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A spectacular solver of low-Mach multiphase Navier-Stokes problems under strong stresses

Philippe Angot, Jean-Paul Caltagirone and Pierre Fabrie

Abstract We present the main features and sharp numerical applications of the *fast vector penalty-projection methods* (VPP_ε) [1, 2, 3], based on three key ideas explained further. In particular, we proposed new fast Helmholtz-Hodge decompositions of L^2 -vector fields in bounded domains by solving vector elliptic problems penalized with suitable adapted right-hand sides [4]. *This procedure, used as an approximate divergence-free velocity projection step, yields a velocity divergence vanishing as $\mathcal{O}(\varepsilon \delta t)$, δt being the time step. It only requires a few iterations of preconditioned conjugate gradients whatever the spatial mesh step h , if the penalty parameter ε is chosen sufficiently small up to machine precision, e.g. $\varepsilon = 10^{-14}$.* These methods prove to be efficient, fast and robust to accurately compute incompressible or low Mach multiphase flows under strong stresses: large mass density, viscosity or anisotropic permeability jumps, strong surface tension inducing large interface deformations, or with open boundary conditions, whereas other methods either cannot reach the suitable mesh convergence and run slower or simply crash.

1 Introduction: time-splitting methods for Navier-Stokes

We consider the numerical solution of unsteady incompressible viscous flows with variable density in a bounded domain $\Omega \subset \mathbb{R}^3$, the frontier $\partial\Omega := \Gamma = \Gamma_D \cup \Gamma_N$ ($\Gamma_D \cap \Gamma_N = \emptyset$) being subjected to a Dirichlet boundary condition $\mathbf{v} = \mathbf{v}_D$ on Γ_D and a given traction stress vector $\boldsymbol{\sigma}(\mathbf{v}, p) \cdot \mathbf{n} := -p\mathbf{n} + \mu(\nabla\mathbf{v} + (\nabla\mathbf{v})^t) \cdot \mathbf{n} = \mathbf{g}$ on Γ_N . Many splitting projection methods [8] of Chorin-Temam's type require, at each time step $t_n = n\delta t$, the solution of the *pressure Poisson equation* to get the divergence-free velocity field \mathbf{v}^{n+1} from a standard first-order velocity prediction step giving $\tilde{\mathbf{v}}^{n+1}$:

$$\begin{cases} \operatorname{div} \left(\frac{\delta t}{\rho^{n+1}} \nabla \phi^{n+1} \right) = \operatorname{div} \tilde{\mathbf{v}}^{n+1}, \\ \nabla \phi^{n+1} \cdot \mathbf{n}|_{\Gamma_D} = 0, \quad \phi|_{\Gamma_N}^{n+1} = 0. \end{cases} \Rightarrow \begin{cases} \rho^{n+1} \frac{\mathbf{v}^{n+1} - \tilde{\mathbf{v}}^{n+1}}{\delta t} + \nabla \phi^{n+1} = 0, \\ \phi^{n+1} = p^{n+1} - p^n, \quad \operatorname{div} \mathbf{v}^{n+1} = 0. \end{cases} \quad (1)$$

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However, our experience with many Navier-Stokes solvers leads us to formulate the following conjecture. We cannot prove it rigorously, but several arguments explained further are likely to confirm it; see also [5] for a more precise analysis.

Conjecture 1 (Numerical solution of Navier-Stokes equations). The main drawbacks of splitting projection methods arise from the introduction of the scalar pressure Poisson equation (1) involving a spatial derivative of mass density which inherently limits the consistency by degrading the original vector formulation of the Navier-Stokes problems.

This yields the first crucial point considered in the development of the new family of vector penalty-projection (VPP) methods.

Key idea 1 (Vector-penalty projection methods for Navier-Stokes equations.)

