

An immersed boundary method with a divergence-free interpolated velocity field

The purpose of this note is to introduce an immersed boundary (IB) method in which the interpolated velocity field is exactly divergence-free, in the continuous sense, that is

$$(1) \quad \nabla \cdot \underline{U} = 0$$

where $\underline{U}(\underline{X}, t)$ is the velocity field in which the Lagrangian points move:

$$(2) \quad \frac{d\underline{X}_k}{dt} = \underline{U}(\underline{X}_k(t), t)$$

This is not the case in existing IB methods, in which $\underline{U}(\underline{X}, t)$ is calculated from a function $\underline{u}(\underline{x}, t)$ that is defined on a fixed mesh \mathcal{I}_h according to

$$(3) \quad \underline{U}(\underline{X}, t) = \sum_{\underline{x} \in \mathcal{I}_h} \underline{u}(\underline{x}, t) \phi_h(\underline{x} - \underline{X}) h^3$$

where $\hat{d}_h(\underline{x})$ is a suitably chosen approximation to the Dirac delta function. No matter how we choose \hat{d}_h , the condition (1) is equivalent to

$$(4) \quad 0 = \sum_{\underline{x} \in g_h} \underline{u}(\underline{x}, t) \cdot (\nabla \hat{d}_h)(\underline{x} - \underline{X}) h^3$$

This amounts to infinitely many linear conditions on the finite number of variables $\underline{u}(\underline{x}, t)$, $\underline{x} \in g_h$, since there is one condition for each \underline{X} , the coordinates of which are real. Thus, it does not seem likely that an interpolation scheme of the form given by (3) can result in divergence-free $\underline{U}(\underline{X})$ for all $\underline{u}(\underline{x})$ in some finite dimensional (discretely divergence-free) space, no matter how the discrete divergence and/or \hat{d}_h may be defined.

Here, we take a different approach. We make use of the fact that $\underline{u}(\underline{x}, t)$ is discretely divergence-free, in a sense to be defined below, and construct an Eulerian vector potential $\underline{a}(\underline{x}, t)$ from which $\underline{u}(\underline{x}, t)$ can be derived by

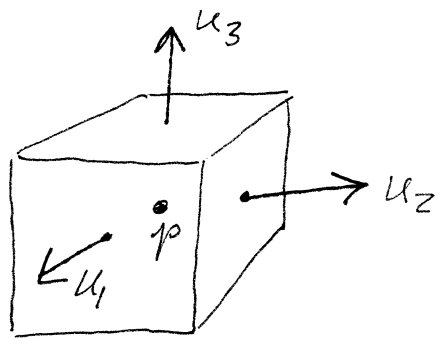
evaluating the discrete curl of $\underline{a}(x, t)$.

We then interpolate $\underline{a}(x, t)$ by a formula analogous to (3) and call the result $\underline{A}(X, t)$. Finally, we take the continuous curl of $\underline{A}(X, t)$ to get a divergence-free $\underline{U}(X, t)$.

An important feature of the IB method is that force-spreading is done in a manner that is adjoint to velocity interpolation. Thus, we also construct a force-spreading scheme that is the adjoint of the interpolation scheme described above.

Both the interpolation and the force-spreading that we construct here are non-local, but they can be implemented efficiently with the help of fast Poisson solvers.

Consider a periodic domain in 3D covered by a uniform Cartesian grid of cubic cells with volume h^3 . We use a staggered grid, in which pressure is defined at cell centers, and each component of velocity is defined at the center of a face to which that velocity component is normal.



Also, the components of the discrete curl of the velocity, and likewise of the vector potential, are defined at the centers of the edges of the cells, with each component being defined on an edge to which it is parallel.

Note that the center of each edge is surrounded by four velocity components that lie in the plane that bisects the edge and is normal to it. Similarly, each velocity component is surrounded by four edges that lie in the plane face to which the velocity component is normal. This is all very suitable for discrete curl.

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We use the notation g_h to refer to the whole staggered grid. In expressions like the right-hand side of equation (3), which involve sums over g_h , it is understood that the sum is over the relevant points. Note in particular that

$$(5) \quad \sum_{\underline{x} \in g_h} \underline{u}(\underline{x}, t) \int_h (\underline{x} - \underline{X}) / h^3$$

is a vector expression. In its 1 component, the sum is over those values of \underline{x} for which u_1 is defined, namely the centers of the faces $x_1 = \text{constant}$, and similarly for the 2 and 3 components. Thus $\underline{x} \in g_h$ has a different meaning depending on the context.

The difference operators D_i , $i=1,2,3$, plays a crucial role in the following. It is defined by

$$(6) \quad (D_i \varphi)(\underline{x}) = \frac{\varphi(\underline{x} + \frac{h}{2} \underline{e}_i) - \varphi(\underline{x} - \frac{h}{2} \underline{e}_i)}{h}$$

where $\{\underline{e}_1, \underline{e}_2, \underline{e}_3\}$ is the standard basis of \mathbb{R}^3 .

We can use D_i to define discrete analogs of gradient, divergence, and curl:

$$(7) \quad \underline{D}\varphi = (D_1\varphi, D_2\varphi, D_3\varphi)$$

$$(8) \quad \underline{D} \cdot \underline{u} = D_i u_i$$

$$(9) \quad \underline{D} \times \underline{u} = \epsilon_{ijk} D_j u_k$$

in which ϵ_{ijk} is the totally antisymmetric tensor and we are using the summation convention.

If φ is defined at cell centers, then the components of $\underline{D}\varphi$ are defined on different grids of points. Indeed, $D_i\varphi$ is defined at precisely the same set of points as u_i .

