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RANDOM VORTEX METHOD FOR THREE DIMENSIONAL FLOWS. PART I: MATHEMATICAL BACKGROUND

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The paper presents a mathematical formulation of the Lagrangian method suitable for numerical simulation of 3D viscous incompressible flows. The vorticity field is approximated by a large ensemble of vortex particles which move with the fluid (advection) and perform random walks (diffusion). The charges of the particles change with time due to the stretching term in the governing equation. The construction of the vortex particles ensures that the approximated vorticity field is strictly divergence-free at any time instant. The boundary condition at the surface of an immersed body is satisfied by the creation of new vortex particles near the surface. Various properties of induced velocity and vorticity fields are also discussed.

Key words: vortex methods, vortex stretching, Fokker-Planck-Kolmogorow equation, Itô stochastic differential equations

1. Introduction: motivation of the paper

The problem of determination of the fluid motion past an immersed body belongs to the most important and challenging problems in fluid mechanics. From the mathematical point of view, the fundamental difficulty lies in the lack of rigorous results concerning the existence and regularity of solutions to the Navier-Stokes and continuity equations in the 3D case with "sensibly" small viscosity or, which is essentially equivalent, a sufficiently large Reynolds number Re. It is commonly known that the flow in the wake behind the immersed body becomes oscillatory with relatively small Reynolds numbers, although the incoming free stream is perfectly steady. Further increase of the Reynolds number Re leads to even more complicated spatio-temporal structure of the fluid motion and, at sufficiently large Reynolds numbers, the flow attains the fully turbulent form.

Investigations of initial stages of the laminar-turbulent transition are of fundamental importance as it is believed that there lies the key to control its development. In geometrically simple cases, remarkable progress has been achieved using linear and/or weakly nonlinear methods of the theory of hydrodynamic stability (see Ref. Schmid and Henningson (2001)). In more complicated (and technically interesting) cases, direct numerical simulations (DNS) are inevitable. During the last twenty years, the DNS methods achieved a high level of sophistication (see, for instance, Peyret, 2000; Deville *et al.*, 2002; Cottet and Koumoutsakos, 2000). In general, the methods can be divided into two classes: the Eulerian (or field) methods and Lagrangian (or particle) methods. Typical methods from the first class are finite difference methods (FDM) or finite element methods (FEM). The Lagrangian methods in fluid mechanics are mostly represented by vortex methods, where the spatio-temporal evolution of the vorticity field is simulated by a large set of discrete vorticity carriers moving as individual, mutually interacting objects. The method described in this work belongs to this class. It should be remarked that the differentiation between Eulerian and Lagrangian is not as strict as it might seem. There is a number of approaches which are in a sense "hybrid" to name only the Large Eddy Simulation (LES) (Sagaut, 2002), methods with moving and/or deforming grids [15] or the arbitrary Lagrangian-Eulerian formulation applied to flows with moving and/or free boundaries (Deville *et al.*, 2002).

While the central idea in the Eulerian approach is a grid (or mesh), the Lagrangian approach is based rather on the usage of moving, spatially localized individuals called particles. The particles are fictitious creatures – they are carriers of the vorticity or magnetization (see Buttke and Chorin, 1993; Styczek and Szumbarski, 2002). The method using vortex particles proved to be especially effective in 2D simulations – in this context it is usually referred to as the method of vortex blobs (see, for instance, Błażewicz and Styczek, 1993; Szumbarski and Styczek, 1997; Styczek and Wald, 1995; Protas and Styczek, 2002). In such a case, the vorticity has only one nonzero component subject only to advection and diffusion (there is no stretching). The generalization for axisymmetric flows was formulated in Hedar and Styczek (1999). Since the governing equation can be cast into the form which formally resembles the 2D case, the axisymmetric vortex method does not differ much from the two dimensional one. For general 3D flows, the situation is much more complex –

there is an additional coupling between the vorticity and local variations of the velocity field. The effect of this coupling is, generically, the stretching of the vorticity due to local velocity gradients.

In the region of the wake behind the immersed body, the velocity field is characterized by immense fine-scale non-uniformity. The velocity-vorticity coupling gives rise to specific synergism, which efficiently breaks up flow structures into even smaller scales. Thus, there is a need for subtle discretization of the wake region, where the spatial scale of the velocity variations is small and time-dependent. The method of the vortex particles meets this demand in an apparently natural way: the vortex particles are born in vicinity of the body, shed from it and gathered in the wake area. This way, higher resolution in the regions with reach kinematics is attained. The other advantage of the vortex method is the elimination of the pressure. It should be remarked that other ways of the pressure elimination (not based on using the curl operator) lead to a complicated integro-differential problem.

The paper is constructed as follows. In Section 2, we formulate the initial boundary problem and transform it to the velocity-vorticity formulation. We derive also some important results concerning the properties of the vorticity in the flow domain. In Section 3, we explain the construction of the 3D vortex particles. In Section 4, the velocity field is constructed and its properties are discussed in some details. In Section5, the splitting of the governing equation into advection/diffusion and the stretching parts are introduced. Next, we explain how the partial problems are solved during each time step of the method. In Section 6, the realization of the no-slip boundary conditions and creation of the vorticity at the material boundary in the form of new particles is considered.

