Exact integration of the unsteady incompressible Navier-Stokes equations, gauge criteria and applications

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An exact first integral of the full, unsteady, incompressible Navier-Stokes equations is achieved in its most general form via the introduction of a tensor potential and parallels drawn with Maxwell's theory. Subsequent to this gauge freedoms are explored, showing that when used astutely they lead to a favourable reduction in the complexity of the associated equation set and number of unknowns, following which the inviscid limit case is discussed. Finally, it is shown how a change in gauge criteria enables a variational principle for steady viscous flow to be constructed having a self-adjoint form.

Use of the new formulation is demonstrated, for different gauge variants of the first integral as the starting point, through the solution of a hierarchy of classical three-dimensional flow problems; two of which are tractable analytically, the third being solved numerically. In all cases the results obtained are found to be in excellent accord with corresponding solutions available in the open literature. Concurrently, the prescription of appropriate commonly occurring physical and necessary auxiliary boundary conditions, incorporating for completeness the derivation of a first integral of the dynamic boundary condition at a free surface, is established, together with how the general approach can be advantageously reformulated for application in solving unsteady flow problems with periodic boundaries.

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I. INTRODUCTION

In classical fluid mechanics, potentials have been used to great effect for the solution of problems considered ideal or Stokes like. Bernoulli's equation is obtained as a first integral of Euler's equations in the absence of vorticity and viscosity, if the velocity vector is taken to be the gradient of a scalar potential. The so-called Clebsch transformation[1,2] and related approaches allow for further extension to flows with non-vanishing vorticity, resulting in a generalised Bernoulli equation complemented with transport equations for the Clebsch potentials[3]. For compressible flow involving volume viscosity but with the shear viscosity neglected – a special case of the general form, see Scholle and Marner[4] – Zuckerwar and Ash[5] obtained a potential-based Lagrangian.

Progress involving the full incompressible Navier-Stokes (NS) equations has been far less fruitful and restricted to the limiting case of steady two-dimensional (2D) flow; the most recent contribution being that of Scholle, Haas, and Gaskell[6] who constructed an exact complex-valued first integral, based on the introduction of an auxiliary potential field. This formulation embodies the classical complex-valued Goursat representation for steady Stokes flow, allowing the streamfunction to be expressed in terms of two analytic functions[7]. While essentially a rediscovery of the result of Legendre[8], along similar lines to the work of Coleman[9] and Ranger[10], a hallmark of Scholle, Haas, and Gaskell[6]'s particular derivation is it provides a clear hint apropos generalisation to unsteady, three-dimensional (3D) viscous flow: the attainment of which has hitherto remained out of reach; providing the impetus for the present work.

Beginning with the transformation of existing 2D theory from a complex formulation to a real-valued one, resulting in the required tensor form, the key aspect leading to the determination of a first integral is recognition that it can be derived using a potential formulation similar to that employed in the reduction of Maxwell's equations. Via the astute use of gauge freedoms, a decrease in the number of equations and unknowns is achieved as well as their transformation to a known, more tractable, equation set in which the differential order of the non-linear terms is reduced. Although consideration is focused on specific gauging of the tensor potential, in order to ensure the equation set has a favourable structure, the theory itself is amenable to alternative development. Some of which offer the prospect of a promising continuation of the research field; for example, it is shown that the gauge freedoms can be utilised intelligently to establish a variational principle for steady viscous flow. The limit case of inviscid flow is also addressed. Since the equations are derived in their most general form, restrictions to special cases such as steady or Stokes flow follows naturally, leading to further simplifications.

Boundary conditions, physical and auxiliary, in the framework of the above are provided, with the condition essential to the investigation of 3D free-surface flow problems derived in the form of a first integral of the usual dynamic boundary condition[6,7]. As a whole the approach followed together with the established first integral, represents an important step forward; demonstrated via the solution of three classical, yet diverse, fluid flow problems of differing complexity, two of which are approached analytically, the other numerically. In all three cases it is found that starting from the first integral, in deference to the NS equations, corresponding established solutions appearing in the open literature are recovered exactly; in one case it provides new theoretical insight. Last but not least, the time-evolution of periodically constrained unsteady flow is addressed as a standard scenario often encountered in relation to the direct numerical simulation (DNS) of viscous flow; using Fourier

decomposition, the first integral formulation proves to be a very elegant approach leading to a reduced set of ordinary differential equations (ODEs).

II. FIRST INTEGRAL DERIVATION

With reference to earlier work concerning the derivation and use of an exact complex-valued first integral for 2D incompressible flow[7,11] a real-valued one for the full unsteady, incompressible NS equations is formulated. Tensor calculus is employed, where vector fields are denoted by their Cartesian components, e.g. the velocity field $\vec{u}$ by u_i, $i = 1, \cdots, 3$, and tensors such as that for stress $\underline{T}$ by T_{ij}. The Einstein summation convention is used throughout: ∂_i denotes a spatial derivative with respect to x_i, i.e. $\partial_i = \partial/\partial x_i$, and ∂_t the time derivative; δ_{ij} is the Kronecker delta function and ε_{ijk} the 3D Levi-Civita symbol.

The beneficial use of potential fields, synonymous with Maxwell's theory[12], underpins the present approach: in that important and essential insight is gained for a similar treatment of the NS equations. The latter together with the Continuity equation, for the unsteady, incompressible flow of a Newtonian fluid, dynamic viscosity η and density ϱ, are given by:

$$\varrho \partial_t u_i + \varrho u_j \partial_j u_i = -\partial_i \left[p + U \right] + \eta \partial_j \partial_j u_i \,, \tag{1}$$

$$\partial_i u_i = 0 \,, \tag{2}$$

where p is the pressure and U the potential energy density of an external conservative force.

A. Preliminaries and introduction of a streamfunction vector

Prior to deriving the 3D form of the first integral, consideration is given to equation (2), which is fulfilled identically by introducing a vector potential Ψ_k for the velocity according to:

$$u_i = \varepsilon_{ijk} \partial_j \Psi_k \,, \tag{3}$$

known in the literature as a 3D generalisation of the 2D streamfunction[13] that can be gauged by an arbitrary gradient field, that is:

$$\Psi_k \longrightarrow \Psi_k + \partial_k \chi \,; \tag{4}$$

leading, according to (3), to the same velocity field u_i.

Within the present context, the above allows reformulation of the time derivative in equation (1) as the divergence of a tensor field, namely: $\partial_t u_i = \varepsilon_{ijk} \partial_t \partial_j \Psi_k = \partial_j \left(\varepsilon_{ijk} \partial_t \Psi_k \right)$. In this way equations (1) can be re-written as:

$$\partial_j \left[\varrho \varepsilon_{ijk} \partial_t \Psi_k + \varrho u_j u_i - T_{ji} + U \delta_{ji} \right] = 0 \,, \tag{5}$$

with the stress tensor given by:

$$T_{ij} = -p \delta_{ij} + \eta \left[\partial_j u_i + \partial_i u_j \right] \,. \tag{6}$$

B. First integral of the field equations

With reference to the above it is clear that the momentum balance (5) is a partial differential equation (PDE) of the same type as equation (2) but for a tensor rather than a vector field. Hence, by introducing the tensor M_{lj} as a new potential, in accordance with:

$$\varrho\varepsilon_{ijk}\partial_t\Psi_k + \varrho u_i u_j - T_{ij} + U\delta_{ij} = \varepsilon_{jlk}\partial_l M_{ki}\,, \tag{7}$$

equation (5) is fulfilled identically; the analogy with (3) being obvious. Since T_{ij} is a symmetric tensor, it is convenient to split the above equation into symmetric:

$$\varrho u_i u_j - T_{ij} + U\delta_{ij} = \frac{1}{2}\left[\varepsilon_{jlk}\partial_l M_{ki} + \varepsilon_{ilk}\partial_l M_{kj}\right]\,, \tag{8}$$

and skew-symmetric parts; the latter, by multiplying (7) with ε_{ijn}, is conveniently represented as a vector equation:

$$2\varrho\partial_t\Psi_n = \partial_n M_{ll} - \partial_l M_{nl}\,. \tag{9}$$

Though not immediately obvious, the above rudimentary form of the first integral corresponds to that of the 2D first integral[7,11]; a more conveniently recognisable form is arrived at via the following reformulation.

First, using the streamfunction (3) the stress tensor (6) can be written as:

$$T_{ij} = -p\delta_{ij} + \eta\left[\varepsilon_{ilk}\partial_l\left(\partial_j\Psi_k\right) + \varepsilon_{jlk}\partial_l\left(\partial_i\Psi_k\right)\right]\,,$$

and, hence, equation (8) as:

$$\varrho u_i u_j + (p+U)\delta_{ij} = \frac{1}{2}\left[\varepsilon_{jlk}\partial_l\left(M_{ki} + 2\eta\partial_i\Psi_k\right) + \varepsilon_{ilk}\partial_l\left(M_{kj} + 2\eta\partial_j\Psi_k\right)\right]\,. \tag{10}$$

The first order potential M_{ki} enters the equations in combination with terms of the form $2\eta\partial_i\Psi_k$ only. Recognising this and following the procedure adopted by Marner, Gaskell, and Scholle[11] for 2D flow the combination $M_{ki} + 2\eta\partial_i\Psi_k$ can be rewritten as:

$$M_{ki} + 2\eta\partial_i\Psi_k = \varepsilon_{ipq}\partial_p a_{kq} + 2\partial_i\varphi_k\,, \tag{11}$$

which for vector fields is the well-known Maxwell decomposition into a divergence-free and a curl-free part; the form of which is a generalisation towards tensors of second rank with vector and tensor potential φ_k and a_{kq}, respectively. Inserting (11) into equations (8) and (9), yields the following relationships:

$$\varrho u_i u_j + (p+U)\delta_{ij} = \frac{1}{2}\varepsilon_{ilk}\varepsilon_{jpq}\partial_l\partial_p\left(a_{kq} + a_{qk}\right) + \partial_i\left(\varepsilon_{jlk}\partial_l\varphi_k\right) + \partial_j\left(\varepsilon_{ilk}\partial_l\varphi_k\right)\,, \tag{12}$$

$$2\varrho\partial_t\Psi_n = \partial_n\partial_k\left[\varepsilon_{kqp}a_{pq} + 2\varphi_k - 2\eta\Psi_k\right] - \partial_k\partial_k\left[2\varphi_n - 2\eta\Psi_n\right]\,, \tag{13}$$

which can be simplified by making use of the gauge transformation (4). The latter has no effect on equation (12) but equation (13) becomes:

$$2\varrho\partial_t\Psi_n = \partial_n\left\{\partial_k\left[\varepsilon_{kqp}a_{pq} + 2\varphi_k - 2\eta\Psi_k\right] - 2\varrho\partial_t\chi\right\} - \partial_k\partial_k\left[2\varphi_n - 2\eta\Psi_n\right]\,. \tag{14}$$

Since the gauge field χ can be chosen arbitrarily, the term $\varepsilon_{kqp}\partial_k a_{pq} - 2\varrho\partial_t\chi$ may be set to any value; in particular, by choosing:

$$\chi = \frac{1}{2\varrho}\int \varepsilon_{kqp}\partial_k a_{pq}\mathrm{d}t + \chi_0(x_i)\,, \tag{15}$$

leads to

$$\varrho\partial_t\Psi_n = \partial_n\partial_k\left[\varphi_k - \eta\Psi_k\right] - \partial_k\partial_k\left[\varphi_n - \eta\Psi_n\right] \; ; \tag{16}$$

showing that the skew-symmetric part of the tensor potential can be eliminated and therefore a_{pq} assumed symmetric from the very outset, leading ultimately to the following simplified form of equation (12):

$$\varrho u_i u_j + (p+U)\delta_{ij} = \varepsilon_{ilk}\varepsilon_{jpq}\partial_l\partial_p a_{kq} + \partial_i\left(\varepsilon_{jlk}\partial_l\varphi_k\right) + \partial_j\left(\varepsilon_{ilk}\partial_l\varphi_k\right) \; . \tag{17}$$

Second, the divergence $\partial_n(\cdots)$ of equation (16) leads to $2\varrho\partial_t\left(\partial_n\Psi_n\right) = 0$, implying that $\partial_n\Psi_n$ is independent of time. Since χ_0 in (15) is arbitrary, it can be chosen such that:

$$\partial_n\Psi_n = 0 \, , \tag{18}$$

analogous to the Coulomb gauge in Maxwell's theory[12]. This, together with the identity $\partial_n\partial_k\varphi_k - \partial_k\partial_k\varphi_n = \varepsilon_{nij}\partial_i\left(\varepsilon_{jlk}\partial_l\varphi_k\right)$, enables equation (16) to be written in the form of an inhomogeneous diffusion equation:

$$\varrho\partial_t\Psi_n - \eta\partial_k\partial_k\Psi_n = \varepsilon_{nij}\partial_i\left(\varepsilon_{jlk}\partial_l\varphi_k\right) \; ; \tag{19}$$

leading simultaneously to a reduction in the numbers of potentials due to the elimination of the skew-symmetric part of a_{pq}.

