BULLETIN OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 79, Number 2, March 1973

AN ALGEBRAIC, ENERGY CONSERVING FORMULATION OF CLASSICAL MOLECULAR AND NEWTONIAN n-BODY INTERACTION

BY DONALD GREENSPAN

Communicated by Fred Brauer, August 14, 1972

1. **Introduction.** In this note we will develop a unifying theory of collisionless n-body problems which includes both Newtonian and classical molecular forces. By using only *differences* to simulate physical concepts and *difference* equations to determine dynamical behavior, the resulting theory will be completely arithmetic in nature. Thus, we will have the advantages of mathematical simplicity and computer compatibility. The formulation will have special value for problems involving large amounts of energy, since it will be energy conserving.

2. **Basic concepts.** For positive time step Δt, let $t_k = k\Delta t$, $k = 0, 1, 2, \ldots$. At time t_k, let particle P_i of mass m_i be located at $\boldsymbol{x}_{i,k} = (x_{i,k}, y_{i,k}, z_{i,k})$, have velocity $\boldsymbol{v}_{i,k} = (v_{i,k,x}, v_{i,k,y}, v_{i,k,z})$, and have acceleration $\boldsymbol{a}_{i,k} = (a_{i,k,x}, a_{i,k,y}, a_{i,k,z})$, for $i = 1, 2, \ldots, n$. Position, velocity, and acceleration are assumed to be related by the fundamental formulas [**2**]:

$$(\boldsymbol{v}_{i,k+1} + \boldsymbol{v}_{i,k})/2 = (\boldsymbol{x}_{i,k+1} - \boldsymbol{x}_{i,k})/(\Delta t), \tag{2.1}$$

$$\boldsymbol{a}_{i,k} = (\boldsymbol{v}_{i,k+1} - \boldsymbol{v}_{i,k})/(\Delta t). \tag{2.2}$$

If $\boldsymbol{F}_{i,k} = (F_{i,k,x}, F_{i,k,y}, F_{i,k,z})$ is the force acting on P_i at time t_k, then force and acceleration are assumed to be related by the discrete dynamical equation

$$\boldsymbol{F}_{i,k} = m_i\,\boldsymbol{a}_{i,k}. \tag{2.3}$$

The work W_i done by $\boldsymbol{F}_{i,k}$ on P_i from initial time t_0 to terminal time t_N is defined by

$$W_i = \sum_{k=0}^{N-1} [(\boldsymbol{x}_{i,k+1} - \boldsymbol{x}_{i,k}) \cdot \boldsymbol{F}_{i,k}], \tag{2.4}$$

while the total work W done on the system from time t_0 to time t_N is defined by

$$W = \sum_{i=1}^{n} W_i. \tag{2.5}$$

AMS(MOS) subject classifications (1970). Primary 70F10, 39A10.

Copyright © American Mathematical Society 1973

3. **Conservation of kinetic energy.** From (2.1)–(2.4), it follows that

$$W_i = m_i \sum_{k=0}^{N-1} [(x_{i,k+1} - x_{i,k})a_{i,k,x} + (y_{i,k+1} - y_{i,k})a_{i,k,y} + (z_{i,k+1} - z_{i,k})a_{i,k,z}]$$

$$= \tfrac{1}{2}m_i \sum_{k=0}^{N-1} [(v_{i,k+1,x}^2 - v_{i,k,x}^2) + (v_{i,k+1,y}^2 - v_{i,k,y}^2) + (v_{i,k+1,z}^2 - v_{i,k,z}^2)]$$

$$= \tfrac{1}{2}m_i(v_{i,N,x}^2 + v_{i,N,y}^2 + v_{i,N,z}^2) - \tfrac{1}{2}m_i(v_{i,0,x}^2 + v_{i,0,y}^2 + v_{i,0,z}^2).$$

Thus, if the kinetic energy $K_{i,k}$ of P_i at t_k is defined by

$$K_{i,k} = \tfrac{1}{2}m_i(v_{i,k,x}^2 + v_{i,k,y}^2 + v_{i,k,z}^2), \tag{3.1}$$

then

$$W_i = K_{i,N} - K_{i,0}. \tag{3.2}$$

Finally, if the kinetic energy K_k of the system at t_k is defined by

$$K_k = \sum_{i=0}^{n} K_{i,k}, \tag{3.3}$$

then (2.5), (3.2), and (3.3) imply

$$W = K_N - K_0, \tag{3.4}$$

which is called the law of conservation of kinetic energy.

It is interesting to note that (3.4) is valid independently of the specific structure of the forces involved.

