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The violation of objectivity in Laplace formulations of the Navier–Stokes equations

A. Limache[1,*,†], S. Idelsohn[1,2,‡], R. Rossi[2] and E. Oñate[2]

[1]*International Center of Computational Methods in Engineering* (*CIMEC*), *INTEC-CONICET-UNL*, *Santa Fe*, *Argentina*
[2]*International Center for Numerical Methods in Engineering* (*CIMNE*), *Barcelona*, *Spain*

SUMMARY

The Navier–Stokes equations written in Laplace form are often the starting point of many numerical methods for the simulation of viscous flows. Imposing the natural boundary conditions of the Laplace form or neglecting the viscous contributions on free surfaces are traditionally considered reasonable and harmless assumptions. With these boundary conditions any formulation derived from integral methods (like finite elements or finite volumes) recovers the pure Laplacian aspect of the strong form of the equations. This approach has also the advantage of being convenient in terms of computational effort and, as a consequence, it is used extensively. However, we have recently discovered that these resulting Laplacian formulations violate a basic axiom of continuum mechanics: the principle of objectivity. In the present article we give an accurate account about these topics. We also show that unexpected differences may sometimes arise between Laplace discretizations and divergence discretizations. Copyright © 2007 John Wiley & Sons, Ltd.

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*Correspondence to: Dr Alejandro Limache, CIMEC, INTEC, Guemes 3450, Santa Fe 3000, Argentina.
†E-mail: alejandrolimache@hotmail.com; http://www.cimec.org.ar/∼alimache
‡ICREA Research Professor.

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1. INTRODUCTION

The incompressible Navier–Stokes (N–S) equations under the approximation of a nearly constant viscosity is probably the most known and one of the most used equation of fluid mechanics. Starting from the equation of conservation of momentum, the N–S equations may be written as the divergence of the Cauchy stress plus the external forces equal to the inertial terms. Nevertheless, taking into account the equation of conservation of mass and supposing that the viscosity is constant or nearly constant, it turns out that the divergence of the Cauchy stress can be simply written as the Laplacian of the velocity field times the viscosity. For this reason, this last form is named the Laplace form of the N–S equations. This form is exactly equivalent to the original divergence form for all cases of incompressible flows with constant viscosity.

The Laplace form is, most of the time, the form in which the N–S equations are presented in the literature, probably because of historical reasons, since its simple form allows to obtain some analytical solutions and probably also for the fact that the three components of the velocity field appear uncoupled being only coupled by the pressure terms. This latter advantage is taken into account in some iterative solution methods, for instance projection methods or fractional step methods, in which each velocity component may be solved separately at each iteration with a large improvement in the computing time and memory.

In the development of modern approaches based on integral/weak forms such as finite elements and finite volumes, a careful analysis shows that the Laplace form introduces some additional boundary terms. This is not a problem *per se*, as long as one manages to incorporate these additional terms into the formulation. Nevertheless, it has become a common practice to introduce seemingly small and reasonable approximations on the boundary so as to neglect these additional terms. The resulting formulation has better property in that the Laplacian nature of the stress terms in the strong form is preserved in the weak form.

Although a number of stabilized fractional-step formulations for different velocity–pressure interpolations were proposed based on the divergence form (see, for example, [1–3]), the Laplace form is what we see most of the time in fractional-step algorithms. Similarly, the Laplace form is what we see most often in pressure-projection methods.

However, Limache and Idelsohn [4] have recently discovered that these Laplacian formulations introduce an error which results in the violation of a main axiom of continuum mechanics: the principle of objectivity. In this article, we will extend the theoretical results presented in [4] and for the first time we will show some of the effects of this violation on real numerical simulations.

2. NAVIER–STOKES EQUATIONS IN DIVERGENCE FORM

The *equations of conservation of mass and conservation of momentum in strong form* of an incompressible fluid material are given by

$$\nabla \cdot \mathbf{v} = 0 \tag{1}$$

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho(\nabla \mathbf{v}) \cdot \mathbf{v} = \nabla \cdot \boldsymbol{\sigma} \tag{2}$$

In the above equations $\mathbf{v}$ is the velocity vector, ρ the density, $\nabla \cdot \boldsymbol{\sigma}$ is the divergence of the Cauchy stress tensor $\boldsymbol{\sigma}$ and we have assumed that there are no external body forces.

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For the particular case of incompressible Newtonian fluids, the Cauchy stress is given by,

$$\boldsymbol{\sigma} = -p\mathbf{I} + \mu\nabla\mathbf{v} + \mu(\nabla\mathbf{v})^{\mathrm{T}} \tag{3}$$

where p is the fluid's pressure, $\mathbf{I}$ is the Identity Tensor and μ the viscosity. Replacing this relationship into Equation (2) we get the divergence form of the N–S equations

$$\rho\frac{\partial\mathbf{v}}{\partial t} + \rho(\nabla\mathbf{v})\cdot\mathbf{v} = \nabla\cdot\boldsymbol{\sigma} = \nabla\cdot(-p\mathbf{I} + \mu\nabla\mathbf{v} + \mu(\nabla\mathbf{v})^{\mathrm{T}}) \tag{4}$$

$$\nabla\cdot\mathbf{v} = 0 \tag{5}$$

3. NAVIER–STOKES EQUATIONS IN LAPLACE FORM

Making use of the following tensor identities:

$$\nabla\cdot(p\mathbf{I}) = \nabla p \tag{6}$$

$$\nabla\cdot(\nabla\mathbf{V}) = \nabla^2\mathbf{v} \tag{7}$$

$$\nabla\cdot(\nabla\mathbf{v})^{\mathrm{T}} = \nabla(\nabla\cdot\mathbf{v}) \tag{8}$$

and assuming that the spatial variation of the viscosity can be neglected, it turns out that the $\nabla\cdot\boldsymbol{\sigma}$ simplifies to

$$\nabla\cdot\boldsymbol{\sigma} = \nabla\cdot(-p\mathbf{I} + \mu\nabla\mathbf{v}) = -\nabla p + \mu\nabla^2\mathbf{v} \tag{9}$$

Replacing this into the right-hand side (RHS) of Equation (4), we get an alternative expression for the N–S equations: the *Incompressible N–S equations in Laplace form*

$$\rho\frac{\partial\mathbf{v}}{\partial t} + \rho\nabla\mathbf{v}\cdot\mathbf{v} = -\nabla p + \mu\nabla^2\mathbf{v} \tag{10}$$

$$\nabla\cdot\mathbf{v} = 0 \tag{11}$$

We call it the *Laplace form* of the N–S equations because the viscous contribution is simply the Laplacian of the velocity components

$$\nabla^2\mathbf{v}$$

Note that both the strong forms, the Laplace form and the Divergence form, are equivalent (under the constant viscosity approximation) and that the $(\nabla\mathbf{v})^{\mathrm{T}}$ term does not contribute to the momentum equations because

$$\nabla\cdot(\nabla\mathbf{v})^{\mathrm{T}} = 0$$

for incompressible fluids.

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4. BOUNDARY CONDITIONS OF NAVIER–STOKES EQUATIONS

In general the fluid moves around and between solid surfaces $\Gamma_{\mathbf{v}}$ and traction surfaces $\Gamma_{\mathbf{t}}$ where suitable boundary conditions have to be prescribed. The set of exact boundary conditions will be presented next.

4.1. Boundary conditions at solid boundaries

At solid boundaries $\Gamma_{\mathbf{v}}$ which may be moving with arbitrary velocity $\bar{\mathbf{v}}$, the flow velocity is imposed

$$\mathbf{v} = \bar{\mathbf{v}} \quad \text{on } \Gamma_{\mathbf{v}} \tag{12}$$

4.2. Boundary conditions at traction surfaces

There are many problems of practical importance where flows are not fully bounded and then have traction surfaces. On traction surfaces, external forces are present but the fluid's motion is not imposed. Consequently, part of the problem consists in determining the position and shape of these surfaces. Examples of traction surfaces are all the cases where there exists interaction between two fluids, this includes multi-phase flows.

At traction surfaces $\Gamma_{\mathbf{t}}$ where arbitrary external forces $\bar{\mathbf{t}}$ are acting, the condition of continuity of forces must hold. So denoting by $\mathbf{n}$ the outward pointing surface's unit normals, the following boundary condition must hold:

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{t}} \quad \text{on } \Gamma_{\mathbf{t}} \tag{13}$$

Then, for Newtonian fluids

$$-p\mathbf{n} + \mu(\nabla \mathbf{v}) \cdot \mathbf{n} + \mu(\nabla \mathbf{v})^{\mathrm{T}} \cdot \mathbf{n} = \bar{\mathbf{t}} \quad \text{on } \Gamma_{\mathbf{t}} \tag{14}$$

4.3. Boundary conditions at free-surfaces

Free-surface flows are a special case of multi-phase flows. They are essentially two-phase flows, usually a liquid phase and a gas phase, where one usually neglects the density and viscous effects of the lighter phase. For a deeper discussion on the subject refer to [5] . Examples of free-surface flows are sea waves, dam breaks, flow over structures, flow around ships, mould filling, flow with bubbles, etc.