2. The velocity-vorticity formulation of the flow problem

Consider a nonstationary flow of a viscous fluid in the exterior of a motionless body with the smooth surface $\varGamma$. The unknowns are the velocity field $\boldsymbol{v}$ and the pressure p. The specific mass is constant and equals to the unity. The fluid motion is governed by the Navier-Stokes equation

$$\partial_t \boldsymbol{v} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{v} = -\nabla p + \nu \varDelta \boldsymbol{v} \tag{2.1}$$

The velocity field is divergent-free

$$\nabla\cdot\boldsymbol{v} = 0 \tag{2.2}$$

and satisfies the following boundary conditions

$$\boldsymbol{v}\Big|_{\boldsymbol{r}\in\Gamma} = \boldsymbol{0} \qquad\qquad \boldsymbol{v}\Big|_{\boldsymbol{r}\to\infty} = \boldsymbol{U}_\infty \tag{2.3}$$

At the initial time, the velocity is given as

$$\boldsymbol{v}\Big|_{t=0} = \boldsymbol{v}_0(\boldsymbol{r}) \tag{2.4}$$

The vector field $\boldsymbol{v}_0$ satisfies conditions (2.2) and $(2.3)_1$, and asymptotic condition $(2.3)_2$ at $t = t_0$. We also assume that at infinity the pressure is spatially homogeneous.

As it was already mentioned, the proof of existence and uniqueness of a regular (smooth) solution to the above problem is not yet available, unless some additional restrictions (symmetry, sufficiently small Reynolds number) are assumed.

We will show that the pressure p is a nonlocal quantity. Indeed, applying the divergence operator to equation (2.1) one gets

$$-\Delta p = \frac{\partial v_i}{\partial x_j}\frac{\partial v_j}{\partial x_i} \tag{2.5}$$

In the above, the summation convention has been applied.

The following Neumann condition can be formulated at the surface Γ

$$\boldsymbol{n}\cdot\nabla p\Big|_{\Gamma} = \nu\boldsymbol{n}\Delta\boldsymbol{v} \equiv -\nu\boldsymbol{n}(\nabla\times\boldsymbol{\omega})\Big|_{\Gamma} \tag{2.6}$$

The vorticity $\boldsymbol{\omega}$ is defined as the curl of the velocity

$$\boldsymbol{\omega} = \nabla\times\boldsymbol{v} \tag{2.7}$$

By definition, the vorticity has zero divergence. Poisson equation (2.5) with boundary condition (2.6) can be formally inverted with the use of the generalized Green function. Then, inserting the pressure gradient into equation (2.1), one obtains the previously mentioned nonlocal, integro-differential form of the governing equation. The other method of the pressure elimination consists in using the equation of vorticity transport (the Helmholtz equation)

$$\partial_t\boldsymbol{\omega} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{\omega} = \nu\Delta\boldsymbol{\omega} + (\boldsymbol{\omega}\cdot\nabla)\boldsymbol{v} \tag{2.8}$$

The velocity field $\boldsymbol{v}$ can be then expressed as follows

$$\boldsymbol{v} = \nabla(\boldsymbol{r}\boldsymbol{U}_\infty(t) + \varphi) + \frac{1}{4\pi}\int\limits_{\operatorname{supp}\boldsymbol{\omega}} \boldsymbol{\omega}(t,\boldsymbol{\xi})\times\frac{\boldsymbol{r}-\boldsymbol{\xi}}{|\boldsymbol{r}-\boldsymbol{\xi}|^3}\,d\boldsymbol{\xi} \tag{2.9}$$

where the potential φ is a harmonic function vanishing at infinity and the symbol $\operatorname{supp}\boldsymbol{\omega}$ denotes the vorticity support (the closure of the subset in $\mathbb{R}^3$, where $\boldsymbol{\omega} \neq \mathbf{0}$).

The initial condition for the vorticity field is implied by condition (2.4)

$$\boldsymbol{\omega}\Big|_{t=0} = \boldsymbol{\omega}_0(\boldsymbol{r}) \equiv \nabla \times \boldsymbol{v}_0(\boldsymbol{r}) \tag{2.10}$$

We also formulate the Neumann boundary condition

$$-\frac{\partial\varphi}{\partial n}\Big|_{\varGamma} = \boldsymbol{n}\boldsymbol{U}_\infty + \frac{\boldsymbol{n}}{4\pi} \int\limits_{\operatorname{supp}\boldsymbol{\omega}} \boldsymbol{\omega}(t,\boldsymbol{\xi}) \times \frac{\boldsymbol{r}-\boldsymbol{\xi}}{|\boldsymbol{r}-\boldsymbol{\xi}|^3}\, d\boldsymbol{\xi} \tag{2.11}$$

which – formally – allows for determination of the harmonic potential φ.

Next, taking the component of the velocity $\boldsymbol{v}$ tangent to the surface $\varGamma$, we get

$$\boldsymbol{n}\times(\boldsymbol{n}\times\boldsymbol{U}_\infty(t)+\boldsymbol{n}\times\nabla\varphi)\Big|_{\varGamma}+\boldsymbol{n}\times\Big\{\frac{\boldsymbol{n}}{4\pi}\times \int\limits_{\operatorname{supp}\boldsymbol{\omega}} \boldsymbol{\omega}(t,\boldsymbol{\xi})\times\frac{\boldsymbol{r}-\boldsymbol{\xi}}{|\boldsymbol{r}-\boldsymbol{\xi}|^3}\, d\boldsymbol{\xi}\Big\}\Big|_{\varGamma} = \mathbf{0} \tag{2.12}$$

The nonlocality of formula (2.11) and (2.12) is evident. In a sense, it has been "shifted" from the equation of motion. However, we will show later that conditions (2.11) and (2.12) are relatively easy and straightforward to implement in the method of vortex particles.

