The Störmer-Verlet method

F. Crivelli (`flcrivel@student.ethz.ch`)

May 8, 2008

Introduction

During this talk I'll introduce the *Störmer-Verlet method*, also known by the name *leap-frog method* or *Newton method* or more extensively *Newton-Störmer-Verlet-leapfrog method*. This method is used in order to find numerical solutions of ordinary differential equations: its various names are due to the different branchs of science in which the method is used. Carl Störmed used this method for his computations of the motion of ionized particles in the earth's magnetic field (aurora borealis) in 1907; in the context of partial differential equations of wave propagation, this method is called leap-frog method; Loup Verlet in 1967 used this method in molecular dynamics and then he discovered that Newton used this method in his *Principia Mathematica* in 1687.

1 Ordinary differential equations

In this paragraph I'll just remind some basis definitions of the language of ordinary differential equations.

Definition 1. *Let*

$$\begin{array}{rccc} y : & \mathbb{R} & \longrightarrow & \mathbb{R} \\ & x & \mapsto & y(x) \end{array}$$

be an unknown function of x and denote by $y^{(i)}$ its i-th derivative. An ***Ordinary Differential Equation (ODE) of order n*** *is an equation of the form*

$$F\left(x, y, y', \ldots, y^{(n-1)}\right) = y^{(n)},$$

where $F : \mathbb{R}^{n+1} \to \mathbb{R}$ is a function.

This leads to the definition of a solution of an ODE.

Definition 2. *A* ***solution*** *of an ODE of dimension n, $F\left(x, y, y', \ldots, y^{(n-1)}\right) = y^{(n)}$, is a function $u : I \subset \mathbb{R} \to \mathbb{R}$ such that u is n-times differentiable on I, F is defined for all $\left(x, u, u', \ldots, u^{(n-1)}\right)$, $x \in I$, and $F\left(x, u, u', \ldots, u^{(n-1)}\right) = u^{(n)}$, $x \in I$.*

Solutions of ODE of order n usually contain n parameters, resulting from the constants of integration. This parameters can be uniquely determined if we give an initial condition at the ODE, i.e., for some $x_0 \in \mathbb{R}$ and $y_0^{(i-1)} \in \mathbb{R}$, $i = 1, \ldots, n$, we want the solution to satisfy the conditions

$$y^{(i)}(x_0) = y_0^{(i)},\ i = 0, \ldots, n-1.$$

We have another important

Definition 3. *Let $y_i : \mathbb{R} \to \mathbb{R}$, $i = 1, \ldots, n$, be unknown functions of the variable x. A **first order system of differential equations of dimension n** is a system of equations of the form*

$$\begin{array}{rcl} y_1' & = & F_1(x, y_1, \ldots, y_n) \\ y_2' & = & F_2(x, y_1, \ldots, y_n) \\ \vdots & \vdots & \vdots \\ y_n' & = & F_n(x, y_1, \ldots, y_n) \end{array}$$

where $F_i : \mathbb{R}^{n+1} \to \mathbb{R}$, $i = 1, \ldots, n$, are functions. Setting

$$y := (y_1, \ldots, y_n)^T,\ \mathbf{F} := (F_1, \ldots, F_n)^T,$$

the system becomes

$$y' = \mathbf{F}(x, y),$$

with y and $\mathbf{F}$ interpreted as vectors. This notation was introduced by Giuseppe Peano in 1890.

Take an ODE of order n, $F\left(x, y, y', \ldots, y^{(n-1)}\right) = y^{(n)}$. If we write $y_i(x) := y^{i-1}(x)$, $i = 1, \ldots, n$, we obtain a first order system of differential equations of dimension n

$$\begin{array}{rcl} y_1' & = & y_2 \\ y_2' & = & y_3 \\ \vdots & \vdots & \vdots \\ y_{n-1}' & = & y_n \\ y_n' & = & F(x, y_1, \ldots, y_n) \end{array}$$

Hence, we can switch from an ODE of dimension n to a first order system of differential equations.

We look at the existence and uniqueness of solutions of a first order system of differential equations of dimension n. We state this theorem without proof.