To keep a fully vector formulation of the numerical methods for the solution of Navier-Stokes problems, it is essential to compute at each time step an accurate and curl-free approximation of the pressure gradient, and then reconstruct the pressure field if necessary. Thus, the primary unknowns should be the velocity and pressure gradient vectors $(\mathbf{v}, \nabla p)$. This is the objective of the VPP methods proposed in [1, 2, 3] to directly calculate the curl-free component $\hat{\mathbf{v}}^{n+1} := \mathbf{v}^{n+1} - \tilde{\mathbf{v}}^{n+1}$ of $\tilde{\mathbf{v}}^{n+1}$.

It is not so surprising remembering that Euler¹ introduces the so-called *Euler equations* from the works of Bernoulli² and D'Alembert³ by defining $\mathbf{F}_p := -\nabla p$ as the pressure force which induces the fluid motion.

2 Fast Helmholtz-Hodge decompositions in bounded domains

For a given vector field $\mathbf{v} \in \mathbf{L}^2(\Omega) := L^2(\Omega)^3$, later chosen as the predicted velocity $(-\tilde{\mathbf{v}}^{n+1})$, let us now consider the orthogonal Helmholtz-Hodge decomposition :

$$\mathbf{v} = \mathbf{v}_\phi + \mathbf{v}_\psi, \quad \text{with} \quad \mathbf{v}_\phi = \nabla \phi, \quad \mathbf{v}_\psi = \mathbf{rot} \psi, \quad \text{div} \psi = 0, \quad \mathbf{v}_\psi \cdot \mathbf{n}|_\Gamma = 0. \quad (2)$$

The last normal boundary condition is necessary to ensure the \mathbf{L}^2 -orthogonality and thus the uniqueness of the components \mathbf{v}_ϕ and \mathbf{v}_ψ , the scalar potential ϕ and vector potential ψ being determined up to an additive constant. Then, for $\mathbf{v} \in \mathbf{H}_{div}(\Omega)$ we have in Ω , supposed to be at least connected and possibly simply connected :

$$\begin{cases} \text{div} \mathbf{v}_\phi = \text{div} \mathbf{v}, & \mathbf{rot} \mathbf{v}_\phi = 0, \\ \mathbf{v}_\phi \cdot \mathbf{n}|_\Gamma = \mathbf{v} \cdot \mathbf{n} \text{ on } \Gamma. \end{cases} \quad \text{and} \quad \begin{cases} \mathbf{rot} \mathbf{v}_\psi = \mathbf{rot} \mathbf{v}, & \text{div} \mathbf{v}_\psi = 0, \\ \mathbf{v}_\psi \cdot \mathbf{n}|_\Gamma = 0 \text{ on } \Gamma. \end{cases} \quad (3)$$

¹ Leonhard Euler, Principes g n raux du mouvement des fluides (1755)

² Daniel Bernoulli, Hydrodynamica (1738)

³ Jean Le Rond d'Alembert, Trait  de dynamique (1743 & 1749)

Key idea 2 (Fast Helmholtz-Hodge decompositions of L^2 -vector fields.)

The curl-free component \mathbf{v}_ϕ and the divergence-free (solenoidal) component \mathbf{v}_ψ of \mathbf{v} satisfying (3) can be accurately and efficiently calculated with a penalization method by respectively solving the vector penalty-projection problem (VPP $_n$) and the rotational penalty-projection (RPP $_\tau$) problem below, as proposed in [4].

Moreover, the computation can be extremely fast whatever the spatial mesh step h if the penalty parameter $\varepsilon > 0$ is chosen sufficiently small up to machine precision. Indeed, these problems take advantage of the splitting penalty method for saddle-point [2] in order to get adapted right-hand sides when $\varepsilon \rightarrow 0$, and the effective conditioning becomes independent of ε and h , as confirmed numerically in [3, 4, 6].