The vorticity $\boldsymbol{\omega}$ subjects to an additional restriction. Let us integrate Helmholtz equation (2.8) in the fixed region D bounded by the material surface $\varGamma$ and the sphere S_∞ of the very large radius R.

$$\frac{d}{dt}\int\limits_D \boldsymbol{\omega}\, d\boldsymbol{r} + \int\limits_{\varGamma\cup S_\infty} (\boldsymbol{n}\boldsymbol{v})\boldsymbol{\omega}\, dS = -\nu \int\limits_{\varGamma\cup S_\infty} \boldsymbol{n}\times(\nabla\times\boldsymbol{\omega})\, dS + \int\limits_{\varGamma\cup S_\infty} (\boldsymbol{n}\boldsymbol{\omega})\boldsymbol{v}\, dS$$

Since $\boldsymbol{v}|_{\varGamma} = \mathbf{0}$ and the vorticity vanishes at S_∞ faster than r^{-2}, one obtains for $R \to \infty$

$$\frac{d}{dt}\int \boldsymbol{\omega}\, d\boldsymbol{r} = -\nu \int\limits_{\varGamma} \boldsymbol{n}\times(\nabla\times\boldsymbol{\omega})\, dS$$

Using equation of motion (2.1) written for $\boldsymbol{r} \to \boldsymbol{r}_{\varGamma} \in \varGamma$, we get

$$\nabla p\Big|_{\varGamma} = -\nu\nabla\times\boldsymbol{\omega}\Big|_{\varGamma}$$

Thus, the equality can be inferred

$$-\nu\int\limits_{\varGamma} \boldsymbol{n}\times(\nabla\times\boldsymbol{\omega})\, dS = \int \nabla\times(\nabla p)\, d\boldsymbol{r} \equiv \mathbf{0}$$

which immediately leads to the following conclusion

$$\frac{d}{dt} \int\limits_{\operatorname{supp} \boldsymbol{\omega}} \boldsymbol{\omega}(t, \boldsymbol{r})\, d\boldsymbol{r} = \boldsymbol{0} \tag{2.13}$$

One can see that the total charge of the vorticity is conserved in the presence of a motionless material boundary (the surface $\mathit{\Gamma}$) of the flow domain.

3. The particles of vorticity

The vorticity field with a bounded support induces the velocity field with the asymptotic behavior

$$\boldsymbol{v} = \boldsymbol{C} \times \frac{\boldsymbol{r}}{r^3} + O(r^{-3})$$

Such behavior can be concluded from the form of the Biot-Savart integral appearing in formula (2.9). The vector constant $\boldsymbol{C}$ is proportional to the charge of vorticity. We will generalize the above expression by postulating the velocity field induced by a single vortex particle placed at the origin in the following form

$$\boldsymbol{v} = \frac{\boldsymbol{\Omega} \times \boldsymbol{r}}{r^3} F(r) = \boldsymbol{\Omega} \times \nabla \mathit{\Phi} = -\nabla \times (\boldsymbol{\Omega} \mathit{\Phi}) \tag{3.1}$$

The time-dependent vector $\boldsymbol{\Omega}(t)$ is an individual characteristic of a particle. and the potential $\mathit{\Phi}$ is spherically symmetric and defined as

$$\mathit{\Phi}(r) = \int\limits_0^r \frac{F(\xi)}{\xi^2}\, d\xi \tag{3.2}$$

The corresponding vorticity field is given as

$$\boldsymbol{\omega} = \boldsymbol{\Omega} \mathit{\Delta} \mathit{\Phi} - \nabla(\boldsymbol{\Omega} \cdot \nabla \mathit{\Phi}) \tag{3.3}$$

The internal structure of the vortex particle is implied by the determination of the Laplacian of $\mathit{\Phi}$

$$\mathit{\Delta} \mathit{\Phi} \equiv \frac{1}{r^2} \frac{d}{dr}\Big(r^2 \frac{d\mathit{\Phi}}{dr} \Big) = f(r) \tag{3.4}$$

If the following function is introduced

$$F(r) = \int_0^r \xi^2 f(\xi)\, d\xi \tag{3.5}$$

the vorticity field of the particle can be expressed in the following manner

$$\boldsymbol{\omega} = \boldsymbol{\Omega}\Big[f(r) - \frac{1}{r^3}F(r)\Big] - \frac{(\boldsymbol{\Omega}\boldsymbol{r})\boldsymbol{r}}{r^2}\Big[f(r) - \frac{3}{r^3}F(r)\Big] \tag{3.6}$$

The total charge of vorticity in the particle can be calculated as

$$\boldsymbol{Q}_\omega = \int \boldsymbol{\omega}\, d\boldsymbol{\xi} = \int_0^\infty \int_{S(\xi)} \boldsymbol{\omega}(\boldsymbol{\xi})\, dS(\xi) d\xi$$

The iterated integration is carried out over the sphere $S(\xi)$ with the radius equal to ξ, and next along the variable ξ. The internal integration can be performed as follows

$$\int_{S(\xi)} \frac{(\boldsymbol{\Omega}\boldsymbol{\xi})\boldsymbol{\xi}}{\xi^2}\, dS(\xi) = \int_{S(1)} (\boldsymbol{\Omega}\boldsymbol{\zeta})\boldsymbol{\zeta}\, dS(1) = \boldsymbol{e}_\beta \int_{S(1)} \varOmega_\alpha \zeta_\alpha \zeta_\beta\, dS(1) =$$

$$= \frac{4\pi}{3}\boldsymbol{e}_\beta \delta_{\beta\alpha} \varOmega_\alpha = \frac{4\pi}{3}\boldsymbol{\Omega}$$

