Chapter I

Examples and Numerical Experiments

This chapter introduces some interesting differential equations and illustrates the different qualitative behaviour of numerical methods. We deliberately consider only very simple numerical methods of orders 1 and 2 in order to emphasize the qualitative aspects of the experiments. The same effects (on a different scale) could be observed with more sophisticated higher order integration schemes. The presented experiments should serve as a motivation for the theoretical and practical investigations of later chapters. Every reader is encouraged to repeat the experiments or to invent similar ones.

I.1 Two-Dimensional Problems

Volterra-Lotka Problem Consider the problem

$$u' = u(v-2), \qquad v' = v(1-u), \tag{1.1}$$

which constitutes an autonomous system of two differential equations. It is a simple model for the development of two populations, where u represents the predator and v the prey. If we divide the two equations of (1.1) by each other and if we consider u as a function of v (or reversed), we get after separation of variables

$$\frac{1-u}{u}\,du - \frac{v-2}{v}\,dv = 0.$$

Integration then leads to

$$I(u,v) = \ln u - u + 2\ln v - v = \mathit{Const}. \tag{1.2}$$

This means that solutions of (1.1) lie on level curves of (1.2) or, equivalently, $I(u,v)$ is a first integral of (1.1). Some of the level curves are drawn in the pictures of Fig. 1.1. Since these level curves are closed, all solutions of (1.1) are periodic. Can we have the same property for the numerical solution?

Simple Numerical Methods The most simple numerical method for the solution of the initial value problem

$$y' = f(y), \qquad y(t_0) = y_0 \tag{1.3}$$

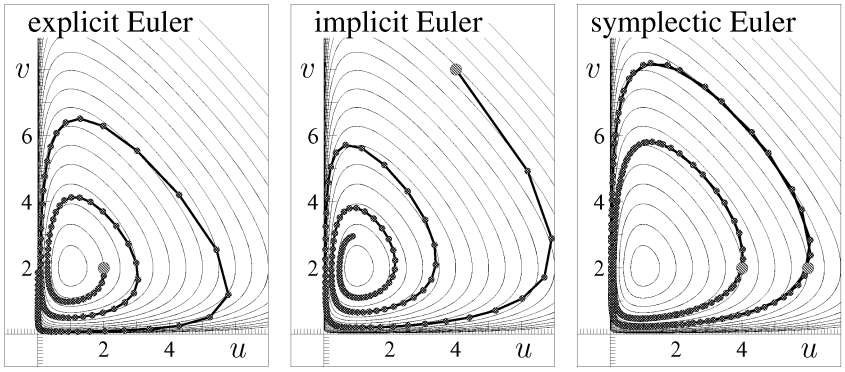


FIG. 1.1: Solutions of the Volterra-Lotka equations (1.1)

is Euler's method

$$y_{n+1} = y_n + hf(y_n). \tag{1.4}$$

It is also called *explicit Euler method*, because the approximation y_{n+1} can be computed in an explicit straight-forward way from y_n and from the step size h. Here, y_n is an approximation to $y(t_n)$ where $y(t)$ is the exact solution of (1.3), and $t_n = t_0 + nh$.

The *implicit Euler method*

$$y_{n+1} = y_n + hf(y_{n+1}), \tag{1.5}$$

which has its name from its similarity to (1.4), is known from its excellent stability properties. In contrast to (1.4), the approximation y_{n+1} is defined implicitly by (1.5), and the implementation needs the resolution of nonlinear systems.

Taking the mean of y_n and y_{n+1} in the argument of f, we get the *implicit midpoint rule*

$$y_{n+1} = y_n + hf\Big(\frac{y_n + y_{n+1}}{2}\Big). \tag{1.6}$$

It is a symmetric method, which means that the formula remains the same if we exchange $y_n \leftrightarrow y_{n+1}$ and $h \leftrightarrow -h$.

For partitioned systems

$$u' = a(u, v), \qquad v' = b(u, v), \tag{1.7}$$

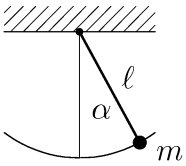
such as the problem (1.1), we also consider the method

$$u_{n+1} = u_n + ha(u_{n+1}, v_n), \qquad v_{n+1} = v_n + hb(u_{n+1}, v_n), \tag{1.8}$$

which treats the u-variable by the implicit and the v-variable by the explicit Euler method. It is called *symplectic Euler method* (in Sect. IV it will be shown that it represents a symplectic transformation).

Numerical Experiment The result of our first numerical experiment is shown in Fig. 1.1. We have applied different numerical methods to (1.1), all with constant step size $h = 0.12$. As initial values (the enlarged symbols in the pictures) we have chosen $(u_0, v_0) = (2, 2)$ for the explicit Euler method, $(u_0, v_0) = (4, 8)$ for the implicit Euler method, and $(u_0, v_0) = (4, 2)$ respectively $(6, 2)$ for the symplectic Euler method. The figure shows the numerical approximations of the first 125 steps. We observe that the

explicit and implicit Euler methods behave qualitatively wrong. The numerical solution either spirals outwards or it spirals inwards. The symplectic Euler method, however, gives a numerical solution that lies on a closed curve as does the exact solution. It is important to remark that the curves of the numerical and exact solution do not coincide, but they will be closer for smaller h. The implicit midpoint rule also shows the correct qualitative behaviour (we did not include it in the figure).



