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Alessandro Franci

Unified Lagrangian Formulation for Fluid and Solid Mechanics, Fluid-Structure Interaction and Coupled Thermal Problems Using the PFEM

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Unified Lagrangian Formulation for Fluid and Solid Mechanics, Fluid-Structure Interaction and Coupled Thermal Problems Using the PFEM

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Dai diamanti non nasce niente,
dal letame nascono i fior.

Nothing grows out of precious diamonds,
Out of dung the flowers do grow.

Fabrizio De André

To my mother and father

Supervisor's Foreword

It is a big pleasure to write a foreword for Dr. Alessandro Franci's thesis. The publication in the Springer Thesis program represents a further recognition of the quality of thesis, which has received the PIONER prize and the SEMNI award conferred in 2015 by the Catalan association CERCA and the Spanish Society of Numerical Methods in Engineering (www.semni.com), respectively.

The objective of Dr. Franci's thesis was the development and experimental validation of a new particle-based computational method termed particle finite element method (PFEM) for the solution of practical fluid–structure interaction (FSI) problems.

The PFEM formulation proposed in the thesis represents an extremely powerful numerical tool that can be used for a wide range of engineering problems. In particular, the PFEM is very adequate to reproduce bulk forming processes, such as the forging and extrusion of metal pieces, among others. The numerical modeling of these industrial problems is useful for the optimization of the manufacturing process and the reduction of the defects in the final products.

The thesis includes many practical engineering applications (not only of forming processes), such as the collapse of a water column against a deformable membrane and the melting of ice block in a tank filled with hot water, among others.

The last chapter of the thesis has been devoted to an industrial application solved with the proposed computational method. The numerical results showed in this chapter were obtained by Dr. Franci as part of an international project sponsored by a Japanese company carried out in the three-month period during June–September of 2014.

The object of the project was to simulate two hypothetical scenarios during a nuclear core melt situation, one of the most severe accident in a nuclear power plant. This kind of analysis belongs to those problems that are difficult to solve with traditional strategies or with laboratory tests and also their numerical simulation is extremely complex. Despite that, with the methodology developed by Dr. Franci in his thesis fine and accurate simulations of this phase-change problem were obtained.

The success of this project was another proof of the applicability of the numerical strategy proposed in the thesis of Dr. Franci for solving industrial problems.

The numerical formulation has been well received also in the scientific community. I highlight that six publications in international peer-reviewed journals have already resulted from Dr. Franci's thesis.

The thesis outcomes leave many open lines of research and future developments. In particular, there is the high interest to couple the PFEM technique developed in the thesis with the discrete element method (DEM) and to extend the proposed formulation to large scale engineering problems.

Knowing the motivation, dedication and capabilities of Dr. Franci, I look forward to seeing him leading these new projects in the next coming years.

Barcelona, Spain
May 2016

Prof. Eugenio Oñate

Parts of this thesis have been published in the following articles:

E. Oñate and A. Franci and J.M. Carbonell, *Lagrangian formulation for finite element analysis of quasi-incompressible fluids with reduced mass losses*, International Journal for Numerical Methods in Fluids, 74 (10), 699–731, 2014;

E. Oñate and A. Franci and J.M. Carbonell, *A particle finite element method (PFEM) for coupled thermal analysis of quasi and fully incompressible flows and fluid-structure interaction problems*, Numerical Simulations of Coupled Problems in Engineering. S.R. Idelsohn (Ed.), 33, 129–164, 2014;

E. Oñate and A. Franci and J.M. Carbonell, *A particle finite element method for analysis of industrial forming processes*, Computational Mechanics, 54, 85–107, 2014;

A. Franci and E. Oñate and J.M. Carbonell, *On the effect of the bulk tangent matrix in partitioned solution schemes for nearly incompressible fluids*, International Journal for Numerical Methods in Engineering, 102, 257–277, 2015;

A. Franci and E. Oñate and J.M. Carbonell, *Unified formulation for solid and fluid mechanics and FSI problems*, Computer Methods in Applied Mechanics and Engineering, 298, 520–547, 2016;

A. Franci and E. Oñate and J.M. Carbonell, *Velocity-based formulations for standard and quasi-incompressible hypoelastic-plastic solids*, International Journal for Numerical Methods in Engineering, 10.1002/nme.5205, 2016.

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I would like to thank all the people that in some way have helped me to complete this doctoral thesis.

