

Chapter 1

Mathematical, Physical, and Computational Preliminaries

1.1. The N-Body Problem

The fundamental mathematical problem considered throughout this book is a non continuum problem called the N-body problem, which is described in complete generality as follows. In cgs units and for $i = 1, 2, \dots, N$, let P_i of mass m_i be at $\vec{r}_i = (x_i, y_i, z_i)$, have velocity $\vec{v}_i = (v_{i,x}, v_{i,y}, v_{i,z})$, and have acceleration $\vec{a}_i = (a_{i,x}, a_{i,y}, a_{i,z})$ at time $t \geq 0$. Let the positive distance between P_i and $P_j, i \neq j$, be $r_{ij} = r_{ji} \neq 0$. Let the force on P_i due to P_j be $\vec{F}_{ij} = \vec{F}_{ij}(r_{ij})$, so that the force depends only on the distance between P_i and P_j . Also, assume that the force \vec{F}_{ji} on P_j due to P_i satisfies $\vec{F}_{ji} = -\vec{F}_{ij}$. Then, given the initial positions and velocities of all the $P_i, i = 1, 2, 3, \dots, N$, the general N -body problem is to determine the motion of the system if each P_i interacts with all the other P_j 's in the system.

The prototype N -body problem was formulated in about 1900. In it the P_i were the Sun and the then known eight planets, and the force on each P_i was gravitational attraction. This problem is exceptionally difficult for $N \geq 3$. The additional difficulties with the problems to be considered in this book arise from the fact that we will be concerned with the interactions of molecules and particles (molecular aggregates), for which the forces are more complex than gravitation.

1.2. Classical Molecular Potentials

Classical molecular forces behave, in general, as follows (Feynman, Leighton and Sands (1973)). When two *close* (to be made precise shortly) molecules are pulled apart, they attract. When pushed together, they repel. And

the force of repulsion is of a greater order of magnitude than the force of attraction.

Perhaps the most important exception to the behavior just described is the basic fluid of all living matter, namely, liquid water, and this will be discussed later.

Example. Consider two hypothetical molecules P_1, P_2 on an X axis as shown in Fig. 1.1. Let P_1 be at the origin and let P_2 be R units from $P_1, R > 0$. Let \vec{F} be the force P_1 exerts on P_2 and let F be the magnitude of \vec{F} . Suppose

$$F = \frac{1}{R^{13}} - \frac{1}{R^7}.$$

Then, if $R = 1, F = 0$, and the molecules are in equilibrium. If $R > 1$, say, $R = 2$, then

$$F = \frac{1}{2^{13}} - \frac{1}{2^7} < 0,$$

so that \vec{F} acts toward the origin, which corresponds to attraction. If $R < 1$, say, $R = 0.1$, then

$$F = \frac{1}{0.1^{13}} - \frac{1}{0.1^7} > 0,$$

so that \vec{F} acts away from the origin, which corresponds to repulsion. Note that F is unbounded as R converges to zero, so that as R converges to zero the interaction of the two molecules can be extremely volatile.

There are a variety of classical molecular potentials for the interactions of molecules and from these classical molecular force formulas can be derived (Hirschfelder, Curtiss and Bird (1967)). There are, for example, Buckingham, Lennard–Jones, Morse, Slater–Kirkwood, Stockmayer, Sutherland, and Yntema–Schneider potentials. The potential which has received the most attention is the Lennard–Jones potential, that is,

$$\phi(r_{ij}) = 4\epsilon \left[\frac{\sigma^{12}}{r_{ij}^{12}} - \frac{\sigma^6}{r_{ij}^6} \right] \text{ erg},$$

some examples of which can be found in Table 1.1.

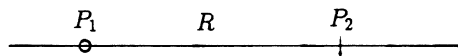


Fig. 1.1. Force interaction.

