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Activity Report 2011

Project-Team CONCHA

Complex Flow Simulation Codes based on High-order and Adaptive methods

IN COLLABORATION WITH: Laboratoire de mathématiques et de leurs applications (LMAP)

RESEARCH CENTER
Bordeaux - Sud-Ouest

THEME
Computational models and simulation

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Project-Team CONCHA

Keywords: Adaptive Algorithm, Fluid Dynamics, Finite Elements, Numerical Methods, Object Oriented Programming, Optimization

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2. Overall Objectives

2.1. Objectives

The main objective of this project is the development of innovative algorithms and efficient software tools for the simulation of complex flow problems. Accurate predictions of physical quantities are of great interest in fluid mechanics, for example in order to analyze instabilities, predict forces acting on a body, estimate the flow through an orifice, or predict thermal conductivity coefficients. Due to the complex and highly nonlinear equations to be solved, it is difficult to know in advance how fine the spatial or temporal resolution should be and how detailed a given physical model has to be represented. We propose to develop a systematic approach to these questions based on auto-adaptive methods.

Most of the physical problems under consideration have a three-dimensional character and involve the coupling of models and extremely varying scales. This makes the development of fast numerical methods and efficient implementation a question of feasibility. Our contributions concern modern discretization methods (high-order and adaptivity) and goal-oriented simulation tools (prediction of physical quantities, numerical sensitivities, and parameter identification). Concrete applications originate from aerodynamics, viscoelastic flows, heat transfer, and porous media.

The goal of the **first phase** of the project is to develop flow solvers based on modern numerical methods such as high-order discretization in space and time and self-adaptive algorithms. Adaptivity based on a posteriori error estimators has become a new paradigm in scientific computing, first because of the necessity to give rigorous error bounds, and second because of the possible speed-up of simulation tools. A systematic approach to these questions requires an appropriate variational framework and the development of a posteriori error estimates and adaptive algorithms, as well as sufficiently general software tools able to realize these algorithms. To this end we develop a single common library written in C++ and study at hand of concrete applications the possible benefits and difficulties related to these algorithms in the context of fluid mechanics. The main ingredients of our numerical approach are adaptive finite element discretizations combined with multilevel solvers and hierarchical modeling. We develop different kinds of finite element methods, such as discontinuous (DGFEM) and stabilized finite element methods (SFEM), either based on continuous or non-conforming finite element spaces (NCFEM). The availability of such tools is also a prerequisite for testing advanced physical models, concerning for example turbulence, compressibility effects, and realistic models for viscoelastic flows.

The goal of the **second phase** is to tackle questions going beyond forward numerical simulations: parameter identification, design optimization, and questions related to the interaction between numerical simulations and physical experiments. It appears that many questions in the field of complex flow problems can neither be solved by experiments nor by simulations alone. In order to improve the experiment, the software has to be able to provide information beyond the results of simple simulation. Here, information on sensitivities with respect to selected measurements and parameters is required. The parameters could in practice be as different in nature as a diffusion coefficient and a velocity boundary condition. It is our long-term objective to develop the necessary computational framework and to contribute to the rational interaction between simulation and experiment.

The interdisciplinary collaboration is at the heart of this project. The team consists of mathematicians and physicists, and we develop collaborations with computer scientists.

2.2. Highlights

- Habilitation thesis of Daniela Capatina.
- Optimality of an adaptive finite element method for the Stokes equations.
- Parallelization of the CONCHA library.

3. Scientific Foundations

3.1. Challenges related to numerical simulations of complex flows

First, we describe some typical difficulties in our fields of application which require the improvement of established and the development of new methods.

- Coupling of equations and models
  The general equations of fluid dynamics consist in a strongly coupled nonlinear system. Its mathematical nature depends on the precise model, but in general contains hyperbolic, parabolic, and elliptic parts. The spectrum of physical phenomena described by these equations is very large: convection, diffusion, waves... In addition, it is often necessary to couple different models in order to describe different parts of a mechanical system: chemistry, fluid-fluid-interaction, fluid-solid-interaction...
- Robustness with respect to physical parameters
  The values of physical parameters such as diffusion coefficients and constants describing different state equations and material laws lead to different behaviour characterized for example by the Reynolds, Mach, and Weissenberg numbers. Optimized numerical methods are available in many situations, but it remains a challenging problem in some fields of applications to develop robust discretizations and solution algorithms.
- Multiscale phenomena

The inherent nonlinearities lead to an interplay of a wide range of physical modes, well-known for example from the study of turbulent flows. Since the resolution of all modes is often unreachable, it is a challenging task to develop numerical methods, which are still able to reproduce the essential features of the physical phenomenon under study.

3.2. Stabilized and discontinuous finite element methods

The discontinuous Galerkin method [69], [66], [37], [36] has gained enormous success in CFD due to its flexibility, links with finite volume methods, and its local conservation properties. In particular, it seems to be the most widely used finite element method for the Euler equations [39]. On the other hand, the main drawback of this approach is the large number of unknowns as compared to standard finite element methods. The situation is even worse if one counts the population of the resulting system matrices. In order to find a more efficient approach, it seems therefore important to study the connections with other finite element methods.

In view of the ubiquous problem of large Péclet numbers, stabilization techniques have been introduced since a long time. They are either based on upwinding or additional terms in the discrete variational formulation. The drawback of the first technique is a loss in consistency which generally leads to large numerical diffusion. The grand-father of the second technique is the SUPG/GLS method [54], [67]. Recently, new approaches have been developed, which try do avoid coupling of the different equations due to the residuals. In this context we cite LPS (local projection stabilization) [61], [52], [43][1] and CIP (continuous interior penalty) [55], [56].

3.3. Finite element methods on quadrilateral and hexahedral meshes

The construction of finite element methods on quadrilateral, and particularly, hexahedral meshes can be a complicated task; especially the development of mixed and non-conforming methods is an active field of research. The difficulties arise not only from the fact that adequate degrees of freedom have to be found, but also from the non-constantness of the element Jacobians; an arbitrary hexahedron, which we define as the image of the unit cube under a tri-linear transformation, does in general not have plane faces, which implies for example, that the normal vector is not constant on a side.

In collaboration with Eric Dubach (Associate professor at LMAP) and Jean-Marie Thomas (Former professor at LMAP) we have built a new class of finite element functions (named pseudo-conforming) on quadrilateral and hexahedral meshes. The degrees of freedom are the same as those of classical iso-parametric finite elements but the basis functions are defined as polynomials on each element of the mesh. On general quadrilaterals and hexahedra, our method leads to a non-conforming method; in the particular case of parallelotopes, the new finite elements coincide with the classical ones [60], [59].

3.4. Finite element methods for interface problems

The NXFEM (Nitsche eXtended finite element method) has been developed in [62] and [63]. It is based on a pure variational formulation with standard finite element spaces, which are locally enriched in such a way that the accurate capturing of an interface not aligned with the underlying mesh is possible, giving a rigorous formulation of the very popular XFEM. A typical computation for the Stokes problem with varying, piecewise constant viscosity is shown in Figure 1. This technology opens the door to many applications in the field of fluid mechanics, such as immiscible flows, free surface flows and so on.

3.5. Adaptivity

Adaptive finite element methods are becoming a standard tool in numerical simulations, and their application in CFD is one of the main topics of Concha. Such methods are based on a posteriori error estimates of the discretization error avoiding explicit knowledge of properties of the solution, in contrast to a priori error estimates. The estimator is used in an adaptive loop by means of a local mesh refinement algorithm. The mathematical theory of these algorithms has for a long time been bounded to the proof of upper and lower bounds, but has made important improvements in recent years. For illustration, a typical sequence of adaptively refined meshes on an L-shaped domain is shown in Figure 2.

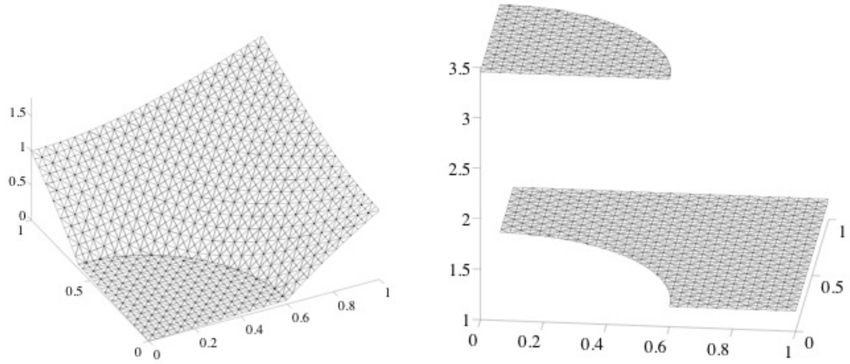


Figure 1. Incompressible elasticity with discontinuous material properties (left: modulus of velocities, right: pressure; from [40]).