$$(VPP_n) \begin{cases} \varepsilon \mathbf{v}_\phi^\varepsilon - \nabla (\operatorname{div} \mathbf{v}_\phi^\varepsilon) = -\nabla (\operatorname{div} \mathbf{v}) & \text{in } \Omega \\ \mathbf{v}_\phi^\varepsilon \cdot \mathbf{n}|_\Gamma = \mathbf{v} \cdot \mathbf{n} & \text{on } \Gamma \end{cases} \Rightarrow \begin{cases} \mathbf{v}_\phi^\varepsilon = \frac{1}{\varepsilon} \nabla (\operatorname{div} (\mathbf{v}_\phi^\varepsilon - \mathbf{v})), \\ \phi^\varepsilon = \frac{1}{\varepsilon} \operatorname{div} (\mathbf{v}_\phi^\varepsilon - \mathbf{v}), \mathbf{v}_\phi^\varepsilon = \nabla \phi^\varepsilon \end{cases}$$

$$(RPP_\tau) \begin{cases} \varepsilon \mathbf{v}_\psi^\varepsilon + \operatorname{rot} (\operatorname{rot} \mathbf{v}_\psi^\varepsilon) = \operatorname{rot} (\operatorname{rot} \mathbf{v}) & \text{in } \Omega \\ (\operatorname{rot} \mathbf{v}_\psi^\varepsilon) \wedge \mathbf{n}|_\Gamma = (\operatorname{rot} \mathbf{v}) \wedge \mathbf{n} & \text{on } \Gamma \end{cases} \Rightarrow \begin{cases} \mathbf{v}_\psi^\varepsilon = \frac{1}{\varepsilon} \operatorname{rot} (\operatorname{rot} (\mathbf{v} - \mathbf{v}_\psi^\varepsilon)), \\ \psi^\varepsilon = \frac{1}{\varepsilon} \operatorname{rot} (\mathbf{v} - \mathbf{v}_\psi^\varepsilon), \mathbf{v}_\psi^\varepsilon = \operatorname{rot} \psi^\varepsilon \end{cases}$$

Theorem 3 (Optimal accuracy for (VPP $_n$) and (RPP $_\tau$) problems).

For any $\mathbf{v} \in \mathbf{H}_{\operatorname{div}}(\Omega) \cap \mathbf{H}_{\operatorname{rot}}(\Omega)$ and all $\varepsilon > 0$, the unique solution $\mathbf{v}_\phi^\varepsilon$ or $\mathbf{v}_\psi^\varepsilon$ to the (VPP $_n$) or (RPP $_\tau$) problems respectively, satisfies the optimal error estimates below:

$$(i) \quad \|\mathbf{v}_\phi - \mathbf{v}_\phi^\varepsilon\|_1 + \|\operatorname{div} (\mathbf{v} - \mathbf{v}_\phi^\varepsilon)\|_1 + \|\phi - \phi^\varepsilon\|_2 \leq c_1(\Omega) \|\mathbf{v}\|_0 \varepsilon,$$

$$(ii) \quad \|\mathbf{v}_\psi - \mathbf{v}_\psi^\varepsilon\|_1 + \|\operatorname{rot} (\mathbf{v} - \mathbf{v}_\psi^\varepsilon)\|_1 + \|\psi - \psi^\varepsilon\|_2 \leq c_2(\Omega) \|\mathbf{v}\|_0 \varepsilon.$$

Proof. See [4], [5, Sect. 3], Ω being connected or simply connected for (RPP $_\tau$). The convergence towards 3-D Navier-Stokes weak solutions for constant density is also proved in [7] for a continuous version of the (VPP $_\varepsilon$) method when $\varepsilon \rightarrow 0$. \square

The condition number κ of the discrete left-hand side operators for these problems varies as $\kappa = \mathcal{O}(1/(\varepsilon h^2))$. Thus, the associated matrices are ill-conditioned in the usual sense for $\varepsilon \ll 1$ since the number of iterations of a preconditioned conjugate gradient solver verifies $\mathcal{N}_{\operatorname{iter}} \leq \mathcal{O}(\sqrt{\kappa})$, which is the bound in the worst case for an arbitrary right-hand side (Arrhs). However, the amazingly fast convergence history observed in [3, Fig. 3] and [4, Fig. 2] for these *P.D.E. problems with adapted right-hand sides (Adrhs)* can be explained by defining the notion of *effective condition number of the whole linear system*; see [2, Corollary 1.2 & 1.3]. Indeed, the linear system itself is extremely well-conditioned in this latter case.