Let us turn attention first to a Lennard–Jones potential for argon vapor. We examine this first because it is thought that for argon, the Lennard–Jones potential is *quantitatively* accurate (Koplik and Banavar (1998)). The potential is

$$\phi(r_{ij}) = (6.848)10^{-14} \left[\frac{3.418^{12}}{r_{ij}^{12}} - \frac{3.418^6}{r_{ij}^6} \right] \text{erg} \left(\frac{\text{grcm}^2}{\text{sec}^2} \right) \quad (1.1)$$

in which r_{ij} is measured in angstroms (\AA). The force \vec{F}_{ij} exerted on P_i by P_j is then

$$\vec{F}_{ij} = (6.848)10^{-14} \left[\frac{12(3.418)^{12}}{r_{ij}^{13}} - \frac{6(3.418)^6}{r_{ij}^7} \right] (10)^8 \frac{\vec{r}_{ji}}{r_{ij}} \text{dynes} \left(\frac{\text{grcm}}{\text{sec}^2} \right). \quad (1.2)$$

Note that in deriving (1.2) from (1.1), one must use the chain rule

$$F_{ij} = -\frac{d\phi(r_{ij})}{dR} = -\frac{d\phi(r_{ij})}{dr_{ij}} \frac{dr_{ij}}{dR}$$

and the fact that $R \text{ cm} = 10^8 R \text{\AA}$, that is, $r_{ij} = 10^8 R$. Hence, (1.2) reduces readily to

$$\vec{F}_{ij} = \left[\frac{209.0}{r_{ij}^{13}} - \frac{0.06551}{r_{ij}^7} \right] \frac{\vec{r}_{ji}}{r_{ij}} \text{dynes} \left(\frac{\text{grcm}}{\text{sec}^2} \right). \quad (1.3)$$

Table 1.1. Lennard–Jones (6–12) Potentials

$$\phi(r_{ij}) = 4\epsilon \left[\frac{\sigma^{12}}{r_{ij}^{12}} - \frac{\sigma^6}{r_{ij}^6} \right] \text{erg}, \quad k = (1.381)10^{-16}.$$

Gas	ϵ/k ($^\circ\text{K}$)	σ (\AA)
Ar	124	3.418
Ne	35.7	2.789
CO	110	3.590
CO ₂	190	3.996
NO	119	3.470
CH ₄	137	3.822
SO ₂	252	4.290
F ₂	112	3.653
Cl ₂	357	4.115
C ₆ H ₆	440	5.270
Air	97.0	3.617

Note also that

$$F_{ij} = \|\vec{F}_{ij}\| = \left[\frac{209.0}{r_{ij}^{13}} - \frac{0.06551}{r_{ij}^7} \right],$$

so that $F_{ij}(r_{ij}) = 0$ implies that $r_{ij} = 3.837 \text{ \AA}$, which is the *equilibrium* distance.

1.3. Molecular Mechanics

Molecular mechanics is the simulation of molecular interaction as an N-body problem using classical molecular potentials and Newtonian mechanics. Most fluid studies using molecular mechanics are concerned with the *physics* of fluids and are concerned with flows at low Reynolds numbers. Recall then that, at *low* Reynolds number, the temperature T on the Kelvin scale of a molecule of mass m gr and speed v cm/sec is given in two dimensions by

$$kT = \frac{1}{2}mv^2 \quad (1.4)$$

and in three dimensions by

$$\frac{3}{2}kT = \frac{1}{2}mv^2, \quad (1.5)$$

in which k is the Boltzmann constant $(1.381)10^{-16}$ erg deg⁻¹. Also recall that T degrees Kelvin and C degrees centigrade are related by

$$T = C + 273. \quad (1.6)$$

But, perhaps most importantly, it must be understood clearly at the outset that statistical mechanics concepts and formulas, including temperature, do *not* apply to turbulent flows, which will be our primary concern and which occur at *high* Reynolds numbers (Batchelor (1960), Bernard (1998), Koplík and Banavar (1998), Speziale and So (1998)). Related details and considerations will be discussed shortly.

1.4. The Leap Frog Formulas

Classical molecular force formulas require small time steps in any numerical simulation in order to yield physically correct results for the effect of repulsion, which is unbounded when the distance between the molecules is close

to zero. Because we are restricted physically to small time steps and because the number of equations is usually exceptionally large, Runge–Kutta and Taylor expansion methods, for example, prove to be unwieldy for related problems. Hence, in this section we will develop a simplistic, efficient, but low order method, called the Leap Frog Method, for molecular mechanics simulations and it is described as follows.