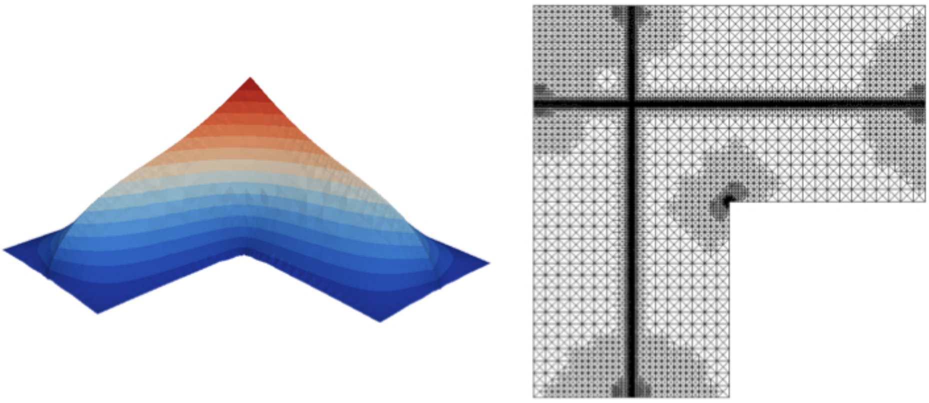


Figure 2. Solution with rough right-hand-side in a corner domain and adaptively refined mesh (from [45]).

The theoretical analysis of mesh-adaptive methods, even in the most standard case of the Poisson problem, is in its infancy. The first important results in this direction concern the convergence of the sequence of solution generated by the algorithm (the standard a priori error analysis does not apply since the global mesh-size does not necessarily go to zero). In order to prove convergence, an unavoidable data approximation term has to be treated in addition to the error estimator [71]. These result do not say anything about the convergence speed, that is the number of unknowns required to achieve a given accuracy. Such complexity estimates are the subject of active research, the first fundamental result in this direction is [50].

Our first contribution [5] to this field has been the introduction of a new adaptive algorithm which makes use of an adaptive marking strategy, which refines according to the data oscillations only if they are by a certain factor larger then the estimator. This algorithm allowed us to prove geometric convergence and quasi-optimal complexity, avoiding additional iteration as used before [75]. We have extended our results to conforming FE without inner node refinement [46] and to mixed FE [45]. In this case, a major additional difficulty arises from the fact that, due to the saddle-point formulation, the orthogonality relation known from continuous FEM does not hold. In addition, we have considered the case of incomplete solution of the discrete systems. To this end, we have developed a simple adaptive stopping criterion based on comparison of the iteration error with the discretization error estimator, see also [44].

Goal-oriented error estimation has been introduced in [48]. It allows to error control and adaptivity directly oriented to the computation of physical quantities, such as the drag and lift coefficient, the Nusselt number, and other physical quantities.

4. Application Domains

4.1. Aerodynamics

Aerodynamics provide a challenging field for numerical simulations in fluid dynamics with a wide range of applications. Robustness of the simulation software with respect to physical parameters as the Reynolds and Mach numbers is necessary condition. In general, realistic simulations need to be done in three dimensions, which makes the efficiency of the numerical approach and implementation a question of feasibility. Therefore, different efforts are made in this project in order to tackle these subjects.

4.2. Viscoelastic flows

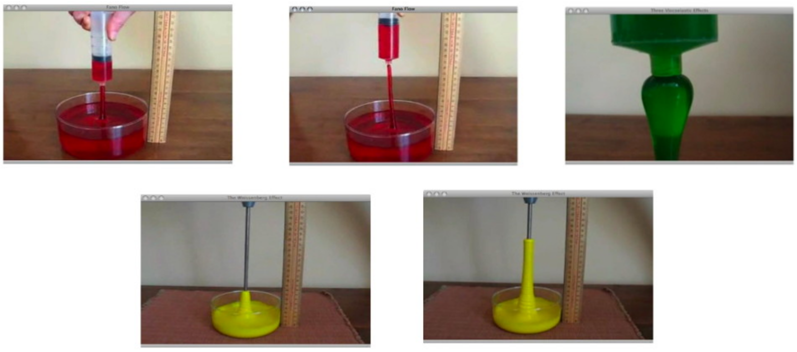


Figure 3. Unexpected behavior of flow of polymer liquids.

Polymeric fluids are, from a rheological point of view, viscoelastic non-Newtonian fluids, see Figure 3. Their specific behavior can be observed in a variety of physical phenomena, which are unseen with Newtonian liquids and which cannot be predicted by the Navier-Stokes equations. The better known examples include the rod climbing Weissenberg effect, die swell and extrusion instabilities (cf. fig. 1). The rheological behavior of polymers is so complex that many different constitutive equations have been proposed in the literature in order to describe these phenomena, see for instance [72]. The choice of an appropriate constitutive law is still a central problem. We consider realistic constitutive equations such as the Giesekus model. In comparison to the classical models used in CFD, such as UCM or Oldroyd B fluids, the Giesekus model is characterized by a quadratic stress term. It is important to understand the theoretical properties of the Giesekus model. As outlined above, energy estimates are crucial for the development of robust numerical schemes, see also the recent work on similar questions in the EPI MICMAC [51], [64].

Our aim is to develop new algorithms for the discretization of polymer models, which should be efficient and robust for $We > 10$. For this purpose, we will develop a mathematical approach based on recent ideas on discretizations preserving the positivity of the conformation tensor. This property is believed to be crucial in order to avoid numerical instabilities associated with large Weissenberg numbers. In order to develop monotone numerical schemes, we use recent discretization techniques such as stabilized finite element and discontinuous Galerkin methods. We have validated our code at hand of academic benchmark problems in comparison with the commercial code PolyFlow®.

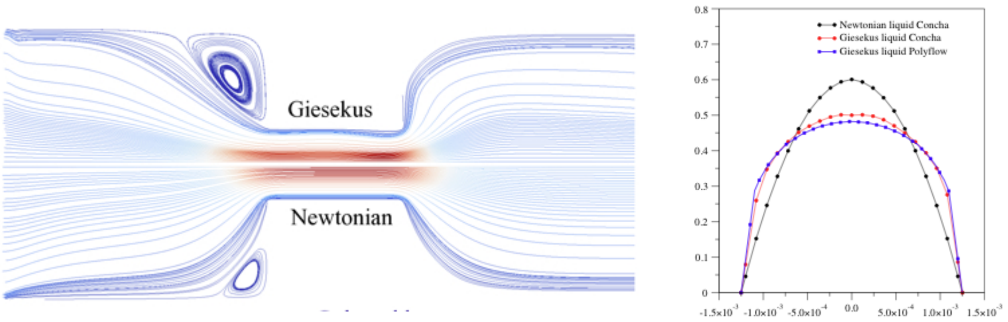


Figure 4. Comparison of Newtonian and Giesekus flow for a contraction flow (left) and comparison with PolyFlow® (right).

The result of a computation of a 4:1-contraction, comparing Newtonian flow with Giesekus model, is shown in Figure 4. In the same figure, a comparison of the computed profile in the channel with the one obtained by the PolyFlow®, both on a relatively coarse mesh, is shown. A precise study shows that the results are in good agreement for moderate Weissenberg numbers We; the computation time is by a factor of two smaller for the preliminary version of our code based on triangular meshes. For $We > 20$, we were not able to get a converged solution with the commercial code, whereas our program yields stationary solutions up to $We \approx 30$.

Further improvements are expected from the use of adaptivity, as well as from the implementation of adequate iterative solvers. The long-term goal is to successively build up robust and efficient software tools in order to tackle design problems, such as the design of mixing devices.

4.3. Heat transfer

Heat transfer problems involve the coupling of the flow field of the fluid with temperature inside the flow and possibly on the boundary of the flow domain. A typical example of a heat transfer problem is the cooling of a combustion engine, see the project Optimal described in Section 7.1.

