Equation-Based Modeling: Simulation of a Flow With Concentrated Vorticity in an Unbounded Domain

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Abstract: The velocity field of a fluid flow in an unbounded domain, $\mathcal{R}$, in which the spin of fluid elements is nonzero only within a bounded subdomain, $\mathcal{R}^i$—namely, the interior of a sphere of radius, a—is simulated by equation-based modeling. A change of independent variable motivated by *Kelvin Inversion* (Ref. 1) maps the region exterior to $\mathcal{R}^i$, hereinafter denoted $\mathcal{R}^e$, to a proxy domain, $\mathcal{Q}$, in the form of a spherical ball whose radius is also a. The simulation involves simultaneous solution of the boundary-value problems for the physical velocty in $\mathcal{R}^i$ and a proxy velocity in $\mathcal{Q}$ and the results recover those of a 19$^{\text{th}}$ century analytical solution known as *Hill's spherical vortex* (Ref. 2).

Keywords: Unbounded domains, Concentrated vorticity, Kelvin Inversion

1. Hill's spherical vortex

Suppose the fluid is inviscid and incompressible. If $\mathbf{u}$ denotes the velocity then the incompressibility condition is

$$\operatorname{div}\mathbf{u} = 0 \, . \tag{1.1}$$

Hill's spherical vortex is axisymmetric. The motion outside of a sphere of radius a is irrotational and steady in time as seen by an observer who moves with the sphere. Consider a circular fluid filament inside the sphere. The filament is centered on the axis of symmetry of the overall motion and its plane is normal to that axis. The radius of the filament and its latitude angle relative to the sphere vary with time and the fluid in the filament is subject to stretching and compression in the azimuthal direction during the motion. By appeal to Helmholtz theorems of vortex motion one may deduce that the intensity of the vorticity—all of which is azimuthal—increases or decreases in direct proportion to the stretching or compression of the filament in the azimuthal direction. Hill's spherical vortex abides by this requirement by postulating a vorticity field of the form

$$\operatorname{curl}\mathbf{u} = \begin{cases} (A\hat{\mathbf{\imath}}_3)\times\mathbf{r} \, , & \text{for } r \le a \\ \mathbf{0} \, , & \text{for } r > a \end{cases} \, . \tag{1.2$_{1,2}$}$$

Here A is a given constant, $\hat{\mathbf{\imath}}_3$ is a constant unit vector parallel to the axis of symmetry, and $\mathbf{r}$ is the position vector, $\overrightarrow{OP}$, from the center, O, of the sphere to a typical point, P, inside it.

Let $\mathbf{v}$ denote a generic vector field and let $\nabla\mathbf{v}$ and $(\nabla\mathbf{v})^T$ denote its gradient the transpose of its gradient, respectivley. If $\mathbf{a}$ is any other vector then

$$[\nabla\mathbf{v} - (\nabla\mathbf{v})^T]\mathbf{a} = \operatorname{curl}\mathbf{v}\times\mathbf{a} \tag{1.3}$$

is an identity. Gurtin (Ref. 3), for example, uses (1.3) as a definition of the curl of a vector. The point here is that there is a one-to-one corresondance between curl $\mathbf{u}$ and the skew tensor $\nabla\mathbf{u} - (\nabla\mathbf{u})^T$. Let W denote the skew tensor that equals $\nabla\mathbf{u} - (\nabla\mathbf{u})^T$ inside Hill's spherical vortex. Within Hill's spherical vortex, then, $\mathbf{u}$ satisfies the equation

$$\nabla\mathbf{u} - (\nabla\mathbf{u})^T = W \, . \tag{1.4}$$

In view of (1.3) W must satisfy $W(\mathbf{a}) = [\nabla\mathbf{u} - (\nabla\mathbf{u})^T](\mathbf{a}) = \operatorname{curl}\mathbf{u}\times\mathbf{a} = [(A\hat{\mathbf{\imath}}_3)\times\mathbf{r}]\times\mathbf{a}$. It follows from the expansion of the vector triple product and the definition of the tensor product* that

$$W = A(\mathbf{r}\otimes\hat{\mathbf{\imath}}_3 - \hat{\mathbf{\imath}}_3\otimes\mathbf{r}) \, . \tag{1.5}$$

2. Variational principle for the flow inside Hill's spherical vortex

In $\mathcal{R}^i$ consider the problem of minimizing the expresson F defined by

$$F := \iiint_{\mathcal{R}^i} \{(\operatorname{div}\mathbf{u})^2 + (1/4)\|\nabla\mathbf{u} - (\nabla\mathbf{u})^T - W]\|^2\}\, dV \tag{2.1}$$

over all smooth functions $\mathbf{r}\mapsto\mathbf{u}$. Here dV is the volume of a typical small part of $\mathcal{R}^i$. Equation (2.1) employs the notation $\|S\|^2 := S\bullet S$ for the square-norm of a tensor, S. The inner product, $A\bullet B$, of tensors A and B is defined by the rule $A\bullet B :=$

* For any two given vectors, $\mathbf{a}$ and $\mathbf{b}$, their tensor product, denoted $\mathbf{a}\otimes\mathbf{b}$, is a linear vector-to-vector operator whose action upon a third vector, $\mathbf{v}$, is defined by the rule $(\mathbf{a}\otimes\mathbf{b})\mathbf{v} = \mathbf{a}(\mathbf{b}\bullet\mathbf{v})$.

