Rigid structure coupling to fluctuating hydrodynamics.

Assume we have a rigid structure composed of $N$ particles / marker points.

Let the velocity of the geometric center of the structure

$$\mathbf{q}_0 = \frac{1}{N} \sum_{i=1}^{N} \mathbf{q}_i$$

be $\dot{\mathbf{q}}_0 = \mathbf{U}$

and the angular velocity of the structure around $\mathbf{q}_0$ be $\mathbf{\Omega}$.

The velocity of each marker obeys the no-slip condition

$$\dot{\mathbf{q}}_i = \mathbf{U}_i = \mathbf{U} + \mathbf{\Omega} \times (\mathbf{q}_i - \mathbf{q}_0)$$

$$\dot{\mathbf{q}}_i = \mathbf{J}_i \cdot \mathbf{v}(r,t) = S_i \cdot \mathbf{v}(r,t)$$

where $\mathbf{v}(r,t)$ is the velocity field of the fluid.
and \( J_i = J(q_i) \) is a local averaging/interpolation operator, while \( S_i = S(q_i) \) is a local spreading operator. The two are adjoints, \( J_i^* = S_i \) and \( S_i^* = J_i \).

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**Kinematics**

For notational simplicity, let us group

\[
W = \begin{bmatrix} U & J \end{bmatrix}
\]

into one vector in \( \mathbb{R}^6 \)

and define the matrix

\[
T_i = \begin{bmatrix} I \\ \Delta Q \end{bmatrix}
\]

\[
= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & \Delta q_i^x & -\Delta q_i^y & \Delta q_i^z \\ \Delta q_i^y & \Delta q_i^z & -\Delta q_i^x & 0 \\ \end{bmatrix}
\]

\( T_i \in \mathbb{R}^{6 \times 3} \)
where $\Delta q_i = q_i - q_0$ is the position of particle $i$ relative to the center.

With the help of this matrix, we can write the no-slip constraint very simply as:

\[
(*) \quad U = \begin{bmatrix}
    u_1 \\
    u_2 \\
    \vdots \\
    u_N
\end{bmatrix} = T^* W
\]

where

\[
T = \begin{bmatrix}
    T_1 & T_2 & \cdots & T_N
\end{bmatrix}
\]

so that $(*)$ is equivalent to the system $U_i = T_i^* W$.
Let an external force $F_i$ be applied to each particle, and let the total force on particle $i$ due to the rigidity forces and fluid forces be $\lambda_i$ (a Lagrange multiplier).

Then, we have that the total force/torque on the structure is zero:

$$\sum_i \lambda_i = \sum_i F_i$$

$$\sum_i \Delta q_i \times \lambda_i = \sum_i \Delta q_i \times F_i$$

This can be written in matrix form as

$$\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_N \end{bmatrix} = T \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_N \end{bmatrix}$$

where $\lambda = \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_N \end{bmatrix}$ and $F = \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_N \end{bmatrix}$.
This is because
\[ \Delta q_i F_i = \Delta q_i \times F_i = -\Delta q_i F_i \]
so the same cross-product matrix \( \Delta q_i \) appears in both statics and kinematics.

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**Fluid equations**

The fluid equation is
\[ \sum \mathbf{ \Psi} = -\nabla \Pi - \nu \mathbf{ \nabla} \cdot \mathbf{ \psi} + \sum_{i=1}^{N} S_i \lambda_i \\
= -\nabla \Pi - \eta \nabla^2 \psi + S \lambda \\
+ \text{thermal forces} \]

where
\[ S = \begin{bmatrix} S_1 & S_2 & \cdots & S_N \end{bmatrix} \]
is a composite spreading operator.
Complete equations

The equations of motion for the coupled fluid-structure system is:

\[ \nabla \cdot \mathbf{u} = 0 \]

\[ \frac{\partial}{\partial t} \mathbf{u} + \nabla \mathbf{F} = \nu \Delta \mathbf{u} + \mathbf{f} \]

\[ \mathbf{q} = \mathbf{S}\cdot \mathbf{u} \quad \text{(no slip)} \]

\[ \mathbf{T}_\lambda = \mathbf{T}_F \quad \text{(force free)} \]

\[ S\cdot \mathbf{u} = T\cdot \mathbf{w} \quad \text{(rigidity)} \]

where we recall that \( S, T, \) and \( F \) depend on \( \mathbf{q} \).