Thus far, a first integral of the unsteady incompressible Navier-Stokes equations has been obtained in the form of a tensor-valued field equation (17) and a vector-valued field equation (19) constrained by (18), involving various unknown fields a_{pq}, Ψ_n, u_n, p and φ_n. Although these remain to be closed mathematically, even at this stage they serve as an insightful starting point for fixing the remaining degrees of freedom in beneficial ways, that is *tuning* the form of the equations. This is explored in detail below.

III. CLOSURE VIA SELECTIVE GAUGE CRITERIA

In general, a gauge transformation of a given set of potentials replaces them by an equivalent set of potentials leading to identical observables. Accordingly, such transformations can be used to simplify corresponding field equations, for the potentials, with respect to their mathematical structure as well as to the number of potentials. In the following, the gauge freedoms of a_{pq} and φ_n are analysed in detail. Obviously, by performing the operations:

$$a_{pq} \longrightarrow a_{pq} + \partial_p\alpha_q + \partial_q\alpha_p \, , \tag{20}$$

$$\varphi_n \longrightarrow \varphi_n + \partial_n\zeta \, , \tag{21}$$

for an arbitrary vector field α_q and an arbitrary scalar field ζ, the field equations (17, 19) remain invariant. The above rules are utilised subsequently to establish bona fide gauging scenarios, ones that lead favourably to a reduction of the order of the established first integral, equations (17) to (19); in this context Scholle, Haas, and Gaskell[6] showed that, by applying a particular gauge, a special form of the first integral of NS equations for steady 3D flow can be obtained based on a minimum number of three potential fields only.

A. Convenient re-ordering of the first integral

Mixed derivatives of the form $\partial_k\partial_l(\cdots)$ are an inconvenience which can be avoided via a specific gauge transformation. This is achieved as follows, beginning with the re-ordering of the first the second order derivatives within the double curl operation $\varepsilon_{ikl}\varepsilon_{jpq}\partial_k\partial_p a_{lq}$ of equation (17). Since the product of two Levi-Civita symbols can be expressed as:

$$\varepsilon_{ikl}\varepsilon_{jpq} = \delta_{ij}\delta_{kp}\delta_{lq} + \delta_{ip}\delta_{kq}\delta_{lj} + \delta_{iq}\delta_{kj}\delta_{lp} - \delta_{ip}\delta_{kj}\delta_{lq} - \delta_{ij}\delta_{kq}\delta_{lp} - \delta_{iq}\delta_{kp}\delta_{lj}\,,$$

the identity:

$$\begin{aligned}\varepsilon_{ikl}\varepsilon_{jpq}\partial_k\partial_p a_{lq} &= -\partial_k\partial_k\left[a_{ij} - a_{ll}\delta_{ij}\right] + \partial_i\partial_k a_{kj} + \partial_j\partial_k a_{ki} - \partial_i\partial_j a_{kk} - \partial_l\partial_k a_{kl}\delta_{ij}\\ &= -\partial_k\partial_k\left[a_{ij} - \frac{a_{ll}}{2}\delta_{ij}\right] + \partial_i\partial_k\left[a_{kj} - \frac{a_{ll}}{2}\delta_{kj}\right] + \partial_j\partial_k\left[a_{ki} - \frac{a_{ll}}{2}\delta_{ki}\right] - \partial_l\partial_k\left[a_{kl} - \frac{a_{nn}}{2}\delta_{kl}\right]\delta_{ij}\,,\end{aligned}$$

results, giving rise to the following reformulation of equation (17):

$$\varrho u_i u_j + (p+U)\delta_{ij} = -\partial_k\partial_k\tilde{a}_{ij} + \partial_i A_j + \partial_j A_i - \partial_k A_k\delta_{ij}, \tag{22}$$

in terms of the modified tensor potential $\tilde{a}_{ij}$ and an auxiliary vector field A_j defined as:

$$\tilde{a}_{ij} := a_{ij} - \frac{a_{kk}}{2}\delta_{ij}\,, \tag{23}$$

$$A_j := \partial_k\tilde{a}_{kj} + \varepsilon_{jlk}\partial_l\varphi_k\,. \tag{24}$$

Note that from the form (22) of the tensor equation, the mathematical structure of the first integral for 2D flows reported in[7,11] is recovered, see Appendix A.

Compared to its original form (17), equation (22) provides a partition of terms: in particular, all mathematical expressions with mixed derivatives of the form $\partial_k\partial_l(\cdots)$ occur exclusively as derivatives of the auxiliary vector field A_j. Now, via a gauge transformation of the form (20), the vector field A_j can be manipulated according to:

$$A_j \to A_j + \partial_k\partial_k\alpha_j\,, \tag{25}$$

which can be set to any arbitrary value by means of the proper choice of the gauge field α_j. The choice:

$$A_j = 0\,, \tag{26}$$

leads to the elimination of all mixed derivatives in (22), and to the simplified form:

$$\varrho u_i u_j + (p+U)\delta_{ij} = -\partial_k\partial_k\tilde{a}_{ij}\,. \tag{27}$$

The gauge condition (26) is reminiscent of the Lorenz gauge or Coulomb gauge in Maxwell's theory[12] which similarly leads to the elimination of mixed terms in the associated field equations. Moreover, via (26) the additional vector potential φ_j is eliminated from equation (27). By writing (26) explicitly as $\varepsilon_{jlk}\partial_l\varphi_k = -\partial_k\tilde{a}_{kj}$, φ_j can also be eliminated from equation (19), which accordingly takes the form:

$$\varrho\partial_t\Psi_n - \eta\partial_k\partial_k\Psi_n = -\varepsilon_{nkl}\partial_k\partial_m\tilde{a}_{ml}\,, \tag{28}$$

of an inhomogeneous diffusion equation; c.f. equation (19). Total elimination of φ_j from the entire set of equations requires the divergence of the gauge condition (26), implying:

$$\partial_j\partial_k\tilde{a}_{kj} = 0\,. \tag{29}$$

The outcome is a favourably reduced equation set comprised of one each of a symmetric tensor equation (27), a vector equation (28) and a scalar equation (29), in terms of the symmetric modified tensor potential $\tilde{a}_{ij} = a_{ij} - a_{kk}\delta_{ij}/2$, the streamfunction vector Ψ_n and the pressure p.

The key features associated with equations (27) to (29) are: (i) though the number of unknown fields (one symmetric tensor, one vector, one scalar) exceeds that of a comparable formulation in primitive variables (one vector and one scalar), their favourably different *structure* off-sets this; (ii) in contrast to the original NS equations (1) which include the material time derivative, a non-linear term involving first order velocity derivatives, equation (27) consists of a non-linear term which depends directly on the velocities – equation (28) is simply a linear inhomogeneous diffusion equation, not a nonlinear diffusion-convection equation – resulting in a reduction of the differential order of the non-linearity.

1. Zero-viscosity limit

Since the zero-viscosity limit leads to a change of problem type, namely from second order PDEs (Navier-Stokes equations) to ones of first order (Euler's equations), it is apposite to explore this special case: applying the limit $\eta \to 0$ to equations (27-29), the following set of PDEs:

$$\partial_k \partial_k \tilde{a}_{ij} = -\varrho u_i u_j - (p+U)\delta_{ij}\,, \tag{30}$$

$$\varrho \partial_t \Psi_n = -\varepsilon_{nkl}\partial_k \partial_m \tilde{a}_{ml}\,, \tag{31}$$

$$\partial_j \partial_k \tilde{a}_{kj} = 0\,, \tag{32}$$

is obtained; containing still, second order derivatives of the tensor potential but only first order derivatives of the streamfunction vector. Taking now the curl $\varepsilon_{pqn}\partial_q$ of (31), in combination with (30, 32) and (3), it follows that:

$$\begin{aligned}\varrho \partial_t \underbrace{(\varepsilon_{pqn}\partial_q \Psi_n)}_{u_p} &= -\left[\delta_{pk}\delta_{ql} - \delta_{pl}\delta_{qk}\right]\partial_q \partial_k \partial_m \tilde{a}_{ml} = \partial_m \partial_k \partial_k \tilde{a}_{mp} - \partial_p \underbrace{\partial_l \partial_m \tilde{a}_{ml}}_{0} \\ &= -\partial_m\left[\varrho u_m u_p + (p+U)\delta_{mp}\right] = -\varrho \overbrace{\partial_m u_m}^{0} u_p - \varrho u_m \partial_m u_p - \partial_p p - \partial_p U\,,\end{aligned}$$

which is a full reproduction of Euler's equations, proving that the PDE set (30-32) is a first integral of Euler's equations, as it should be. Also in this case conservation of energy, momentum (in absence of external forces, $U = 0$), angular momentum and helicity is fulfilled[13].

2. Steady flow case

By employing the two gauge conditions (18, 29), together with the well known identity $\partial_k \partial_k \Psi_n = \partial_n \partial_k \Psi_k - \varepsilon_{nkl}\partial_k\left(\varepsilon_{lpq}\partial_p \Psi_q\right)$ and the definition of the streamfunction vector (3), equation (28) takes the form: $\varrho \partial_t \Psi_n + \varepsilon_{nkl}\partial_k\left[\eta u_l + \partial_m \tilde{a}_{ml}\right] = 0$. Hence, for steady flow, $\partial_t \Psi_n = 0$, the term in square brackets can be written as the gradient of a scalar field, that is:

$$\eta u_l + \partial_m \tilde{a}_{ml} = \partial_l \Phi\,;$$

by proper gauging of the tensor potential $\tilde{a}_{ml}$, Φ can be set equal to zero, resulting in the identity:

$$u_l = -\frac{1}{\eta}\partial_m \tilde{a}_{ml}\,, \tag{33}$$

via which the streamfunction vector is eliminated. The remaining fields are the symmetric tensor potential $\tilde{a}_{ml}$ and the pressure p; the field equations for steady flow being simply (27) and (29).

B. Traceless form

Two of the scalar fields, namely the pressure p and the trace of the tensor potential, can be eliminated as follows. The trace of equation (27):

$$\partial_k \partial_k \tilde{a}_{ii} = -\varrho u_i u_i - 3(p+U)\,, \tag{34}$$

enables direct calculation of the pressure from the other fields, c.f. Bernoulli's equation in potential theory. Equation (34) can be used to express $p+U$ in terms of the square of the velocity and second order derivatives of the tensor potential; this allows elimination of the pressure from equation (27), resulting in the following traceless symmetric tensor equation:

$$\partial_k \partial_k \bar{a}_{ij} = -\varrho \left[u_i u_j - \frac{u_k u_k}{3}\delta_{ij} \right]\,, \tag{35}$$

in terms of the traceless tensor potential:

$$\bar{a}_{ij} = \tilde{a}_{ij} - \frac{\tilde{a}_{kk}}{3}\delta_{ij}\,. \tag{36}$$

Equation (35) is supplemented by equation (28) which in terms of the traceless tensor potential reads:

$$\varrho \partial_t \Psi_n - \eta \partial_k \partial_k \Psi_n = -\varepsilon_{nkl}\partial_k \partial_m \bar{a}_{ml}\,. \tag{37}$$

Together, expressions (35) and (37) comprise eight independent equations for the eight independent components of $\bar{a}_{ij}$ and Ψ_n, which is the minimum number in the case of unsteady flow.

Steady flow case: As above, a traceless and therefore reduced version of the field equations is achieved by inserting the identity (33) into (35) and taking (29) as the second equation, leading to six independent PDEs for six unknown fields.

C. Self-adjoint form

Finding variational formulations for physical systems is beneficial with respect to a deeper understanding of the system and for establishing new solution methods, both analytical and numerical. In fluid mechanics two major routes have emerged: (i) the stochastic variational description corresponding to the Lagrangian equations of motion in terms of material path lines, making use of a statistical treatment of kinetic models, see e.g.[14–16] and[17]; (ii) in the framework of a field description involving the recovery of the NS equations by variation of an action integral in the classical deterministic sense. In terms of the latter, it was Millikan[18] who showed the non-existence of a Lagrangian, in terms of the velocity u_i, the pressure p

and their first order derivatives, that would enable the NS equations to be written as Euler-Lagrange equations. An analogue situation is found in Maxwell's theory, where it is not possible to establish a Lagrangian in terms of an electric field E_i and magnetic flux density B_i; however, a Lagrangian can be found in terms of a scalar potential φ and vector potential A_i. It is the latter that has prompted the search for a variational description for viscous flow in terms of potentials rather than velocity and pressure.

A variety of suggestions from different authors have appeared based on different potential formulations: Zuckerwar and Ash [5] used the Clebsch transformation[1,2] to establish a Lagrangian for flows with volume viscosity, while latterly Scholle and Marner [4] consider shear viscosity in a similar manner. A variational description based on a vector potential for the velocity was proposed by Bendali, Dominguez, and Gallic [19]. In the present work the field equations are comprised of vector and tensor potentials, posing the question as to whether they are self-adjoint. As demonstrated below for the case of steady flow, a special gauge criteria is required to achieve a self-adjoint first integral of the NS equations.