The exact free-surface boundary conditions of free-surface flows are obtained as a special case of the general interface condition (13), assuming that external tangential forces are negligible and that only external normal pressures are applied. In such case and in the absence of surface tension, we can write the imposed external forces simply as

$$\bar{\mathbf{t}} = -\bar{p}\mathbf{n} \tag{15}$$

where $\bar{p}$ is an imposed known external pressure, such as the atmospheric pressure. Replacing (15) into the traction boundary condition (13) we get

$$\boldsymbol{\sigma} \cdot \mathbf{n} = -\bar{p}\mathbf{n} \tag{16}$$

Then, for Newtonian fluids

$$-p\mathbf{n} + \mu(\nabla \mathbf{v}) \cdot \mathbf{n} + \mu(\nabla \mathbf{v})^{\mathrm{T}} \cdot \mathbf{n} = -p\mathbf{n} \quad \text{on } \Gamma_{\mathbf{t}} \tag{17}$$

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Observation 1
It is important to note then that in general the internal pressure does not match the imposed external pressure $\bar{p}$ on the free surface.

If we consider a two-dimensional flow and decompose the traction forces and the velocity vector in a tangential and a normal component

$$\mathbf{v} = v_t \mathbf{e}_t + v_n \mathbf{e}_n \quad \text{no sum}$$

The exact boundary condition (14) becomes

$$\bar{t}_n \mathbf{e}_n + \bar{t}_t \mathbf{e}_t = -p\mathbf{e}_n + \mu \frac{\partial v_t}{\partial x_n}\mathbf{e}_t + \mu \frac{\partial v_n}{\partial x_n}\mathbf{e}_n + \mu \frac{\partial v_n}{\partial x_n}\mathbf{e}_n + \mu \frac{\partial v_n}{\partial x_t}\mathbf{e}_t \quad \text{no sum} \tag{18}$$

Separating in components

$$\bar{t}_n = -p + 2\mu \frac{\partial v_n}{\partial x_n} \quad \text{no sum} \tag{19}$$

$$\bar{t}_t = \mu \frac{\partial v_t}{\partial x_n} + \mu \frac{\partial v_n}{\partial x_t} \quad \text{no sum} \tag{20}$$

In case, only normal loads are applied

$$-\bar{p} = -p + 2\mu \frac{\partial v_n}{\partial x_n} \quad \text{no sum} \tag{21}$$

$$0 = \mu \frac{\partial v_t}{\partial x_n} + \mu \frac{\partial v_n}{\partial x_t} \quad \text{no sum} \tag{22}$$

From (21)–(22) we see that even in 2D pressures do not match.

4.4. Inviscid approximations

For many practical applications (such as the ones involving liquids with free surfaces), it is a common assumption (see [6, p. 3429; 7, Chapter 1]) that the viscous terms in the RHS of Equations (14) and (17) are negligible

$$\mu(\nabla \mathbf{v}) \cdot \mathbf{n} \approx 0 \quad \text{and} \quad \mu(\nabla \mathbf{v})^{\mathrm{T}} \cdot \mathbf{n} \approx 0 \quad \text{on } \Gamma_{\mathbf{t}} \tag{23}$$

This seems reasonable because one expects the velocity gradients in the fluid to be small on the free surface. Under this *inviscid* assumption, the internal pressure p matches the external pressure $\bar{p}$ (say the atmospheric pressure)

$$p = \bar{p} \quad \text{on } \Gamma_{\mathbf{t}} \tag{24}$$

The matching of internal and external pressures is a classical assumption, see, for example, [8–14], etc.

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4.5. Pseudo-tractions approximations

In their book, Donea and Huerta [15] mention an alternative approach for boundary conditions. The idea is to use a seemingly less restrictive approximation than the inviscid approximation, i.e. to neglect just the second viscous term of the LHS of Equations (14) and (17):

$$\mu(\nabla \mathbf{v})^{\mathrm{T}} \cdot \mathbf{n} \approx \mathbf{0} \quad \text{on } \Gamma_{\mathbf{t}} \tag{25}$$

Under this assumption the traction boundary condition (14) becomes

$$-p\mathbf{n} + \mu(\nabla \mathbf{v}) \cdot \mathbf{n} = -p\mathbf{n} + \mu(\mathbf{n} \cdot \nabla)v = \bar{\mathbf{t}} \quad \text{on } \Gamma_{\mathbf{t}} \tag{26}$$

They call this boundary condition the *pseudo-traction* boundary condition.

Note that the pseudo-traction condition (26) does not necessarily imply that the internal pressure should match the imposed external pressure $\bar{p}$ on the free surface. Effectively for the case of free surfaces (26) becomes

$$-p\mathbf{n} + \mu(\nabla \mathbf{v}) \cdot \mathbf{n} = -\bar{p}\mathbf{n} \quad \text{on } \Gamma_{\mathbf{t}} \tag{27}$$

and then

$$p \neq \bar{p} \quad \text{on } \Gamma_{\mathbf{t}} \tag{28}$$

unless also

$$\mu(\nabla \mathbf{v}) \cdot \mathbf{n} \approx \mathbf{0} \quad \text{on } \Gamma_{\mathbf{t}} \tag{29}$$

From this it follows that the inviscid assumption is equivalent to assume the pseudo-traction condition plus the condition of matching external pressure.

5. DIVERGENCE WEAK FORM OF NAVIER–STOKES EQUATIONS

Nowadays most people solve the N–S equations, not by discretization of the *strong form*s (Equations (10)–(11) or Equations (4)–(5)) presented in Sections 2 and 3, but by discretization of a *weak form* of the differential equations. The most popular methods to get such weak form are the finite-element method (FEM) and the finite-volume method (FVM). In the present paper we will assume that we are interested in solving the N–S equations using a FEM formulation. However, the results are not restricted to FEM. Similar implications are obtained for FVM.

In this section we will derive the weak form of the N–S equations when they are written in divergence form (i.e. Equations (4)–(5)). For the sake of simplicity we will call it the divergence weak form of the N–S equations or just the divergence weak form.

5.1. Divergence weak form

To find the weak form of the Equations (4)–(5) we proceed as it is usual in FEM [16]. We multiply both sides of Equation (4) by a weighting function w and integrate over the whole fluid domain Ω to get

$$\int_{\Omega} w\rho \frac{\partial \mathbf{v}}{\partial t} \, \mathrm{d}\Omega + \int_{\Omega} w\rho(\nabla \mathbf{v}) \cdot \mathbf{v} \, \mathrm{d}\Omega = \int_{\Omega} w \nabla \cdot \boldsymbol{\sigma} \, \mathrm{d}\Omega \tag{30}$$

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Integration by parts of the divergence terms leads to

$$\int_\Omega w\nabla\cdot[\boldsymbol{\sigma}]\,\mathrm{d}\Omega = -\int_\Omega [\boldsymbol{\sigma}]\cdot\nabla w\,\mathrm{d}\Omega + \int_\Gamma w[\boldsymbol{\sigma}]\cdot\mathbf{n}\,\mathrm{d}\Gamma \tag{31}$$

So we get

$$\int_\Omega w\rho\frac{\partial\mathbf{v}}{\partial t}\,\mathrm{d}\Omega + \int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega$$
$$= -\int_\Omega [-p\mathbf{I} + \mu\nabla\mathbf{v} + \mu(\nabla\mathbf{v})^{\mathrm{T}}]\cdot\nabla w\,\mathrm{d}\Omega + \int_{\Gamma_\mathbf{t}} w\boldsymbol{\sigma}\cdot\mathbf{n}\,\mathrm{d}\Gamma \tag{32}$$

where we have used also that

$$w = 0 \quad \text{on } \Gamma_\mathbf{v} \tag{33}$$

Observation 2
Note that the integrand of the boundary integral in the momentum equation (32) is exactly the physical traction condition (13). This means that the traction condition is *the natural boundary condition* of the N–S equations written in divergence form.

Since we have got the natural boundary condition on the boundary integral, it is straightforward to impose the boundary conditions (13). Then, for the general traction problem we have

$$\int_\Omega w\rho\frac{\partial\mathbf{v}}{\partial t}\,\mathrm{d}\Omega + \int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega$$
$$= \int_\Omega p\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu\nabla\mathbf{v}\cdot\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu(\nabla\mathbf{v})^{\mathrm{T}}\cdot\nabla w\,\mathrm{d}\Omega + \int_{\Gamma_\mathbf{t}} w\bar{\mathbf{t}}\,\mathrm{d}\Gamma \tag{34}$$

Note that there are not unknowns in the boundary integral. For the particular case of free surfaces we get

$$\int_\Omega w\rho\frac{\partial\mathbf{v}}{\partial t}\,\mathrm{d}\Omega + \int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega$$
$$= \int_\Omega p\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu\nabla\mathbf{v}\cdot\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu(\nabla\mathbf{v})^{\mathrm{T}}\cdot\nabla w\,\mathrm{d}\Omega - \int_{\Gamma_\mathbf{t}} w\bar{p}\mathbf{n}\,\mathrm{d}\Gamma \tag{35}$$

We can perform a similar approach for the continuity equation with a weighting function q to get:

$$\int_\Omega q\nabla\cdot\mathbf{v}\,\mathrm{d}\Omega = 0 \tag{36}$$

Equations (34) or (35) supplemented with Equation (36) are what we called the divergence weak form of the N–S equations.