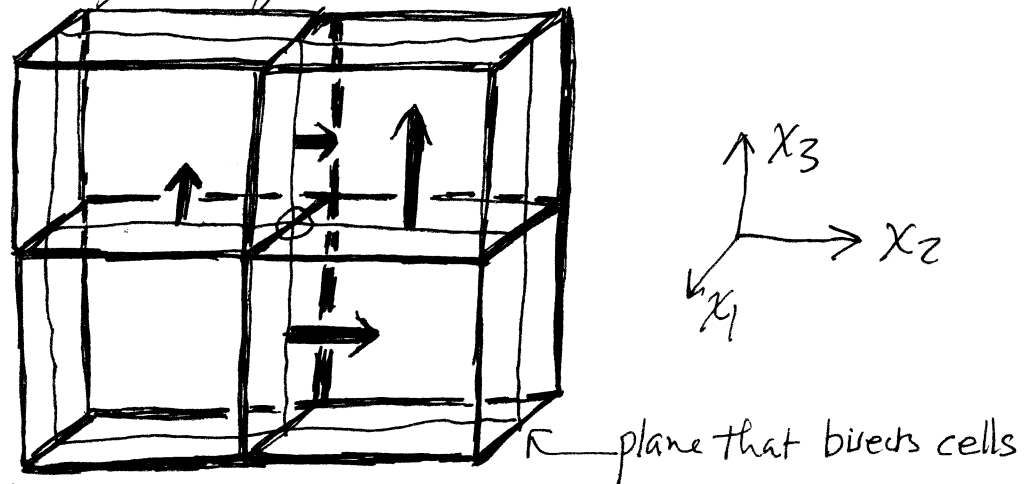
With u_i defined at centers of cell faces, as described above, then $\underline{D} \cdot \underline{u}$ is defined at cell centers. Note, however, that it is also possible to apply $\underline{D} \cdot$ to vectors whose components ^{are} at the centers of cell edges, with the x_j components located on the edges that run parallel to the x_j axis. If such a vector is denoted \underline{a} , then $\underline{D} \cdot \underline{a}$ is defined at the cell corners.

As for $(\underline{D} \times)$, each component of $(\underline{D} \times)$ involves vectors that lie in a plane normal to the axis parallel to that component. Thus, for example

$$(10) \quad (\underline{D} \times \underline{u})_1 = D_2 u_3 - D_3 u_2$$

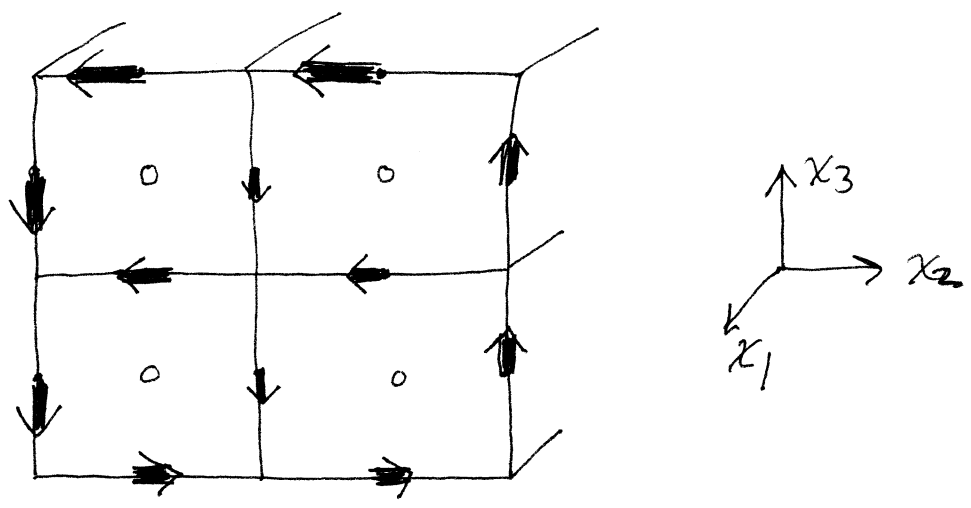
$$(11) \quad (\underline{D} \times \underline{u})_1(\underline{x}) = \frac{u_3(\underline{x} + \frac{h}{2} \underline{e}_2) - u_3(\underline{x} - \frac{h}{2} \underline{e}_2)}{h} - \frac{u_2(\underline{x} + \frac{h}{2} \underline{e}_3) - u_2(\underline{x} - \frac{h}{2} \underline{e}_3)}{h}$$

The above computation takes place in a plane perpendicular to the x_1 axis that bisects the cells of the grid



Thus $(\underline{D} \times \underline{u})_1$ is defined at the centers of the cell edges that run parallel to the x_1 axis.

The same operation $(\underline{D} \times)$ can also be applied to vectors of the type \underline{a} defined above, in which the components are located at the centers of the cell edges, with each component having a direction parallel to the edge. In that case the computations take place on the cell faces. For example $(\underline{D} \times \underline{a})_1$ looks like this:



Thus $(\underline{D} \times \underline{a})_1$ is defined at the centers of the cell faces $x_1 = \text{constant}$, that is, at the same points where u_1 is defined.

The operator \underline{D} has many properties that reflect those of ∇ . We list them here, with proofs to follow

(12) $\underline{D} \times \underline{D} \varphi = 0$

(13) $\underline{D} \cdot (\underline{D} \times \underline{u}) = 0$

(14) $\sum_{\underline{x} \in \mathcal{G}_h} \underline{u}(\underline{x}) \cdot (\underline{D} \varphi)(\underline{x}) h^3 = - \sum_{\underline{x} \in \mathcal{G}_h} (\underline{D} \cdot \underline{u})(\underline{x}) \varphi(\underline{x}) h^3$

(15) $\sum_{\underline{x} \in \mathcal{G}_h} \underline{a}(\underline{x}) \cdot (\underline{D} \times \underline{u})(\underline{x}) h^3 = + \sum_{\underline{x} \in \mathcal{G}_h} (\underline{D} \times \underline{a})(\underline{x}) \cdot \underline{u}(\underline{x}) h^3$

Also, if

$$(16) \quad \sum_{\underline{x} \in \mathcal{G}_h} \underline{u}(\underline{x}) h^3 = 0$$

Then

$$(17) \quad \underline{D} \times \underline{u} = 0 \Rightarrow \exists \varphi \text{ such that } \underline{u} = \underline{D} \varphi$$

$$(18) \quad \underline{D} \cdot \underline{u} = 0 \Rightarrow \exists \underline{a} \text{ such that } \underline{u} = \underline{D} \times \underline{a}$$

To prove (12) and (13) we rely on the easily-checked fact that D_i and D_j commute. We have

$$(19) \quad (\underline{D} \times \underline{D} \varphi)_i = \varepsilon_{ijk} D_j D_k \varphi$$

$$(20) \quad \underline{D} \cdot \underline{D} \times \underline{u} = D_i \varepsilon_{ijk} D_j u_k$$

Both right-hand sides are obviously zero because of the antisymmetry of ε_{ijk} and the symmetry of $D_j D_k$ and $D_i D_j$.

