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DISCRETE MECHANICS FOR ANISOTROPIC POTENTIALS

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ABSTRACT

In previous work, a new type of numerical method for the solution of equations of motion was derived, denoted "discrete mechanics", which has the unique property of conserving the additive constants of motion exactly. The discrete mechanics' "forces" were obtained for the case of a general, separable potential with radial dependences. In the present work, discrete mechanics is extended to include potentials with anisotropy.

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In previous work [1], an energy and angular momentum conserving numerical method--"discrete mechanics"--was derived for the case of a separable, radially dependent potential ϕ : i.e., ϕ is of the form

$$\phi(r_1,r_2,\ldots,r_n) = \phi_1(r_1)\phi_2(r_2)\ldots\phi_n(r_n) \tag{1}$$

or is composed of a sum of terms of this type. Here $\vec{r}_i$ is the coordinate vector of a particle i of a system of n particles, and r_i is its magnitude. For a complete description of the mechanics of the motion of the n particles subject to the potential ϕ , as well as the basic formulae of "discrete mechanics", see [1]. The "discrete mechanics" solution is specified in terms of the implicit formulae for the "forces" $\vec{F}_i^{\,*}$ (see equation (5.71) of [1]):

$$\vec{F}_i^{\,*} = -\frac{\tilde{\Delta\phi_i}}{\Delta r_i}\,\frac{\vec{r}_i{}'+\vec{r}_i}{r_i'+r_i} \tag{2}$$

where the primes denote values at the new time $t' = t + \Delta t$, and where

$$\Delta r_i = r_i' - r_i \tag{3}$$

and

$$\tilde{\Delta\phi_i} = \frac{\phi_i'-\phi_i}{n}\sum_{\ell=0}^{n-1}\frac{1}{\binom{n-1}{\ell}}\sum_{1}^{\binom{n-1}{\ell}}\left(\prod_{s=1}^{\ell}\phi_{i_s}'\right)\left(\prod_{s=\ell+1}^{n-1}\phi_{i_s}\right) \tag{4}$$

In equation (4),

$$\phi_j' = \phi_j(r_j') \tag{5}$$

and the inner sum is over all combinations of the ϕ_{i_s} $(i_s \neq i)$ of which ℓ are primed and $n - 1 - \ell$ are unprimed.[5] (The notation is such that null products with upper limits smaller than lower limits have value unity.) For example, if $n = 1$, then

$$\tilde{\Delta\phi_i} = \phi_i' - \phi_i \tag{6}$$

For $n = 2$,

$$\tilde{\Delta\phi_i} = \frac{\phi_i'-\phi_i}{2} [\phi_j'+\phi_j] \qquad (j \neq i) \tag{7}$$

Finally, if $n = 3$,

$$\tilde{\Delta\phi_i} = \frac{\phi_i'-\phi_i}{3} [\phi_j'\phi_k' + \tfrac{1}{2}(\phi_j'\phi_k+\phi_j\phi_k') + \phi_j\phi_k] \qquad (j \neq i\ ,\ k \neq i,j) \tag{8}$$

Although many fundamental interactions are expressible in the separable form of equation (1), in certain problems "anisotropic" potentials arise which depend directly upon the angles between the radius vectors $\vec{r}_i$. Such potentials are usually obtained from the perturbation of a spherical distribution of mass or charge: e.g., the oblateness of the sun [2], or the shapes of molecules [3]. As an illustration, a typical case might have a potential term of the form

$$\phi(r_1,r_2) = \phi_1(r_1)\phi_2(r_2)\phi_{12}(\alpha_{12}) \tag{9}$$

where $n = 2$ and

$$\alpha_{12} = \vec{r}_1 \cdot \vec{r}_2 \tag{10}$$

For ϕ given by equation (9), the exact forces are

$$\vec{F}_1 = -\frac{\partial\phi}{\partial\vec{r}_1} \tag{11a}$$

$$= -\phi_2\phi_{12}\frac{d\phi_1}{dr_1}\frac{\vec{r}_1}{r_1} - \phi_1\phi_2\frac{d\phi_{12}}{d\alpha_{12}}\vec{r}_2 \tag{11b}$$

and

$$\vec{F}_2 = -\frac{\partial\phi}{\partial\vec{r}_2} \tag{12a}$$

$$= -\phi_1\phi_2\frac{d\phi_{12}}{d\alpha_{12}}\vec{r}_1 - \phi_1\phi_{12}\frac{d\phi_2}{dr_2}\frac{\vec{r}_2}{r_2} \tag{12b}$$

