A Numerical Model for Inertial and Lagrangian Particles in Inertial and Rotating Frames

AMCG, Department of Earth Science and Engineering, Imperial College London, South Kensington, London, SW7 2AZ

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Chapter 1

Governing equations

1.1 Force balance for an immersed body

The inertial frame equations of motion for a rigid body of finite size and mass immersed in a fluid are

$$\frac{d\boldsymbol{r}}{dt} := \boldsymbol{v}. \qquad \text{(particle motion)}$$

$$m\frac{d\boldsymbol{v}}{dt} = \oint_{\text{boundary}} \boldsymbol{f} dS - m\boldsymbol{g}, \qquad \text{(linear momentum)}$$

$$m\frac{d\boldsymbol{\omega}}{dt} = \oint_{\text{boundary}} (\boldsymbol{x} - \boldsymbol{r}) \times \boldsymbol{f} dS \qquad \text{(angular momentum)}$$

here $\boldsymbol{r}$ is the location of the particle's centre of mass,

$$\boldsymbol{r} = \frac{1}{m}\int_{\text{body}} \rho_p \boldsymbol{x} dV,$$

m is the body mass, a function of the body density, ρ_p

$$m = \int_{\text{body}} \rho_p dV,$$

$\boldsymbol{v}$ is the particle's linear velocity,

$$\boldsymbol{v} = \frac{1}{m}\int_{\text{body}} \rho_p \frac{d\boldsymbol{x}}{dt} dV,$$

$\boldsymbol{\omega}$ is the particle's angular velocity,

$$\boldsymbol{\omega} = \frac{1}{m}\int_{\text{body}} \rho_p \left(\boldsymbol{x} - \boldsymbol{r}\right) \times \frac{d}{dt}\left(\boldsymbol{x} - \boldsymbol{r}\right) dV,$$

$\boldsymbol{f}$ are the surface forces applied by the fluid on the body and $\boldsymbol{g}$ is the acceleration. Since the system is closed, the force applied to the body by the fluid match the force applied to the fluid by the body, hence

$$\boldsymbol{f} = p\boldsymbol{n} + \boldsymbol{n} \cdot \underline{\boldsymbol{\sigma}},$$

where p is the fluid pressure, $\boldsymbol{n}$ is a unit vector normal to the body surface and $\underline{\boldsymbol{\sigma}}$ is the fluid stress tensor. The relevant equations for the fluid are the Navier-Stokes equations,

$$\rho_f \frac{\partial \boldsymbol{u}}{\partial t} + \rho_f \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \nabla \cdot \underline{\boldsymbol{\sigma}} - \rho \boldsymbol{g}, \qquad \text{(momentum)}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \boldsymbol{u} = 0. \qquad \text{(continuity)}$$

along with a jump condition across the interface

$$\boldsymbol{v} = \boldsymbol{u} \text{ on } \delta S. \qquad \text{(no slip)}$$

The exact solution has a boundary layer in the viscinity of the body.

1.2 The Basset-Boussinesq-Oseen equation

In the limit that the body is small compared to the length scales of the fluid, it is desirable to parameterise the viscous forces in terms of far field fluid velocity. In the low Reynolds number limit we obtain (for spherical particles) the Basset-Boussinesq-Oseen equation,

$$\frac{\pi}{6}\rho_p d_p^3 \frac{d\boldsymbol{v}}{dt} = 3\pi\mu d_p \left(\boldsymbol{U}-\boldsymbol{v}\right) - \frac{\pi}{6} d_p^3 \left.\nabla p\right|_{\boldsymbol{x}=\boldsymbol{r}} + \frac{\pi}{12}\rho_f d_p^3 \frac{d}{dt}\left(\boldsymbol{U}-\boldsymbol{v}\right) + \frac{3}{2} d_p^2 \sqrt{\pi\rho_f\mu} \int_{t_o}^{t} \frac{1}{\sqrt{t-\tau}} \frac{d}{d\tau}\left(\boldsymbol{U}-\boldsymbol{v}\right) - \frac{\pi}{6}\rho_p d_p^3 \boldsymbol{g}$$

These are the drag law (Stokes drag, in the low Reynolds number limit), Froude-Krylov force, added (or virtual) mass, Basset force and the force due to gravity respectively. Here d_p is the diameter of the particle, and $\boldsymbol{U} = \boldsymbol{u}\left(\boldsymbol{r}\left(t\right), t\right)$, where p and $\boldsymbol{r}$ are the *undisturbed* fluid pressure and velocity.