When the flow is steady, $\partial_t \Psi_n = 0$, equation (16) is fulfilled identically by writing:

$$\varphi_n = \eta \Psi_n \,, \tag{38}$$

the insertion of which in equation (12) and making use of the relationship $a_{kq} + a_{qk} = 2\bar{a}_{kq} + 2a_{nn}\delta_{kq}/3$ from equation (36), leads to the following tensor equation:

$$\varrho u_i u_j + (p+U)\delta_{ij} = \varepsilon_{ilk}\varepsilon_{jpq}\partial_l\partial_p\bar{a}_{kq} + \frac{1}{3}\left[\partial_l\partial_l a_{nn}\delta_{ij} - \partial_i\partial_j a_{nn}\right] + \eta\left[\partial_i u_j + \partial_j u_i\right] \,, \tag{39}$$

as the most general form of the first integral for steady flow; valid for any gauging of the tensor potential. On elimination of the isotropic part and hence the pressure, its associated traceless form results:

$$\varrho\left[u_i u_j - \frac{u_k u_k}{3}\delta_{ij}\right] - \eta\left[\partial_i u_j + \partial_j u_i\right] = \left[\varepsilon_{ilk}\varepsilon_{jpq} - \varepsilon_{nlk}\varepsilon_{npq}\frac{\delta_{ij}}{3}\right]\partial_l\partial_p\bar{a}_{kq} + \frac{1}{3}\left[\partial_l\partial_l a_{nn}\delta_{ij} - \partial_i\partial_j a_{nn}\right] \,, \tag{40}$$

in terms of the traceless symmetric tensor potential $\bar{a}_{kq}$, the trace a_{nn} of the tensor potential and the velocity field $u_i = \varepsilon_{inm}\partial_n\Psi_m$. Suggesting a Lagrangian of the form:

$$\ell = \varrho\bar{a}_{ij}u_i u_j + \left[2\eta u_j - \frac{1}{3}\partial_j a_{nn}\right]\partial_i\bar{a}_{ij} + \frac{1}{2}\varepsilon_{ilk}\varepsilon_{jpq}\partial_l\bar{a}_{ij}\partial_p\bar{a}_{kq} + f\left(u_i, a_{nn}, \partial_i a_{nn}\right) \,, \tag{41}$$

which, because $u_i = \varepsilon_{inm}\partial_n\Psi_m$, is a function of the fields $\bar{a}_{kq}$, a_{nn}, Ψ_m and their associated first order derivatives, i.e. $\ell = \ell\left(\bar{a}_{kq}, a_{nn}, \partial_n\Psi_m, \partial_p\bar{a}_{kq}, \partial_i a_{nn}\right)$. f remains to be specified, its significance being discussed below.

Variation of the action integral:

$$\delta \iiint_V \ell\left(\bar{a}_{kq}, a_{nn}, \partial_n\Psi_m, \partial_p\bar{a}_{kq}, \partial_i a_{nn}\right) \mathrm{d}V = 0 \,, \tag{42}$$

with respect to $\bar{a}_{ij}$ results in the required Euler-Lagrange equations (40); whereas variation with respect to Ψ_m and a_{nn} lead to:

$$-2\varepsilon_{mni}\partial_n\left[\varrho\bar{a}_{ij}u_j + \eta\partial_j\bar{a}_{ji} + \frac{1}{2}\frac{\partial f}{\partial u_i}\right] = 0 \,, \tag{43}$$

$$\frac{1}{3}\partial_i\partial_j\bar{a}_{ij} + \frac{\partial f}{\partial a_{nn}} - \partial_i\left(\frac{\partial f}{\partial(\partial_i a_{nn})}\right) = 0 \,. \tag{44}$$

The meaning of equations (43) and (44) becomes much clearer after a substitution and rearrangement of terms: use of the definitions (23, 24) and (36) together with $\varepsilon_{jlk}\partial_l\varphi_k = \eta u_j$ following from (3) and (38), leads to the identity:

$$\partial_j \bar{a}_{ji} = A_i - \eta u_i + \frac{1}{6}\partial_i a_{nn}\,, \tag{45}$$

which, when substituted into (43, 44), yields:

$$\varepsilon_{mni}\partial_n A_i = \varepsilon_{mni}\partial_n \left[\eta u_i - \frac{1}{2\eta}\frac{\partial f}{\partial u_i} - \frac{\varrho}{\eta}\bar{a}_{ij}u_j\right]\,, \tag{46}$$

$$\partial_i A_i = \partial_i \left[3\frac{\partial f}{\partial(\partial_i a_{nn})} - \frac{1}{2}\partial_i a_{nn}\right] - 3\frac{\partial f}{\partial a_{nn}}\,. \tag{47}$$

Since any vector field A_i can be reconstructed from its divergence $\partial_i A_i$ and its curl $\varepsilon_{mni}\partial_n A_i$, the reformulated Euler-Lagrange equations (46) and (47) is identifiable as an *alternative gauge* to that given by (26), the latter leading to the favourable formulation developed at the end of Section III A for steady flow having a reduced number of unknown fields.

Hence, for steady flow a choice is available between the use of gauge (26) leading to a reduced set of fields and a favourable mathematical form of the field equations or gauge (43, 44) supplementing equations (40) to form a self-adjoint set of equations. The availability of a self-adjoint form can be useful for particular problems, e.g. when trying to compute normal forms around singular bifurcation points since it is necessary to make projections onto the eigenfunction of an adjoint problem, see Dijkstra *et al.*[20] and references therein.

Via a proper choice of the yet unknown function f in (41) the gauge conditions (46) and (47) are tuneable to some extent. For example, by choosing:

$$f\left(u_i, \partial_i a_{nn}\right) = \eta^2 u_i^2 + \frac{1}{12}\left(\partial_i a_{nn}\right)^2 \tag{48}$$

they simplify to:

$$\varepsilon_{mni}\partial_n A_i = -\frac{\varrho}{\eta}\varepsilon_{mni}\partial_n\left(\bar{a}_{ij}u_j\right)\,, \tag{49}$$

$$\partial_i A_i = 0\,. \tag{50}$$

In principle any arbitrary choice of f is possible.

For completeness it is important to mention that for the case of 2D flow the first integral formulation for steady, incompressible and inviscid conditions proposed by He[21,22] with the aim of establishing a variational formulation, features unresolved issues[23]. In contrast, the variational principle above recovers, for $\eta \to 0$, the traceless version of the first integral of Euler's equations for steady flow.

IV. APPLICATION OF THE METHODOLOGY

Having derived the first integral and explored its versatility in detail and on different levels, its use as a starting point to solve viscous fluid flow problems is now demonstrated. Not all of the gauge variants described in Section III are analysed further; rather the focus is those formulated in Section III A and the solution of three different classical, benchmark

viscous flows, which exhibit a hierarchy of sufficient complexity for such purposes – geometry, unsteadiness, non-linearity, inertia – and are solved analytically where analysis permits, otherwise numerically. The necessary, and related, boundary conditions required to do so are outlined below.

A. Boundary conditions

Depending on the problem of interest, the physical boundary conditions involved have to be formulated appropriately; a good example of this is the kinematic and dynamic boundary conditions required to solve 3D free surface flow problems which, although not utilised, are included for completeness.

1. Boundary conditions at solid walls, inlets and outlets

Along solid walls, for the velocity field the no-slip condition:

$$u_i = U_{Bi} \ , \tag{51}$$

has to be fulfilled, where U_{Bi} is the velocity of the boundary; inlet and outlet boundary conditions with fixed velocity profile have the same mathematical form as does the specification and advantageous use of symmetry and periodic boundary conditions. The latter type is discussed in more detail in Section IV C 2.

2. Boundary conditions at a free surface

Although a free surface condition does not appear in the problems solved below, the required attendant boundary conditions are provided. Their full derivation is given in Appendix B but in summary two conditions must be fulfilled at a free surface: (i) the kinematic boundary condition, $u_i n_i = 0$, related to mass conservation; (ii) the dynamic boundary condition related to stress equilibrium at the surface. The latter can be described by the vector equation:

$$T_{ij} n_j = \sigma_s \kappa n_i \, , \tag{52}$$

involving the stress tensor T_{ij}, the normal vector n_i, the surface tension σ_s and the curvature κ. Using the potential representation for the respective physical quantities, equation (52) can be reformulated into a more convenient form – see Appendix B, where it is also shown that for steady flow a first integral of the dynamic boundary itself can be constructed leading to a first order condition for the tensor potential entries only:

$$\varepsilon_{ikl} \left[\partial_k a_{lm} \mathrm{d}x_m + \left(\sigma_s n_k - \frac{U_k}{2} \right) \mathrm{d}x_l \right] = 0 \, , \tag{53}$$

with the auxiliary functions U_k implicitly defined by (B.11).

3. Auxiliary boundary conditions

Irrespective of the physical boundary conditions present, e.g. walls or free surfaces, an insufficient number can be prescribed to ensure a uniquely solvable system. An example of this is flow problems in which wall boundary conditions are prescribed on *all* parts of the boundary, as in the case of the lid-driven cavity flow explored below. Exactly three velocity conditions exist, which is less than the number of unknown fields. Even in the case of steady flow, where according to (33) the velocity can be expressed via the divergence of the tensor potential, 6 independent fields have to be considered – with at least three additional boundary conditions having to be formulated although there are no more physical conditions to be fulfilled; these necessary additional boundary conditions are subsequently termed *auxiliary boundary conditions* since they exert no influence on the physics.

While the options available for specifying these auxiliary boundary conditions appears wide, the two provided below are the only possible auxiliary Dirichlet conditions which appear reasonable:

1. Let n_j be the normal vector of the respective boundary. Then, three Dirichtlet boundary conditions are given by:
$$\tilde{a}_{ij} n_j = 0\,. \tag{54}$$

2. Let $t_i^{(1)}$ and $t_i^{(2)}$ be two orthogonal tangential vectors at the boundary. Then, three independent Dirichlet boundary conditions are given by:
$$t_i^{(1)} \tilde{a}_{ij} t_j^{(1)} = 0\,, \tag{55}$$
$$t_i^{(1)} \tilde{a}_{ij} t_j^{(2)} = 0\,, \tag{56}$$
$$t_i^{(2)} \tilde{a}_{ij} t_j^{(2)} = 0\,. \tag{57}$$

The decisive criterion for the choice of auxiliary boundary conditions is that they must not contradict the physically prescribed boundary conditions. For example, consider boundary conditions (54) for a steady flow; by integration over the entire boundary ∂V of the system's volume V and making use of Gauss's theorem, the following identities:
$$0 = \oiint_{\partial V} \tilde{a}_{ij} n_j \mathrm{d}S = \iiint_V \partial_j \tilde{a}_{ij} \mathrm{d}V = -\eta \iiint_V u_i \mathrm{d}V \tag{58}$$
are obtained, where relationship (33) has been utilised. Equation (58) implies the vanishing of the global momentum, which is clearly an inadmissible physical restriction.

While the above example demonstrates the choice of auxiliary boundary conditions to be neither arbitrary nor intuitive, heuristic considerations lead to conditions (55-57) which do not conflict with the physics; although no proof is given at this point, the comparatively accurate numerical results obtained below for the lid-driven cavity problem suggest the postulated conditions (55-57) to be both admissible *and* sufficient to mathematically close the boundary value problem, at least in the steady case.

B. Unsteady stagnation flow

Consider the unsteady non-axisymmetric stagnation flow, depicted in to Figure 1, as a prototype example embodying both inertia and time dependence. It is assumed that:

$$\vec{u} = xf'(z,t)\vec{e}_x + yg'(z,t)\vec{e}_y - [f(z,t)+g(z,t)]\,\vec{e}_z = \nabla\times[yg(z,t)\vec{e}_x - xf(z,t)\vec{e}_y]\,,$$

where the prime denotes differentiation with respect to z. Accordingly, the Continuity equation (2) is fulfilled identically and in which case the velocity can be obtained from a streamfunction vector, according to equation (3), with:

$$\vec{\Psi} = yg(z,t)\vec{e}_x - xf(z,t)\vec{e}_y\,; \tag{59}$$

note too, that the streamfunction vector fulfils the Coulomb gauge (18). The traceless form of the first integral is utilised, equations (35) and (37); written in component form equation (35) reads:

$$-\varrho^{-1}\Delta\bar{a}_{11} = \frac{2}{3}x^2f'^2 - \frac{1}{3}y^2g'^2 - \frac{1}{3}(f+g)^2\,, \tag{60}$$

$$-\varrho^{-1}\Delta\bar{a}_{22} = \frac{2}{3}y^2g'^2 - \frac{1}{3}x^2f'^2 - \frac{1}{3}(f+g)^2\,, \tag{61}$$

$$-\varrho^{-1}\Delta\bar{a}_{12} = xyf'g'\,, \tag{62}$$

$$-\varrho^{-1}\Delta\bar{a}_{13} = -x(f+g)f'\,, \tag{63}$$

$$-\varrho^{-1}\Delta\bar{a}_{23} = -y(f+g)g'\,, \tag{64}$$

while equation (37) gives:

$$-y\varrho\,[\dot{g} - \nu g''] = \partial_1\partial_2\bar{a}_{13} - \partial_1\partial_3\bar{a}_{12} + \{\partial_2\partial_2 - \partial_3\partial_3\}\bar{a}_{23} + \partial_2\partial_3[\bar{a}_{33} - \bar{a}_{22}]\,, \tag{65}$$

$$x\varrho\left[\dot{f} - \nu f''\right] = \partial_1\partial_3[\bar{a}_{11} - \bar{a}_{33}] + \partial_3\partial_2\bar{a}_{12} - \partial_1\partial_2\bar{a}_{23} + \{\partial_3\partial_3 - \partial_1\partial_1\}\bar{a}_{13}\,, \tag{66}$$

$$0 = \{\partial_1\partial_1 - \partial_2\partial_2\}\bar{a}_{12} + \partial_1\partial_2[\bar{a}_{22} - \bar{a}_{11}] + \partial_1\partial_3\bar{a}_{23} - \partial_2\partial_3\bar{a}_{13}\,, \tag{67}$$

the dot above a symbol, here and subsequently, denoting differentiation with respect to time.