4.4. Turbulence

Turbulent flows are ubiquitous in industrial applications. Direct numerical simulation (DNS), which aims at complete resolution of the flow field up to the Kolmogorov scale, has historically been limited to very simple geometries. The increase of computational power and the development of specialized numerical methods open the door to a wider range of applications. However, for most applications of practical interest, the use of some kind of turbulence modeling is unavoidable in order to obtain the prediction of averaged values and commercial software is in general based on such approaches combined with wall laws. In many applications, such as the project Optimal, see Section 7.1, the Reynolds number is at an intermediate level, which means that the turbulence is not fully developed, and the heuristics behind most turbulence models are questionable. Especially, in heat transfer problems, the usage of wall laws seems to considerably lower the accuracy of the predicted mean values. In order to improve the computation of such values, we are particularly interested in variational multiscale methods and its relations to stabilized finite element methods.

4.5. Flows in porous media

Flows in fractured pourous media are very important in petroleum engineering. They represent a good framework for the application of the tools developed in the CONCHA library such as the NXFEM method, goal oriented adaptivity, multiscale coupling of different models and multilevel solvers.

5. Software

5.1. C++ library Concha

Participants: Roland Becker, Daniela Capatina, Robert Luce, David Trujillo.

The objectives of our library CONCHA are to offer a flexible and extensible software with respect to:

- Numerical methods and
- Physical models.

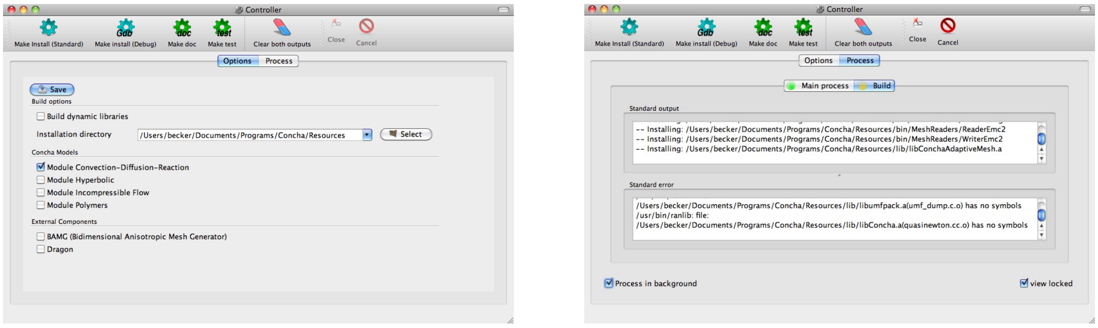
The aim is to have a flexible code which could easily switch between the different discretizations, in order to provide a toolbox for rapid testing of new ideas.

The software architecture is designed in such a way that a group of core developers can contribute in an efficient manner, and that independent development of different physical applications is possible. Further, in order to accelerate the integration of new members and in order to provide a basis for our educational purposes (see Section 9.3), the software proposes different entrance levels. The basic structure consists of a common block, and several special libraries which correspond to the different fields of applications described in Sections 4.1–4.4 Hyperbolic solvers, Low-Mach number flow solvers, DNS, and viscoelastic flows. A more detailed description of each special library may be found below. In order to coordinate the cooperative development of the library, Concha is based on the INRIA-Gforge.

5.2. User interface and python interface

Participants: Roland Becker, David Trujillo.

A graphical user-interface facilitate the use of the C++-library. It has been developed by Guillaume Baty (former technical staff) in collaboration with Pierre Puiseux (associate professor at LMAP). All members of the team have been involved in the testing of the interface. The first objective is to provide an easy way of installation and to facilitate the usage. To this end we use the python language with Qt in order to take advantage of higher level libraries, which allow us to reduce development time.



Build options

☐ Build dynamic libraries

Installation directory /Users/becker/Documents/Programs/Concha/Resources

Concha Models

☑ Module Convection-Diffusion-Reaction
☐ Module Hyperbolic
☐ Module Incompressible Flow
☐ Module Polymers

External Components

☐ BAMG (Bidimensional Anisotropic Mesh Generator)
☐ Dragon

Standard output

```
-- Installing: /Users/becker/Documents/Programs/Concha/Resources/bin/MeshReaders/ReaderEmc2
-- Installing: /Users/becker/Documents/Programs/Concha/Resources/bin/MeshReaders/WriterEmc2
-- Installing: /Users/becker/Documents/Programs/Concha/Resources/lib/libConchaAdaptiveMesh.a
```

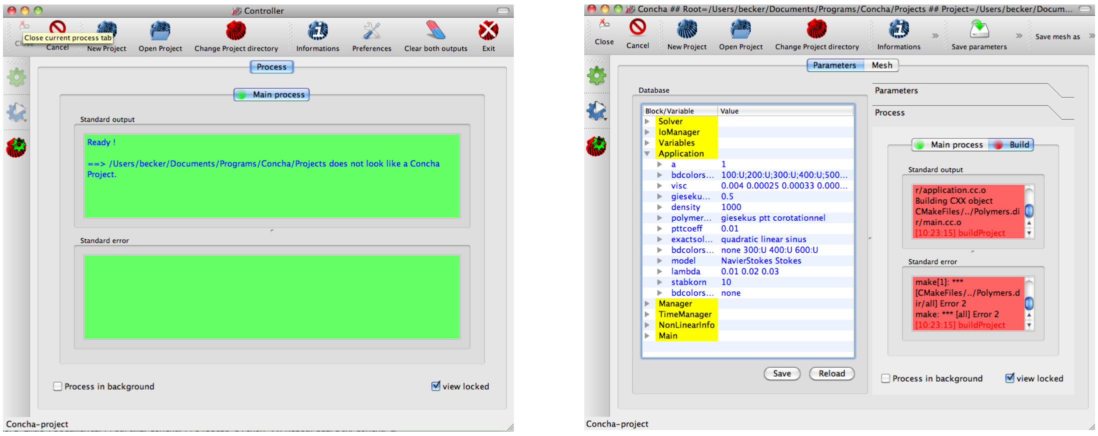
Standard error

```
/Users/becker/Documents/Programs/Concha/Resources/lib/libumfpack.a(umf_dump.c.o) has no symbols
/usr/bin/ranlib: file:
/Users/becker/Documents/Programs/Concha/Resources/lib/libConcha.a(quasinewton.cc.o) has no symbols
```

☑ Process in background ☑ view locked

Figure 5. Graphical user interface: option panel (left) and process panel (right) of the install tool.

We are confronted with heterogenous backgrounds and levels of implication of the developers and users. It seems therefore crucial to be able to respond to the different needs. Our aim is to facilitate the development of the library, and at the same time, to make it possible that our colleagues involved in physical modeling can have access to the functionality of the software with a reasonable investment of time. Two graphical user interfaces have been developed: one for the installation of the library and another one for the building and execution of projects. They are based on common database and scripts written in python. The scripts can also be launched in a shell. In Figure 5 the user interface of the install tool is shown. The option panel allows to choose the components for conditional compilation and the compilation type (debug and release).



Standard output

```
Ready !

==> /Users/becker/Documents/Programs/Concha/Projects does not look like a Concha
Project.
```

Standard error

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Block/Variable	Value
Solver	
IoManager	
Variables	
Application	
a	1
bdcolors...	100:U;200:U;300:U;400:U;500...
visc	0.004 0.00025 0.00033 0.000...
gieseku...	0.5
density	1000
polymer...	giesekus ptt corotationnel
pttcoeff	0.01
exactsol...	quadratic linear sinus
bdcolors...	none 300:U 400:U 600:U
model	NavierStokes Stokes
lambda	0.01 0.02 0.03
stabkorn	10
bdcolors...	none
Manager	
TimeManager	
NonLinearInfo	
Main	

Standard output

```
r/application.cc.o
Building CXX object
CMakeFiles/../Polymers.di
r/main.cc.o
[10:23:15] buildProject
```

Standard error

```
make[1]: ***
[CMakeFiles/../Polymers.d
ir/all] Error 2
make: *** [all] Error 2
[10:23:15] buildProject
```

☐ Process in background ☑ view locked

Figure 6. Graphical user interface: project build panel (left) and parameter panel (right) of the project tool.

