Long-term Conservation of Geometric Invariants by Newmark Beta methods

Numerical Computation Structured Projects

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Introduction

Geometric Numerical Integration

- Relatively young field - came into limelight around 40 years ago
- Study of numerical solutions to ordinary differential equations had begun in the late 19^{th} Century
- The focus had been on quantity - making the solutions as accurate as possible
- Interest in computer simulations over a longer time frame raised an important question

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What about the quality of solutions?

Example: Lotka-Volterra Equations

$$\frac{du}{dt} = u \cdot (1 - v),$$
$$\frac{dv}{dt} = (u - 2) \cdot v,$$

where $u(t)$ is the population of the prey over time, and $v(t)$ is that of the predator. Dividing the two equations, we get that

$$\left(1 - \frac{2}{u}\right) du = \left(\frac{1}{v} - 1\right) dv.$$

Integrating the two sides of the equation, we get that

$$I(u, v) = u - 2 \ln u + v - \ln v = const$$

Example: Lotka-Volterra Equations

Defining $a(u, v) := u \cdot (1 - v)$, and $b(u, v) := (u - 2) \cdot v$

- Explicit Euler Method

$$u_{n+1} = u_n + h \cdot a(u_n, v_n),$$
$$v_{n+1} = v_n + h \cdot b(u_n, v_n).$$

- Implicit Euler Method

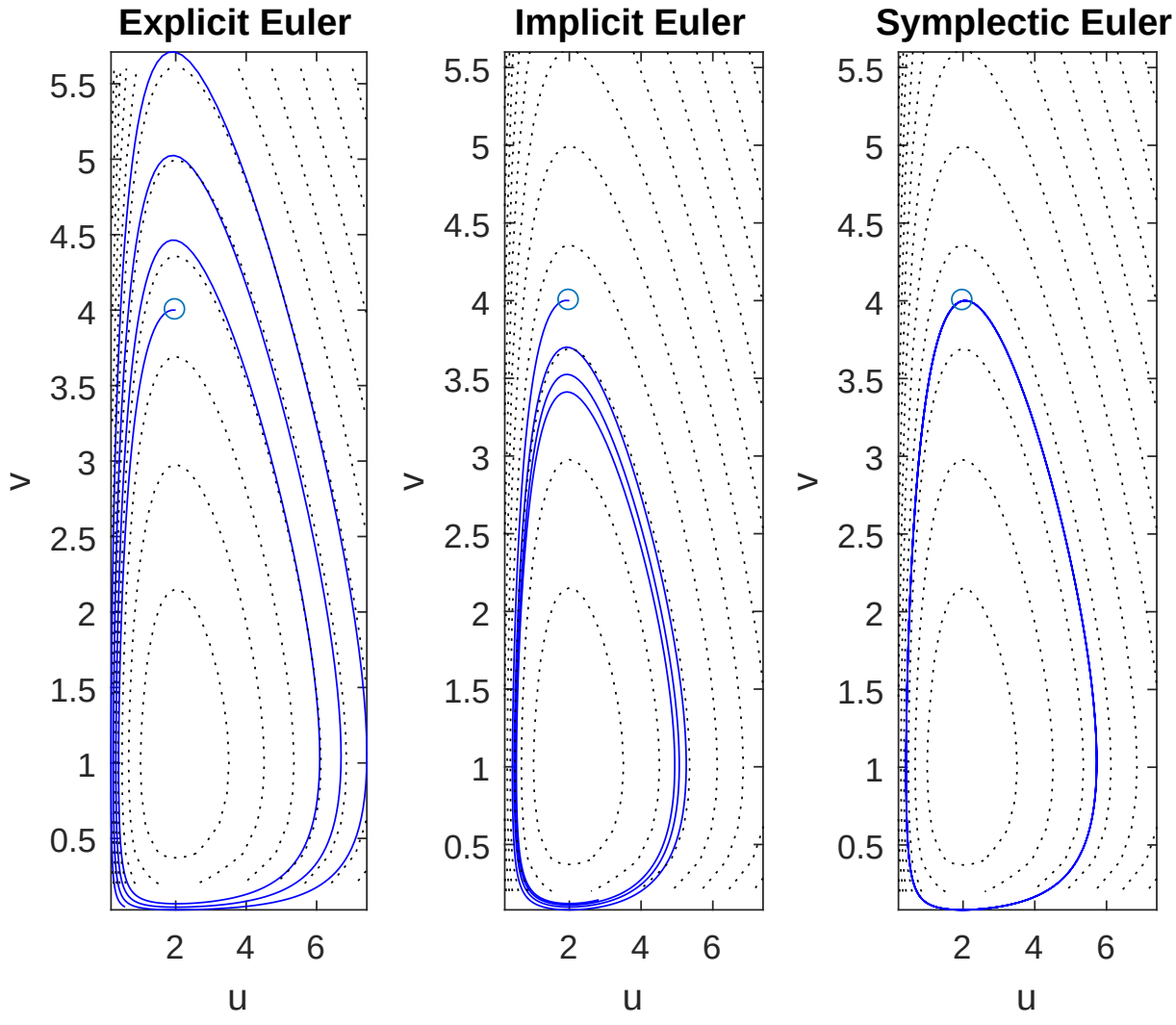
$$u_{n+1} = u_n + h \cdot a(u_{n+1}, v_{n+1}),$$
$$v_{n+1} = v_n + h \cdot b(u_{n+1}, v_{n+1}).$$

- Symplectic Euler Method

$$u_{n+1} = u_n + h \cdot a(u_{n+1}, v_n),$$
$$v_{n+1} = v_n + h \cdot b(u_{n+1}, v_n).$$

Example: Lotka-Volterra Equations

Initial Conditions: $N = 1000, h = 0.02, (u_0, v_0) = (2, 4)$



Newmark Beta methods

Newmark Beta methods

$$\mathbf{v}_{i+1} = \mathbf{v}_i + h\left[(1-\gamma)\,\mathbf{a}_i + \gamma \mathbf{a}_{i+1}\right],$$
$$\mathbf{x}_{i+1} = \mathbf{x}_i + h\mathbf{v}_i + \frac{h^2}{2}\left[(1-2\beta)\,\mathbf{a}_i + 2\beta \mathbf{a}_{i+1}\right],$$

where $\gamma \in [0,1]$ and $\beta \in \left[0, \frac{1}{2}\right]$.

