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A Spectacular Vector Penalty-Projection Method for Darcy and Navier-Stokes Problems

Philippe Angot, Jean-Paul Caltagirone and Pierre Fabrie

Abstract We present a new *fast vector penalty-projection method* (VPP_ε), issued from noticeable improvements of previous works [7, 3, 4], to efficiently compute the solution of unsteady Navier-Stokes/Brinkman problems governing incompressible multiphase viscous flows. The method is also efficient to solve anisotropic Darcy problems. The key idea of the method is to compute at each time step an accurate and curl-free approximation of the pressure gradient increment in time. This method performs a *two-step approximate divergence-free vector projection* yielding a velocity divergence vanishing as $\mathcal{O}(\varepsilon \delta t)$, δt being the time step, with a penalty parameter ε as small as desired until the machine precision, e.g. $\varepsilon = 10^{-14}$, whereas the solution algorithm can be extremely fast and cheap. The method is numerically validated on a benchmark problem for two-phase bubble dynamics where we compare it to the Uzawa augmented Lagrangian (UAL) and scalar incremental projection (SIP) methods. Moreover, a new test case for fluid-structure interaction problems is also investigated. That results in a robust method running faster than usual methods and being able to efficiently compute accurate solutions to sharp test cases whatever the density, viscosity or anisotropic permeability jumps, whereas other methods crash.

Key words: Vector penalty-projection; Penalty method; Splitting method; Multiphase Navier-Stokes/Brinkman; Anisotropic Darcy problem; Incompressible flows
MSC 2010: 35Q30, 35Q35, 65M12, 65M85, 65N12, 65N85, 74F10, 76D05, 76D45, 76M25, 76R10, 76S05, 76T10

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1 Introduction to model incompressible multiphase flows

Let $\Omega \subset \mathbb{R}^d$ ($d=2$ or 3 in practice) be an open bounded and connected domain with a Lipschitz continuous boundary $\Gamma = \partial\Omega$ and $\mathbf{n}$ be the outward unit normal vector on Γ . For $T > 0$, we consider the following unsteady Navier-Stokes/Brinkman problem [9] governing incompressible non-homogeneous or multiphase flows where Dirichlet boundary conditions for the velocity $\mathbf{v}|_{\Gamma} = 0$ on Γ , the volumic force $\mathbf{f}$ and initial data $\mathbf{v}(t=0) = \mathbf{v}_0$, $\varphi(t=0) = \varphi_0 \in L^\infty(\Omega)$ with $\varphi_0 \geq 0$ *a.e.* in Ω , are given. For sake of brevity here, we just focus on the model problem (1-3) where $\mathbf{d}(\mathbf{v}) = (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)/2$, as a part of more complex fluid mechanics problems.

$$\rho (\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v}) - 2 \nabla \cdot (\mu \mathbf{d}(\mathbf{v})) + \mu \mathbf{K}^{-1} \mathbf{v} + \nabla p = \mathbf{f} \quad \text{in } \Omega \times (0, T) \quad (1)$$

$$\nabla \cdot \mathbf{v} = 0 \quad \text{in } \Omega \times (0, T) \quad (2)$$

$$\partial_t \varphi + \mathbf{v} \cdot \nabla \varphi = 0 \quad \text{in } \Omega \times (0, T). \quad (3)$$

The permeability tensor $\mathbf{K}$ in the Darcy term is supposed to be symmetric, uniformly positive definite and bounded in Ω . We refer to [1, 9] for the modeling of flows inside complex fluid-porous-solid heterogeneous systems with the Navier-Stokes/Brinkman or Darcy equations. The equation (3) for the positive phase function φ governs the transport by the flow of the interface between two phases, either fluid or solid, respectively in the case of two-phase fluid flows or fluid-structure interaction problems. The force $\mathbf{f}$ may include some volumic forces like the gravity force $\rho \mathbf{g}$ as well as the surface tension force to describe the capillarity effects at the phase interfaces Σ . The advection-diffusion equation for the temperature $\mathcal{T}$ is not precised here and we assume some given state laws: $\rho = \rho(\varphi, \mathcal{T})$ and $\mu = \mu(\varphi, \mathcal{T})$ for each phase, where the functions are continuous and positive.