4. **The n-body force law.** In order to simulate Newtonian gravitation and various classical laws of molecular interaction ([**1**], [**5**]), we will structure the force between each pair of particles to consist of a component of attraction which behaves like $p/(r^\alpha)$ and a component of repulsion which behaves like $q/(r^\beta)$, where p, q, α, and β are nonnegative parameters and r is the distance between the particles, as follows. Let $r_{ij,k}$ be the distance between P_i and P_j at time t_k. Then $\boldsymbol{F}_{i,k}$, the force exerted on P_i by P_j, is defined by

$$\boldsymbol{F}_{i,k} = m_i \sum_{j=1;j\neq i}^{n} \left\{ m_j \left(-\frac{p\sum_{\xi=0}^{\alpha-2}(r_{ij,k}^{\xi}\, r_{ij,k+1}^{\alpha-\xi-2})}{r_{ij,k}^{\alpha-1}\, r_{ij,k+1}^{\alpha-1}\,(r_{ij,k+1} + r_{ij,k})} + \frac{q\sum_{\xi=0}^{\beta-2}(r_{ij,k}^{\xi}\, r_{ij,k+1}^{\beta-\xi-2})}{r_{ij,k}^{\beta-1}\, r_{ij,k+1}^{\beta-1}\,(r_{ij,k+1} + r_{ij,k})} \right) (\boldsymbol{x}_{i,k+1} + \boldsymbol{x}_{i,k} - \boldsymbol{x}_{j,k+1} - \boldsymbol{x}_{j,k}) \right\}. \tag{4.1}$$

In particular, (4.1) defines discrete Newtonian gravitation when $p = G$, $q = 0$, $\alpha = 2$, while it defines a force with discrete Lennard-Jones potential when $\alpha = 7$, $\beta = 13$.

5. **Conservation of energy.** Consider now formula (2.5) with force defined by (4.1). In this connection the following lemma will be of value.

LEMMA. *For $n \geqq 2$, the following identity is valid:*

$$\sum_{j=1;j\neq i}^{n}\sum_{i=1}^{n}\left[\frac{m_i m_j \sum_{\xi=0}^{\alpha-2}(r_{ij,k}^{\xi}\, r_{ij,k+1}^{\alpha-\xi-2})}{r_{ij,k}^{\alpha-1}\, r_{ij,k+1}^{\alpha-1}(r_{ij,k+1}+r_{ij,k})}(\boldsymbol{x}_{i,k+1}+\boldsymbol{x}_{i,k}-\boldsymbol{x}_{j,k+1}-\boldsymbol{x}_{j,k})\cdot(\boldsymbol{x}_{i,k+1}-\boldsymbol{x}_{i,k})\right] \tag{5.1}$$
$$\equiv \sum_{i,j=1;i<j}^{n}\left\{m_i m_j\left(\frac{r_{ij,k+1}^{\alpha-1}-r_{ij,k}^{\alpha-1}}{r_{ij,k}^{\alpha-1}\, r_{ij,k+1}^{\alpha-1}}\right)\right\}.$$

PROOF. The proof follows readily by mathematical induction on n. From (2.5), (4.1), and (5.1), then,

$$W = \sum_{k=0}^{N-1}\sum_{i,j=1;i<j}^{n}\left\{m_i m_j\left(-p\frac{r_{ij,k+1}^{\alpha-1}-r_{ij,k}^{\alpha-1}}{r_{ij,k}^{\alpha-1}\, r_{ij,k+1}^{\alpha-1}}+q\frac{r_{ij,k+1}^{\beta-1}-r_{ij,k}^{\beta-1}}{r_{ij,k}^{\beta-1}\, r_{ij,k+1}^{\beta-1}}\right)\right\}$$
$$= \sum_{i,j=1;i<j}^{n}\left\{m_i m_j\left[-p\left(\frac{1}{r_{ij,0}^{\alpha-1}}-\frac{1}{r_{ij,N}^{\alpha-1}}\right)+q\left(\frac{1}{r_{ij,0}^{\beta-1}}-\frac{1}{r_{ij,N}^{\beta-1}}\right)\right]\right\}.$$

Defining the potential energy $V_{ij,k}$ of the pair P_i and P_j at time t_k by

$$V_{ij,k} = (-p/r_{ij,k}^{\alpha-1} + q/r_{ij,k}^{\beta-1})m_i m_j$$

then yields

$$W = \sum_{i,j=1;i<j}^{n} V_{ij,0} - \sum_{i,j=1;i<j}^{n} V_{ij,N}.$$

Defining the potential energy V_k of the system at t_k by

$$V_k = \sum_{i,j=1;i<j}^{n} V_{ij,k}$$

then implies

$$W = V_0 - V_N. \tag{5.2}$$

Finally, elimination of W between (3.4) and (5.2) yields

$$K_N + V_N = K_0 + V_0, \qquad N = 0, 1, 2, \ldots, \tag{5.3}$$

which is the classical law of conservation of energy.