In the above, the integrals for $\alpha \neq \beta$ vanish identically, and the remaining three integrals are equal. Since their sum is simply the surface of the unitary sphere, each integral is equal to $4\pi/3$. Using this fact, the calculation of the integral with respect to ζ finally gives

$$\boldsymbol{Q}_\omega = \frac{8\pi}{3}\boldsymbol{\Omega} \int_0^\infty \xi^2 f(\xi)\, d\xi = \frac{8\pi}{3}\boldsymbol{\Omega} F(\infty) \tag{3.7}$$

Note that if $F(r)$ vanishes for $r > r_0$, the vortex particle carries zero total vorticity charge, and there is no induction in this area. We will postulate that the function $f(r)$ vanishes for $r > \sigma$. The quantity σ will be referred to (conventionally) as the particle radius. The function $f(r)$ can be unbounded for $r \to 0$. However, to avoid singularity in the velocity field at the particle center, the function $f(r)$ should satisfy the inequality $|f(r)| < \mathrm{const} \cdot r^{-\alpha}$ with $\alpha < 1$. In such a case $\boldsymbol{v}(0) = \boldsymbol{0}$, and, additionally, the value of the potential $\varPhi(r)$ exists in the particle center. If the function f vanishes for $r > \sigma$, then

$$F(\infty) = \int_0^\sigma \xi^2 f(\xi)\, d\xi = F(\sigma) \tag{3.8}$$

We will normalize the function f so that $F(\infty) = 1$. For $r > \sigma$, the potential Φ can be expressed as follows

$$\Phi(r) = \int\limits_0^\sigma \frac{F(\xi)}{\xi^2}\, d\xi + \int\limits_\sigma^r \frac{1}{\xi^2}\, d\xi = \Phi(\sigma) + \frac{1}{\sigma} - \frac{1}{r} = \Phi(\infty) - \frac{1}{r} \tag{3.9}$$

Note also that the induced vorticity field outside the particle "core" (the interior of the sphere with the radius σ) is the potential vector field. Indeed, one can write

$$\boldsymbol{\omega} = \nabla \times \Big(\frac{\boldsymbol{\Omega} \times \boldsymbol{r}}{r^3}\Big) = -\nabla \frac{\boldsymbol{\Omega}\boldsymbol{r}}{r^3} = \nabla\Big(\boldsymbol{\Omega} \cdot \nabla \frac{1}{r}\Big) \tag{3.10}$$

For a particularly simple function $f(r)$, namely

$$f(r) = \begin{cases} \dfrac{3}{\sigma^3} & \text{for} \quad r < \sigma \\ 0 & \text{for} \quad r > \sigma \end{cases} \tag{3.11}$$

we get

$$\boldsymbol{v} = \boldsymbol{\Omega} \times \begin{cases} \dfrac{\boldsymbol{r}}{\sigma^3} & \text{for} \quad r \leqslant \sigma \\ \dfrac{\boldsymbol{r}}{r^3} & \text{for} \quad r > \sigma \end{cases} \tag{3.12}$$

and

$$\boldsymbol{\omega} = \begin{cases} \dfrac{2\boldsymbol{\Omega}}{\sigma^3} \equiv \nabla\Big(2\dfrac{\boldsymbol{\Omega}\boldsymbol{r}}{\sigma^3}\Big) & \text{for} \quad r < \sigma \\ -\dfrac{\boldsymbol{\Omega}}{r^3} + 3\dfrac{(\boldsymbol{\Omega}\boldsymbol{r})\boldsymbol{r}}{r^5} \equiv -\nabla\Big(\dfrac{\boldsymbol{\Omega}\boldsymbol{r}}{r^3}\Big) & \text{for} \quad r > \sigma \end{cases} \tag{3.13}$$

The induced velocity field is continuous in space. The vorticity field is constant inside the particle core and discontinuous across the core boundary $r = \sigma$. The jump across the discontinuity $[\omega]$ is tangent to the core boundary (the normal component is continuous) and can be evaluated as follows

$$[\boldsymbol{\omega}] = \boldsymbol{\omega}\Big|_+ - \boldsymbol{\omega}\Big|_- = \frac{3}{\sigma^3}\Big[\frac{(\boldsymbol{\Omega}\boldsymbol{r})\boldsymbol{r}}{\sigma^2} - \boldsymbol{\Omega}\Big] \tag{3.14}$$

If the function $f(r)$ is continuous then the tangent component of the vorticity is continuous as well. If we "mollify" the jump attained by step function (3.11) at $r = \sigma$, we obtain the vorticity field with a rapid variation in vicinity of $r = \sigma$. Note that zero-divergence constraint imposed on the field $\boldsymbol{\omega}$ implies that any vortex particle which induces in the whole space must have an unbounded vorticity support. In such a case, the total charge of the particle $\boldsymbol{Q}_\omega$

defined by (3.7) is always different from zero. If the total charge of an ensemble of the vortex particles is zero then, for a sufficiently large radius r (reaching beyond all particle cores in the ensemble), the induced velocity and vorticity fields will decay at a rate proportional to r^{-3} and r^{-4}, respectively.