2 The fast vector-penalty projection method (VPP $_\varepsilon$)

2.1 The (VPP $_\varepsilon$) method for multiphase Navier-Stokes/Brinkman

We describe hereafter the two-step vector penalty-projection (VPP $_\varepsilon$) method with a penalty parameter $0 < \varepsilon \ll 1$; see more details in [5]. For φ^0 with $\varphi^0 \geq 0$ *a.e.* in Ω , $\mathbf{v}^0$ and $p^0 \in L_0^2(\Omega)$ given, the method reads as below with usual notations for the semi-discrete setting in time, $\delta t > 0$ being the time step. For all $n \in \mathbb{N}$ such that $(n+1)\delta t \leq T$, find $\tilde{\mathbf{v}}^{n+1}$, $\mathbf{v}^{n+1}$, $p^{n+1} \in L_0^2(\Omega)$, $\varphi^{n+1} \in L^\infty(\Omega)$, such that:

$$\rho^n \left(\frac{\tilde{\mathbf{v}}^{n+1} - \mathbf{v}^n}{\delta t} + (\mathbf{v}^n \cdot \nabla) \tilde{\mathbf{v}}^{n+1} \right) - 2 \nabla \cdot (\mu^n \mathbf{d}(\tilde{\mathbf{v}}^{n+1})) + \mu^n \mathbf{K}^{-1} \tilde{\mathbf{v}}^{n+1} + \nabla p^n = \mathbf{f}^n \quad (4)$$

$$\frac{\varepsilon}{\delta t} \rho^n \hat{\mathbf{v}}^{n+1} - \nabla (\nabla \cdot \hat{\mathbf{v}}^{n+1}) = \nabla (\nabla \cdot \tilde{\mathbf{v}}^{n+1}) \quad (5)$$

$$\mathbf{v}^{n+1} = \tilde{\mathbf{v}}^{n+1} + \hat{\mathbf{v}}^{n+1}, \quad \text{and} \quad \nabla(p^{n+1} - p^n) = -\frac{\rho^n}{\delta t} \hat{\mathbf{v}}^{n+1} \quad (6)$$

$$p^{n+1} = p^n + \phi^{n+1} \quad \text{with } \phi^{n+1} \text{ reconstructed from } \nabla \phi^{n+1} = -\frac{\rho^n}{\delta t} \hat{\mathbf{v}}^{n+1} \quad (7)$$

$$\frac{\varphi^{n+1} - \varphi^n}{\delta t} + \mathbf{v}^{n+1} \cdot \nabla \varphi^n = 0 \quad (8)$$

with: $\tilde{\mathbf{v}}|_{\Gamma}^{n+1} = 0$, or for non homogeneous Dirichlet conditions: $\tilde{\mathbf{v}}|_{\Gamma}^{n+1} = \mathbf{v}_D^{n+1}$, and $\hat{\mathbf{v}}^{n+1} \cdot \mathbf{n}|_{\Gamma} = 0$. Here $\mathbf{v}^n, p^n$ are desired to be first-order approximations of the exact velocity and pressure solutions $\mathbf{v}(t_n), p(t_n)$ at time $t_n = n \delta t$. Since the end-of-step velocity divergence is not exactly zero, the additional spherical part $\lambda \nabla \cdot \mathbf{v} \mathbf{I}$ of the Newtonian stress tensor is included within the dynamical pressure gradient ∇p . Once the equations (4-8) have been solved, the advection-diffusion equation of temperature can be solved too for $\mathcal{T}^{n+1}$ and we can find: $\rho^{n+1} = \rho(\varphi^{n+1}, \mathcal{T}^{n+1})$ and $\mu^{n+1} = \mu(\varphi^{n+1}, \mathcal{T}^{n+1})$.