The boundary conditions at $z = 0$ are the usual no-slip/no-penetration conditions $f'(0,t) = g'(0,t) = 0$ and $f(0,t) = g(0,t) = 0$. Since stagnation flows are classified as boundary layer flows[24], they have to match the associated potential flow as $z\to\infty$. Accordingly, the tensor potential for an inviscid boundary layer flow has to be constructed *a priori*.

1. Associated potential flow

In the case of 3D stagnation flow, the corresponding potential flow is given[24] by: $f(z) = a_1z$, $g(z) = a_2z$, fulfilling the no-penetration condition $f(0) = g(0) = 0$, but not so the no-slip condition. For the construction of the associated traceless tensor potential, equations (60-64) have to be solved. One such particular solution is given by:

$$\bar{a}^{\rm p}_{11} = -\frac{\varrho}{6}\left[2a_1^2x^2z^2 - a_2^2y^2z^2 - \frac{1}{6}(3a_1^2+2a_1a_2)z^4\right]\,, \tag{68}$$

$$\bar{a}^{\rm p}_{22} = -\frac{\varrho}{6}\left[2a_2^2y^2z^2 - a_1^2x^2z^2 - \frac{1}{6}(3a_2^2+2a_1a_2)z^4\right]\,, \tag{69}$$

$$\bar{a}^{\rm p}_{12} = -\frac{\varrho}{2}a_1a_2xyz^2\,,\quad \bar{a}^{\rm p}_{13} = \frac{\varrho}{6}a_1(a_1+a_2)xz^3\,,\quad \bar{a}^{\rm p}_{23} = \frac{\varrho}{6}a_2(a_1+a_2)yz^3\,; \tag{70}$$

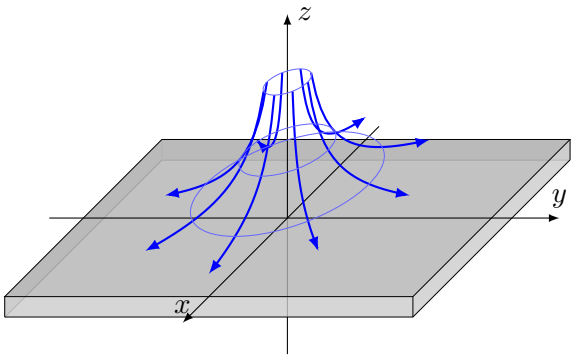

FIG. 1. Schematic of the non-axisymmetric, unsteady stagnation flow problem.

which fulfils equation (67), but not equations (65, 66); a superposition of the form $\bar{a}_{ij} = \bar{a}^{\mathrm{h}}_{ij} + \bar{a}^{\mathrm{p}}_{ij}$ with $\Delta\bar{a}^{\mathrm{h}}_{ij} = 0$ is required in order to fulfil all of the equations. By choosing $\bar{a}^{\mathrm{h}}_{12} = \bar{a}^{\mathrm{h}}_{13} = \bar{a}^{\mathrm{h}}_{23} = 0$ and

$$\bar{a}^{\mathrm{h}}_{11} = A_1\left[x^4 + z^4 - 6x^2z^2\right] , \qquad \bar{a}^{\mathrm{h}}_{22} = A_2\left[y^4 + z^4 - 6y^2z^2\right] ,$$

equations (65, 66) results in: $0 = [48A_2 + \varrho a_2^2]yz\,, \quad 0 = -[48A_1 + \varrho a_1^2]xz\,$, implying $A_1 = -\varrho a_1^2/48$ and $A_2 = -\varrho a_2^2/48$; the other equations are not affected. Hence, the resulting solutions of the homogeneous equations read:

$$\bar{a}^{\mathrm{h}}_{11} = -\varrho\frac{a_1^2}{48}\left[x^4 + z^4 - 6y^2z^2\right] , \tag{71}$$

$$\bar{a}^{\mathrm{h}}_{22} = -\varrho\frac{a_2^2}{48}\left[y^4 + z^4 - 6y^2z^2\right] . \tag{72}$$

2. General case

Assume the following analogous form of the traceless tensor potential:

$$\begin{aligned}
\bar{a}^{\mathrm{p}}_{11} &= -\varrho\left[F_{110}(z,t) + x^2F_{111}(z,t) + y^2F_{112}(z,t)\right] ,\\
\bar{a}^{\mathrm{p}}_{22} &= -\varrho\left[F_{220}(z,t) + x^2F_{221}(z,t) + y^2F_{222}(z,t)\right] ,\\
\bar{a}^{\mathrm{p}}_{12} = -\varrho xyF_{12}(z,t)\,, &\quad \bar{a}^{\mathrm{p}}_{13} = \varrho xF_{13}(z,t)\,, \quad \bar{a}^{\mathrm{p}}_{23} = \varrho yF_{23}(z,t)\,,
\end{aligned}$$

for the particular solution of (60-64); while remembering that as above the flow is of a boundary-layer type. In order to fulfil the matching condition, this particular solution has to be supplemented by equations (71, 72). In this way, equations (60-64) are reduced as follows:

$$F''_{110} + 2F_{111} + 2F_{112} = -\frac{1}{3}(f+g)^2\,, \qquad F''_{111} = \frac{2}{3}f'^2\,, \qquad F''_{112} = -\frac{1}{3}g'^2\,, \tag{73}$$

$$F''_{220} + 2F_{221} + 2F_{222} = -\frac{1}{3}(f+g)^2\,, \qquad F''_{221} = -\frac{1}{3}f'^2\,, \qquad F''_{222} = \frac{2}{3}g'^2\,, \tag{74}$$

$$F''_{12} = f'g'\,, \quad F''_{13} = (f+g)f'\,, \quad F''_{23} = (f+g)g'\,, \tag{75}$$

written in terms of functions $F_{110}, F_{111}, F_{112}, F_{220}, F_{221}, F_{222}, F_{12}, F_{13}, F_{23}$. By inserting the above solution into equations (65) to (67), it is found that equation (67) is fulfilled identically

whereas equations (65) and (66) yield:

$$\dot{g} - \nu g'' = a_2^2 z + F_{23}'' - F_{12}' - 4F_{222}' - 2F_{112}' = a_2^2 z + gg' + \int \left[fg'' - 2g'^2 \right] \mathrm{d}z, \qquad (76)$$

$$\dot{f} - \nu f'' = a_1^2 z + F_{13}'' - F_{12}' - 4F_{111}' - 2F_{221}' = a_1^2 z + ff' + \int \left[gf'' - 2f'^2 \right] \mathrm{d}z, \qquad (77)$$

which, upon taking their derivative with respect to z, leads to a coupled set of third order equations for the functions $f(z,t)$ and $g(z,t)$, namely:

$$\dot{g}' - \nu g''' = a_2^2 - g'^2 + (f+g)g'', \qquad (78)$$

$$\dot{f}' - \nu f''' = a_1^2 - f'^2 + (f+g)f''. \qquad (79)$$

These have to be solved numerically; the special case of a steady flow, $\dot{f} = \dot{g} = 0$, results in a set of ODEs as reported and solved by Howarth[25].

C. Flow within a cubic domain:

1. Steady flow within a lid-driven cavity

The case of stationary viscous flow in a square-sided 3D lid-driven cavity of equal edge length, L, and a constant upper lid velocity of U_0[26], is explored through the numerical solution of the primitive variable form of the first integral for steady flow tuned as per the corresponding gauge criterion of Section III A – a key feature being that the essential equation (27) is devoid of mixed derivatives, with the consequent benefit it simplifies and accelerates the use of iterative solvers. The equations to be solved, namely (27), (29) and (33), when non-dimensionalised in terms of L and U_0, read:

$$\partial_k \partial_k \tilde{a}_{ij} + \mathrm{Re}\, u_i u_j + (p+U)\delta_{ij} = 0 \qquad \text{in } \Omega, \qquad (80)$$

$$\partial_l \partial_k \tilde{a}_{kl} = 0 \qquad \text{in } \Omega, \qquad (81)$$

$$-\partial_k \tilde{a}_{kl} = u_l \qquad \text{in } \overline{\Omega}, \qquad (82)$$

where $\mathrm{Re} = \frac{\varrho U_0 L}{\eta}$ is the Reynolds number. $\overline{\Omega}$ in equation (82) denotes the closed set of the solution domain $\Omega = [0,1]^3$ with boundary $\partial\Omega$ (the moving lid lying in the plane $z = 1$) and indicates that (82) is valid both in the inner domain defining the velocities from the known tensor potential entries and at the boundary where the velocities are prescribed in the form of Dirichlet conditions, that is by $u_l = g_l$ on $\partial\Omega$ for appropriate g_l. Equations (80-82) are complemented by the three auxiliary Dirichlet boundary conditions (55-57) for the tensor potential entries in order to obtain a uniquely solvable equation set: although this remains to be proven formally, the numerical results indicate the above system to be mathematically closed.

Newton's method is employed to generate a sequence of $n \in \mathbb{N}_0$ linearised systems based on the following steps:

Step 1:

$$\partial_k \partial_k \tilde{a}_{ij}^{(n+1)} - \mathrm{Re}\left[u_i^{(n)} \partial_k \tilde{a}_{kj}^{(n+1)} + u_j^{(n)} \partial_k \tilde{a}_{ki}^{(n+1)} \right] + (p^{(n+1)} + U)\delta_{ij} = \mathrm{Re}\, u_i^{(n)} u_j^{(n)} \quad \text{in } \Omega, \qquad (83)$$

$$\partial_l \partial_k \tilde{a}_{kl}^{(n+1)} = 0 \qquad \text{in } \Omega, \qquad (84)$$

$$-\partial_k \tilde{a}_{kl}^{(n+1)} = g_l \qquad \text{on } \partial\Omega, \qquad (85)$$

