Scientific report: Mixed kinematics

The authors

Implementation details for mixed kinematic problems. Our implementation works for combinations of free and fixed (i.e. $\boldsymbol{U} = 0$) bodies.

I. MOBILITY-RESISTANCE PROBLEM

We write in this section the linear systems that appear in the free and prescribed kinematics problems (see Ref. [1] for details and notation). In the free kinematics problem the linear system is

$$\begin{bmatrix} \boldsymbol{M} & -\boldsymbol{K} \\ \boldsymbol{K}^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \boldsymbol{U} \end{bmatrix} = \begin{bmatrix} \tilde{\boldsymbol{u}} + \boldsymbol{W}_1 \\ -\boldsymbol{F} + \boldsymbol{W}_2 \end{bmatrix}, \tag{1}$$

where the value of the noise terms ($\boldsymbol{W}_1$ and $\boldsymbol{W}_2$) is different for each stochastic integrator.

The linear system for prescribed kinematics is

$$\begin{bmatrix} \boldsymbol{M} & 0 \\ \boldsymbol{K}^T & \boldsymbol{I} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \boldsymbol{F} \end{bmatrix} = \begin{bmatrix} \tilde{\boldsymbol{u}} + \boldsymbol{K}\boldsymbol{U} + \boldsymbol{W}_1 \\ 0 \end{bmatrix}. \tag{2}$$

Note that the second equation ($\boldsymbol{K}^T\boldsymbol{\lambda} + \boldsymbol{F} = 0$) is redundant and therefore it is not necessary to include it. However, having linear systems of the same size for both the free and prescribed kinematic simplifies the bookkeeping of variables in the code, therefore, we include it in our implementation. Note also that in our implementation $\boldsymbol{K}\boldsymbol{U} = 0$.

The only coupling between bodies in (1) and (2) is through the blob mobility matrix $\boldsymbol{M}$. Since that term is the same in both equations is trivial to combine them to simulate bodies with free and prescribed kinematics simultaneously

$$\begin{bmatrix} \boldsymbol{M} & -\boldsymbol{K}_{\text{free}} & 0 \\ \boldsymbol{K}_{\text{free}}^T & 0 & 0 \\ \boldsymbol{K}_{\text{presc}}^T & 0 & \boldsymbol{I} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda} \\ \boldsymbol{U}_{\text{free}} \\ \boldsymbol{F}_{\text{presc}} \end{bmatrix} = \begin{bmatrix} \tilde{\boldsymbol{u}} + \boldsymbol{K}_{\text{presc}}\boldsymbol{U}_{\text{presc}} + \boldsymbol{W}_1 \\ -\boldsymbol{F}_{\text{free}} + \boldsymbol{W}_2 \\ 0 \end{bmatrix}, \tag{3}$$

where $\boldsymbol{\lambda}$ is the constraint force acting on all blobs in the system.

We use GMRES with a block diagonal preconditioner to solve these linear systems. In all cases the preconditioner is an exact solver for a single body but it does not include any coupling between bodies.

II. STOCHASTIC INTEGRATOR

Our implementation of obstacles works with the deterministic schemes *Forward Euler* and *Adams-Basforth* and with the stochastic integrators *Trapezoidal Slip* and *Midpoint Slip*, see Ref. [2].

In the stochastic integrators the only modification that we do, besides using the linear system (3), is to fix the position of bodies with prescribed kinematics. We do not update their positions neither to perform RFD nor to update the middle or final configurations.

[1] F. Balboa Usabiaga, B. Kallemov, B. Delmotte, A. P. S. Bhalla, B. E. Griffith, and A. Donev, Communications in Applied Mathematics and Computational Science **11**, 217 (2016).

[2] B. Sprinkle, F. Balboa Usabiaga, N. A. Patankar, and A. Donev, The Journal of Chemical Physics **147**, 244103 (2017), https://doi.org/10.1063/1.5003833, URL `https://doi.org/10.1063/1.5003833`.