Theorem 1. *Let $y' = \mathbf{F}(x, y)$ be a first order system of differential equations of dimension n with $y = (y_1, \ldots, y_n)^T$ and $\mathbf{F} = (F_1, \ldots, F_n)^T$ and initial conditions $y_i(x_0) = y_{i0}$, $x_0, y_{i0} \in \mathbb{R}$, $i = 1, \ldots, n$. Assume that $\mathbf{F}$ is continuous and that F_i is Lipschitz in the variables y_j for all $i, j = 1, \ldots, n$, i.e.,*

$$\mid F_i(x, y_1, \ldots, y_n) - F_i(x, \tilde{y}_1, \ldots, \tilde{y}_n) \mid \leq M \max_{1 \leq j \leq n} \mid y_j - \tilde{y}_j \mid,\ \forall\ i = 1, \ldots, n,$$

where $M > 0$ is a positive constant. Then the first order system of differential equations $y' = \mathbf{F}(x, y)$ has a unique solution $y_1(x), \ldots, y_n(x)$ on the interval

$$I := \{x \in \mathbb{R} \text{ s.t. } \mid x - x_0 \mid \leq \delta\}$$

for some $\delta > 0$.

2 Runge-Kutta methods

We are interested in solving numerically ODE and in how different numerical methods behave on ODE's, especially the Störmer-Verlet method. In order to do that, we introduce a family of methods, called *Runge-Kutta methods* in honor to the German mathematicians Carl Runge and Martin Kutta who developed these methods. One thing should always be in the mind of the reader, looking to a numerical method for solving an ODE: the expression of the derivative of a function g

$$g'(a) = \lim_{h \to 0} \frac{g(a+h) - g(a)}{h},$$

because this gives an approximation of the function at the point $a + h$, for small h,

$$g(a+h) \approx g(a) + hg'(a).$$

This leads to the Taylor series of g, that gives a good approximation of a function. We will now define the Runge-Kutta methods' family and concentrate on two of the most famous methods of this type: the *midpoint method* and the *Euler method*. We give just the definition for an ODE of first order, since we know that if the ODE is of order greater than 1, we can always translate the ODE on to a first order system of differential equations.

Definition 4. *Let* $F(x, y) = y'$ *be an ODE with initial condition* $y(x_0) = y_0$*. Let* $h > 0$ *be a positive real, called* ***step size****, and* s *a positive integer, called* ***number of stages****. Define* $x_n := x_0 + nh$ *and let* y_n *be the approximation of* $y(x_n)$*,* $n \geq 0$*. Then a* ***s-stage explicit Runge-Kutta method*** *is of the form*

$$y_{n+1} = y_n + h \sum_{j=1}^{s} b_j k_j$$

where

$$\begin{array}{rcl} k_1 & = & F(x_n, y_n) \\ k_2 & = & F(x_n + c_2 h, y_n + h a_{21} k_1) \\ k_3 & = & F\left(x_n + c_3 h, y_n + h(a_{31} k_1 + a_{32} k_2)\right) \\ \vdots & \vdots & \vdots \\ k_s & = & F\left(x_0 + c_s, y_n + h(a_{s1} k_1 + \cdots + a_{s,s-1} k_{s-1})\right) \end{array}$$

and $a_{21}, a_{31}, a_{32}, \ldots, a_{s1}, \ldots, a_{s,s-1}, b_1, \ldots, b_s, c_1, \ldots, c_s \in \mathbb{R}$.

Remark:

1. A method is often denoted by Φ_h, with $h > 0$ the step size, in order to say the $y_{n+1} = \Phi_h(y_n)$. Φ_h is called an **one-step method** because we approximate $y(x_{n+1})$ just by y_n and not by other previous approximation (e.g. by y_n and y_{n-1}). The function $\Phi_h : \mathbb{R} \to \mathbb{R}$ is called the **numerical flow**.

2. The term explicit refers to the fact that we compute directly the approximation y_{n+1} from y_n, i.e., $y_{n+1} = \Phi(y_n)$ and not that we can find y_{n+1} solving an equation, i.e., $y_{n+1} = \Phi_h(y_{n+1}, y_n)$. In the latter case the method is called implicit.

It is easy to extend the definition and the remarks in the case of a first order system of differential equations of finite dimension.
We will not discuss the convergence of a method, i.e., if the approximate solution approaches the exact solution when h goes to 0, in details because it will require some "advanced" definitions...

Definition 5. *The **local error** of a method is the error made by a step of the method, assuming that no error was made in earlier steps:*

$$\delta_h := ||y(x_n + h) - y_{n+1}|| = ||y(x_0 + h) - y_1|| \,.$$

*A method is said to be **consistent** if*

$$\lim_{h \to 0} \frac{\delta_h}{h} = 0$$

*and to have **order p** if $\delta_h = \mathcal{O}(h^{p+1})$ as $h \to 0$. Clearly if a method is of order $p \geq 1$, it is also consistent.*