The key feature of our method is to calculate an accurate and curl-free approximation of the momentum vector correction $\rho^n \hat{\mathbf{v}}^{n+1}$ in (5). Indeed (5-6) ensures that $\rho^n \hat{\mathbf{v}}^{n+1}$ is exactly a gradient which justifies the choice for $\nabla \phi^{n+1} = \nabla(p^{n+1} - p^n)$ since we have:

$$\rho^n \hat{\mathbf{v}}^{n+1} = \frac{\delta t}{\varepsilon} \nabla (\nabla \cdot \mathbf{v}^{n+1}) \Rightarrow \nabla(p^{n+1} - p^n) = -\frac{\rho^n}{\delta t} \hat{\mathbf{v}}^{n+1} = -\frac{1}{\varepsilon} \nabla (\nabla \cdot \mathbf{v}^{n+1}). \quad (9)$$

The (VPP $_{\varepsilon}$) method effectively takes advantage of the splitting method proposed in [4] for augmented Lagrangian systems or general saddle-point computations to get a very fast solution of (5); see Theorem 1. When we need the pressure field itself, e.g. to compute stress vectors, it is calculated in an incremental way as an auxiliary step. We propose to reconstruct $\phi^{n+1} = p^{n+1} - p^n$ from its gradient $\nabla \phi^{n+1}$ given in (6) with the following method.

Reconstruction of $\phi^{n+1} = p^{n+1} - p^n$ from its gradient.

By circulating on a suitable path starting at a point on the border where $\phi^{n+1} = 0$ is fixed and going through all the pressure nodes in the mesh, we get with the gradient formula between two neighbour points A and B using the mid-point quadrature:

$$\phi^{n+1}(B) - \phi^{n+1}(A) = \int_A^B \nabla \phi^{n+1} \cdot d\mathbf{l} = - \int_A^B \frac{\rho^n}{\delta t} \hat{\mathbf{v}}^{n+1} \cdot d\mathbf{l} \approx -\frac{\rho^n}{\delta t} |\hat{\mathbf{v}}^{n+1}| h_{AB} \quad (10)$$

with h_{AB} = distance (A, B) . The field ϕ^{n+1} is calculated point by point from the boundary and then passing successively by all the pressure nodes. This fast algorithm is performed at each time step to get the pressure field p^{n+1} from the known field p^n . We refer to [5] for more details and validations on the present method.

2.2 The (VPP $_{\varepsilon}$) method for anisotropic Darcy problems

We present below the fast solution to incompressible Darcy flow problems in porous media with the (VPP $_{\varepsilon}$) method. The model problem reads in dimensionless form:

$$s \partial_t \mathbf{v} + \mu \mathbf{K}^{-1} \mathbf{v} + \nabla p = \mathbf{f} \quad \text{in } \Omega \times (0, T) \quad (11)$$

$$\nabla \cdot \mathbf{v} = 0 \quad \text{in } \Omega \times (0, T) \quad (12)$$

$$\mathbf{v} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma \times (0, T) \quad (13)$$

where the viscosity $\mu > 0$ is constant and the permeability tensor $\mathbf{K}$ is supposed to be symmetric, bounded in Ω and uniformly positive definite. The dimensionless stationarity parameter $s > 0$ includes the Darcy number: $Da = K_{ref}/L_{ref}^2$ and thus we have $s \ll 1$ for most practical problems or even $s = 0$ for the steady anisotropic Darcy problem. The equations (11-13) also model flows inside heterogeneous porous-solid systems by letting the permeability tend to zero inside the impermeable media; see also [1, 9] for the analysis and validations of the so-called L^2 volume penalty method.

The (VPP $_{\varepsilon}$) method with $r = \mathcal{O}(\varepsilon) > 0$ and $0 < \varepsilon \ll 1$ to solve (11-13) reads as follows. For all $n \in \mathbb{N}$ such that $(n+1)\delta t \leq T$, find $\tilde{\mathbf{v}}^{n+1}$, $\mathbf{v}^{n+1}$ and p^{n+1} such that:

$$s \frac{\tilde{\mathbf{v}}^{n+1} - \mathbf{v}^n}{\delta t} + \mu \mathbf{K}^{-1} \tilde{\mathbf{v}}^{n+1} - r \nabla (\nabla \cdot \tilde{\mathbf{v}}^{n+1}) + \nabla p^n = \mathbf{f}^n \quad (14)$$

$$\varepsilon \left(\frac{s}{\delta t} + \mu \mathbf{K}^{-1} \right) \hat{\mathbf{v}}^{n+1} - \nabla (\nabla \cdot \hat{\mathbf{v}}^{n+1}) = \nabla (\nabla \cdot \tilde{\mathbf{v}}^{n+1}) \quad (15)$$

