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A numerical study of the settling of non-spherical particles in quiescent water: Supplementary material

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Dual-Euler whole-attitude solver

A dual-Euler whole-attitude solver is used to simulate the variation in particle orientation during settling. The inherent singularity of a single Euler sequence is avoided by switching between two different Euler angle sets (Singla et al., 2005).

Euler angles are one of the most commonly used sets of attitude parameters. They describe the attitude of the body frame relative to the inertial frame by means of three successive rotation angles (ψ, θ, γ) about the body fixed axes. Given that all rotations are performed about the principal axes of the body frame, three elementary rotation matrices can be given as

$$C_\psi = \begin{bmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{S1}$$

$$C_\theta = \begin{bmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{bmatrix}, \tag{S2}$$

$$C_\gamma = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\gamma & \sin\gamma \\ 0 & -\sin\gamma & \cos\gamma \end{bmatrix}. \tag{S3}$$

The order of the axes about which the body frame is rotated is important. When the rotation sequence follows $\psi \to \theta \to \gamma$, the attitude matrix from the inertial frame to the body frame is calculated as

$$C_n^b = C_\gamma C_\theta C_\psi . \tag{S4}$$

Accordingly, the attitude matrix from the body frame to the inertial frame is given by

$$C_b^n = \left(C_n^b\right)^{\mathrm{T}} = \begin{bmatrix} \cos\psi\cos\theta & \cos\psi\sin\theta\sin\gamma - \sin\psi\cos\gamma & \cos\psi\sin\theta\cos\gamma + \sin\psi\sin\gamma \\ \sin\psi\cos\theta & \sin\psi\sin\theta\sin\gamma + \cos\psi\cos\gamma & \sin\psi\sin\theta\cos\gamma - \cos\psi\sin\gamma \\ -\sin\theta & \cos\theta\sin\gamma & \cos\theta\cos\gamma \end{bmatrix}. \tag{S5}$$

Furthermore, the relation between the angular velocities of the body frame and the Euler angle velocities can be expressed as

$$\begin{bmatrix}\omega_x\\ \omega_y\\ \omega_z\end{bmatrix}=\begin{bmatrix}\dot{\gamma}\\ 0\\ 0\end{bmatrix}+C_\gamma\begin{bmatrix}0\\ \dot{\theta}\\ 0\end{bmatrix}+C_\gamma C_\theta\begin{bmatrix}0\\ 0\\ \dot{\psi}\end{bmatrix}, \tag{S6}$$

where $\left[\omega_x,\omega_y,\omega_z\right]^{\mathrm{T}}$ are angular velocity components of the body frame. From Eq. (S6), differential equations for the Euler angles can be derived as

$$\begin{bmatrix}\dot{\gamma}\\ \dot{\theta}\\ \dot{\psi}\end{bmatrix}=\frac{1}{\cos\theta}\begin{bmatrix}\cos\theta & \sin\gamma\sin\theta & \cos\gamma\sin\theta\\ 0 & \cos\gamma\cos\theta & -\sin\gamma\cos\theta\\ 0 & \sin\gamma & \cos\gamma\end{bmatrix}\begin{bmatrix}\omega_x\\ \omega_y\\ \omega_z\end{bmatrix}. \tag{S7}$$

Based on the time series of $\left[\omega_x,\omega_y,\omega_z\right]^{\mathrm{T}}$, Equation (S7) can be solved using the fourth-order Runge-Kutta method, with singularities occurring when $\theta=\pm\pi/2$. To avoid such singularities, another set of Euler angles, where the rotation sequence follows $\psi_r\rightarrow\gamma_r\rightarrow\theta_r$, is introduced. The corresponding attitude matrix from the body frame to the inertial frame and differential equations for the Euler angles are obtained as