In this formulation, \( \lambda \) is the Lagrange multiplier for the rigidity constraint, and \( \mathbf{w} \) is the Lagrange multiplier for the force and torque-free constraint, and \( T \) is the multiplier for divergence-free
An implicit second-order discretization for these equations is the following algorithm:

\[ \frac{q_{n+1} - q_n}{\Delta t} + \nabla \cdot \mathbf{U} = 0 \]

1. Move the structure to midpoint

\[ q_{n+\frac{1}{2}} = q_n + \frac{\mathbf{U} \Delta t}{2} + R^m \left( \frac{\Delta t}{2} \right) (q_n - q_0) \]

where \( R^m(\theta) \) is a rotation matrix with angular rotation \( \mathbf{R}^n \Delta t \), where

\[ \mathbf{R}^n = \begin{bmatrix} \mathbf{U}^n \\ \mathbf{J}^n \end{bmatrix} \]

This simply means move and rotate to midpoint.
Then, evaluate forces at $g^{n+1/2}$

2. Now solve the fluid problem with constraints

$$S \frac{u^{n+1} - u^n}{\Delta t} + \nabla \cdot \mathbf{u}^{n+1/2} = \frac{1}{\Delta t} \left( \frac{1}{2} (u^{n} + u^{n+1}) \right)$$

$$+ S^{n+1/2} \lambda^{n+1/2} + \text{thermal}$$

where $L$ is the Laplacian

3. $(S^*)^{u^{n+1}} = (T^*)^{n+1/2} u^{n+1}$

Note: This is not second-order but we can try to fix it later

4. $T^{n+1/2} \lambda^{n+1/2} = T^{n+1/2} F^{n+1/2}$

5. $\nabla \cdot \mathbf{u}^{n+1} = 0$
2) Finally, move the structure again with linear velocity and angular velocity at midpoint:

\[ \omega^{n+1/2} = \frac{1}{2} (\omega^n + \omega^{n+1}) \]

\[ q^{n+1} = q_0 + U^{n+1/2} \Delta t + R^{n+1/2} (\Delta t)(q - q_0) \]

Note that even if one wants only first-order accuracy to be robust in the Brownian or overdamped limit the fluid solver has to be implicit (Backward Euler) so the same fluid solver is needed.

Therefore, now I focus entirely on the fluid solver.
Fluid Solver

In matrix notation, the fluid solver we need is to solve the linear system:

\[
\begin{bmatrix}
\frac{3}{4}I - \frac{\nu}{2}D & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
U^{n+1/2} \\
V^{n+1/2} \\
W^{n+1} \\
\end{bmatrix}
= \begin{bmatrix}
f^{n+1/2} \\
0 \\
0 \\
0 \\
\end{bmatrix}
\]

everything evaluated at \( n+1/2 \)

Here \( D \) is discrete divergence

\( G \) is discrete gradient

\( D^* = -G \) so the system is symmetric
How do we solve this system?

The right approach is to use an iterative preconditioned solver.

As a preconditioner, we can use the procedure Amreit is using now.

Let me summarize this procedure in my notation:

\[ \text{Amreit's approximation} \]

1. First, solve the fluid ignoring the terms with \( \lambda_1 \):

\[
\begin{bmatrix}
\frac{3 I}{A} & -\frac{1}{2} & 0 \\
-\frac{1}{2} & \lambda_1 & 0 \\
0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
x_{n+1} \\
x_{n+1/2} \\
0
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
0 \\
0
\end{bmatrix}
\]

