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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

$$q_0 = \frac{1}{N} \sum_{i=1}^{N} q_i \leftarrow \text{positions of markers}$$

be $\dot{q}_0 = U$

and the angular velocity of the structure around q_0 be Ω.

The velocity of each marker obeys the no-slip condition

$$\dot{q}_i = u_i = U + \Omega \times (q_i - q_0)$$

$$\dot{q}_i = J_i\, v(r,t) = S_i^{*}\, v(r,t)$$

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

$$J_i^* = S_i \quad \text{and} \quad S_i^* = J_i$$

Kinematics

For notational simplicity, let us group

$$W = \begin{bmatrix} U \\ \Omega \end{bmatrix}$$

into one vector in $\mathbb{R}^6$

and define the matrix

$$T_i = \begin{bmatrix} I \\ \hline \Delta Q \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \hline 0 & \Delta q_z^i & -\Delta q_y^i \\ -\Delta q_z^i & 0 & \Delta q_x^i \\ \Delta q_y^i & -\Delta q_x^i & 0 \end{bmatrix}$$

$$T_i \in \mathbb{R}^{6\times 3}$$

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:

$$(*) \quad u = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{bmatrix} = T^* \omega$$

where

$$T = \left[T_1 \mid T_2 \mid \dots \mid T_N \right]$$

so that $(*)$ is equivalent to the system $u_i = T_i^* \omega$

Statics

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 λ_i (a Lagrange multiplier).

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

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

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

This can be written in matrix form as

$$(**) \quad T\lambda = TF$$

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 ΔQ_i appears in both statics and kinematics

Fluid Equations

The fluid equation is

$$\rho \partial_t v = -\nabla \Pi - \nabla \cdot \sigma + \sum_{i=1}^{N} S_i \lambda_i$$

$$= -\nabla \Pi - \eta \nabla^2 v + S\lambda$$

+ thermal forces

where $S = [\, S_1 \,|\, S_2 \,|\, \ldots \,|\, S_N \,]$

is a composite spreading operator.

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Complete equations

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

$$
\begin{cases}
\nabla \cdot v = 0 \\
\rho \partial_t v + \nabla \Pi = \eta \nabla^2 v + S\lambda + f_{th} \\
\dot{q} = S^* v & \text{(no slip)} \\
T\lambda = TF & \text{(force ~~balance~~ free)} \\
S^* v = T^* w & \text{(rigidity)}
\end{cases}
$$

where we recall that S, T and F depend on q

In this formulation λ is the Lagrange ~~constraint~~ multiplier for the rigidity constraint, and w is the Lagrange multiplier for the force and torque-free constraint, and Π is the multiplier for divergence-free

Temporal Discretization

An implicit second-order discretization for these equations is the following algorithm

1. Move the structure to midpoint

$$q^{n+1/2} = q_0^n + \bar{U}^n \frac{\Delta t}{2} + R^n\left(\frac{\Delta t}{2}\right)\left(q^n - q_0^n\right)$$

where $R^n(\Delta t)$ is a rotation matrix with angular rotation $\Omega^n \Delta t$, where

$$w^n = \begin{bmatrix} \bar{U}^n \\ \Omega^n \end{bmatrix}$$

This simply means move and rotate to midpoint

~~Fluid solver~~

Then, evaluate forces at $q^{n+1/2}$

2. Now solve the fluid problem with constraints

a. $$\rho \frac{u^{n+1} - u^{n}}{\Delta t} + \nabla \Pi^{n+1/2} = \frac{\eta L}{2}\left(u^{n} + u^{n+1}\right) + S^{n+1/2} \lambda^{n+1/2} + \text{thermal}$$

where L is the Laplacian

b. $$\left(S^{*}\right)^{n+1/2} u^{n+1} = \left(T^{*}\right)^{n+1/2} w^{n+1}$$

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

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

d. $$\nabla \cdot u^{n+1} = 0$$

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Finally, move the structure again with linear velocity and angular velocity at midpoint:

$$\omega^{n+1/2} = \frac{1}{2}\left(\omega^{n} + \omega^{n+1}\right)$$

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

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

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Fluid Solver

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

$$\begin{bmatrix} \frac{\rho}{\Delta t} I - \mu \frac{L}{2} & G & 0 & -S \\ -D & 0 & 0 & 0 \\ 0 & 0 & 0 & T \\ -S^* & 0 & T^* & 0 \end{bmatrix} \begin{bmatrix} u^{n+1} \\ \pi^{n+1/2} \\ w^{n+1} \\ \lambda^{n+1/2} \end{bmatrix} = \begin{bmatrix} f^{n+1/2} \\ 0 \\ TF^{n+1/2} \\ 0 \end{bmatrix}$$

everything evaluated at $n+1/2$

Here D is discrete divergence

G is discrete gradient

$D^* = -G$ so the system is symmetric

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How do we solve this system?