A Runge-Kutta method is consistent if we have

$$c_i = \sum_{j=1}^{i-1} a_{ij}, \; 2 \leq i \leq s.$$

2.1 The explicit Euler method

The explicit Euler method is a 1 stage Runge-Kutta method of the form

$$y_{n+1} = y_n + hF(x_n, y_n).$$

This method is simplest Runge-Kutta's method. Indeed, for small $h > 0$, we have

$$y'(x) \approx \frac{y(x+h) - y(x)}{h},$$

and this gives

$$y(x+h) \approx y(x) + hF\left(x, y(x)\right).$$

Hence, this method is just the simplest approximation given by the definition of derivative.
We have that

$$y(x_0 + h) = y(x_0) + hy'(x_0) + \mathcal{O}(h^2)$$

using the Taylor series of y. We know that

$$y'(x_0) = F(x_0, y) = F(x_0, y_0) \text{ and } y(x_0) = y_0,$$

therefore

$$\begin{aligned} y(x_0+h) - y_1 &= y(x_0) + hy'(x_0) - y_0 - hF(x_0, y_0) + \mathcal{O}(h^2) \\ &= y_0 + hF(x_0, y_0) - y_0 - hF(x_0, y_0) + \mathcal{O}(h^2) \\ &= \mathcal{O}(h^2), \end{aligned}$$

so the Euler methods has order 1.

2.2 The explicit midpoint method

The midpoint method is a 2 stages Runge-Kutta method given by the formula

$$y_{n+1} = y_n + hF\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}F(x_n, y_n)\right).$$

Geometrically, the midpoint method can be viewed in the following way: assuming that y_n is the exact value of $y(x_n)$, the midpoint method gives y_{n+1} such that the segment between y_n and y_{n+1} is approximatively parallel to the tangent line at the midpoint $y(x_n + h/2)$.
We look at the Taylor expansions of $y(x_0 + h)$ and $F\left(x_0 + \frac{h}{2}, y_0 + \frac{h}{2}F(x_0, y_0)\right)$:

$$y(x_0 + h) = y(x_0) + hy'(x_0) + \frac{h^2}{2}y''(x_0) + \mathcal{O}(h^3)$$

and

$$F\left(x_0 + \frac{h}{2}, y_0 + \frac{h}{2}F(X_0, y_0)\right) = F(x_0, y_0) + \frac{h}{2}F_x(x_0, y_0) + \frac{h}{2}F(x_0, y_0)F_y(x_0, y_0) + \mathcal{O}(h^2),$$

where F_x, resp. F_y, denotes the partial derivative of F with respect to the variable x, resp. to the variable y. This gives

$$\begin{aligned} y_1 &= y_0 + hF\left(x_0 + \tfrac{h}{2}, y_0 + \tfrac{h}{2}F(x_0, y_0)\right) \\ &= y_0 + h\left(F(x_0, y_0) + \tfrac{h}{2}F_x(x_0, y_0) + \tfrac{h}{2}F(x_0, y_0)F_y(x_0, y_0) + \mathcal{O}(h^2)\right) \\ &= y_0 + hF(x_0, y_0) + \tfrac{h^2}{2}F_x(x_0, y_0) + \tfrac{h^2}{2}F(x_0, y_0)F_y(x_0, y_0) + h\mathcal{O}(h^2) \\ &= y_0 + hF(x_0, y_0) + \tfrac{h^2}{2}F_x(x_0, y_0) + \tfrac{h^2}{2}F(x_0, y_0)F_y(x_0, y_0) + \mathcal{O}(h^3). \end{aligned}$$

On the other side, we know that $y(x_0) = y_0$ and $y'(x_0) = F(x_0, y_0)$. Moreover, we find that

$$y''(x_0) = F_x(x_0, y_0) + F(x_0, y_0)F_y(x_0, y_0).$$

Finally, we get

$$y(x_0 + h) - y_1 = \mathcal{O}(h^3),$$

hence, the midpoint method has order 2.

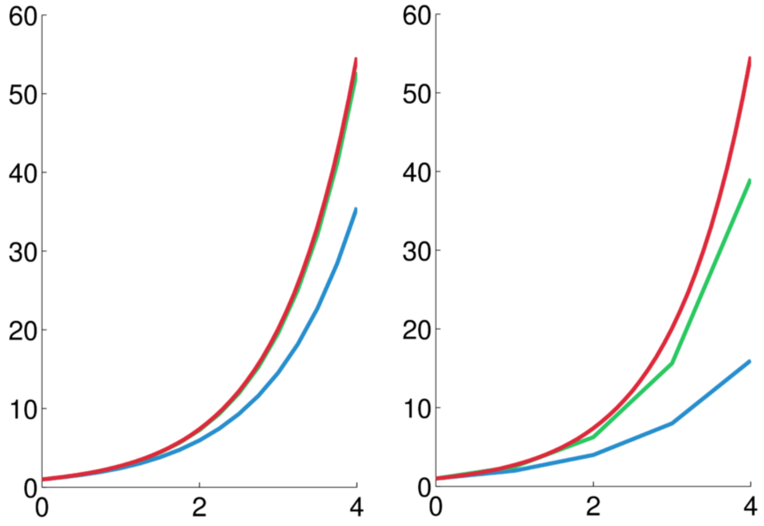

Figure 1: The exact solution e^x of the ODE $y' = y, y(0) = 1$ is the red line, in green we have the midpoint approximation and in blue the Euler approximation. The step size in the left picture is $h = 1$, in the right picture $h = 0.25$. The right picture shows that the midpoint method converges faster than the Euler method.

