Interface capturing method and two-phase flow using phase-field Cahn–Hilliard and stabilized Navier–Stokes coupling in a mixed finite element framework

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Mots Clés : PDEs Mixed Problem, Finite Element, Interface Capturing Method, Cahn–Hilliard Equations, Computational Fluid Dynamics, Multiphase Flow, Industrial Applications

Biographie – After being graduated from Masters of Science in Mathematical Modeling at Sorbonne Université (Jussieu), I started my PhD in Applied Mathematics at Cemef laboratory in Mines ParisTech at Sophia Antipolis campus. My thesis relies on the development of a unified solver for industrial process in multiphase flow. It is part of the ANR chair INFINITY, a 4 year a project bringing together academic and industrial partners which aims to develop a numerical tool for the quenching process simulation.

Resumé :

In order to meet the challenges of competitiveness and technological innovations in the energy and automotive, air and space transport sectors, manufacturers have a strong demand for obtaining a quality material for their productions. This demand varies according to the structure of the material, its size and geometry due to the diversity of applications envisaged such as car production, airplanes or power plants. Today, to change the quality of the material, manufacturers employ a metallurgical process : the quenching process. The quenching process is a heat treatment operation consisting in heating a material at high temperature for a while and then suddenly cool it down by dipping it into a liquid (water, polymer, ...) at a lower temperature to give it certain mechanical properties. In contact with the liquid, the high temperature difference creates a boiling point, revealing a film of vapor enveloping the material. This vapor film acts as a thermal mantle which decreases the cooling rate of the material. Controlling the cooling during the quenching process is therefore a major issue. The approach currently followed by manufacturers to study material cooling relies on models based on averaged semi-empirical parameters, called exchange coefficients. These are limited to particular scenarios and for a specific evolution of the flow geometry. They are determined experimentally and accumulating these experiments is not an economically viable strategy because of the cost of this process.

So a physical modeling of the system coupled with numerical simulation is therefore a promising alternative since Computational Fluid Dynamics (CFD) offers powerful numerical tools thanks to the increase computing performance. Despite numerical simulation is starting to be used in industry metallurgy, there is to date no software to reliably simulate a quenching because of the complexity of the physical phenomena involved. In order to develop this numerical tool, the INFINITY industrial ANR chair, a 4-year project bringing together academic and industrial partners, was initiated and a contribution of which is distributed by my thesis. This software allows manufacturers to speed up decision support to obtain a high quality material, without cracks and with the desired properties. However, a clear understanding of physical phenomena is required and remains today a major challenge both industrially and academically. Modeling the liquid/vapor phase change taking place during quenching because of the temperature difference is one of the many challenges. To carry out this modeling, it is necessary to describe the evolution

of the liquid/vapor interface and of precise way. The development of efficient methods to simulate complex two-fluid flows remains a challenge.

Amongst interface capturing methods the use of Cahn-Hilliard equations [2] has gained attention for the simulation of large-scale industrial problems. In this contribution, we describe a recently developed mixed finite element methods for the Cahn-Hilliard equations. Details on the Cahn-Hilliard model with constant mobility, a positive diffusion coefficient describing the movement of species from a phase to another, and its weak and full discrete finite element formulations will be presented, as well as a convergence analysis and a series of numerical tests, assessing the performance of the implemented algorithm. Then coupling of the Cahn-Hilliard and Navier-Stokes equations [1] for an incompressible two-fluid mixture with different densities will be established in a fractional step sheme. The incompressible Navier–Stokes equations are solved using the Variational Multiscale Method [4]. Adaptive anisotropic meshing [3] is leveraged with a free energy based criteria to improve accuracy. The numerical method is implemented in a massively parallel finite element framework. A series of 2D and 3D tests cases are proposed for validation of the coupled method as well as comparison with a level-set approach. The mathematical and numerical difficulty in studying the Cahn–Hilliard equations for realistic multiphase flows lies in the degeneration of this mobility, vanishing in the pure phases. A generalization of the study to degenerated mobility is envisaged.

Références

- [1] H Abels, D Depner, and H Garcke. On an incompressible Navier–Stokes/Cahn–Hilliard system with degenerate mobility. Annales de l'I.H.P. Analyse non linéaire, 30(6):1175–1190, 2013.
- [2] JW Cahn and JE Hilliard. Free Energy of a Nonuniform System. I. Interfacial Free Energy. Journal of Chemical Physics, 28(2):258–267, 1958.
- [3] T. Coupez and E. Hachem. Solution of high-reynolds incompressible flow with stabilized finite element and adaptive anisotropic meshing. *Computer Methods in Applied Mechanics* and Engineering, 267:65–85, 2013.
- [4] Thomas J. R. Hughes. Multiscale phenomena: Green's functions, the dirichlet-to-neumann formulation, subgrid scale models, bubbles and the origins of stabilized methods. *Computer Methods in Applied Mechanics and Engineering*, 127(1):387–401, 1995.