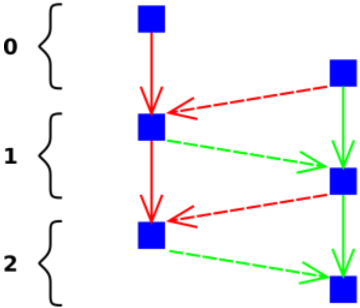
Molecular Dynamics and simple pendulum



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Content

Arithmetic-Geometrical Mean

1 - Carl Friedrich Gauss (1809) AGM - Algorithm

2 - Arithmetical-geometrical mean were and is used to compute π to billions and trillions of digits.

3 - AGM for exact values of the pendulum’s period.

Naive Integration

1 - Time reversible - do not work

$$\theta' = \theta + p\Delta t, \quad p' = p + F(\theta')\Delta t$$

$$\theta \leftrightarrow \theta', \quad p \leftrightarrow -p'$$

2 - Conservation of Phase Volume - do not work

$$\triangle J = \begin{vmatrix} \frac{\partial\theta'}{\partial\theta} & \frac{\partial\theta'}{\partial p} \\ \frac{\partial p'}{\partial\theta} & \frac{\partial p'}{\partial p} \end{vmatrix} = \begin{vmatrix} 1 & \Delta t \\ F'(\theta)\Delta t & 1 \end{vmatrix} = 1 - F'(\theta)(\Delta t)^2$$

3 - Conservation of Hamiltonian - do not work

$$H' \equiv H(\theta', p') = H(\theta, p) \equiv H + O(\Delta t^2)$$

Introduction to Leapfrog

1 - Method for solving dynamical system problems, and it is used in many fields like physics, chemistry, numerical analysis, biology, etc.

2 - Leapfrog is a second-order differential method, wich we choose to solve the equation of harmonic motion:

$$\ddot{\theta} + \omega_0^2 sin(\theta) = 0$$

3 - Leapfrog method updates position at step θ_{n+1} and it's momentum on step p_{n+1}, it comes from Verlett-Algorithm.

The Algorithm

The leapfrog integrator should be able to find a numerical solution to these equations:

$$
\begin{aligned}
\tilde{p} &= p - (\omega_0^2 \sin\theta)\frac{\Delta t}{2} \\
\theta' &= \theta + \tilde{p}\Delta t \\
p' &= \tilde{p} - (\omega_0^2 \sin\theta')\frac{\Delta t}{2}
\end{aligned}
$$

Limitation of Leapfrog

1 - The limitation of leapfrog algorithm is that the hamiltonian is not conserved:

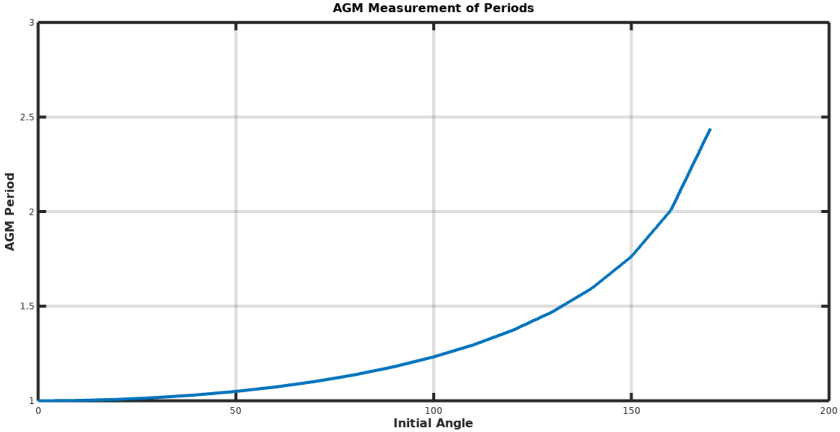
$$H' \equiv H(\theta', p') = H(\theta, p) \equiv H + O(\Delta t^2)$$

2 - The leapfrog algorithm satisfies only two of three hamiltonian dynamics properties.

3 - Approaching to a solution we set the Δt constant to get results.

Periods by Arithmetic-Geometrical mean

Leapfrog produces the same periods as AGM algorithm.



Conclusions

1 - Molecular dynamics can give a solution to dynamical system through Leapfrog algorithm.

2 - Leapfrog is ”symplectic” for harmonic motion, meaning that motion preserve volume and is time reversible in phase space.

3 - Leapfrog approx with error to 10^{-7} digits besides AGM.

4 - The integrator can not calculate chaos.


QUESTIONS