Let us look at a simple example where $f \in H^{-1}(\Omega)$ or $u \in H_0^1(\Omega)$ are given:

$$(Arrhs) \begin{cases} \varepsilon u_\varepsilon - \Delta u_\varepsilon = f & \text{in } \Omega, \\ u_\varepsilon = 0 & \text{on } \Gamma. \end{cases} \quad \text{or} \quad (Adrhs) \begin{cases} \varepsilon u_\varepsilon - \Delta u_\varepsilon = -\Delta u & \text{in } \Omega, \\ u_\varepsilon = 0 & \text{on } \Gamma. \end{cases} \quad (4)$$

In this simple case, since the operator $-\Delta : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$ is a (bi-continuous) isomorphism between Hilbert spaces, we can even take here $\varepsilon = 0$ and it is clear that $u_0 = u$ and $\|u_\varepsilon - u\|_1 \leq c(\Omega) \|u\|_0 \varepsilon$ for (Adrhs). Now, let $A_h := -\Delta_h$, a symmetric positive definite matrix, be the discrete Laplacian operator with homogeneous

Dirichlet boundary condition, e.g. by standard finite differences. Then, the matrix system $\mathcal{A}_{\varepsilon,h} := \varepsilon I + A_h$ verifies $\kappa := \text{cond}_2(\mathcal{A}_{\varepsilon,h}) \xrightarrow{\varepsilon \rightarrow 0} \text{cond}_2(A_h) = \mathcal{O}(1/h^2)$. Nevertheless using Neumann series, since $\mathcal{A}_{\varepsilon,h} = A_h(I + \varepsilon A_h^{-1})$, we get the asymptotic expansion of the discrete solution $u_{\varepsilon,h}$ in both cases when $\varepsilon < 1/\|A_h^{-1}\|$:

$$(\text{Arrhs}) \begin{cases} (\varepsilon I + A_h) u_{\varepsilon,h} = f_h, \\ \Rightarrow u_{\varepsilon,h} = A_h^{-1} f_h + \mathcal{O}(\varepsilon). \end{cases} \quad \text{or} \quad (\text{Adrhs}) \begin{cases} (\varepsilon I + A_h) u_{\varepsilon,h} = A_h u_h, \\ \Rightarrow u_{\varepsilon,h} = u_h + \mathcal{O}(\varepsilon). \end{cases} \quad (5)$$

Hence for $\varepsilon \ll 1$, the zero-order term in these expansions is a good approximation of $u_{\varepsilon,h}$, but its computation for *(Arrhs)* requires the solution of the linear system $A_h u_{0,h} = f_h$ with a condition number as $\mathcal{O}(1/h^2)$, whereas $u_{0,h} = u_h$ for *(Adrhs)* and therefore, the effective condition number is bounded independently on both ε and h in this case.

In [2, Theorem 1.1 & Corollary 1.3], a generalization of such a result is proved for *(VPP_n)* problems, although the $\nabla(\text{div})$ operator is not invertible. A similar result also holds for *(RPP_{\tau})* problems using the identity $-\Delta \mathbf{u} = \text{rot}(\text{rot} \mathbf{u}) - \nabla(\text{div} \mathbf{u})$ for all vector field \mathbf{u} in 3-D.

3 Vector penalty-projection methods for Navier-Stokes equations

Let us now consider the incompressible multiphase Navier-Stokes model during the time interval $(0, T)$ and supplemented with suitable initial and boundary conditions:

$$\begin{cases} \rho (\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v}) - 2 \text{div} (\mu(\rho) \mathbf{d}(\mathbf{v})) + \nabla p = \mathbf{f} & \text{in } \Omega \times (0, T), \\ \text{div} \mathbf{v} = 0 & \text{in } \Omega \times (0, T), \\ \partial_t \rho + \text{div}(\rho \mathbf{v}) = 0 & \text{in } \Omega \times (0, T). \end{cases} \quad (6)$$

