The Sub-Mesh Penalty Method

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ABSTRACT. *The Sub-Mesh Penalty (SMP) method, a new fictitious domain method of high order is presented. The final aim 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 Lagrangian surface elements. Several validation problems in 2D and 3D are presented to demonstrate the interest and accuracy of the method.*

KEYWORDS: *High-order penalty methods, fictitious domains, Eulerian/Lagrangian grid coupling*

1. Introduction

Many works have been devoted to the interaction between multiphase flows and solid obstacles such as the Arbitrary Lagrangian Eulerian (ALE) method [Mau 99], the Immersed Boundary Method (IBM) [PES 00] or the Immersed Interface Method (IIM) [LE 07], the Distributed Lagrangian Multiplier (DLM) approach [GLO 99] or the Ghost Fluid method [FED 99]. 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 CFD code with minor modifications of the standard discretization schemes. The main interest of this new method is to account for complex solid shapes or immersed interfaces on non-conforming structured grids with second-order accuracy, while former penalty methods are generally of first order only since they consider the projected shape of the fluid-solid interface on the Eulerian grid to define the penalty parameters [RAM 07]. Among the existing methods, we can cite the Darcy Penalty Method (DPM) for the Navier-Stokes equations that can be used to treat fixed obstacles by adding a Darcy term [KHA 00] in the momentum equations. Concerning obstacles moving under flow action the derivatives of the velocity are penalized through a new formulation of the viscous stress tensor ([RAN 05] and [VIN 07]) 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).

As a first step, we present the method for a fixed Cartesian grid in finite volumes, even if the method can *a priori* be applied to finite elements and unstructured grids. The article recalls the principles of the penalty methods. The new high-order method which 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*

Let us consider the following model scalar problem with a Dirichlet boundary condition on the interface Σ :

$$\left\{ \begin{array}{rl} -\nabla \cdot (a \nabla u) = f & \text{in } \Omega_0 \\ u_{|\Sigma} = u_D & \text{on } \Sigma \end{array} \right. \quad [1]$$

Some boundary conditions are also imposed on the other part of the boundary $\partial\Omega_0$ such that the whole problem is well-posed. The penalty methods consist adding specific terms in the conservation equations to play with the order of magnitude of existing physical contributions so as to obtain at the same time and with the same set of equations two different physical properties. The Volumic Penalty Method (VPM) ([KHA 00] and the references therein) consists the addition of a penalty term $b(u-u_D)$ in the conservation equations, such that:

$$\left\{ \begin{array}{l} -\nabla \cdot (a \nabla u) + b(u - u_D) = f \text{ in } \Omega \\ \text{with } b_{|\Omega_0} = 0, b_{|\Omega_1} = \frac{1}{\varepsilon}, \text{ for } 0 < \varepsilon \ll 1 \end{array} \right. \quad [2]$$

where ε denotes the penalty parameter which tends to 0.

2.2. *Sub Mesh Penalty algorithm with Dirichlet boundary conditions*

A simple version of the SMP algorithm for problem [2] was first proposed in [SAR 08]. Let us consider the original domain of interest denoted by Ω_0, typically the fluid domain, which is embedded inside a simple computational domain $\Omega \subset \mathbb{R}^d$. The auxiliary domain Ω_1, typically a solid particle or an obstacle, is then such that : $\Omega = \Omega_0 \cup \Sigma \cup \Omega_1$ where Σ is an immersed interface (see Fig. 1 left). Let $\mathbf{n}$ be the unit outward normal vector to Ω_0 on Σ. Our objective is to numerically impose the adequate boundary conditions on the interface Σ. These conditions will be discretized in space with second order schemes on an Eulerian structured mesh covering Ω.