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5.2. Divergence discretization (FEM)

With the divergence weak form expressions (35)–(36) for free surfaces in our hands we can obtain the divergence discretization using standard FEM procedures [16].

If we identify the following discrete operators in Equation (35):

$$\int_\Omega w\rho\frac{\partial \mathbf{v}}{\partial t}\,\mathrm{d}\Omega + \int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega = \mathbb{M}\frac{\Delta\mathbf{v}}{\Delta t} + \mathbb{C}(\mathbf{v}) \tag{37}$$

$$\int_\Omega p\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu\nabla\mathbf{v}\cdot\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu(\nabla\mathbf{v})^{\mathrm{T}}\cdot\nabla w\,\mathrm{d}\Omega - \int_{\Gamma_{\mathbf{t}}} w\bar{p}\mathbf{n}\,\mathrm{d}\Gamma$$
$$= -\mathbb{G}p + \mu\mathbb{L}\mathbf{v} + \mu\mathbb{T}\mathbf{v} + \mathbb{F} \tag{38}$$

and in Equation (36) as:

$$\int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\mathrm{d}\Omega = \mathbb{D}(\mathbf{v}) \tag{39}$$

We can use different forms of the discrete operators to get different numerical schemes. For example, a fully implicit (see [17]) scheme at time $(n+1)$ will look like

$$\begin{bmatrix} \mathbb{M}\mathbf{v}^{n+1} + \Delta t\mathbb{C}(\mathbf{v}^{n+1}) + \Delta t\mathbb{G}p^{n+1} - \Delta t\mu(\mathbb{L}+\mathbb{T})\mathbf{v}^{n+1} \\ \mathbb{D}\mathbf{v}^{n+1} \end{bmatrix} = \begin{bmatrix} \mathbb{M}\mathbf{v}^n + \Delta t\mathbb{F} \\ 0 \end{bmatrix} \tag{40}$$

Similarly, if we use (see [18]) a second–order Crank–Nicholson for the diffusive terms and the convective terms are updated using a second-order Adams–Bashforth method our discrete system of equations will look something like

$$\begin{bmatrix} \mathbb{M} - \dfrac{\Delta t\mu}{2}(\mathbb{L}+\mathbb{T}) & \Delta t\mathbb{G} \\ \mathbb{D} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}^{n+1} \\ p^{n+1} \end{bmatrix}$$
$$= \begin{bmatrix} -\Delta t\left(\dfrac{3}{2}\mathbb{C}(\mathbf{v}^n) - \dfrac{1}{2}\mathbb{C}(\mathbf{v}^{n-1})\right) + \dfrac{\Delta t\mu}{2}(\mathbb{L}+\mathbb{T})\mathbf{v}^n + \mathbb{M}\mathbf{v}^n + \Delta t\mathbb{F} \\ 0 \end{bmatrix} \tag{41}$$

It is worth to make the following observations:

Observation 3
The operator

$$\mathbb{K} = \mathbb{L} + \mathbb{T} \tag{42}$$

is the stiffness matrix of linear elasticity.

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Observation 4
The operator

$$\mathbb{T}\mathbf{v}$$

produces a full coupling of velocity components.

6. LAPLACE WEAK FORMS OF NAVIER–STOKES EQUATIONS

In this section we will derive the weak form of the N–S equations when written in Laplace form (i.e. Equations (10)–(11)). We proceed in a similar way as done for the divergence form. Since both forms are supposed to be equivalent we expect to get the same results.

6.1. Exact Laplace weak form

Multiplying both sides of Equation (10) by the weighting function w and integrating over the whole fluid domain Ω we get

$$\int_\Omega w\rho\frac{\partial \mathbf{v}}{\partial t}\,\mathrm{d}\Omega + \int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega = \int_\Omega w[-\nabla p + \mu\nabla^2\mathbf{v}]\,\mathrm{d}\Omega \tag{43}$$

After integration by parts of the pressure term and the Laplacian term, we get that

$$\begin{aligned}&\int_\Omega w\rho\frac{\partial \mathbf{v}}{\partial t}\,\mathrm{d}\Omega + \int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega\\ &\quad= \int_\Omega p\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu\nabla\mathbf{v}\cdot\nabla w\,\mathrm{d}\Omega + \int_{\Gamma_\mathbf{t}} w[-p\mathbf{I} + \mu\nabla\mathbf{v}]\cdot\mathbf{n}\,\mathrm{d}\Gamma\end{aligned} \tag{44}$$

Observation 5
As opposed to what we might have expected, in Equation (44) we do not get back in the boundary integral the exact traction condition. This means that the physical boundary condition is not *the natural boundary condition* of the N–S equations written in Laplace Form. If we look carefully, we can see that *the natural boundary conditions* of the Laplace form of the N–S equations are actually the *pseudo-tractions* conditions presented in Equation (26).

Some of the issues related to the boundary conditions associated with the divergence and Laplace forms were addressed in [19, 20].

In order to be completely accurate we should be careful in not to replace the integrand of the boundary integral by $\boldsymbol{\sigma}\cdot\mathbf{n}$, instead we should make use of the relationship (14)

$$\bar{\mathbf{t}} - \mu(\nabla\mathbf{v})^{\mathrm{T}}\cdot\mathbf{n} = [-p\mathbf{I} + \mu\nabla\mathbf{v}]\cdot\mathbf{n} \quad \text{on } \Gamma_\mathbf{t} \tag{45}$$

Replacing Equation (45) in the boundary integral of Equation (44), we see that *the Laplace weak form of the N–S equations* is

$$\begin{aligned}&\int_\Omega w\rho\frac{\partial \mathbf{v}}{\partial t}\,\mathrm{d}\Omega + \int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega\\ &\quad= \int_\Omega p\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu\nabla\mathbf{v}\cdot\nabla w\,\mathrm{d}\Omega + \int_{\Gamma_\mathbf{t}} w\bar{\mathbf{t}}\,\mathrm{d}\Gamma - \int_{\Gamma_\mathbf{t}} w[\mu(\nabla\mathbf{v})^{\mathrm{T}}]\cdot\mathbf{n}\,\mathrm{d}\Gamma\end{aligned} \tag{46}$$

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supplemented with the weak form of the incompressibility condition (36). In particular, for free surfaces we have

$$\int_\Omega w\rho\frac{\partial \mathbf{v}}{\partial t}\,\mathrm{d}\Omega + \int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega = \int_\Omega p\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu\nabla\mathbf{v}\cdot\nabla w\,\mathrm{d}\Omega - \int_{\Gamma_\mathbf{t}} w\bar{p}\mathbf{n}\,\mathrm{d}\Gamma - \int_{\Gamma_\mathbf{t}} w[\mu(\nabla\mathbf{v})^{\mathrm{T}}]\cdot\mathbf{n}\,\mathrm{d}\Gamma \tag{47}$$

6.2. *Exact Laplace discretization*

If we define the discrete operator $\mathbb{V}$ as

$$\mathbb{V}\mathbf{v} = -\int_{\Gamma_\mathbf{t}} w[\mu(\nabla\mathbf{v})^{\mathrm{T}}]\cdot\mathbf{n}\,\mathrm{d}\Gamma \tag{48}$$

we can get the Laplace discretizations of the N–S equations that are the counterpart the divergence discretization Equations (40) and (41). The exact fully implicit Laplace scheme at time $(n+1)$ that corresponds to (40) is

$$\begin{bmatrix} \mathbb{M}\mathbf{v}^{n+1} + \Delta t\mathbb{C}(\mathbf{v}^{n+1}) + \Delta t\mathbb{G}p^{n+1} - \Delta t\mu(\mathbb{L}+\mathbb{V})\mathbf{v}^{n+1} \\ \mathbb{D}\mathbf{v}^{n+1} \end{bmatrix} = \begin{bmatrix} \mathbb{M}\mathbf{v}^n + \Delta t\mathbb{F} \\ 0 \end{bmatrix} \tag{49}$$

Similarly, the semi-implicit second-order case that corresponds to (41) is

$$\begin{bmatrix} \mathbb{M} - \dfrac{\Delta t\mu}{2}(\mathbb{L}+\mathbb{V}) & \Delta t\mathbb{G} \\ \mathbb{D} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} -\Delta t\left(\dfrac{3}{2}\mathbb{C}(\mathbf{v}^n) - \dfrac{1}{2}\mathbb{C}(\mathbf{v}^{n-1})\right) + \dfrac{\Delta t\mu}{2}(\mathbb{L}+\mathbb{V})\mathbf{v}^n + \mathbb{M}\mathbf{v}^n + \Delta t\mathbb{F} \\ 0 \end{bmatrix} \tag{50}$$