4. Properties of the velocity field

The velocity field defined by expression (2.9) is divergence-free. Similarly, the divergence of the vorticity induced component determined by the Biot-Savart integral is zero. In can be concluded that the following equality holds for any closed surface immersed in the flow domain

$$\int \boldsymbol{n} \cdot \nabla\varphi \, dS \equiv \int \frac{\partial\varphi}{\partial n} \, dS = 0 \tag{4.1}$$

which ensures correctness of Neumann boundary problem (2.11). Using the Green formula, the harmonic function φ can be expressed as follows

$$4\pi\varphi(\boldsymbol{r}) = \int\limits_{\Gamma} \Big(\varphi(\boldsymbol{\xi})\frac{\partial}{\partial n_\xi}\frac{1}{|\boldsymbol{r}-\boldsymbol{\xi}|} - \frac{\partial\varphi}{\partial n_\xi}\frac{1}{|\boldsymbol{r}-\boldsymbol{\xi}|}\Big)\, dS_\Gamma \tag{4.2}$$

The expansion of the integral kernels and use of equality (4.1) yield the following asymptotic behavior with $r \to \infty$

$$\varphi(\boldsymbol{r}) = \frac{\text{const}}{r^2} + O(r^{-3}) \tag{4.3}$$

The velocity field, which is the sum of the uniform stream, potential component $\nabla\varphi$ and the component induced by the set of vortex particles, can be written in the form

$$\boldsymbol{v} = \boldsymbol{U}_\infty + \nabla\varphi + \sum_{k=1}^{N} \frac{\boldsymbol{\Omega}_k \times (\boldsymbol{r}-\boldsymbol{r}_k)}{|\boldsymbol{r}-\boldsymbol{r}_k|^3} F(|\boldsymbol{r}-\boldsymbol{r}_k|) \tag{4.4}$$

In the above, $\boldsymbol{r}_k$ denotes the location of the center of the kth particle ($k = 1, .., N$).

The asymptotic form of the velocity field for $r \to \infty$ can be obtained by expanding the denominator $|\boldsymbol{r}-\boldsymbol{r}_k|^{-3}$ and using (4.3). The resulting form is

$$\begin{aligned} \boldsymbol{v} \;&=\; \boldsymbol{U}_\infty + \frac{\boldsymbol{r}}{r^4}\,\text{const} + \frac{(\sum \boldsymbol{\Omega}_k)\times \boldsymbol{r}}{r^3} - \frac{\sum(\boldsymbol{\Omega}_k \times \boldsymbol{r}_k)}{r^3} + \\ &+\; 3\frac{\sum[\boldsymbol{\Omega}_k \times \boldsymbol{r}_k(\boldsymbol{r}\boldsymbol{r}_k)]}{r^5} + O(r^{-4}) \end{aligned} \tag{4.5}$$

The velocity field, (4.5), has to be compatible with the constraint imposed on the total vorticity charge, see (2.13). In view of (3.7), we conclude that the following equality must hold

$$\boldsymbol{\Omega}_0 = \sum_{k=1}^{N} \boldsymbol{\Omega}_k = \text{const}$$

If the velocity vanishes at the initial time instant, then obviously

$$\boldsymbol{\Omega}_0 = \sum_{k=1}^{N} \boldsymbol{\Omega}_k = \mathbf{0} \tag{4.6}$$

The zero value of the total vorticity charge means that the total amount of the angular momentum in the flow is finite. To show this, let us calculate the total angular momentum of the fluid outside the ball containing all vortex particles. In the course of the calculations we will obtain the following integrals

$$\int\limits_{|\boldsymbol{r}|>R} \frac{\boldsymbol{r} \times [\boldsymbol{\Omega}_k \times (\boldsymbol{r} - \boldsymbol{r}_k)]}{|\boldsymbol{r} - \boldsymbol{r}_k|^3}\, d\boldsymbol{r} = \int\limits_{|\boldsymbol{\xi}|>R} \frac{\boldsymbol{\xi} \times (\boldsymbol{\Omega}_k \times \boldsymbol{\xi})}{\xi^3}\, d\boldsymbol{\xi} + \boldsymbol{r}_k \times \int\limits_{|\boldsymbol{\xi}|>R} \frac{\boldsymbol{\Omega}_k \times \boldsymbol{\xi}}{\xi^3}\, d\boldsymbol{\xi}$$

The second integral in the right-hand side is zero. The first one can be transformed to the form

$$\frac{8\pi}{3}\boldsymbol{\Omega}_k \int\limits_{|\boldsymbol{\xi}|>R} \xi\, d\xi$$

Summing up the contributions from all vortex particles one concludes that the total amount of the angular momentum will remain finite only if condition (4.6) is satisfied. Note that the potential component can be transformed to the surface integral $\int_{\Gamma} \boldsymbol{n} \times \boldsymbol{r}\varphi\, dS_{\Gamma}$, which is also finite and therefore cannot prevent infinity in the momentum when condition (4.6) is violated.

If the restriction was not imposed, an infinite amount of the angular vorticity would be produced in the flow within a finite time. This singularity cannot be avoided in a way similar to how it is done in the case of the infinite momentum. The latter difficulty can be removed simply by choosing the reference frame related to the motionless fluid at infinity – in such a case the immersed body moves with respect to the ambient fluid.

It is reasonable to use the "corrected" form of the velocity

$$\boldsymbol{v} = \boldsymbol{U}_\infty + \nabla\varphi + \sum_{k=1}^{N} \frac{\boldsymbol{\Omega}_k \times (\boldsymbol{r} - \boldsymbol{r}_k)}{|\boldsymbol{r} - \boldsymbol{r}_k|^3} F(|\boldsymbol{r} - \boldsymbol{r}_k|) - \frac{\boldsymbol{\Omega}_0 \times \boldsymbol{r}}{r^3} \tag{4.7}$$

and the vorticity

$$\boldsymbol{\omega} = \sum_{k=1}^{N} \boldsymbol{\omega}_k(t, \boldsymbol{r} - \boldsymbol{r}_k) - \boldsymbol{\omega}_0(t, \boldsymbol{r}) \tag{4.8}$$

where

$$\boldsymbol{\omega}_k(t, \boldsymbol{\xi}) = \boldsymbol{\Omega}_k(t)\Big[f(\xi) - \frac{1}{\xi^3}F(\xi)\Big] - \frac{(\boldsymbol{\Omega}_k\boldsymbol{\xi})\boldsymbol{\xi}}{\xi^2}\Big[f(\xi) - \frac{3}{\xi^3}F(\xi)\Big]$$

In the above, the symbol $\boldsymbol{\omega}_0$ denotes the vorticity field induced by the additional vortex particle located inside the immersed body (outside the flow domain).

