Nondimentionalization

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Force balance equation

The following force balance equation is considered here;

$$\boldsymbol{F}_{\mathrm{H}} + \boldsymbol{F}_{\mathrm{R}} = 0. \tag{1}$$

The hydrodynamic interaction is assumed to be linear form of velocities.

$$\boldsymbol{F}_{\mathrm{H}} = -\boldsymbol{R} \cdot \boldsymbol{U}. \tag{2}$$

Once we set unit of force, force balance equations can be nondimensionalized. Then, we also need to select relation between force unit and velocity unit. Since our force balance equations include Stokes hydrodynamic interactions (2), the simplest way is use of Stokes drag formula for any force units:

$$F^{*} = 6\pi\eta_0 a U^{*}. \tag{3}$$

Thanks to this, the hydrodynamic interaction is nondimensionalized as follows,

$$\boldsymbol{F}_{\mathrm{H}}/F^{*} = -(\boldsymbol{R}/6\pi\eta_0 a) \cdot (\boldsymbol{U}/U^{*}) = -\boldsymbol{R}' \cdot (\boldsymbol{U}/U^{*}), \tag{4}$$

and the resistance matrix in our codes is the identity matrix in the dilute limit: $\boldsymbol{R}'(\phi \to 0) = \boldsymbol{I}$

Representative quantities

Particle radius is commonly considered as the representative length in our particle simulations: $L^{*} = a$.

From shear rate

One way to give the representative particle velocity in a sheared suspension is

$$U^{*}_{\mathrm{H}} = L^{*}\dot{\gamma}. \tag{5}$$

The typical hydrodynamic force is given by the typical velocity U^{*}_{H} and Stokes-drag form;

$$F^{*}_{\mathrm{H}} = 6\pi\eta_0 a U^{*}_{\mathrm{H}}. \tag{6}$$

Here, we indicate nondimensionalized variables in the hydrodynamic unit by using 'tilde', i.e., $\tilde{\boldsymbol{F}} = \boldsymbol{F}/F_{\mathrm{H}}^{*}$, etc.

[note] Since F_{H}^{*} is a function of shear rate $\dot{\gamma}$, it is not constant in stress controlled simulations and zero if system is not sheared.

From repulsive force

The repulsive force $\boldsymbol{F}_{\mathrm{R}}$ is a function of particle-to-particle distance. We take the amplitude F_{R}^{*} to represent its typical strength:

$$\boldsymbol{F}_{\mathrm{R}} = F_{\mathrm{R}}^{*}\hat{\boldsymbol{F}}_{\mathrm{R}}, \tag{7}$$

where 'hat' indicates nondimensionalized variables based on this repulsive force. The corresponding velocity can also be given via the Stokes-drag form;

$$U_{\mathrm{R}}^{*} \equiv \frac{F_{\mathrm{R}}^{*}}{6\pi\eta_0 a}. \tag{8}$$

Hydrodynamic (or shear-rate) unit

In the hydrodynamic unit, the nondimensionalized force balance equation is

$$\frac{\boldsymbol{F}_{\mathrm{H}}}{F_{\mathrm{H}}^{*}} + \frac{\boldsymbol{F}_{\mathrm{R}}}{F_{\mathrm{H}}^{*}} = 0 \quad \Longrightarrow \quad -\boldsymbol{R}' \cdot \tilde{\boldsymbol{U}} + \tilde{\boldsymbol{F}}_{\mathrm{R}} = 0, \tag{9}$$

where $\boldsymbol{R}' \equiv \boldsymbol{R}/6\pi\eta_0 a$.

The origin of shear-rate dependence becomes clear if the repulsive force is expressed with the typical value F_{R}^{*};

$$-\tilde{\boldsymbol{R}} \cdot \tilde{\boldsymbol{U}} + \frac{1}{\alpha}\hat{\boldsymbol{F}}_{\mathrm{R}} = 0. \tag{10}$$

This α indicates the competition between two representative forces:

$$\alpha \equiv \frac{\boldsymbol{F}_{\mathrm{H}}^{*}}{\boldsymbol{F}_{\mathrm{R}}^{*}} = \frac{\dot{\gamma}}{F_{\mathrm{R}}^{*}/6\pi\eta_0 a^2}. \tag{11}$$