- Second order accurate $\Leftrightarrow \gamma = \frac{1}{2}$
- Conditionally stable $\Leftrightarrow 2\beta \geq \gamma \geq \frac{1}{2}$

Newmark Beta methods

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where $\gamma \in [0,1]$ and $\beta \in \left[0, \frac{1}{2}\right]$.

- Average Acceleration Method $\left(\gamma = \frac{1}{2},\ \beta = \frac{1}{4}\right)$
- Linear Acceleration Method $\left(\gamma = \frac{1}{2},\ \beta = \frac{1}{6}\right)$
- Velocity Verlet Method $\left(\gamma = \frac{1}{2},\ \beta = 0\right)$

Computational Application of Newmark Beta methods

Application of the General Procedure

In general unless β is 0 we may proceed with our calculation as follows:

(1) Assume values of the acceleration of each mass at the end of the interval.

(2) Compute the velocity and the displacement of each mass at the end of the interval from Eqs. (4) and (3), respectively. (Unless damping is present it is not necessary to compute the velocity at the end of the interval until step (5) is completed.)

(3) For the computed displacements at the end of the interval compute the resisting forces R which are required to hold the structural framework in the deflected configuration.

(4) From Eq. (1) and the applied loads and resisting forces at the end of the interval recompute the acceleration at the end of the interval.

(5) Compare the derived acceleration with the assumed acceleration at the end of the interval. If these are the same the calculation is completed. If these are different, repeat the calculation with a different value of assumed acceleration. It will usually be best to use the derived value as the new acceleration for the end of the interval.

Computational Application of Newmark Beta methods

$$\mathbf{v}_{i+1} = \mathbf{v}_i + h\left[(1-\gamma)\,\mathbf{a}_i + \gamma \mathbf{a}_{i+1}\left(\mathbf{x}_{i+1}\right)\right],$$

$$\mathbf{x}_{i+1} = \mathbf{x}_i + h\mathbf{v}_i + \frac{h^2}{2}\left[(1-2\beta)\,\mathbf{a}_i + 2\beta \mathbf{a}_{i+1}\left(\mathbf{x}_{i+1}\right)\right].$$

Computational Application of Newmark Beta methods

$$\mathbf{v}_{i+1} = \mathbf{v}_i + h\left[(1-\gamma)\,\mathbf{a}_i + \gamma \mathbf{a}_{i+1}\left(\mathbf{x}_{i+1}\right)\right],$$
$$\mathbf{x}_{i+1} = \mathbf{x}_i + h\mathbf{v}_i + \frac{h^2}{2}\left[(1-2\beta)\,\mathbf{a}_i + 2\beta \mathbf{a}_{i+1}\left(\mathbf{x}_{i+1}\right)\right].$$

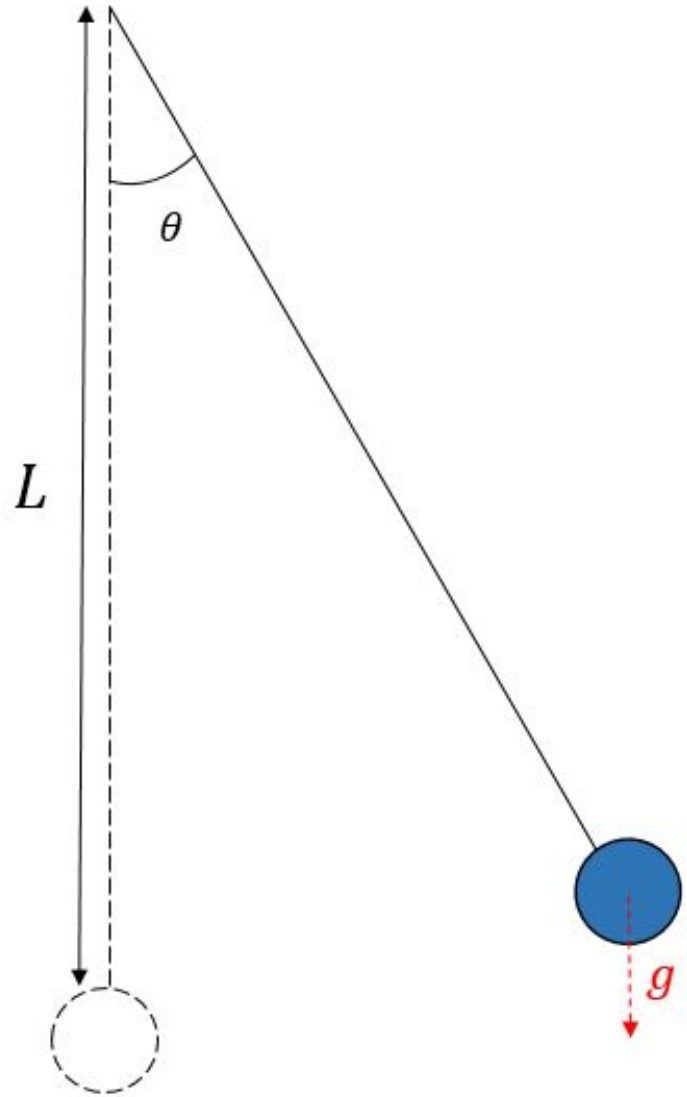
$$\tilde{\mathbf{F}}\left(\mathbf{x}_{i+1}\right) = \mathbf{x}_{i+1} - \mathbf{x}_i - h\mathbf{v}_i - \frac{h^2}{2}\left[(1-2\beta)\,\mathbf{a}_i + 2\beta \mathbf{a}_{i+1}\left(\mathbf{x}_{i+1}\right)\right],$$
$$D_{\mathbf{x}_{i+1}}\tilde{\mathbf{F}}\left(\mathbf{x}_{i+1}\right) = \mathbf{I} - \beta h^2 \mathbf{J}_{\mathbf{a}_{i+1}},$$
$$\mathbf{x}_{i+1} = \mathbf{x}_i - D\tilde{\mathbf{F}}\left(\mathbf{x}_i\right)^{-1}\tilde{\mathbf{F}}\left(\mathbf{x}_i\right).$$