If (4.6) holds exactly, both velocity and vorticity remain unchanged. However, in the course of numerical computation, inaccuracies are inevitable. Then, the correction terms in (4.7) and (4.8) ensure that condition (4.6) is verified.

5. Evolution of the vorticity field

According to the Lie-Trotter Theorem (see Chorin and Marsden, 1997), we split Helmholtz equation (2.8) into the equation of advection/diffusion

$$\partial_t\boldsymbol{\omega} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{\omega} = \nu\Delta\boldsymbol{\omega} \tag{5.1}$$

and the "stretching" equation

$$\partial_t\boldsymbol{\omega} = (\boldsymbol{\omega} \cdot \nabla)\boldsymbol{v} \tag{5.2}$$

The evolution operator corresponding to the Helmholtz equation can be expressed by a formal composition of the resolvents of equations (5.1) and (5.2)

$$H_t = \lim_{n\to\infty}(S_{t/n} \circ A_{t/n})^n \tag{5.3}$$

The emergence of the vorticity at material boundaries of the flow domain introduces an additional element in composition (5.3) – the operator of the vorticity creation Ψ_t (Chorin and Marsden, 1997)

$$H_t = \lim_{n\to\infty}(S_{t/n} \circ \Psi_{t/n} \circ A_{t/n})^n \tag{5.4}$$

We will determine the resolvent operators used in (5.4). Equation (5.1) formally resembles the Fokker-Planck-Kolmogorov equation (see Gardiner, 1990), governing the spatio-temporal evolution of the density of the conditional probability $p(t, \boldsymbol{r}|t_0, \boldsymbol{r}_0)$ for the stochastic process determined by the Itô differential equations

$$d\boldsymbol{r}_i = \boldsymbol{v}_i \, dt + \sqrt{2\nu} \, d\boldsymbol{W}_i \qquad \boldsymbol{r}_i\Big|_{t=t_0} = \boldsymbol{r}_{i0} \tag{5.5}$$

In the above, $\boldsymbol{v}_i$ denotes an instantaneous velocity at the location of the ith "diffusive particle", while $d\boldsymbol{W}_i$ denotes the infinitesimal increment of the vector Wiener process modeling the diffusion of the particles.

In view of this interpretation, the vorticity field at the time instant $t > t_0$ can be calculated as a conditional expectation as follows

$$\boldsymbol{\omega}(t, \boldsymbol{r}) = \int\limits_{\operatorname{supp} \boldsymbol{\omega}_0} p(t, \boldsymbol{r}|t_0, \boldsymbol{r}_0) \boldsymbol{\omega}_0(\boldsymbol{r}_0) \, d\boldsymbol{r}_0 \tag{5.6}$$

The vorticity field determined by (5.6) satisfies equation (5.1) and the initial condition

$$\boldsymbol{\omega}\Big|_{t=t_0} = \boldsymbol{\omega}_0(\boldsymbol{r})$$

Equation (5.2) can be re-written using directional differentiation as follows

$$\partial_t \boldsymbol{\omega} = (\boldsymbol{\omega} \cdot \nabla)\boldsymbol{v} \equiv \frac{d}{d\lambda} \boldsymbol{v}(t, \boldsymbol{r} + \lambda \boldsymbol{\omega})\Big|_{\lambda=0} \tag{5.7}$$

For a given velocity field, formula (5.7) defines a parameterized family of ordinary differential equations. The parameters of this family are spatial coordinates (or, simply, the vector $\boldsymbol{r}$).

The resolvent operator for equation (5.2) is defined by the transformation $\boldsymbol{\omega}(t, \boldsymbol{r}) \to \boldsymbol{\omega}(t + \Delta t, \boldsymbol{r})$ ($\boldsymbol{r}$ plays the role of the parameter), which is simply the process of numerical integration of the ordinary differential equations.

Finally, the operator of the vorticity creation for the time period Δt describes production of such a boundary distribution of the vorticity so that the boundary condition for the velocity field (no-slip condition) is satisfied. An instantaneous vorticity distribution at the boundary is related via certain integral operation to the vorticity field in the whole flow domain. If the particle representation of the vorticity field is used the integral relation is, as we will show in the next Section, approximated by an algebraic one.

Summarizing, the vorticity field at the time instant $t + \Delta t$ is determined due to:

- Modification of the vorticity field at the instant t caused by the vortex particles displacement during the time interval $(t, t + \Delta t)$, accordingly to Itô equations (5.5)
- Transformation of the vorticity field by integrating ordinary differential equations (5.7) describing the effect of the "stretching"
- Creation of the vorticity at the material boundary so that condition (2.12) is verified.