11

The proofs of (14-15) rely on the corresponding property of D_j in "summation by parts"

$$\begin{aligned}
 (21) \quad & \sum_{\underline{x} \in \mathcal{G}_h} \varphi(\underline{x}) (D_j \psi)(\underline{x}) h^3 \\
 &= \sum_{\underline{x} \in \mathcal{G}_h} \varphi(\underline{x}) \frac{\psi(\underline{x} + \frac{h}{2} \underline{e}_j) - \psi(\underline{x} - \frac{h}{2} \underline{e}_j)}{h} h^3 \\
 &= \sum_{\underline{x} \in \mathcal{G}_h} \frac{\varphi(\underline{x} - \frac{h}{2} \underline{e}_j) - \varphi(\underline{x} + \frac{h}{2} \underline{e}_j)}{h} \psi(\underline{x}) h^3 \\
 &= - \sum_{\underline{x} \in \mathcal{G}_h} (D_j \varphi)(\underline{x}) \psi(\underline{x}) h^3
 \end{aligned}$$

As mentioned above, we are using the notation " $\underline{x} \in \mathcal{G}_h$ " loosely. In fact, the set of values of \underline{x} that is denoted \mathcal{G}_h changes from line 2 to line 3 of the foregoing. The change is a shift of $\frac{h}{2}$ in the \underline{e}_j direction.

Making use of (21), we can easily prove (14) and (15) by writing everything in components:

$$\begin{aligned}
 (22) \quad & \sum_{\underline{x} \in \mathcal{J}_h} \underline{u}(\underline{x}) \cdot (\underline{D}\varphi)(\underline{x}) h^3 \\
 &= \sum_{\underline{x} \in \mathcal{J}_h} u_i(\underline{x}) (D_i \varphi)(\underline{x}) h^3 \\
 &= - \sum_{\underline{x} \in \mathcal{J}_h} (D_i u_i)(\underline{x}) \varphi(\underline{x}) h^3 \\
 &= - \sum_{\underline{x} \in \mathcal{J}_h} (\underline{D} \cdot \underline{u})(\underline{x}) \varphi(\underline{x}) h^3
 \end{aligned}$$

which proves (14). Similarly

$$\begin{aligned}
 (23) \quad & \sum_{\underline{x} \in \mathcal{J}_h} \underline{a}(\underline{x}) \cdot (\underline{D} \times \underline{u})(\underline{x}) h^3 \\
 &= \varepsilon_{ijk} \sum_{\underline{x} \in \mathcal{J}_h} a_i(\underline{x}) (D_j u_k)(\underline{x}) h^3
 \end{aligned}$$

$$= -\varepsilon_{ijk} \sum_{\underline{x} \in \mathcal{G}_h} (D_j a_i)(\underline{x}) u_k(\underline{x}) h^3$$

$$= +\varepsilon_{kji} \sum_{\underline{x} \in \mathcal{G}_h} (D_j a_i)(\underline{x}) u_k(\underline{x}) h^3$$

$$= + \sum_{\underline{x} \in \mathcal{G}_h} (\underline{D} \times \underline{a})(\underline{x}) \cdot \underline{u}(\underline{x}) h^3$$

which proves (15).

To prove (16-18), we start by deriving an identity that will also be useful later:

$$\begin{aligned} (24) \quad (\underline{D} \times (\underline{D} \times \underline{u}))_i &= \varepsilon_{ijk} D_j \varepsilon_{klm} D_l u_m \\ &= (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) D_j D_l u_m \\ &= D_i D_j u_j - D_j^2 u_i \end{aligned}$$

or in vector notation

$$(25) \quad \underline{D} \times (\underline{D} \times \underline{u}) = \underline{D}(\underline{D} \cdot \underline{u}) - D_j^2 \underline{u}$$

Now we use (25) to prove the following lemma

$$(26) \quad \underline{D} \cdot \underline{u} = 0 \quad \& \quad \underline{D} \times \underline{u} = 0 \quad \Rightarrow \quad \underline{u} = \text{constant}$$

To prove this, note that

$$\sum_{\underline{x} \in \mathcal{J}_h} (\underline{D} \times \underline{u}) \cdot (\underline{D} \times \underline{u}) h^3 = \sum_{\underline{x} \in \mathcal{J}_h} \underline{u} \cdot (\underline{D} \times (\underline{D} \times \underline{u})) h^3$$

$$= \sum_{\underline{x} \in \mathcal{J}_h} \underline{u} \cdot \underline{D} (\underline{D} \cdot \underline{u}) h^3 - \sum_{\underline{x} \in \mathcal{J}_h} \underline{u} \cdot \underline{D}_j^2 \underline{u} h^3$$

$$= - \sum_{\underline{x} \in \mathcal{J}_h} (\underline{D} \cdot \underline{u})^2 h^3 + \sum_{\underline{x} \in \mathcal{J}_h} (\underline{D}_j u_i)^2 h^3$$

Thus

$$(27) \quad \sum_{\underline{x} \in \mathcal{J}_h} (\underline{D}_j u_i)^2 h^3 = \sum_{\underline{x} \in \mathcal{J}_h} (\underline{D} \cdot \underline{u})^2 h^3 + \sum_{\underline{x} \in \mathcal{J}_h} |\underline{D} \times \underline{u}|^2 h^3$$

Now if $\underline{D} \cdot \underline{u} = 0$ and $\underline{D} \times \underline{u} = 0$, the right-hand side of (27) is zero, and therefore so is the left-hand side. But this implies that u_i is constant for $i=1,2,3$.