Choose a positive time step h and let $t_k = kh, k = 0, 1, 2, \dots$. For $i = 1, 2, 3, \dots, N$, let P_i have mass m_i and at t_k let it be at $\vec{r}_{i,k} = (x_{i,k}, y_{i,k}, z_{i,k})$, have velocity $\vec{v}_{i,k} = (v_{i,k,x}, v_{i,k,y}, v_{i,k,z})$, and have acceleration $\vec{a}_{i,k} = (a_{i,k,x}, a_{i,k,y}, a_{i,k,z})$. The leap frog formulas, which relate position, velocity and acceleration are

$$\frac{\vec{v}_{i,\frac{1}{2}} - \vec{v}_{i,0}}{\frac{1}{2}h} = \vec{a}_{i,0}, \quad (\text{Starter}) \tag{1.10}$$

$$\frac{\vec{v}_{i,k+\frac{1}{2}} - \vec{v}_{i,k-\frac{1}{2}}}{h} = \vec{a}_{i,k}, \quad k = 1, 2, 3, \dots \tag{1.11}$$

$$\frac{\vec{r}_{i,k+1} - \vec{r}_{i,k}}{h} = \vec{v}_{i,k+\frac{1}{2}}, \quad k = 0, 1, 2, 3, \dots, \tag{1.12}$$

or, explicitly,

$$\vec{v}_{i,\frac{1}{2}} = \vec{v}_{i,0} + \frac{1}{2}h\vec{a}_{i,0}, \quad (\text{Starter}) \tag{1.13}$$

$$\vec{v}_{i,k+\frac{1}{2}} = \vec{v}_{i,k-\frac{1}{2}} + h\vec{a}_{i,k}, \quad k = 1, 2, 3, \dots \tag{1.14}$$

$$\vec{r}_{i,k+1} = \vec{r}_{i,k} + h\vec{v}_{i,k+\frac{1}{2}}, \quad k = 0, 1, 2, 3, \dots \tag{1.15}$$

Note that (1.11) and (1.12) are two point central difference formulas. The name *leap frog* derives from the way position and velocity are defined at alternate, sequential time values. As shown in Fig. 1.2, the r values are defined at the times $t_0, t_1, t_2, t_3, \dots$, while the v values are defined at the times $t_{\frac{1}{2}}, t_{\frac{3}{2}}, t_{\frac{5}{2}}, t_{\frac{7}{2}}, \dots$, and indeed the figure is symbolic of the children’s game *leap frog*.

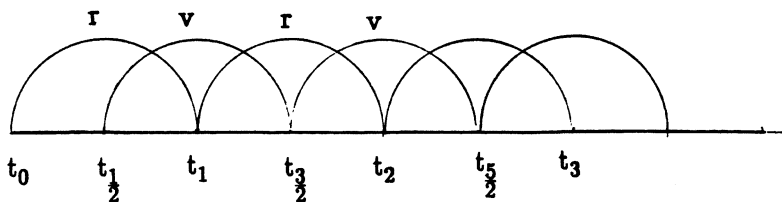


Fig. 1.2. Leap frog.

In formulas (1.13)–(1.15), the values $\vec{a}_{i,k}$ are determined from

$$\vec{a}_{i,k} = \frac{\vec{F}_{i,k}}{m_i}.$$

Example. For illustrative purposes only, let us consider the following simple example. On an X axis, let P_1, P_2 , with respective masses $m_1 = 2$, $m_2 = 1$ be located initially at $x_{1,0} = 0, x_{2,0} = 1$ and have initial velocities $v_{1,0} = -1, v_{2,0} = 3$. Let $h = 0.1$ and assume that the forces on P_1 and P_2 at t_k are given by

$$F_{1,k} = \left(-\frac{1}{|x_{2,k} - x_{1,k}|^3} + \frac{2}{|x_{2,k} - x_{1,k}|^6} \right) \frac{x_{1,k} - x_{2,k}}{|x_{2,k} - x_{1,k}|} \quad (1.16)$$