The computational domain Ω is meshed with a set of cell-centered finite volumes $(\mathcal{V}_I)$ for $I \in \mathcal{E}$, $\mathcal{E}$ being the set of index of the Eulerian structured mesh (typically a Cartesian mesh uniform or not). Let x_I be the vector coordinates of the center of each volume $\mathcal{V}_I$. The local space step of the volume $\mathcal{V}_I$ defined as the maximum length

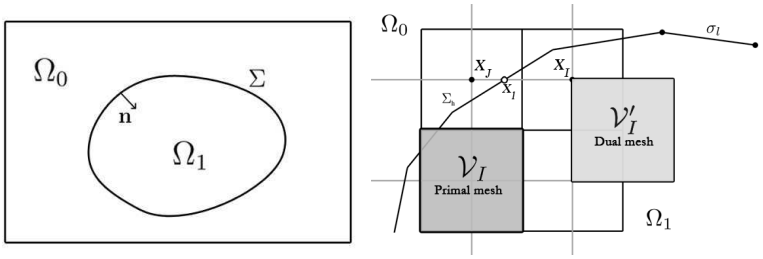

Figure 1. *Definition of the domains-discretization for the SMP method*

of $\mathcal{V}_I$ in each direction is denoted by h_I, whereas h denotes the Eulerian mesh step: $h = \sup_{I\in\mathcal{E}} h_I$. This grid is used to discretized the conservation equations. A dual grid is introduced for the management of the penalty method. The grid lines of this dual cell-vertex mesh are defined by the network of the cell centers x_I. The volumes of the dual mesh are denoted by $(\mathcal{V}'_I)$ We note the Eulerian unknowns u_I which are the approximated values of $u(x_I)$, i.e. the solution at the cell centers x_I.
The discrete interface Σ_h, hereafter called the Lagrangian mesh, is given by a discretization of the original interface Σ. It is described by a piecewise linear approximation of Σ : $\Sigma_h = \{\sigma_l \in \mathbb{P}_1^{d-1}, l \in \mathcal{L}_f\}$, $\mathcal{L}_f$ being the set of index of the Lagrangian mesh, and $\mathbb{P}_n^d$ being the space of polynomial of n degrees in d dimensions. Typically, σ_l are segments in $2D$ and triangles in $3D$. The vertices of each face σ_l are denoted by $x_{l,i}$ for $i = 1, d$ and the set of all vertices is : $\{x_l, l \in \mathcal{L}_v\}$. The intersection points between the grid lines of the Eulerian dual mesh and the faces σ_l of the Lagrangian mesh are denoted by $\{x_i, i \in \mathcal{N}\}$ (see Fig. 1 right). Our objective is to discretize the boundary conditions at these interface points with a second-order approximation.
The cell centers x_I are sorted according to their location inside Ω_0 or Ω_1 by defining the color fonction C defined by : $C_I = C(x_I) = 1$ if $x_I \in \Omega_1$, and $C_I = 0$ if $x_I \in \Omega_0$. We introduce new sets of Eulerian points x_I near the interface such that there it exists one neighbor x_J verifying $C_J \neq C_I$, i.e. the segment $[x_I; x_J]$ is cut by Σ_h. These Eulerian "interface" points are also sorted according to their location inside Ω_0 or Ω_1. So we have the two sets $\{x_I, I \in \mathcal{N}_0\}$ and $\{x_I, I \in \mathcal{N}_1\}$. The previous equation [2] is then discretized with finite volumes on the Eulerian mesh covering Ω. For each control volume $\mathcal{V}_I$, we get a discrete equation formally written as:

$$-\{\nabla \cdot (a\nabla u)\}_I + \{b(u - u_D)\}_I = \{f\}_I, \forall I \in \mathcal{E} \qquad [3]$$

where $\{\}_I$ denotes the spatial approximation of a quantity. The SMP algorithm introduces a specific discretization procedure for the points x_I which are near the interface and inside the fictitious domain Ω_1, i.e. for $I \in \mathcal{N}_1$. We first describe the case when x_I has only one neighbor in Ω_0.
Let us consider one point x_I of this type, x_J its neighbor in Ω_0 and x_l the intersection between $[x_I; x_J]$ and Σ_h (Fig. 1 right). Then, the interface unknown u_l is approximated by the $\mathbb{P}_1^1$-interpolation between the Eulerian unknowns u_I and u_J :

$$u_l = \lambda_I u_I + \lambda_J u_J \text{ with } 0 < \lambda_I, \lambda_J < 1 \text{ and } \lambda_I + \lambda_J = 1 \qquad [4]$$