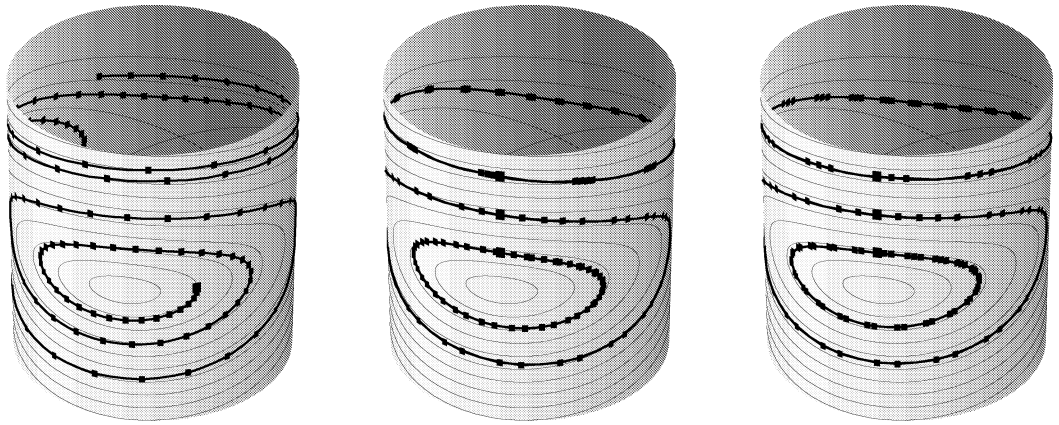
Pendulum Our next problem is the mathematical pendulum with a massless rod of length $\ell = 1$ and mass $m = 1$. Its movement is described by the equation $\alpha'' + \sin\alpha = 0$. With the coordinates $q = \alpha$ and $p = \alpha'$ this becomes the two-dimensional system

$$q' = p, \qquad p' = -\sin q. \tag{1.9}$$

As in the example above we can find a first integral, so that all solutions satisfy

$$H(p,q) = \frac{1}{2}\,p^2 - \cos q = \mathit{Const.} \tag{1.10}$$

Since the vector field (1.9) is 2π-perdiodic in q, it is natural to consider q as a variable on the circle S^1. Hence, the phase space of elements (p,q) becomes the cylinder $\mathbb{R} \times S^1$. In Fig. 1.2 level curves of $H(p,q)$ are drawn. They correspond to solution curves of the problem (1.9).



explicit Euler symplectic Euler implicit midpoint

FIG. 1.2: Solutions of the pendulum problem (1.9)

Again we apply our numerical methods: the explicit Euler method with step size $h = 0.2$ and initial value $(p_0, q_0) = (0, 0.5)$; the symplectic Euler method and the implicit midpoint rule with $h = 0.3$ and three different initial values $q_0 = 0$ and $p_0 \in \{0.7, 1.4, 2.1\}$. Similar to the computations for the Volterra-Lotka equations we observe that only the symplectic Euler method and the implicit midpoint rule exhibit the correct qualitative behaviour. The numerical solution of the midpoint rule is closer to the exact solution, because it is a method of order 2, whereas the other methods are only of order 1.

Conclusion We have considered two-dimensional problems with the property that all solutions are periodic. In general, a discretization of the differential equation destroys this property. Surprisingly, there exist methods for which the numerical flow shows the same qualitative behaviour as the exact flow of the problem.

I.2 Kepler's Problem and the Outer Solar System

> The evolution of the entire planetary system has been numerically integrated for a time span of nearly 100 million years. This calculation confirms that the evolution of the solar system as a whole is chaotic, ...
>
> (G.J. Sussman and J. Wisdom 1992)

The Kepler problem (also called the two-body problem) describes the motion of two bodies which attract each other. If we choose one of the bodies as the center of our coordinate system, the motion will stay in a plane (Exercise 2). Denoting the position of the second body by $q = (q_1, q_2)^T$, Newton's law yields a second order differential equation which, with a suitable normalization, is given by

$$\ddot{q}_1 = -\frac{q_1}{(q_1^2 + q_2^2)^{3/2}}, \qquad \ddot{q}_2 = -\frac{q_2}{(q_1^2 + q_2^2)^{3/2}}. \tag{2.1}$$

One can check that this is equivalent to a Hamiltonian system

$$\dot{q} = H_p(p, q), \qquad \dot{p} = -H_q(p, q) \tag{2.2}$$

(H_p and H_q are the vectors of partial derivatives) with total energy

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}\,(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}. \tag{2.3}$$