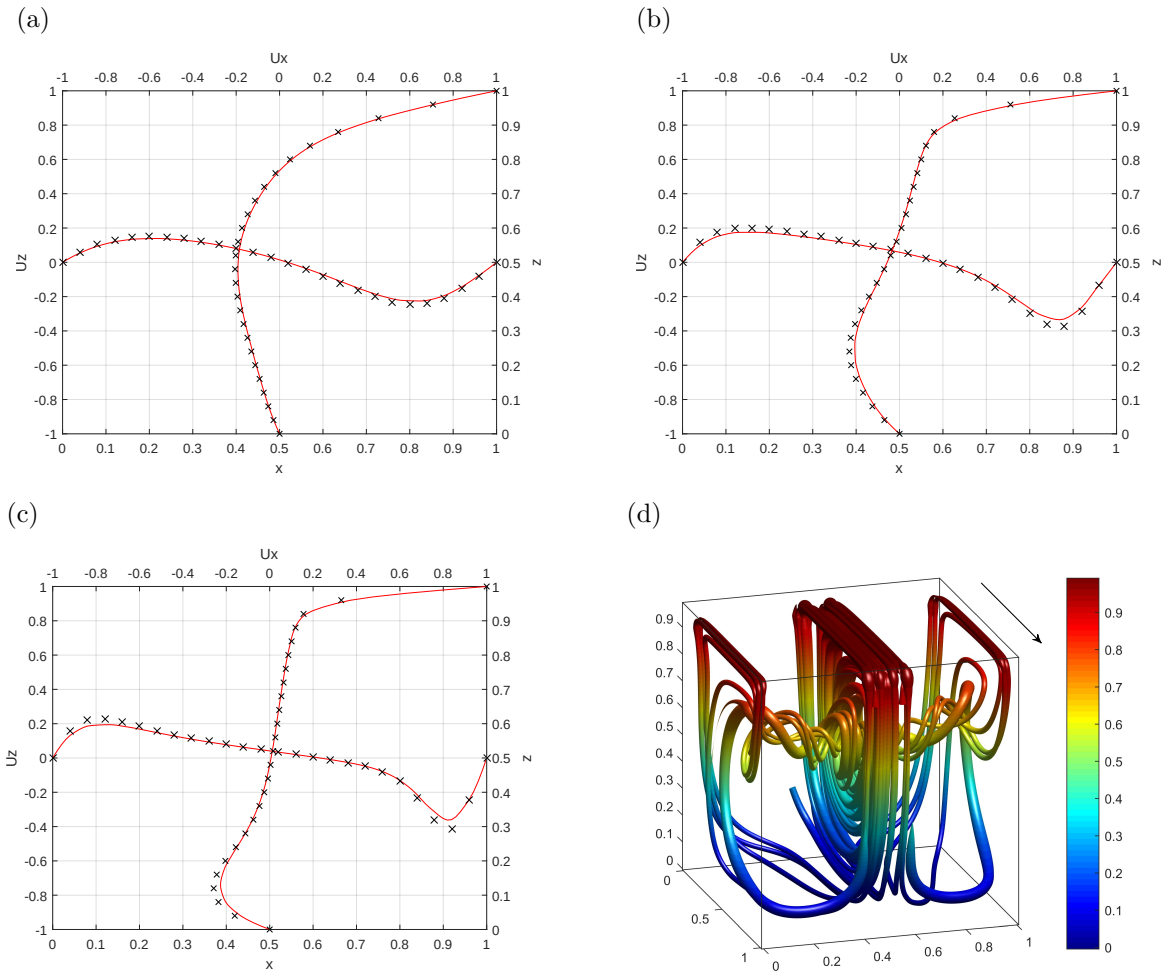

FIG. 2. 3D lid-driven cavity flow. Centre-line velocity profiles for u_x and u_z in the plane intersections $x = y = 0.5$ and $y = z = 0.5$, respectively, for Reynolds numbers of (a) 100, (b) 400 and (c) 1000; the results from the present work are shown as solid red curves and compared to those of Ding *et al.*[26] shown as black crosses. (d) Shows selected stream tubes for the case Re = 400, the arrow indicating the direction of motion of the upper moving lid.

Step 2:

$$u_l^{(n+1)} := -\partial_k \tilde{a}_{kl}^{(n+1)} \qquad \text{in } \Omega\,, \tag{86}$$

in which (82) has been used to replace the velocities in (83) as primary unknowns with index $(n+1)$; the velocities $u_i^{(n)}$ in (83) are assumed known from the previous iterative step having been calculated from the tensor potential via (86). As such, the above equations only involve the six tensor potential entries and the pressure as independent primary variables, with the velocities appearing as secondary variables. Iteration starts from $n = 0$ where the unknown fields are initialised with respect to the linear Stokes flow solution.

For demonstration purposes the cubic nature of the flow field is well suited to solution via a finite difference methodology and structured Cartesian grid system which is the approach adopted. In doing so the well-known oscillatory pressure instability problem linked with

the discretisation of flow problems in terms of primitive variables is avoided by employing a velocity-pressure staggered grid arrangement[27] which is extended to encompass the remaining unknowns, namely the tensor potential entries, in a consistent way. Accordingly, central difference stencils and therefore the discrete equations are well defined everywhere. Although the numerical scheme itself is not the focus of the present work, as it is the first such implementation of the same in the present context the details are summarised in Appendix C. The above equations are similarly amenable to solution utilising, for example, a more complex irregular grid structure and finite element methodology that satisfies a compatibility condition between solution spaces when employing mixed finite elements[28]. Solutions are presented for three different Reynolds numbers up to and including $\mathrm{Re} = 1000$.

Figure 2 shows the results obtained with a grid containing $30 \times 30 \times 30$ points for $\mathrm{Re} = 100$, 400 and 1000 which prove to be in very good agreement with those of Ding *et al.*[26], Ku, Hirsh, and Taylor[29], Jiang, Lin, and Povinelli[30]. Figure 2d shows selected stream tubes for $\mathrm{Re} = 400$ while Figure 3 visualises the corresponding tensor potential entries. Identification of the diagonal tensor entries as volume quantities and the off-diagonal entries as edge quantities (see Appendix C), when compared with the stress discretisation by Graves[31], suggests a close relationship between the tensor entries and the stresses which opens up the opportunity to calculate the stresses from a_{ij}, an option that would justify the additional effort in calculating the tensor entries; this is left as a topic for future investigation. Finally Figure 4 displays the projected streamlines on the three mid-planar cross-sections for $\mathrm{Re} = 100$, 400 and 1000; the results are consistent with, for example, those of Wang *et al.*[32].

2. Unsteady flow and periodic boundary conditions

In relation to the DNS of viscous flow problems using a primitive variable formulation of the governing NS and Continuity equations, the use of periodic geometries/domains - ones with boundaries that are periodic in each and every coordinate direction - can prove particularly advantageous. The pressure can be readily eliminated from the NS equations leading to a Poisson equation for the pressure which lends itself well to solution using pseudospectral methods since the pressure at the boundaries is easily specified. It results in the NS equations preserving the divergence free nature of the velocity field; as shown theoretically by Frisch[33] for what he equivalently terms a 3D periodicity cube.

Within the framework of the first integral the problem of having to solve a Poisson equation for the pressure can be avoided elegantly beginning with its traceless form, equations (35) and (37), from which the pressure field is completely absent.

Consider periodic boundary conditions for the stream function vector written as:

$$\Psi\left(x_1 + L, x_2, x_3, t\right) = \Psi\left(x_1, x_2 + L, x_3, t\right) = \Psi\left(x_1, x_2, x_3 + L, t\right) = \Psi\left(x_1, x_2, x_3, t\right) \,,$$

together with multi-index notation for Greek letters, e.g. $\lambda = (\lambda_1, \lambda_2, \lambda_3) \in \mathbb{Z}^3$ with $\lambda^2 = \lambda_p \lambda_p = \lambda_1^2 + \lambda_2^2 + \lambda_3^2$, followed by adopting a Fourier representation for both the stream function vector and the traceless tensor potential, namely:

$$\Psi_i(x_j, t) = \sum_{\lambda} \Psi_i^{\lambda}(t) \exp\left(\mathrm{i} k_0 \lambda_j x_j\right) \,, \tag{87}$$

$$\bar{a}_{pq}(x_j, t) = \sum_{\lambda} \bar{a}_{pq}^{l}(t) \exp\left(\mathrm{i} k_0 \lambda_j x_j\right) + \bar{a}_{pq}^{0}(t) x_m x_m \,, \tag{88}$$

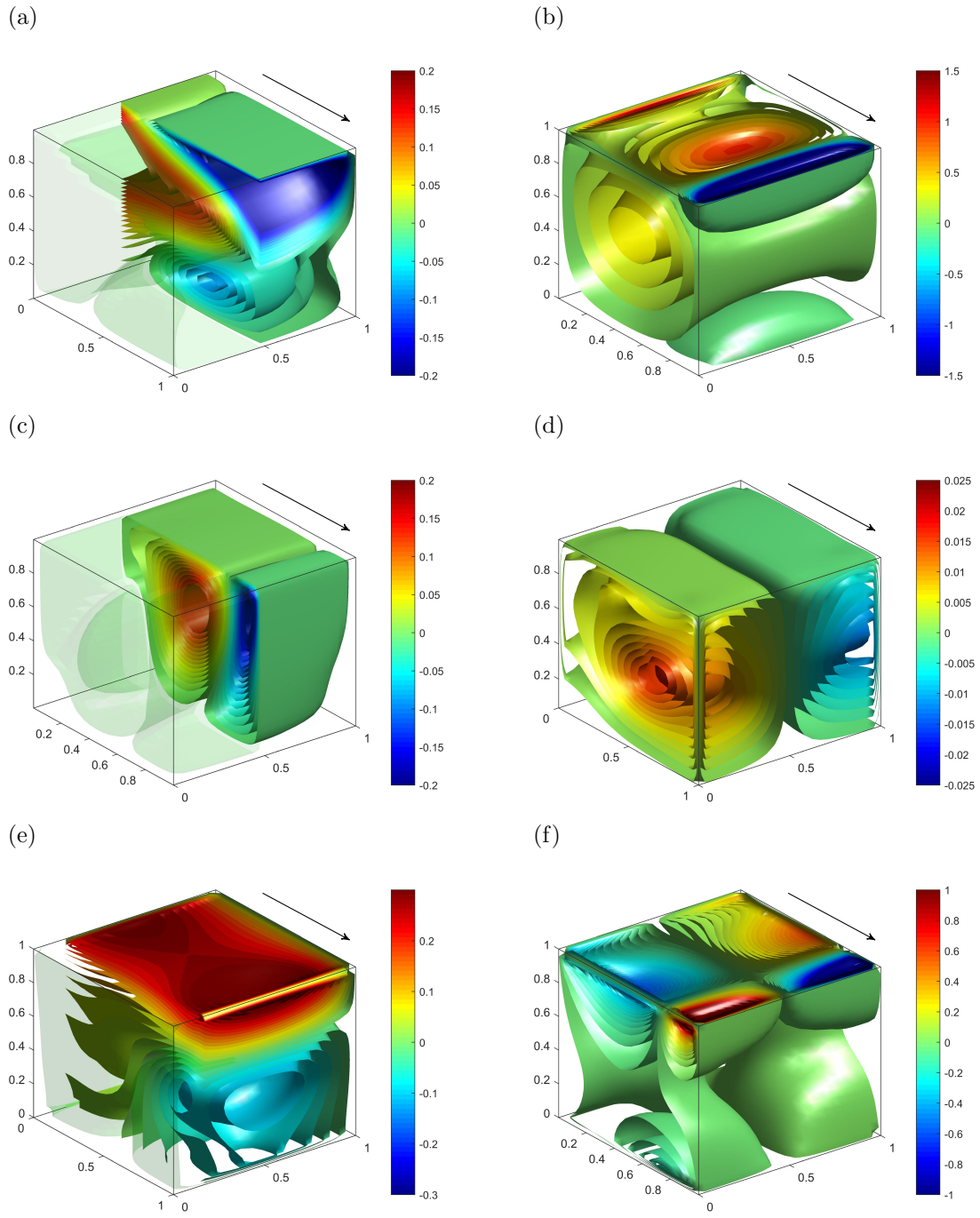

FIG. 3. Visualisation of the six tensor potential entries for the 3D lid-driven cavity flow problem, for the case Re = 400: (a) a_{11}; (b) a_{22}; (c) a_{33}; (d) a_{12}; (e) a_{13}; (f) a_{23}. The arrow indicates the direction of motion of the upper moving lid.

with $k_0 = 2\pi/L$, fulfilling periodic boundary conditions for the stream function vector

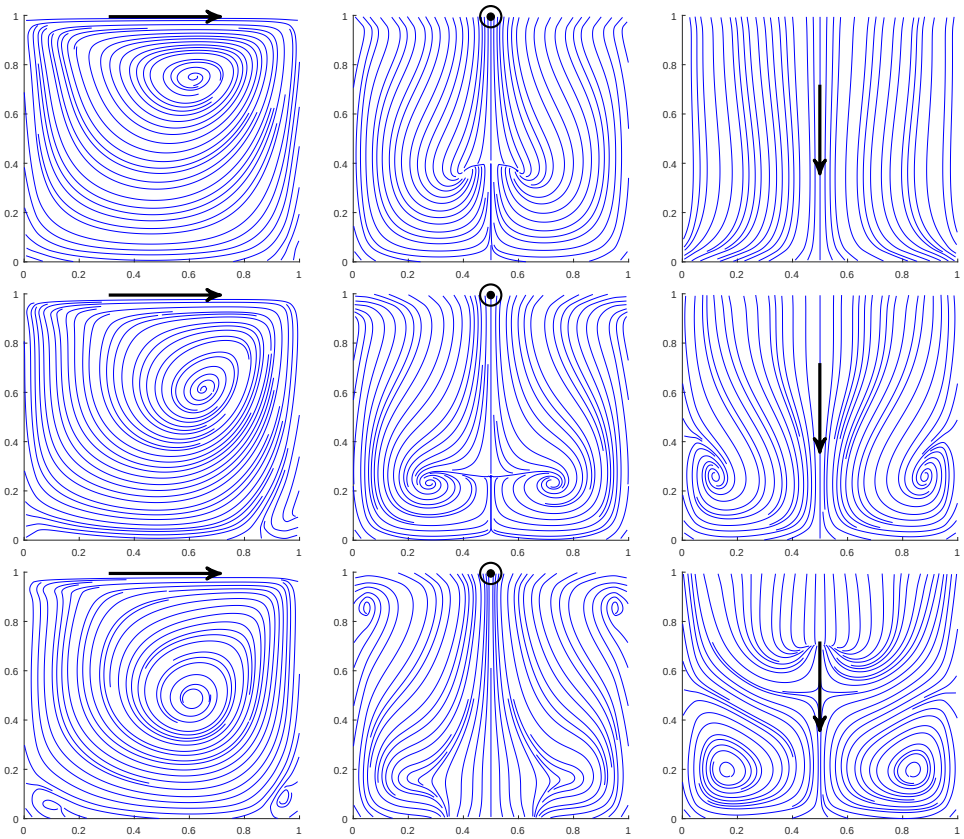

FIG. 4. Streamline projections onto fixed planes for flow in a 3D lid-driven cavity at different Reynolds numbers. The planes $y = 0.5$, $x = 0.5$ and $z = 0.5$ are displayed from left to right; the Reynolds numbers concerned are Re = 100 (top), 400 (middle) and 1000 (bottom). The arrow indicates the associated direction of motion of the upper moving lid.

automatically. The velocity field (3) then takes the form:

$$u_i = \sum_{\lambda} \underbrace{\mathrm{i}k_0 \varepsilon_{ijn} \lambda_j \Psi_n^{\lambda}}_{u_i^{\lambda}} \exp\left(\mathrm{i}k_0 \lambda_j x_j\right) . \tag{89}$$

Note that, the summation convention adopted for multi-indices is that summation is invoked only if the entire index, e.g. λ, occurs twice in a product; a single component of it, e.g. λ_i, acts as a factor only and therefore does not affect summation.