I would like to express my gratitude to Prof. Eugenio Oñate for many reasons. Thanks to him, four years ago I could come to Barcelona and start my Ph.D. at CIMNE. He gave me the balanced doses of freedom and pressure and he encouraged me to test innovative technologies. I would like thank Prof. Oñate also for giving me the opportunity and the material support to spend a three-month period at the College of Engineering of Swansea.

Special thanks go to Dr. Josep Maria Carbonell. Without his support I could not realize this work. He devoted me innumerable hours of his time and he gave me technical and non-technical suggestions that helped me to make the right choices during my Ph.D.

I would like to thank Prof. Javier Bonet for giving me the possibility to work with his group during my stay at Swansea. Special thanks go to Prof. Antonio Gil y Dr. Aurelio Arranz for their very kind treatment, for improving my knowledge of the Immersed boundary potential method and for the useful discussions about FSI strategies. I really hope that this is just the first step for a future fruitful collaboration.

I also acknowledge the Agencia de Gestió d'Ajuts Universitaris i de Recerca (AGAUR) for the financial support.

I would like to thank also Riccardo, Antonia, Jordi, Pablo, Lorenzo and Stefano for their contributions to this thesis.

This thesis is dedicated to my parents who still represent to me a fundamental and unique support.

Finally, I would like to thank Lucía simply for staying by my side during these years. Her smile has been the gasoline I used for dealing with all this work.

Contents

Abbreviations

AL	Augmented Lagrangian
ASGS	Algebraic SubGrid Scale
FCM	Fuel Containing Material
FEM	Finite Element Method
FIC	Finite Increment Calculus
FSI	Fluid–Structure Interaction
GLS	Galerkin Least Squares
IBM	Immersed Boundary Method
IFEM	Immersed Finite Element Method
ISPM	Immersed Structural Potential Method
LBB	Ladyzenskaya–Babuzka–Brezzi
LFCM	Lava-like Fuel Containing Material
NPP	Nuclear Power Plant
OSS	Orthogonal SubScale
PFEM	Particle Finite Element Method
SPH	Smooth Particle Hydrodynamics
SUPG	Streamline Upwind Petrov Galerkin
TL	Total Lagrangian
UL	Updated Lagrangian
V	Velocity
VMS	Variational Multi-Scale
VP	Velocity-Pressure
VPS	Velocity-Pressure-Stabilized

Chapter 1
Introduction

The objective of this work is to develop a unified formulation for the solution of fluid and solid mechanics, Fluid-Structure Interaction (FSI) and thermal coupled problems and to prove its efficacy by solving both academic and industrial problems.

Due to their complexity, generally FSI problems cannot be solved with the traditional engineering methodology and numerical methods represent the best alternative to the expansive laboratory tests and even, in same cases, the unique possibility to face them.

FSI problems involve a large number of physical phenomena characterizing many fields of engineering, technology and also biology. An example of problem of interest in civil engineering is the safety study of civil constructions to water-induced hazards. These constructions include: buildings, bridges, harbors, dams, dykes, breakwaters, and similar infrastructures in water hazard scenarios such as flooding, large sea waves, tsunamis and water spills due to the collapse of dams, dykes and reservoirs, among others. Also industrial engineering is full of example of complex FSI problems. For example, this is the case of many manufacturing processes in which complicated thermo-coupled interactions occur between different materials at different phases. This list could be further extended considering other branches of engineering, from aeronautics to mechanical and naval engineering.

The numerical method developed in this work is designed for solving a big part of the mentioned situations.

From the theoretical point of view, the aim is to analyze the continuum in a unified manner trying to reduce at minimum the differences between the analysis of fluids and solids. For this purpose the numerical model has been designed in order to meet the specific requirements of solid and fluid mechanics and their approximation with the FEM, but without limiting excessively the capability of the model. In fact the computational method should be capable to deal with critical problems such as those involving elastic-plastic solids, quasi-incompressible materials, free-surface fluids and phase change.

A. Franci, *Unified Lagrangian Formulation for Fluid and Solid Mechanics, Fluid-Structure Interaction and Coupled Thermal Problems Using the PFEM*, Springer Theses, DOI 10.1007/978-3-319-45662-1_1

Following these considerations, the computational model has been designed according to a stabilized Velocity–Pressure formulation. The numerical method has been applied for solving hypoelasto-plastic, compressible and quasi-incompressible solids and quasi-incompressible Newtonian fluids. The algorithm for the FSI problems has been inspired by the analogous unified strategy presented in [1]. For the fluid phase, the Particle Finite Element Method (PFEM) [2] has been used, while for the solid the classical Finite Element Method (FEM) [3] is adopted.