Exact Integration Kepler's problem can be solved analytically, i.e., it can be reduced to the computation of integrals. This is possible, because the system has not only the total energy $H(p, q)$ as invariant, but also the angular momentum

$$L(p_1, p_2, q_1, q_2) = q_1 p_2 - q_2 p_1. \tag{2.4}$$

This can be checked by differentiation. Hence, every solution of (2.1) satisfies the two relations

$$\frac{1}{2}\,(\dot{q}_1^2 + \dot{q}_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} = H_0, \qquad q_1\dot{q}_2 - q_2\dot{q}_1 = L_0,$$

where the constants H_0 and L_0 are determined by the initial values. Using polar coordinates $q_1 = r\cos\varphi$, $q_2 = r\sin\varphi$, this system becomes

$$\frac{1}{2}\,(\dot{r}^2 + r^2\dot{\varphi}^2) - \frac{1}{r} = H_0, \qquad r^2\dot{\varphi} = L_0. \tag{2.5}$$

For its solution we consider r as a function of φ (assuming that $L_0 \neq 0$ so that φ is a monotonic function). Hence, we have $\dot{r} = \frac{dr}{d\varphi} \cdot \dot{\varphi}$ and the elimination of $\dot{\varphi}$ in (2.5) yields

$$\frac{1}{2}\left(\left(\frac{dr}{d\varphi}\right)^2 + r^2\right)\frac{L_0^2}{r^4} - \frac{1}{r} = H_0.$$

With the abbreviations

$$d = L_0^2, \qquad e^2 = 1 + 2H_0L_0^2 \tag{2.6}$$

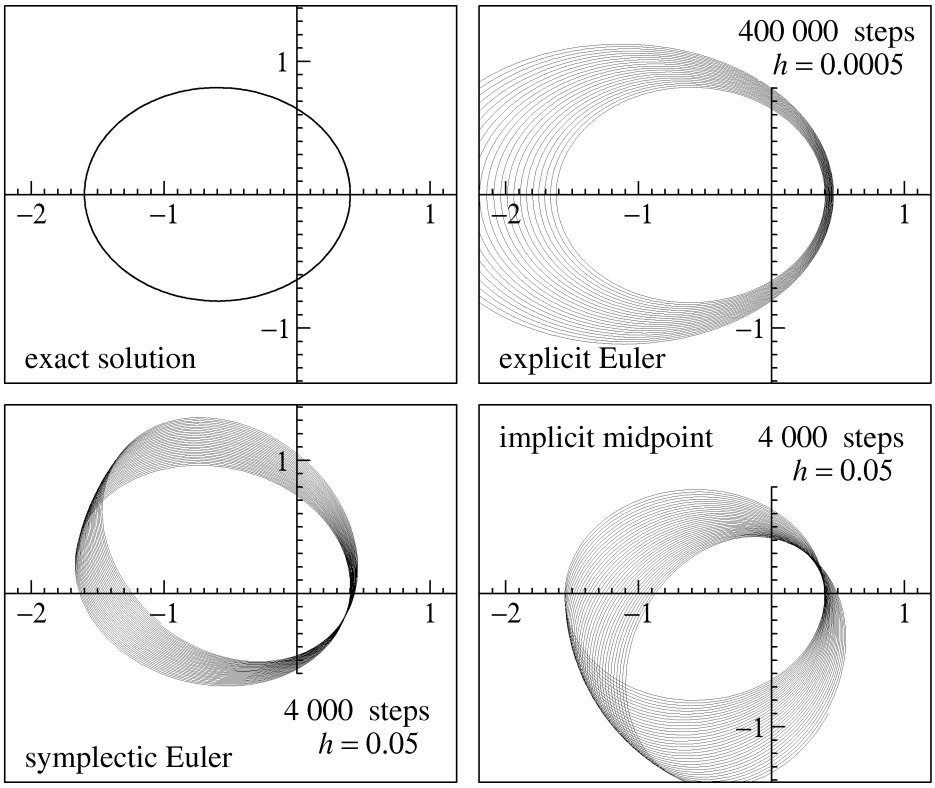


FIG. 2.1: Exact and numerical solutions of Kepler's problem

and the substitution $u(\varphi) = 1/r(\varphi)$ we get

$$\Big(\frac{du}{d\varphi}\Big)^2 = \frac{e^2}{d^2} - \Big(u - \frac{1}{d}\Big)^2.$$

This differential equation can be solved by separation of variables and yields

$$r(\varphi) = \frac{d}{1 + e\cos(\varphi - \varphi^*)}, \tag{2.7}$$

where φ^* is determined by the initial values r_0 and φ_0. In the original coordinates this relation becomes

$$\sqrt{q_1^2 + q_2^2} + e(q_1 \cos\varphi^* + q_2 \sin\varphi^*) = d.$$

Eliminating the square root, this gives a quadratic relation for (q_1, q_2) which represents an ellipse with eccentricity e for $H_0 < 0$ (see Fig. 2.1), a parabola for $H_0 = 0$, and a hyperbola for $H_0 > 0$. With the relation (2.7), the second equation of (2.5) gives

$$\frac{d^2}{(1 + e\cos(\varphi - \varphi^*))^2}\, d\varphi = L_0\, dt \tag{2.8}$$

which, after integration, gives an implicit equation for $\varphi(t)$.