Before we can prove (16-18), we need one more lemma

(28) If ψ is such that

$$(28a) \quad \sum_{\underline{x} \in \mathcal{J}_h} \psi(\underline{x}) h^3 = 0$$

then $\exists \phi$ such that

$$(28b) \quad \underline{D} \cdot \underline{D} \phi = \psi$$

This is an exercise in linear algebra. Since $\underline{D} \cdot \underline{D}$ is symmetric with respect to the inner product

$$(29) \quad (\phi, \psi) = \sum_{\underline{x} \in \mathcal{J}_h} \phi(\underline{x}) \psi(\underline{x}) h^3$$

what we have to show is that any ψ satisfying (28a) is orthogonal to any ϕ_0 in the null space of $\underline{D} \cdot \underline{D}$, that is, any ϕ_0 such that

$$(30) \quad \underline{D} \cdot \underline{D} \phi_0 = 0$$

But (30) \Rightarrow

$$(31) \quad \sum_{\underline{x} \in \mathcal{J}_h} \phi_0(\underline{x}) (\underline{D} \cdot \underline{D} \phi_0)(\underline{x}) h^3 = 0$$

which implies

$$(32) \quad - \sum_{\underline{x} \in J_h} (\underline{D}\phi_0)(\underline{x}) \cdot (\underline{D}\phi_0)(\underline{x}) h^3 = 0$$

which implies that $\phi_0 = \text{constant}$, and hence that

$$(33) \quad (\psi, \phi_0) = 0$$

because of 28a, as required.

Now to prove (17), we choose φ as any solution of

$$(34) \quad \underline{D} \cdot \underline{D} \varphi = \underline{D} \cdot \underline{u}$$

Such φ exist, by the lemma (28), since

$$(35) \quad \sum_{\underline{x} \in \mathcal{J}_h} (\underline{D} \cdot \underline{u}) h^3 = \sum_{\underline{x} \in \mathcal{J}_h} 1 (\underline{D} \cdot \underline{u}) h^3 \\ = - \sum_{\underline{x} \in \mathcal{J}_h} (\underline{D} 1) \cdot \underline{u} h^3 = 0$$

We still have to prove that $\underline{u} = \underline{D} \varphi$.
To show this, consider $\underline{u} - \underline{D} \varphi$. We have

$$(36) \quad \underline{D} \cdot (\underline{u} - \underline{D} \varphi) = 0$$

directly from (34), and

$$(37) \quad \underline{D} \times (\underline{u} - \underline{D} \varphi) = \underline{D} \times \underline{u} = 0$$

by hypothesis. It follows from the lemma (26), then, that

$$(38) \quad \underline{u} - \underline{D} \varphi = \text{constant}$$

This constant must be zero, however, since \underline{u} satisfies (16) by hypothesis, and also

$$(39) \quad \sum_{\underline{x} \in \mathcal{G}_h} D_i \varphi h^3 = - \sum_{\underline{x} \in \mathcal{G}_h} (D_i 1) \varphi h^3 = 0$$

This completes the proof of (17).

The proof of (18) is similar. We choose \underline{a} as any solution of

$$(40) \quad -D_j^2 \underline{a} = \underline{D} \times \underline{u}$$

Such \underline{a} exist because

$$(41) \quad \sum_{\underline{x} \in \mathcal{G}_h} (\underline{D} \times \underline{u})_i = \varepsilon_{ijk} \sum_{\underline{x} \in \mathcal{G}_h} 1 \cdot D_j u_k h^3 \\ = - \varepsilon_{ijk} \sum_{\underline{x} \in \mathcal{G}_h} (D_j 1) u_k h^3 = 0$$

Notice, too, that

$$(42) \quad -\underline{D}_j^2 (\underline{D} \cdot \underline{a}) = \underline{D} \cdot (\underline{D} \times \underline{u}) = 0$$

We have seen previously that the null space of \underline{D}_j^2 contains only the constants, so it follows from 42 that

$$(43) \quad \underline{D} (\underline{D} \cdot \underline{a}) = 0$$

This tells us that (40) can be rewritten as

$$(44) \quad \underline{D} \times (\underline{D} \times \underline{a}) = \underline{D} \times \underline{u}$$

or

$$(45) \quad \underline{D} \times (\underline{D} \times \underline{a} - \underline{u}) = 0$$

But we also have

$$(46) \quad \underline{D} \cdot (\underline{D} \times \underline{a} - \underline{u}) = 0$$

since $\underline{D} \cdot (\underline{D} \times \underline{a}) = 0$ for any \underline{a} , and since $\underline{D} \cdot \underline{u} = 0$ by hypothesis. From (45-46) and lemma (26), it follows that

$$(47) \quad \underline{D} \times \underline{a} - \underline{u} = \text{constant}$$

The constant must be zero, however, since $\underline{D} \times \underline{a}$ has zero sum for any \underline{a} , and \underline{u} has zero sum

by hypothesis. This completes the proof of (18).

