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Eulerian–Lagrangian grid coupling and penalty methods for the simulation of multiphase flows interacting with complex objects

A. Sarthou[1,*,†], S. Vincent[1], J. P. Caltagirone[1] and Ph. Angot[2]

[1] *Université Bordeaux I, TREFLE-ENSCPB, UMR 8508, 16, avn Pey-Berland, 33607 Pessac Cedex, France*
[2] *Université de Provence, LATP-CMI, UMR 6632, 39, rue F. Joliot Curie, 13453 Marseille Cedex 13, France*

SUMMARY

Our purpose is to develop an efficient coupling between incompressible multiphase flows and fixed or moving obstacles of complex shape. The flow is solved on a fixed Cartesian grid and the solid objects are represented by surface elements. Our strategy is based on two main originalities: the generation and management of the objects are ensured by computer graphics software and front-tracking methods, while the coupling between the flow and the obstacle grids is ensured by a fictitious domain approach and new high-order penalty techniques. Several validation problems are presented to demonstrate the interest and accuracy of the method. Copyright © 2007 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Many works have been devoted to the interaction between multiphase flows and solid obstacles such as the arbitrary Lagrangian–Eulerian (ALE) method [1], the immersed boundary method (IBM) [2] or the immersed interface method (IIM) [3], the distribute Lagrangian multiplier (DLM) approach [4] or the ghost fluid method [5]. In order to deal with fluid/solid interactions, our objective is to propose a new penalty-based numerical method, spatially of second order, which can be easily implemented in an implicit finite volume computational fluid dynamics (CFD) code with minor modifications of the standard discretization. The main interest of the method is to account for complex solid shapes or immersed interfaces on non-conforming structured grids with second-order accuracy. As a first step, we present the method for a fixed Cartesian grid in finite

*Correspondence to: A. Sarthou, TREFLE-ENSCPB, UMR 8508, 16, avn Pey-Berland, 33607 Pessac Cedex, Université de sciences Bordeaux I, France.
†E-mail: sarthou@enscpb.fr

volumes, even if the method can *a priori* be applied to finite elements and unstructured grids. The article recalls existing first-order penalty methods. The new high-order method that is based on a sub-mesh penalty approach is then detailed. The last section presents validations dedicated to scalar and vector problems. Perspectives and conclusions are finally drawn.

2. PENALTY METHODS FOR IMMERSED INTERFACES

2.1. Low-order penalty methods

First-order methods are first presented. They are used to penalize control volumes in solid media approximating the solid–fluid interface with stair-steps. They can be applied to both scalar and Navier–Stokes equations. The penalty methods consist in adding specific terms in the conservation equations to play with the order of magnitude of existing physical contributions so as to solve at the same time and with the same set of equations the fluid and solid mechanics (see [6] for example). Among the existing methods, we can cite the Darcy penalty method (DPM) that can be used to treat fixed obstacles by adding a Darcy term [7] in the momentum equations. The volumic penalty method (VPM) (see [7] and the references therein) consists in the addition of a penalty term $\beta_u(\mathbf{u}-\mathbf{u}_\infty)$ in conservation equations, such that

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}-\nabla\cdot D\nabla\mathbf{u}=F+\beta_u(\mathbf{u}-\mathbf{u}_\infty)\longrightarrow\begin{cases}\dfrac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}-\nabla\cdot D\nabla\mathbf{u}=F & \text{if } \beta_u\to 0\\ \mathbf{u}=\mathbf{u}_\infty & \text{if } \beta_u\to\infty\end{cases}\tag{1}$$

where $\mathbf{u}$ is a unknown scalar or vector, F a source term, β_u the penalty coefficient and $\mathbf{u}_\infty$ the value of a Dirichlet condition to be imposed in the given media. Concerning obstacles moving under flow action, the derivatives of the velocity are penalized through a new formulation of the viscous stress tensor [8] in order to impose no deformation with a velocity resulting from the effect of the surrounding fluid. This method is called the implicit tensorial penalty method (ITPM). The space convergence of these VPMs is only first order since they consider the projected shape of the fluid–solid interface on the Eulerian grid to define the penalty parameters (see [9, 10]).