Convergence Tests

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\sin\theta$$

Initial Conditions:

$$\theta_0 = 0$$
$$g = 10 \text{ m s}^{-2}$$
$$L = 5 \text{ m}$$
$$T = 5 \text{ s}$$



Molecular Dynamics

Hamiltonian System

We have to solve the Hamiltonian

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{N} m_i^{-1} p_i^T p_i + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} V\left(\|q_i - q_j\|_2\right).$$

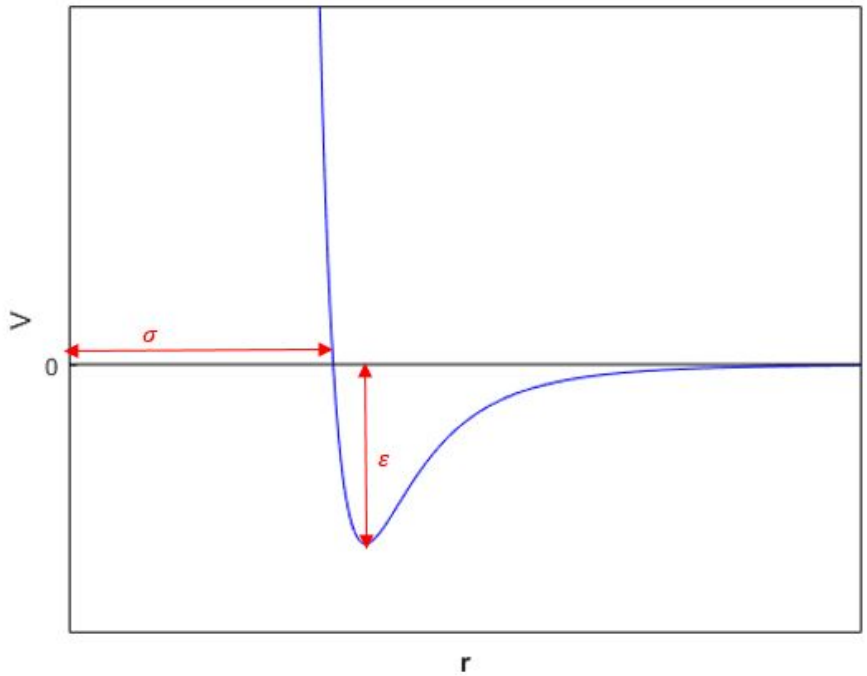
This is equivalent to

$$\dot{q}_i = \frac{1}{m_i} p_i, \qquad \dot{p}_i = \sum_{j=1}^{N} \nu_{ij}\left(q_i - q_j\right),$$

$$\text{where } \nu_{ij} = \begin{cases} 0 & , \text{ if } i = j \\ -\dfrac{V'\left(\|q_i - q_j\|_2\right)}{\|q_i - q_j\|_2} & , \text{ otherwise} \end{cases}$$

Lennard-Jones Potential

$$V(\mathbf{r}_{ij}) = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right],$$



where

$\mathbf{r}_{ij}$ is the displacement between the i^{th} and the j^{th} atoms
$r_{ij} = \|\mathbf{r}_{ij}\|_2$
ε is the potential well depth
σ is the distance at which the potential between two atoms is 0

Calculation of Forces

We have that force $\mathbf{f}$ along the vector $\mathbf{r}_{ij}$ is given by

$$\begin{aligned}\mathbf{f}\left(\mathbf{r}_{ij}\right) &= -\frac{dV}{d\mathbf{r}_{ij}} \\ &= 48 \cdot \varepsilon \cdot \sigma^6 \left[\sigma^6 \left(\frac{1}{r_{ij}}\right)^{14} - \frac{1}{2}\left(\frac{1}{r_{ij}}\right)^{8}\right] \mathbf{r}_{ij}\end{aligned}$$

Adding these terms up, the force exterted on particle i, $\mathbf{F}_i$ is given by

$$\mathbf{F}_i = \sum_{i \neq j} \mathbf{f}_{ij}.$$

Reduced Units

Physical Quantity	Reduced Unit	Value
Length	σ^*	3.40×10^{-10} m
Energy	ε^*	1.65×10^{-21} J
Mass	m^*	6.69×10^{-23} kg
Time	s^*	3.125×10^{-13} s
Temperature	K^*	119.6 K