6. **Remarks.** Let us note first that the algebraic formulation of this paper

yields other basic classical results. With regard to initial value problems, for example, (2.3) and (4.1) imply

$$\sum_{i=1}^{n} m_i \boldsymbol{a}_{i,k} = \boldsymbol{0}, \tag{6.1}$$

so that, from (2.2),

$$\sum_{i=1}^{n} m_i(\boldsymbol{v}_{i,k+1} - \boldsymbol{v}_{i,k}) = \boldsymbol{0}. \tag{6.2}$$

Summing both sides of (6.2) over k from 0 to $s - 1$, where $s \geqq 1$, yields

$$\sum_{i=1}^{n} m_i(\boldsymbol{v}_{i,s} - \boldsymbol{v}_{i,0}) = \boldsymbol{0}. \tag{6.3}$$

Since (6.3) is valid also for $s = 0$, then

$$\sum_{i=1}^{n} m_i \boldsymbol{v}_{i,s} = \boldsymbol{c}_1, \qquad s \geqq 0, \tag{6.4}$$

where $\boldsymbol{c}_1$ is a constant vector. Formula (6.4) is, of course, the law of conservation of linear momentum. From (6.4) it then follows that

$$\sum_{i=1}^{n} m_i \left(\frac{\boldsymbol{v}_{i,s+1} + \boldsymbol{v}_{i,s}}{2} \right) = \boldsymbol{c}_1, \qquad s \geqq 0. \tag{6.5}$$

Thus, from (2.1),

$$\sum_{i=1}^{n} m_i(\boldsymbol{x}_{i,s+1} - \boldsymbol{x}_{i,s}) = (\Delta t)\boldsymbol{c}_1, \qquad s \geqq 0. \tag{6.6}$$

Summing both sides of (6.6) over s from 0 to $r - 1$, for $r \geqq 1$, implies

$$\sum_{i=1}^{n} m_i(\boldsymbol{x}_{i,r} - \boldsymbol{x}_{i,0}) = t_r \boldsymbol{c}_1. \tag{6.7}$$

However, (6.7) is valid also for $r = 0$, so that

$$\sum_{i=1}^{n} m_i \boldsymbol{x}_{i,r} = t_r \boldsymbol{c}_1 + \boldsymbol{c}_2, \tag{6.8}$$

where $\boldsymbol{c}_2$ is a constant vector. Finally, set $M = \sum_{i=1}^{n} m_i$ and let $\boldsymbol{X}_r$ be the center of gravity of the system at time t_r. Then (6.8) implies

$$M\boldsymbol{X}_r = t_r \boldsymbol{c}_1 + \boldsymbol{c}_2,$$

from which it follows that the motion of the centroid is linear.

Finally, note that analogous techniques ([**3**], [**4**]) yield the same results of this paper for discrete mechanical systems in which (2.2) is replaced by either

$$(a_{i,k+1} + a_{i,k})/2 = (v_{i,k+1} - v_{i,k})/(\Delta t),$$

or

$$\tfrac{1}{2}(3a_{i,k} - a_{i,k-1}) = (v_{i,k+1} - v_{i,k})/(\Delta t).$$

REFERENCES

1. R. P. Feynman, R. B. Leighton and M. Sands, *The Feynman lectures on physics*. Vol. 1: *Mainly mechanics, radiation, and heat*, Addison-Wesley, Reading, Mass., 1963. MR **35** #3942.

2. D. Greenspan, *Introduction to numerical analysis and applications*, Markham, Chicago, Ill., 1971. MR **42** #7028.

3. ———, *New forms of discrete mechanics*, Kybernetes **1** (1972), 87–101.

4. ———, *A new explicit discrete mechanics with applications*, TR 23, Computing Center, University of Wisconsin, Madison, Wis., 1971; J. Franklin Inst. **294** (1972), 231–240.

5. J. O. Hirschfelder, C. F. Curtiss and R. B. Bird, *Molecular theory of gases and liquids*, Wiley, New York, 1954.

COMPUTER SCIENCE DEPARTMENT, UNIVERSITY OF WISCONSIN, MADISON, WISCONSIN 53706