6. Vortex particle approximation of the vorticity field

Assume that we have N vortex particles in the flow domain at the time instant t. The vortex charges $\boldsymbol{\Omega}_k^O$ and coordinate vectors $\boldsymbol{r}_k^O$ $(k = 1, ..., N)$ of all particles are known. During a short time interval Δt the particles move accordingly with the Itô equations

$$\Delta \boldsymbol{r}_k^0 = \boldsymbol{v}_k \Delta t + \sqrt{2\nu}\, \Delta \boldsymbol{W}_k \tag{6.1}$$

and their vorticity charges change due to the stretching effect. Since at the particle central point, i.e. for $\boldsymbol{r} = \boldsymbol{r}_k^O$, the vorticity carried by the particle is

$$\boldsymbol{\omega}\Big|_0 = \frac{2}{3} f(0) \boldsymbol{\Omega} \tag{6.2}$$

then the stretching equation takes the form

$$\frac{d\boldsymbol{\Omega}_k^0}{dt} = \frac{3}{2f(0)} \frac{d}{d\lambda} \boldsymbol{v}(t, \boldsymbol{r} + \lambda \boldsymbol{\omega}(t, \boldsymbol{r}_k))\Big|_{\lambda=0} \tag{6.3}$$

and a new vorticity charge of the particle can be evaluated

$$\boldsymbol{\Omega}_k^0(t + \Delta t) = \boldsymbol{\Omega}_k^0(t) + \Delta \boldsymbol{\Omega}_k^0 \tag{6.4}$$

Since the vortex particles change both their positions and vorticity charges, condition $(2.3)_1$ imposed on the velocity field is violated at the time instant $t + \Delta t$. In order to ensure $(2.3)_1$, it is necessary to modify the boundary (or near-boundary) value of the vorticity field and calculate a new potential φ. The former can be achieved by introducing new vortex particles in a closed vicinity of the surface of the immersed body. The potential φ is sought in the form of the sum

$$\varphi = \varphi_U + \varphi_O + \varphi^* \tag{6.5}$$

Each term in (6.5) represents a harmonic function, specified by appropriate boundary conditions of the Neumann type. These conditions for two first functions in (6.5) are

$$\begin{aligned} \frac{\partial \varphi_U}{\partial n}\Big|_\Gamma &= -\boldsymbol{n}\boldsymbol{U}_\infty \\ \frac{\partial \varphi_O}{\partial n}\Big|_\Gamma &= \boldsymbol{n}\Big(\sum_{k=1}^{N} \boldsymbol{\Omega}_k^0\Big) \times \frac{\boldsymbol{r}}{r^3}F(r) - \boldsymbol{n}\sum_{k=1}^{N} \boldsymbol{\Omega}_k^0 \times \frac{\boldsymbol{r}-\boldsymbol{r}_k}{|\boldsymbol{r}-\boldsymbol{r}_k|^3}F(|\boldsymbol{r}-\boldsymbol{r}_k|) \end{aligned} \tag{6.6}$$

It can be verified that both (6.6) verify the solvability condition of the Neumann boundary problem, and hence the functions φ_U and φ_O can be found using standard methods.

The third harmonic potential φ^* is connected to newly created vortex particles. We will assume that M such particles are born at the fixed positions $\boldsymbol{r}_k^{new}$ near the material surface at each time step. In general, each new particle induces the velocity with nonzero tangent and normal components at the body surface. The role of the potential φ^* is to compensate the induction normal to the surface incurred by the new vortex particles. To achieve this, the potential is defined in the form of the sum

$$\varphi^* = \sum_{k=1}^{M} (\Omega_{k1}^{new}\varphi_{k1} + \Omega_{k2}^{new}\varphi_{k2} + \Omega_{k3}^{new}\varphi_{k3}) \tag{6.7}$$

where $\varphi_{k\alpha}$, $\alpha = 1, 2, 3$, are harmonic functions fulfilling the Neumann boundary conditions as follows

$$\frac{\partial \varphi_{k\alpha}}{\partial n}\Big|_\Gamma = \boldsymbol{n}\frac{\boldsymbol{e}_\alpha \times \boldsymbol{r}}{r^3}F(r) - \boldsymbol{n}\frac{\boldsymbol{e}_\alpha \times (\boldsymbol{r}-\boldsymbol{r}_k^{new})}{|\boldsymbol{r}-\boldsymbol{r}_k^{new}|^3}F(|\boldsymbol{r}-\boldsymbol{r}_k^{new}|)\Big|_{r\in\Gamma} \tag{6.8}$$

Using the same standard procedure as in the case of φ_U and φ_O, we can calculate $3M$ potentials related individually to all newly created vortex particles. The velocity field induced by these particles is given as

$$\boldsymbol{v}^{new} = \sum_{k=1}^{M}\sum_{\alpha=1}^{3} \Omega_{k\alpha}^{new}\Big[\nabla\varphi_{k\alpha} - \frac{\boldsymbol{e}_\alpha \times \boldsymbol{r}}{r^3}F(r) + \frac{\boldsymbol{e}_\alpha \times (\boldsymbol{r}-\boldsymbol{r}_k^{new})}{|\boldsymbol{r}-\boldsymbol{r}_k^{new}|^3}F(|\boldsymbol{r}-\boldsymbol{r}_k^{new}|)\Big] \tag{6.9}$$

Note that if the places of creation of the new particles are fixed, all potentials $\varphi_{k\alpha}$, $\alpha = 1, 2, 3$ can be calculated once and forever. For brevity, let us write formula (6.9) as

$$\boldsymbol{v}^{new} = \sum_{k=1}^{M} \widehat{\mathbf{K}}(\boldsymbol{r}, \boldsymbol{r}_k^{new})\boldsymbol{\Omega}_k \tag{6.10}$$

Note that the following equality holds

$$\boldsymbol{n}\widehat{\mathbf{K}}(\boldsymbol{r}, \boldsymbol{r}_k^{new})\Big|_{\boldsymbol{r}\in\Gamma} = \mathbf{0} \tag{6.11}$$