Initializing Positions

We initialize the atoms as face-centered cubic lattice:

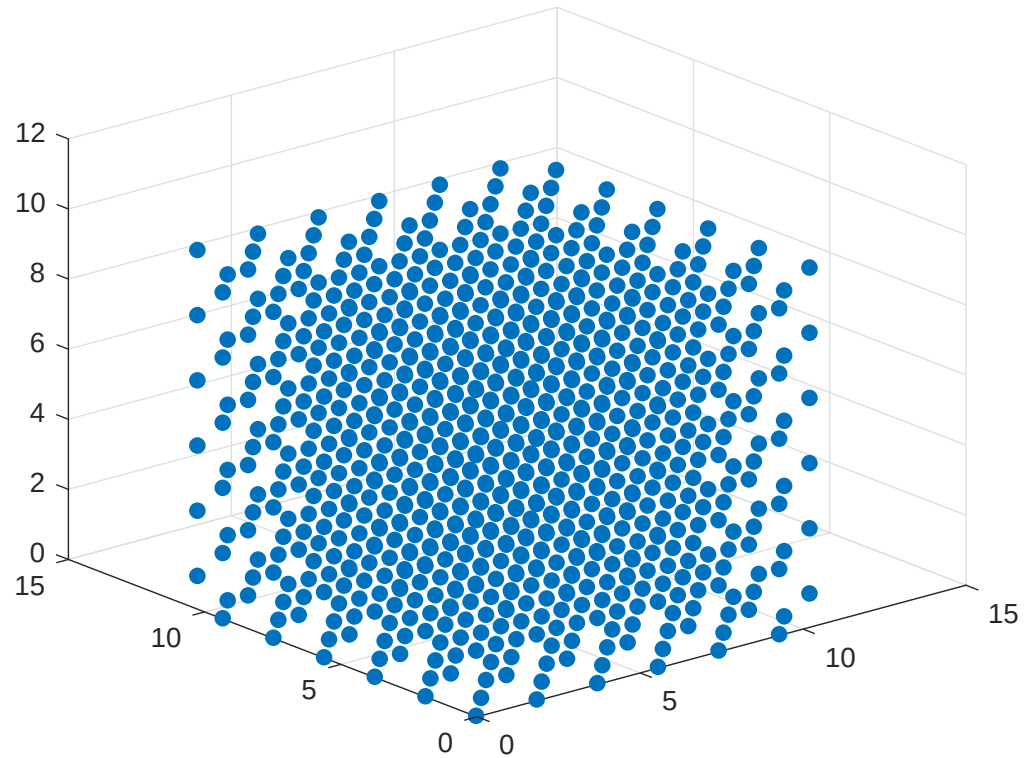


Figure: Initial cubic lattice for 864 particles at a density of 1.374 $\mathrm{g} \cdot \mathrm{cm}^{-3}$

Initializing Velocities

The probablity density function for velocities under the Maxwellian distribution is given by

$$f_{\mathbf{v}}\left(v_x, v_y, v_z\right) = \left(\frac{m}{2\pi k_B T}\right)^{\frac{3}{2}} \exp\left[-\frac{m\left(v_x^2 + v_y^2 + v_z^2\right)}{2k_B T}\right].$$

Assuming that the velocity in a direction is independent of the velocities in the other directions, we get that the probability density function for velocity v_i in direction i is

$$f_{\mathbf{v}}\left(v_i\right) = \left(\frac{m}{2\pi k_B T}\right)^{\frac{1}{2}} \exp\left[-\frac{m v_i^2}{2k_B T}\right].$$

So, $v_i \sim \mathcal{N}\left(0, \frac{k_B T}{m}\right)$.