$$\mathbf{v}^{n+1} = \tilde{\mathbf{v}}^{n+1} + \hat{\mathbf{v}}^{n+1},$$

$$\text{and } \nabla(p^{n+1} - p^n) = - \left(\frac{s}{\delta t} + \mu \mathbf{K}^{-1} \right) \hat{\mathbf{v}}^{n+1} - r \nabla (\nabla \cdot \tilde{\mathbf{v}}^{n+1}) \quad (16)$$

$$p^{n+1} = p^n + \phi^{n+1} \quad \text{with } \phi^{n+1} \text{ reconstructed from its gradient } \nabla \phi^{n+1} \quad (17)$$

with the boundary conditions: $\tilde{\mathbf{v}}^{n+1} \cdot \mathbf{n}|_{\Gamma} = 0$ and $\hat{\mathbf{v}}^{n+1} \cdot \mathbf{n}|_{\Gamma} = 0$ on Γ . The space discrete solution to the prediction step (14) is explicit for s and r sufficiently small to invert a perturbation of the Identity matrix with a Neumann asymptotic expansion.

3 On the fast discrete solution to the (VPP $_{\varepsilon}$) method

The great interest for solving (5) or (15) instead of a usual augmented Lagrangian problem lies in the following result issued from [4] which shows that the method can be ultra-fast and very cheap if $\eta = \varepsilon/\delta t$ is sufficiently small.

Let us now consider any space discretization of our problem. We denote by $B = -\text{div}_h$ the $m \times n$ matrix corresponding to the discrete divergence operator, $B^T = \text{grad}_h$ the $n \times m$ matrix corresponding to the discrete gradient operator, whereas I denotes the $n \times n$ identity matrix with $n > m$ and D the $n \times n$ diagonal nonsingular matrix containing all the discrete density values of $\rho^n > 0$ a.e. in Ω . Here n is the

number of velocity unknowns whereas m is the number of pressure unknowns. Then, the discrete vector penalty-projection problem corresponding to (5) with $\varepsilon = \eta \delta t$ reads:

$$\left(D + \frac{1}{\eta} B^T B\right) \hat{v}_\eta = -\frac{1}{\eta} B^T B \tilde{v}, \quad \text{with} \quad v_\eta = \tilde{v} + \hat{v}_\eta. \quad (18)$$

We proved in [4] the crucial result below due to the *adapted right-hand side* in the correction step (18) which lies in the range of the limit operator $B^T B$. Indeed, (18) can be viewed as a singular perturbation problem with well-suited data in the right-hand side. More precisely, we give in Theorem 1 the zero-order term of the solution $\hat{v}_\eta$ to (18):

$$\hat{v}_\eta = -\frac{1}{\eta} \left(D + \frac{1}{\eta} B^T B\right)^{-1} B^T B \tilde{v} \quad (19)$$

when the penalty parameter η is chosen sufficiently small; see the asymptotic expansion of $\hat{v}_\eta$ and the proof in [4, Theorem 1.1 and Corollary 1.3].

Theorem 1 (Fast solution of the discrete vector penalty-projection). *Let D be an $n \times n$ positive definite diagonal matrix, I the $n \times n$ identity matrix and B an $m \times n$ matrix. If the rows of B are linearly independent, $\text{rank}(B) = m$, then for all η small enough, $0 < \eta < 1/\|S^{-1}\|$ where $S = BD^{-1}B^T$, there exists an $n \times n$ matrix C_1 bounded independently on η such that the solution of the correction step (19) writes for any vector $\tilde{v} \in \mathbb{R}^n$:*

$$\hat{v}_\eta = C_0 \tilde{v} + \eta C_1 \tilde{v} \quad \text{with} \quad C_0 = -D^{-1}B^T S^{-1}B = -D^{-1}B^T (BD^{-1}B^T)^{-1}B. \quad (20)$$

If $\text{rank}(B) = p < m$, there exists a surjective $p \times n$ matrix T such that $B^T B = T^T T$ and a similar result holds replacing B by T .

