

AN EFFICIENT ALGORITHM FOR CONSTRAINT DYNAMICS

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In constraint dynamics one solves the Newton equations of motion of the particles along with the holonomic constraints on a given set of particles. The holonomic constraints are generally of the form

$$(\vec{r}_i - \vec{r}_j)^2 - d_{ij}^2 = 0 \quad (1)$$

where \vec{r}_i and \vec{r}_j are the positions of particle i and j of the given set and d_{ij} is the preassigned bond length between these particles constituting the molecule.

The numerical technique used in constraint dynamics is:

1. First to solve the unconstrained Newton equations using some convenient algorithm, e.g. Verlet or leapfrog and thereby obtain the unconstrained positions from the initial constrained positions;
2. Then to use these unconstrained positions in eq.(1) to find constrained positions, the difference in unconstrained and constrained positions are used to calculate the velocities of the constrained particles from the unconstrained velocities. The details of the numerical procedure is given in ref.1 and 2.

Basically, if the unconstrained positions are \vec{r}_i^u and \vec{r}_j^u and the corresponding constrained positions are \vec{r}_i^c and \vec{r}_j^c such that

$$\vec{r}_i^c = \vec{r}_i^u + \delta\vec{r}_i$$

and $\vec{r}_j^c = \vec{r}_j^u + \delta\vec{r}_j$

then one has to solve

$$((\vec{r}_i^u - \delta\vec{r}_i) - (\vec{r}_j^u - \delta\vec{r}_j))^2 - d_{ij}^2 = c_k = 0 \quad (2)$$

In fact there will be a set of simultaneous equations of the above type, each constraining a pair of particles in the molecule.

An approximate solution of these equations can be obtained by using an iterative method of root finding (Newton iteration). It is well known that the convergence of such an iterative method depends very much on the curvature of hyper-surface given by eqn.(2).

Another form of holonomic constraint which can lead to a faster convergence than eqn.(1) is

$$|\vec{r}_i - \vec{r}_j| - d_{ij} = 0 \quad (3)$$

The simultaneous equations corresponding to eqn.(2), for this constraint are

$$|(\vec{r}_i - \delta\vec{r}_i) - (\vec{r}_j - \delta\vec{r}_j)| - d_{ij} = c_k = 0 \quad (4)$$

Faster convergence in this case is possible because the hypersurface given by eqn.(4) is much flatter than the former.

In fact in the iterative calculation of eqn.(4) one need not calculate the first derivative of c_k at each and every iteration. Considerable computational time can be saved by using the initial value of this derivative calculated at the beginning of the iteration for negligibly small sacrifice of convergence.

These constraints (eqn.(2) and eqn.(4)) are used to simulate a system of water molecules ($2H^+$ and O^{2-}) at very high temperature. Typically first method (eqn.(2)) requires 10 iterations as compared to 5 iterations by second method (eqn.(4)) to achieve $10^{-7}\%$ accuracy in the position.

References

- ¹ J.P. Ryckaert, G. Ciccotti and H.J.C. Berendsen, *J. Comput. Phys.* 23 (1977) 327.
- ² M.K. Memon, R.W. Hockney and S.K. Mitra, *J. Comput. Phys.* (1981) In press.