Initializing Velocities - Equilibration

Scaling the velocities

$$\mathbf{v}_{new} = \sqrt{\frac{T_{target}}{T_{old}}} \cdot \mathbf{v}_{old}.$$

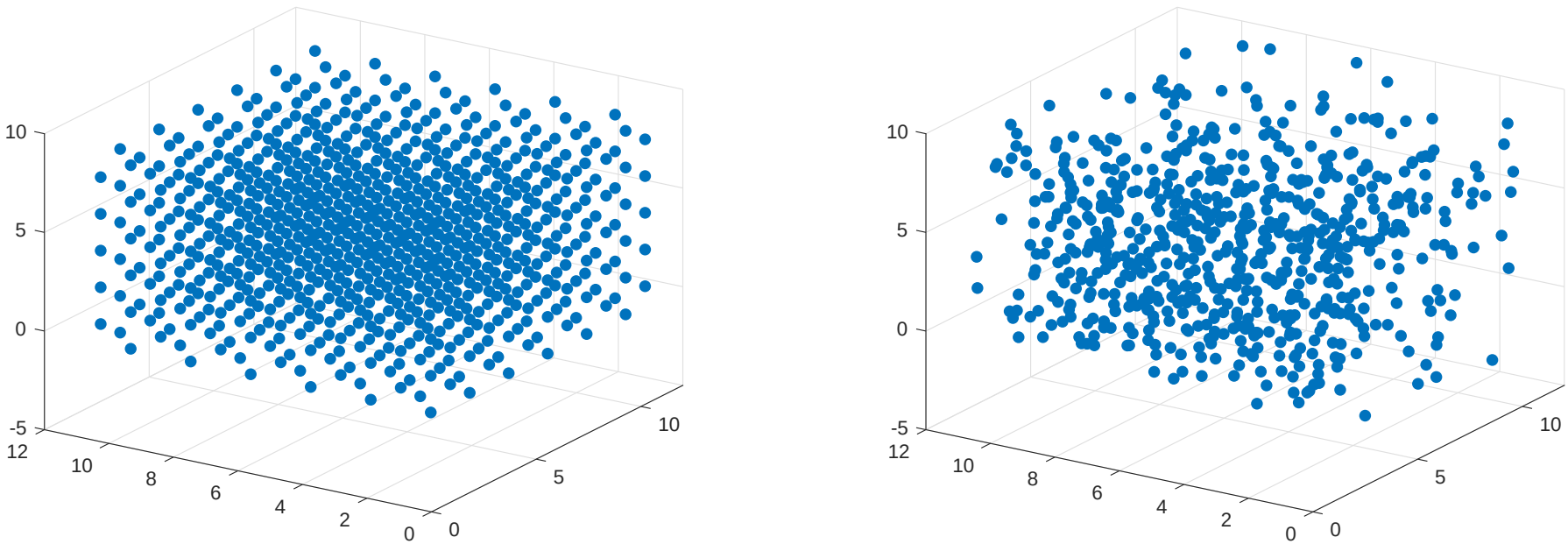


Figure: Change in the position of particles after 500 steps of equilibration

Periodic Boundary Conditions

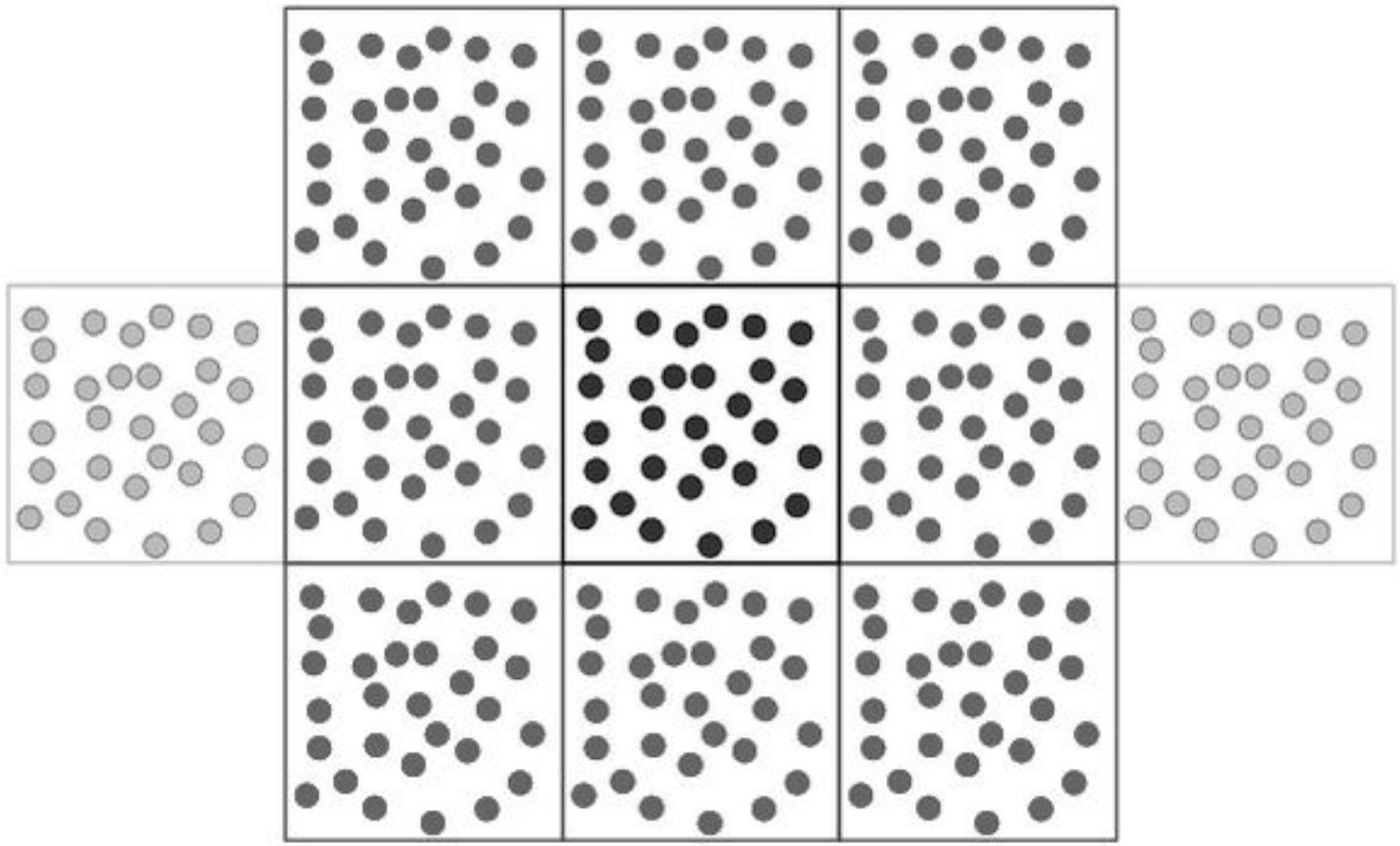


Figure: Periodic Boundary Conditons in 2-d

Conservation of Geometric Invariants

Time Reversibility

Theorem

A Hamiltonian system is time reversible.

Proof.