In Figure 6 the user interface of the project tool is shown. A project consists of a number of sources files and a parameter file used by the C++-executable. The sources define classes derived from the library, which are used to specify certain data such as boundary conditions and employed finite element spaces. The parameter file contains algorithmic information and physical parameters. It is generated from a database by the python utilities.

The tools offered by this development platform are based on a python interface for the library, called pyConcha. It offers a common interface, based on a pluggin-system, which allows the devloppement of command line tools in parallel. This year the consolidation of the interface part of pyConcha has been an important task. The pyConcha library is now a framework rather than a simple interface to Concha C++ library. It allows now creation of plugins, so that each user-programmer can customize pyConcha to his own goals. Previously, two main programs where working: concha-install.py to install library, and concha-project.py for (semi-)end-users. Both are now plugins of pyConcha, and can be launched by pyConcha at startup. A plugin visualization could now be developped in an independant way, and launched by pyConcha on demand.

The structure of pyConcha framework is clearly splitted in various modules(layers): Command Line Interface module, Graphical User Interface module and Handlers modules, see Figure 7. A great effort has been made for internationalization of pyConcha.

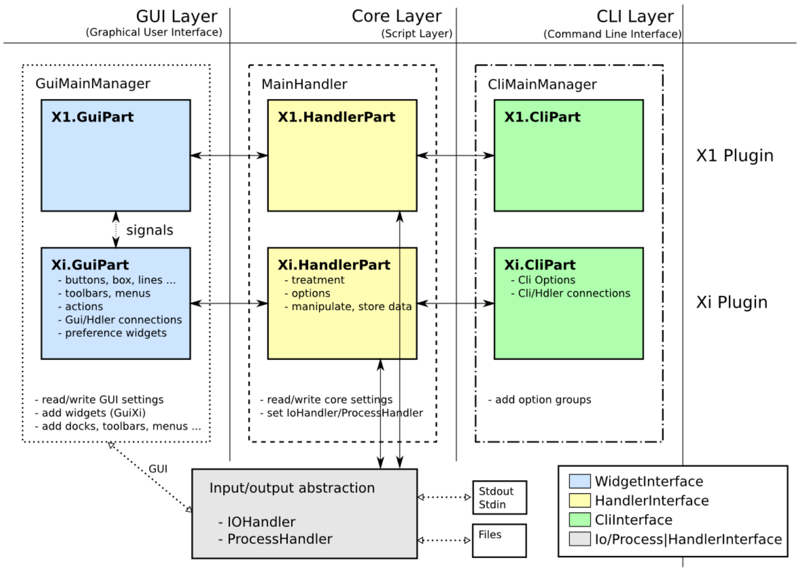


Figure 7. Structure of the pyConcha framework.

5.3. Parallelization

Participants: Roland Becker, Elies Bergounioux, David Trujillo.

The parallelization of the library is done in collaboration with the INRIA-team Runtime, Marie-Christine Counilh and Olivier Aumage and with Séphanie Delage (CRI, UPPA). Elies Bergounioux worked on this topic and was financed as an IJD by the ADT AMPLI. The strategy for the parallelization is based on a hybrid approach using OpenMP and MPI.

5.4. Euler equations

Participants: Roland Becker, Robert Luce, Eric Schall, David Trujillo.

Based on the library CONCHA we have develop a solver for hyperbolic PDE's based on DGFEM. So far different standard solvers for the Euler equations such as Lax-Friedrichs, Steger-Warming, and HLL have been implemented for test problems. A typical example is the scram jet test case shown in Figure 8.

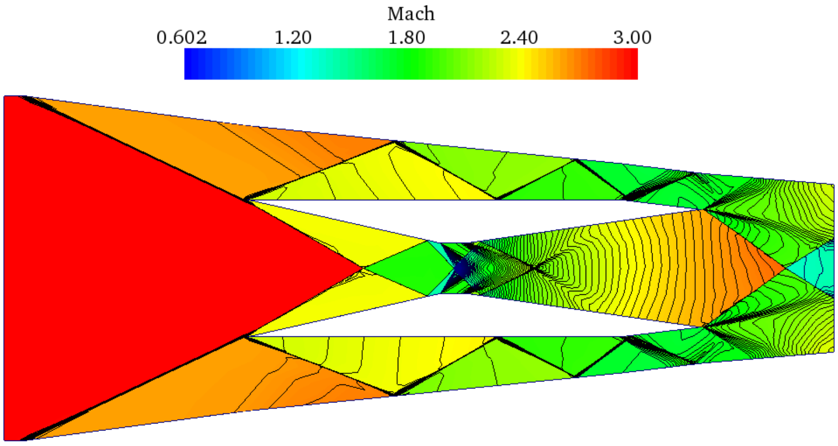


Figure 8. Computed Mach-number distribution for the Scramjet test problem.

5.5. Incompressible flow solvers

Participants: Roland Becker, Daniela Capatina, Robert Luce, David Trujillo.

We have started the validation of the implementation of different finite element methods for incompressible flows at hand of standard benchmark problems as the Stokes flow around a symmetric cylinder [65] and the stationary flow around a slightly non symmetric cylinder [74], see Figure 9.

5.6. DNS

Participants: Roland Becker, David Trujillo, Elies Bergounioux.

For the direct numerical simulation of incompressible turbulent flows, we have started to develop a special solver based on structured meshes with a fast multigrid algorithm incorporating projection-like schemes. The main idea is to use non-conforming finite elements for the velocities with piecewise constant pressures, leading to a special structure of the discrete Schur complement, when an explicit treatment of the convection and diffusion term is used.

5.7. Polymer flow

Participants: Roland Becker, Daniela Capatina, Julie Joie, Didier Graebling.

Based on our library CONCHA we have implemented a three-field formulation with unknowns (u, p, τ) for the two-dimensional Navier-Stokes equations, based on nonconforming finite elements. The extension to the Giesekus-model for polymers has been achieved, see Section 6.7. In the case of Newtonian flows, the extra-tensor can be eliminated in order to reduce storage and computing time. This procedure serves as a preconditioner in the general case. The aim is to provide software tools for the problems in Section Viscoelastic flows.

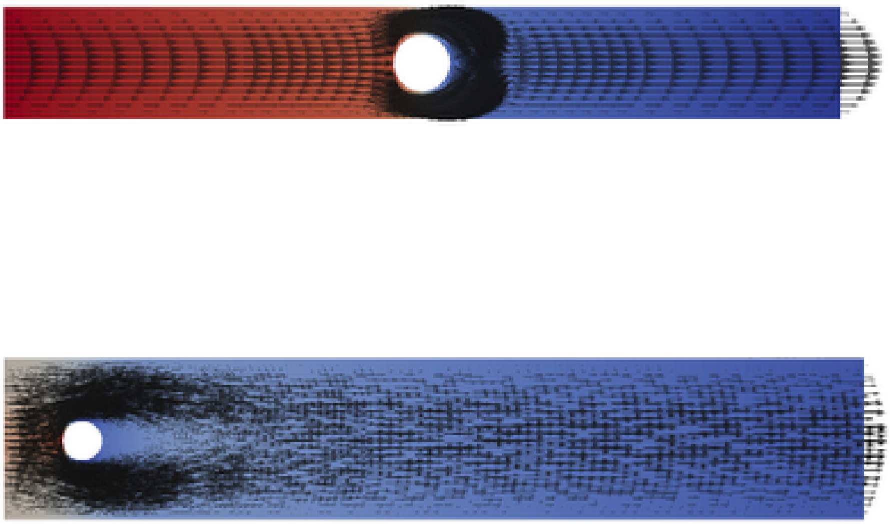


Figure 9. Flow fields for the Stokes (above) and Navier-Stokes (below) benchmark.

5.8. Validation and comparison with other CFD-software

Participants: Daniela Capatina, Didier Graebling, Julie Joie, Eric Schall.

We intend to compare computations based on CONCHA with other codes at hand of the prototypical test problems described above. This allows us to evaluate the potential of our numerical schemes concerning accuracy, computing time and other practical expects such as integration with mesh generators and post-processing. At the same time, this, unfortunately very time-consuming, benchmarking activity allows us to validate our own library. The following commercial and research tools might be considered: *Aéro3d (INRIA-Smash), AVBP (CERFACS), ELSA (ONERA), Fluent (ANSYS), and OpenFOAM (OpenCfd), and Polyflow® (ANSYS)*. So far, we have compared our code for the Giesekus model of polymer flows with the commercial software Polyflow®, see Section 4.2.