2.3 Example

We want to solve numerically, using the two methods presented above, the ODE

$$y' = y, y(0) = 1.$$

The exact solution is e^x. Fix $h > 0$. For the Euler method we get

$$y_n = (1+h)^n,\ n \geq 0$$

while for the midpoint method we get

$$y_n = \left(1 + h + \frac{h^2}{2}\right)^n,\ n \geq 0.$$

3 Störmer-Verlet method

In this section, the Störmer-Verlet method is presented, with some of its interesting properties, in the special case of a second order ODE of the form

$$\ddot{q} = F(q),$$

where the right-hand side does not depend on $\dot{q}$. This equation is common in physics. There are variations of the Störmer-Verlet method for a genereal second order ODE.

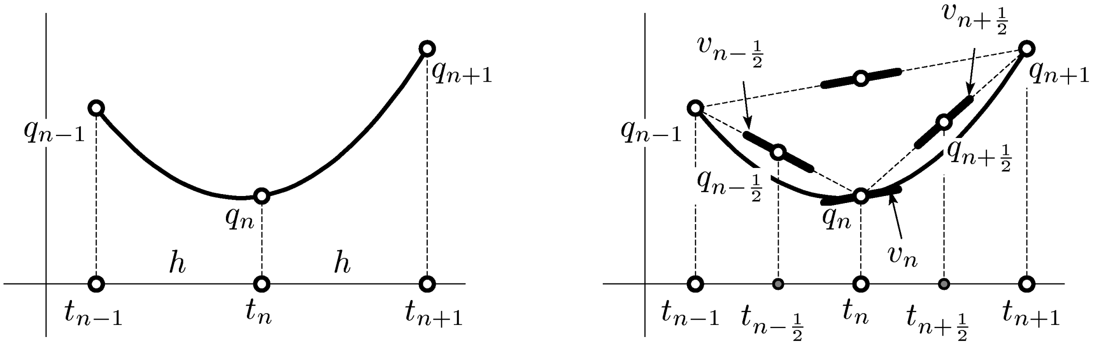

Figure 2: Störmer-Verlet method. Left: two-step formulation. Right: one-step formulation.

3.1 Definition

Let $h > 0$ be the step size. The simplest case is just the discretisation of the ODE, i.e.,

$$q_{n+1} - 2q_n + q_{n-1} = h^2 F(q_n).$$

It is a two-step method since q_{n+1} is computed using q_n and q_{n-1}. This formulation is not very interesting. We know that we can transform a second order ODE into a first order system of differential equations of dimension 2, in order to do so, we introduce the unknown function $v = \dot{q}$ and the system becomes

$$v = \dot{q}, \quad \dot{v} = F(q).$$

In physics often this type of system is closely related to the motion of a physical body. In this sense, we can see v as the velocity, q as the displacement (as functions of the time) and F describes some kind of force acting on the physical body.
We set

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

Inserting these expressions in the two-step formulation gives a one-step method Φ_h : $(q_n, v_n) \mapsto (q_{n+1}, v_{n+1})$ of the form

$$\begin{aligned} q_{n+1} &= q_n + h\left(v_n + \tfrac{h}{2}F(q_n)\right), \\ v_{n+1} &= v_n + \tfrac{h}{2}F(q_n) + \tfrac{h}{2}F(q_{n+1}). \end{aligned}$$

This formulation of the Störmer-Verlet method is more economic to implement for numerical calculation and is also numerically more stable than the two-step formulation.