We apply the transformation $t \mapsto -t$.

$$q \mapsto q = \tilde{q}, \qquad p \mapsto -p = \tilde{p}.$$

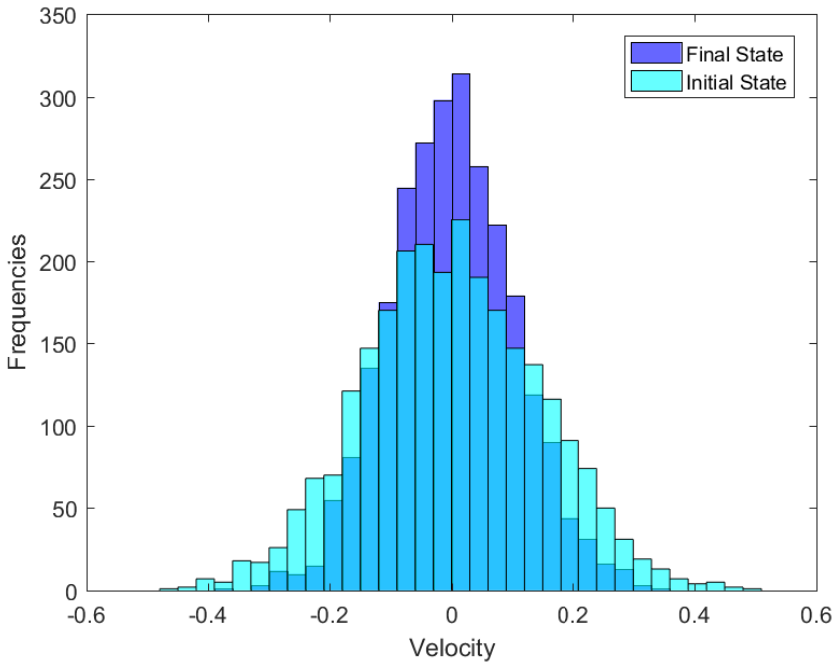
Then

$$\begin{aligned}
\dot{\tilde{q}} = \frac{d\tilde{q}}{d(-t)} &= -\nabla_{\tilde{p}} H &&= \nabla_p H &&= \dot{q}, \\
\dot{\tilde{p}} = \frac{d\tilde{p}}{d(-t)} &= -\nabla_{\tilde{q}} H &&= -\nabla_q H &&= \dot{p}. \quad \square
\end{aligned}$$

Time Reversibility

- A numerical one-step method $\Phi_h : (\mathbf{x}_i, \mathbf{v}_i) \mapsto (\mathbf{x}_{i+1}, \mathbf{v}_{i+1})$ is time reversible if $\Phi_h = \Phi_{-h}^{-1}$.
- Informally, this means that if we exchange $i \leftrightarrow i+1$ and replace h by $-h$ in our original method, then we should get the same method back.
- Any Newmark Beta method with $\gamma = \frac{1}{2}$ is reversible.
- No other Newmark Beta method is reversible.
- However, rounding-off errors in practice mean that we may not get back the initial state of the system after reversing the velocities.

Time Reversibility



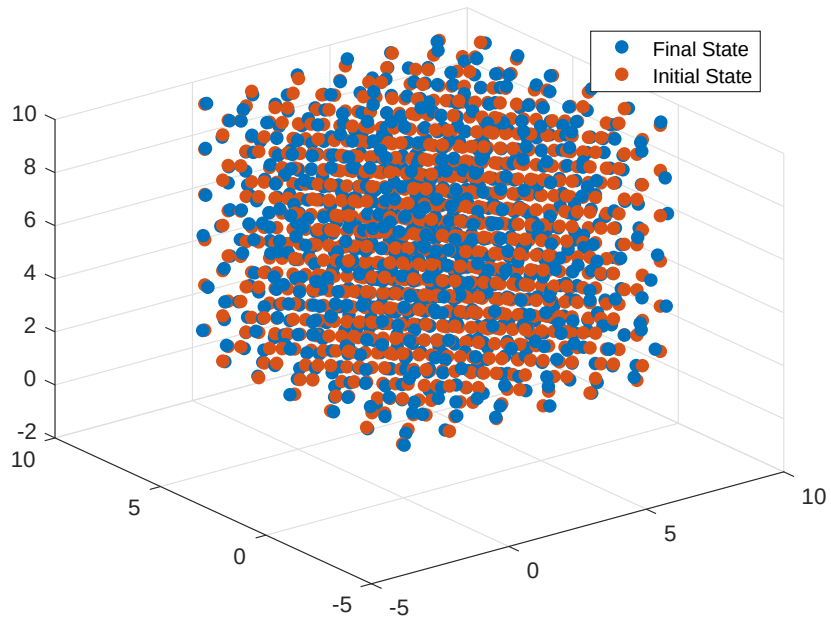
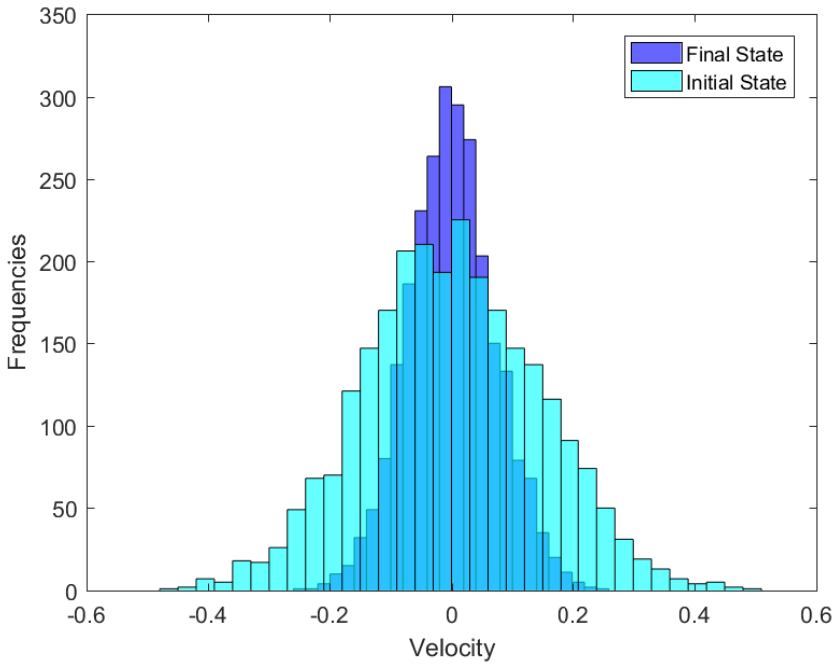