2.2. High-order penalty method: the sub-mesh penalty method

The order of the standard VPMs is limited since they approach at first order the topology of the real interface by fitting its shape to the control volumes. Thus, these penalty methods have to be improved near the fluid–solid interface. Instead of strongly constraining the mean value of the solution in Eulerian control volumes, we decide to impose the local value of the Dirichlet condition at the Lagrangian interface location and so to define implicit penalty functions that are no longer constant into the control volumes. The key points of the method lie on the following concepts. First, the interface Σ is accurately piecewise reconstructed using a Lagrangian mesh coupled with front-tracking methods. This discrete interface Σ_h is used to build the penalty terms. As the interface is described at a smaller scale than the Eulerian grid scale, the method is called the sub-mesh penalty (SMP) method. The method is fully implicit and the same model, like (1) applies in all domains by adding a penalty term in the conservation equations. The discrete operators are not modified, contrary to ghost fluid or IIM methods. The method uses interpolation functions f_p of various support $\mathscr{S}_p$ (typically P_1 or Q_1) according to the local interface topology.

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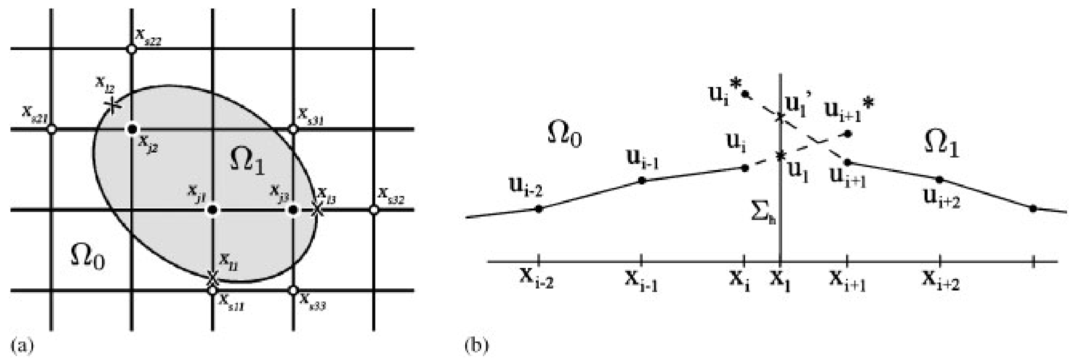

Figure 1. (a) Location of the kind of nodes used for the SMP method and (b) illustration of the symmetric SMP method.

In two dimensions, let $\mathbf{u}$ be the solution of (1) in a domain $\Omega=\Omega_0\cup\Omega_1$, Ω_1 being an embedded domain (solid media for example) of frontier Σ on which the Dirichlet condition $\mathbf{u}=\mathbf{u}_\infty$ must be satisfied. We discretize $\mathbf{u}$ over the computational domain by a set of unknowns $\mathbf{u}_i$ located at the nodes $\mathbf{x}_i$, with $i\in\{1,2,\ldots,N_x\times N_y\}$. We first explain the non-symmetric version used to impose Dirichlet boundary conditions on Ω_0 only, the solution in Ω_1 being known or without interest. That is the case if Ω_0 is a fluid domain and Ω_1 a fixed obstacle of complex shape. Then, we generalize the method for Dirichlet conditions on immersed interfaces.

An Eulerian volume of fluid (VOF) fraction C is built with a front-tracking Lagrangian–Eulerian projection method [11] that solves a Poisson equation and uses Peskin discrete Dirac functions. The color function C admits the value 0 in Ω_0 and 1 in Ω_1. The interface is easily located on the Eulerian grid by stating $C=0.5$. In all the control volumes V_i, where $C_i=1$ and $\nabla C_i.=0$, a standard VPM is used to impose $\mathbf{u}=\mathbf{u}_\infty$. In our case, we use the VPM and state $\beta_{u_i}=1/\eta$ with $\eta\approx O(10^{-40})$. The SMP functions f_p are built in all V_i where $\nabla C\geqslant 0.5/h_i$, with h_i the local space step. We define $\mathscr{P}$ the set containing each node $\mathbf{x}_j\in\Omega_1$ having at least one neighbor in Ω_0, and $\mathscr{I}$ the set containing each node in Ω_1 but not in $\mathscr{P}$. Each node of $\mathscr{P}$ is associated with a specific penalty function f_p. If $\mathbf{x}_j$ (x_{j1} in Figure 1(a)) has one neighbor in Ω_0 (x_{s11} in Figure 1(a)), the support of f_p is the segment composed of the two nodes (x_{j1} and x_{s11}) and the interpolation is linear in one direction. If $\mathbf{x}_j$ (x_{j2} in Figure 1(a)) has two neighbors in Ω_0, the support of f_p is the Q_1 or P_1 cell containing $\mathbf{x}_j$ and its two neighbors in Ω_0. The interpolation is then linear/bilinear. If $\mathbf{x}_j$ (x_{j3} in Figure 1(a)) has three neighbors in Ω_0, the support of f_p is again a segment formed by $\mathbf{x}_j$ and the median point of the three neighbors (x_{s32} in Figure 1(a)).