$\mathrm{tr}\,(A^T B)$, in which $\mathrm{tr}\,(\,.\,)$ denotes the *trace* operator and $(\,.\,)^T$ denotes the transpose. Note that F is non-negative by construction. Moreover, F attains the value zero when $\mathbf{u}$ satisfies equations (1.1) and (1.4). By requiring the first variation, δF, of F to be zero for arbitrary variations, $\delta\mathbf{u}$, of $\mathbf{u}$ within $\mathcal{R}^i$ and on $\partial\mathcal{R}^i$ one my derive a the differential equation for $\mathbf{u}$ in $\mathcal{R}^i$ (a.k.a. the EULER-LAGRANGE equation) for the variational problem and a natural (a.k.a. flux-source) boundary condition for $\mathbf{u}$ on $\partial\mathcal{R}^i$.

To be specific, if one takes the first variation of (2.1), applies some identites*, and introduces the abbreviation

$$\Gamma := 2(\mathrm{div}\,\mathbf{u})I + \nabla\mathbf{u} - (\nabla\mathbf{u})^T - W \tag{2.2}$$

one may arrange the result in the form

$$\delta F - \iiint_{\mathcal{R}^i} \Gamma \bullet \nabla(\delta\mathbf{u})\, dV = 0\ . \tag{2.3}$$

If one sets δF to zero (as is appropriate when F attains a minimum) and interprets the first variation, $\delta\mathbf{u}$, of $\mathbf{u}$ as what the COMSOL documentation denotes by $\mathbf{v}$ and calls a *test function* then equation (2.3) becomes what that documentation calls *the weak form*.

By application of some more identities† one may write (2.3) in the equivalent form

$$\delta F + \iint_{\partial\mathcal{R}^i} \delta\mathbf{u} \bullet [-\Gamma(\hat{\mathbf{n}})] dA + \iiint_{\mathcal{R}^i} \delta\mathbf{u} \bullet \mathrm{div}\,\Gamma\, dV = 0\ . \tag{2.4}$$

Here dA is the area of a typical small part of $\partial\mathcal{R}^i$ and $\hat{\mathbf{n}}$ is the outward unit normal vector on that surface. If F is a minimum then $\delta F = 0$ subject to arbitrary variations $\delta\mathbf{u}$ on $\partial\mathcal{R}^i$ and in $\mathcal{R}^i$. Equation (2.4) then implies that

$$\mathrm{div}\,\Gamma = \mathbf{0} \quad , \quad -\Gamma(\hat{\mathbf{n}}) = \mathbf{0}\ , \qquad (2.5)_{1,2}$$

which constitute the EULER-LAGRANGE equation and the natural boundary condition, respectively. The system consisting of (2.2) and $(2.5)_1$ is suitable for input to the COMSOL general form PDE physics interface and $(2.5)_2$ is the corresponding *null flux* boundary conditon.

The solution for $\mathbf{u}$ of the minimization problem as posed thus far is not unique. To see why note that replacement of $\mathbf{u}$ by $\mathbf{u} + \nabla\varphi$ will leave the expression under the integral sign in (2.1) unchanged provided $\nabla\nabla\varphi - (\nabla\nabla\varphi)^T = O$—which is always the case—and $\mathrm{div}\,(\nabla\varphi) = 0$. There are, of course, infinitely many solutions of $\mathrm{div}\,(\nabla\varphi) = 0$ in $\mathcal{R}^i$ so if there is one vector field $\mathbf{u}$ in $\mathcal{R}^i$ for which F is zero there must be infintely many of them. To remove this ambiguity one may recall that the most general solution of the problem consisting of the equation $\mathrm{div}\,(\nabla\varphi) = 0$ subject to the boundary condition $\nabla\varphi \bullet \hat{\mathbf{n}} = 0$ in a simply connected domain (a.k.a. the homogeneous NEUMANN problem) is a constant. But the gradient of a constant is the zero vector so $\nabla\varphi$ must reduce to $\mathbf{0}$ in that case. Now a boundary condition that specifies $\nabla\varphi \bullet \hat{\mathbf{n}}$ in classical potential theory corresponds one that specifies $\mathbf{u} \bullet \hat{\mathbf{n}}$ in the problem of minimizing F, *i.e.* to a boundary condition of the form

$$\mathbf{u} \bullet \hat{\mathbf{n}} = m\ , \tag{2.6}$$

in which $\mathbf{r} \mapsto m$ is subject to the constraint that the total volumetric outflow across $\partial\mathcal{R}^i$ be zero (as incompressiblity requires) but is otherwise arbitrary. If the observer for whom $\mathbf{u}$ is the fluid velocity is at rest relative to the boundary sphere then m in (2.6) is identically zero.