Because of the form of equations (11) and (12), the discrete mechanics "forces", in order to maintain consistency, may reasonably be expected to be composed also of two contributions, or:

$$\vec{F}_1^{\,*} = \vec{F}_{11}^{\,*} + \vec{F}_{12}^{\,*} \tag{13a}$$

$$\vec{F}_2^{\,*} = \vec{F}_{21}^{\,*} + \vec{F}_{22}^{\,*} \tag{13b}$$

where $\vec{F}_{11}^{\,*}$ and $\vec{F}_{12}^{\,*}$ are approximations to the two terms in equation (11b) and $\vec{F}_{21}^{\,*}$ and $\vec{F}_{22}^{\,*}$ are approximations to the two terms of equation (12b).

The forms of the $\vec{F}_{ij}^{\,*}$ may be ascertained via consideration of the requirement of conservation of angular momentum. From equation (5.39) of [1], this condition requires

$$\frac{\vec{r}_1{}'+\vec{r}_1}{2} \times \vec{F}_1{}^* + \frac{\vec{r}_2{}'+\vec{r}_2}{2} \times \vec{F}_2 = \vec{0} \qquad (14)$$

which must hold for all values of $\vec{r}_1$, $\vec{r}_2$, $\vec{r}_1{}'$ and $\vec{r}_2{}'$. The general solution to equation (14) is given by

$$\vec{F}_1{}^* = F_{11}{}^* \ (\vec{r}_1{}'+\vec{r}_1) + F_{12}{}^* \ (\vec{r}_2{}'+\vec{r}_2) \qquad (15a)$$

$$\vec{F}_2{}^* = F_{21}{}^* \ (\vec{r}_1{}'+\vec{r}_1) + F_{22}{}^* \ (\vec{r}_2{}'+\vec{r}_2) \qquad (15b)$$

with $F_{12}{}^* = F_{21}{}^*$ and the $F_{ij}{}^*$ otherwise unrestricted. By comparison of equations (13) and (15), satisfactory choices for the $\vec{F}_{ij}{}^*$ are

$$\vec{F}_{11}{}^* = F_{11}{}^* \ (\vec{r}_1{}'+\vec{r}_1) \qquad (16a)$$

$$\vec{F}_{12}{}^* = F_{12}{}^* \ (\vec{r}_2{}'+\vec{r}_2) \qquad (16b)$$

$$\vec{F}_{21}{}^* = F_{21}{}^* \ (\vec{r}_1{}'+\vec{r}_1) \qquad (16c)$$

$$\vec{F}_{22}{}^* = F_{22}{}^* \ (\vec{r}_2{}'+\vec{r}_2) \qquad (16d)$$

The symmetric matrix of coefficients $F_{ij}{}^*$ remains to be determined. From equation (5.24b) of [1], conservation of energy requires

$$\vec{F}_1{}^* \cdot (\vec{r}_1{}'-\vec{r}_1) + \vec{F}_2{}^* \cdot (\vec{r}_2{}'-\vec{r}_2) = \phi_1\phi_2\phi_{12} - \phi_1{}'\phi_2{}'\phi_{12}{}' \qquad (17)$$