Each penalty function is associated with a Lagrangian point $\mathbf{x}_l$ of Σ_h included in the support of f_p. Once the support $\mathscr{S}_p$ and the corresponding interpolation type are defined, f_p is built. Each f_p is a polynomial function that satisfies $f_p(x_s)=\mathbf{u}_s$, with $\mathbf{u}_s$ the solution at the nodes x_s of $\mathscr{S}_p$. In this way, f_p can be expressed as a linear combination of unknowns $\mathbf{u}_s$, such as $f_p(x)=\sum_{k/x_k\in\mathscr{S}_p}\alpha_k(x)\mathbf{u}_k$. Once f_p is defined, the constraint $f_p(x_l)=\mathbf{u}_\infty$ defines the penalty constraint. Hence, the penalty term $\beta_u(\mathbf{u}-\mathbf{u}_l)$ from the VPM is replaced by $\beta_u(f_p(\mathbf{u})-\mathbf{u}_\infty)$. The support $\mathscr{S}_p$ of each f_p contains some nodes in Ω_0 but only one node in Ω_1. The penalty term is acting only for the discretization of (1) at this node in Ω_1. The penalty term locally crushes the physical equation in Ω_1 where we are not interested by the solution. Equation (1) is then

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equivalent to a penalty constraint acting on all the nodes of $\mathscr{P}$. Hence, the computation of the physical solution in Ω_0 does not require the unknowns located at the nodes of $\mathscr{I}$. This version of the method is then adapted to take account of complex immersed boundaries of Ω_0. For vector problems, each component is treated as described before.

To allow an immersed Dirichlet condition from both sides of the interface (that is to say to compute the solution both in Ω_0 and Ω_1), we symmetrize the procedure previously described. Now we have to consider two unknowns at each node near the interface: a 'physical unknown' is used for the physical equation and is seen only by the node of the same subdomain and an 'auxiliary unknown' that supports the penalty constraint and is seen only by unknowns in the other subdomain (Figure 1(b)). The auxiliary unknowns are marked with $*$. The creation of auxiliary unknowns near the interface increases the size of the linear system. A way to avoid the creation of auxiliary unknowns is to use nodes only from the same side of the interface for a given penalty constraint. The interface is no more included in the support of the penalty function. The Dirichlet value at the interface becomes an implicit extrapolation of the solution in the support. Instead of being activated for nodes in Ω_1, penalty terms are now active for the discretization of (1) at nodes in Ω_0, where the physical solution is required. An implementation of this method for scalar problems has showed that convergence order remains the same, but the error grows two orders in magnitude.

3. VALIDATION AND APPLICATIONS

3.1. Sub-mesh penalty method for scalar equation

We solve the homogeneous Laplace equation in a square numerical domain $[-2;2]\times[-2;2]$ with a Dirichlet condition of $\mathbf{u}_1=10$ on a first circular interface ($R_1=1$) and an analytical solution on the boundary of the Eulerian grid. Practically, the analytical solution that accounts for the presence of the second circle with a radius $R_2=4$ and $\mathbf{u}_2=0$ is imposed on the boundary conditions. Figure 2(1) (left) shows a second order of convergence in space for the L^2 relative error on velocity. Figures 2(2) and (3) represent the isovalue $\mathbf{u}=10$ (i.e. the Dirichlet value imposed on R_1. Analytically, the isovalue is a circle) obtained from the simulations with the VP method (center) and the SMP method (right). As can be seen, the SMP method greatly improves the shape of the isovalue.

3.2. Sub-mesh penalty method for the Navier–Stokes equations on a MAC grid

The simulation of Eulerian two-phase flows is based on staggered Cartesian grid, implicit finite volumes, one fluid model, VOF interface tracking and augmented Lagrangian velocity–pressure coupling. Details on the discretizations and the validations have previously been published by Vincent and Caltagirone [12]. Concerning the management of the objects, their generation is achieved using a computer graphics software and a specific algorithm has been developed to interpret the Lagrangian grid of these objects on the Eulerian flow grid. We use a front-tracking method [11] to obtain phase functions C_i of objects. This Eulerian description of the objects allows us to define the characteristics of the whole fluid/solid medium, such as the density and the viscosity, and the penalty terms are added to the motion equations according to the Eulerian description C of the object (low-order approach) or to their Lagrangian position (high-order