Figure: Changes in position and velocities for $\beta = 0.00$ and $\gamma = 0.50$ after reversing 500 steps

Time Reversibility



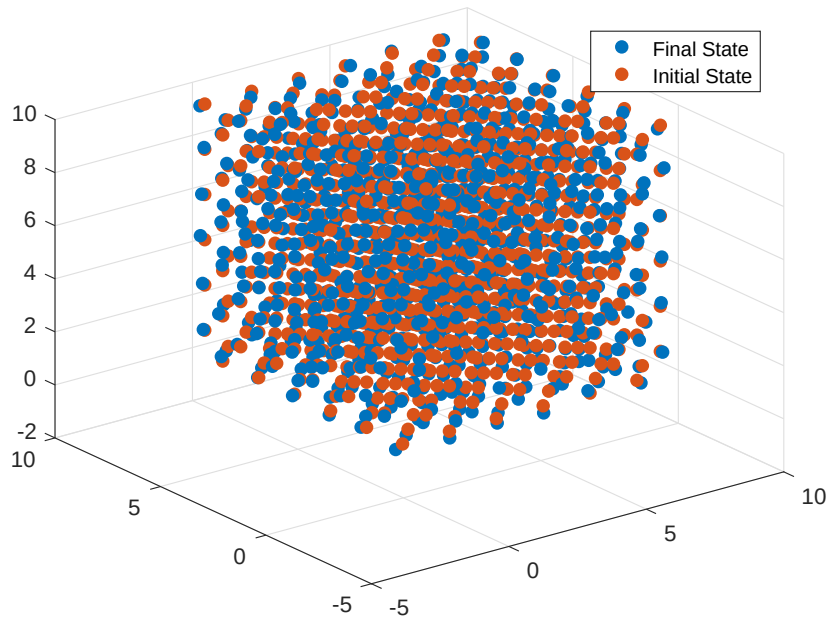
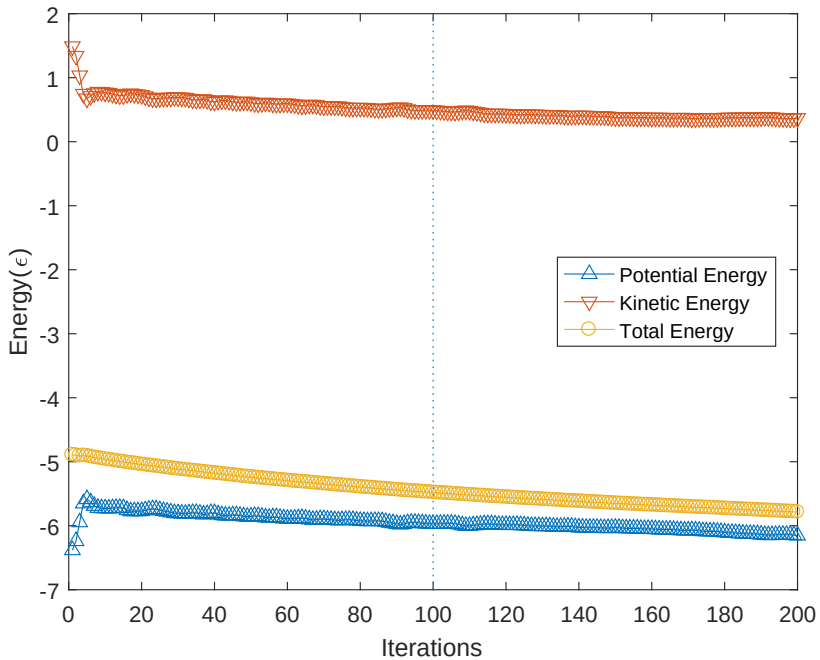


Figure: Changes in position and velocities for $\beta = 0.00$ and $\gamma = 0.75$ after reversing 500 steps