Hence, for this point, the corresponding penalty term $\{b(u-u_D)\}_I$ is approximated by $\{b(u_l-u_D(x_l))\}_I$ with $b=1/\varepsilon$ and the discrete equation becomes

$$-\{\nabla\cdot(a\nabla u)\}_I+\left\{\frac{1}{\varepsilon}\left(\lambda_I u_I+\lambda_J u_J-u_D(x_l)\right)\right\}_I=\{f\}_I,\forall I\in\mathcal{N}_1 \qquad [5]$$

So, u_l tends to u_D when ε tends to 0.
Let us consider an additional point x_K such as u_J is between u_I and u_K. For the sake of simplicity, $h=1$. The discretization of the Laplacian operator at x_J using a centered scheme is $(u_I-2u_J+u_K)$. The discretization of [2] at x_I tends to $(\lambda_I u_I+\lambda_J u_J-u_D(x_l))=0$. We recall that $\lambda_I+\lambda_J=1$, and for $h=1$, $\lambda_I=d(x_J,x_l)$, d being the distance function. Hence, the discretization at x_J of the Laplacian operator can be rewritten as $(-(\lambda_J u_J+u_D(x_l))/\lambda_I-2u_J+u_K)=((u_D-u_J)/\lambda_I-(u_J-u_K))$. We can notice that the term $(u_D-u_J)/\lambda_I$ is the centered spatial derivative between x_D and x_J, and the method is equivalent to rewriting the discretization of spatial operators using a modified boundary mesh fitting the objects. If x_I has more than one neighbor in different directions, we build a penalty constraint using higher dimension P_1 or Q_1 interpolation. If x_I has more than one neighbor in a given direction, the Eulerian mesh is considered as too coarse to accurately describe the interface and VPM is used. In any case, by decreasing the Eulerian mesh step h, we also decrease the number of points x_I near Σ_h where VPM is used. Hence, the present method is suitable to impose a Dirichlet boundary condition on Σ for Ω_0, when the solution in Ω_1 has no interest. For nodes in this domain, the penalty term has crushed the initial conservation equation and the solution $u_I(x_I)$ for $I\in\mathcal{N}_1$ is only useful to build the physical solution in Ω_0. The solution in Ω_1 far from the interface is obtained using VPM. The imposed solution can be analytical, when possible, or a constant value. The uselessness of the calculation of the solution for these nodes can be treated numerically by switching the solving of $u(x_I), x_I\in\{\Omega_1\}$, $I\notin\mathcal{N}_1$ off, or by totally removing these nodes. Future investigations will be devoted to these topics. The SMP method can be extended to any scalar or vector equations, such as the Navier-Stokes model.

2.3. *Management of the Lagrangian points*

The generation of the Lagrangian mesh of the obstacles is achieved using a computer graphics software. Specific algorithms have been developed to interpret this Lagrangian grid on the Eulerian physical grid. We use a fast ray-casting method (working row by row) to obtain the binary phase functions C_i of objects (strictly 0 or 1). These phase-functions are used to localize the immersed obstacles. These binary C_i functions are used to build an Eulerian Level-Set function near the interface by estimating the distance between the Eulerian points and the neighbor Lagrangian points. The Lagrangian points used to couple the Lagrangian surface of the complex object and the Eulerian grid used to solve the conservation equations are the points x_l of Σ_h. We use two different methods to determine these points.
The first method (SMP-LS) uses the Level-Set function which indicates the signed