$$\left(C_b^n\right)_r=\begin{bmatrix}\cos\theta_r\cos\psi_r-\sin\theta_r\sin\gamma_r\sin\psi_r & -\cos\gamma_r\sin\psi_r & \sin\theta_r\cos\psi_r+\cos\theta_r\sin\gamma_r\sin\psi_r\\ \cos\theta_r\sin\psi_r+\sin\theta_r\sin\gamma_r\cos\psi_r & \cos\gamma_r\cos\psi_r & \sin\theta_r\sin\psi_r-\cos\theta_r\sin\gamma_r\cos\psi_r\\ -\sin\theta_r\cos\gamma_r & \sin\gamma_r & \cos\theta_r\cos\gamma_r\end{bmatrix}, \tag{S8}$$

$$\begin{bmatrix}\dot{\gamma}_r\\ \dot{\theta}_r\\ \dot{\psi}_r\end{bmatrix}=\frac{1}{\cos\gamma_r}\begin{bmatrix}\cos\theta_r\cos\gamma_r & 0 & \sin\theta_r\cos\gamma_r\\ \sin\theta_r\sin\gamma_r & \cos\gamma_r & -\cos\theta_r\sin\gamma_r\\ -\sin\theta_r & 0 & \cos\theta_r\end{bmatrix}\begin{bmatrix}\omega_x\\ \omega_y\\ \omega_z\end{bmatrix}. \tag{S9}$$

Given that the attitude matrix from the body frame to the inertial frame is identical for different rotation sequences, the two distinct Euler angle sets can be transformed to each other by equating C_b^n to $\left(C_b^n\right)_r$:

$$C_b^n=\left(C_b^n\right)_r=\begin{bmatrix}\zeta_{11} & \zeta_{12} & \zeta_{13}\\ \zeta_{21} & \zeta_{22} & \zeta_{23}\\ \zeta_{31} & \zeta_{32} & \zeta_{33}\end{bmatrix}. \tag{S10}$$

And the transformation relations are derived as

$$\begin{cases} \theta_r = \arctan\left(-\dfrac{\zeta_{31}}{\zeta_{33}}\right) = \arctan\left(\dfrac{\tan\theta}{\cos\gamma}\right) \\ \gamma_r = \arcsin\zeta_{32} = \arcsin(\cos\theta\sin\gamma) \\ \psi_r = \arctan\left(-\dfrac{\zeta_{12}}{\zeta_{22}}\right) = \arctan\left(\dfrac{\sin\psi\cos\gamma - \cos\psi\sin\theta\sin\gamma}{\cos\psi\cos\gamma + \sin\psi\sin\theta\sin\gamma}\right) \end{cases}, \tag{S11}$$

$$\begin{cases} \gamma = \arctan\left(\dfrac{\zeta_{32}}{\zeta_{33}}\right) = \arctan\left(\dfrac{\tan\gamma_r}{\cos\theta_r}\right) \\ \theta = -\arcsin\zeta_{31} = \arcsin(\sin\theta_r\cos\gamma_r) \\ \psi = \arctan\left(\dfrac{\zeta_{21}}{\zeta_{11}}\right) = \arctan\left(\dfrac{\cos\theta_r\sin\psi_r + \sin\theta_r\sin\gamma_r\cos\psi_r}{\cos\theta_r\cos\psi_r - \sin\theta_r\sin\gamma_r\sin\psi_r}\right) \end{cases}. \tag{S12}$$

Notably, the singularity condition for Eq. (S9) is $\gamma_r = \pm\pi/2$, which should correspond to $\theta = 0$ or $\theta = \pm\pi$. Based on such characteristics, Equation (S7) is solved if $|\theta| \le \pi/4$ or $|\theta| > 3\pi/4$, otherwise Equation (S9) is solved. Thus, singularities are avoided, and the orientation of the body frame can be readily inferred using the calculated Euler angles and attitude matrix.

References

Singla, P., Mortari, D., and Junkins, J.L., "How to avoid singularity when using Euler angles ?," Adv. Astron. Sci. **119**, 1409-1426 (2005).