Integration of the Rigid Body Equations of Motion

The net translational force acting upon the rigid unit is

$$\underline{F} = \sum_{\alpha} \underline{f}_{\alpha} \tag{2.204}$$

where $\underline{f}_{\alpha}$ is the force on a rigid unit site, and the sum includes all sites α in the body. The translational motion can be integrated by the standard leapfrog algorithm.

$$\underline{V}(t + \frac{\Delta t}{2}) = \underline{V}(t - \frac{\Delta t}{2}) + \Delta t\ M^{-1} \underline{F}(t) \tag{2.205}$$

$$\underline{X}(t + \Delta t) = \underline{X}(t) + \Delta t\ \underline{V}(t + \frac{\Delta t}{2}) \tag{2.206}$$

where M is the mass of the rigid unit, $\underline{V}$ is the rigid bodies c.o.m. velocity and $\underline{X}$ is the c.o.m. position. The cartesian components of these quantitites are stored in the arrays: `gvxx`, `gvyy`, and `gvzz` for c.o.m. velocity; and `gcmx`, `gcmy`, and `gcmz` for c.o.m. position.

The torque acting upon the body in the space fixed frame is

$$\underline{\tau} = \sum_{\alpha} \underline{d}_{\alpha} \times \underline{f}_{\alpha}. \tag{2.207}$$

Transformed to the local body frame (and including the centrifugal terms) this is

$$\hat{\underline{\tau}} = \underline{\underline{\mathbf{R}}}^{T} \underline{\tau} + \underline{\eta}. \tag{2.208}$$

where

$$\eta_x = ((\hat{I})_{yy} - (\hat{I})_{zz}) \hat{\omega}_y \hat{\omega}_z \tag{2.209}$$

plus cyclic permutations for y and z components. The angular velocity transformed to the local body frame, $\hat{\omega}$, can then be integrated using the leapfrog algorithm and the diagonal rotational inertia tensor.

$$\hat{\omega}(t+\frac{\Delta t}{2}) = \hat{\omega}(t-\frac{\Delta t}{2}) + \Delta t\, \hat{\underline{\underline{\mathbf{I}}}}^{-1} \hat{\underline{\tau}}(t) \tag{2.210}$$

The new quaternions cannot be found so simply. DL_POLY_2 uses Fincham's implicit quaternion algorithm (FIQA) to do this [14]. In this algorithm the new quaternions are found by solving the implicit equation

$$\underline{q}(t+\Delta t) = \underline{q}(t) + \frac{\Delta t}{2} \left(\underline{\underline{\mathbf{Q}}}[\underline{q}(t)]\underline{\hat{w}}(t) + \underline{\underline{\mathbf{Q}}}[\underline{q}(t+\Delta t)]\underline{\hat{w}}(t+\Delta t) \right) \tag{2.211}$$

where $\underline{\hat{w}} = [0, \hat{\omega}]^T$ and $\underline{\underline{\mathbf{Q}}}[\underline{q}]$ is

$$\underline{\underline{\mathbf{Q}}} = \frac{1}{2} \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & -q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \tag{2.212}$$

The above equation is solved iteratively with

$$\underline{q}(t+\Delta t) = \underline{q}(t) + \Delta t\ \underline{\underline{\mathbf{Q}}}[\underline{q}(t)]\underline{\hat{w}}(t) \tag{2.213}$$

as the first guess. Typically no more than 3 or 4 iterations are needed for convergence. At each step the constraint

$$\|\underline{q}(t+\Delta t)\| = 1 \tag{2.214}$$

is imposed.

The quaternions are stored in the arrays `q0, q1, q2` and `q3`. The angular velocity (transformed to the body fixed frame) is stored in the arrays `omx, omy` and `omx`, while the work arrays `opx, opy, opz, oqx, oqy, oqz` hold values of $\hat{\omega}(t)$ and $\hat{\omega}(t+\Delta t)$. The torques, $\hat{\tau}(t)$ are held in the work arrays `tqx, tqy` and `tqz`.

The NVE algorithm is implemented in NVEQ_1 which allows for a system containing a mixture of rigid bodies and atomistic species, provided the rigid bodies are not linked to other species by constraint bonds.

Thermostats and Barostats It is straightforward to couple the rigid body equations of motion to a thermostat and/or barostat. The thermostat is coupled to both the translational and rotational degrees of freedom and so both the translational and rotational velocities are propagated in an analogous manner to the thermostated atomic velocities. The barostat, however, is coupled only to the translational degrees of freedom, not to the rotational ones.DL_POLY_2 supports both Hoover type and Berendsen thermostats and barostats for systems containing rigid bodies. The Hoover thermostat is implemented in NVTQ/SMALL>_H1, the Hoover isotropic barostat (plus themostat) in NPTQ/SMALL>_H1 and the anisotropic barostat in NSTQ/SMALL>_H1. The analogous routines for the Berendsen algorithms are NVTQ/SMALL>_B1, NPTQ/SMALL>_B1 and NSTQ/SMALL>_B1.

Next Up Previous Contents Index
Next: Linked Rigid Bodies **Up:** Rigid Bodies and Rotational **Previous:** Description of Rigid Body **Contents** **Index**
W Smith 2003-05-12