3. Variational principle for the flow outside Hill's spherical vortex

In $\mathcal{R}^e$ consider the problem of minimizing the expresson F defined by

$$F := \iiint_{\mathcal{R}^e} \left[(\mathrm{div}\,\mathbf{u})^2 + (1/4)\|\nabla\mathbf{u} - (\nabla\mathbf{u})^T]\|^2\right] dV \tag{3.1}$$

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* Three such identities are: (i), the divergence of a vector field equals the trace of its gradient; (ii) the trace of any tensor equals the inner product of that tensor with the identity, I; and (iii), the inner product of two tensors equals zero whenever one factor is symmetric and the other is skew.

† One such identity [*cf.* GURTIN (Ref. 3), equation $(4.2)_5$ on p30] is the differentiation formula $\mathrm{div}\,[S^T(\mathbf{v})] = S \bullet \nabla\mathbf{v} + \mathbf{v} \bullet \mathrm{div}\,S$ (in which $\mathbf{v}$ and S are generic vector and tensor fields); another is the divergence theorem; and third is the definition of the transpose, according to which $S^T(\mathbf{a}) \bullet \mathbf{b} = \mathbf{a} \bullet S(\mathbf{b})$.

over all smooth functions $\mathbf{r} \mapsto \mathbf{u}$. The fact that $\mathcal{R}^e$ is unbounded poses both practical and mathematical challenges. One way of addressing these challenges is precede the treatment of the minimization problem for F by a change of independent variable $\mathbf{r} \to \mathbf{q}$, which maps points in the original domain, $\mathcal{R}^e$—which is not bounded—to points in proxy domain, $\mathcal{Q}$, which is. To this end, let $a > 0$ be a given constant length and let r and q denote the magnitudes of the vectors $\mathbf{r}$ and $\mathbf{q}$, respectively. One may then define a change of variable $\mathbf{r} \to \mathbf{q}$ by the following equations:

$$\mathbf{r}/r = -\mathbf{q}/q \quad , \quad a^2 = rq \; . \qquad (3.2)_{1,2}$$

One may visualize $\mathbf{r}$ and $\mathbf{q}$ as position arrows springing from a common point, namely the center of the *boundary sphere* $r = a$ or $q = a$. If the minus sign in $(3.2)_1$ were replaced by a plus sign then the resulting change variable $\mathbf{r} \to \mathbf{q}$ would represent Kelvin inversion, as introduced by Kelvin in 1845 (Ref. 1) and employed in classical treatises on potential theory since then [*e.g.* Kellogg (Ref. 4, Chapter IX, §2]. I will postpone the discussion of my reason for introducing the minus sign in $(3.2)_1$ until after I have discussed an orthogonal curvilinear coordinate system that arises naturally in this problem.

I introduced the constant unit vector, $\hat{\mathbf{i}}_3$, in $(1.2)_1$ above. Now let $\hat{\mathbf{i}}_1$ and $\hat{\mathbf{i}}_2$ be any two constant unit vectors chosen such that $\{\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3\}$ forms a right-handed orthogonal system. One may expand a generic vector $\mathbf{v}$ into components with respect to $\{\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3\}$, *viz.* $\mathbf{v} = \sum_{i=1}^3 v_i \hat{\mathbf{i}}_i$. Here and elsewhere, italic symbols with numerical subscripts denote the scalar components with respect to $\{\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3\}$ of a vector denoted by the corresponding letter, without subscripts, in bold face.

According to this convention once $\{\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3\}$ is fixed the list $(q_1.q_2, q_3)$ determines $\mathbf{q}$, and the system $(3.2)_{1,2}$ then determines $\mathbf{r}$, so $(q_1, q_2, q_3) \mapsto \mathbf{r}$ is now a known function and (q_1, q_2, q_3) constitutes a set of *curvilinear coordinates*. One may show that this curvilinear coordinate system is *orthogonal, i.e.*

$$(\partial \mathbf{r}/\partial q_i) \bullet (\partial \mathbf{r}/\partial q_j) = 0 \quad \text{for } i \neq j \qquad (3.3)$$

It will be convenient at this point to recall some textbook results that apply to all orthogonal curvilinear coordinate systems [*i.e* ones which satisfies (3.3)]. Given any orthogonal curvilinear coordinate system, one may associate each coordinate, q_i, with a corresponding *scale factor*, h_i, defined by

$$h_i := \|\partial \mathbf{r}/\partial q_i\| \quad , \quad i \in \{1, 2, 3\} \; . \qquad (3.4)$$

From (3.3) and (3.4) one may construct a system of unit vectors $\hat{\mathbf{e}}_i := (1/h_i)(\partial \mathbf{r}/\partial q_i)$ $i \in \{1, 2, 3\}$ belonging to any orthogonal curvilinear coordinate system. Having the system $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\}$ one may expand a generic vector $\mathbf{v}$ into components with respect to that system, *i.e.* $\mathbf{v} = \sum_{i=1}^3 v_i^e \hat{\mathbf{e}}_i$, in which the scalar components (v_1^e, v_2^e, v_3^e) are not to be confused with the scalars (v_1, v_2, v_3) in the expansion $\mathbf{v} = \sum_{i=1}^3 v_i \hat{\mathbf{i}}_i$. Textbooks that treat orthogonal curvilinear coordinates [*e.g.* Phillips (Ref. 5, pp 88–90) and Hildebrand (Ref. 6, pp 306–311)] include derivations of expansions of the divergence and curl of a generic vector, $\mathbf{v}$, and of the gradient of a generic scalar, φ, with respect to orthogonal curvilinear coordinates. These authors, and others, assume in their derivations that the system $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\}$ is right-handed. It so happens that the omission of the minus sign in the definition $(3.2)_1$ above would result in a left-handed system. This fact drove my decision to employ an inversion rule motivated by Kelvin's but not Kelvin Inversion *proper*. Returning, now, to the textbook results one may write them in the following forms:

$$\operatorname{div} \mathbf{v} = \frac{1}{h_1 h_2 h_3} \sum_{i=1}^{3} \frac{\partial}{\partial q_i} \left(\frac{(h_1 h_1 h_3 \, v_i^e)}{h_i} \right) , \qquad (3.5)$$

$$\operatorname{curl} \mathbf{v} = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{\hat{\mathbf{e}}_i \times \hat{\mathbf{e}}_j}{h_i h_j} \frac{\partial (h_j v_j^e)}{\partial q_i} , \qquad (3.6)$$

and

$$\nabla \varphi = \sum_{i=1}^{3} \frac{\hat{\mathbf{e}}_i}{h_i} \frac{\partial \varphi}{\partial q_i} \; . \qquad (3.7)$$

One may employ (1.3) to deduce the corresponding representation of $\nabla \mathbf{v} - (\nabla \mathbf{v})^T$ with respect to orthogonal curviliner coordinates as follows. If $\mathbf{a}$ is any vector equation (3.6) implies that

$$\operatorname{curl} \mathbf{v} \times \mathbf{a} = \sum_{i=1}^{3} \sum_{j=1}^{3} \frac{[(\hat{\mathbf{e}}_i \times \hat{\mathbf{e}}_j) \times \mathbf{a}]}{h_i h_j} \frac{\partial (h_j v_j^e)}{\partial q_i} , \qquad (3.8)$$

But $(\hat{\mathbf{e}}_i \times \hat{\mathbf{e}}_j) \times \mathbf{a} = (\hat{\mathbf{e}}_i \bullet \mathbf{a})\hat{\mathbf{e}}_j - (\hat{\mathbf{e}}_j \bullet \mathbf{a})\hat{\mathbf{e}}_i = (\hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_i - \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j)\mathbf{a}$, so (3.8) is equivalent to

$$\left[\sum_{i=1}^{3}\sum_{j=1}^{3}\frac{(\hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_i - \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j)}{h_i h_j}\frac{\partial(h_j v_j^e)}{\partial q_i}\right](\mathbf{a}) = \operatorname{curl}\mathbf{v} \times \mathbf{a}. \tag{3.9}$$

Since the right members of (1.3) and (3.9) are equal their left members must be equal as well for all $\mathbf{a}$. The operators that act upon $\mathbf{a}$ must then be equal, *i.e.*

$$\nabla\mathbf{v} - (\nabla\mathbf{v})^T = \sum_{i=1}^{3}\sum_{j=1}^{3}\frac{(\hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_i - \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j)}{h_i h_j}\frac{\partial(h_j v_j^e)}{\partial q_i}. \tag{3.10}$$

The discussion in the paragraphs containing (3.4) through (3.10) applies to all orthogonal curvliner coordinates systems. I will now revert to the discussion of the particular orthogonal curvilinear coordinate system defined by $(3.2)_{1,2}$ and the system $\{\hat{\mathbf{i}}_1, \hat{\mathbf{i}}_2, \hat{\mathbf{i}}_3\}$. Here, one finds that

$$h_1 = h_2 = h_3 := h = (a/q)^2 . \tag{3.11}$$

Equations (3.5), (3.10), and (3.7) then take the simpler forms

$$\operatorname{div}\mathbf{v} = \frac{1}{h^3}\sum_{i=1}^{3}\frac{\partial(h^2 v_i^e)}{\partial q_i}, \tag{3.12}$$

$$\nabla\mathbf{v} - (\nabla\mathbf{v})^T = \frac{1}{h^2}\sum_{i=1}^{3}\sum_{j=1}^{3}(\hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_i - \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j)\frac{\partial(h v_j^e)}{\partial q_i}, \tag{3.13}$$

$$\nabla\varphi = \sum_{i=1}^{3}\frac{\hat{\mathbf{e}}_i}{h}\frac{\partial\varphi}{\partial q_i}, \tag{3.14}$$

respectively.