The Unified formulation is based on a stabilized Velocity–Pressure Lagrangian procedure. Each time step increment is solved using a two-step Gauss–Seidel scheme: first the linear momentum equations are solved for the velocity increments, next the continuity equation is solved for the pressure in the updated configuration.

Linear shape functions are used for both the velocity and the pressure fields. In order to deal with the incompressibility of the materials, the formulation has been stabilized using an updated version of the Finite Calculus (FIC) method [4]. The procedure has been derived for quasi-incompressible Newtonian fluids. In this work, the FIC stabilization procedure has been extended also to the analysis of quasi-incompressible hypoelastic solids [5].

Specific attention has been given to the study of free surface flow problems. In particular, the mass preservation feature of the PFEM-FIC stabilized procedure has been deeply studied with the help of several numerical examples. Furthermore, the conditioning of the problem has been analyzed in detail describing the effect of the bulk modulus on the numerical scheme. A strategy based on the use of a pseudo bulk modulus for improving the conditioning of the linear system is also presented.

The Unified formulation has been validated by comparing its numerical results to experimental tests and other numerical solutions for fluid and solid mechanics, and FSI problems. The convergence of the scheme has been also analyzed for most of the problems presented.

The Unified formulation has been coupled with the heat transfer problem using a staggered scheme. A simple algorithm for simulating phase change problems is also described. The numerical solution of several FSI problems involving the temperature is given.

The thermal coupled scheme has been used successfully for the solution of an industrial problem. The objective of study was to analyze the damage of a nuclear power plant pressure vessel induced by a high viscous fluid at high temperature, the corium. The numerical study of this industrial problem has been included in the thesis.

The whole formulation has been implemented in a C++ code.

1.1 State of the Art

In this section, an overview of the numerical methods used for simulating a free surface fluid flow interacting with deformable solids is given. For the sake of clarity, the section is divided in three parts representing the main topics raised by this work. First the Eulerian and Lagrangian approaches for free surface fluid dynamics problems are presented. Then an overview of the stabilization for incompressible, or quasi-incompressible, material is given. Finally, the principal algorithms for solving FSI problems are described.

1.1.1 Eulerian and Lagrangian Approaches for Free Surface Flow Analysis

Consider the description of the motion of a general continuum represented in Fig. 1.1. The domain Ω_0 represents the body at the initial state at time $t = t_0$ while the domain Ω represents the same body at time $t = t_n$ after deformation. The domain Ω_0 is called *initial configuration*, whereas Ω is the *current,* or *deformed*, *configuration*. In order to describe the kinematics and the deformation of the body, the *reference configuration* has to be defined because the motion is defined with respect to this configuration.

In solid mechanics, the stresses generally depend on the history of deformation and the undeformed configuration must be specified in order to define the strains. Due to the history dependence, Lagrangian descriptions are prevalent in solid mechanics. In Newtonian fluids however, the stresses do not depend on the history and it is often unnecessary to describe the motion with respect to a reference configuration. For this reason an Eulerian description represents the most reasonable choice. Furthermore, in problems where the fluid contours are fixed, Eulerian meshes are generally preferred to the Lagrangian ones. This is because Eulerian grids are fixed and they do not deform according to the fluid motion, as shown in Fig. 1.2.

Conversely, in the Lagrangian description, the mesh nodes coincide with the fluid particles and the discretization moves and deforms as the fluid flow (Fig. 1.3).