Recall that the **flow** of a first order system of differential equations $y = \mathbf{F}(x, y)$ of dimension n is the function $\varphi_x : \mathbb{R}^n \to \mathbb{R}^n$ which associates, for a given x, to the initial condition $y_0 = y(x_0)$ the corresponding solution value at x

$$\varphi_x(y_0) = y(x),$$

where y depends on the choice of the initial value y_0. Sometimes φ_x is called the *exact* flow, in order to avoid confusion between the flow of a first order system of differential equations and the numerical flow of a method.
Let us look at the order of the Störmer-Verlet method. Recall that $\delta_h = ||y(x_0 + h) - y_1||$, where $y(x)$ is the solution of the system

$$\dot{y} = \left(\begin{array}{c} \dot{q} \\ \dot{v} \end{array} \right) = \left(\begin{array}{c} v \\ F(q) \end{array} \right) = \mathbf{F}(y).$$

with initial conditions $v_0 = v(x_0)$, $q_0 = q(x_0)$. We have

$$y_1 = \left(\begin{array}{c} q_1 \\ v_1 \end{array} \right) = \left(\begin{array}{c} q_0 + h\left(v_0 + \frac{h}{2}F(q_0)\right) \\ v_0 + \frac{h}{2}F(q_0) + \frac{h}{2}F(q_1) \end{array} \right) \text{ and } y(x_0+h) = \left(\begin{array}{c} q(x_0+h) \\ v(x_0+h) \end{array} \right)$$

We have also the following Taylor expansions

$$\begin{array}{rcl} q(x_0+h) & = & q_0 + hv_0 + \frac{h^2}{2}F(q_0) + \mathcal{O}(h^3), \\ v(x_0+h) & = & v_0 + hF(q_0) + \frac{h^2}{2}\ddot{v}(x_0) + \mathcal{O}(h^3), \\ F(q_1) & = & F(q_0) + h\left(v_0 + \frac{h}{2}F(q_0)\right)\dot{F}(q_0) + \mathcal{O}(h^2). \end{array}$$

Note that $\ddot{v}(x_0) = \dot{F}(q_0)v_0$ since $\dot{v}(x) = F\left(q(x)\right)$ gives $\ddot{v}(x) = \dot{F}\left(q(x)\right)\dot{q}(x) = \dot{F}\left(q(x)\right)v(x)$. We have

$$q(x_0+h) - q_1 = \mathcal{O}(h^3) \text{ and } v(x_0+h) - v_1 = \mathcal{O}(h^3)$$

and this implies that the Störmer-Verlet method has order 2.

3.2 Properties

We introduce some notions.

Definition 6. *Let $\Phi_h : (q_n, v_n) \mapsto (q_{n+1}, v_{n+1})$ be a one-step method for the first order system of differential equations $v = \dot{q}$, $\dot{v} = F(q)$.*

- *Φ_h is called* ***symmetric*** *if*

$$\Phi_h = \Phi_{-h}^{-1},$$

  where Φ_{-h}^{-1} denotes the method $\tilde{\Phi}_{-h} : (q_{n+1}, v_{n+1}) \mapsto (q_n, v_n)$, i.e, we invert the subscripts n and $n+1$, as a reflection based on $x_{n+\frac{1}{2}}$.

- *the numerical flow Φ_h is called* ***reversible*** *if*

$$\Phi_h(q, v) = (\hat{q}, \hat{v}) \text{ implies } \Phi_h(\hat{q}, -\hat{v}) = (q, -v),$$

  for all q, v and for all h.

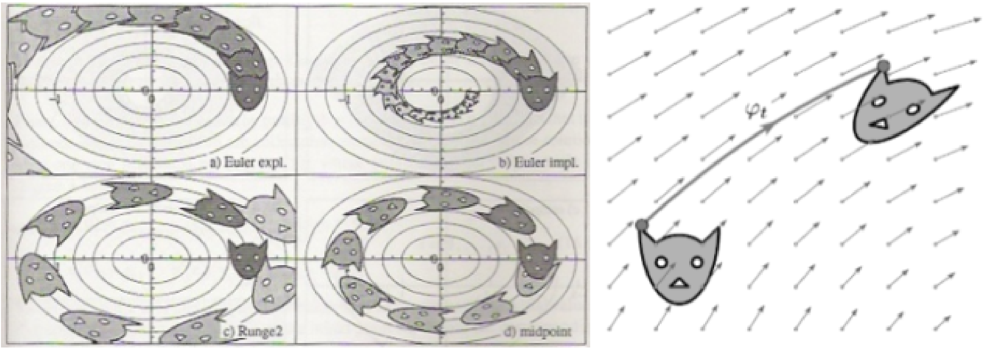

Figure 3: On the right some non-symplectic methods. On the left the simplecticity of the Störmer-Verlet method.