We are now ready to state the proposed velocity interpolation scheme. Suppose we are given $\underline{u}(\underline{x})$ such that $\underline{D} \cdot \underline{u} = 0$. Let

$$(48) \quad \underline{u}_0 = \frac{1}{V} \sum_{\underline{x} \in \mathcal{T}_h} \underline{u}(\underline{x}) h^3$$

where

$$(49) \quad V = \sum_{\underline{x} \in \mathcal{T}_h} h^3$$

is the volume of the domain. Thus \underline{u}_0 is the mean of \underline{u} . We have shown above that $\exists \underline{a}$ such that

$$(50) \quad \underline{u} - \underline{u}_0 = \underline{D} \times \underline{a}$$

$$(51) \quad 0 = \underline{D} \cdot \underline{a}$$

and that such an \underline{a} can be found by

solving the (vector) Poisson problem

$$(52) \quad -(\underline{D} \cdot \underline{D}) \underline{a} = \underline{D} \times \underline{u}$$

The next step is to interpolate \underline{a} to get

$$(53) \quad \underline{A}(\underline{X}) = \sum_{\underline{x} \in \mathcal{S}_h} \underline{a}(\underline{x}) \delta_h(\underline{x} - \underline{X}) h^3$$

Next, we evaluate the curl of \underline{A} with respect to the continuous variable \underline{X} :

$$(54) \quad (\nabla \times \underline{A})_i(\underline{X}) = \varepsilon_{ijk} \frac{\partial}{\partial X_j} \sum_{\underline{x} \in \mathcal{S}_h} a_k(\underline{x}) \delta_h(\underline{x} - \underline{X}) h^3$$

$$= - \varepsilon_{ijk} \sum_{\underline{x} \in \mathcal{S}_h} a_k(\underline{x}) \frac{\partial \delta_h(\underline{x} - \underline{X})}{\partial x_j} h^3$$

$$= + \varepsilon_{ikj} \sum_{\underline{x} \in \mathcal{S}_h} a_k(\underline{x}) \frac{\partial \delta_h(\underline{x} - \underline{X})}{\partial x_j} h^3$$

$$= \left(\sum_{\underline{x} \in \mathcal{S}_h} \underline{a}(\underline{x}) \times (\nabla \delta_h)(\underline{x} - \underline{X}) h^3 \right)_i$$

The last step is to set

$$(55) \quad \underline{U}(\underline{X}) = \underline{u}_0 + (\nabla \times \underline{A})(\underline{X})$$

$$= \underline{u}_0 + \sum_{\underline{X} \in \mathcal{J}_h} \underline{a}(\underline{x}) \times (\nabla d_h)(\underline{x} - \underline{X}) h^3$$

This completes the statement of the interpolation scheme. To complete the design of this new IB method, we now need a force-spreading scheme that is adjoint to the velocity-interpolation scheme. Suppose we have a collection of Lagrangian points

$$(56) \quad \{ \underline{X}_n, n=1, 2, \dots, N \}$$

$$(57) \quad \text{Let } \underline{U}_n = \underline{U}(\underline{X}_n)$$

and let \underline{F}_n be the force (not force density) which is applied to the fluid by the Lagrangian point at \underline{X}_n . We seek a

grid function $\underline{f}(\underline{x})$ such that

$$(58) \quad \sum_{\underline{x} \in \mathcal{J}_h} \underline{u}(\underline{x}) \cdot \underline{f}(\underline{x}) h^3 = \sum_{n=1}^N \underline{U}_n \cdot \underline{F}_n$$

In this equation, it is understood that $\underline{u}(\underline{x})$ and \underline{U}_n are related as described above but otherwise arbitrary.

Since $\underline{D} \cdot \underline{u} = 0$, we do not expect $\underline{f}(\underline{x})$ to be uniquely determined by (58) alone. In fact, given an $\underline{f}(\underline{x})$ that satisfies (58), we can get another such $\underline{f}(\underline{x})$ by adding a discrete gradient to $\underline{f}(\underline{x})$.

To see what (58) implies about $\underline{f}(\underline{x})$, we rewrite both sides in terms of $\underline{a}(\underline{x})$. On the left-hand side, we have

$$(59) \quad \sum_{\underline{x} \in \mathcal{J}_h} \underline{u}(\underline{x}) \cdot \underline{f}(\underline{x}) h^3 \\ = \underline{u}_0 \cdot \sum_{\underline{x} \in \mathcal{J}_h} \underline{f}(\underline{x}) h^3 + \sum_{\underline{x} \in \mathcal{J}_h} (\underline{D} \times \underline{a})(\underline{x}) \cdot \underline{f}(\underline{x}) h^3$$

$$= \underline{u}_0 \cdot \underline{f}_0 V + \sum_{\underline{x} \in \mathcal{G}_h} \underline{a}(\underline{x}) \cdot (\underline{D} \times \underline{f})(\underline{x}) h^3$$

where

$$(60) \quad \underline{f}_0 = \frac{1}{V} \sum_{\underline{x} \in \mathcal{G}_h} \underline{f}(\underline{x}) h^3$$

Meanwhile, on the right-hand side of (58), we have

$$(61) \quad \sum_{n=1}^N \underline{U}_n \cdot \underline{F}_n =$$

$$\underline{u}_0 \cdot \sum_{n=1}^N \underline{F}_n + \sum_{n=1}^N \sum_{\underline{x} \in \mathcal{G}_h} \underline{a}(\underline{x}) \times (\nabla \hat{d}_h)(\underline{x} - \underline{X}_n) \cdot \underline{F}_n h^3$$

$$= \underline{u}_0 \cdot \sum_{n=1}^N \underline{F}_n + \sum_{\underline{x} \in \mathcal{G}_h} \underline{a}(\underline{x}) \cdot \sum_{n=1}^N (\nabla \hat{d}_h)(\underline{x} - \underline{X}_n) \times \underline{F}_n h^3$$

Now \underline{u}_0 and $\underline{a}(\underline{x})$ are arbitrary, except that $\underline{D} \cdot \underline{a} = 0$. Thus, comparison of (59) and (61) shows that (58) will be satisfied if and only if

$$(62) \quad \underline{f}_0 = \frac{1}{V} \sum_{n=1}^N \underline{F}_n$$

and

$$(63) \quad \underline{D} \times \underline{f} = \sum_{n=1}^N (\nabla \phi_h^n)(\underline{x} - \underline{X}_n) \times \underline{F}_n + \underline{D} \phi$$