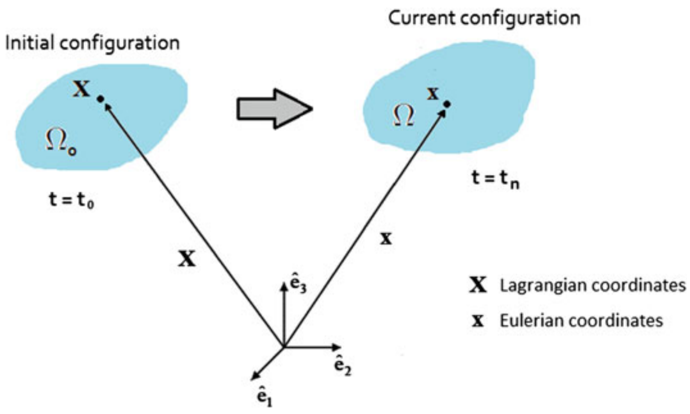

Fig. 1.1 Description of the motion of a general continuum body

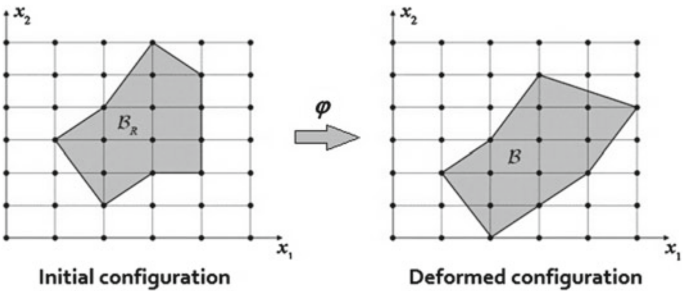

Fig. 1.2 Motion description using an Eulerian mesh

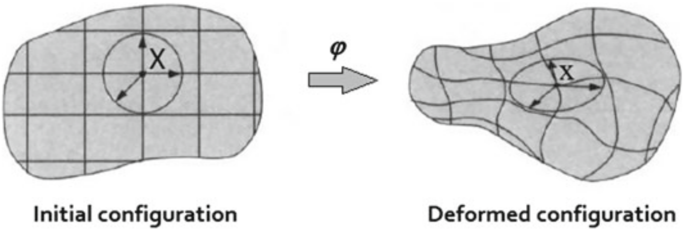

Fig. 1.3 Motion description using a Lagrangian mesh

Consequently, on the one hand the non-linear convective term disappears from the problem and on the other hand the mesh undergoes large distortions and it requires to be regenerated.

In the analysis of free surface flows, the detection of free surface contours represents a crucial task. Its position is unknown a priori and it has to be determined at each time increment in order to solve properly the boundary value problem. For these problems, the Lagrangian description may be preferred to the Eulerian one. In fact, with a Lagrangian approach the free surface is automatically detected by the position of the mesh nodes, while an Eulerian approach requires the implementation of a specific technology for this task.

Several strategies have been developed and presented in the literature for tracking the free surface in an Eulerian framework. One of the earliest contributions was given by the so called *marker and cell* method [6]. In this approach a set of marker particles that move according the flow are used to detect which regions are occupied by the fluid and which not. An evolution of this technique is the *volume of fluid* method [7]. In this case the free surface boundary is detected using a scalar function that assumes the unit value in the fluid cells and the value zero in those ones with no fluid. The cells with an intermedium value are the ones that contain the free surface. Another possibility is the *level set* method [8]. This technique is used in various fields, not only in continuum mechanics, and it allows for detecting shapes or surfaces on a fixed grid without making any parametrization of them. For this reason, this procedure has been also used for matching the free surface contour on an Eulerian mesh [9]. A similar idea was used in [10] where the position of the free surface is detected using a cloud of Lagrangian particles moving over an Eulerian mesh.

The free surface flows can be solved also using an hybrid Eulerian-Lagrangian technique. This is the so termed *Arbitrary Lagrangian-Eulerian (ALE)* approach [11]. The aim of this method is to exploit the best features of the Eulerian and the Lagrangian procedures and to combine them. The mesh nodes can arbitrary be fixed or can move with the fluid [12]. Generally, far from the moving boundaries a fixed Eulerian grid is used, while near to the interface the mesh moves according to the motion of the boundary [13]. However if the boundary motion is large or unpredictable, also in the ALE methods the grid may suffer large distortions and may require a proper remeshing procedure [14].

In purely Lagrangian approaches, the mesh needs to be regenerated whenever a threshold limit for the distortion is exceeded. This is the basis of a particular class of Lagrangian finite element formulation called the *Particle Finite Element Method (PFEM)*. The method was initially developed by the group of professors Idelsohn and Oñate [15, 16]. The PFEM treats the mesh nodes of the domain as particles which can freely move and even separate from the rest of the fluid domain representing, for instance, the effect of water drops. A mesh connects the nodes discretizing the domain where the governing equations are solved using a classical finite element method. These features make the PFEM the ideal numerical procedure to model and simulate free surface flows. In the last years, many scientific publications have shown the efficacy of the PFEM for solving free surface flow problems, see among others [17–19]. The PFEM has also successfully been tested in other kind of problems, such as fluid mechanics including thermal convection-diffusion [20–22], multi-fluids [23, 24], granular materials [25], bed erosion [26], FSI [27, 28] and excavation [29].