Observation 6

Note that exact Laplace discretizations and divergence discretizations are similar. They would be identical if the discrete operators $\mathbb{T}\mathbf{v}$ and $\mathbb{V}\mathbf{v}$ would be equal. This is the case in the continuum because from the identity

$$\int_\Omega w\nabla(\nabla\cdot\mathbf{v})\,\mathrm{d}\Omega = -\int_\Omega (\nabla\mathbf{v})^{\mathrm{T}}\cdot\nabla w\,\mathrm{d}\Omega + \int_\Gamma w(\nabla\mathbf{v})^{\mathrm{T}}\cdot\mathbf{n}\,\mathrm{d}\Gamma \tag{51}$$

and the incompressibility condition, it follows that

$$-\int_\Omega (\nabla\mathbf{v})^{\mathrm{T}}\cdot\nabla w\,\mathrm{d}\Omega = -\int_\Gamma w(\nabla\mathbf{v})^{\mathrm{T}}\cdot\mathbf{n}\,\mathrm{d}\Gamma \tag{52}$$

Then

$$\mathbb{T}\mathbf{v} = \mathbb{V}\mathbf{v} \quad \text{in the continuum} \tag{53}$$

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However, in a real discretization one should be careful to state a *strict* equality because $\mathbb{T}$ involves volume integration while $\mathbb{V}$ involves contributions of boundary elements, and because the incompressibility condition is satisfied weakly. So in general

$$\mathbb{T}\mathbf{v} \neq \mathbb{V}\mathbf{v} \quad \text{in the discrete} \tag{54}$$

7. STANDARD LAPLACE WEAK FORMS

In our previous derivations we did not make any approximation (except of course the assumption of negligible spatial variation of the viscosity). Usually the use of approximations are convenient, for example, so as to increase performance and reduce complexity without loosing accuracy. One traditional way of obtaining helpful approximations for simulations of viscous flows is the one that combines the Laplace weak form derived in the previous section with the 'reasonable' approximations on the boundary conditions described in Sections 4.4 and 4.5. This leads to simplified classical formulations as shown below.

If we assume that the physical boundary conditions can be safely replaced with the Laplace natural boundary conditions (27) (i.e. pseudo-tractions) or with the inviscid boundary conditions, the exact Laplace form (47) reduces to the *standard Laplace form*

$$\int_\Omega w\rho\frac{\partial \mathbf{v}}{\partial t}\,\mathrm{d}\Omega + \int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega = \int_\Omega p\nabla w\,\mathrm{d}\Omega - \int_\Omega \mu\nabla\mathbf{v}\cdot\nabla w\,\mathrm{d}\Omega - \int_{\Gamma_\mathbf{t}} w\bar{p}\mathbf{n}\,\mathrm{d}\Gamma\cdot\mathbf{n}\,\mathrm{d}\Gamma \tag{55}$$

So because of Equation (25), in the standard Laplace form the internal viscous contribution on the traction boundary disappears. In this case, the semi-implicit Laplace discretization (50) reduces to

$$\begin{bmatrix} \mathbb{M} - \dfrac{\Delta t\mu}{2}\mathbb{L} & \Delta t\mathbb{G} \\ \mathbb{D} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} -\Delta t\left(\dfrac{3}{2}\mathbb{C}(\mathbf{v}^n) - \dfrac{1}{2}\mathbb{C}(\mathbf{v}^{n-1})\right) + \dfrac{\Delta t\mu}{2}\mathbb{L}\mathbf{v}^n + \mathbb{M}\mathbf{v}^n + \Delta t\mathbb{F} \\ 0 \end{bmatrix} \tag{56}$$

Observation 7

Standard Laplace formulations (like the one given in Equation (56)) can be easily recognized by the fact that the viscous contributions come exclusively from the Laplacian operator $\mathbb{L}$.

Note that Laplacian discrete operator $\mathbb{L}$ has been defined to be

$$\mathbb{L}\mathbf{v} = -\int_\Omega \nabla\mathbf{v}\cdot\nabla w\,\mathrm{d}\Omega$$

it is symmetric and block-diagonal (decoupled) by velocity components. Because of this, the matrix

$$\mathbb{A} = \mathbb{M} - \frac{\Delta t\mu}{2}\mathbb{L}$$

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appearing in projection/fractional-step methods is block-diagonal and can be decoupled in velocity components.

8. THE VIOLATION OF OBJECTIVITY BY STANDARD LAPLACE FORMULATIONS

The boundary term (48) is the only difference between the standard Laplace form and the exact Laplace form derived in Sections 7 and 6, respectively. In the previous section we showed that if we use the natural boundary conditions of the Laplace form such term is not longer part of the formulation. Note that by making use of such approximation one expects to make improvements in the performance of the resulting algorithms (see Observation 7).

The boundary term (48) can be written in component form as

$$\mathbb{V}v = -\mu \int_{\Gamma_{\mathbf{t}}} w(\nabla \mathbf{v})^{\mathrm{T}} \cdot \mathbf{n}\, \mathrm{d}\Gamma = -\mu \int_{\Gamma_{\mathbf{t}}} w \left(\frac{\partial v_i}{\partial x_j} n_i \mathbf{e}_j \right) \mathrm{d}\Gamma \tag{57}$$

From this we see that the jth component involves components v_i with $j \neq i$ then this term fully couples all the components of the velocity. The above coupling is a coupling due to viscosity, i.e. a *viscous coupling*. The corresponding discrete operator $\mathbb{V}$ then produces a coupling in velocity components. It is not a block-diagonal operator.

In this section we will explain why it is a bad idea to simulate viscous flows with standard Laplace formulations (such as the one given in Equation (56)).

We will show that the lack of the boundary term (48) causes the violation of *the principle of objectivity or invariance under a change of observer* which is a main axiom of continuum mechanics (see [21, 22]).

To demonstrate this, we will prove that the absence of the boundary term (48) is equivalent to writing the Cauchy stress $\boldsymbol{\sigma}$ (Equation (3)) without the contribution due to $\mu(\nabla \mathbf{v})^{\mathrm{T}}$

$$\tilde{\boldsymbol{\sigma}} = -p\mathbf{I} + \tilde{\boldsymbol{\sigma}}_{\text{viscous}} = -p\mathbf{I} + \mu(\nabla \mathbf{v}) \tag{58}$$

and then prove that (58) is an *incorrect or incomplete* constitutive law: it violates the principle of objectivity.

The demonstration that the absence of (48) is equivalent to using the constitutive law (58) is as follows. First note that a material whose constitutive law is given by (58) still satisfies the strong form of the N–S equations

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \nabla \mathbf{v} \cdot \mathbf{v} = \nabla \cdot \tilde{\boldsymbol{\sigma}} = -\nabla p + \mu \nabla^2 \mathbf{v} \tag{59}$$

The only change being a slightly different traction boundary condition

$$\tilde{\boldsymbol{\sigma}} \cdot \mathbf{n} = \bar{\mathbf{t}} \quad \text{on } \Gamma_{\mathbf{t}} \tag{60}$$

$$\Downarrow$$

$$[-p\mathbf{I} + \mu(\nabla \mathbf{v})] \cdot \mathbf{n} = \bar{\mathbf{t}} \quad \text{on } \Gamma_{\mathbf{t}} \tag{61}$$

Now, if we redo the steps followed in Section 6.1 with $\tilde{\boldsymbol{\sigma}}$ instead of $\boldsymbol{\sigma}$ we obtain again Equation (44), then inserting the boundary condition (61) we get back the standard Laplace form given in

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Equation (55):

$$\int_\Omega w\rho\frac{\partial \mathbf{v}}{\partial t}\,\mathrm{d}\Omega+\int_\Omega w\rho(\nabla\mathbf{v})\cdot\mathbf{v}\,\mathrm{d}\Omega=\int_\Omega p\nabla w\,\mathrm{d}\Omega-\int_\Omega \mu\nabla\mathbf{v}\cdot\nabla w\,\mathrm{d}\Omega+\int_{\Gamma_\mathbf{t}} w\bar{\mathbf{t}}\,\mathrm{d}\Gamma\cdot\mathbf{n}\,\mathrm{d}\Gamma \tag{62}$$

This proves that the use of standard Laplace formulations is equivalent to the use of a Cauchy stress $\tilde{\boldsymbol{\sigma}}$.

Now, let us show that (58) violates *the principle of objectivity*.