Here, $\mathbf{d}(\mathbf{v}) := (\nabla \mathbf{v} + (\nabla \mathbf{v})^t)/2$ denotes the strain rate tensor and $\mathbf{f} = \rho \mathbf{g} + \sigma_{st} \kappa \mathbf{n}_\Sigma \delta_\Sigma$ includes the gravity force and surface tension on interfaces Σ , κ being the curvature of Σ and δ_Σ the Dirac measure supported on Σ , which yields the immersed stress jump interface condition on Σ : $\llbracket \sigma(\mathbf{v}, p) \cdot \mathbf{n} \rrbracket_\Sigma = \sigma_{st} \kappa \mathbf{n}_\Sigma$.

Then as proposed in [1, 3], using a phase function φ to track the motion and deformation of Σ by VOF-PLIC or level-set methods, e.g. [10] and the references therein, the fast *(VPP_{\varepsilon})* method reads with a first-order linearly implicit scheme:

$$\begin{cases} \rho(\varphi^n) \left(\frac{\tilde{\mathbf{v}}^{n+1} - \tilde{\mathbf{v}}^n}{\delta t} + (\mathbf{v}^n \cdot \nabla) \tilde{\mathbf{v}}^{n+1} \right) - 2 \text{div} (\mu(\varphi^n) \mathbf{d}(\tilde{\mathbf{v}}^{n+1})) + \nabla p^n = \mathbf{f}^n, \\ \rho(\varphi^n) \frac{\hat{\mathbf{v}}^{n+1} - \hat{\mathbf{v}}^n}{\delta t} - \frac{1}{\varepsilon} \nabla (\text{div} \hat{\mathbf{v}}^{n+1}) = \frac{1}{\varepsilon} \nabla (\text{div} \tilde{\mathbf{v}}^{n+1}), \text{ with } \hat{\mathbf{v}}^{n+1} \cdot \mathbf{n}|_\Gamma = 0, \\ \mathbf{v}^{n+1} = \tilde{\mathbf{v}}^{n+1} + \hat{\mathbf{v}}^{n+1}, \quad \text{velocity and pressure gradient corrections} \\ \varphi^{n+1} = p^{n+1} - p^n \text{ from: } \nabla \varphi^{n+1} = \nabla (p^{n+1} - p^n) = -\rho(\varphi^n) \frac{\hat{\mathbf{v}}^{n+1} - \hat{\mathbf{v}}^n}{\delta t} \\ \frac{\varphi^{n+1} - \varphi^n}{\delta t} + \mathbf{v}^{n+1} \cdot \nabla \varphi^n = 0. \end{cases} \quad (7)$$

Key idea 4 (Vector penalty-projection methods for variable density flows.)

In the fast (VPP $_{\varepsilon}$) prediction-correction method (7) for non-homogeneous Navier-Stokes equations, the mass density ρ is only included in the diagonal of the discrete velocity penalty-projection step and a cheap diagonal preconditioning is therefore recommended. This ensures not only the space-time consistency with the pressure gradient correction by keeping a fully vector formulation of the scheme, but also does not introduce any spatial derivative of ρ . This important feature makes the robustness of the method insensitive to large variations of density [1, 3].

Besides, the fully vector formulation of (VPP $_{\varepsilon}$) versions with a formally second-order time scheme yields a natural expression of outflow boundary conditions with a given stress vector (traction or pseudo-traction). It ensures the optimal second-order accuracy in time and space, both for the velocity and pressure fields [6].

For low-Mach number flows, typically when $M < 0.2$, the parameter ε has a physical meaning since it can be related as below [5] to the Mach number $M := V/c$ (V being a given reference velocity and c the speed of acoustic waves), the velocity divergence vanishing as $\mathcal{O}(\chi_T)$ where χ_T, χ_S are the isothermal or isentropic compressibility coefficients of the fluid and $\gamma := c_p/c_v \geq 1$:

$$\varepsilon \delta t = \chi_T = \gamma \chi_S = \frac{\gamma M^2}{\rho V^2}, \quad \text{or also} \quad \gamma M^2 = \rho V^2 (\varepsilon \delta t) \ll 1. \quad (8)$$

4 Sharp test cases with large density jumps or surface tension

The (VPP $_{\varepsilon}$) method, spatially discretized with the finite volume method on the cartesian staggered MAC grid or generalized MAC unstructured meshes, was tested and validated in [1, 3] against usual standard benchmark problems. In particular, the comparison with the scalar incremental projection (SIP) or Uzawa augmented Lagrangian (UAL) methods was excellent for the first benchmark in [9]; see [3, Fig. 4].