The unit of time is

$$t_{\mathrm{H}}^{*} \equiv \frac{L^{*}}{U_{\mathrm{H}}^{*}} = \frac{1}{\dot{\gamma}}. \tag{12}$$

Therefore, the nondenominational time $\tilde{t}$ is shear strain (when shear rate is constant):

$$\tilde{t} \equiv \frac{t}{t_{\mathrm{H}}^{*}} = t\dot{\gamma} = \gamma. \tag{13}$$

The nondimensionalized shear rate is

$$\tilde{\dot{\gamma}} = \frac{\dot{\gamma}}{1/t_{\mathrm{H}}^{*}} = 1. \tag{14}$$

[note] We call this unit system "hydrodynamic". But, the essential origin for this unit system is the way to give typical velocity, i.e., $U^* = a\dot{\gamma}$. "Shear-rate" unit might be proper name.

Repulsive force unit

In the repulsive unit, the nondimensionalized force balance equation is

$$\frac{\boldsymbol{F}_{\mathrm{H}}}{F_{\mathrm{R}}^*} + \frac{\boldsymbol{F}_{\mathrm{R}}}{F_{\mathrm{R}}^*} = 0 \quad \Longrightarrow \quad -\boldsymbol{R}' \cdot \hat{\boldsymbol{U}} + \hat{\boldsymbol{F}}_{\mathrm{R}} = 0. \tag{15}$$

The time unit is

$$t_{\mathrm{R}}^* \equiv \frac{L^*}{U_{\mathrm{R}}^*} = \frac{6\pi\eta_0 a^2}{F_{\mathrm{R}}^*}. \tag{16}$$

The nondimensionalized shear rate is

$$\hat{\dot{\gamma}} = \dot{\gamma} t_{\mathrm{R}}^* = \alpha. \tag{17}$$

In rate-controlled simulations, the relation between the nondimensionalized time $\hat{t} \equiv t/t_{\mathrm{R}}^*$ and shear strain γ is

$$\gamma \equiv \dot{\gamma} t = \dot{\gamma} t_{\mathrm{R}}^* \hat{t} = \frac{F_{\mathrm{H}}^*}{F_{\mathrm{R}}^*} \hat{t} = \alpha \hat{t}, \tag{18}$$

where α is defined in (11).

In stress controlled simulations, the strain is simply given by

$$\gamma = \int^{t} \dot{\gamma} dt = \int^{\hat{t}} \alpha d\hat{t}. \tag{19}$$

Simulation data

In both ways of nondimensionalization, we can unify the output data with ones nondimensionalized by repulsive force.

	Output	**Output in H.U.**	**Calc in H.U.**	**Output in R.U.**	**Calc in R.U.**
strain	γ	$\tilde{t}$		γ	
relative viscosity	η_{r}	$6\pi\tilde{\sigma}$		$6\pi\hat{\sigma}/\alpha$	
time	$\hat{t}$	$\tilde{t}/\alpha$	$\tilde{t}$	$\hat{t}$	$\hat{t}$
shear rate	$\hat{\dot{\gamma}}$	α	$\tilde{\dot{\gamma}} = 1$	$\hat{\dot{\gamma}}$	$\hat{\dot{\gamma}}$
shear stress	$\hat{\sigma}$	$\alpha\tilde{\sigma}$	$\tilde{\sigma}$	$\hat{\sigma}$	$\hat{\sigma}$

Note

This choice of relating velocity scale and force scale (3) is specific. This is why we see numerical factor 6π at several places.

This may generate a little confusion on nondimensionalization of stresses. In viscous suspensions, the representative value of stress can be given by the solvent viscosity η_0 and shear rate.

$$\sigma^* = \eta_0 \dot{\gamma}^*. \tag{20}$$

We need to give a typical shear rate in the system. If a repulsive force plays the critical role on the shear rate dependence, we can set the corresponding shear rate $\dot{\gamma}_{\mathrm{R}}^*$:

$$F_{\mathrm{R}}^* = 6\pi\eta_0 a^2 \dot{\gamma}_{\mathrm{R}}^* \tag{21}$$

So, the unit of stress can be given as follows,

$$\begin{aligned} \sigma_{\mathrm{R}}^* &= \eta_0 \dot{\gamma}_{\mathrm{R}}^* \\ &= F_{\mathrm{R}}^*/6\pi a^2 \end{aligned} \tag{22}$$

Thus, the numerical factor 6π comes from the way to relate force and velocity.