We have the freedom to add the term $\underline{D} \phi$ because

$$(64) \quad \sum_{\underline{x} \in \mathcal{S}_h} (\underline{a}(\underline{x}) \cdot \underline{D} \phi) h^3 = - \sum_{\underline{x} \in \mathcal{S}_h} (\underline{D} \cdot \underline{a})(\underline{x}) \phi(\underline{x}) h^3 = 0$$

and we are required to include such a term since the left-hand side of (63) is discretely divergence-free but there is no reason to expect that the first term on the right-hand side will be discretely divergence free. It would be

straightforward to solve for ϕ by taking the discrete divergence of both sides of (63) and solving the resulting Poisson equation for ϕ . We will not actually do this, however, since our next step is to eliminate ϕ by taking the discrete curl of both sides of (63) to obtain

$$(65) \quad \underline{D} \times (\underline{D} \times \underline{f}) = \underline{D} \times \left(\sum_{n=1}^N (\nabla d_h^n) (\underline{x} - \underline{X}_n) \times \underline{F}_n \right)$$

Also, we make \underline{f} unique by imposing

$$(66) \quad \underline{D} \cdot \underline{f} = 0$$

Because of (66), equation (65) reduces to the vector Poisson equation

$$(67) \quad -(\underline{D} \cdot \underline{D}) \underline{f} = \underline{D} \times \left(\sum_{n=1}^N (\nabla d_h^n) (\underline{x} - \underline{X}_n) \times \underline{F}_n \right)$$

This determines \underline{f} up to an arbitrary constant, and that constant is determined by equations (60) and (62), which may be combined to yield

$$(68) \quad \sum_{\underline{x} \in \mathcal{J}_h} \underline{f}(\underline{x}) h^3 = \sum_{n=1}^N \underline{F}_n$$

This is simply the statement that the total Eulerian force (integral of the force density) and the total Lagrangian force should agree.

Finally, we note that the right-hand side of (67) can be simplified by writing it in components. We have

$$\begin{aligned} & \left(\underline{D} \times \left(\sum_{n=1}^N (\nabla d_h) (\underline{x} - \underline{X}_n) \times \underline{F}_n \right) \right)_i \\ &= \epsilon_{ijk} D_j \sum_{n=1}^N \epsilon_{klm} \frac{\partial d_h}{\partial x_l} (\underline{x} - \underline{X}_n) F_{n,m} \\ &= (d_{il} d_{jm} - d_{im} d_{jl}) \sum_{n=1}^N \left(D_j \frac{\partial d_h}{\partial x_l} \right) (\underline{x} - \underline{X}_n) F_{n,m} \\ &= \sum_{n=1}^N \left(D_j \frac{\partial d_h}{\partial x_i} \right) (\underline{x} - \underline{X}_n) F_{n,j} - \left(D_j \frac{\partial d_h}{\partial x_j} \right) (\underline{x} - \underline{X}_n) F_{n,i} \\ &= \sum_{n=1}^N C_{ij} (\underline{x} - \underline{X}_n) F_{n,j} \end{aligned}$$

where

$$(69) \quad C_{ij} = D_j \frac{\partial d_h}{\partial x_i} - \delta_{ij} \underline{D} \cdot \nabla d_h$$

A remarkable feature of the above scheme is that it calculates an $\underline{f}(\underline{x})$ which is discretely divergence-free. That is, $\underline{f}(\underline{x})$ includes the pressure gradient that is generated by the Laprasim forces, and I don't see any way to separate this pressure gradient (or the associated pressure) from \underline{f} in case it is needed for output purposes. This may be an important advantage of the scheme from the standpoint of accuracy, since it means that jumps in pressure across surfaces do not require any explicit representation. (Thanks to Griffith for pointing this out.)

In summary, we have the following two procedures:

Interpolation

Given a grid function $\underline{u}(\underline{x})$, solve the vector Poisson equation

such that $\underline{D} \cdot \underline{u} = 0$

$$(70) \quad -(\underline{D} \cdot \underline{D}) \underline{a} = \underline{D} \times \underline{u}$$

for the grid function $\underline{a}(\underline{x})$. Then, for any \underline{X} , let

$$(71) \quad \underline{U}(\underline{X}) = \sum_{\underline{x} \in \mathcal{G}_h} \left(\frac{1}{V} \underline{u}(\underline{x}) + \left(\underline{a}(\underline{x}) \times \nabla_{\mathcal{G}_h} (\underline{x} - \underline{X}) \right) \right) h^3$$

where

$$(72) \quad V = \sum_{\underline{x} \in \mathcal{G}_h} h^3 = \text{volume of domain}$$

(An arbitrary constant vector can be added to any solution $\underline{a}(\underline{x})$ of (70), but it makes no difference. Do you see why?)

Force Spreading

Given forces \underline{F}_n applied to the fluid at locations \underline{X}_n , let $\underline{f}(\underline{x})$ be the solution of the vector Poisson equation

$$(73) \quad -(\underline{D} \cdot \underline{D}) \underline{f} = \underline{D} \times \sum_{n=1}^N \left((\nabla_{\underline{D}_h}^{\wedge}) (\underline{x} - \underline{X}_n) \times \underline{F}_n \right)$$

with the arbitrary constant in the solution determined by

$$(74) \quad \sum_{\underline{x} \in \mathcal{S}_h} \underline{f}(\underline{x}) h^3 = \sum_{n=1}^N \underline{F}_n$$

As a check, we should show that

$$(75) \quad \sum_{n=1}^N \underline{F}_n \cdot \underline{U}(\underline{X}_n) = \sum_{\underline{x} \in \mathcal{I}_h} \underline{u}(\underline{x}) \cdot \underline{f}(\underline{x}) h^3$$

To prove this, we first recall that

$$(70) \Rightarrow \underline{D} \cdot \underline{a} = 0, \text{ and that } (73) \Rightarrow \underline{D} \cdot \underline{f} = 0$$

Because of this, (70) and (73) can be rewritten

$$(76) \quad \underline{D} \times (\underline{D} \times \underline{a}) = \underline{D} \times \underline{a}$$

$$(77) \quad \underline{D} \times (\underline{D} \times \underline{f}) = \underline{D} \times \sum_{n=1}^N \left((\nabla \underline{d}_h^n) (\underline{x} - \underline{X}_n) \times \underline{F}_n \right)$$

or

$$(78) \quad \underline{D} \times (\underline{D} \times \underline{a} - \underline{u}) = 0$$

$$(79) \quad \underline{D} \times \left(\underline{D} \times \underline{f} - \sum_{n=1}^N (\nabla \delta_h) (\underline{x} - \underline{X}_n) \times \underline{F}_n \right) = 0$$

Besides (78), we also have

$$(80) \quad \underline{D} \cdot (\underline{D} \times \underline{a} - \underline{u}) = 0,$$

and (78) & (80) \Rightarrow

$$(81) \quad \underline{u} = \underline{u}_0 + \underline{D} \times \underline{a}$$

where \underline{u}_0 is a constant vector, and this constant must be equal to the mean of $\underline{u}(\underline{x})$, since the mean of $(\underline{D} \times \underline{a})(\underline{x})$ is zero.