6. New Results

6.1. Convergence of adaptive finite element algorithms

Participants: Roland Becker, Shipeng Mao, David Trujillo.

The theoretical analysis of mesh-adaptive methods is a very active field of research. We have generalized our previous results concerning optimality of adaptive methods to nonconforming finite elements [49]. Our results include the error due to iterative solution of the system matrices by means of a simple stopping criterion related to the error estimator. The main difficulty was the treatment of the nonconformity which leads to a perturbation of the orthogonality relation at the heart of the proofs for conforming finite elements. We have been able to extend this result to the Stokes equations, considering different lowest-order nonconforming finite elements on triangular and quadrilateral meshes [16].

In [17] we have shown that the smallness assumption required in all former proofs of optimality of adaptive finite element methods can be overcome, at least in some situations.

Finally, we have shown optimality of a new goal-oriented method in [19].

Our theoretical studies, which are motivated by the aim to develop better adaptive algorithms, have been accompanied by software implementation with the Concha library, see Section 5.1. It hopefully opens the door to further theoretical and experimental studies.

6.2. Finite element methods for interface problems

Participants: Nelly Barrau, Roland Becker, Robert Luce, Erik Burman, Peter Hansbo.

The original formulation of NXFEM [62] is based on the doubling of elements. In some situations, as the case of a moving interface, it is computationally more convenient to have a method with local enrichment, as for the standard XFEM. In [41] we have developed such an approach based on NXFEM. We have developed an hierarchical formulation for a fictitious domain formulation in [13]

One of the technical difficulties is the simultaneous robustness of the method with respect to the size of the intersection of a mesh cell with the interface and with respect to the discontinuous diffusion parameters. This is the subject of the thesis of Nelly Barrau, supervised by Robert Luce and Eric Dubach (LMAP).

6.3. Discontinous finite element methods

Participants: Roland Becker, Daniela Capatina, Julie Joie.

We have developed a new discontinuous Galerkin scheme for the Stokes equations and corresponding three-fields formulation. In this work, which is part of the Phd Thesis of Julie Joie, we introduce a modification of the stabilization term in the standard DG-IP method. This allows for a cheaper implementation and has a more robust behavior with respect to the stabilization parameter; we have shown convergence towards the solution of non-conforming finite element methods for linear, quadratic and cubic polynomial degrees. This scheme has been extended to the three-field formulation of the Stokes problem, which is a further step towards the polymer project of Section 4.2. Since it is well known that the non-conforming finite element approximations do not verify the discrete Korn inequality, an appropriate further stabilization term is introduced, see [42].

6.4. Stabilized finite element methods

Participants: Roland Becker, Erik Burman, Peter Hansbo.

We have developed a new stabilized finite element formulation based on implicit penalization of the singularities of higher-order derivatives of continuous finite element spaces in [12]. It has been applied to the convection-diffusion problem as well as to the incompressible Euler equations.

6.5. A posteriori error estimators based on $H(\mathrm{div})$-reconstructed fluxes

Participants: Roland Becker, Daniela Capatina, Robert Luce.

Mesh adaptivity is nowadays an essential tool in numerical simulations; in order to achieve it, reliable and efficient, easily computable *a posteriori* error estimators are needed. Such estimators obtained by reconstructing locally conservative fluxes in the Raviart-Thomas finite element space have been largely employed in the past years.

We have so far considered the convection-diffusion equation and proposed a unified framework for several finite element approximations (conforming, nonconforming and discontinuous Galerkin). The main advantage of our approach is to use, contrarily to the existing references, only the primal mesh for the flux reconstruction, which presents certain facilities from a computational point of view.

For this purpose, the construction of the $H(\mathrm{div})$-vector involved in the error estimator is inspired by the hypercircle method cf. [53] and is achieved on patches, which may overlap. A patch depends on the type of the employed finite elements and is defined as the support of a basis function.

Our first results were presented in [26]. We are working on the extension to higher-order approximations, to quadrilateral meshes and to other model problems.

6.6. A posteriori error analysis of sensitivities

Participants: Roland Becker, Daniela Capatina, Robert Luce, David Trujillo.

Most practical applications involve parameters $q=(q_i)_{1\leq i\leq N}$ of different origins: physical (viscosity, heat conduction), modeling (computational domain, boundary conditions) and numerical (mesh, stabilization parameters, stopping criteria, values of a turbulence model). Numerical simulations can provide information related to the (first order) sensitivity of a quantity of physical interest $I(q)$ with respect to different parameters: $\partial I/\partial q_i$. Their computation can help to validate the physical model, to explain unexpected behaviour and also to guide efforts to improve both the physical and the computational models.

A posteriori error estimates for the functional itself, for fixed values of the parameters q, are well-known, cf. for example [47] where a goal-oriented error control is achieved by introducing an adjoint problem. Our goal is to provide a general framework for the *a posteriori* error estimation of sensitivities $\partial I/\partial q_i - \partial I_h/\partial q_i$, which has not been given yet in the literature.

So far, we have applied the proposed method to the computation of the Nusselt number measuring the efficiency of a cooling process, described in the project Optimal. A cold liquid is injected in a annular domain through several inlets in order to cool a heated interior stator.

First numerical results, including adaptation with respect to the functional and to the sensitivity, have been carried out with the library Concha. They have been presented in [33], [30]. In Figure 10 one may see the computed temperature and velocity field, while the *a posteriori* error estimator for the sensitivity of the Nusselt number with respect to the inflow speed at the right-hand side inlet, as well as the adapted mesh, are given in Figure 11.

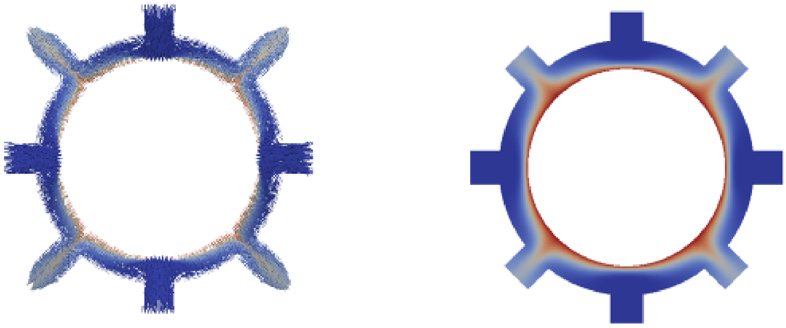


Figure 10. Computed velocity and temperature fields.

In the future, several important aspects related to the adaptive method are still to be investigated such as design of an appropriate adaptive algorithm, proof of its convergence and optimality etc.

6.7. Viscoelastic fluids modeling and numerical simulation

Participants: Roland Becker, Daniela Capatina, Didier Graebling, Julie Joie.

We have continued our activities with respect to numerical simulations of polymer flows.

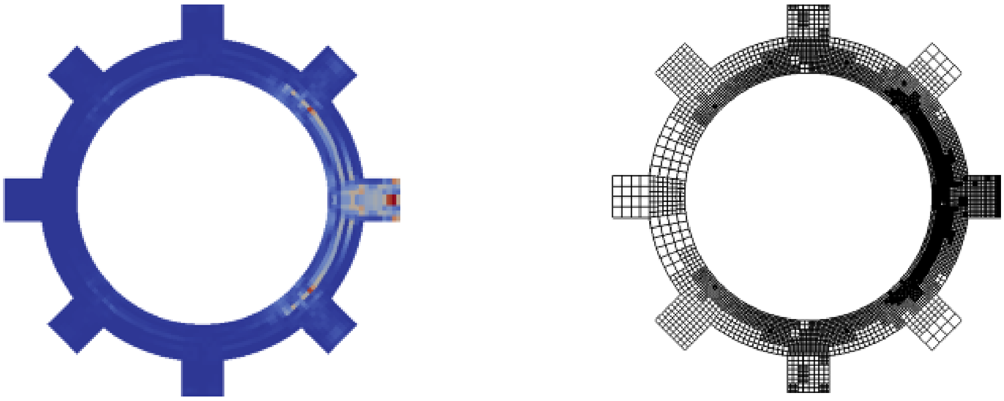


Figure 11. Error estimator for the sensitivity and adapted mesh.