Substitution of equation (15) into equation (17) yields

$$\Delta T_1 + \Delta T_2 + \Delta T_{12} = \phi_1\phi_2\phi_{12}-\phi_1{}'\phi_2{}'\phi_{12}{}' \qquad (18)$$

where

$$\Delta T_1 = F_{11}^* \; [(r_1')^2 - r_1^2] \tag{19a}$$

$$\Delta T_2 = F_{22}^* \; [(r_2')^2 - r_2^2] \tag{19b}$$

$$\Delta T_{12} = 2F_{12}^* \; (\alpha_{12}' - \alpha_{12}) \tag{19c}$$

Now, equation (18) is identical in form to equation (5-50) of [1] for $n = 3$ (i.e., <u>three</u> particles) if a pseudoradius $r_3 = \alpha_{12}$ is defined. Therefore, the solution obtained in [1] for equation (5.50) also suffices for equation (17), if α_{12} is substituted for r_3 :

$$\Delta T_1 = -\Delta\tilde{\phi}_1 \tag{20a}$$

$$\Delta T_2 = -\Delta\tilde{\phi}_2 \tag{20b}$$

$$\Delta T_{12} = -\Delta\tilde{\phi}_{12} \tag{20c}$$

where the $\Delta\tilde{\phi}$ are given by equation (8), i.e.,

$$\Delta\tilde{\phi}_1 = \frac{1}{3}[\phi_2'\phi_{12}' + \frac{1}{2}(\phi_2'\phi_{12} + \phi_2\phi_{12}') + \phi_2\phi_{12}] \; (\phi_1' - \phi_1) \tag{21a}$$

$$\Delta\tilde{\phi}_2 = \frac{1}{3}[\phi_1'\phi_{12}' + \frac{1}{2}(\phi_1'\phi_{12} + \phi_1\phi_{12}') + \phi_1\phi_{12}] \; (\phi_2' - \phi_2) \tag{21b}$$

$$\Delta\tilde{\phi}_{12} = \frac{1}{3}[\phi_1'\phi_2' + \frac{1}{2}(\phi_1'\phi_2 + \phi_1\phi_2') + \phi_1\phi_2] \; (\phi_{12}' - \phi_{12}) \tag{21c}$$

Substituting equations (20) and (21) into equations (19) then gives the discrete mechanics "forces" corresponding to ϕ of the form of equation (9):

$$\vec{F}_1^{\,*} = -\frac{\Delta\tilde{\phi}_1}{\Delta r_1}\,\frac{\vec{r}_1{}'+\vec{r}_1}{r_1{}'+r_1} - \frac{\Delta\tilde{\phi}_{12}}{\Delta\alpha_{12}}\,\frac{\vec{r}_2{}'+\vec{r}_2}{2} \qquad (22a)$$

$$\vec{F}_2^{\,*} = -\frac{\Delta\tilde{\phi}_{12}}{\Delta\alpha_{12}}\,\frac{\vec{r}_1{}'+\vec{r}_1}{2} - \frac{\Delta\tilde{\phi}_2}{\Delta r_2}\,\frac{\vec{r}_2{}'+\vec{r}_2}{r_2{}'+r_2} \qquad (22b)$$

where $\Delta\alpha_{12} = \alpha_{12}{}' - \alpha_{12}$. In the limit $\Delta t \to 0$, equations (22) of course reduce to equations (11) and (12).

In summary, for the case of a potential ϕ of the form given by equation (9), the discrete mechanics forces are obtained by considering the r_1 and r_2 terms in the energy and angular momentum simultaneously. The resulting implicit expressions for $\vec{F}_1^{\,*}$ and $\vec{F}_2^{\,*}$ are given by equations (22) and (21). The $\vec{F}_i^{\,*}$ for the general case of an n-body system with a more complicated form of ϕ may be obtained in an analogous way by treating the $\vec{r}_i \cdot \vec{r}_j$ the same as radial dependences, with vector directions determined as above in equations (15).

As remarked in [1], the same discrete mechanics solution holds for the case of ϕ dependent upon the distances $\vec{r}_{ij}$ <u>between</u> particles, if the $\vec{r}_{ij}$ are used as the $\vec{r}_i$ and n is replaced by $N = n(n-1)/2$.

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3. See, e.g., J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, Molecular Theory of Gases and Liquids, Wiley, N.Y., 1967, Chapters 12-14.

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16. Abstracts

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