Kee Boyce has already developed a solver for this in IBM MKR.
Now, obtain $\tilde{w}^{n+1}$ from:

$$S^{*} \tilde{w}^{n+1} = T^{*} \tilde{w}^{n+1}$$

This is an overdetermined system for more than two markers, so we solve it in the least-squares sense, by multiplying both sides by $T^{*}$:

$$T S^{*} \tilde{w}^{n+1} = (T T^{*}) \tilde{w}^{n+1}$$

$$\Rightarrow \tilde{w}^{n+1} = (T T^{*})^{-1} T S^{*} \tilde{w}^{n+1}$$

To see that this is the same as what Am neet does, observe that:

$$T T^{*} = \begin{bmatrix} N I & \Sigma \Delta Q_{i}^{*} \\ \Sigma \Delta Q_{i} & \Sigma \Delta Q \Delta Q^{*} \end{bmatrix}$$
But, from our definition of \( \Delta q_i \), we have

\[
\sum \Delta q_i = 0 = \sum \Delta q_i^*
\]

because \( q_0 \) is the geometric center, \( q_0 = \frac{1}{N} \sum q_i \).

Also, observe that

\[
\sum_{i=1}^{N} \Delta q_i \Delta q_i^* = \sum_{i=1}^{N} \begin{bmatrix}
\Delta q_i^2 + \Delta q_i^2 \\
-\Delta q_i \Delta q_i^* \\
-\Delta q_i \Delta q_i^* \\
\end{bmatrix}
\]

which is exactly the moment of inertia that Amreet is using!

So we have:

\[
\begin{bmatrix}
N & I \\
0 & J
\end{bmatrix}
\]
where $J$ is the moment of inertia of the structure.

Therefore we get

$$\mathbf{U} = \frac{1}{N} \sum_{i=1}^{N+1} S_i \mathbf{U}$$

which is a simple arithmetic average, and

$$\mathbf{S} = J^{-1} \sum_{i=1}^{N+1} \Delta q_i \mathbf{U}$$

which is what Amnest is doing now.

Notice that we can add volume to each marker by using weighted least squares to solve

$$\mathbf{S} = \mathbf{T} \mathbf{W}$$
The next step is to set
\[ \lambda^{n+1/2} = \frac{\delta}{\Delta t} \left( T^* w^{n+1} - S^* u^{n+1} \right) \]
(this is for the case \( F = 0 \), which is what Ammeet did)

Now resolve the fluid equation
\[
\begin{align*}
S \frac{u^{n+1} - u^n}{\Delta t} &= S \lambda^{n+1/2} \\
\n\end{align*}
\]
\[ v^{n+1} = 0 \]

I believe Ammeet sets
\[ w^{n+1} = \tilde{w}^{n+1} \]
i.e. there is no correction to obtain an improved \( w^{n+1} \) from \( \tilde{u}^{n+1} \) (Why not?)
Let's see how good of an approximation Ammeet's solution is:

First, check

\[ T \lambda = \frac{\dot{q}}{\Delta t} \left( T T^* \dot{w}^{n+1} - T S^* \omega \right) \]

\[ = 0 \quad \text{by definition of } \dot{w}^{n+1} \]

So the force and torque free constraint is obeyed.

Now, the real difficulty is whether no-slip is obeyed

\[ S^* \dot{w}^{n+1} = I^* w = I^* w \]

If we do the calculation, we get

\[ S^* \dot{w}^{n+1} = S^* \dot{w}^{n+1} + (S^* S)^T (T T^*)^{-1} S^* \omega^{n+4} \]

\[ = \left[ -S S^* I + (S^* S)^T (T T^*)^{-1} \right] S^* \omega^{n+1} \]
We want this to be equal to
\[ T^* W = T^* (TT^*)^{-1} S^* \sim^{n+1} \]
that is, we want
\[ (I - S^* S) + (S^* S) T^* (TT^*)^{-1} T = T(TT^*)^{-1} \]
The only way this is true in general is if
\[ S^* S = I \]
which is NOT true for the Peshin operator $S$ (but maybe it is if the number of marker points goes to infinity?!!)
For our particle marker
\[ S S S = 8 I \]