$$F_{2,k} = -F_{1,k}. \quad (1.17)$$

Then (1.13)–(1.15) yield for P_1

$$v_{1,\frac{1}{2}} = v_{1,0} + (0.05) a_{1,0}, \quad (\text{Starter})$$

$$v_{1,k+\frac{1}{2}} = v_{1,k-\frac{1}{2}} + (0.1) a_{1,k}, \quad k = 1, 2, 3, \dots$$

$$x_{1,k+1} = x_{1,k} + (0.1) v_{1,k+\frac{1}{2}}, \quad k = 0, 1, 2, 3, \dots,$$

or, equivalently,

$$v_{1,\frac{1}{2}} = -1 + (0.05) \left(\frac{1}{2} \right) F_{1,0} = -1 + (0.025) F_{1,0} \quad (1.18)$$

$$v_{1,k+\frac{1}{2}} = v_{1,k-\frac{1}{2}} + (0.1) \left(\frac{1}{2} \right) F_{1,k} = v_{1,k-\frac{1}{2}} + (0.05) F_{1,k} \quad (1.19)$$

$$x_{1,k+1} = x_{1,k} + (0.1) v_{1,k+\frac{1}{2}}. \quad (1.20)$$

From (1.16), then,

$$F_{1,0} = \left(-\frac{1}{1^3} + \frac{2}{1^6} \right) \left(-\frac{1}{1} \right) = -1,$$

so that (1.18) implies

$$v_{1,\frac{1}{2}} = -1.025.$$

In an analogous fashion, one finds that

$$v_{2,\frac{1}{2}} = v_{2,0} + (0.05) a_{2,0} \quad (\text{Starter})$$

$$v_{2,k+\frac{1}{2}} = v_{2,k-\frac{1}{2}} + (0.1) a_{2,k}, \quad k = 1, 2, 3, \dots$$

$$x_{2,k+1} = x_{2,k} + (0.1) v_{2,k+\frac{1}{2}}, \quad k = 0, 1, 2, 3, \dots,$$

and

$$v_{2,\frac{1}{2}} = 3 + (0.05)\frac{F_{2,0}}{1} = 3 + (0.05)F_{2,0}, \quad \text{(Starter)} \quad (1.21)$$

$$v_{2,k+\frac{1}{2}} = v_{2,k-\frac{1}{2}} + (0.1)\frac{F_{2,k}}{1} = v_{2,k-\frac{1}{2}} + (0.1)F_{2,k}, \quad k = 1, 2, 3, \dots \quad (1.22)$$

$$x_{2,k+1} = x_{2,k} + (0.1)v_{2,k+\frac{1}{2}}, \quad k = 0, 1, 2, \dots \quad (1.23)$$

Then, (1.16) and (1.21) yield

$$v_{2,\frac{1}{2}} = 3.05.$$

Since $v_{1,\frac{1}{2}}, v_{2,\frac{1}{2}}$ are now known, we can determine $x_{1,1}, x_{2,1}$ from (1.20) and (1.23) to yield

$$x_{1,1} = x_{1,0} + (0.1)v_{1,\frac{1}{2}} = -0.1025$$

$$x_{2,1} = x_{2,0} + (0.1)v_{2,\frac{1}{2}} = 1.305.$$

Next, knowing $x_{1,1}, x_{2,1}$, we can use (1.19) and (1.22) to determine $v_{1,\frac{3}{2}}, v_{2,\frac{3}{2}}$ as follows. For $k = 1$,

$$\begin{aligned} F_{1,1} &= \left(-\frac{1}{|x_{2,1}-x_{1,1}|^3} + \frac{2}{|x_{2,1}-x_{1,1}|^6} \right) \frac{x_{1,1}-x_{2,1}}{|x_{2,1}-x_{1,1}|} \\ &= \left(-\frac{1}{(1.305+0.1025)^3} + \frac{2}{(1.305+0.1025)^6} \right) \frac{-0.1025-1.305}{1.305+0.1025} \\ &= 0.101396 \end{aligned}$$