Numerical Integration We consider the problem (2.1) and we choose

$$q_1(0) = 1 - e, \quad q_2(0) = 0, \quad \dot q_1(0) = 0, \quad \dot q_2(0) = \sqrt{\frac{1+e}{1-e}}, \tag{2.9}$$

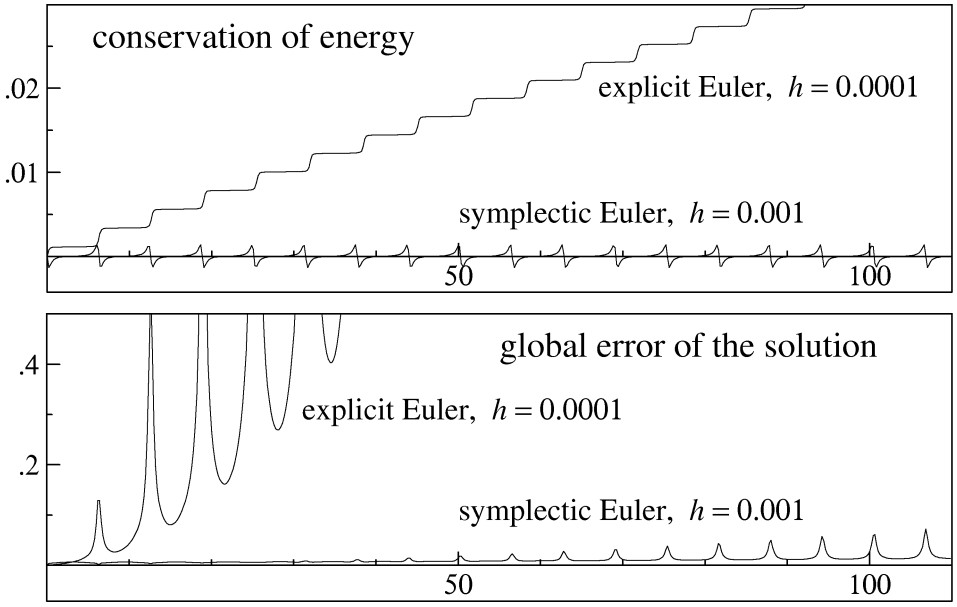


FIG. 2.2: Energy conservation and global error for Kepler's problem

with $0 \leq e < 1$ as initial values. This implies that $H_0 = -1/2$, $L_0 = \sqrt{1-e^2}$, $d = 1 - e^2$ and $\varphi^* = 0$. The period of the solution is 2π (Exercise 4). Fig. 2.1 shows the exact solution with eccentricity $e = 0.6$ and some numerical solutions. After our previous experience, it is no longer a surprise that the explicit Euler method spirals outwards and gives a completely wrong answer. For the symplectic Euler method and the implicit midpoint rule we take a step size 100 times larger in order to better observe their qualitative behaviour. We see that the numerical solution lies close to an ellipse which turns slowly around its focus, clockwise for the symplectic Euler method and anticlockwise for the implicit midpoint rule. The same behaviour can be observed for the exact solution of perturbed Kepler problems (Exercise 6).

Our next experiment (Fig. 2.2) studies the conservation of invariants and the global error. The main observation is that the error in the energy grows linearly for the explicit Euler method, and it remains bounded and small (no secular terms) for the symplectic Euler method. The global error, measured in the Euclidean norm, shows a quadratic growth (explicit Euler) compared to a linear growth (symplectic Euler and implicit midpoint rule). The findings of this experiment are collected in Table 2.1. We remark that the angular momentum $L(p, q)$ is exactly conserved for the symplectic Euler and the implicit midpoint rule.

TABLE 2.1: Qualitative long-time behaviour for Kepler's problem

method	error in H	error in L	global error
explicit Euler	$\mathcal{O}(th)$	$\mathcal{O}(th)$	$\mathcal{O}(t^2h)$
symplectic Euler	$\mathcal{O}(h)$	0	$\mathcal{O}(th)$
implicit midpoint	$\mathcal{O}(h^2)$	0	$\mathcal{O}(th^2)$

TABLE 2.2: Data for the outer solar system

planet	mass	initial position	initial velocity
Jupiter	$m_1 = 0.000954786104043$	-3.5023653 -3.8169847 -1.5507963	0.00565429 -0.00412490 -0.00190589
Saturn	$m_2 = 0.000285583733151$	9.0755314 -3.0458353 -1.6483708	0.00168318 0.00483525 0.00192462
Uranus	$m_3 = 0.0000437273164546$	8.3101420 -16.2901086 -7.2521278	0.00354178 0.00137102 0.00055029
Neptune	$m_4 = 0.0000517759138449$	11.4707666 -25.7294829 -10.8169456	0.00288930 0.00114527 0.00039677
Pluto	$m_5 = 1/(1.3 \cdot 10^8)$	-15.5387357 -25.2225594 -3.1902382	0.00276725 -0.00170702 -0.00136504