In (79), the vector for which the discrete curl is zero also has mean zero (why?), and it follows that

$$(82) \quad \underline{D} \times \underline{f} = \sum_{n=1}^N (\nabla \delta_h)(\underline{x} - \underline{X}_n) \times \underline{F}_n + \underline{D} \phi$$

for some scalar grid function $\phi(\underline{x})$.

We now have everything we need to show that the left-hand side of (75) is equal to the right-hand side:

$$\begin{aligned}
 (83) \quad & \sum_{n=1}^N \underline{F}_n \cdot \underline{U}(\underline{X}_n) \\
 &= \sum_{n=1}^N \underline{F}_n \cdot \sum_{\underline{x} \in \mathcal{G}_h} \left(\frac{1}{V} \underline{u}(\underline{x}) + (\underline{a}(\underline{x}) \times (\nabla \delta_h)(\underline{x} - \underline{X}_n)) \right) h^3 \\
 &= \underline{u}_0 \cdot \sum_{n=1}^N \underline{F}_n + \sum_{\underline{x} \in \mathcal{G}_h} \underline{a}(\underline{x}) \cdot \left(\sum_{n=1}^N (\nabla \delta_h)(\underline{x} - \underline{X}_n) \times \underline{F}_n \right) h^3
 \end{aligned}$$

$$= \underline{u}_0 \cdot \sum_{n=1}^N \underline{F}_n + \sum_{\underline{x} \in \mathcal{I}_h} \underline{a}(\underline{x}) \cdot (\underline{D} \times \underline{f} - \underline{D} \phi)(\underline{x}) h^3$$

$$= \underline{u}_0 \cdot \sum_{n=1}^N \underline{F}_n + \sum_{\underline{x} \in \mathcal{I}_h} (\underline{D} \times \underline{a})(\underline{x}) \cdot \underline{f}(\underline{x}) h^3$$

~~$$+ \sum_{\underline{x} \in \mathcal{I}_h} (\underline{D} \cdot \underline{a})(\underline{x}) \phi(\underline{x}) h^3$$~~

~~$$= \underline{u}_0 \cdot \sum_{n=1}^N \underline{F}_n + \sum_{\underline{x} \in \mathcal{I}_h} (\underline{u}(\underline{x}) - \underline{u}_0) \cdot \underline{f}(\underline{x}) h^3$$~~

See (74)

$$= \sum_{\underline{x} \in \mathcal{I}_h} \underline{u}(\underline{x}) \cdot \underline{f}(\underline{x}) h^3$$

as required.

A numerical scheme that makes use of the above interpolation and force spreading procedures is as follows.

Let superscript m be a time-step index. We are given

$$(84) \quad \begin{cases} \underline{u}^m(\underline{x}), \quad \underline{x} \in \mathcal{G}_h & \text{with } \underline{D} \cdot \underline{u}^m = 0 \\ \underline{x}_n^m, \quad n=1, 2, \dots, N \end{cases}$$

The first step is to evaluate $\underline{a}^m(\underline{x})$ by solving

$$(85) \quad -(\underline{D} \cdot \underline{D}) \underline{a}^m = \underline{D} \times \underline{u}^m$$

Then we have the function:

$$(86) \quad \underline{u}^m(\underline{X}) = \sum_{\underline{x}' \in \mathcal{G}_h} \left(\frac{1}{V} \underline{u}^m(\underline{x}') + \left(\underline{a}^m(\underline{x}') \times \nabla \delta_h(\underline{x}' - \underline{X}) \right) \right) h^3$$

We write \underline{x}' here since later it will be useful to set $\underline{X} = \underline{x}$.

Next, we evaluate

$$(87) \quad \underline{X}_n^{m+1/2} = \underline{X}_n^m + \frac{\Delta t}{2} \underline{U}^m \left(\underline{X}_n^m \right)$$

$$(88) \quad \underline{F}_n^{m+1/2} = - \frac{\partial E}{\partial \underline{X}_n} \left(\dots \underline{X}_{n'}^{m+1/2} \dots \right)$$

Remark: If E is translation-invariant,

then $\sum_{n=1}^N \underline{F}_n^{m+1/2} = 0$, but we do

not assume that here.

Now we apply the force-spreading procedure by solving the following equations for $\underline{f}^{m+1/2}(\underline{x})$:

$$(89) \quad -\underline{D} \cdot \underline{D} \underline{f}^{m+1/2} =$$

$$\underline{D} \times \sum_{n=1}^N (\nabla \underline{d}_h) (\underline{x} - \underline{X}_n) \times \underline{F}^{m+1/2}$$

with

$$(90) \quad \sum_{\underline{x} \in \mathcal{G}_h} \underline{f}^{m+1/2}(\underline{x}) h^3 = \sum_{n=1}^N \underline{F}_n^{m+1/2}$$

The next step is to update the fluid velocity to the middle of the time step by solving the following system

$$(91) \left\{ \begin{aligned} & \rho \left(\frac{\underline{u}^{m+1/2} - \underline{u}^m}{(\Delta t/2)} + S(\underline{v}^m) \underline{u}^m \right) + \underline{D} \tilde{p}^{m+1/2} \\ & = \mu (\underline{D} \cdot \underline{D}) \underline{u}^{m+1/2} + \underline{f}^{m+1/2} \\ & \underline{D} \cdot \underline{u}^{m+1/2} = 0 \end{aligned} \right.$$

