Integrador simpléctico I: Muestre que el método de Verlet es simpléctico, es decir, el Jacobiano inducido en el método es igual a uno.

Sea f una función vectorial:

$$f(x_1, x_2, \dots) = (y_1, y_2, \dots)$$

Entonces, el jacobiano se define como:

$$J = \begin{vmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots \\ \vdots & \vdots & \ddots \end{vmatrix}$$

En este caso se tiene la siguiente función:

$$f(x_n, v_n) = (x_{n+1}, v_{n+1})$$

El método de Verlet indica lo siguiente:

$$x_{n+1} = 2x_n - x_{n-1} + a(x_n)\Delta t^2, \qquad v_n = \frac{x_{n+1} - x_{n-1}}{2\Delta t}$$

Se pueden hacer unas operaciones para poner estas ecuaciones en términos de las variables que nos interesan:

$$v_n = \frac{x_{n+1} - x_{n-1}}{2\Delta t} \to v_n = \frac{(2x_n - x_{n-1} + a(x_n)\Delta t^2) - x_{n-1}}{2\Delta t} \to v_n = \frac{2x_n - 2x_{n-1} + a(x_n)\Delta t^2}{2\Delta t} \to$$

$$\to v_n = \frac{x_n - x_{n-1}}{\Delta t} + \frac{a(x_n)\Delta t}{2}$$

$$x_{n+1} = 2x_n - x_{n-1} + a(x_n)\Delta t^2 \to x_{n+1} = x_n + x_n - x_{n-1} + \frac{a(x_n)\Delta t^2}{2} + \frac{a(x_n)\Delta t^2}{2} \to$$

$$\to x_{n+1} = x_n + \left(\frac{x_n - x_{n-1}}{\Delta t} + \frac{a(x_n)\Delta t}{2}\right)\Delta t + \frac{a(x_n)\Delta t^2}{2} \to$$

$$\to x_{n+1} = x_n + v_n\Delta t + \frac{a(x_n)\Delta t^2}{2}$$

$$v_n = \frac{x_n - x_{n-1}}{\Delta t} + \frac{a(x_n)\Delta t}{2} \to v_{n+1} = \frac{x_{n+1} - x_n}{\Delta t} + \frac{a(x_{n+1})\Delta t}{2} \to$$

$$\to v_{n+1} = \frac{\left(x_n + v_n\Delta t + \frac{a(x_n)\Delta t^2}{2}\right) - x_n}{\Delta t} + \frac{a(x_{n+1})\Delta t}{2} \to v_{n+1} = \frac{v_n\Delta t + \frac{a(x_n)\Delta t^2}{2}}{\Delta t} + \frac{a(x_{n+1})\Delta t}{2} \to$$

$$\to v_{n+1} = v_n + \frac{a(x_n)\Delta t}{2} + \frac{a(x_{n+1})\Delta t}{2}$$

Entonces se tienen estas ecuaciones:

$$x_{n+1} = x_n + v_n\Delta t + \frac{a(x_n)\Delta t^2}{2}, v_n + \frac{a(x_n) + a(x_{n+1})}{2}\Delta t$$

Se calculan las derivadas:

$$\frac{\partial x_{n+1}}{\partial v_n} = \Delta t, \qquad \frac{\partial v_{n+1}}{\partial v_n} = 1 + \frac{a'(x_{n+1})(\Delta t)}{2}\Delta t = 1 + \frac{a'(x_{n+1})\Delta t^2}{2}, \qquad \frac{\partial x_{n+1}}{\partial x_n} = 1 + \frac{a'(x_n)\Delta t^2}{2}$$

$$\frac{\partial v_{n+1}}{\partial x_n} = \frac{a'(x_n) + a'(x_{n+1})\left(1 + \frac{a'(x_n)\Delta t^2}{2}\right)}{2}\Delta t = \frac{a'(x_n) + a'(x_{n+1})}{2}\Delta t + \frac{a'(x_{n+1})a'(x_n)\Delta t^3}{4}$$

Por lo tanto, el jacobiano es:

$$J = \begin{vmatrix} 1 + \frac{a'(x_n)\Delta t^2}{2} & \Delta t \\ \frac{a'(x_n) + a'(x_{n+1})}{2}\Delta t + \frac{a'(x_{n+1})a'(x_n)\Delta t^3}{4} & 1 + \frac{a'(x_{n+1})\Delta t^2}{2} \end{vmatrix} =$$

$$= \left(1 + \frac{a'(x_n)\Delta t^2}{2}\right)\left(1 + \frac{a'(x_{n+1})\Delta t^2}{2}\right) - \left(\frac{a'(x_n) + a'(x_{n+1})}{2}\Delta t + \frac{a'(x_{n+1})a'(x_n)\Delta t^3}{4}\right)(\Delta t) =$$

$$= 1 + \frac{a'(x_n)\Delta t^2}{2} + \frac{a'(x_{n+1})\Delta t^2}{2} + \frac{a'(x_n)a'(x_{n+1})\Delta t^4}{4} - \frac{a'(x_n) + a'(x_{n+1})}{2}\Delta t^2 - \frac{a'(x_{n+1})a'(x_n)\Delta t^4}{4} = 1$$

Y como el jacobiano es 1, se concluye que el algoritmo es simpléctico.