A necessary condition for a constitutive law to satisfy the principle of objectivity is that a rigid motion should not generate viscous stresses and preserve incompressibility on the material. Expressed mathematically this implies that under a velocity field $\mathbf{v_R}$ corresponding to a rigid motion we should have

$$\tilde{\boldsymbol{\sigma}}_{\text{viscous}}=\mathbf{0} \tag{63}$$

$$\Downarrow$$

$$\mu\nabla\mathbf{v_R}=\mathbf{0} \tag{64}$$

and

$$\nabla\cdot\mathbf{v_R}=0 \tag{65}$$

Mathematically the velocity field of a rigid motion is given by

$$\mathbf{v_R}=\boldsymbol{\omega}\times\mathbf{x}$$

In component form

$$\mathbf{v_R}=\varepsilon_{ijk}\omega_j x_k\mathbf{e}_i$$

Then

$$\nabla\cdot\mathbf{v_R}=\frac{\partial}{\partial x_i}(\varepsilon_{ijk}\omega_j x_k)=\varepsilon_{ijk}\omega_j\frac{\partial}{\partial x_i}x_k=\varepsilon_{ijk}\omega_j\delta_{ki}=\varepsilon_{iji}\omega_j=0 \tag{66}$$

which proves that the incompressibility condition is preserved. On the other hand,

$$\begin{aligned}\nabla\mathbf{v_R}&=\frac{\partial}{\partial x_l}(\varepsilon_{ijk}\omega_j x_k)\mathbf{e}_i\mathbf{e}_l=\varepsilon_{ijk}\omega_j\frac{\partial}{\partial x_l}(x_k)\mathbf{e}_i\mathbf{e}_l=\varepsilon_{ijk}\omega_j\delta_{kl}\mathbf{e}_i\mathbf{e}_l\\ \nabla\mathbf{v_R}&=\varepsilon_{ijl}\omega_j\mathbf{e}_i\mathbf{e}_l\neq\mathbf{0}\end{aligned} \tag{67}$$

In Cartesian coordinates we can write the components of $\nabla\mathbf{v_R}$ in matrix form as

$$[\nabla\mathbf{v_R}]=\begin{pmatrix}0 & -\omega_z & \omega_y\\ \omega_z & 0 & -\omega_x\\ -\omega_y & \omega_x & 0\end{pmatrix} \tag{68}$$

Then it follows from (67) that

$$\tilde{\boldsymbol{\sigma}}_{\text{viscous}}\neq\mathbf{0}$$

so the principle of objectivity is violated.

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However, if we consider the correct expression for the stress

$$\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\sigma}_{\text{viscous}} = -p\mathbf{I} + \mu(\nabla \mathbf{v}) + \mu(\nabla \mathbf{v})^{\mathrm{T}} \tag{69}$$

we get that

$$\boldsymbol{\sigma}_{\text{viscous}} = \mu(\nabla \mathbf{v}_{\mathbf{R}}) + \mu(\nabla \mathbf{v}_{\mathbf{R}})^{\mathrm{T}} = \mathbf{0} \tag{70}$$

Because

$$\begin{aligned} (\nabla \mathbf{v}_{\mathbf{R}})^{\mathrm{T}} &= \frac{\partial}{\partial x_l}(\varepsilon_{ijk}\omega_j x_k)\mathbf{e}_l\mathbf{e}_i = \varepsilon_{ijk}\omega_j\delta_{kl}\mathbf{e}_l\mathbf{e}_i = \varepsilon_{ijl}\omega_j\mathbf{e}_l\mathbf{e}_i \\ (\nabla \mathbf{v}_{\mathbf{R}})^{\mathrm{T}} &= \varepsilon_{lji}\omega_j\mathbf{e}_i\mathbf{e}_l = -\varepsilon_{ijl}\omega_j\mathbf{e}_i\mathbf{e}_l \end{aligned} \tag{71}$$

and then

$$\nabla \mathbf{v}_{\mathbf{R}} + (\nabla \mathbf{v}_{\mathbf{R}})^{\mathrm{T}} = \varepsilon_{ijl}\omega_j\mathbf{e}_i\mathbf{e}_l - \varepsilon_{ijl}\omega_j\mathbf{e}_i\mathbf{e}_l \equiv \mathbf{0}$$

This proves then that one must use the entire tensor in order to preserve objectivity and, as a consequence, the term (48) cannot be neglected if the main axioms of continuum mechanics are wanted to be preserved.

8.1. An error estimation of standard Laplace formulations

Note that

$$(\nabla \mathbf{v}_{\mathbf{R}})^{\mathrm{T}} \cdot \mathbf{n} = -\varepsilon_{ijl}\omega_j n_l \mathbf{e}_i = -\boldsymbol{\omega} \times \mathbf{n} \tag{72}$$

Replacing this into the expression of the neglected surface integral, we see that

$$\text{Neglected term} = -\int_{\Gamma_\sigma} w\mu(\nabla \mathbf{v}_{\mathbf{R}})^{\mathrm{T}} \cdot \mathbf{n}\, \mathrm{d}\Gamma = \int_{\Gamma_\sigma} w\mu\boldsymbol{\omega} \times \mathbf{n}\, \mathrm{d}\Gamma = \mu\boldsymbol{\omega} \times \int_{\Gamma_\sigma} w\mathbf{n}\, \mathrm{d}\Gamma \tag{73}$$

The above expression can be used to provide a good estimation for the magnitude of the error made when using standard Laplace formulations.

Observation 8
From (73) it is clear that in flow simulations where the flow experiences rotations, curvature changes and twisting may be affected the most. The approximation may be valid for simulations like flow in a straight channel.

Note also from (73) that due to the cross-product with the surface normal ($\ldots \times \mathbf{n}$), the neglected term generates a force tangent to the surface of prescribed tractions. This force has the direction $\boldsymbol{\omega} \times \mathbf{n}$, and in the case of a two-dimensional flow with an external free surface, because $\mathbf{v}_{\mathbf{R}} \cdot \boldsymbol{\omega} \times \mathbf{n} \geqslant 0$, this neglected term generates a force in a direction that helps to keep the rigid motion.

9. FULLY BOUNDED DOMAINS AND CAVITY FLOWS

In the previous sections we obtained both Laplace discretizations and divergence discretizations for general cases of flow motion. There we centred the discussion on the handling of traction surfaces and the contribution of traction boundary integrals for flows with free surfaces.

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Now let us consider the case of flows in fully bounded domains (i.e. no free surfaces) such as the one of the cavity flow problem [15, 23; Section 6.8].

In such cases the velocity is prescribed in the whole boundary surface Γ of the volume domain Ω so

$$\mathbf{v} = \bar{\mathbf{v}} \quad \text{on } \Gamma = \Gamma_{\mathbf{v}} \tag{74}$$

and there are no traction boundaries

$$\Gamma_{\mathbf{t}} = 0 \tag{75}$$

As a consequence the following operators become zero:

$$\mathbb{F} = -\int_{\Gamma_{\mathbf{t}}} w\bar{p}\mathbf{n}\,\mathrm{d}\Gamma = \mathbf{0}$$

$$\mathbb{V}\mathbf{v} = -\int_{\Gamma_{\mathbf{t}}} w[\mu(\nabla\mathbf{v})^{\mathrm{T}}]\cdot\mathbf{n}\,\mathrm{d}\Gamma = \mathbf{0}$$

Then, for the fully bounded case the Laplace discretization (i.e. Equation (50)) reduces to

$$\begin{bmatrix} \mathbb{M} - \dfrac{\Delta t\,\mu}{2}(\mathbb{L}) & \Delta t\,\mathbb{G} \\ \mathbb{D} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} -\Delta t\left(\dfrac{3}{2}\mathbb{C}(\mathbf{v}^n) - \dfrac{1}{2}\mathbb{C}(\mathbf{v}^{n-1})\right) + \dfrac{\Delta t\,\mu}{2}(\mathbb{L})\mathbf{v}^n + \mathbb{M}\mathbf{v}^n \\ 0 \end{bmatrix} \tag{76}$$

However, note that because of Equation (54) we have that

$$\mathbb{T}\mathbf{v} \neq \mathbf{0} \quad \text{in the discrete} \tag{77}$$

so, for the divergence discretization (50) we can just say that

$$\begin{bmatrix} \mathbb{M} - \dfrac{\Delta t\,\mu}{2}(\mathbb{L}+\mathbb{T}) & \Delta t\,\mathbb{G} \\ \mathbb{D} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}^{n+1} \\ p^{n+1} \end{bmatrix}$$

$$= \begin{bmatrix} -\Delta t\left(\dfrac{3}{2}\mathbb{C}(\mathbf{v}^n) - \dfrac{1}{2}\mathbb{C}(\mathbf{v}^{n-1})\right) + \dfrac{\Delta t\,\mu}{2}(\mathbb{L}+\mathbb{T})\mathbf{v}^n + \mathbb{M}\mathbf{v}^n \\ 0 \end{bmatrix} \tag{78}$$

Observation 9

Note then that in the case of fully bounded domains with bounded solutions the Laplace discretization and the standard Laplace discretization match. However, none of the Laplace discretizations match with the divergence discretization.

The common approach in publications dealing with projection methods is to start with the standard Laplace formulation in fully bounded domains [18, 24–29]. However, the divergence formulation is a more accurate and general approach. Then such projections methods should be studied from the divergence discretization perspective. At present we (the authors) do not know if

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using a divergence formulation instead of the commonly used standard Laplace formulation would have a sensible effect on the performance characteristics of such methods, probably it will. It may also be the case that the coupling effect of operator $\mathbb{T}$ will complicate the analysis.