Hence, for a constant density $\rho > 0$ and choosing now $\eta = \rho \varepsilon / \delta t$, we have: $D = I$, $S = BB^T$ and $C_0 = -B^T S^{-1}B = -B^T (BB^T)^{-1}B$. Moreover, if $\text{rank}(B) = p \leq m \leq n$, the zero-order solution $\hat{v} = C_0 \tilde{v}$ in (20) is the solution of minimal Euclidean norm in $\mathbb{R}^n$ to the linear system: $B \hat{v} = -B \tilde{v}$ by the least-squares method, and the matrix $B^\dagger = B^T (BB^T)^{-1}$ is the Moore-Penrose pseudo-inverse of B such that $C_0 = -B^\dagger B$. Indeed, a singular value decomposition (SVD) or a QR factorization of B yields: $C_0 = -I_0$ where I_0 is the $n \times n$ diagonal matrix having only 1 or 0 coefficients, the zero entries in the diagonal being the $n - p$ null eigenvalues of the operator $B^T B$.

Hence, for η small enough, the computational effort required to solve (18) amounts to approximate the matrix C_0 which includes both D and D^{-1} inside non commutative products. Thus, we always use the diagonal preconditioning in the case of a variable density which makes the effective condition number quasi-independent on the density or permeability jumps. We also use the Jacobi preconditioner in the prediction step (4) to cope with the viscosity or permeability jumps as performed in [9]. However, for a constant density when $D = I$, we get $C_0 = -I_0$. This explains why the solution can be obtained with only one iteration of a suitable preconditioned Krylov solver whatever the size of the mesh step or the dimension n ; see the numerical results in [4].

4 Numerical validations with discrete operator calculus

The (VPP_ε) method has been implemented with discrete exterior calculus (DEC) methods, see the recent review in [6], for the space discretization of the Navier-Stokes equations on unstructured staggered meshes. The (DEC) methods ensure primary and secondary discrete conservation properties. In particular, the space discretization satisfies for the discrete operators: $\nabla_h \times (\nabla_h \phi) = 0$ and $\nabla_h \cdot (\nabla_h \times \psi) = 0$, which is not usually verified by other methods; see [6]. Hence, the (VPP_ε) method is now validated on unstructured meshes both in 2-D or 3-D.

The structure and solver of the computational code are issued from previous works, originally implemented with a Navier-Stokes finite volume solver on the staggered MAC mesh and using the Uzawa augmented Lagrangian (UAL) method to deal with the divergence-free constraint; see [9]. We refer to [1, 2, 9] and the references therein for the analysis and numerical validations of the fictitious domain model using the so-called L^2 or H^1 -penalty methods to take account of obstacles in flow problems with the Navier-Stokes/Brinkman equations. Hence, our approach is essentially Eulerian with a Lagrangian front-tracking of the sharp interfaces accurately reconstructed on the fixed Eulerian mesh, see e.g. [10, 11] and the references therein. Thus we use no Arbitrary Lagrangian-Eulerian (ALE) method, no global remeshing nor moving mesh method.

Fig. 1 Benchmark for 2-D bubble dynamics with (VPP_ε) method, $\varepsilon = 10^{-8}$: motion of a circular bubble with surface tension at time $t = 3$ and $Re = 35$ - bubble initial diameter $\phi = 0.05$, $\rho_1/\rho_2 = 1000/100 = 10$, $\mu_1/\mu_2 = 10/1 = 10$, domain 0.1×0.2 , mesh size 128×256 , $\delta t = 0.007143$, circular bubble initially with no motion at height $y = 0.05$. LEFT: isobars and isoline $\phi = 0.5$ of the phase function at interface. RIGHT: superposition of isoline $\phi = 0.5$ at interface for (UAL), (SIP), (VPP) and vertical velocity field (in absolute referential).