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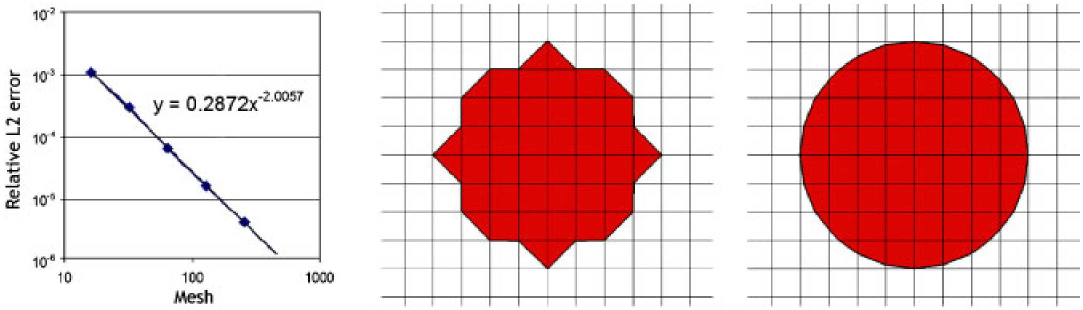

Figure 2. Relative L^2 convergence of the SMP method and comparison between solutions obtained with VP method and SMP method on a 16×16 grid.

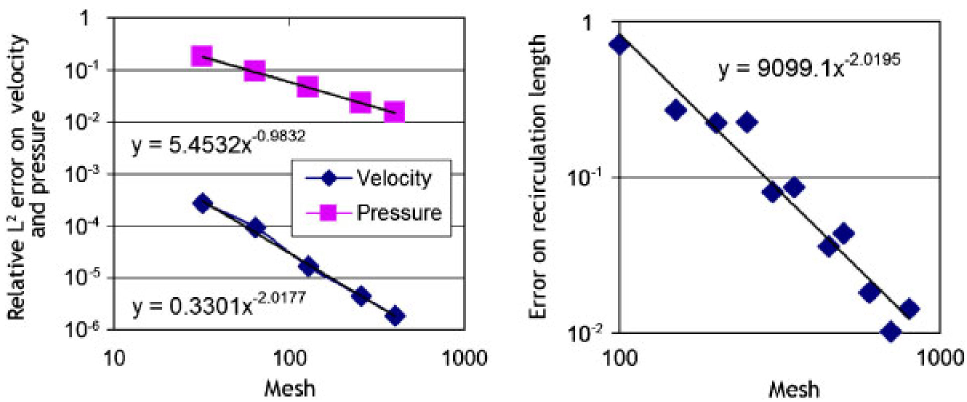

Figure 3. Relative L^2 error of the SMP method for a Couette flow (1) and error on recirculation length for a flow past a cylinder (2).

method). Finally, the unsteady flow is simulated with a single fluid model and penalty methods dedicated to incompressible and solid behavior.

We simulate the cylindrical Couette flow in a square numerical domain $[-0.15;0.15]\times[-0.15;0.15]$. The inner circle has a rotation speed $\omega_1 = 1\,\mathrm{rad/s}$ and radius $R_1 = 0.05\,\mathrm{m}$. We impose the analytical solution on the numerical boundary as the domain is surrounded by a second circle whose rotation speed is $\omega_2 = 2\,\mathrm{rad/s}$ and radius is $R_2 = 2\,\mathrm{m}$. In Figure 3(1), the convergence of the L^2 relative error is presented. A second order is reached for velocity, whereas a first order is observed for pressure. For all meshes, the maximum divergence of the flow is about 10^{-14} with a velocity correction of projection type. As a second test case, we simulate flow past a circular cylinder of radius 0.05 m immersed in a rectangular domain $[-1.6;1.4]\times[-0.75;0.75]$ at Reynolds 40. Figure 3(2) shows the convergence of the recirculation length against the length for a 2000×1000 mesh for which $L/d = 2.37$. A second order is obtained. Regular velocity and pressure field are observed near the interface (Figure 4(1)).

