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

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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

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

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