Outer Solar System We next apply our methods to the system which describes the motion of the five outer planets relative to the sun. This system has been studied extensively by astronomers, who integrated it for a time span of nearly 100 million years and concluded the chaotic evolution of the solar system [SW92]. The problem is a Hamiltonian system (2.2) with

$$H(p,q) = \frac{1}{2}\sum_{i=0}^{5} m_i^{-1} p_i^T p_i - G\sum_{i=1}^{5}\sum_{j=0}^{i-1} \frac{m_i\, m_j}{\|q_i - q_j\|}. \tag{2.10}$$

Here p and q are the supervectors composed by the vectors $p_i, q_i \in I\!R^3$ (momenta and positions), respectively. The chosen units are: masses relative to the sun, so that the sun has mass 1. We have taken

$$m_0 = 1.00000597682$$

in order to take account of the inner planets. Distances are in astronomical units (1 [A.U.] = 149 597 870 [km]), times in earth days, and the gravitational constant is

$$G = 2.95912208286 \cdot 10^{-4}.$$

The initial values for the sun are taken as $q_0(0) = (0,0,0)^T$ and $\dot{q}_0(0) = (0,0,0)^T$. All other data (masses of the planets and the initial positions and initial velocities) are given in Table 2.2. The initial data are taken from "Ahnerts Kalender für Sternfreunde 1994", Johann Ambrosius Barth Verlag 1993, and they correspond to September 5, 1994 at 0h00.[1]

To this system we applied our four methods, all with step size $h = 10$ (days) and over a time period of 200 000 days. The numerical solution (see Fig. 2.3) behaves similarly to

[1]We thank Alexander Ostermann, who provided us with all these data.

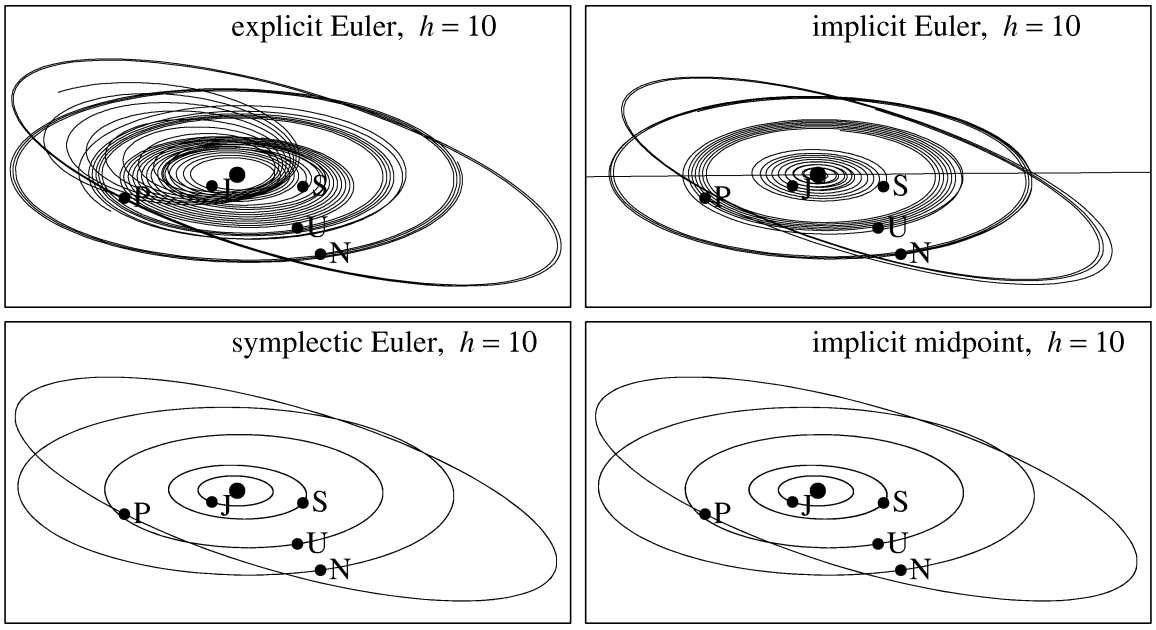


FIG. 2.3: Solutions of the outer solar system

that for the Kepler problem. With the explicit Euler method the planets increase their energy, they spiral outwards, Jupiter approaches Saturn which leaves the plane of the two-body motion. With the implicit Euler method the planets (first Jupiter and then Saturn) fall into the sun and are thrown far away. Both the symplectic Euler method and the implicit midpoint rule show the correct behaviour. An integration over a much longer time of say several million of years does not deteriorate this behaviour. Let us remark that Sussman & Wisdom [SW92] have integrated the outer solar system with special methods which will be discussed in Chap. IV.