distance of an Eulerian point from the interface. Using this Eulerian function, we can quite accurately determine the intersection between an edge of $\mathcal{V}_i'$ and the interface. For example, let us consider two Eulerian points $x_I \in \Omega_0$ and $x_J \in \Omega_1$. We denote by $d_I = d(x_I, \Sigma_h)$ and $d_J = d(x_J, \Sigma_h)$ the unsigned distances between Eulerian points and the interface Σ_h. Then, we obtain $x_l = (x_I d_J + x_J d_I)/(d_I + d_J)$. The efficiency of this method increases with the regularity of the Lagrangian interface. The second method (SMP-GI) calculates the geometric intersection between an edge of $\mathcal{V}_i'$ crossing the interface and the interface. This last method is very accurate but a lot slower.

2.4. *Discretization and solvers*

Details on the discretizations and the validations have previously been published by Vincent *et al.* [VIN 00]. All simulations are based on implicit finite volumes on staggered Cartesian grids. For the Navier-Stokes equations, velocity/pressure coupling is obtained using an Augmented Lagrangian (AL) method. In [SAR 08], the use of 1D linear interpolations only was incompatible with the minimization of the divergence provided by the AL operator. This problem has been solved using multidimensional linear interpolations. Concerning the penalty terms, they are added to the motion equations according to the Eulerian description C_i of the object (low order approach) or to their Lagrangian position x_l (high order method). The penalization parameter ϵ is chosen according to C_i independently of any other numerical or physical parameters. Numerically, $b = 1/\epsilon = 10^{40} C_i$. A particular class of IBM methods, the direct-forcing method [TSE 03] for the Navier-Stokes equations, uses a technique quite similar to SMP to treat the fluid/solid interface. The main difference lies in the integration of the interfacial constraint into the conservation equation. Our technique lies in an implicit penalty method whereas the IBM direct-forcing approach builds a source term. Direct forcing methods uses fractional step methods to ensure pressure/velocity coupling. The AL ensure in only one step both divergence free and penalty constraint, whereas the time splitting approach requires a corrector step to ensure the divergence free constraint which must be adapted to each fictitious domain method. Gibou *et al*. have proposed a fictitious domain approach for scalar equations [GIB 05]. The method uses 1D interpolations which are taken into account by directly modifying the discretization of the operators. [TSE 03] and [GIB 05] explain that their methods requires special treatment of the interpolation when a Lagrangian point is very close to an Eulerian point. In fact, implicit constraints modify the matrix which can loose its diagonal dominance. Numerical problems occurs with SMP method too if coupled with a basic solver such as a Jacobi method. When coupled with a PARDISO direct solver or an iterative BiCG-Stab method and an ILU preconditioning, our method correctly impose the interfacial constraint, no matter the matrix coefficients.

3. Validations and applications

3.1. *Sub Mesh Penalty method for scalar equation*

We solve the homogenous Laplace equation in a numerical square of side 4 with a Dirichlet condition of $u_1 = 10$ on a first circular interface ($R_1 = 1$) and an analytical solution on the boundary of the Eulerian grid. Practically, the analytical solution which accounts for the presence of a second circle with a radius $R_2 = 4$ and $u_2 = 0$ is imposed on the boundary conditions. Fig. 2 left shows a second order of convergence in space for the L^2 relative error. Fig. 2 center and right represent the isovalue $u = 10$, i.e. the Dirichlet value imposed on R_1, obtained from the simulations with the VPM (center) and the SMP method (right). Analytically, the isovalue is a circle. As can be seen, the SMP method greatly improves the shape of the isovalue.