10. LEVEL-SET METHODS USING LAPLACE FORMULATIONS OF THE NAVIER–STOKES EQUATIONS

Level-set methods, also named pseudo-concentration methods, have been largely used to solve flow problems with free surfaces [30]. The idea is very simple: to solve a fully bounded domain containing two different flows, the true one, with the appropriate viscosity and density and a pseudo-fluid with a much smaller viscosity and density. For example, for the case of a problem involving water the second fluid will be air. Both fluids are solved in a unique fully bounded domain with the original free surface being now inside the domain and defining the interface between the two fluids. The position of the interface, i.e. the position of the free surface, being determined in a Lagrangian way using an auxiliary level set or pseudo-concentration function.

Some researchers using level sets argue that the error signalled in Section 8 about the use of standard Laplace formulations with free-surface problems disappears with this technique. They claim that because the domain under consideration is a fully bounded domain there is no longer an error (as discussed in Section 9). Unfortunately this is not true. We will show in this section that the introduction of an internal discontinuity (i.e. a jump in the viscosity) results in the same magnitude of error as in the open domains with a free surfaces.

In order to analyse the level-set method in a general way, suppose the domain is divided in two sub-domains: Ω_1 were the true fluid is and Ω_2 were the pseudo-fluid is.

10.1. The divergence weak form

Taking into account the divergence form for the stress tensor from Equation (4)

$$\nabla \cdot \boldsymbol{\sigma} = \nabla \cdot (-p\mathbf{I} + \mu\nabla\mathbf{v} + \mu(\nabla\mathbf{v})^{\mathrm{T}}) \tag{79}$$

and applying Green's theorem

$$\begin{aligned}\int_{\Omega} w\nabla\cdot[\boldsymbol{\sigma}]\,\mathrm{d}\Omega &= \int_{\Omega_1} w\nabla\cdot[\boldsymbol{\sigma_1}]\,\mathrm{d}\Omega + \int_{\Omega_2} w\nabla\cdot[\boldsymbol{\sigma_2}]\,\mathrm{d}\Omega \\ &= -\int_{\Omega_1}[\boldsymbol{\sigma_1}]\cdot\nabla w\,\mathrm{d}\Omega - \int_{\Omega_2}[\boldsymbol{\sigma_2}]\cdot\nabla w\,\mathrm{d}\Omega \\ &\quad + \int_{\Gamma_{e1}} w\mathbf{t_1}\,\mathrm{d}\Gamma + \int_{\Gamma_{e2}} w\mathbf{t_2}\,\mathrm{d}\Gamma + \int_{\Gamma_{1,2}} w(\mathbf{t_1}-\mathbf{t_2})\,\mathrm{d}\Gamma \end{aligned} \tag{80}$$

Where $\Gamma_{1,2}$ is the boundary surface forming the interface between the two fluids, and, Γ_{e1} and Γ_{e2} are the remaining portion of traction boundary surfaces of Ω_1 and Ω_2, respectively. We use the notation $\boldsymbol{\sigma_1}$ and $\boldsymbol{\sigma_2}$ for the stresses, and, $\mathbf{t_1}$ and $\mathbf{t_2}$ for the surface-tractions corresponding to fluids 1 and 2, respectively.

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Considering that the pseudo-fluid does not produce any stress ($\boldsymbol{\sigma_2} = \mathbf{t_2} = 0$), we conclude that the divergence form is

$$\int_\Omega w\nabla \cdot [\boldsymbol{\sigma}]\,\mathrm{d}\Omega = -\int_{\Omega_1} [\boldsymbol{\sigma_1}] \cdot \nabla w\,\mathrm{d}\Omega + \int_{\Gamma_{e1}} w\mathbf{t_1}\,\mathrm{d}\Gamma + \int_{\Gamma_{1,2}} w\mathbf{t_1}\,\mathrm{d}\Gamma \tag{81}$$

And, for the fully bounded domain of the level-set method where the surface tractions are only on the fluid's interface

$$\int_\Omega w\nabla \cdot [\boldsymbol{\sigma}]\,\mathrm{d}\Omega = -\int_{\Omega_1} [\boldsymbol{\sigma_1}] \cdot \nabla w\,\mathrm{d}\Omega + \int_{\Gamma_{1,2}} w\mathbf{t_1}\,\mathrm{d}\Gamma \tag{82}$$

We conclude that the natural condition for the divergence form of the N–S equations remains the zero-traction condition:

$$\boldsymbol{\sigma_1} \cdot \mathbf{n} = \mathbf{t_1} = 0$$

10.2. The Laplace weak form

Taking the Laplace form of Equation (79)

$$\nabla \cdot \boldsymbol{\sigma} = -\nabla p\mathbf{I} + \mu\nabla^2\mathbf{v} \tag{83}$$

The weak equation becomes

$$\begin{aligned}\int_\Omega w\nabla \cdot [\boldsymbol{\sigma}]\,\mathrm{d}\Omega &= \int_{\Omega_1} w[-\nabla p\mathbf{I} + \mu_1\nabla^2\mathbf{v}]\,\mathrm{d}\Omega + \int_{\Omega_2} w[-\nabla p\mathbf{I} + \mu_2\nabla^2\mathbf{v}]\,\mathrm{d}\Omega \\ &= \int_{\Omega_1} p\nabla w\,\mathrm{d}\Omega - \int_{\Omega_1} \mu_1\nabla\mathbf{v} \cdot \nabla w\,\mathrm{d}\Omega + \int_{\Omega_2} p\nabla w\,\mathrm{d}\Omega - \int_{\Omega_2} \mu_2\nabla\mathbf{v} \cdot \nabla w\,\mathrm{d}\Omega \\ &\quad + \int_{\Gamma_{e1}} w[\mathbf{t_1} - \mu_1(\nabla\mathbf{v})^{\mathrm{T}}]\,\mathrm{d}\Gamma + \int_{\Gamma_{e2}} w[\mathbf{t_2} - \mu_2(\nabla\mathbf{v})^{\mathrm{T}}]\,\mathrm{d}\Gamma \\ &\quad + \int_{\Gamma_{e1}} w[\mathbf{t_1} - \mathbf{t_2} - \mu_1(\nabla\mathbf{v})^{\mathrm{T}} + \mu_2(\nabla\mathbf{v})^{\mathrm{T}}]\,\mathrm{d}\Gamma\end{aligned} \tag{84}$$

Again, considering the pseudo-fluid does not produce stress and that the surface tractions are only on the fluid's interface

$$\int_\Omega w\nabla \cdot [\boldsymbol{\sigma}]\,\mathrm{d}\Omega = \int_{\Omega_1} p\nabla w\,\mathrm{d}\Omega - \int_{\Omega_1} \mu_1\nabla\mathbf{v} \cdot \nabla w\,\mathrm{d}\Omega + \int_{\Gamma_{e1}} w[\mathbf{t_1} - \mu_1(\nabla\mathbf{v})^{\mathrm{T}}]\,\mathrm{d}\Gamma \tag{85}$$

This shows that the natural condition

$$[\mathbf{t_1} - \mu_1(\nabla\mathbf{v})^{\mathrm{T}}] = 0$$

of the Laplace form is not any more the physical condition of free surface ($\mathbf{t_1} = 0$). Then level-set methods based on Laplace formulations have exactly the same inconvenience presented previously for standard open domains with free surface problems.

We conclude that in both methods, either the one tracking the free surface or the one using the level-set idea to transform the problem to a bounded-domain problem, one must use the divergence

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form of the N–S equations. Otherwise, if a standard Laplace form is used one will have to deal with the dangerous consequences of violating objectivity. Note that if an exact Laplace form (i.e. a non-violating form) is used, it will be necessary to introduce additional terms on the free surface or interface. These terms coupled the three components of the velocity and, for this reason, most of the advantages of the Laplacian approach are lost.

11. NUMERICAL RESULTS

In order to show numerically the importance of using the divergence form of the N–S equations instead of standard Laplace formulations, three examples will be presented. As explained before, standard Laplace formulations are particularly wrong in the case of viscous flow with free surfaces. Theory tells us that in the case of fully bounded domains (cavity flows) the errors should not be so significant. We expect also that errors should decrease proportionally to the viscosity and increase proportionally with rotational flow velocities. Since in the problems presented here we are dealing with moving free surfaces, we chose particle finite element method (PFEM) [31] to carry out our numerical experiments. With PFEM the free surface is tracked in a Lagrangian way and a new triangulation is generated at each time step. The free surface is determined using the alpha-shape concept [32]. Nevertheless, the differences in the results that we are going to show are independent of the particular integral method used to solve the differential equations. The errors are related to the theoretical formulation itself and not to the discretization of the problem.

11.1. Viscous flow in a spinning cylindrical container

The first example considered is the case of a spinning cylindrical container partially full with a viscous fluid and without gravitational forces, as shown in Figures 1 and 2. Due to the centrifugal forces, the fluid is pushed towards the outer portions of cylinder and in the steady-state it takes the form of a cylindrical ring with an internal free surface having the form of a circular tube.