$$F_{2,1} = -0.101396.$$

Thus, from (1.19),

$$v_{1,\frac{3}{2}} = v_{1,\frac{1}{2}} + (0.05)F_{1,1} = -1.019930,$$

while, from (1.22),

$$v_{2,\frac{3}{2}} = v_{2,\frac{1}{2}} + (0.1)F_{2,1} = 3.039860.$$

One next determines $x_{1,2}$ and $x_{2,2}$ from (1.20) and (1.23) to yield

$$x_{1,2} = x_{1,1} + (0.1)v_{1,\frac{3}{2}} = -0.204493.$$

$$x_{2,2} = x_{2,1} + (0.1)v_{2,\frac{3}{2}} = 1.608986.$$

The computation then continues in the indicated fashion until one has calculated for a fixed time period, which is usually prescribed by the constraints of the problem under consideration.

Note that in later discussions, confusion in notation will be avoided by using either h or Δt to represent a time step in a calculation.

Specific FORTRAN programs will be provided in later chapters. At present, however, a generic computer program for implementing the leap frog formulas is given as follows.

ALGORITHM — PROGRAM LEAP FROG

- Step 1. Set a time step h .
- Step 2. Let distinct times t_k be given by $t_k = kh$, $k = 0, 1, 2, \dots$
- Step 3. Let $P(I)$ of mass $m(I)$ be N given bodies, $I = 1, 2, \dots, N$.
- Step 4. For each I , let $P(I)$ be initially at $x(I, 0), y(I, 0), z(I, 0)$ with velocity components $vx(I, 0), vy(I, 0), vz(I, 0)$.
- Step 5. For each I , let the force on $P(I)$ at any time t be $(Fx(I, t), Fy(I, t), Fz(I, t))$ and let the acceleration be $(Ax(I, t), Ay(I, t), Az(I, t))$, with
- $$Ax(I, t) = Fx(I, t)/m(I)$$
- $$Ay(I, t) = Fy(I, t)/m(I)$$
- $$Az(I, t) = Fz(I, t)/m(I).$$
- Step 6. For each I , apply the starter formulas
- $$vx(I, 0.5) = vx(I, 0) + \frac{1}{2}hAx(I, 0)$$
- $$vy(I, 0.5) = vy(I, 0) + \frac{1}{2}hAy(I, 0)$$
- $$vz(I, 0.5) = vz(I, 0) + \frac{1}{2}hAz(I, 0)$$
- Step 7. For each I , determine positions and velocities sequentially by
- $$x(I, t_k + h) = x(I, t_k) + (h)vx(I, t_k + 0.5h), k = 0, 1, 2, \dots$$
- $$y(I, t_k + h) = y(I, t_k) + (h)vy(I, t_k + 0.5h), k = 0, 1, 2, \dots$$
- $$z(I, t_k + h) = z(I, t_k) + (h)vz(I, t_k + 0.5h), k = 0, 1, 2, \dots$$
- $$vx(I, t_p + 0.5h) = vx(I, t_p - 0.5h) + (h)Ax(I, t_p), p = k + 1.$$
- $$vy(I, t_p + 0.5h) = vy(I, t_p - 0.5h) + (h)Ay(I, t_p), p = k + 1.$$
- $$vz(I, t_p + 0.5h) = vz(I, t_p - 0.5h) + (h)Az(I, t_p), p = k + 1.$$
- Step 8. Stop when $k = 999$.

1.5. Turbulence

Turbulence is the most common, yet least understood, form of fluid motion. Let us the first describe some related concepts, views, and results from the points of view of engineering, fluid theory, and numerical analysis. As will be clear from the discussion, overlapping between any two of these areas is relatively common.

1.5.1. *Engineering*

From an engineering point of view, turbulent flow may be characterized qualitatively as fluid motion displaying seemingly random behavior. More precisely, if a fluid flow is one realization of repeatable experiment, then the flow is called turbulent if the velocity field, either in whole or in part, changes to a degree greater than experimental error each time the experiment is performed. Even though the flow is deterministic, turbulence results because the flow is acutely sensitive to minute, uncontrollable differences in boundary and/or initial data, whose effects are amplified in time to a measurable scale. *The flow is characterized also by the random appearance and disappearance of many vortices.* However, even though understanding the dynamics of these vortical structures is considered to be an important part of current turbulence research, many related physical and mathematical issues are unresolved. (Bernard (1998), Speziale and So (1998)).