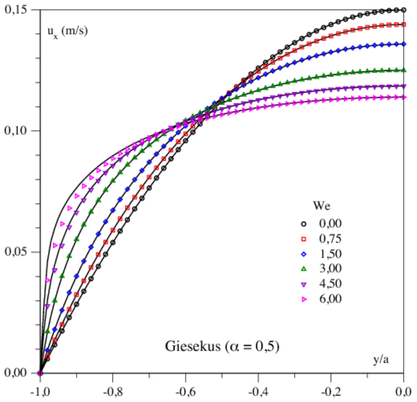


Figure 12. Comparison with semi-analytical solution for different Weissenberg numbers.

We have further validated [32] the code on both triangular and quadrilateral 2D meshes, by using a mixed non-conforming/DG method. In the case of Giesekus model, comparisons of velocity profile with semi-analytical solutions for Poiseuille flow [70] and with experimental data [73] for the 4:1 contraction are respectively shown in Figures 12 and 13).

The quadrilateral scheme needs an additional stabilization term, in order to ensure uniform consistency and stability for the underlying linear problem. It has been tested in particular on the benchmark case of flow around a 2D cylinder, for which our code converged for high values of the Weissenberg number (We > 70). We have computed the drag and compared it, see Figure 14, with numerical data found in the literature [58], [65], [76], [57] in the case of the Oldroyd-B model.

The system associated to this quasi-linear model has been solved on rather fine meshes (of about 10^6 elements) thanks to a multigrid solver based on a Vanka type preconditionner. We have worked on the extension of the multigrid method to more complex and more realistic polymer models, involving nonlinear terms in the constitutive law such that Phan Thien-Tanner and Giesekus models.

The unsteady case has also been treated for different geometries.

The parallelization of the library is ongoing work as described in the section 5.3; first tests have been carried on in the case of viscoelastic liquids.

In order to better describe real polymer flows, the thermal aspects have to be taken into account. As a first step, the coupling of the flow with the energy equation in the Newtonian case was considered in [38], by using a conservative variable. Our next objective is to simulate anisothermal viscoelastic flows, including typical effects such that thermo-dependent viscosity and viscous heating.

With these tools, the long-term goal is to successively build up robust and efficient software in order to tackle design problems.

Moreover, we intend to consider other models of non-Newtonian fluids employed in other application domains such as biomedecine.

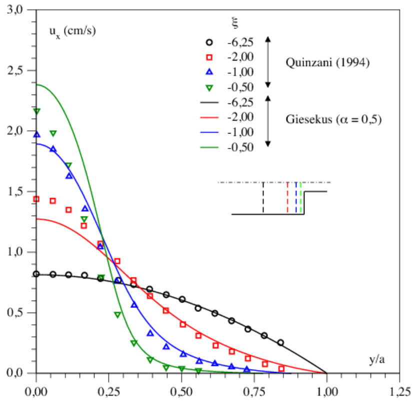


Figure 13. Comparison with experimental data for the 4:1 contraction.

6.8. Positivity preserving schemes

Participants: Roland Becker, Daniela Capatina.

λ	CONCHA	Dou *et al.*	Hulsen *et al.*	Étienne *et al.*	Damanik *et al.*
0	132,357	131,809	132,358	132,33	-
0,3	123,190	123,514	123,193	123,41	123,194
0,6	117,780	120,485	117,792	-	117,779

Figure 14. Comparison of drag coefficients with the literature.

The stability and robustness with respect to physical parameters of numerical schemes for polymer flows is a challenging question. Indeed, most algorithms encounter serious convergence problems for large Weissenberg numbers. In the recent years, this issue has been asscociated to the discrete positive definiteness of the so-called conformation tensor. It seems therefore essential for the numerical simulations to employ positivity preserving schemes.

In order to develop such schemes, we have adopted the approach proposed by Lee and Xu [68] in the case of the quasi-linear Oldroyd-B model, based on the similarities between its constitutive equation and differential Riccati equations. We have applied it to a more general matrix equation; a typical example is the nonlinear Giesekus constitutive law. In agreement with our code (see Section 6.7), we have discretized it by a discontinuous Galerkin method combined with an upwinding of the transport terms, whereas the approach of Lee and Xu relies essentially on the characteristics method.

We have shown that a modification of Newton's method yields a monotone and positive scheme, under certain hypothesis, and we have applied this study to both Oldroyd-B and Giesekus polymer models. This allowed us to better understand and explain the better behaviour of the latter for large Weissenberg numbers. These results have been presented in [24],[31].

We are working on several challenging questions such as the extension to other discretization methods, the improvement of the iterative method or the derivation of energy estimates for the coupled system.

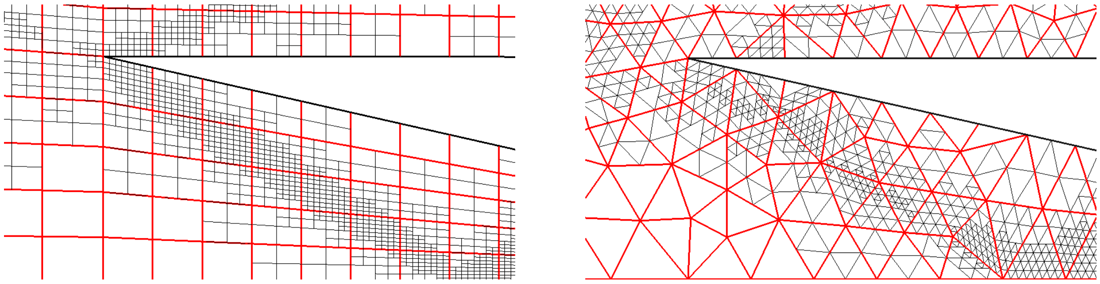
6.9. Discretization of Euler's equations

Participants: Roland Becker, Kossivi Gopki, Eric Schall, David Trujillo.

Over the past years, significant advances have been made in developing discontinuous Galerkin finite element methods (DGFEM) for applications in fluid flow and heat transfer. Certain features of the method have made it attractive as an alternative to other popular methods such as finite volume and more convenient finite element methods in thermal fluid engineering analyses. The DGFEM has been used successfully to solve hyperbolic systems of conservation laws. It makes use of the same local function space as the continuous method, but with relaxed continuity at inter-element boundaries. Since it uses discontinuous piecewise polynomial bases, the discretization is locally conservative and in the considered lowest-order case, the method preserves the maximum principle for scalar equations.

One of the challenges in Computational Fluid Dynamic (CFD) is to obtain as accurate as possible the solution of the problem under consideration at very low cost in terms of computational time. So our principal work is to find some relevant and robust strategies and technics of meshes adaptation in order to concentrate just the calculation where there are physical phenomena to capture. From Industrial point of view, the aim is to get the stationary solution as quick as possible with as much accuracy as possible. The main limitation of these results in CFD concern the underlying models: for example, nearly nothing seems to be known for (even linear) first-order systems or for realistic nonlinear equations. We therefore have developed different modern techniques, especially adaptive methods, to tackle this kind of problems in compressible CFD. The strategy is to iteratively improve the quality of the approximate solutions based on computed information (a posteriori error analysis). In this way, a sequence of locally refined meshes is constructed, which allows for better efficiency as compared to more classical approaches in the presence of different kind of singularities. The main goal is to improve the aerodynamical design process for complex configurations by significantly reducing the time from geometry to solution at engineering-required accuracy using high-order adaptive methods.

One of our strategies of refinement is based on the creation of hanging nodes commonly called non-conforming refinement. The figures 15 show superposition of two kinds of meshes. One is a non-conforming refined mesh (black color) and the other one is the initial grid (red color) on which the refinement has been performed. It shows the technic of cutting the cells where singularities occur in the scramjet inlet.



(a) (b)

Figure 15. Superposition of non-conforming adapted black color) grid and initial grid (red color) – (a) quadrangles and (b) triangles.

The mesh adaptation is designed using some criteria as a posteriori error estimates. We have designed criteria based on the calculation of the jump of physical quantities like density, pressure, entropy, temperature and mach number at the inter-element. This criteria seems to be a very good indicator for the mesh adaptation. Figure 16 is the comparison of isoline of the density in scramjet internal flow at mach 3 of the initial mesh, the third and the sixth mesh after refinement.The indicator used is the density jump. It shows the impact and the accuracy of the solution obtained after the sixth iteration of the refinement.