Next, from equations (35, 37) the following set of equations result:

$$6\bar{a}_{ij}^{0} = -\varrho \left[u_i^{-\mu} u_j^{\mu} - \frac{u_p^{-\mu} u_p^{\mu}}{3} \delta_{ij} \right] , \tag{90}$$

$$-k_0^2 \lambda^2 \bar{a}_{ij}^{\lambda} = -\varrho \left[u_i^{\lambda-\mu} u_j^{\mu} - \frac{u_p^{\lambda-\mu} u_p^{\mu}}{3} \delta_{ij} \right] , \tag{91}$$

$$\varrho \dot{\Psi}_n^{\lambda} + \eta k_0^2 \lambda^2 \Psi_n^{\lambda} = k_0^2 \varepsilon_{npq} \lambda_p \lambda_m \bar{a}_{mq}^{\lambda} . \tag{92}$$

Note that via equation (91) the coefficients of the traceless tensor potential can be expressed in terms of the coefficients of the velocity. Hence, all occurrences of $\bar{a}_{mq}^{\lambda}$ in equation (92)

can be replaced, leading to:

$$\varrho\dot{\Psi}_n^\lambda + \eta k_0^2\lambda^2\Psi_n^\lambda = \frac{\varrho}{\lambda^2}\varepsilon_{npq}\lambda_p\lambda_m\left[u_m^{\lambda-\mu}u_q^\mu - \frac{u_k^{\lambda-\mu}u_k^\mu}{3}\delta_{mq}\right]$$
$$= \frac{\varrho}{\lambda^2}\left[\varepsilon_{npq}\lambda_p u_q^\mu\lambda_m u_m^{\lambda-\mu} - \underbrace{\varepsilon_{npq}\lambda_p\lambda_q}_{0}\frac{u_k^{\lambda-\mu}u_k^\mu}{3}\right].$$

In addition, making use of the following identities:

$$\varepsilon_{npq}\lambda_p u_q^\mu = \mathrm{i}k_0\varepsilon_{npq}\varepsilon_{qjk}\lambda_p\mu_j\Psi_k^\mu = \mathrm{i}k_0\left[\delta_{jn}\delta_{kp} - \delta_{jp}\delta_{kn}\right]\lambda_p\mu_j\Psi_k^\mu = \mathrm{i}k_0\left[\lambda_p\mu_n\Psi_p^\mu - \lambda_j\mu_j\Psi_n^\mu\right],$$
$$\lambda_i u_i^{\lambda-\mu} = \mathrm{i}k_0\varepsilon_{ijq}\lambda_i(\lambda_j - \mu_j)\Psi_q^{\lambda-\mu} = -\mathrm{i}k_0\varepsilon_{ijq}\lambda_i\mu_j\Psi_q^{\lambda-\mu},$$

leads to:

$$\varrho\dot{\Psi}_n^\lambda + \eta k_0^2\lambda^2\Psi_n^\lambda - \frac{\varrho k_0^2}{\lambda^2}\left[\lambda_p\mu_n - \lambda_k\mu_k\delta_{np}\right]\varepsilon_{qij}\lambda_i\mu_j\Psi_q^{\lambda-\mu}\Psi_p^\mu = 0, \tag{93}$$

and therefore a set of quadratic equations for the coefficient functions $\Psi_n^\lambda(t)$. By truncating the set of equations after a finite number of modes corresponding to the values of the multi index λ, it can be solved numerically, to reveal the time evolution of the flow for a given initial state, e.g. a Taylor-Green vortex[33]; a topic of fundamental interest and for future exploration.

The attractiveness associated with periodic geometries has been mirrored in the interest shown in the use of pseudospectral methods for the solution of 3D viscous flows in non-periodic ones based on a primitive variable formulation – see, for example, the work of Ku, Hirsh, and Taylor[29] – having at least one coordinate direction in which the boundaries are not periodic. The key related issues of deriving equations and boundary conditions for the pressure there which ensure satisfaction of the divergence free constraint on the velocity are comprehensively discussed by Tuckerman[34] with particular emphasis on the influence matrix method. However, as is rightly pointed out in the same article, the solution of a Poisson equation for the pressure can be avoided completely by solving for the governing equations for the velocity and pressure fields together in a manner similar to the numerical scheme outlined in Appendix C, augmented with a suitably accurate temporal discretisation of the relevant terms in the governing equations. The same is clearly true if a solution based on a primitive variable formulation is preferred for unsteady flow in a periodic geometry.

D. Steady Stokes flow

The well known problem of the broadside translation of a thin disc through a viscous fluid[35], is considered. The unit disc $D = \{x \in \mathbb{R}^3 \,|\, (x_1^2 + x_2^2)^{1/2} \leq 1, x_3 = 0\}$ is located in the plane $P = \{x \in \mathbb{R}^3 \,|\, x_3 = 0\}$ and a constant disc velocity U_0 assumed, so that a steady unbounded and decaying velocity field (33) under conditions:

$$u_3(x) = U_0, x \in D \quad \text{and} \quad \partial_3 u_3(x) = 0, x \in P \setminus D, \tag{94}$$

is sought.

By assuming the potential energy density U to be zero and the vector $\mathcal{A}$ to be defined by:

$$\mathcal{A}_l = -\eta u_l - \partial_k\mathcal{D}(\tilde{a})_{kl} = \partial_k\tilde{a}_{kl} - \partial_k\mathcal{D}(\tilde{a})_{kl}, \tag{95}$$

with $\mathcal{D}(\tilde{a})$ denoting the diagonal part of the tensor $\tilde{a}$, then, from (27), it follows that $\partial_k\partial_k\mathcal{A}_l = 0$. The remaining gauge freedoms in (33) signify $\tilde{a}_{11} = \tilde{a}_{22} = \tilde{a}_{33}$, reducing the number of unknown fields from six to just four. As a consequence, using (29), the divergence of (95) results in $\partial_l\mathcal{A}_l = -\partial_l\partial_k\mathcal{D}(\tilde{a})_{kl} = -\partial_k\partial_k\tilde{a}_{11} = p$, providing a useful guide for the construction of a particular solution $\tilde{a}_{11}$; which is that the relationship:

$$\partial_k\partial_k x_l\mathcal{A}_l = x_l\partial_k\partial_k\mathcal{A}_l + 2\partial_l\mathcal{A}_l = 2p \tag{96}$$

facilitates the following decomposition involving an arbitrary harmonic field χ: $\tilde{a}_{11} = -\frac{1}{2}x_l\mathcal{A}_l + \chi$. What remains to be found is an overall solution procedure for obtaining four harmonic unknown fields $\mathcal{A}_l$ and χ for which the continuity equation is fulfilled identically and the velocity components are given by:

$$u_l = -\frac{1}{\eta}\left[\mathcal{A}_l + \partial_l\left(\chi - \frac{1}{2}x_k\mathcal{A}_k\right)\right] . \tag{97}$$

The pressure can be reconstructed subsequently via $p = \partial_l\mathcal{A}_l$. Equation (97) is equivalent to the Papkovich-Neuber representation known from elasticity theory[36] which generally allows for the analytical solution of various axis-symmetric problems as, for instance, shown by Rudge[37], Woodhouse and Goldstein[38] or Tran-Cong and Blake[39]; moreover, it is closely related to the Clebsch transformation[1,2,40]. The above considerations lead to the representation of Papkovich and Neuber directly as a special case of the first integral of the NS equations, illustrating the elegance of this generalised theory.

Inspection of the flow geometry and imposition of the missing azimuthal dependency in the solution being sought leads to a reduced approach, that is equation (97) with $\mathcal{A}_1 = \mathcal{A}_2 = \chi = 0$; a manageable task utilising potential theory which can conveniently be written in cylindrical coordinates as:

$$\Delta\mathcal{A}(r,z) = \frac{\partial^2\mathcal{A}}{\partial r^2} + \frac{1}{r}\frac{\partial\mathcal{A}}{\partial r} + \frac{\partial^2\mathcal{A}}{\partial z^2} = 0 \quad \text{and} \quad \begin{cases} \mathcal{A} = -\eta U_0\,, & z = 0\,,\ r \le 1 \\ \frac{\partial\mathcal{A}}{\partial z} = 0\,, & z = 0\,,\ r > 1 \end{cases} \tag{98}$$

involving $\mathcal{A} := \mathcal{A}_3$, $r := \sqrt{x_1^2 + x_2^2}$ and $z := x_3$. Problem (98) can be solved by either Hankel transform methods, see e.g. Tanzosh and Stone[35] and references therein, or through a Green's function representation combined with a clever reformulation of the fundamental singularity as provided by Ramm and Fabrikant[41]. A Hankel transform involving Bessel functions of the first kind leads to:

$$\mathcal{H}_\nu[\mathcal{A}] = \int_0^\infty \mathcal{A}rJ_\nu\left(tr\right)\,\mathrm{d}r\,, \quad \mathcal{H}_\nu[\Delta\mathcal{A}] = \left(\frac{\partial^2}{\partial z^2} - t^2\right)\mathcal{H}_\nu[\mathcal{A}]\,, \tag{99}$$

resulting in $\mathcal{H}_\nu[\mathcal{A}] = A(t)\exp(-tz) + B(t)\exp(tz)$ with A and B independent of z. Symmetry considerations enable the calculation to be restricted to $z > 0$, giving $B = 0$ due to the decay condition. After performing an inverse Hankel transform:

$$\mathcal{A}(r,z) = \mathcal{H}_\nu^{-1}[A(t)\exp(-tz)] = \int_0^\infty A(t)t\exp\left(-tz\right)J_\nu\left(tr\right)\,\mathrm{d}t\,, \tag{100}$$

the boundary conditions on the right-hand side of (98) become:

$$\mathcal{A}(r,0) = \int_0^\infty A(t)tJ_\nu\left(tr\right)\,\mathrm{d}t = -\eta U_0\,, \quad r \le 1\,, \tag{101}$$

$$\frac{\partial\mathcal{A}}{\partial z}(r,0) = -\int_0^\infty A(t)t^2J_\nu\left(tr\right)\,\mathrm{d}t = 0\,, \quad r > 1\,, \tag{102}$$

which, with reference to Gradshteyn and Ryzhik [42] (6.671 and 6.693) gives $A(t) = -\frac{2\eta U_0}{\pi}\frac{\sin(t)}{t^2}$ in the case of $\nu = 0$. Making use of integral calculus, see again Gradshteyn and Ryzhik [42] (6.752), an analytical solution of the form (100) is finally obtained:

$$\begin{aligned}\mathcal{A}(r,z) &= -\frac{2\eta U_0}{\pi}\int_0^\infty \frac{\sin(t)}{t}\exp\left(-tz\right)J_0\left(tr\right)\,\mathrm{d}t \\ &= -\frac{2\eta U_0}{\pi}\arcsin\left(\frac{2}{\sqrt{z^2+(r+1)^2}+\sqrt{z^2+(r-1)^2}}\right),\end{aligned} \tag{103}$$

enabling the velocity components to be written down via (97), leading to the same result as reported by Tanzosh and Stone [35].

V. SUMMARY AND OUTLOOK

At outset, the principal aim was to derive a first integral representation of the full unsteady incompressible NS equations, for use as an alternative starting point for the solution of 3D viscous flow problems. Although representing a novel achievement in itself, not unexpectedly the emphasis was broadened to encompass a number of related topics; these have been explored and reported in tandem, in some cases representing a future research area in its own right and thus left as such with a constructive way forward having been provided.