I.3 Molecular Dynamics

> We do not need exact classical trajectories to do this, but must lay great emphasis on energy conservation as being of primary importance for this reason. (M.P. Allen and D.J. Tildesley 1987)

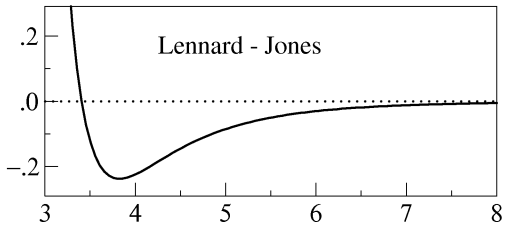
Molecular dynamics requires the solution of Hamiltonian systems (2.2), where the total energy is given by

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{N} m_i^{-1} p_i^T p_i + \sum_{i=2}^{N}\sum_{j=1}^{i-1} V_{ij}\big(\|q_i - q_j\|\big), \tag{3.1}$$

and $V_{ij}(r)$ are given potential functions. Here, q_i and p_i denote the positions and momenta of atoms and m_i is the atomic mass of the ith atom. We remark that the outer solar system (2.10) is such an N-body system with $V_{ij}(r) = -Gm_im_j/r$. In molecular dynamics the Lennard-Jones potential

$$V_{ij}(r) = 4\varepsilon_{ij}\Big(\big(\frac{\sigma_{ij}}{r}\big)^{12} - \big(\frac{\sigma_{ij}}{r}\big)^{6}\Big), \tag{3.2}$$

is very popular (ε_{ij} and σ_{ij} are suitable constants depending on the atoms). This potential has an absolute minimum at distance $r = \sigma_{ij}\sqrt[6]{2}$. The force due to this potential strongly repulses the atoms when they are closer than this value, and they attract each other when they are farther.



Störmer-Verlet Scheme The Hamiltonian of (3.1) is of the form $H(p,q) = T(p)+V(q)$, where $T(p)$ is a quadratic function. Hence, the Hamiltonian system is of the form

$$\dot{q} = M^{-1}p, \qquad \dot{p} = -V'(q),$$

where $M = \mathrm{diag}(m_1 I, \ldots, m_N I)$ and I is the 3-dimensional identity matrix. This system is equivalent to the special second order differential equation

$$\ddot{q} = f(q), \tag{3.3}$$

where the right-hand side $f(q) = M^{-1}V'(q)$ does not depend on $\dot{q}$. The most natural discretization of (3.3) is[2]

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n). \tag{3.4}$$

This formula is either called *Störmer's method* (C. Störmer in 1907 used higher order variants for the numerical computation concerning the aurora borealis) or *Verlet method*. L. Verlet [Ver67] proposed this method for computations in molecular dynamics. An approximation to the derivative $v = \dot{q}$ is simply obtained by

$$v_n = \frac{q_{n+1} - q_{n-1}}{2h}. \tag{3.5}$$

For the second order problem (3.3) one usually has given initial values $q(0) = q_0$ and $\dot{q}(0) = v_0$. However, one also needs q_1 in order to be able to start the integration with the 3-term recursion (3.4). Putting $n = 0$ in (3.4) and (3.5), an elimination of q_{-1} gives

$$q_1 = q_0 + hv_0 + \frac{h^2}{2} f(q_0)$$

for the missing starting value.

The Störmer-Verlet method admits an interesting *one-step formulation* which is useful for numerical computations. Introducing the velocity approximation at the midpoint $v_{n+1/2} := v_n + \frac{h}{2} f(q_n)$, an elimination of q_{n-1} (as above) yields

$$\begin{aligned} v_{n+1/2} &= v_n + \frac{h}{2} f(q_n) \\ q_{n+1} &= q_n + hv_{n+1/2} \\ v_{n+1} &= v_{n+1/2} + \frac{h}{2} f(q_{n+1}) \end{aligned} \tag{3.6}$$

[2] *Attention.* In (3.4) and in the subsequent formulas q_n denotes an approximation to $q(nh)$, whereas q_i in (3.1) denotes the ith subvector of q.

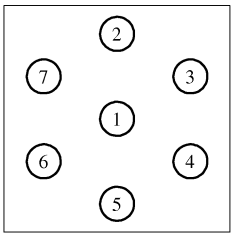
which is an explicit one-step method $\Psi_h^V : (q_n, v_n) \mapsto (q_{n+1}, v_{n+1})$ for the first order system $\dot{q} = v, \dot{v} = f(q)$. If one is not interested in the values v_n of the derivative, the first and third equations in (3.6) can be replaced with

$$v_{n+1/2} = v_{n-1/2} + h\, f(q_n).$$

Finally, let us mention an interesting connection between the Störmer-Verlet method and the symplectic Euler method (1.8). If the variable q is discretized by the explicit Euler and v by the implicit Euler method, we denote it by Ψ_h^{ei}; if q is discretized by the implicit Euler and v by the explicit Euler method, we denote it by Ψ_h^{ie}. Introducing $q_{n+1/2} := q_n + \frac{h}{2}\, v_{n+1/2}$ as an approximation at the midpoint, one recognizes the mapping $(q_n, v_n) \mapsto (q_{n+1/2}, v_{n+1/2})$ as an application of $\Psi_{h/2}^{ei}$, and $(q_{n+1/2}, v_{n+1/2}) \mapsto (q_{n+1}, v_{n+1})$ as an application of $\Psi_{h/2}^{ie}$. Hence, the Störmer-Verlet method satisfies