Meshfree methods are other class of Lagrangian techniques. In this strategy the remeshing is not required because the governing equations are solved over a set of nodes without referring to a mesh. One of the first meshfree techniques is the *Smooth Particle Hydrodynamics (SPH)* method. This method was introduced independently by Gingold and Monaghan [30] and Lucy [31] for the simulation of astrophysical problems such as fission of stars. SPH is a particle-based Lagrangian technique where discrete smoothed particles are used to compute approximate values of needed physical quantities and their spatial derivatives. The particles have assigned a characteristic distance, called 'smoothing length', over which their properties are "smoothed" by a kernel function. A typical drawback of the SPH method is that it is hard to reproduce accurately the incompressibility of the materials. The SPH technique has been used successfully for solving fluid-structure interaction problems [32].

1.1.2 Stabilization Techniques

A FEM-based procedure may require to be stabilized when incompressible, or quasi-incompressible, materials are analyzed. In the FEM solution of the Navier Stokes problem numerical instabilities may arise from two sources. The first one is due to the presence of the convective term in the linear momentum equations. This term introduces a non-linearity in the equations and it needs a proper stabilization for solving high Reynolds number flows with the FEM [12]. Furthermore, the orders of interpolation of pressure and velocity fields cannot be chosen freely but they have to satisfy the so called *Ladyzenskaya–Babuzka–Brezzi* (LBB), or *inf–sup*, condition [33]. If the orders of interpolation of the unknown fields do not satisfy this restriction, a stabilization technique is required in order to avoid numerical instabilities, as the spurious oscillations of the pressure field.

It is well known that the weak form generated by Galerkin approximation leads to a less diffusive solution than the strong problem. So the main idea of many stabilization techniques consists of adding an artificial diffusion to the problem. The first attempt was made by Von Neumann and Richtmyer [34]. Their solution adds an artificial diffusion to the strong form of the problem. However, this technique introduces an excessive dissipation to the problem because the diffusivity is added in every direction. An important evolution of this approach was the *Streamline Upwind Petrov Galerkin (SUPG)* [35]. In this approach, the artificial diffusion is added by means of the test functions and only on the direction of the streamlines. Furthermore, this is performed in a consistent way: the stabilization terms vanish when the solution is reached. An extension of the SUPG method is the *Galerking Least-Squares (GLS)* method [36]. In the GLS method the stabilization terms are applied not only to the convective term but to all the terms of the equation. The *Variational Multi-Scale (VMS)* methods [37] split the problem variables in a large-scale and a subscale terms. The large-scale terms represent the part of the solution that can be captured by the finite element mesh, while the subscale part consists of an approximate solution that has to be added to the large-scale term in order to obtain the correct solution. This idea represents the basis of other stabilization methods. Among these, the most largely used are the *Algebraic Subgrid Scale Formulation (ASGS)* and the *Orthogonal Subscales (OSS)* methods, respectively introduced in [38, 39]. Another efficient stabilization technique is the *Finite Calculus* (also termed *Finite Increment Calculus*) (*FIC*) approach (see among others [40–43]). This method has some analogies with the SUPG technique (for a comparison between these methods see [44]). The FIC approach is based on expressing the equations of balance of mass and momentum in a space-time domain of finite size and retaining higher order terms in the Taylor series expansion typically used for expressing the change in the transported variables within the balance domain. In addition to the standard terms of infinitesimal theory, the FIC form of the momentum and mass balance equations contains derivatives of the classical differential equations in mechanics multiplied by characteristic distances in space and time. In this work an updated version of the FIC method has been derived and tested.

In solid mechanics a stabilization procedure may be required for the solution of problems involving incompressible, or quasi-incompressible solids. Situations of this type are common in forming processes or in the analysis of rubber-type materials. Many of the mentioned stabilization procedures for fluid dynamics have been also used also for solid dynamics. For example, the VMS method has been applied in quasi-incompressible solid mechanics in [45, 46], the OSS in [47]. In [48, 49] a stabilized multi-field Petrov–Galerkin procedure is used. Finally, the application of the FIC in solid mechanics is reported [50, 51].

