Internal report: Mixed kinematics

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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

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

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

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

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

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

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. We show the convergence for several number of particles in Fig. 1.

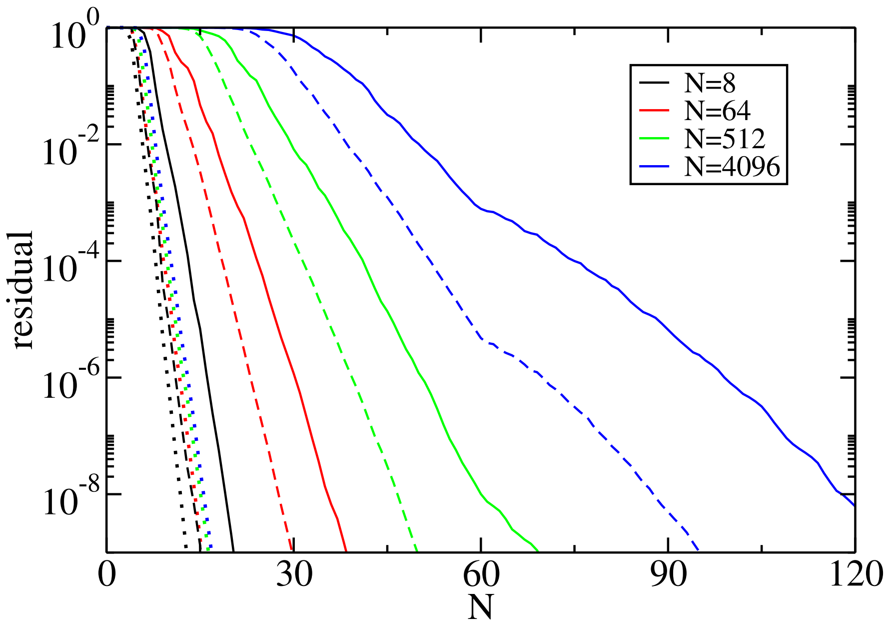

FIG. 1: True residual versus number of GMRES iteration for solving the mixed kinematics problem for N spheres forming a simple cubic lattice (distance between first neighbors $d = 3.6R_h$) and spheres discretized with $N_b = 42$ blobs. In the system there are N_{free} spheres following free kinematics and $N_{\text{presc}} = N - N_{\text{free}}$ following prescribed kinematics. Results for $N_{\text{free}} = 1$ (continuous lines), $N_{\text{free}} = N/2$ (dashed lines) and $N_{\text{free}} = N - 1$ (dotted lines).

II. STOCHASTIC INTEGRATOR

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.

III. IMPLEMENTATION

So far we have only implemented mixed kinematics in the *Trapezoidal Slip Scheme* [2]; it is easy to implement the changes in the other schemes. The files and functions that we modified are

1. **read_input.py:** it is possible to specify in the input file if some structures obey prescribed kinematics. If the option *structure* is followed by four file names (vertex, clones, slip and prescribed

velocity files) the bodies defined on those files will obey prescribed kinematics.

2. **quaternion_integrator_multi_bodies.py:** we modified the following functions
   (a) **stochastic_Slip_Trapz:** small modifications to not update bodies during RFD.
   (b) **solve_mobility_problem:** the right hand side of the linear system is different for prescribed kinematics. Also, after the linear system is solved the solution vector is modified to return the array $(\boldsymbol{\lambda}, \boldsymbol{U})$ even for bodies that follow prescribed kinematics (instead of $(\boldsymbol{\lambda}, \boldsymbol{F})$ as given by (2)).
3. **multi_bodies.py:** we modified the following functions
   (a) **linear_operator_rigid:** the linear operator is different for bodies that follow prescribed kinematics.
   (b) **build_block_diagonal_preconditioners_det_stoch:** in the block-diagonal preconditioner we only build and factorize the matrices associated with bodies with prescribed kinematics one time per simulation. The matrices can be reused because those bodies do not move.
   (c) **main:** small modifications to label bodies that follow prescribed kinematics.
4. **body.py:** we added a few additional variables for prescribed kinematics.

IV. NUMERICAL RESULTS

We do a simple test to confirm that the trajectories generated by this scheme follows the Gibbs-Boltzmann distribution. We simulate two boomerang colloidal particles connected by an harmonic spring. One is fixed at position $\boldsymbol{q} = (0, 0, 100)$ and orientation $\boldsymbol{\theta} = (1, 0, 0, 0)$ while the other is free to move. In the plots we compare the configuration generated by the stochastic integrator to one generated by a Monte Carlo method.