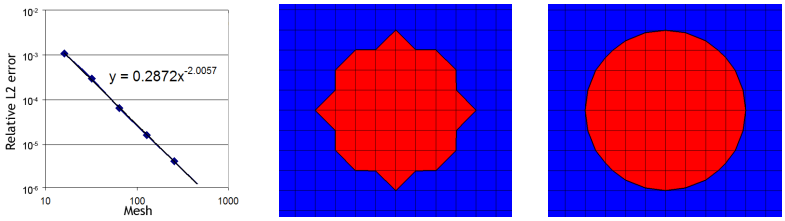

Figure 2. *Relative L^2 convergence of the SMP method and comparison between solutions obtained with VPM and SMP method on a 16×16 grid*

3.2. *Sub Mesh Penalty method for the Navier-Stokes equations on a MAC grid*

We simulate the cylindrical Couette flow in a numerical square of side $0.30\,m$. The inner circle has a rotation speed $\omega_1 = 1\,rad/s$ and a radius $R_1 = 0.05\,m$. We impose the analytical solution on the numerical boundary as the domain is surrounded by a second circle whose rotation speed is $\omega_2 = 2\,rad/s$ and radius is $R_2 = 2\,m$. In Fig. 3 left, 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. The third curve (Velocity LS) shows the convergence rate of the method using the Level-Set function to define x_l (SMP-LS). This method is less accurante than SMP-GI which take the true intersection, and an average order of only 1.55 is obtained. As a second test case, using SMP-GI, we simulate the 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. Fig. 3 right 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. The last case, using SMP-GI, is the measurement of the recirculation length for a 3D flow past a sphere for $Re = 100$. The domain is a box $\Omega = [\,-10\,;10\,] \times [\,-5\,;5\,] \times [\,-5\,;5\,]$

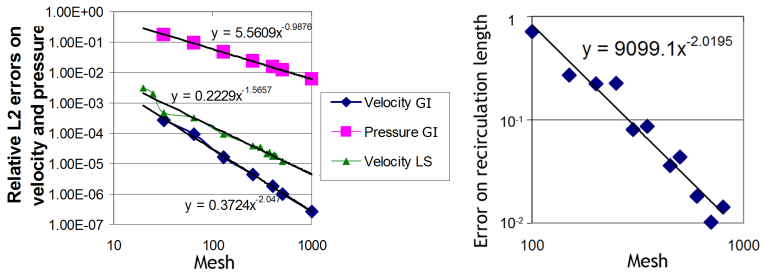

Figure 3. *Relative L^2 error of the SMP method for a Couette flow-Error on recirculation length for a flow past a cylinder*

discretized with a $120 \times 100 \times 100$ Cartesian mesh with irregular space step. A slice of the mesh is presented in Fig. 4 left. Fig. 4 center shows the axisymmetric streamtraces for this case. The ratio $L/d = 0.75$ is in very good agreement with [JOH 99].

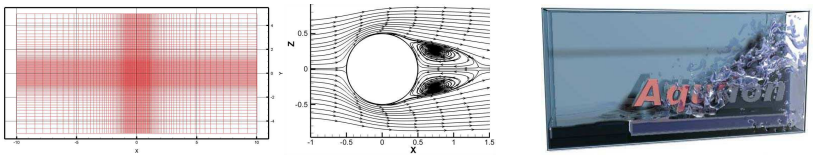

Figure 4. *Mesh and streamtraces for the flow past a sphere-dam break flow over an obstacle*

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 Fig. 4 right). These obstacles are managed using Lagrangian meshes easily generated with 3D computer graphic softwares. Several penalty methods have been implemented and coupled to obtain the interaction between fluid and solid media. The SMP method is second order for both scalar diffusion and the Navier-Stokes equations. The interest of the interpretation and management of triangularized surface of obstacles can be seen in [MKF 07]. This Web site contain several three-dimensional realistic multiphase flow simulations involving the SMP method with Q_0 interpolations. Future works will be devoted to extending the SMP method, coupled to ITPM or VPM, to moving obstacle of arbitrary motion. 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, Adaptive Mesh Refinement (AMR [DEL 06]) techniques will be associated with the tracking of boundary layers in penalized fluid/solid cells.

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