Let Q denote the linear vector-to-vector operator—*i.e.* the tensor—that takes $\hat{\mathbf{i}}_i$ to $\hat{\mathbf{e}}_i$, $i \in \{1,2,3\}$. Then $\hat{\mathbf{e}}_i = Q(\hat{\mathbf{i}}_i)$. Since Q takes unit vectors to unit vectors, it must have the feature that the magnitude of its input must equal the magnitude of its output. Such an tensor is called *orthogonal* and has the feature that its transpose equals its inverse. In view of the identities $\hat{\mathbf{e}}_i = Q(\hat{\mathbf{i}}_i)$ we have

$$v_i^e = \hat{\mathbf{e}}_i \bullet \mathbf{v} = Q(\hat{\mathbf{i}}_i) \bullet \mathbf{v} = \hat{\mathbf{i}}_i \bullet Q^T(\mathbf{v}), \tag{3.15}$$

so (3.12)–(3.14) are equivalent to

$$\operatorname{div}\mathbf{v} = \frac{1}{h^3}\sum_{i=1}^{3}\frac{\partial[\hat{\mathbf{i}}_i \bullet Q^T(h^2\mathbf{v})]}{\partial q_i}, \tag{3.16}$$

$$\nabla\mathbf{v} - (\nabla\mathbf{v})^T = \frac{1}{h^2}\sum_{i=1}^{3}\sum_{j=1}^{3}\Big[Q(\hat{\mathbf{i}}_j) \otimes Q(\hat{\mathbf{i}}_i) - Q(\hat{\mathbf{i}}_i) \otimes Q(\hat{\mathbf{i}}_j)\Big]\frac{\partial[\hat{\mathbf{i}}_j \bullet Q^T(h\mathbf{v})]}{\partial q_i}, \tag{3.17}$$

$$\nabla\varphi = \frac{1}{h}\sum_{i=1}^{3}Q(\hat{\mathbf{i}}_i)\frac{\partial\varphi}{\partial q_i}, \tag{3.18}$$

respectively. If $\mathbf{a}$ and $\mathbf{b}$ are any two vectors and S is any tensor then two rules of tensor algebra state that $S(\mathbf{a}\otimes\mathbf{b}) = S(\mathbf{a})\otimes\mathbf{b}$ and $(\mathbf{a}\otimes\mathbf{b})S = \mathbf{a}\otimes S^T(\mathbf{b})$ [See *e.g.* GURTIN (Ref. 3, p9, Exercises 6 a,b)]. From these general rules one may deduce, for example, that $Q(\hat{\mathbf{i}}_j) \otimes Q(\hat{\mathbf{i}}_i) = Q(\hat{\mathbf{i}}_j \otimes \hat{\mathbf{i}}_i)Q^T$, Thus (3.17) is equivalent to

$$\nabla\mathbf{v} - (\nabla\mathbf{v})^T = \frac{1}{h^2}Q\left[\sum_{i=1}^{3}\sum_{j=1}^{3}(\hat{\mathbf{i}}_j \otimes \hat{\mathbf{i}}_i - \hat{\mathbf{i}}_i \otimes \hat{\mathbf{i}}_j)\frac{\partial[\hat{\mathbf{i}}_j \bullet Q^T(h\mathbf{v})]}{\partial q_i}\right]Q^T. \tag{3.19}$$

One may express these results more compactly by introducing some abbreviations. To this end, let

$$\sum_{i=1}^{3}\frac{\partial v_i}{\partial q_i} = \sum_{i=1}^{3}\frac{\partial(\hat{\mathbf{i}}_i \bullet \mathbf{v})}{\partial q_i} := \operatorname{div}_q\mathbf{v}, \tag{3.20}$$

$$\sum_{i=1}^{3}\hat{\mathbf{i}}_i\frac{\partial\varphi}{\partial q_i} := \nabla_q\varphi, \tag{3.21}$$

$$\sum_{i=1}^{3}\sum_{j=1}^{3}(\hat{\mathbf{i}}_i \otimes \hat{\mathbf{i}}_j)\frac{\partial v_i}{\partial q_j} = \sum_{i=1}^{3}\sum_{j=1}^{3}(\hat{\mathbf{i}}_i \otimes \hat{\mathbf{i}}_j)\frac{\partial(\hat{\mathbf{i}}_i \bullet \mathbf{v})}{\partial q_j} := \nabla_q\mathbf{v}. \tag{3.22}$$

Then equations (3.16), (3.19), (3.18) takes the more compact forms

$$\operatorname{div}\mathbf{v} = \frac{1}{h^3}\operatorname{div}_q[Q^T(h^2\mathbf{v})], \tag{3.23}$$

$$\nabla \mathbf{v} - (\nabla \mathbf{v})^T = \frac{1}{h^2} Q\{\nabla_q [Q^T(h\mathbf{v})] - \nabla_q [Q^T(h\mathbf{v})]^T\} Q^T \ , \quad (3.24)$$

$$\nabla \varphi = \frac{1}{h} Q(\nabla_q \varphi) \ , \quad (3.25)$$

respectively.

Returning, now, to the variational principle (3.1) one may transform the right member from an integral over the physical exterior domain, $\mathcal{R}^e$, to one over the proxy domain, $\mathcal{Q}$, by application of the transformation rules (3.23) and (3.24) in the case when the generic vector, $\mathbf{v}$, is the fluid velocity, $\mathbf{u}$. In carrying out this transformation the volume element transforms according to the rule $dV = h^3 dV_q$, in which dV_q is the volume of a typical small part of $\mathcal{Q}$. The simplicity of this rule is due to both the orthogonality of the coordinates and the equality of three scale factors, as stated in (3.11). Equation (3.1) thus becomes

$$F := \iiint_{\mathcal{Q}} \left[\frac{1}{h^6} \{ \mathrm{div}_q [Q^T(h^2 \mathbf{u})] \}^2 + \frac{1}{4} \left\| \frac{Q\{\nabla_q [Q^T(h\mathbf{u})] - \nabla_q [Q^T(h\mathbf{u})]^T\} Q^T}{h^2} \right\|^2 \right] h^3 dV_q, \quad (3.26)$$