Here \underline{v}^m is the grid function defined by evaluating the interpolated velocity field at grid points

$$(92) \quad \underline{v}^m(\underline{x}) = \underline{U}^m(\underline{x}) \\ = \sum_{\underline{x}' \in g_h} \left(\frac{1}{V} \underline{u}(\underline{x}') + (\underline{a}(\underline{x}') \times (\nabla \phi_h)(\underline{x}' - \underline{x})) \right) h^3$$

Note that all components of \underline{v} are defined whenever any one component of \underline{u} is defined. (or anywhere else, but we use it at those locations)

The expression $S(\underline{v})\underline{u}$ is defined by

$$(93) \quad (S(\underline{v})\underline{u})_i = S(\underline{v})u_i$$

$$(94) \quad S(\underline{v})\phi = \frac{1}{2} v_j D_j^{(2)} \phi \\ + \frac{1}{2} D_j^{(2)} (v_j \phi)$$

where

$$(95) \quad (D_j^{(2)} \phi)(\underline{x}) = \frac{\phi(\underline{x} + h \underline{e}_j) - \phi(\underline{x} - h \underline{e}_j)}{2h}$$

With $\underline{u}^{m+1/2}$ defined, we repeat the interpolation procedure, so that $\underline{a}^{m+1/2}$ is defined by solving

$$(96) \quad -(\underline{D} \cdot \underline{D}) \underline{a}^{m+1/2} = \underline{D} \times \underline{u}^{m+1/2}$$

and then we have the function

$$(97) \quad \underline{U}^{m+1/2}(\underline{X}) = \sum_{\substack{\underline{x}' \in \mathcal{G}_h \\ \underline{V}}} \left(\frac{1}{V} \underline{u}^{m+1/2}(\underline{x}') + \left(\underline{a}^{m+1/2}(\underline{x}') \times (\nabla \hat{d}_h)(\underline{x}' - \underline{X}) \right) \right) h^3$$

This function is used in the update of \underline{X}_n and also to define the grid function

$$\underline{v}^{m+1/2}(\underline{x}) = \underline{U}^{m+1/2}(\underline{x}).$$

The time step is then completed by

solving the system

$$(98) \left\{ \begin{aligned} & P \left(\frac{\underline{u}^{m+1} - \underline{u}^m}{\Delta t} + S(\underline{v}^{m+1/2}) \underline{u}^{m+1/2} \right) + \underline{D} p^{m+1/2} \\ &= \frac{\underline{u}}{2} (\underline{D} \cdot \underline{D}) (\underline{u}^{m+1} + \underline{u}^m) + \underline{f}^{m+1/2} \\ &\underline{D} \cdot \underline{u}^{m+1} = 0 \end{aligned} \right.$$

and by evaluating

$$(99) \quad \underline{x}_n^{m+1} = \underline{x}_n^m + (\Delta t) \underline{v}^{m+1/2} \left(\underline{x}_n^{m+1/2} \right)$$

for $n = 1 \dots N$

It remains to discuss how to solve the linear systems (91) & (98). This is complicated by the staggered grid. It is possible to define a discrete Fourier transform for the staggered grid, and then to solve for all components of \underline{u} and p simultaneously. It is simpler, however, to exploit the fact that each component of \underline{u} , and also p , lives on a standard Cartesian grid. These grids are simply shifted relative to each other.

With this in mind, we solve for p first, and then with p known we solve separately for each component of \underline{u} .

To get the equation for p , we apply $\underline{D} \cdot$ in the momentum equation of (91) or (98), and in each case we get an equation of the form

$$(100) \quad -(\underline{D} \cdot \underline{D}) p = \rho \underline{D} \cdot (S(v) \underline{u})$$

in which the right hand side is known.

The right-hand side of (100) does not involve \underline{f} because $\underline{D} \cdot \underline{f} = 0$ in the special IB method under consideration here. The above numerical scheme, however, is also applicable to the standard IB method on a staggered grid, and in that case there would be an additional term

$$(101) \quad - \frac{\Delta t}{\rho} \underline{D} \cdot \underline{f}$$

on the right-hand side of (100).

Note that the operator $\underline{D} \cdot \underline{D}$ is the standard discrete Laplacian

$$(102) \quad (\underline{D} \cdot \underline{D} \phi)(\underline{x}) = \sum_{j=1}^3 \frac{\phi(\underline{x} + h \underline{e}_j) - 2\phi(\underline{x}) + \phi(\underline{x} - h \underline{e}_j)}{h^2}$$

So equation (100) can be solved for ψ by discrete Fourier transform in the standard way.

Note that the same operator $-\underline{D} \cdot \underline{D}$ appears in the equations that need to be solved for velocity interpolation (70) and force spreading (73). In those cases, the operator is applied to each component separately, and the components live on different grids.

In equation (100), the unknown ψ lives on the grid of cell centers. In equation (70), the unknown a_i lives on the grid of edge centers for those cell edges that are parallel to the i th coordinate direction. In equation (73), the unknown f_i lives on the grid of face centers of those cell faces that are normal to the i th coordinate direction. Each of these grids considered separately is a regular cubic lattice, and they all have the same meshwidth h .

After solving for \hat{p} in Fourier space, we come back to the physical space by an inverse discrete Fourier transform, and then we can evaluate $\underline{D}p$.

With $\underline{D}p$ known, the momentum equations in (91) & (98) decouple into separate equations for each of the three spatial components. In both cases, we get equations of the form

$$(103) \quad \left(\underline{I} - \frac{\Delta t}{2} \frac{\mu}{\rho} (\underline{D} \cdot \underline{D}) \right) \underline{u} = \underline{W}$$

with each spatial component on its own regular cartesian grid, and these equations can again be solved by discrete Fourier transform.