1.1.3 Algorithms for FSI Problems

Many approaches have been developed for solving FSI problems. Typically the computational techniques for FSI are distinguished in *monolithic* and *staggered*, or *partitioned*, approaches. In a monolithic approach fluid and solid domains are solved in a single system of equations (see among others [52], or [53]). In this technique the flow of information between the solid and the fluid parts is implicitly performed by the procedure. On the contrary, in staggered schemes the fluid and the solid dynamics are solved separately and boundary conditions are transferred from a domain to the other at the interface. From the algebraic point of view, the solution is achieved by solving two different linear systems which are coupled by means of the boundary conditions defined along the interface. Within partitioned schemes, a further classification can be done depending on the level of coupling between the fluid and the solid dynamics. In *weakly coupled* segregated methods the transfer of information at the interface is performed only once for each time step, (for example see [54]), whereas in *strongly coupled* schemes this operation is performed within a convergence iterative loop (as a reference see [55]). Clearly, a weakly coupled scheme has a lower computational cost but it can be used only when the interaction between the solid and the fluid domains is not strong or complex. Otherwise the algorithm may not find the correct numerical solution of the problem.

Partitioned methods allow the reutilization of existing solvers. Furthermore, the solid and the fluid solvers can be updated independently. Staggered schemes lead to smaller and better conditioned linear systems than the ones obtained with monolithic approaches. On the other hand, monolithic strategies are generally more stable than staggered schemes, and they lead to a more accurate solution of FSI problems, because a stronger coupling is ensured.

Another general classification of the FSI algorithms is based upon the treatment of meshes. In *conforming mesh* methods, the fluid and the solid meshes must have in common the nodes along the interface in order to allow the transfer of information. Consequently, if the position of the interface nodes changes in a material domain, also the other domain must modify its grid in order to guarantee the conformity of the two meshes along the interface. On the contrary, in *non-conforming mesh* methods the interface and the related conditions are treated as constraints imposed on the model equations so that the fluid and solid equations can be solved independently from each other with their respective grids [56]. This represents an important advantage because, typically, the mesh used for the fluid has an average size lower than the one used for the solid and so it is not necessary to refine the solid finite element grid near to the interface. However, non-conforming mesh algorithms are more complex to implement and it is not trivial to guarantee their robustness.

In the so-called *Immersed Boundary Method* (*IBM*), the fluid is solved using an Eulerian grid and the solids are immersed on top of this mesh [57, 58]. The interaction is ensured by penalizing the Navier–Stokes equations with the momentum forcing sources of the immersed structures. An evolution of the IBM is the *Immersed Structural Potential Method* (*ISPM*) where the structure is modeled as a potential energy functional solved over a cloud of integration points that move within the fixed fluid mesh [58, 59]. Also in the *Immersed Finite Element Method* (*IFEM*) [60, 61] the structure acts as a momentum forcing source for the fluid governing equations, but in this case a Lagrangian mesh is employed for the solid domains.

1.2 Numerical Model

The aim of this work is to derive a finite element formulation capable to solve, through a unique set of equations and unknown variables, the mechanics of a general continuum. The term ‘general continuum’ refers to a domain that may include compressible and quasi-incompressible solids, fluids or both interacting together. For this reason, the formulation is termed *Unified*. The Unified formulation is based on a mixed Velocity–Pressure Stabilized procedure and it has been implemented in a sequential C++ code.

1.2.1 Reasons

There are many reasons for undertaking the above objective.

The first advantage of the Unified formulation is that it allows for solving fluid and solid dynamics problems by implementing and using a single calculation code.

Furthermore, if solids and fluids are solved via the same scheme, it is simpler to implement the solver for FSI problems because it is not required neither changing the variables, neither implementing the transfer of transmission conditions through the interface. With this formulation solids and fluids represent regions of the same continuum and they differ only by the specific values of the material parameters. As a consequence, the FSI solver requires a small computational effort and it can be implemented by introducing just a few specific functions. This will be explained in detail in the section dedicated to FSI problems.

Additionally, with the Unified formulation the most natural approach for solving FSI problem is the monolithic one. This brings in the further advantage that the coupling is ensured strongly and an iteration loop is not required, as for staggered procedures.

Finally, using the same set of unknowns for the fluid and the solid domains reduces the ill-conditioning of the FSI solver, because the solution system does not include variables of different units of measure.