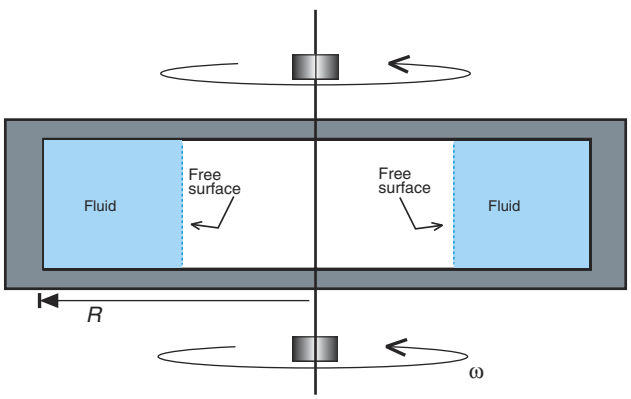

Figure 1. Side view of a cylindrical container of radius R partially full with fluid. The cylinder is rotating with a constant angular velocity ω about its axis under no gravity. The steady motion makes the fluid to fill the outer portions of the container forming an internal free surface with a cylindrical shape.

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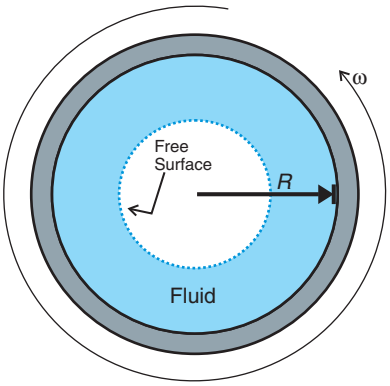

Figure 2. Top view of a cylindrical container partially full with fluid. The cylinder is rotating with a constant angular velocity ω about its axis under no gravity. The spinning motion makes the fluid to fill the outer portions of the container forming an internal free surface with circular shape. The motion is steady.

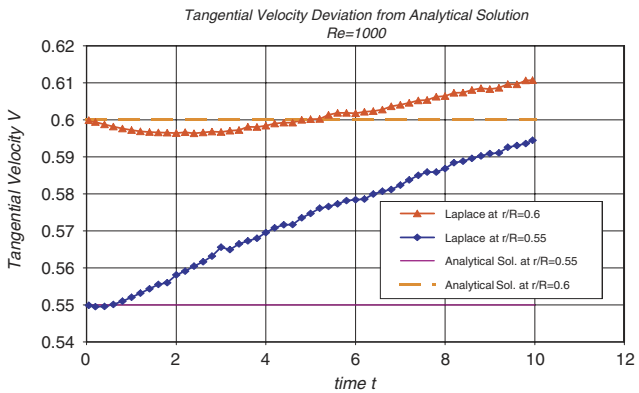

Figure 3. Deviation of the tangential velocity of two points inside the flow with respect to the true steady velocity when the standard Laplace form is used.

Figure 1 shows a side view while Figure 2 shows a top view of the spinning cylinder. For steady viscous flow, the result should be a flow turning as a rigid body. The tangent velocity along a radius becomes perfectly lineal as well as the pressure field.

The problem was solved using the steady-state solution as initial configuration. Then if a correct formulation is used to simulate the spinning cylinder the flow field should remain equal to the initial configuration. It must be noted that the stationary solution to this problem is independent of the value of viscosity (of course as long as $\mu>0$) and the corresponding velocity should be tangential and increase linearly along the radial coordinate.

Using the divergence form of the N–S equations the resulting flow remains all the time in the same position as in the stationary solution. Nevertheless, if the standard Laplace form is used the

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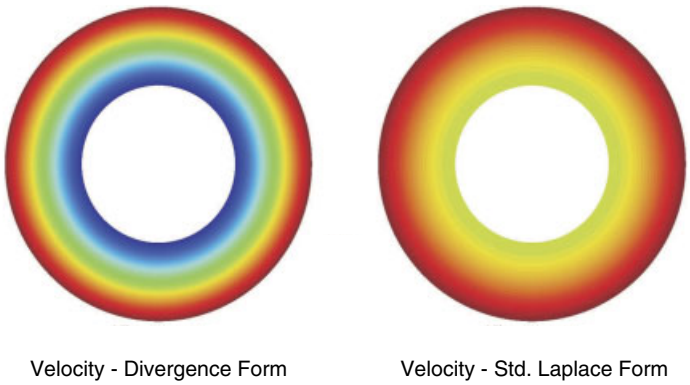

Figure 4. Comparison of velocity distributions for the spinning cylinder at $Re = 1$.

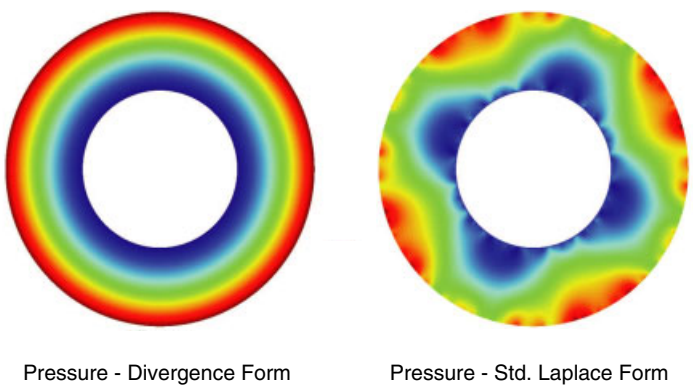

Figure 5. Comparison of pressure distributions for the spinning cylinder at $Re = 1$.

flow changes with time, it does not remain at the correct stationary initial configuration and goes to a wrong result. See, for example, in Figure 3 how the flow tangential velocity does not remain constant for two arbitrary points of the fluid in the spinning cylinder. We clearly see that when the standard Laplace form is used the tangential velocity starts increasing steadily instead of remaining constant. This result is in agreement with the fact that the missing boundary term of the standard Laplace form produces tangential forces that accelerate the flow. We tested three cases at different Reynolds numbers $Re = VR/\nu = \omega R^2/\nu$. In Figures 4 and 5 we can see how the resulting solutions of the two formulations clearly differ for a Reynolds number $Re = 1$. In Figure 6 we see how for highly viscous motions ($Re = 0.000001$ and 1) the velocity matches the expected analytical solution when the divergence form is used while, on the contrary, the velocity is not any more lineal and departs widely from the analytical solution when the standard Laplace form is used. If the viscosity of the flow is decreased so $Re = 1000$, the wrong behaviour of the standard Laplace form is still noticeable as shown in Figure 7. Note that as we decrease the fluid viscosity, it takes more time to see the wrong effects of the Laplace solution but they are still present.

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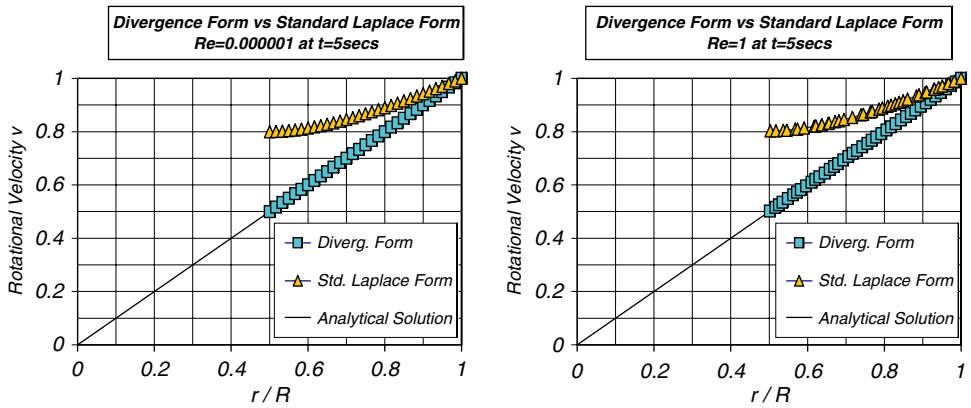

Figure 6. Comparison of the flow rotational velocities v as a function of the radial position r/R obtained using either the divergence form or the standard Laplace form for the case of the spinning cylinder for very viscous flows ($Re = 0.000001$ and 1). Note how the results corresponding to the divergence form match the analytical solution: $v = \omega r = Vr/R$ while the simulations corresponding to the standard Laplace form separate widely from the analytical solution.

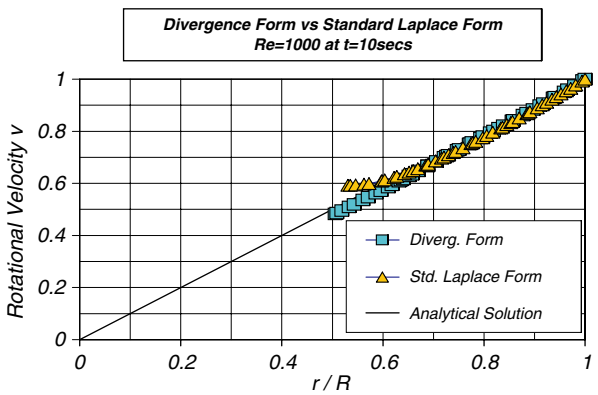

Figure 7. Comparison of the flow rotational velocities v as a function of the radial position r/R obtained using either the divergence form or the standard Laplace form for the case of the spinning cylinder for moderate viscous flows. After 10 s, the results corresponding to the divergence form still match well the analytical solution: $v = Vr/R$. On the other hand, the simulations with the standard Laplace form steadily and visibly deviate from the steady solution.