The first integral is derived in an analogous fashion to Maxwell's use of potential fields in developing his classical electro-magnetic theory and governing equations[12]. A tensor potential is introduced as an auxiliary unknown allowing the NS equations to be recast as the divergence of a tensor quantity set to zero. Integration leads to a tensor equation that splits conveniently into symmetric and skew-symmetric parts. Following this it is shown that the gauge freedoms present can be exploited in an astute way leading to a re-ordering of the first integral via the elimination of mixed derivatives resulting in a more tractable equation set consisting of a vector-valued linear inhomogeneous diffusion equation and a tensor-valued generalised Poisson equation possessing the distinguishing feature of reduced non-linearity for both unsteady and steady flows. Furthermore, traceless forms of the same are derived, leading for unsteady (steady) flow to just eight (six) independent PDEs for eight (six) unknowns. Steady Stokes flow leads to a further reduction still, to simply four independent PDEs for four unknowns.

The inviscid (zero viscosity) limit of the first integral is investigated showing that, starting with its re-ordered form, the Euler equations are recovered proving that it satisfies this important subset together with the requirement that energy, momentum (in the absence of external forces), angular momentum and helicity are all conserved. In addition, for the case of steady flow it is shown in the context of finding a variational formulation how the first integral can be used to define a Lagrangian enabling it to be written in a self-adjoint form which can be useful in relation to representing particular flow problems.

Starting with the first integral three well known 3D classical benchmark viscous flow problems are solved for. The boundary conditions required to do so are defined and although not featuring in the present work, the boundary conditions to be applied at a free surface are derived in full with the dynamic condition itself taking the form of a first integral. Two of the problems investigated are amenable to analysis – that of (i) a translating disc in a viscous fluid and (ii) a non-axisymmetric stagnation flow. In both cases the new approach leads to

a non-conventional but straight forward solution procedure yielding results consistent with counterparts available in the open literature. In addition, for the translating disc problem the well-known potential representation of Papkovich and Neuber[36], known from linear elasticity theory, is reproduced; validating the calculations carried out and demonstrating the use of such a general formulation as a versatile means of representing viscous flow.

The third problem, that of viscous flow in a cubic domain, is considered from two perspectives: (iii) as a classical lid-driven cavity; (iv) from the point of view of evolving flow in periodic geometries synonymous with the DNS of viscous flow. Both situations require a numerical approach to solve them. Since (iii) involves the satisfactory use of a discrete version of the equation set defining the first integral – finite difference, volume or element, any one of which will suffice – attention was directed at this problem for validation purposes. A finite difference methodology was used to obtain solutions for three different Reynolds number flows, yielding results in very good agreement with, for example, the corresponding predictions of Ding *et al.*[26]. A satisfactory outcome in itself, but just as importantly the auxiliary boundary conditions for the tensor potential entries, derived in Section IV A 3, are shown to confirm the establishment of a system of equations that are uniquely solvable. For (iv) the traceless form of the first integral proves to be extremely beneficial since the pressure, in addition to typically causing regularity problems in the numerical treatment[34] of evolving flows in non-periodic geometries, is not involved pointing to an alternative formulation. By Fourier decomposition a set of uniquely solvable quadratic equations for the coefficient functions is obtained, describing the time evolution of the flow and therefore a promising starting point for future exploration.

It is clear that there remains considerable scope for further advancement, since the principle focus of the present work has been the new approach and theory underpinning the establishment of the first integral and its subsequent validation via the solution of a number of benchmark test problems; the investigation of a problem requiring the application of a free-surface boundary condition, such as that of thin film flow over surface topography[43,44], represents an obvious avenue to explore. Similarly, the new approach promises to be other than just useful for deriving different existing potential formulations from within a unified framework but able to serve as a source for further representative formulas with reference to specific applications, as sketched out for the case unsteady flow involving periodic boundary conditions. Such formulas can serve as the starting point for both new analytical solutions and numerical techniques; in this sense the variational principle established in Section III C points a promising way forward for further research.

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Appendix A: Derivation of the 2D form of the first integral from its 3D counterpart

In the following, proof is given that the equations derived in[7,11] for 2D flow uniquely result from equation (22) as a special case of general 3D flow. For steady flow with $\partial_t \Psi_n = 0$ equation (16) is fulfilled via the identity $\varphi_n = \eta \Psi_n$, while the auxiliary vector field defined by (24) reads:

$$A_j = \partial_k \tilde{a}_{kj} + \varepsilon_{jlk} \partial_l \varphi_k = \partial_k \tilde{a}_{kj} + \eta \varepsilon_{jlk} \partial_l \Psi_k = \partial_k \tilde{a}_{kj} + \eta u_j \, .$$

Thus, equations (22) yields:

$$\varrho u_i u_j + (p+U)\delta_{ij} = -\partial_k \partial_k \tilde{a}_{ij} - \partial_l \partial_k \tilde{a}_{kl} \delta_{ij} + \partial_i \left[\partial_k \tilde{a}_{kj} + \eta u_j \right] + \partial_j \left[\partial_k \tilde{a}_{ki} + \eta u_i \right] \, . \tag{A.1}$$

Considering now $u_3 = 0$ and a completely vanishing x_3-dependence of all fields for a 2D flow, i.e. $\partial_3 (\cdots) = 0$, it is obvious that in case of the special choice $\tilde{a}_{ij} = -\Phi \delta_{ij}$ for $i, j = 1, \cdots, 2$ for the modified tensor potential the three field equations for steady 2D flow are reproduced.

For the remaining components of the modified tensor potential, on the assumption that $\tilde{a}_{13} = \tilde{a}_{23} = 0$ and $\tilde{a}_{33} = -\zeta(x_1, x_2)$, equation (A.1) is fulfilled identically for indices $i = 1$, $j = 3$ and $i = 2$, $j = 3$; whereas when the indices are $i = j = 3$ it gives:

$$\partial_k \partial_k \zeta = p + U - \partial_k \partial_k \Phi \, , \tag{A.2}$$

which is a Poisson equation for ζ and therefore solvable. Note that ζ has no influence on the other equations and therefore has no physical effect.

Appendix B: Free surface boundary conditions

Consider the kinematic and dynamic boundary conditions at a free surface. Assuming a parametrisation of the free surface in terms of:

$$x_i = f_i(s_1, s_2, t) \, , \; i = 1, 2, 3 \, , \tag{B.1}$$

the two tangential vectors $t_i^{(1)}$, $t_i^{(2)}$ given by:

$$t_i^{(\lambda)} := \frac{\partial f_i}{\partial s_\lambda}, \tag{B.2}$$

are orthogonal and normalised. Together with the normal vector $\vec{n}$, an orthonormal basis exists locally fulfilling the relations:

$$n_j = \varepsilon_{jpq} t_p^{(1)} t_q^{(2)} \, , \tag{B.3}$$

$$t_i^{(1)} = -\varepsilon_{ikl} n_k t_l^{(2)} \, , \tag{B.4}$$

$$t_i^{(2)} = \varepsilon_{ikl} n_k t_l^{(1)} \, . \tag{B.5}$$

The kinematic boundary condition at a free surface is given by:

$$0 = [\dot{f}_j - u_j] n_j = \dot{f}_j n_j - [\delta_{kp}\delta_{lq} - \delta_{kq}\delta_{lp}] t_p^{(1)} t_q^{(2)} \partial_k \Psi_l = \dot{f}_j n_j + \{ f_l, \Psi_l \} \, , \tag{B.6}$$

with Poisson brackets defined as:

$$\{f,g\} := \frac{\partial f}{\partial s_1}\frac{\partial g}{\partial s_2} - \frac{\partial f}{\partial s_2}\frac{\partial g}{\partial s_1}\,. \tag{B.7}$$

The classical form of the dynamic boundary condition:

$$T_{ij}n_j = \sigma_s \kappa n_i\,, \tag{B.8}$$

involving the stress tensor T_{ij}, surface tension σ_s and curvature κ, can be reformulated in terms of the tensor potential: substituting the term $-p\delta_{ij}$ in the stress tensor (6) by means of (12) and then replacing $\varepsilon_{jlk}\partial_l\varphi_k$ according to (26) by $-\partial_k\tilde{a}_{kj}$, the identity:

$$T_{ij} = \varrho u_i u_j + U\delta_{ij} - \varepsilon_{ilk}\varepsilon_{jpq}\partial_l\partial_p a_{kq} + \partial_i\left[\eta u_j + \partial_k\tilde{a}_{kj}\right] + \partial_j\left[\eta u_i + \partial_k\tilde{a}_{ki}\right] \tag{B.9}$$

results. Inserting (B.9) into (B.8), results in the general form of the dynamic boundary condition for unsteady flows.

In the case of steady flow, the kinematic boundary condition simplifies to: $0 = u_i n_i = \{f_l, \Psi_l\}$. Utilising this and (33), the dynamic boundary condition resulting from (B.8) and (B.9) takes the form:

$$\varepsilon_{ikl}\varepsilon_{jpq}\partial_k\partial_p a_{lq}n_j = (U - \sigma_s\kappa)n_i\,. \tag{B.10}$$

Next, the left-hand side of equation (B.10) can be written as:

$$\varepsilon_{ikl}\varepsilon_{jpq}\varepsilon_{jnm}\partial_k\partial_p a_{lq}t_n^{(1)}t_m^{(2)} = \varepsilon_{ikl}\left[\delta_{pn}\delta_{qm} - \delta_{pm}\delta_{qn}\right]\partial_k\partial_p a_{lq}t_n^{(1)}t_m^{(2)}$$
$$= \varepsilon_{ikl}\left[t_m^{(2)}\frac{\partial}{\partial s_1}\left(\partial_k a_{lm}\right) - t_n^{(1)}\frac{\partial}{\partial s_2}\left(\partial_k a_{ln}\right)\right] = \varepsilon_{ikl}\left[\frac{\partial}{\partial s_1}\left(\partial_k a_{lm}t_m^{(2)}\right) - \frac{\partial}{\partial s_2}\left(\partial_k a_{lm}t_m^{(1)}\right)\right],$$

in which the relationships:

$$t_m^{(\lambda)}\partial_m(\cdots) = \frac{\partial}{\partial s_\lambda}(\cdots)\,, \qquad \frac{\partial t_m^{(1)}}{\partial s_2} - \frac{\partial t_m^{(2)}}{\partial s_1} = 0\,,$$

have been used. Making use of the following relationship for the curvature:

$$-\kappa n_i = \frac{\partial^2 f_i}{\partial s_1^2} + \frac{\partial^2 f_i}{\partial s_2^2} = \frac{\partial t_i^{(1)}}{\partial s_1} + \frac{\partial t_i^{(2)}}{\partial s_2} = -\varepsilon_{ikl}\left[\frac{\partial}{\partial s_1}\left(n_k t_l^{(2)}\right) - \frac{\partial}{\partial s_2}\left(n_k t_l^{(1)}\right)\right],$$

together with the introduction of auxiliary functions $U_j(s_1, s_2)$ implicitly as solutions of the condition:

$$Un_i = \varepsilon_{ijk}\left[\frac{\partial U_j}{\partial s_1}t_k^{(2)} - \frac{\partial U_j}{\partial s_2}t_k^{(1)}\right], \tag{B.11}$$

enables the dynamic boundary condition (B.10) to be written mathematically in the following integral form:

$$\frac{\partial}{\partial s_1}\left\{\varepsilon_{ikl}\left[\partial_k a_{lm}t_m^{(2)} + \left(\sigma_s n_k - \frac{U_k}{2}\right)t_l^{(2)}\right]\right\} - \frac{\partial}{\partial s_2}\left\{\varepsilon_{ikl}\left[\partial_k a_{lm}t_m^{(1)} + \left(\sigma_s n_k - \frac{U_k}{2}\right)t_l^{(1)}\right]\right\} = 0\,,$$

yielding:

$$\varepsilon_{ikl}\left[\partial_k a_{lm}t_m^{(\lambda)} + \left(\sigma_s n_k - \frac{U_k}{2}\right)t_l^{(\lambda)}\right] = \frac{\partial\chi_i}{\partial s_\lambda}\,, \qquad \lambda = 1,2 \tag{B.12}$$

as the first integral of the dynamic boundary condition; containing the yet to be determined integration function $\chi_i = \chi_i(s_1, s_2)$. On applying the gauge transformation (20):

$$\begin{aligned}\varepsilon_{ikl}\partial_k a_{lm} t_m^{(\lambda)} &\to \varepsilon_{ikl}\partial_k a_{lm} t_m^{(\lambda)} + \varepsilon_{ikl}\partial_k\partial_l \alpha_m t_m^{(\lambda)} + t_m^{(\lambda)}\partial_m \varepsilon_{ikl}\partial_k\alpha_l \\ &= \varepsilon_{ikl}\partial_k a_{lm} t_m^{(\lambda)} + \frac{\partial}{\partial s_\lambda}\left(\varepsilon_{ikl}\partial_k\alpha_l\right) ,\end{aligned}$$

equation (B.12) becomes:

$$\varepsilon_{ikl}\left[\partial_k a_{lm} t_m^{(\lambda)} + \left(\sigma_s n_k - \frac{U_k}{2}\right) t_l^{(\lambda)}\right] = \frac{\partial}{\partial s_\lambda}\left[\chi_i - \varepsilon_{ikl}\partial_k\alpha_l\right] , \qquad \lambda = 1, 2 . \tag{B.13}$$

Via a proper choice of α_l, the right hand of equation (B.13) can be gauged to zero, leading to the simplified form:

$$\varepsilon_{ikl}\left[\partial_k a_{lm} t_m^{(\lambda)} + \left(\sigma_s n_k - \frac{U_k}{2}\right) t_l^{(\lambda)}\right] = 0 , \qquad \lambda = 1, 2 . \tag{B.14}$$

From a numerical standpoint the above formulation of the dynamic boundary condition contains an inconvenience, namely the necessity of having to construct the two tangent vectors $t_i^{(\lambda)}$. A more convenient and therefore more general formulation is obtained by contraction of (B.14) with $\mathrm{d}s_\lambda$, resulting in:

$$\varepsilon_{ikl}\left[\partial_k a_{lm}\mathrm{d}x_m + \left(\sigma_s n_k - \frac{U_k}{2}\right)\mathrm{d}x_l\right] = 0 , \tag{B.15}$$

where the fact that $t_l^{(\lambda)}\mathrm{d}s_\lambda = \mathrm{d}x_l$ has been introduced. Note that the above parametrisation (B.1) of the free surface is not required for the general form (B.15) of the first integral of the dynamic boundary condition. For instance, the free surface may equally well be given in an explicit form such as $x_3 = f(x_1, x_2)$, leading to $\mathrm{d}x_3 = (\partial f/\partial x_1)\,\mathrm{d}x_1 + (\partial f/\partial x_2)\,\mathrm{d}x_2$.