[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`.

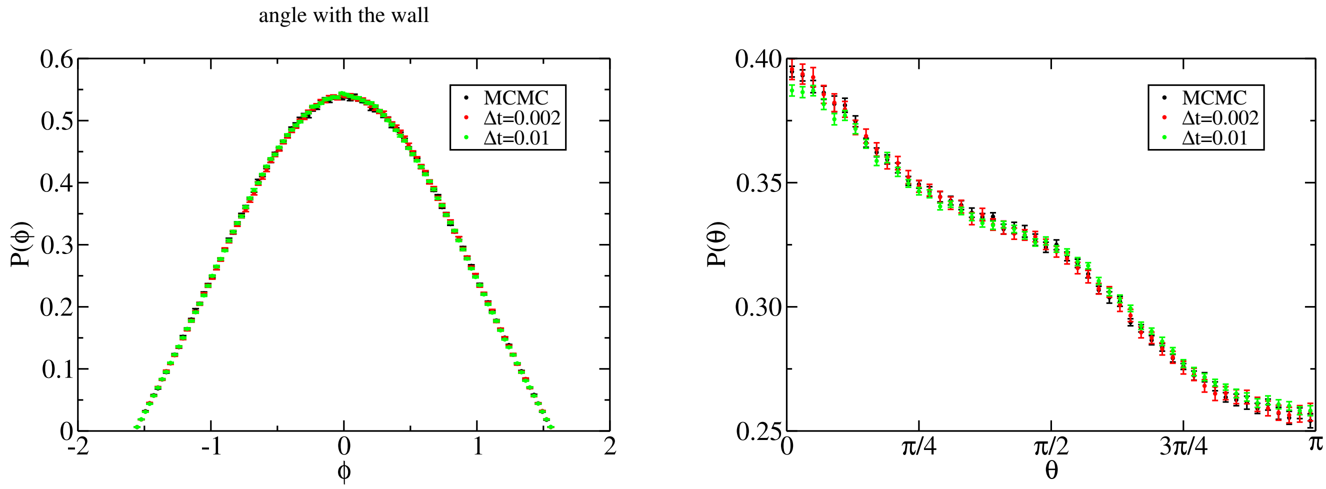

FIG. 2: PDF of the angle between the boomerang's bisector and the xy plane (left) or the x axis (right). Comparison between MCMC results and the stochastic integrator with two time steps.

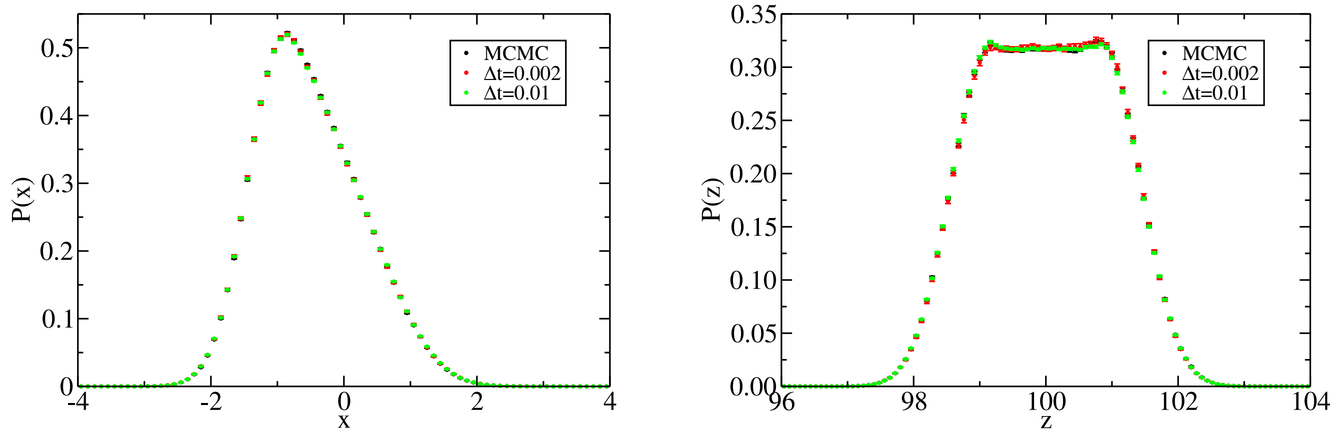

FIG. 3: Histogram of the boomerang position along the x (left) and z axis (right). Comparison between MCMC results and the stochastic integrator with two time steps.