11.2. Container with a viscous fluid falling down

A rectangular container open on the upper side and partially filled with a viscous fluid, as shown in Figure 8, is analysed for the case in which it is subject to gravity forces and just supported in one of the bottom corners. The container must fall down with a rotatory motion around the fixed corner. In the case of a highly viscous material, the fluid must turn as a rigid body with the container. Figure 9 shows the results at different time steps for the case of a kinematic viscosity of

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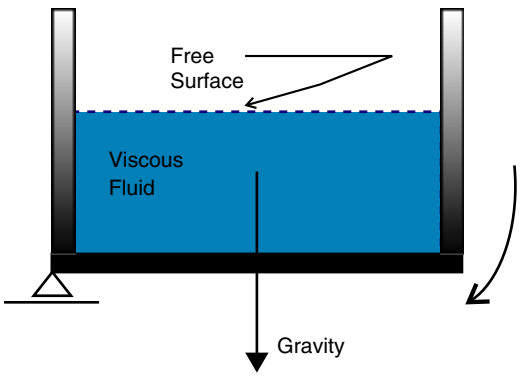

Figure 8. A rectangular container is filled with a viscous fluid subject to gravity g and fixed at the lower left corner.

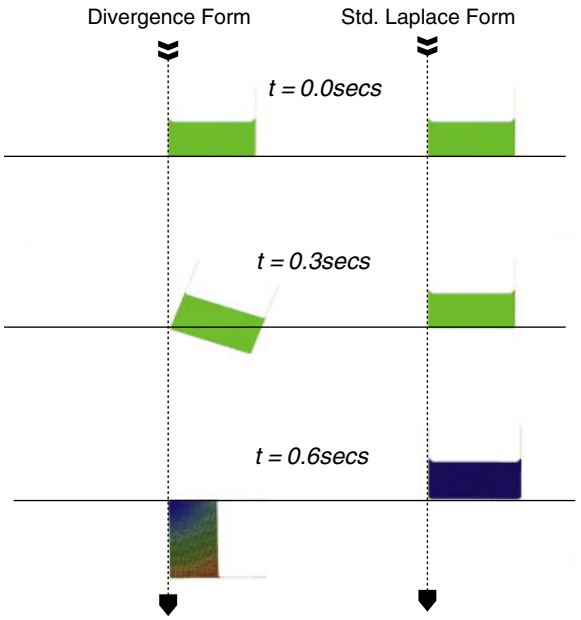

Figure 9. Numerical simulations of the rectangular container shown in Figure 8 filled with extremely high viscosity. Due to the high values of viscosity the fluid should behave as a solid block and fall and rotate around the fixed corner. This is what occurs when the divergence form is used. On the contrary, if the standard Laplace form is used, the fluid remains almost horizontal forcing the container to remain in that position too.

$v = 1000$. Since the viscosity is extremely high the fluid should behave almost as a solid block and fall and rotate with the container around the fixed corner. This is what occurs when the divergence form is used. On the contrary, if the standard Laplace form is used, the fluid completely losses its capacity to achieve rotations and remains almost horizontal forcing the container to remain in that position too.

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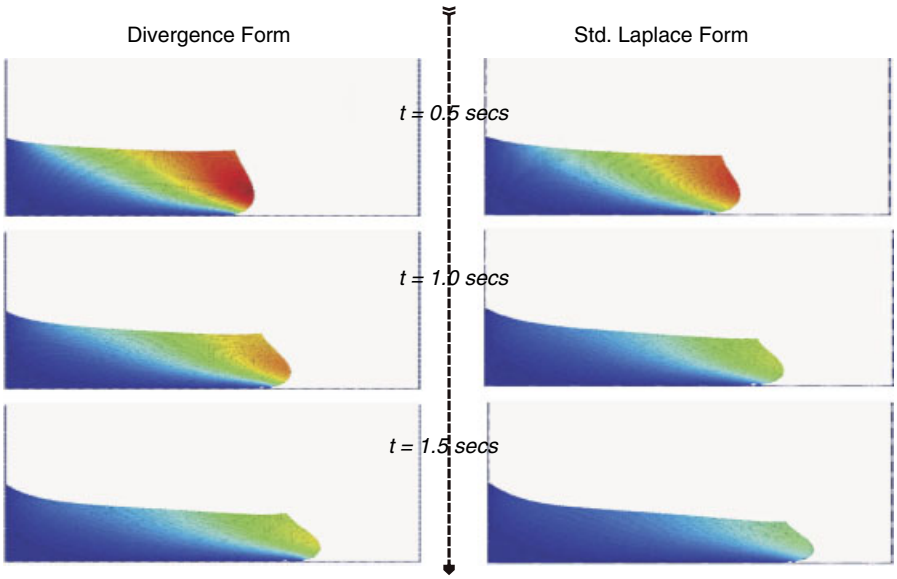

Figure 10. Numerical simulations of a dam break of a viscous fluid $Re = 1$.

11.3. Viscous dam break

The collapse of a water column representing the breaking of a dam has been largely solved in the literature for inviscid or almost inviscid cases. The viscous case is probably not so important in hydraulic engineering but becomes more current in other applications as the cooling of a polymer, fluid concrete, oils, etc. Figure 10 shows the numerical results at different time steps for the standard Laplace form and for the divergence form. The kinematic viscosity was chosen to be $\nu = 1$. From the images of Figure 10 we can note that the shape of the falling fluid column is different. Also, the front of the fluid moves faster for the case of the standard Laplace form than for the divergence case. We do not have experimental results to compare with the numerical simulations but taking into account our theoretical results we expect the simulations corresponding to the divergence form to be closer to reality. The differences between the results of the standard Laplace form and the results of the divergence form are at least worrisome.

12. DISCUSSION AND CONCLUSIONS

Standard Laplace discretizations are recognized by the fact that the viscous contribution comes only from the Laplacian operator $\mathbb{L}$. Since one can arrive to this type of discretization by using classical assumptions, there is a chance that some people may be using them without noting that they have a extremely serious defect. They violate a main axiom of continuum mechanics: the principle of objectivity.

In [15] Donea and Huerta present pseudo-tractions as convenient forms to impose boundary conditions. Particularly, they use them to describe formulations of the unsteady N–S equations [15, Section 6.7]. In this article we have shown that such proposed formulations violate objectivity.

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As a consequence, pseudo-tractions (i.e. natural boundary conditions of the Laplace form) should be avoided. Inviscid assumptions on free surface boundaries should be avoided too.

Standard Laplace discretizations are commonly used in combination with fractional-step methods [6, 33]. Fractional-step methods allow a decoupling of the pressure variable from the velocity components. The use of an equation like (56) allows to decouple the velocity components too. This is advantageous because instead of solving a system containing $3 * N_V$ unknown velocity components, one would solve three smaller systems of size N_V (one system per velocity component). However, as explained in Section 9 this approach is incorrect by the violation of objectivity in such formulations.

Violation of objectivity by standard Laplace discretizations gives another reason to prefer the divergence approach (i.e. weak forms derived from the divergence form of the N–S equations) over the Laplace approach. Note that the use of divergence discretizations forces the computation of a discrete operator $\mathbb{T}$ which automatically produces a linkage between velocity components.

One way to remove the linkage would be to evaluate explicitly the terms associated to $\mathbb{T}$. In such case, Equation (50) would change to

$$\begin{bmatrix} \mathbb{M} - \dfrac{\Delta t\,\mu}{2}\mathbb{L} & \Delta t\,\mathbb{G} \\ \mathbb{D} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}^{n+1} \\ p^{n+1} \end{bmatrix} = \begin{bmatrix} -\Delta t \left(\dfrac{3}{2}\mathbb{C}(\mathbf{v}^{n+1}) - \dfrac{1}{2}\mathbb{C}(\mathbf{v}^{n-1}) \right) + \dfrac{\Delta t\,\mu}{2}(\mathbb{L} + 2\mathbb{T})\mathbf{v}^n + \mathbb{M}\mathbf{v}^n + \Delta t\,\mathbb{F} \\ 0 \end{bmatrix} \tag{86}$$

Numerical simulations and convergence and stability analysis is required to see if the linkage can be removed without loss of convergence, accuracy and performance. We doubt that this will be possible at least for low Reynolds numbers.

Divergence discretization is the modern approach chosen by many researchers for the simulation of incompressible viscous flows with free surfaces (see, for example, [34–39]). It is also general and compatible with the approach used in solid mechanics. So in case of doubt... choose the divergence path.

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