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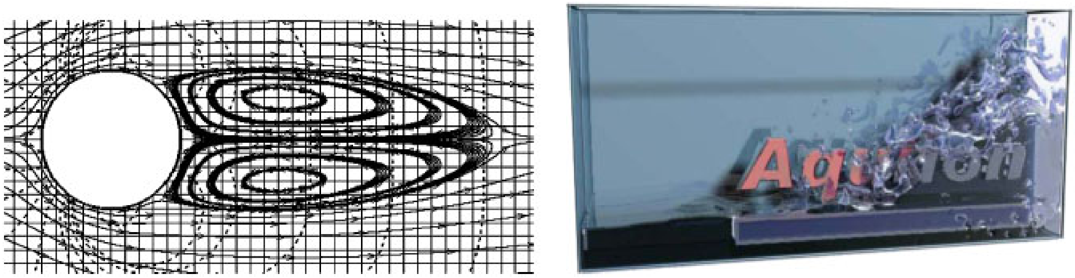

Figure 4. Streamtraces and pressure field on a 64×64 grid for this last case (1) and Dam break flow over an obstacle (2).

4. DISCUSSION AND CONCLUSION

On fixed staggered Cartesian grids, a new sub-mesh penalty method has been proposed for the simulation of free surface flows interacting with complex shape obstacles (see an example of dam break flow over an obstacle in Figure 4(2)). The Lagrangian mesh of these objects is generated in 3D computer graphic softwares and interpreted as a front-tracking surface in an Eulerian formulation of the Navier–Stokes equations for multiphase flows. Several penalty methods have been implemented and coupled to obtain the interaction between fluid and solid media. In two dimensions, the SMP method is second order for both scalar diffusion and Navier–Stokes equations. The interest of the interpretation and management of triangularized surface of obstacles by means of front-tracking procedures can be seen in [13]. This website contains several 3D realistic multiphase flow simulations involving SPM method with Q_0 interpolations. Future works will be devoted to extending the SMP method, coupled to ITPM or VPM, to three-dimensions with Q_1 interpolations. The formal proof of the second order of the SMP method is under consideration, as well as its compatibility with various approaches dealing with incompressibility, in order to reach the second-order convergence on pressure. In addition, adaptative mesh refinement (AMR [14]) techniques will be associated to the tracking of boundary layers in penalized fluid/solid cells.

REFERENCES

1. Maury B. Direct simulation of 2D fluid-particle flows in biperiodic domains. *Journal of Computational Physics* 1999; **156**:325–351.
2. Peskin C. The immersed boundary method. *Acta Numerica* 2000; **11**:479–517.
3. Le BV, Khoo BC, Peraire J. An immersed interface method for viscous incompressible flows involving rigid and flexible boundaries. *Journal of Computational Physics* 2006; **220**:109–138.
4. Glowinski R, Pan TW, Hesla TI, Joseph DD. A distributed Lagrange multiplier/fictitious domain method for particulate flows. *International Journal of Multiphase Flow* 1999; **25**:755–794.
5. Fedkiv R, Aslam T, Merriman B, Osher S. A non-oscillatory Eulerian approach to interfaces in multimaterial flows (the ghost fluid method). *Journal of Computational Physics* 1999; **152**:457–492.
6. Vincent S, Randrianarivelo TN, Pianet G, Caltagirone JP. Local penalty methods for flow interacting with moving solids at high Reynolds numbers. *Computers and Fluids* 2007; **36**:902–913.
7. Khadra K, Angot P, Parneix S, Caltagirone JP. Fictitious domain approach for numerical modelling of Navier–Stokes equations. *International Journal for Numerical Methods in Fluids* 2000; **34**:651–684.
8. Randrianarivelo TN, Pianet G, Vincent S, Caltagirone JP. Numerical modelling of solid particle motion using a new penalty method. *International Journal for Numerical Methods in Fluids* 2005; **47**:1245–1251.

DOI: 10.1002/fld

9. Ramière I, Angot P, Belliard M. A fictitious domain approach with spread interface for elliptic problems with general boundary conditions. *Computer Methods in Applied Mechanics and Engineering* 2007; **196**:766–781.
10. Ramière I, Angot P, Belliard M. A general fictitious domain method with immersed jumps and multilevel nested structured meshes. *Journal of Computational Physics* 2007; **225**:1347–1387.
11. Shin S, Juric D. Modelling three-dimensional multiphase flow using a level contour reconstruction method for front tracking without connectivity. *Journal of Computational Physics* 2002; **180**:427–470.
12. Vincent S, Caltagirone JP. A one-cell local multigrid method for solving unsteady incompressible multiphase flows. *Journal of Computational Physics* 2000; **163**:172–215.
13. MKF Project—Fluid Mechanics and Computer Graphics. Available from: http://projetmkf.free.fr (30 July 2007).
14. Delage S, Vincent S, Caltagirone JP, Heliot JP. A hybrid linking approach for solving the conservation equations with an adaptative mesh refinement method. *Journal of Computational and Applied Mathematics* 2006; **191**: 280–296.