In order to find the M vector quantities $\boldsymbol{\Omega}_k^{new}$ (or, which is equivalent, $3M$ scalar values $\Omega_{k\alpha}^{new}$), we write the expression for the velocity as follows

$$\begin{aligned} \boldsymbol{v} = \boldsymbol{U}_\infty + \nabla\varphi_U + \nabla\varphi_O + \sum_{k=1}^{N} \frac{\boldsymbol{\Omega}_k^{old} \times (\boldsymbol{r} - \boldsymbol{r}_k)}{|\boldsymbol{r} - \boldsymbol{r}_k|^3} F(|\boldsymbol{r} - \boldsymbol{r}_k|) - \\ - \sum_{k=1}^{N} \boldsymbol{\Omega}_k^{old} \times \frac{\boldsymbol{r}}{r^3} F(r) + \sum_{k=1}^{M} \widehat{\mathbf{K}}(\boldsymbol{r}, \boldsymbol{r}_k^{new})\boldsymbol{\Omega}_k^{new} \end{aligned} \tag{6.12}$$

On the surface Γ the normal component of the velocity $\boldsymbol{v}$ is zero identically. One has to eliminate also the tangent component. To this end, we multiple equation (6.12), written for $\boldsymbol{r} \in \Gamma$, by the orthogonal tangent versors $\boldsymbol{\eta}_{\beta j}$, $\beta = 1, 2$, and enforce the no-slip condition at the collocation points $\boldsymbol{r}_j^\Gamma \in \Gamma$, $j = 1, ..., M$. Moving all terms with the known quantities to the right-hand sides, we obtain an algebraic linear system of $2M$ equations

$$\begin{aligned} \sum_{k=1}^{M} \boldsymbol{\eta}_{\beta j} \widehat{\mathbf{K}}(\boldsymbol{r}_j^\Gamma, \boldsymbol{r}_k^{new})\boldsymbol{\Omega}_k^{new} = -\boldsymbol{\eta}_{\beta j}\Big[\boldsymbol{U}_\infty + \nabla\varphi_U + \nabla\varphi_O + \\ + \sum_{k=1}^{N} \frac{\boldsymbol{\Omega}_k^{old} \times (\boldsymbol{r}_j^\Gamma - \boldsymbol{r}_k)}{|\boldsymbol{r}_j^\Gamma - \boldsymbol{r}_k|^3} F(|\boldsymbol{r}_j^\Gamma - \boldsymbol{r}_k|) - \sum_{k=1}^{N} \boldsymbol{\Omega}_k^{old} \times \frac{\boldsymbol{r}_j^\Gamma}{r^3} F(r_j^\Gamma)\Big] \end{aligned} \tag{6.13}$$

In order to get a solvable system of equations, we postulate M additional conditions in the form of

$$\sum_{k=1}^{M} \boldsymbol{n}\boldsymbol{\Omega}_k^{new}\Big|_{\boldsymbol{r}=\boldsymbol{r}_k^\Gamma} = 0 \tag{6.14}$$

It can be shown that the matrix of the full system is not singular. Moreover, if the vectors $\boldsymbol{r}_k^{new}$ and $\boldsymbol{r}_k^\Gamma$, $k = 1, ..., M$, are fixed, than the coefficient matrix of the obtained linear system can be evaluated and LU-factored once and forever.

7. Final remarks

The three dimensional generalization of the Vortex Blobs Method, formulated originally for 2D fluid motion, has been presented. The dynamics of vorticity in three dimensions is essentially more complex than in the 2D case, which makes the construction of the vortex method a nontrivial task. Three dimensional vorticity fields must obey restriction (2.13). The governing equation contains the stretching term giving rise to additional variations of the vorticity due to local nonuniformity of the velocity field, (5.2). Therefore, the 3D vortex particles (analogues of two dimensional vortex blobs) evolve individually in time, while the total charge of the vorticity is constant in time. In two dimensional motion, there is a restriction imposed on the pressure field (corresponding to the conservation of the total vorticity), but the stretching effect is not involved.

The proposed method of accounting for the stretching term is not the only possible. Nevertheless, it is algorithmically simple and seems to be appropriate for the vortex particles with small cores with highly concentrated vorticity.

One of the main problems with the vortex methods is how to maintain computational efficiency during long-time simulations. Note that the new vortex particles are continually generated at the material boundaries of the flow domain, and thus their number gets larger from one step to another. In effect, the CPU time required to evaluate the velocity field at each time step grows in the course of computations. Known algorithms for fast summation can reduce the numerical cost, however, not as spectacularly as in the 2D case. In addition, they are too complex to implement. The other method of cost reduction is to put bounds on the number of particles in the flow domain, which is achieved by selective removal and/or gluing. To this end various strategies can be proposed, but their reasonable application is limited by the lack of rigorous relation between the number of particles and the approximation order. Since these issues are still open, the evaluation of the results consists mostly in comparison with the experimental evidence (if available) and with other methods.

The implementation details of the proposed vortex method and discussion of the obtained results will be presented in Part II of the paper.

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Stochastyczna metoda wirowa dla przepływów trójwymiarowych. Część I: Podstawy matematyczne

Streszczenie

W pracy sformułowano lagranżowską metodę wirową dla trójwymiarowych przepływów cieczy lepkiej. Pole wirowści jest w niej aproksymowane zbiorem cząstek poruszających się wraz z płynem oraz wykonujących ruch losowy (dyfyzja). Ładunki wirowości niesione przez cząstki zależą od czasu (efekt "strechingu"). Konstrukcja cząstek zapewnia, że pole wirowości pozostaje bezźródłowe w trakcie symulacji. Warunek dla pola prędkości stawiany na powierzchni opływanego ciała jest realizowany drogą generacji nowych cząstek w sąsiedztwie tej powierzchni. W pracy przedyskutowano również własności indukowanego pola prędkości i wirowości.

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