4.1 Multiphase flows: dispersed two-phase bubble dynamics

The (VPP_ε) method is numerically validated for multiphase incompressible flows by performing with the three methods (UAL), (SIP) and (VPP), the benchmark problem studied in [8] for 2-D bubble dynamics. In that problem, we compute the first test case which considers an initial circular bubble of diameter $0.05m$ with density and viscosity ratios equal to 10 which undergoes moderate shape deformation. In this

case, the bubble is driven up by the external gravity force $\mathbf{f} = \rho \mathbf{g}$, whereas the surface tension effect on the interface Σ between the two fluid phases is taken into account through the following force balance at the interface Σ :

$$[[\mathbf{v}]]_{\Sigma} = 0 \quad \text{and} \quad [[(-p\mathbf{I} + \mu(\nabla\mathbf{v} + (\nabla\mathbf{v})^T)) \cdot \mathbf{n}]]_{\Sigma} = \sigma \kappa \mathbf{n}_{|\Sigma}, \quad \text{or} \quad \mathbf{f}_{st} = \sigma \kappa \mathbf{n}_{|\Sigma} \delta_{\Sigma}$$

where $\sigma = 24.5$ is the surface tension coefficient, κ the local curvature of the interface, $\mathbf{n}_{|\Sigma}$ the outward unit normal to the interface and δ_{Σ} the Dirac measure supported by the interface Σ . The solution of the phase transport (3) is carried out by the so-called *VOF-PLIC* method, *i.e.* the famous *VOF* method using a piecewise linear interface construction proposed in [12] to precisely reconstruct the sharp interface Σ at the isoline $\varphi = 0.5$, with $\varphi^0 = 0$ in Ω_1 and $\varphi^0 = 1$ in Ω_2 ; see [10, 11].

The results of the three methods (UAL), (SIP) and (VPP) after 420 time iterations are presented in Figure 1 by superposing the different fields to get a more precise comparison. We observe an excellent agreement both between the three methods and the reference solution in [8]. However, the (VPP) method runs faster.

Fig. 2 ACF11-ball with (VPP $_{\varepsilon}$) method, $\varepsilon = 10^{-6}$: free fall of a heavy solid body in air at time $t = 0.15$ and $\text{Re} = 7358$ - Cylinder diameter $\varnothing = 0.05$, $\rho_s = 10^6$, $\rho_f = 1$, $\mu_s = 10^{12}$, $\mu_f = 10^{-5}$, domain 0.1×0.2 , mesh size 256×512 , $\delta t = 0.0002$, cylinder initially with no motion at height $y = 0.15$. LEFT: isobars and isoline $\varphi = 0.5$ of the phase function at interface. RIGHT: vertical velocity field and horizontal velocity isolines.

4.2 A test case for fluid-structure interaction problems

To evaluate the robustness of the (VPP $_{\varepsilon}$) method with respect to large density or viscosity ratios, we compute the motion of an heavy solid body which freely falls vertically in air with the gravity force $\mathbf{f} = \rho_s \mathbf{g}$. The rigid behaviour of the body is obtained by letting the viscosity μ_s tend to infinity inside the ball in order to penalize the tensor of deformation rate $\mathbf{d}(\mathbf{v})$. This fictitious domain method using a penalty

was studied in [1] (see the references therein) to design a numerical wind-tunnel, then numerically validated in several works, e.g. [11], and also analyzed theoretically in [1, 2] where optimal global error estimates are proved for the H^1 penalty method. Moreover, this fictitious domain method allows us to easily compute the forces applied on the obstacle, see [9]; the error estimate being proved in [1] when the nonlinear convection term is neglected inside the solid obstacle.

The results obtained by the (VPP_ε) method are presented in Figure 2 at time $t = 0.15s$ after 750 time iterations when the ball velocity reaches: $V_b = gt = 1.4715 m/s$. The computation shows that the strain rate tensor inside the ball Ω_s vanishes as $\|\mathbf{d}(\mathbf{v})\|_{L^2(\Omega_s)} = \mathcal{O}(\mu_f/\mu_s)$, i.e. of the order of the machine precision. Hence, the (VPP_ε) method efficiently ensures both the rigidity of the solid body and a velocity divergence vanishing as $\mathcal{O}(\varepsilon \delta t)$ [5], whereas it avoids the blocking effect observed with other methods; see e.g. [11].

The (SIP) method crashes after a few time iterations. The (UAL) method is still able to compute the flow with a larger velocity divergence and the computation is far more expensive than with the (VPP_ε) method.

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The paper is in final form and no similar paper has been or is being submitted elsewhere.