As shown in the video during the talk, we have computed with the (VPP $_{\varepsilon}$) method combined with VOF-PLIC [10], the dispersed two-phase dynamics of air bubbles in a liquid melted steel at a temperature of about 850°C. Here we have a large mass density ratio $\rho_l/\rho_g = 8000$, a viscosity ratio of $\mu_l/\mu_g = 6$ and a large surface tension constant $\sigma_{st} = 1.5 \text{ N/m}$ which induces very large shape deformations of the bubble. A few results are shown in Fig. 1, either with an initial cylindrical bubble centered inside the steel column which is then rising along the median, or with a non centered initial bubble which rises by oscillating from the left to the right side.

Nevertheless for dispersed bubbly flows, it is difficult to compare our numerical method with others since most of them have difficulties to compute results with a suitable mesh convergence when the mass density ratio exceeds several hundreds; see [9, second benchmark]. Thus, to evaluate and validate the robustness of the (VPP $_{\varepsilon}$) method with respect to large density or viscosity ratios, we computed in [3, Fig. 5] the motion of a heavy solid ball which freely falls vertically in air with the gravity force $\mathbf{f} = \rho_s \mathbf{g}$. Here we have : $\rho_s/\rho_g = 10^6$ and $\mu_s/\mu_g = 10^{17}$.

Indeed, the SIP method crashes after a few time iterations. The UAL method is still able to compute the flow but with a larger velocity divergence and the computation is far more expensive than with (VPP $_{\varepsilon}$).

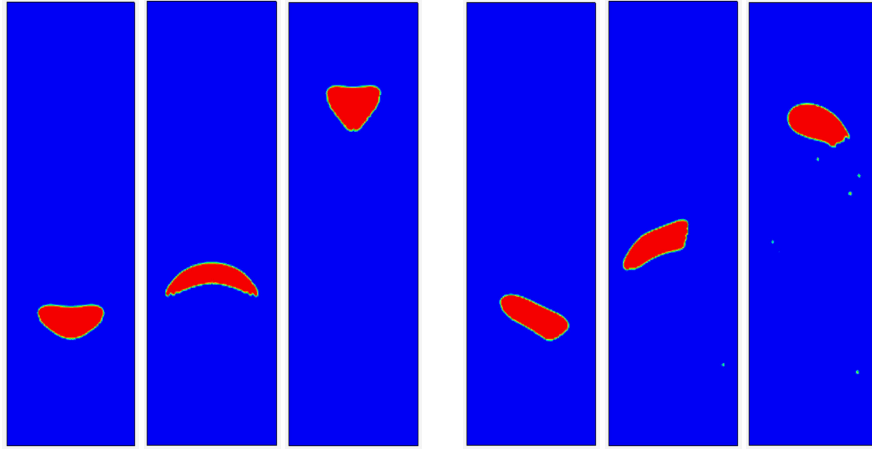


Fig. 1 2-D air bubble dynamics in melted steel (at about 850°C) with $(\text{VPP}_{\varepsilon})$ method, $\varepsilon = 10^{-8}$: cylindrical initial diameter $d = 1\text{ cm}$ in a steel column $L = 3\text{ cm} \times H = 10\text{ cm}$, $\rho_l/\rho_g = 8000$, $\mu_l/\mu_g = 6$, $\sigma_{st} = 1.5\text{ N/m}$, $g = 9.81\text{ m/s}^2$ – Isolines of the VOF-PLIC function at different times: LEFT: bubble initially centered in the column — RIGHT: bubble initially non-centered.

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