- *the method* Φ_h *is called* ***symplectic*** *if it satisfies*

$$\Phi_h'(q,v)^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \Phi_h'(q,v) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

  for all q, v, h *and where* Φ_h' *denotes the Jacobian of* Φ_h*.*

For a method Φ_h, to be symmetric means that when we have computed an approximation y_n, starting with initial condition y_0, if we apply the method Φ_{-h} with initial condition $\tilde{y}_0 = y_n$, after n steps we have that $\tilde{y}_n = y_0$. Intuitively, this means that if we reverse the time, we return where we started.
The reversibility is a very important, because in the case of the above system the flow satisfies the same condition and in the case of physics equations this means that inverting the initial velocity does not change the trajectory, it just inverts the direction of the motion.
The property of being symplectic is also very important, because it implies the preservation of the volume: if the flow of a first order system of differential equations is symplectic, we have that, for a given x, $\operatorname{vol}(\varphi_x(\mathcal{U})) = \operatorname{vol}(\mathcal{U})$, for any open bounded set $\mathcal{U}$ such that the flow is defined in $\mathcal{U}$. Indeed, the fact to be symplectic implies that $|\det \Phi_h'(q,v)| = 1$, for all q, v and h, therefore

$$\operatorname{vol}(\varphi_x(\mathcal{U})) = \int_{\varphi_x(\mathcal{U})} dy = \int_{\mathcal{U}} |\det \Phi_h'(q,v)|\, dy_0 = \int_{\mathcal{U}} dy_0 = \operatorname{vol}(\mathcal{U}).$$

We can see this in the figure 3: the cats denotes a set of initial values; if a method is symplectic the cats have always the same area.
Remark that the midpoint and the Euler methods haven't any of these properties, although they can have one or more of these properties in the case of a particular system of differential equations.

We prove now that the Störmer-Verlet method satisfies the above conditions.

Theorem 2. *The Störmer-Verlet method is symmetric.*

Proof: We have $\Phi_{-h} \ : \ (q_n, v_n) \mapsto (q_{n+1}, v_{n+1})$

$$\begin{aligned} q_{n+1} &= q_n - h\left(v_n - \tfrac{h}{2}F(q_n)\right), \\ v_{n+1} &= v_n - \tfrac{h}{2}F(q_n) - \tfrac{h}{2}F(q_{n+1}). \end{aligned}$$

Inverting n and $n+1$ we get $\Phi_{-h}^{-1} \ : \ (q_{n+1}, v_{n+1}) \mapsto (q_n, v_n)$, explicitly

$$\begin{aligned} q_n &= q_{n+1} - h\left(v_{n+1} - \tfrac{h}{2}F(q_{n+1})\right), \\ v_n &= v_{n+1} - \tfrac{h}{2}F(q_{n+1}) - \tfrac{h}{2}F(q_n). \end{aligned}$$

Finally

$$\begin{aligned} q_{n+1} &= q_n + h\left(v_{n+1} - \tfrac{h}{2}F(q_{n+1})\right) \\ &= q_n + h\left(v_n + \tfrac{h}{2}F(q_n)\right), \\ v_{n+1} &= v_n + \tfrac{h}{2}F(q_n) + \tfrac{h}{2}F(q_{n+1}), \end{aligned}$$

hence $\Phi_h = \Phi_{-h}^{-1}$ and Φ_h is symmetric.

$\square$

Theorem 3. *The Störmer-Verlet method is reversible.*

Proof: We have

$$\Phi_h(q,v) = (\hat{q}, \hat{v}) = \left(q + h\left(v + \frac{h}{2}F(q)\right), v + \frac{h}{2}F(q) + \frac{h}{2}F\left(q + h\left(v + \frac{h}{2}F(q)\right)\right)\right)$$

and so

$$\Phi_h(\hat{q}, -\hat{v}) \ = \ \left(\underbrace{\hat{q} + h\left(-\hat{v} + \frac{h}{2}F(\hat{q})\right)}_{\alpha} \ , \ \underbrace{-\hat{v} + \frac{h}{2}F(\hat{q}) + \frac{h}{2}F\left(\hat{q} + h\left(-\hat{v} + \frac{h}{2}F(\hat{q})\right)\right)}_{\beta}\right).$$

We get

$$\begin{aligned} \alpha &= q + h\left(v + \tfrac{h}{2}F(q)\right) + h\left(-v - \tfrac{h}{2}F(q) - \tfrac{h}{2}F(\hat{q}) + \tfrac{h}{2}F(\hat{q})\right) \\ &= q \end{aligned}$$

and

$$\begin{aligned} \beta &= -v - \tfrac{h}{2}F(q) - \tfrac{h}{2}F(\hat{q}) + \tfrac{h}{2}F(\hat{q}) + \\ &+ \tfrac{h}{2}F\left(\hat{q} + h\left(-v - \tfrac{h}{2}F(q) - \tfrac{h}{2}F(\hat{q}) + \tfrac{h}{2}F(\hat{q})\right)\right) \\ &= -v - \tfrac{h}{2}F(q) + \tfrac{h}{2}F\left(q + h\left(v + \tfrac{h}{2}F(q)\right) + h\left(-v - \tfrac{h}{2}F(q)\right)\right) \\ &= -v. \end{aligned}$$

This gives $\Phi_h(\hat{q}, -\hat{v}) = (q, -v)$, hence Φ_h is reversible.

