientific seminars by expert guests.
- Friday: scientific seminars & discussion on industrial experiences related to Section 4.
- Each participant arrives with a laptop (there will be a limited number of computers to lend). The computer implementation will be done in a code that each installs beforehand. Most likely FreeFem++.

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