which one may simplify in three ways, namely: (i) by cancellation of common powers of h in the numerator and denominator under the integral sign; (ii), by introducing the change of variable $\mathbf{u} \to \mathbf{U}$ defined by $Q^T(h\mathbf{u}) := \mathbf{U}$; and (iii), by appealing to an algebraic rule according to which $\|QSQ^T\|^2 = \|S\|^2$ for any tensor, S, and orthogonal tensor, Q. The resulting simplified form of (3.26) is

$$F := \iiint_{\mathcal{Q}} \left[\frac{1}{h^3} \{ \mathrm{div}_q (h\mathbf{U}) \}^2 + \frac{1}{4h} \left\| [\nabla_q (\mathbf{U}) - \nabla_q (\mathbf{U})^T] \right\|^2 \right] dV_q \ . \quad (3.27)$$

At this point the reasoning follows logic similar to that described in the text containing (2.1)–(2.5) above. By requiring the first variation, δF, of F to be zero for arbitrary variations, $\delta \mathbf{U}$, of $\mathbf{U}$ within $\mathcal{Q}$ and on $\partial\mathcal{Q}$ one my derive a the differential equation for $\mathbf{U}$ in $\mathcal{Q}$ (a.k.a. the EULER-LAGRANGE equation) for the variational problem and a natural (a.k.a. flux-source) boundary condition for $\mathbf{u}$ on $\partial\mathcal{Q}$.

To be specific, if one takes the first variation of (3.27) and applies some identites as described in the footnote prior to equation (2.2) one may arrange the result in the form

$$\delta F - \iiint_{\mathcal{Q}} \Big[\frac{2}{h^3} \mathrm{div}\,(h\mathbf{U}) I \bullet \nabla_q (h\,\delta\mathbf{U}) + \frac{1}{h} \big[\nabla_q \mathbf{U} - (\nabla_q \mathbf{U})^T \big] \bullet \nabla_q (\delta\mathbf{U}) \Big] dV_q = 0 \, . \quad (3.28)$$

Three identities are useful here. The first asserts that $\nabla(\varphi\mathbf{v}) = \varphi\nabla\mathbf{v} + \mathbf{v} \otimes \nabla\varphi$ for a generic scalar φ and vector $\mathbf{v}$ [*cf.* GURTIN (Ref. 3, equation $(4.2)_1$, p30] and the second and third assert that $I \bullet (\mathbf{a} \otimes \mathbf{b}) = \mathrm{tr}\,(\mathbf{a} \otimes \mathbf{b}) = \mathbf{a} \bullet \mathbf{b}$ [*cf.* GURTIN (Ref. 3, pp 5–6)]. With the aid of these identities one may deduce that

$$I \bullet \nabla_q (h\,\delta\mathbf{U}) = hI \bullet \nabla_q (\delta\mathbf{U}) + \delta\mathbf{U} \bullet \nabla_q h \ . \quad (3.29)$$

If one substitutes (3.29) into (3.28) and introduces the abbreviations

$$\Gamma := \frac{2}{h^2} \mathrm{div}\,(h\mathbf{U}) I + \frac{1}{h} \big[\nabla_q \mathbf{U} - (\nabla_q \mathbf{U})^T \big] \quad (3.30)$$

$$\mathbf{f} := \frac{2}{h^3} \mathrm{div}\,(h\mathbf{U}) \nabla_q h \quad (3.31)$$

that equation becomes

$$\delta F - \iiint_{\mathcal{Q}} \big[\Gamma \bullet \nabla_q (\delta\mathbf{U}) + \mathbf{f} \bullet \delta\mathbf{U} \big] dV_q = 0 \quad (3.32)$$

If one sets δF to zero (as is appropriate when F attains a minimum) and interprets the first variation, $\delta\mathbf{U}$, of $\mathbf{U}$ as what the COMSOL documentation denotes by $\mathbf{v}$ and calls a *test function* then equation (3.32) becomes what that documentation calls *the weak form.*

By application of the identities described in the footnote preceding (2.4) above one may write (3.32) in the equivalent form

$$\delta F + \iint_{\partial\mathcal{Q}} \delta\mathbf{U} \bullet [-\Gamma(\hat{\mathbf{n}}_q)] dA_q + \iiint_{\mathcal{Q}} \delta\mathbf{U} \bullet (\mathrm{div}_q \Gamma - \mathbf{f}) \, dV_q = 0 \ . \quad (3.33)$$