□

Theorem 4. *The Störmer-Verlet method is symplectic.*

Proof: Write Φ_h in the following way:

$$\Phi_h(q,v) = (\Phi_1(q,v), \Phi_2(q,v))\,.$$

The Jacobian $\Phi_h'(q,v)$ is the matrix

$$\begin{pmatrix} \partial_q\Phi_1(q,v) & \partial_v\Phi_1(q,v) \\ \partial_q\Phi_2(q,v) & \partial_v\Phi_2(q,v) \end{pmatrix}.$$

We get

$$\Phi_h'(q,v)^T \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \Phi_h'(q,v) = \begin{pmatrix} 0 & \partial_q\Phi_1\partial_v\Phi_2 - \partial_v\Phi_1\partial_q\Phi_2 \\ -(\partial_q\Phi_1\partial_v\Phi_2 - \partial_v\Phi_1\partial_q\Phi_2) & 0 \end{pmatrix}(q,v).$$

We have

$$\begin{aligned} \partial_q\Phi_1(q,v) &= 1 + \tfrac{h^2}{2}F'(q), \\ \partial_q\Phi_2(q,v) &= \tfrac{h}{2}F'(q) + \tfrac{h}{2}F'\left(q + h\left(v + \tfrac{h}{2}F(q)\right)\right)\left(1 + \tfrac{h^2}{2}F'(q)\right), \\ \partial_v\Phi_1(q,v) &= h \\ \partial_v\Phi_2(q,v) &= 1 + \tfrac{h^2}{2}F'\left(q + h\left(v + \tfrac{h}{2}F(q)\right)\right). \end{aligned}$$

This gives

$$\begin{aligned} (\partial_q\Phi_1\partial_v\Phi_2 - \partial_v\Phi_1\partial_q\Phi_2)(q,v) &= \left(1 + \tfrac{h^2}{2}F'(q)\right)\left(1 + \tfrac{h^2}{2}F'\left(q + h\left(v + \tfrac{h}{2}F(q)\right)\right)\right) - \\ &- h\left(\tfrac{h}{2}F'(q) + \tfrac{h}{2}F'\left(q + h\left(v + \tfrac{h}{2}F(q)\right)\right)\left(1 + \tfrac{h^2}{2}F'(q)\right)\right) \\ &= 1 + \tfrac{h^2}{2}F'(q) + \tfrac{h^2}{2}F'(q+\ldots) + \tfrac{h^4}{4}F'(q)F'(q+\ldots) - \\ &- \tfrac{h^2}{2}F'(q) - \tfrac{h^2}{2}F'(q+\ldots)\left(1 + \tfrac{h^2}{2}F'(q)\right) \\ &= 1 \end{aligned}$$

and therefore Φ_h is symplectic.

□

3.3 Examples

Let us look at two example: the Kepler problem and the aurora borealis.
The first example is very famous, known as *Kepler problem* because Johannes Kepler (1571-1630) proposed a similar formula for the celestial orbits, i.e., the equations that define the displacements of two celestial bodies that interact by a force. Explicitly

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

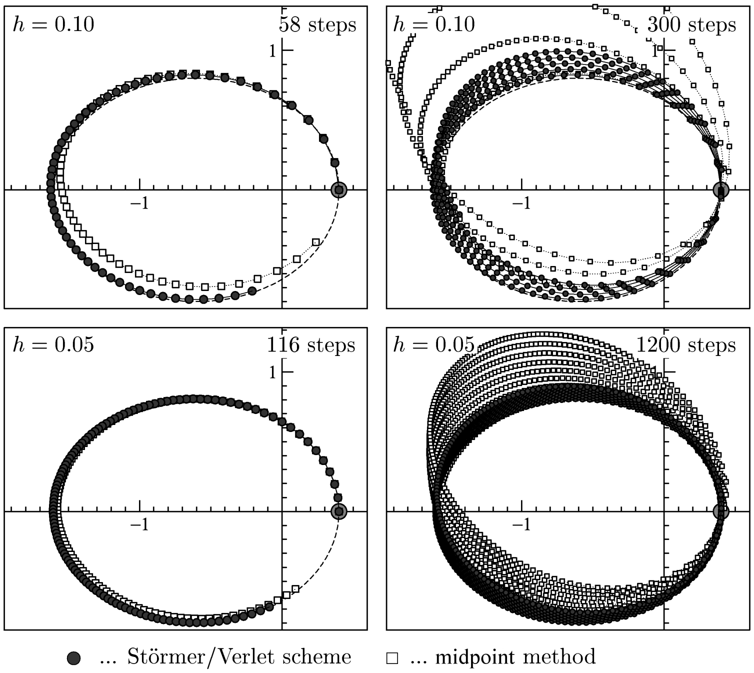

Figure 4: Kepler problem; dashed: exact solution.