Appendix C: Finite difference scheme

A classical velocity-pressure staggered-grid scheme for the finite difference solution of viscous flow problems[27] is extended to encompass the tensor entries a_{ij} in a consistent way which is partly inspired by a common numerical method for solving the velocity-stress-formulation of wave propagation through elastic media, as for example utilised by Graves [31]. As well as the stabilising effect inherent with the use of a staggered grid arrangement, the method also economises on the number of unknowns in contrast to the use of any alternative non-staggered grid scheme. The resulting 3D grid arrangement, see Fig. 5, is such that the diagonal tensor components and the pressure are discretised at identical cell centred grid points (i, j, k), the velocities at face centred grid points $(i{+}1, j, k)$, $(i, j{+}1, k)$, $(i, j, k{+}1)$ and the off-diagonal tensor components at cell edges $(i{+}1, j{+}1, k)$, $(i, j{+}1, k{+}1)$, $(i{+}1, j, k{+}1)$.

In contrast to classical discretisation of the vector-valued Navier-Stokes equations, in the present case the "mapping" between equations and unknown fields is less obvious. Here, the six equations of (83) are discretised at the grid points of the corresponding tensor potential entries, equation (84) at the pressure grid points and equations (85) at the boundary velocity grid points only; correspondingly, recovery of the velocities, equation (86), is also performed

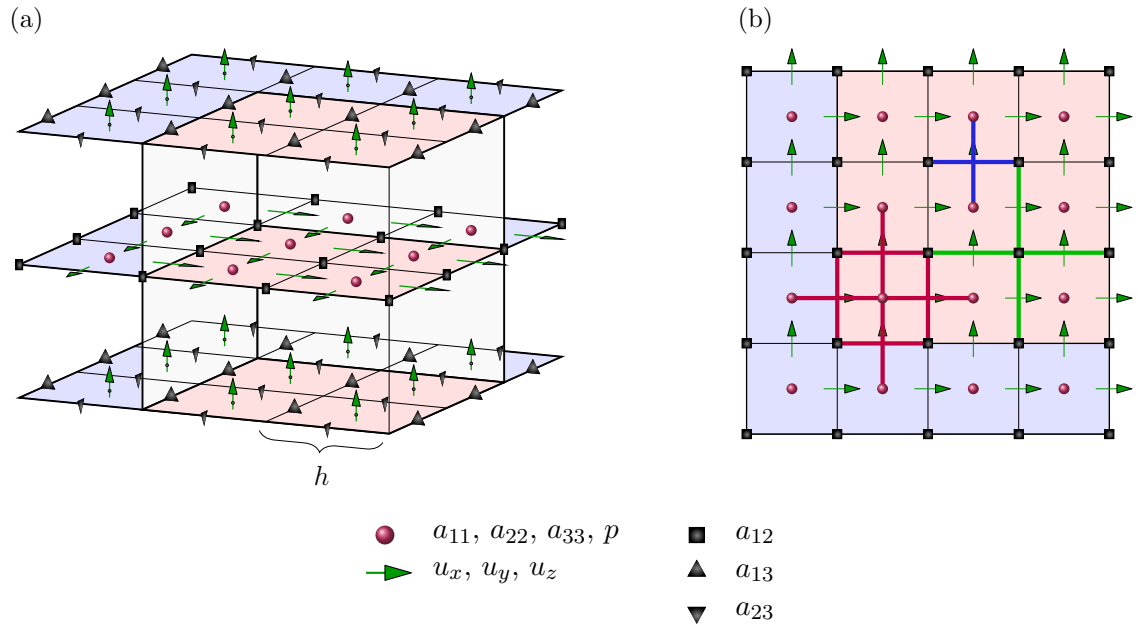

FIG. 5. Schematic of the 3D staggered grid arrangement used to solve the lid-driven cavity problem. (a) Shows three contiguous grids with the pressure and the diagonal tensor entries located at, and identified by, the red spheres, velocities at the sites indicated by green arrows, the off-diagonal tensor entries at the corresponding black squares and triangles. The solution domain of interest is shaded red while the associated boundary region containing the necessary ghost points is shaded blue. (b) View of just one xy-plane, with the dependencies of selected finite difference stencils highlighted at different grid points for the sake of clarity: the stencil for Eq. (83) (for a_{12}) is shown in green, that for Eq. (84) in red and that for Eq. (86) (for u_2) in blue.

at the velocity grid points. Boundary conditions are incorporated via an appropriate ghost cell method involving two grid levels of additional boundary points where conditions (55-57) are similarly specified. Figure 5a highlights a section of the solution domain, shaded red, with the associated boundary region, shaded blue, illustrating the staggered grid arrangement in terms of the various grid point locations.

With reference to the above defined correlation between equations and unknowns, equations (83) to (85) are discretised at different subgrids as indicated in Fig. 5a and all occurring derivatives are approximated by second order central difference stencils in which the nearest available grid points are utilised; the staggered grid arrangement accounts for varying step lengths for the diverse stencils, as illustrated in Figure 5b. The velocities u_i, used iteratively in equation (83), are calculated from the tensor potential entries subsequent to each iteration step, which is achieved by application of equation (86) at all points indicated by a green arrow. The resulting velocity field is then interpolated onto the remaining grid points by a simple weighting of neighbouring points.

The finite difference analogues of the system (83)-(86) can be written in a compact way by defining a number of discrete operators for an arbitrary three-dimensional scalar function $f : \Omega \to \mathbb{R}$; these are valid point-wise for a given set of indices $[i, j, k]$ belonging to grid coordinates (x_i, y_j, z_k). Note, that in the finite difference description provided a grid with uniform step length h in all three coordinate directions is assumed for convenience only (see

Fig. 5); generalisation to a more complex grid pattern follows in a straightforward manner. The standard second order central difference operators for the first and second order partial derivatives of f are given by:

$$\partial_{h,1}[i,j,k]f := \frac{1}{h}\big[f(x_i + h/2, y_j, z_k) - f(x_i - h/2, y_j, z_k)\big]\,, \tag{C.1}$$

$$\partial_{h,2}[i,j,k]f := \frac{1}{h}\big[f(x_i, y_j + h/2, z_k) - f(x_i, y_j - h/2, z_k)\big]\,, \tag{C.2}$$

$$\partial_{h,3}[i,j,k]f := \frac{1}{h}\big[f(x_i, y_j, z_k + h/2) - f(x_i, y_j, z_k - h/2)\big]\,, \tag{C.3}$$

$$\partial_{h,11}[i,j,k]f := \frac{1}{h^2}\big[f(x_i + h, y_j, z_k) - 2f(x_i, y_j, z_k) + f(x_i - h, y_j, z_k)\big]\,, \tag{C.4}$$

$$\partial_{h,22}[i,j,k]f := \frac{1}{h^2}\big[f(x_i, y_j + h, z_k) - 2f(x_i, y_j, z_k) + f(x_i, y_j - h, z_k)\big]\,, \tag{C.5}$$

$$\partial_{h,33}[i,j,k]f := \frac{1}{h^2}\big[f(x_i, y_j, z_k + h) - 2f(x_i, y_j, z_k) + f(x_i, y_j, z_k - h)\big]\,, \tag{C.6}$$

which allows the discrete Laplacian to be written as:

$$\Delta_h[i,j,k]f := \sum_{l=1}^{3} \partial_{h,ll}[i,j,k]f\,. \tag{C.7}$$

Second order discretisation of the mixed derivatives is performed in the standard way, giving:

$$\begin{aligned}\partial_{h,12}[i,j,k]f := \frac{1}{h^2}\big[&f(x_i + h/2, y_j + h/2, z_k) - f(x_i + h/2, y_j - h/2, z_k)\\ &-f(x_i - h/2, y_j + h/2, z_k) + f(x_i - h/2, y_j - h/2, z_k)\big]\,,\end{aligned} \tag{C.8}$$

$$\begin{aligned}\partial_{h,13}[i,j,k]f := \frac{1}{h^2}\big[&f(x_i + h/2, y_j, z_k + h/2) - f(x_i + h/2, y_j, z_k - h/2)\\ &-f(x_i - h/2, y_j, z_k + h/2) + f(x_i - h/2, y_j, z_k - h/2)\big]\,,\end{aligned} \tag{C.9}$$

$$\begin{aligned}\partial_{h,23}[i,j,k]f := \frac{1}{h^2}\big[&f(x_i, y_j + h/2, z_k + h/2) - f(x_i, y_j + h/2, z_k - h/2)\\ &-f(x_i, y_j - h/2, z_k + h/2) + f(x_i, y_j - h/2, z_k - h/2)\big]\,.\end{aligned} \tag{C.10}$$

In addition to the above well-known finite difference stencils the following interpolation operators for functions and their first order derivatives are introduced for convenience:

$$I_{h,1}[i,j,k]f := \frac{1}{2}\big[f(x_i + h/2, y_j, z_k) + f(x_i - h/2, y_j, z_k)\big]\,, \tag{C.11}$$

$$I_{h,2}[i,j,k]f := \frac{1}{2}\big[f(x_i, y_j + h/2, z_k) + f(x_i, y_j - h/2, z_k)\big]\,, \tag{C.12}$$

$$I_{h,3}[i,j,k]f := \frac{1}{2}\big[f(x_i, y_j, z_k + h/2) + f(x_i, y_j, z_k - h/2)\big]\,, \tag{C.13}$$

$$J_h^{r,s}[i,j,k]f := I_{h,r}[i,j,k]\partial_{h,s}f\,; \tag{C.14}$$

with (C.14) in particular facilitating a very compact discrete form of the tensor-valued equation (83), i.e., for $\alpha, \beta = 1, 2, 3$ it is:

$$\begin{aligned}\Delta_h[\gamma]a_{\alpha\beta}^{(n+1)} - \mathrm{Re}\left[I_{h,\beta}[\gamma]u_\alpha^{(n)}\sum_{l=1}^{3} J_h^{\alpha,l}[\gamma]a_{\beta l}^{(n+1)} + I_{h,\alpha}[\gamma]u_\beta^{(n)}\sum_{l=1}^{3} J_h^{\beta,l}[\gamma]a_{\alpha l}^{(n+1)}\right]\\ + \big[p^{(n+1)}(x_i, y_j, z_k) + U(x_i, y_j, z_k)\big]\,\delta_{\alpha\beta} = \mathrm{Re}\, I_{h,\beta}[\gamma]u_\alpha^{(n)} I_{h,\alpha}[\gamma]u_\beta^{(n)}\,,\end{aligned} \tag{C.15}$$

with the abbreviation $\gamma = (i, j, k)$ used for a given index set. Recall, that equations (C.15) are not formed at all grid points (i, j, k), but rather at the respective subsets of grid points belonging to $a_{\alpha\beta}$ according to Fig. 5, whereas the discrete form of equation (84):

$$\sum_{k,l=1}^{3} \partial_{h,kl}[\gamma] a_{kl}^{(n+1)} = 0\,, \tag{C.16}$$

is collocated at the pressure grid points only. Finally, the discrete form of the vector-valued equation (86), similar to that of (85), is given by:

$$u_{\alpha}^{(n+1)} = -\sum_{l=1}^{3} \partial_{h,l}[\gamma] a_{\alpha l}^{(n+1)}\,, \tag{C.17}$$

for $\alpha = 1, 2, 3$ and collocated at the u_α velocity grid points.

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