Two approaches simulating Brownian motion in fluid suspensions

Yasuya Nakayama\textsuperscript{a} \textsuperscript{1}, Takuya Iwashita\textsuperscript{b}, Ryoichi Yamamoto\textsuperscript{b,c}

\textsuperscript{a}Department of Chemical Engineering, Kyushu University
\textsuperscript{b}Department of Chemical Engineering, Kyoto University
\textsuperscript{c}CREST, Japan Science and Technology Agency

Dynamics of sub-micron/nanoscale objects offers many intriguing physical problems since both hydrodynamic interactions and thermal fluctuation are equally influence the motion of such objects. Among such objects, colloids and/or macromolecules have been typical targets of research. We propose a simple and applicable way for simulating colloidal suspensions incorporating hydrodynamic interactions and thermal fluctuation.

Before introducing our new scheme, we observe what we already know in the set of basic equations to describe the Brownian motion in fluid suspensions \cite{1} \cite{2}, viz.,
\begin{align}
\nabla \cdot v &= 0, \quad \rho \ddot{v} = \nabla \cdot \sigma + \nabla \cdot s, \\
M \dot{V}_i &= F_i + F_i', \quad I \cdot \dot{\Omega}_i = N_i + N_i', \\
F_i &= \int dS_i \cdot \sigma, \quad F_i' = \int dS_i \cdot s, \\
N_i &= \int (x - \mathbf{R}_n) \times dS_i \cdot \sigma, \quad N_i' = \int (x - \mathbf{R}_n) \times dS_i \cdot s,
\end{align}

\textsuperscript{1}E-mail: ynakayama-w@chem-eng.kyushu-u.ac.jp
where \( \rho, v \) are the mass density and the velocity of the host fluid, respectively. \( M_i, I_i, R_i, V_i, \Omega_i \) are the mass, the moment of inertia, the center of mass, velocity, and angular velocity of the \( i \)th colloid, respectively. Thermal fluctuation of the system is incorporated through the random stress \( s \) which is white-in-time and white-in-space,

\[
\langle s(x, t)s(x', t') \rangle = 2k_B T \zeta \delta(x - x') \delta(t - t'),
\]

where the fourth rank friction tensor \( \zeta \) should be identified from the structure of the viscous stress \( \sigma \).

Equations (1) and (2) consist a large Markovian Langevin system. Therefore, not only Brownian motion of colloids but that of fluid particles is solved by this set of equations.

We propose another set of working equations by focusing to solve the Brownian motion solely of what we are interested in, colloids and/or macromolecules. Fluctuation–Dissipation theorem (FDT) on colloids states that velocity correlation of hot system \( (k_B T > 0) \) is equal to the velocity response function of the cold system \( (k_B T = 0) \). Thus, we omit the random stress in the equation of the host fluid but retain the viscous stress which is necessary for solving the velocity response. In the hot system, random stress \( s \) plays a role in sustaining the temperature of the whole system, but has no coherent effect on average regression of the velocity correlation of colloids since \( s \) is white-in-time and white-in-space. To agitate colloids, we need to impose random forces on colloids. These new random forces should be white-in-time in order not to have no coherent effect on the regression of the velocity correlation of colloids. The discussion above leads our set of working equations that is described Eq.(1) with,

\[
\begin{align*}
F'_i &= G'_i^V, \quad \langle G'_i^V(t)G'_i^V(0) \rangle \propto \delta(t), \\
N'_i &= G'_i^\Omega, \quad \langle G'_i^\Omega(t)G'_i^\Omega(0) \rangle \propto \delta(t),
\end{align*}
\]

Since FDT was not applied to the whole system, the amplitudes of the fluctuating forces \( G'_i^V \) and \( G'_i^\Omega \) need to be determined implicitly. This is done by controlling \( \langle V^2 \rangle(t), \langle \Omega^2 \rangle(t) \) to certain target values.

By considering the FDT or Onsager's regression hypothesis on colloids, we derived a new set of equations for simulating Brownian motion in fluid suspensions. We conclude the presentation by making two remarks. Our scheme is highly efficient since simulation with Eqs.(1) and (3) requires much less degrees of freedom for random forces than Eqs.(1) and (2). Moreover, we note that our scheme is highly applicable to various type of host fluids since Eqs.(1) and (3) do not depend on a specific constitutive equation of the host fluid. Numerical results based on our scheme are reported elsewhere [3].

References