with initial condition

$$q_1(0) = 1 - e,\ q_2(0) = 0,\ \dot{q}_1(0) = 0,\ \dot{q}_2(0) = \sqrt{\frac{1+e}{1-e}}$$

and $e = 0.6$. In a two-body problem, the exact solution (q_1, q_2) describes the orbit of a body with respect to the other body and has period 2π. Figure 4 shows the behavior of the Störmer-Verlet method with different step-size and different number of steps compared to the explicit midpoint method presented above. We know that the midpoint method has the same order of the Störmer-Verlet method, but the figure shows us that the Störmer-Verlet method approximate pretty well the exact solution in the two cases, instead the midpoint method deteriorates rapidly when the step-size increases and in both cases is less accurate than the Störmer-Verlet method. We remark the fact that the Kepler problem was the foundation of Newton's theory of universal gravitation.

The second example is the original problem that Carl Störmer tried to solve numerically in 1907. Störmer tried to confirm numerically a previous conjecture, that says that the phenomenon known as aurora borealis (figure 5) is produced by electrical particles emanating from the sun and moving in the earth's magnetic field. We are not interested in all the detailed calculations, we hope to convince the reader that using the Störmer-Verlet method we obtain a solution that approaches the real behavior of these particles as shown in the figure 6. This picture shows 125 solution curves in the 3-dimensional space with neighboring initial values: this gives an impression of how an aurora borealis comes into being.

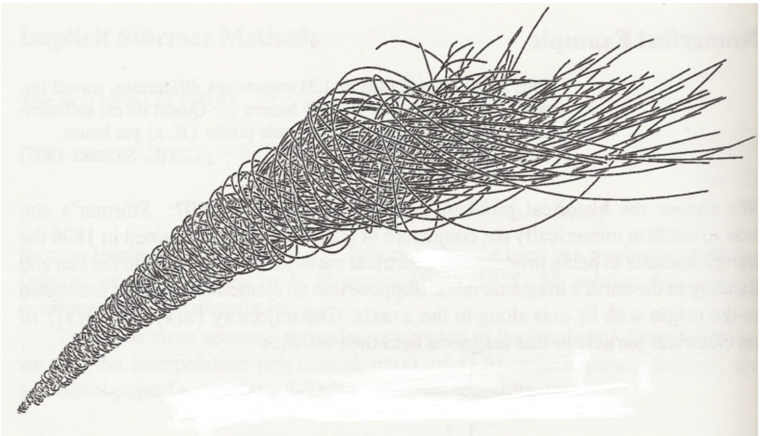

Figure 5: 125 solution curves using the Störmer method.

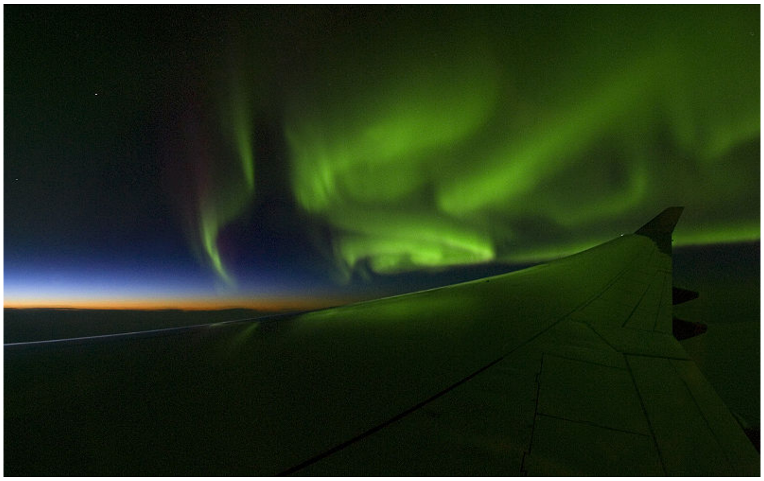

Figure 6: The aurora borealis.

Contents

References

- *Solving Ordinary Differential Equations Vol. I*, E. Hairer, S.P. Nørsett, G. Wanner, *Springer, 1993.*

- *Geometric numerical integration illustrated by the Störmer/Verlet method* (Acta Numerica (2003) pp. 1-51), E. Hairer, C. Lubich, G. Wanner, *Cambridge University Press, 2003.*