Here dA_q is the area of a typical small part of $\partial\mathcal{Q}$ and $\hat{\mathbf{n}}_q$ is the outward unit normal vector on that boundary surface. If F is a minimum then $\delta F = 0$ subject to arbitrary variations $\delta\mathbf{U}$ on $\partial\mathcal{Q}$ and in $\mathcal{Q}$. Equation (3.33) then implies that

$$\operatorname{div}_q \Gamma = \mathbf{f} \quad , \quad -\Gamma(\hat{\mathbf{n}}_q) = \mathbf{0} \, , \qquad (3.34)_{1,2}$$

which constitute the EULER-LAGRANGE equation and the natural boundary condition, respectively. The system consisting of (3.30), (3.31) and $(3.34)_1$ is not quite suitable for input to the COMSOL general form PDE physics interface owing to the presence of the derivative of a product, namely $\operatorname{div}_q(h\mathbf{U})$. If one substitutes $h = a^2/q^2$ [*cf.* (3.11) above] and evaluates the indicated derivatives one finds that (3.31) and (3.32) are equivalent to

$$\Gamma = \left(\frac{2q^2}{a^2}\operatorname{div}_q \mathbf{U} - \frac{4}{a^2}\mathbf{q}\bullet\mathbf{U}\right) I + \frac{q^2}{a^2}\left[\nabla_q \mathbf{U} - (\nabla_q \mathbf{U})^T\right] \qquad (3.35)$$

and

$$\mathbf{f} = -\frac{4}{a^2}\frac{\mathbf{q}}{q}\left(q \operatorname{div}_q \mathbf{U} - \frac{2}{q}\mathbf{q}\bullet\mathbf{U}\right) . \qquad (3.36)$$

The system consisting of $(3.34)_{1,2}$, (3.35), and (3.36) is now suitable for input to the COMSOL general form PDE physics interface.

4. Conditions on normal and slip velocities; Results

As noted in the discussion of the flow in $\mathcal{R}^i$ [see the paragraph containing (2.6) above] the EULER-LAGRANGE equation and natural boundary condition are not sufficient, by themselves, to ensure uniqueness of $\mathbf{u}$, or, in the present context, $\mathbf{U}$. One can determine $\mathbf{U}$ uniquely by augmenting the natural boundary condition $(3.34)_2$, with a condition analogous to (2.6), namely a specification of the value of $\mathbf{U}\bullet\hat{\mathbf{n}}_q$ on $\partial\mathcal{Q}$. If the observer for whom $\mathbf{u}$ is the fluid velocity in $\mathcal{R}^e$ is at rest relative to the boundary sphere, $\partial\mathcal{R}^e$, then the impermeable-sphere boundary condition takes the form $\mathbf{u}\bullet\hat{\mathbf{n}} = 0$. Nontrival solutions are possible if the fluid at a remote distance from the sphere is in uniform motion, with, say, a downward fluid velocity $w_\infty\hat{\mathbf{i}}_3$ with $w_\infty < 0$. in that case $\mathbf{U} = Q^T(h\mathbf{u}) = Q^T[(a^2/q^2)w_\infty\hat{\mathbf{i}}_3]$, whose rightmost member goes to infinity as $q \to 0$. Such a behavior for the unknown $\mathbf{U}$ is unsatisfactory for computation.

A alternative approach is to frame the impermeable-sphere boundary condition on $\partial\mathcal{R}^e$ under the assumption that the observer for whom $\mathbf{u}$ is the velocity in $\mathcal{R}^e$ is *at rest relative to the remote undisturbed fluid.* In such a reference frame the bounding sphere, $\partial\mathcal{R}^e$, translates upward with velocity $-w_\infty\hat{\mathbf{i}}_3$ and the impermeable sphere boundary condition becomes $\mathbf{u}\bullet\hat{\mathbf{n}} = (-w_\infty\hat{\mathbf{i}}_3)\bullet\hat{\mathbf{n}}$ on $\partial\mathcal{R}^e$.

To relate $\mathbf{u}\bullet\hat{\mathbf{n}}$ at a typical point on $\partial\mathcal{R}^e$ to $\mathbf{U}\bullet\hat{\mathbf{n}}_q$ at its image on $\partial\mathcal{Q}$ let Ψ be a scalar-valued function of position with the feature that both $\partial\mathcal{R}^e$ and $\partial\mathcal{Q}$ are surfaces of constant Ψ, say $\Psi = 0$. For definiteness let Ψ be negative valued in both $\mathcal{R}^e$ and $\mathcal{Q}$. Then the outward unit normal vectors on $\partial\mathcal{R}^e$ and $\partial\mathcal{Q}$ satisfy

$$\hat{\mathbf{n}} = (\nabla\Psi/\|\nabla\Psi\|)_{\Psi=0} \ , \ \hat{\mathbf{n}}_q = (\nabla_q \Psi/\|\nabla_q \Psi\|)_{\Psi=0} \ , \qquad (4.1)_{1,2}$$

respectively. If one re-expresses $\nabla\Psi$ in the right member of $(4.1)_1$ by means of (3.25), cancels the factors $1/h$ in the numerator and denominator, and notes that $\|Q(\mathbf{a})\| = \|\mathbf{a}\|$ for every vector $\mathbf{a}$ and orthogonal tensor, Q, equation $(4.1)_1$ becomes

$$\hat{\mathbf{n}} = \left[Q(\nabla_q \Psi)/\|\nabla_q \Psi\|\right]_{\Psi=0} . \qquad (4.2)$$