$$\Psi_h^V = \Psi_{h/2}^{ie} \circ \Psi_{h/2}^{ei}. \tag{3.7}$$

Numerical Experiment with a Frozen Argon Crystal As in [BS93] we consider the interaction of seven argon atoms in a plane, where six of them are arranged symmetrically around a center atom. As mathematical model we take the Hamiltonian (3.1) with $N = 7$, $m_i = m = 66.34 \cdot 10^{-27}$ [kg],



$$\varepsilon_{ij} = \varepsilon = 119.8\, k_B \text{ [J]}, \qquad \sigma_{ij} = \sigma = 0.341 \text{ [nm]},$$

where $k_B = 1.380658 \cdot 10^{-23}$ [J/K] is Boltzmann's constant (see [AT87, page 21]). As units for our calculations we take masses in [kg], distances in nanometers ($1\,[\text{nm}] = 10^{-9}\,[\text{m}]$), and times in nanoseconds ($1\,[\text{nsec}] = 10^{-9}\,[\text{sec}]$). Initial positions (in [nm]) and initial velocities (in [nm/nsec]) are given in Table 3.1. They are chosen such that neighbouring atoms have a distance that is close to the one with lowest potential energy, and such that the total momentum is zero and therefore the centre of gravity does not move. The energy at the initial position is $H(p_0, q_0) \approx -1260.2\, k_B$ [J].

For computations in molecular dynamics one is usually not interested in the trajectories of the atoms, but one aims at macroscopic quantities such as temperature, pressure, internal energy, etc. We are interested in the total energy, given by the Hamiltonian, and in the temperature which can be calculated from the formula [AT87, page 46]

$$T = \frac{1}{2Nk_B} \sum_{i=1}^{N} m_i \|\dot{q}_i\|^2. \tag{3.8}$$

We apply the explicit and symplectic Euler methods and also the Verlet method to this problem. Observe that for a Hamiltonian such as (3.1) all three methods are explicit, and

TABLE 3.1: Initial values for the simulation of a frozen Argon crystal

atom	1	2	3	4	5	6	7
position	0.00	0.02	0.34	0.36	−0.02	−0.35	−0.31
	0.00	0.39	0.17	−0.21	−0.40	−0.16	0.21
velocity	−30	50	−70	90	80	−40	−80
	−20	−90	−60	40	90	100	−60

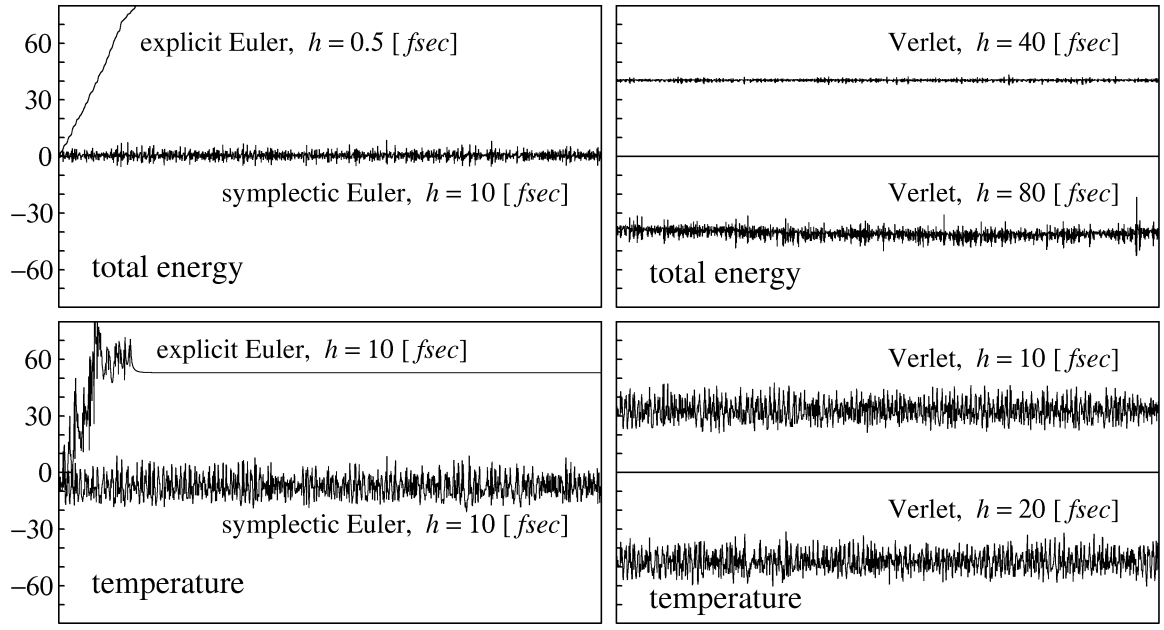


FIG. 3.1: Computed total energy and temperature of the Argon crystal

all of them need only one force evaluation per integration step. In Fig. 3.1 we present the numerical results of our experiments. The integrations are done over an interval of length 0.2 [nsec]. The step sizes are indicated in femtoseconds ($1\,[\text{fsec}] = 10^{-6}\,[\text{nsec}]$).