1.3 Alternative drag laws

Generic drag laws for small particles take the form.

$$\boldsymbol{F}_{\text{drag}} = C\left(d_p, \boldsymbol{u}-\boldsymbol{v}\right)\left[\boldsymbol{u}-\boldsymbol{v}\right].$$

For example, the classic turbulent drag law for spheres,

$$\boldsymbol{F}_{\text{turbulent drag}} = \frac{0.44\pi\rho d_p^2}{8}\left\|\boldsymbol{u}-\boldsymbol{v}\right\|\left[\boldsymbol{u}-\boldsymbol{v}\right],$$

or the transitional drag law,

$$\boldsymbol{F}_{\text{transitional drag}} = \begin{cases} 3\pi\mu d_p\left(\boldsymbol{U}-\boldsymbol{v}\right) & \text{Re} < 10^{-4}, \\ \frac{c_d\pi\rho d_p^2}{8}\left\|\boldsymbol{u}-\boldsymbol{v}\right\|\left[\boldsymbol{u}-\boldsymbol{v}\right] & \text{Re} < 1000, \\ \frac{0.44\pi\rho d_p^2}{8}\left\|\boldsymbol{u}-\boldsymbol{v}\right\|\left[\boldsymbol{u}-\boldsymbol{v}\right] & \text{otherwise,} \end{cases}$$

where Re is a particle Reynolds number,

$$\text{Re}{:=}\tfrac{\rho_f\|\boldsymbol{u}-\boldsymbol{v}\|d_p}{\mu},$$

and the empirically determined transitional drag coeffient is

$$c_d = \frac{24}{\text{Re}}\left(1+0.15\text{Re}^{0.687}\right)$$

1.4 Pure Lagrangian particles

In the “pure” Lagrangian limit the ratio of particle diameter and the fluid length scale vanishes, $\frac{d_p}{\ell}\to 0$, in this limit $C\to\infty$, hence force balance requires $\boldsymbol{v}\to\boldsymbol{U}$. This simplies the equations of motion to

$$\frac{d\boldsymbol{r}}{dt} = \boldsymbol{u}\left(\boldsymbol{r}, t\right).$$

1.5 The hydrostatic limit

For slow flows in the Boussinesq limit, $|\rho_f - \rho_0| \ll 1$, and small aspect ratio, the pressure is dominated by the hydrostatic component,

$$p \approx p_H := \rho_0 g z,$$

Substituting into the particle Froude-Krylov term we see that the principal effect is to modify the force due to gravity into a reduced buoyancy term,

$$\boldsymbol{F}_{\text{gravity}} \approx -\frac{\pi d_p^3}{6}\left(\rho_f-\rho_0\right)\boldsymbol{g}.$$

1.6 Virtual Mass

1.7 Basset Force

1.8 Particles in a rotational frame

Replacing the original inertial frame, $\boldsymbol{x}, t$, with a new frame, $\boldsymbol{x}', t$, rotating at a spatially constant angular velocity $\boldsymbol{\Omega}\,(t)$ around around an axis passing through a point $\boldsymbol{x}_0$ gives new temporal derivatives for the particles

$$\left.\frac{d\boldsymbol{v}}{dt}\right|_{\boldsymbol{x},t} = \left.\frac{d\boldsymbol{v}'}{dt}\right|_{\boldsymbol{x}',t} + 2\boldsymbol{\Omega}\times\boldsymbol{v}' + \boldsymbol{\Omega}\times\left(\boldsymbol{\Omega}\times\left[\boldsymbol{r}'-\boldsymbol{x}_0\right]\right) + \frac{d\boldsymbol{\Omega}}{dt}\times\left[\boldsymbol{r}'-\boldsymbol{x}_0\right],$$

$$\frac{d\boldsymbol{r}'}{dt} = \boldsymbol{v}',$$

and for the fluid of

$$\left.\frac{\partial\boldsymbol{u}}{\partial t}\right|_{\boldsymbol{x},t} = \left.\frac{d\boldsymbol{u}'}{dt}\right|_{\boldsymbol{x}',t} + 2\boldsymbol{\Omega}\times\boldsymbol{u}' + \boldsymbol{\Omega}\times\left(\boldsymbol{\Omega}\times\left[\boldsymbol{x}'-\boldsymbol{x}_0\right]\right) + \frac{d\boldsymbol{\Omega}}{dt}\times\left[\boldsymbol{x}'-\boldsymbol{x}_0\right].$$