Also, it is known that *a strong current across a customary laminar flow initiates turbulent flow* (Schlichting (1960)).

It is also thought by some (Yakhot and Orszag (1986)) that sub-continuum perturbations, such as those responsible for Brownian motion, may initiate instabilities which lead to turbulence.

1.5.2. *Theoretical*

A fundamental pure number, called the Reynolds number Re , is defined as follows:

$$Re = UL/\nu,$$

in which U and L are reference velocity and length scales and ν is the kinematic viscosity of the fluid under consideration, is assumed to be related to turbulence. It is believed that Re large results in turbulent flow. Note that the Reynolds number is not related to any assumed equations of fluid flow.

As for the overall theoretical modelling of turbulent flow, several major approaches have been formulated and explored. Beginning with Taylor's seminal paper (Taylor (1921)), one school of study (Favre (1964)) has emphasized the statistical approach. A second major school of thought, following fundamental papers of Landau (1944), Hopf (1948), and Ruelle and Takens (1971) uses Galerkin approximations to simplify the Navier–Stokes equations and bifurcation theory to analyze the resulting ordinary differential system (Barenblatt, Iooss, and Joseph (1983)). A still third approach

utilizes statistical thermodynamics (Chorin (1994), Malkus (1960)). Unfortunately, important and realistic aspects of turbulent motions have defied inclusion in all the models just described (Barenblatt, Iooss, and Joseph (1983), Markatos (1986), Zabusky (1968)). Thus, for example, whereas homogeneous turbulence has received intensive theoretical study (Batchelor (1960)), it is not known to exist anywhere in Nature.

1.5.3. Numerical

The dominant numerical approaches to the simulation of turbulent flow have centered on computational solution of the Navier–Stokes equations for large Reynolds numbers. This has been shown to be invalid if one uses the classical (non averaged) Navier–Stokes equations. In the words of Ladyzhenskaya (1969): “The results given in this book support the belief that it is reasonable to use the Navier–Stokes equations to describe the motions of a viscous fluid in the case of Reynolds numbers which do not exceed certain limits. They partially refute the statements described above concerning the properties of solutions of the Navier–Stokes equations, and they force us to find other explanations for observed phenomena in real fluids, in particular, for the familiar paradoxes involving viscous fluids. Apparently, in seeking these explanations, one must ignore the fact that if a large force \mathbf{f} acts on the fluid for an extended interval of time, then the quantities $D_x^m v_k$ (where $\mathbf{v} = (v_1, v_2, v_3)$ is the solution) can become so large that the assumption that they are comparatively small, made in deriving the Navier–Stokes equations from the statistical Maxwell–Boltzmann equations, will no longer be satisfied, just as other assumptions of the Stokes theory, i.e. the assumption that the kinematic viscosity and the thermal regime are constant, will be far from valid. Because of this, it is hardly possible to explain the transition from laminar to turbulent flows within the framework of the classical Navier–Stokes theory.”

Replacement of a numerical solution of the classical Navier–Stokes equations by a numerical solution of averaged fluid equations using large Reynolds numbers leave many related mathematical issues unresolved and have also led to results which are contradicted by experiment (Bernard (1998)).

1.6. Overview

In order not to spread our attention too broadly, we will concentrate, primarily, in both two and three dimensions on a prototype fluid flow called

cavity flow. For such problems we will use two significant markers discussed in Section 1.5, namely, that turbulent flow follows when a strong cross-current develops and imposes itself on a laminar flow (Schlichting (1960)), and that turbulent flow exhibits the rapid appearance and disappearance of many vortices (Kolmogorov (1964)). However, initially, we will work in the spirit of nano physics and will proceed into the large only in a later chapter, Chapter 6. On the molecular level, we may find somewhat different results at first that one might expect in the large. Indeed, researchers in both nano physics and nano technology are finding that this is exactly the case. However, our results will confirm the conjecture of Yakhot and Orszag (1986) that sub continuum perturbations, such as those responsible for Brownian motion, do initiate instabilities which lead to turbulence. Indeed, by working first on the molecular level we will show clearly the mechanisms by which turbulence develops.