If one substitutes $(4.1)_2$ into the right member of (4.2) that equation becomes

$$\hat{\mathbf{n}} = Q(\hat{\mathbf{n}}_q) . \qquad (4.3)$$

But $Q^T(h\mathbf{u}) = \mathbf{U}$, so $\mathbf{u} = (1/h)Q(\mathbf{U})$. If one evaluates this last equation on the boundary sphere $q = a$ and notes that $h = 1$ there one gets

$$\mathbf{u} = Q(\mathbf{U}) \qquad (4.4)$$

Now the inner product of the left members of (4.3) and (4.4) must equal the inner product of their right members, so

$$\mathbf{u}\bullet\hat{\mathbf{n}} = Q(\mathbf{U})\bullet Q(\hat{\mathbf{n}}_{\mathbf{q}}) = \mathbf{U}\bullet\hat{\mathbf{n}}_q \ , \qquad (4.5)$$

in which the last equality follows from the orthogonality of Q. In view of (4.5) the impermeable-sphere boundary condition $\mathbf{u} \bullet \hat{\mathbf{n}} = (-w_\infty \hat{\mathbf{i}}_3) \bullet \hat{\mathbf{n}}$ on $\partial \mathcal{R}^e$ is equivalent to

$$\mathbf{U} \bullet \hat{\mathbf{n}}_q = (-w_\infty \hat{\mathbf{i}}_3) \bullet \hat{\mathbf{n}} \,. \tag{4.6}$$

The system consisting of the differential equation $(3.34)_1$ subject to the natural boundary condition $(3.34)_2$ and the impermeable-sphere condition (4.6) is now sufficient to ensure a unique solution for $\mathbf{U}$. Having $\mathbf{U}$ in $\mathcal{Q}$, one could compute $\mathbf{u}$ in $\mathcal{R}^e$ from $\mathbf{u} = (1/h)Q(\mathbf{U})$, which would represent the velocity relative to the remote undisturbed fluid. If, alternativley one wants $\mathbf{u}$ to represent the velocity as seen by an observer who moves with the sphere then one may take $\mathbf{u} = (1/h)Q(\mathbf{U}) + w_\infty \hat{\mathbf{i}}_3$.

The vorticity constant, A, for the flow in $\mathcal{R}^i$ and the free-stream velocity, $w_\infty \hat{\mathbf{i}}_3$ cannot be specified independently without causing a discontinuity in the tagential velocity, or slip, across the boundary sphere. To avoid this slip one specifies only one of the two parameters A and w_∞ and computes the other. The present COMSOL model implements no-slip by requiring that the average around the equator of the $\hat{\mathbf{i}}_3$-component computed from the $\mathbf{u}$-solutions in $\mathcal{R}^i$ and $\mathcal{R}^e$ agree.

The present COMSOL model employs three components: the first contains a General Form PDF interface to solve for $\mathbf{u}$ in $\mathcal{R}^i$; the second contains a General Form PDF interface to solve for $\mathbf{U}$ in $\mathcal{Q}$; and the third calculates $\mathbf{u}$ in a subrgion of $\mathcal{R}^e$—namely the region $a < r < 2a$—from $\mathbf{U}$ in the corresponding subregion of $\mathcal{Q}$. This third component enables graphical illustration of $\mathbf{u}$ in the immediate neighborhood of the spherical vortex. To accomplish this calculation from the identity $\mathbf{u} = (1/h)Q(\mathbf{U})$ one requires an explicit representation of Q, namely $Q = 2(\mathbf{q}/q) \otimes (\mathbf{q}/q) - I$. These three components employ General Extrusion Model Coupling Operators to exchage information between components. The first component contains a node which enforces no-slip by means of a Global ODE and DAE node. There are two Study Steps: the first carries out the computations in components 2 and 3; and the second carries them out in component 1. Fig. 5.1 nearby illustrates the results.

5. Conclusion

COMSOL's General Form PDE interface enables computation of the three-dimensional velocity field of a fluid flow with nonzero vorticity in a bounded subdomain of a larger domain that lacks any exterior boundary.

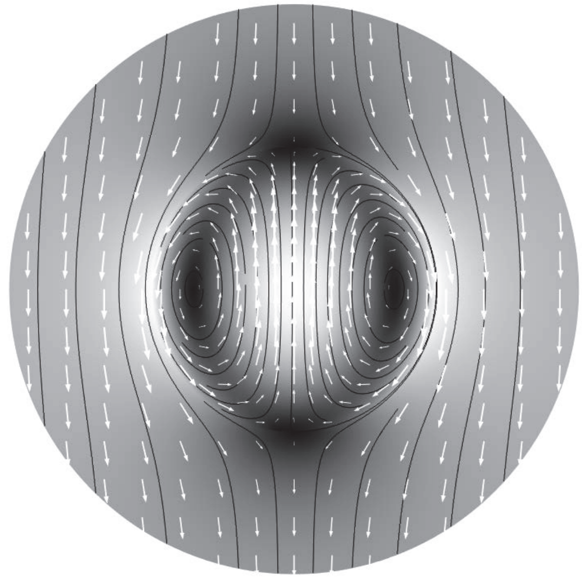

Figure 4.1 Computed velocity field in Hill's spherical vortex in a cut plane containing the axis of symmetry: shading represents fluid speed; solid lines represent streamlines; and arrows represent velocity vectors.

6. References

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