Chapter 2

Particle-Wall Collisions and Wear Modelling

2.1 A Collision Event

Chapter 3

Numerical implementation

3.1 Timestepping

Following the approximations in the previous section, the transitional particle model with can be written as

$$\frac{d\boldsymbol{r}}{dt} = \boldsymbol{v},$$

$$\frac{(2\rho_p + \rho_f)\,d_p}{12}\left(\frac{d\boldsymbol{v}}{dt} + 2\boldsymbol{\Omega}\times 2\rho_p\boldsymbol{v}\right) = \frac{\rho_f d_p}{12} - \frac{d_p}{6}\left[(\rho_p - \rho_f)\,\boldsymbol{\Omega}\times(\boldsymbol{\Omega}\times[\boldsymbol{r}-\boldsymbol{x}_0]) - (\rho_p-\rho_f)\,\frac{d\boldsymbol{\Omega}}{dt}\times[\boldsymbol{r}-\boldsymbol{x}_0]\right],$$

The terms on the right hand side involve evaluations of $\boldsymbol{u}$ at the location $\boldsymbol{r}$. If an implicit timestepping scheme is used, this will require solving an implicitly defined geometric problem to calculate $\boldsymbol{r}^{n+1}$. This is generally a computationally expensive undertaking, hence an explicit timestepping scheme is used for this term. Unlike in Eulerian fluid modelling side, for inertial particles this does not impose a stability constraint on the problem, but merely one of accurracy.

3.1.1 Adams-Bashforth schemes

The family of Adams-Bashforth timestepping schemes for first order ordinary differential equations(ODEs), are a collection of explicit linear multistep methods, with the kth scheme, ABk, accurate to kth order in time. Consider an ODE for an independent variable, t, and a dependent variable, $y(t)$,

$$\frac{dy}{dt} = f(y,t),$$

with discretized time levels t_n, and discretized solutions $y_n \approx y(t_n)$The Adams-Bashforth methods represent the $k-1$ order accurate extrapolation of y_{n+1} from the data for y_n at the previous time level and the values of f derived from the data at the previous k time levels. These methods are particularly suited to particles which collide, since a collision event means that multistage methods would be polluted with inaccurate data.

3.1.1.1 The first order AB1 scheme

The first order method, AB1, is simply the forward Euler method, so AB1 sets

$$y_n = y_n + \Delta t_{n+\frac{1}{2}} f(y_n, t_n).$$

where $\Delta t_{n+\frac{1}{2}} = t_{n+1} - t_n$.

3.1.1.2 The second order AB2 scheme

For unequally spaced time levels the second order scheme, AB2, sets

$$y_{n+1} = y_n + \Delta t_{n+\frac{1}{2}}\left(\frac{2\Delta t_{n-\frac{1}{2}} + \Delta t_{n+\frac{1}{2}}}{2\Delta t_{n-\frac{1}{2}}} f(y_n, t_n) - \frac{\Delta t_{n+\frac{1}{2}}}{2\Delta t_{n-\frac{1}{2}}} f(y_{n-1}, t_{n-1})\right),$$

where $\Delta t_{n+\frac{1}{2}} = t_{n+1} - t_n$, $\Delta t_{n-\frac{1}{2}} = t_n - t_{n-1}$.

3.1.1.3 The third order AB3 scheme

The third order scheme, AB3 sets

$$y_n = y_n + \Delta t_{n+\frac{1}{2}} \left(af\left(y_n, t_n\right) - bf\left(y_{n-1}, t_{n-1}\right) + cf\left(y_{n-1}, t_{n-2}\right) \right),$$

where

$$a = 1 + \frac{\Delta t_{n+\frac{1}{2}}}{6\Delta t_{n-\frac{3}{2}}} \left[\frac{\left(5\Delta t_{n+\frac{1}{2}} + 3\Delta t_{n-\frac{1}{2}}\right)}{\Delta t_{n-\frac{1}{2}}} - \frac{\left(2\Delta t_{n+\frac{1}{2}} + 3\Delta t_{n-\frac{1}{2}}\right)}{\left(\Delta t_{n-\frac{1}{2}} + \Delta t_{n-\frac{3}{2}}\right)} \right],$$

$$b = \frac{\Delta t_{n+\frac{1}{2}} \left(5\Delta t_{n+\frac{1}{2}} + 3\Delta t_{n-\frac{1}{2}}\right)}{6\Delta t_{n-\frac{1}{2}}\Delta t_{n-\frac{3}{2}}},$$

$$c = \frac{\Delta t_{n+\frac{1}{2}} \left(2\Delta t_{n+\frac{1}{2}} + 3\Delta t_{n-\frac{1}{2}}\right)}{6\left(\Delta t_{n-\frac{1}{2}} + \Delta t_{n-\frac{3}{2}}\right)\left(\Delta t_{n-\frac{3}{2}}\right)}.$$