The right approach is to use an iterative preconditioned solver.

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

Let me summarize this procedure in my notation

$\boxed{\text{Amneet's approximation}}$

(1) First, solve the fluid ignoring the terms with λ:

$$\left[\begin{array}{c|c} \rho\frac{I}{\Delta t}-\frac{L}{2} & G \\ \hline -D & 0 \end{array}\right]\begin{bmatrix}\tilde{u}^{n+1}\\ \tilde{\pi}^{n+1/2}\end{bmatrix}=\begin{bmatrix}f^{n+1/2}\\ 0\end{bmatrix}$$

~~Boyce~~ Boyce has already developed a solver for this in IBAMR

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Now, obtain $\tilde{w}^{n+1}$ from:

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

This is an <u>overdetermined</u> system for more than two markers, so we solve it in the least-squares sense, by multiplying both sides by T:

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

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

To see that this is the same as what Amneet does, observe that

$$T T^* = \left[\begin{array}{c|c} N I & \sum \Delta Q_i^* \\ \hline \sum \Delta Q_i & \sum \Delta Q_i \Delta Q_i^* \end{array}\right]$$

(13) But, from our definition of ΔQ_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

$$\sum_i \Delta Q \Delta Q_i^* = \sum_{i=1}^{N} \begin{bmatrix} \Delta q_z^2 + \Delta q_y^2 & \cdots \\ -\Delta q_y \Delta q_x & \cdots \\ -\Delta q_z \Delta q_x & \cdots \text{ etc} \end{bmatrix}$$

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

So we have:

$$T T^* = \left[\begin{array}{c|c} N I & 0 \\ \hline 0 & J \end{array}\right]$$

where J is the moment of inertia of the structure.

Therefore we get

$$\tilde{U}^{n+1} = \frac{1}{N} \sum \overbrace{S_i^* \tilde{v}^{n+1}}^{\tilde{u}_i^{n+1}}$$

which is a simple arithmetic average, and

$$\tilde{\Omega}^{n+1} = J^{-1} \sum \Delta q_i \times \tilde{u}_i^{n+1}$$

which is what Ameet is doing now.

Notice that we can add volume to each marker by using <u>weighted</u> least squares to solve

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

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3. The next step is to set

$$\lambda^{n+1/2} = \frac{\rho}{\Delta t}\left(T^{*}\tilde{w}^{n+1} - S^{*}\tilde{v}^{n+1}\right)$$

(This is for the case $F=0$, which is what Anmeet did)

4. Now re-solve the fluid equation

$$\begin{cases} \rho \dfrac{v^{n+1} - \tilde{v}^{n+1}}{\Delta t} = S\lambda^{n+1/2} \\ \nabla \cdot v^{n+1} = 0 \end{cases}$$

I believe Anmeet sets

$$w^{n+1} = \tilde{w}^{n+1}$$

i.e. there is no correction to obtain an improved w^{n+1} from v^{n+1} (why not?)

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Let's see how good of an approximation Anmeets solution is:

First, check

$$T\lambda^{n+1/2} = \frac{\rho}{\Delta t}\left(TT^*\tilde{w}^{n+1} - TS^*\tilde{v}^{n+1}\right)$$

$$= 0 \quad \text{by definition of } \tilde{w}^{n+1}$$

So the force and torque free constraint is obeyed.

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

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

If we do the calculation, we get

$$S^* v^{n+1} = S^* \tilde{v}^{n+1} + (S^*S)T^*(TT^*)^{-1}TS^*\tilde{v}^{n+1}$$

$$-(S^*S)S^*\tilde{v}^{n+1}$$

$$= \left[-S^*S + I + (S^*S)T^*(TT^*)^{-1}T\right]S^*\tilde{v}^{n+1}$$

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We want this to be equal to

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

that is, we want

$$(I - S^* S) + (S^* S) T^* (T T^*)^{-1} T = T (T T^*)^{-1} T$$

The only way this is true in general is if

$\cancel{S S^* = I}$ $\boxed{S^* S = I}$

which is <u>NOT</u> true for the Peskin operator S (but maybe it is if the number of marker points goes to infinity ?!?)

For one particle marker

$S^* S = 8 I$ for the 3 pt function!