The figure 17 shows the streamlines of the density in the scramjet inlet after the seventh iteration. This shows how the adaptation depicts almost clearly and accurately the shock waves and the expansion waves and their interactions in the domain.

Figure 18 represent the density isolines of a flow past cylinder test case using the non-conforming mesh adaptation with quadrangular an triangular girds.

We have also settled another indication which is hierarchical. It measures the difference of g_h with the physical quantity $g_{h/2}$ obtained by computation on a globally refined mesh $h/2$. This allows us the make comparison with the previous indicator. The case test considered for this comparison is an external flows past a cylinder airfoil at fixed free stream conditions : $M_\infty = 3$. The result is quite surprising the way one type of indicator can capture phenomenon that are not capture by the another one. In fact the hierarchical indicator seems to capture recirculation downstream to the obstacle which was not capture by the jump indicator (see figure 19)

We compare the computational time between a non-conforming mesh refinement and a globally mesh refined with nearly the same amount of cells. The meshes contain quadrangles or triangles. We can observe trough the following tables that the adapted meshes wether triangular or quadrangular meshes allow to save 20 to 90 times the computational time than the normal globally refined mesh. (see tables 1 and 2)

In table 1, the gain in time is 35 times in quadrangular grid case and 90 times triangular ones and in table 2, the gain in time: 18 times in quadrangular grid case and 58 times triangular ones. So one can say that the adaptive mesh with the strategies and technics we have settled are efficient and robust in capturing physical phenomenon at a very reasonable low cost.

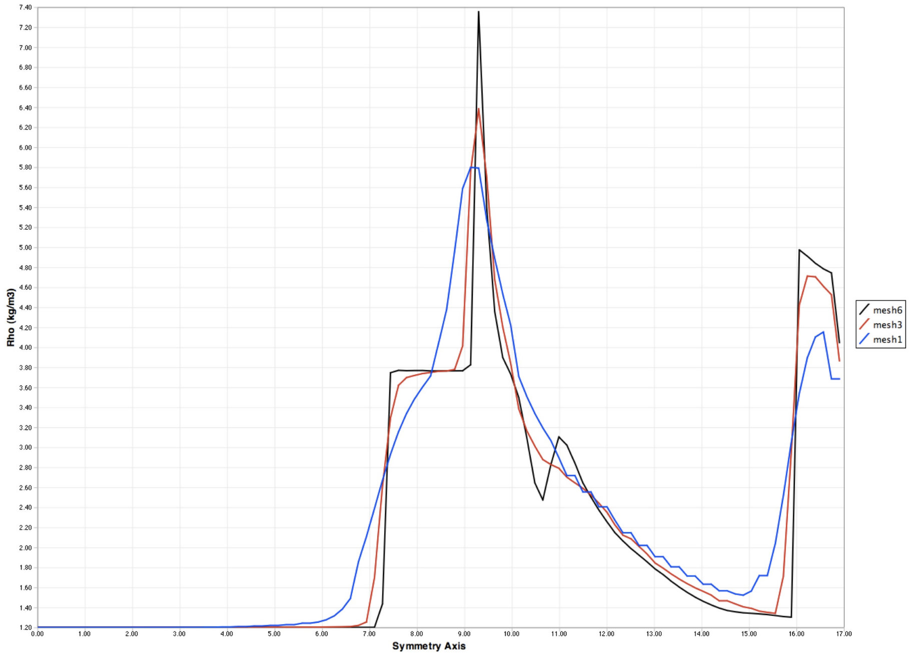


Figure 16. Cutlines along the symmetry axis of various meshes for the scramjet test case

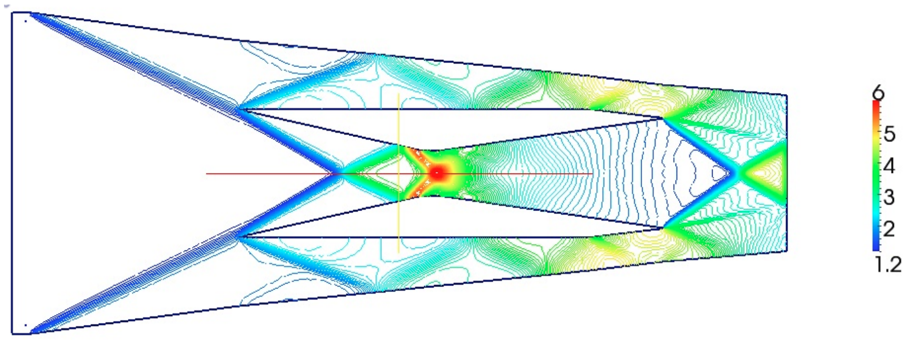
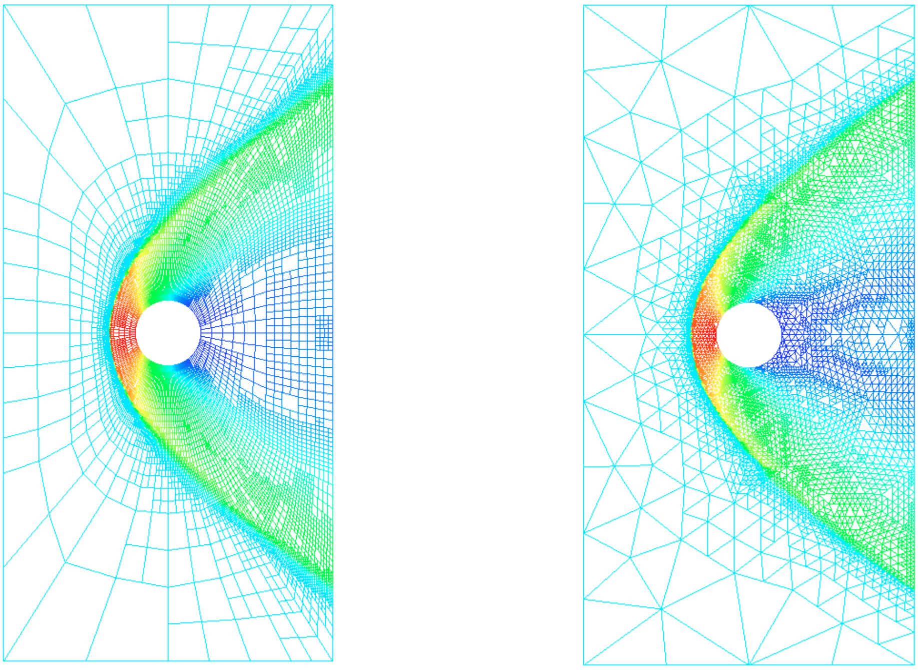
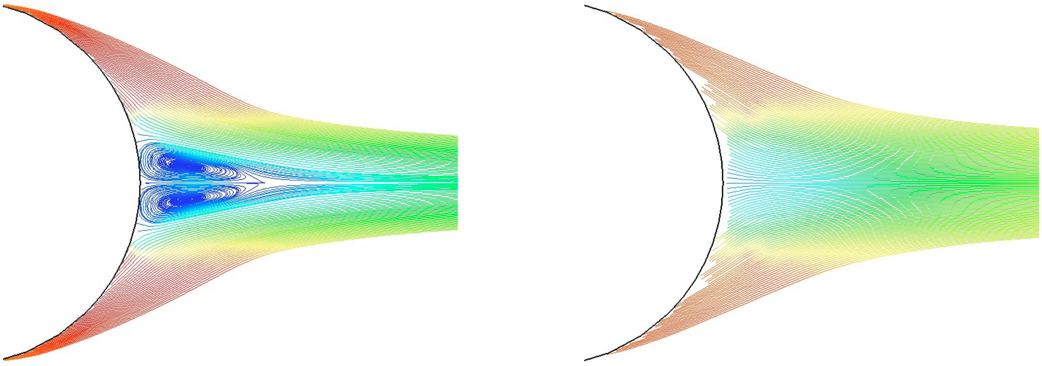


Figure 17. Density streamlines on grid obtained after the seveneth iteration of adaptive refinement procedure with density jump as indicator



(a) (b)