3.1.1.4 The generic order k scheme

The generic scheme takes the form

$$y_{n+1} = y_n + \Delta t_{n+\frac{1}{2}} \sum_{i=0}^{k-1} a_i f\left(y_{n-i}, t_{n-i}\right),$$

where the coefficients, a_i, can be found by matching terms to the order k in the Taylor expansions of y_{n+1}, y_n and of the $f_{n-i} := f\left(y_{n-i}, t_{n-i}\right)$, i.e

$$y_{n+1} = y_n + \Delta t_{n+\frac{1}{2}} f_n + \sum_{s=1}^{\infty} \frac{\left(\Delta t_{n+\frac{1}{2}}\right)^{s+1}}{(s+1)!} \frac{d^s f}{dt^s},$$

$$f_{n-i} = f_n + \sum_{s=1}^{\infty} \frac{\left(t_{n-i} - t_n\right)^s}{s!} \frac{d^s f}{dt^s}.$$

This gives relations

$$a_0 = 1 - \sum_{i=1}^{k-1} a_i,$$

$$\sum_{j=1}^{k-1} A_{ij} a_j = \frac{\left(\Delta t_{n+\frac{1}{2}}\right)^{i+1}}{(i+1)!}$$

where

$$A_{ij} = \frac{\left(t_{n-j} - t_n\right)^i}{i!}.$$

3.1.2 Explicit Runge-Kutta Schemes

The family of Runge-Kutta timestepping schemes are a collection of multi-stage iterative methods for the solution of first order ODEs. Generically for an ODE for a variable, $y\left(t\right)$,

$$\frac{dy}{dt} = f\left(y, t\right),$$

they take the form of a set of coefficients $\boldsymbol{A}$, $\boldsymbol{b}$, $\boldsymbol{c}$, with relations

$$k_i = f\left(y_n + \sum_{j=1}^{s} A_{ij} k_j, t_n + b_i \Delta t\right),$$

$$y_{n+1} = y_n + \sum_{i=1}^{s} c_i k_i,$$

The family of explicit methods have $\boldsymbol{A}$ strictly lower triangular, so that the k_i can be built sequentially.

3.1.2.1 A first order scheme

This is just the forward Euler scheme

$$k_1 = f(y_n, t_n),$$
$$y_{n+1} = y_n + \Delta t_{n+\frac{1}{2}} k_1,$$

3.1.2.2 The second order RK2 scheme

Also known as the midpoint method,

$$k_1 = f(y_n, t_n),$$
$$k_2 = f\left(y_n + \frac{\Delta t_{n+\frac{1}{2}}}{2} k_1, t_n + \frac{\Delta t_{n+\frac{1}{2}}}{2}\right),$$
$$y_{n+1} = y_n + \Delta t_{n+\frac{1}{2}} k_2,$$

3.1.2.3 The third order RK3 scheme,

This scheme is sometimes used in TVD methods,

$$k_1 = f(y_n, t_n),$$
$$k_2 = f\left(y_n + \frac{\Delta t_{n+\frac{1}{2}}}{2} k_1, t_n + \frac{\Delta t_{n+\frac{1}{2}}}{2}\right),$$
$$k_3 = f\left(y_n + \Delta t_n (2k_2 - k_1), t_n + \Delta t_{n+\frac{1}{2}}\right),$$
$$y_{n+1} = y_n + \frac{\Delta t_{n+\frac{1}{2}}}{6}(k_1 + 4k_2 + k_3).$$

3.1.2.4 The fourth order RK4 scheme

This is probably the most famous method, aka "the Runge-Kutta method", which appears in the original paper,

$$k_1 = f(y_n, t_n),$$
$$k_2 = f\left(y_n + \frac{\Delta t_{n+\frac{1}{2}}}{2} k_1, t_n + \frac{\Delta t_{n+\frac{1}{2}}}{2}\right),$$
$$k_3 = f\left(y_n + \frac{\Delta t_{n+\frac{1}{2}}}{2} k_2, t_n + \frac{\Delta t_{n+\frac{1}{2}}}{2}\right),$$
$$k_4 = f\left(y_n + \Delta t_{n+\frac{1}{2}} k_3, t_n + \Delta t_{n+\frac{1}{2}}\right),$$
$$y_{n+1} = y_n + \frac{\Delta t_{n+\frac{1}{2}}}{6}(k_1 + 2k_2 + 2k_3 + k_4).$$

3.1.3 Timestep splitting

For reasons of stability

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