The two upper pictures show the values $(H(p_n, q_n) - H(p_0, q_0))/k_B$ as a function of time $t_n = nh$. For the exact solution, this value is precisely zero for all times. Similar to earlier experiments we see that the symplectic Euler method is qualitatively correct, whereas the numerical solution of the explicit Euler method, although computed with a much smaller step size, is completely useless (see the citation of the beginning of this section). The Verlet method is qualitatively correct and gives much more accurate results than the symplectic Euler method (we shall see later that the Verlet method is of order 2). The two computations with the Verlet method show that the energy error decreases by a factor of 4, if the step size is reduced by a factor of 2 (second order convergence).

The two lower pictures of Fig. 3.1 show the numerical values of the temperature difference $T - T_0$ with T given by (3.8) and $T_0 \approx 22.72\,[\text{K}]$ (initial temperature). In contrast to the total energy, this is not an exact invariant, but for our problem it fluctuates around a fixed value. The explicit method gives wrong results, but the symplectic Euler and the Verlet methods show the desired behaviour. This time a reduction of the step size does not reduce the amplitude of the oscillations.

I.4 Highly Oscillatory Problems

Fermi-Pasta-Ulam ...

I.5 Exercises

1. Apply the symplectic Euler method (or the implicit midpoint rule) to problems such as
$$\begin{pmatrix} u \\ v \end{pmatrix}' = \begin{pmatrix} (v-2)/v \\ (1-u)/u \end{pmatrix}, \qquad \begin{pmatrix} u \\ v \end{pmatrix}' = \begin{pmatrix} u^2 v(v-2) \\ v^2 u(1-u) \end{pmatrix}$$
which both have the same first integral (1.2) as the Volterra-Lotka problem and therefore also periodic solutions. Do the numerical solutions also show this behaviour?

2. A general two-body problem (sun and planet) is given by the Hamiltonian
$$H(p, p_S, q, q_S) = \frac{1}{2M} p_S^T p_S + \frac{1}{2m} p^T p - \frac{GmM}{\|q - q_S\|},$$
where $q_S, q \in I\!R^3$ are the positions of sun (mass M) and the planet (mass m), $p_S, p \in I\!R^3$ are their momenta, and G is the gravitational constant.
a) Prove that, in heliocentric coordinates $Q := q - q_S$, the equations of motion are
$$\ddot{Q} = -G(M+m) \frac{Q}{\|Q\|^3}.$$
b) Prove that $\frac{d}{dt}(Q(t) \times \dot{Q}(t)) = 0$, so that $Q(t)$ stays for all times t in the plane $E = \{q\,;\, d^T q = 0\}$, where $d = Q(0) \times \dot{Q}(0)$.
Conclusion. The coordinates corresponding to a basis in E satisfy the two-dimensional equations (2.1).

3. In polar coordinates, the two-body problem (2.1) becomes
$$\ddot{r} = -V'(r) \qquad \text{with} \qquad V(r) = \frac{L_0^2}{2r^2} - \frac{1}{r}$$
which is independent of φ. The angle $\varphi(t)$ can be obtained by simple integration from $\dot{\varphi}(t) = L_0/r^2(t)$.

4. Compute the period of the solution of Kepler's problem (2.1).
Result. $T = 2\pi(2|H_0|)^{-3/2}$, see e.g. [Ar78, page 40].

5. Whatever the initial values for the Kepler problem are, $1 + 2H_0 L_0^2 \geq 0$ holds. Hence, the value e is well defined by (2.6).
Hint. L_0 is the area of the parallelogram spanned by the vectors $q(0)$ and $\dot{q}(0)$.

6. Study numerically the solution of the perturbed Kepler problem with Hamiltonian
$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} - \frac{\varepsilon}{2\sqrt{(q_1^2 + q_2^2)^3}},$$
where ε is a positive or negative small number, e.g., $\varepsilon = \pm 0.01$ (see [SC94, page 8]). A closely related problem is the "main problem of artificial satellite theory" [Ki88].

7. Consider the *harmonic oscillator* $\ddot{q} + \omega^2 q = 0$. Prove that the exact solution and the numerical solution can be written as
$$\begin{pmatrix} \omega q(t) \\ \dot{q}(t) \end{pmatrix} = \begin{pmatrix} \cos \omega t & \sin \omega t \\ -\sin \omega t & \cos \omega t \end{pmatrix} \begin{pmatrix} \omega q(0) \\ \dot{q}(0) \end{pmatrix}, \qquad \begin{pmatrix} \omega q_{n+1} \\ \dot{q}_{n+1} \end{pmatrix} = M(\omega h) \begin{pmatrix} \omega q_n \\ \dot{q}_n \end{pmatrix}.$$
Compute $M(\omega h)$ for all numerical methods considered in this chapter, and investigate for which methods $\det M(\omega h) = 1$.

8. Show that not only the symplectic Euler and the implicit midpoint rule preserve exactly the angular momentum for Kepler's problem (see Table 2.1), but also the Störmer-Verlet scheme preserves it.

9. *Implementation of the Störmer-Verlet scheme.* Explain why the use of the one-step formulation (3.6) is numerically more stable than that of the two-term recursion (3.4).