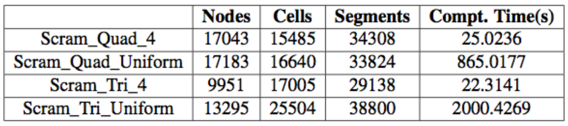
Figure 18. Locally adapted mesh on quadrilaterals (a) and triangles (b)



(a) (b)

Figure 19. Streamlines coloured by the density on meshes generated with hierarchical indicator (a) and with jump indicator (b)

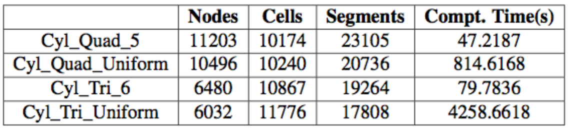
Scramjet test case at mach=3



	Nodes	Cells	Segments	Compt. Time(s)
Scram_Quad_4	17043	15485	34308	25.0236
Scram_Quad_Uniform	17183	16640	33824	865.0177
Scram_Tri_4	9951	17005	29138	22.3141
Scram_Tri_Uniform	13295	25504	38800	2000.4269

Table 1

Flow past cylinder test case at mach=3



	Nodes	Cells	Segments	Compt. Time(s)
Cyl_Quad_5	11203	10174	23105	47.2187
Cyl_Quad_Uniform	10496	10240	20736	814.6168
Cyl_Tri_6	6480	10867	19264	79.7836
Cyl_Tri_Uniform	6032	11776	17808	4258.6618

Table 2

Figure 20. Comparison of computational times

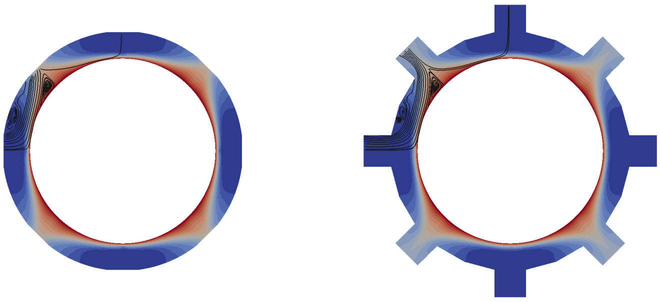
In concluding, the procedure of refinement permit to save computational time and have good accuracy of the approximated solution computed. Our focus is to continue the improve our methods and strategies in order to meet the requirement of accuracy, robustness and efficiency. Many other works are in hand such as slope limiters for high-order Discontinous Galerkin, low mach number computation with some remarkable approaches.

7. Contracts and Grants with Industry

7.1. Optimal (Aerospace Valley)

Participants: Roland Becker, Kossivi Gokpy, Robert Luce, Eric Schall, David Trujillo.

Optimal is a research project related to the cooling of the stator of a turbomachinery. Both physical experiments and numerical simulations are employed. This project has three industrial (Liebherr, Epsilon, and SIBI) and three academic partners (Universities of Pau, Poitiers, and Toulouse). It has been evaluated by the cluster Aerospace Valley. The PhD-thesis of Kossivi Gokpy is financed by this project.



v_{in}	geo1	geo2
10	135,97	130,53
20	216,73	213,59
50	352,61	341,47

Figure 21. Temperature field and recirculation for two geometries and computed Nusselt numbers for different inflow velocities.

Our contributions concern the numerical simulation of the viscous flow in different geometrical configurations. Comparison with experimental data will be investigated with respect to the Nusselt number. The computed temperature and streamlines for typical geometries are shown in Figure 21. In addition, the computed Nusselt numbers for the two configurations and varying inflow velocities are given.

Among the different questions concerning modeling such as the boundary conditions at the in- and outlets and the sensitivity to the geometry, a particular point of interest is the study of compressibility effects.

The experimental part of the product is conducted in collaboration with Mathieu Mory, professor at UPPA, and the post-doctoral position of Stéphane Soubacq, who started to work in 10/2009, is financed by the project. The modeling and numerical simulation is done in collaboration with Abdellah Saboni, professor at UPPA.

7.2. Fractured reservoir (Total)

Participants: Robert Luce, David Trujillo.

We have developped specific meshing tools in order to take into account the interaction between faults and a petroleum reservoir for the company Total. This work was done in collaboration with Eric Dubach and Pierre Puiseux from LMA.

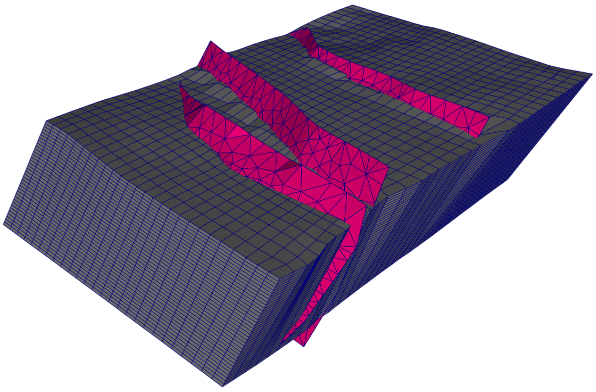


Figure 22. Fractured reservoir

8. Partnerships and Cooperations

8.1. European Initiatives

We have long-standing the following international collaborations:

- Chalmers University of Technology, Sweden (Prof. Peter Hansbo)
  This collaboration concerns the following subjects: stabilized finite element methods, NXFEM, adaptivity.
- University of Sussex, UK (Prof. Erik Burman)
  This collaboration concerns the following subjects: stabilized finite element methods, NXFEM, adaptivity.
- University of Kiel, Germany (Prof. Malte Braack)
  This collaboration concerns the following subjects: stabilized finite element methods, fluid-acoustic interaction.

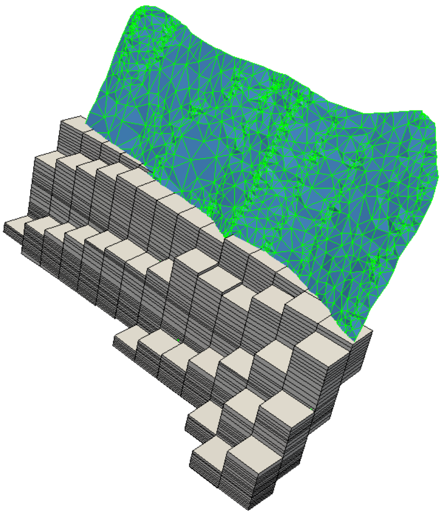


Figure 23. Intersection between fault and reservoir

8.2. International Initiatives

We have a collaboration with the Institute of Computational Mathematics of the Chinese Academy of Sciences CAS (Prof. Lin Qun, Prof Li Yuan, Dr. Shipeng Mao, Dr. Mingxia Li, Dr. Chunguang Xiong, Qin Li) on finite element methods and numerical fluid mechanics. The team leader has been invited by Prof. Yuan for a one-month during summer 2010 at CAS in Bejing. Dr. Chunguang Xiong is working as a post-doc since june 2011 in the team. Since october 2012 Qin Li is staying as a common doctoral student (supervised by Prof. Lin Qun and the team leader) in the frame of a joint CAS-INRIA program.

9. Dissemination

9.1. Animation of the scientific community

We have organized the sixth VMS (Variational MultiScale Methods) workshop https://sites.google.com/site/conchapau/vms, which has allowed the scientific exchange of about 40 experts in the field of numerical methods for multiscale problems mostly related to CFD.

9.2. Phd and Habilitation theses

Daniela Capatina has defended her Habilitation in november 2011 [11].

9.3. Teaching

The LMA has proposed a new Master program starting in 2007, which is called MMS (Mathématiques, Modélisation et Simulation) and has a focus on analysis, modeling, and numerical computations in PDEs; Robert Luce and R. Becker are co-responsables of this Master program. The core of this education is formed by lectures in four fields : PDE-theory, mechanics, numerical analysis, and simulation tools.

This master program includes lectures on physical applications, one of the three proposed application fields is CFD; lectures are provided by the members of the project; especially the following lectures have been given:

- Simulation numérique 1, Robert Luce and Eric Dubach,
- Analyse numérique des EDP, R. Becker and D. Capatina,
- Simulation numérique 2, Robert Luce and Eric Dubach,
- Méthodes numériques pour les EDP, R. Becker,
- Mécanique des fluides, R. Becker,
- Simulation numérique 3, P. Puiseux
- Mécanique des Fluides et Turbulence, Eric Schall, D. Graebling

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