Time Reversibility



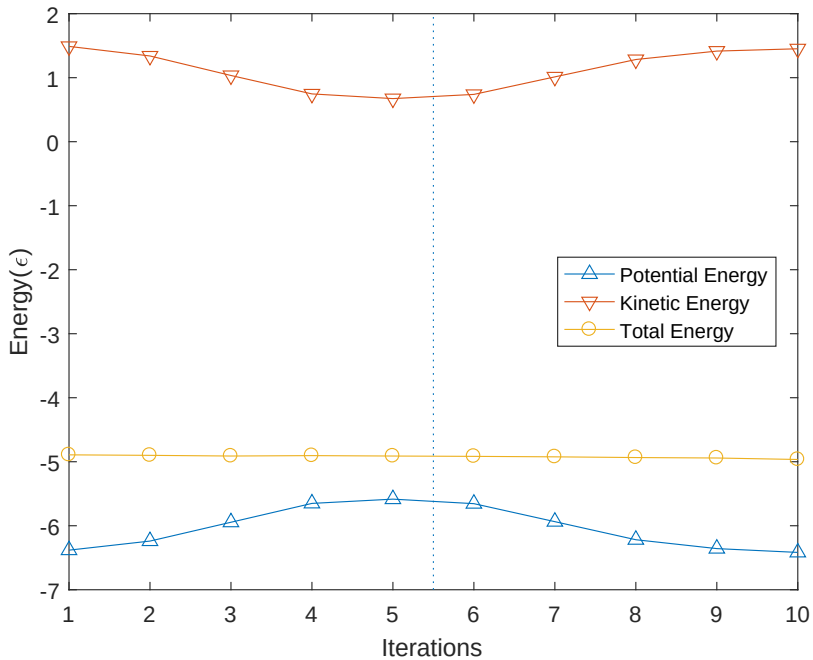
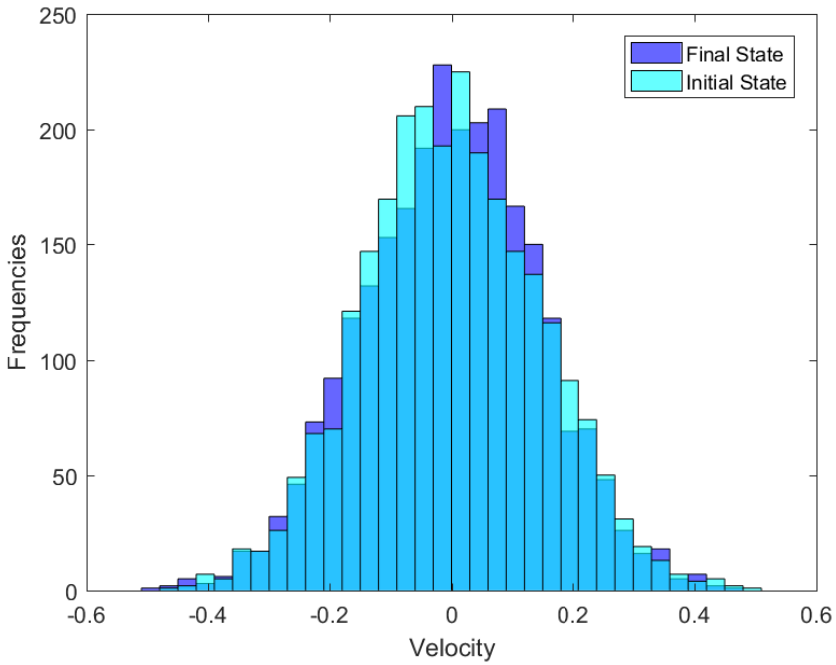


Figure: Difference in behaviour of total energy for $\beta = 0.00$ and $\gamma = 0.75$ over different timesteps

Time Reversibility



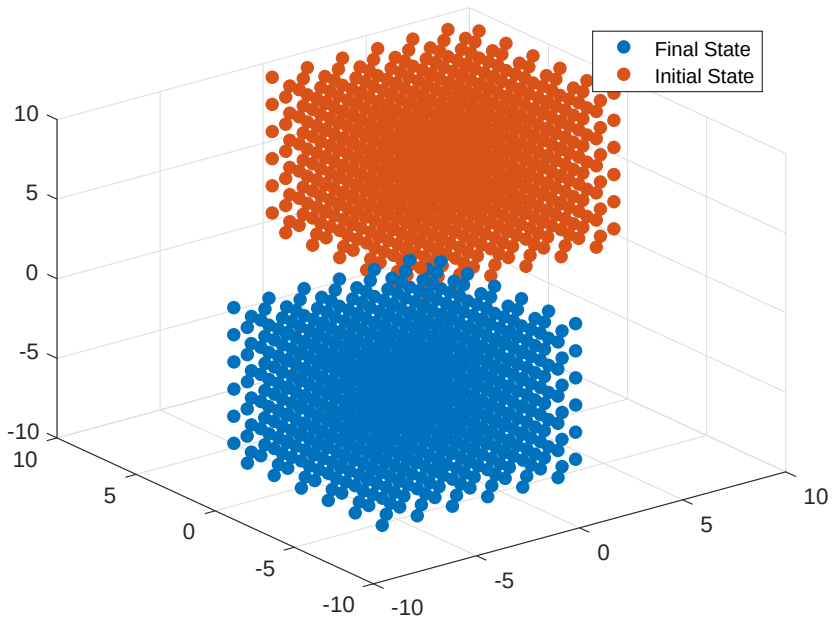


Figure: Changes in position and velocities for $\beta = 0.25$ and $\gamma = 0.50$ after reversing 125 steps

Aside: First Integrals

Definition

A non-constant function $I(y)$ is a *first integral* (or an invariant) of the differential equation $\dot{y} = F(y)$ if $I(y(t))$ is constant along every solution, or equivalently, if

$$\nabla I(y) F(y) = 0 \qquad \forall y.$$

Total Linear Momentum

Theorem

Total linear momentum $P = \sum_{i=1}^{N} p_i$ is a first integral.

Proof.

$$\begin{aligned}
\nabla P &= \frac{dP}{dt} = \sum_{i=1}^{N} \frac{dp_i}{dt} \\
&= \sum_{i=1}^{N} \sum_{j=1}^{N} \nu_{ij} \left(q_i - q_j\right) \\
&= 0 \qquad \cdots \text{ as } \nu_{ij} = \nu_{ji} \, \forall i, j
\end{aligned}$$

Total Linear Momentum

Claim

All Newmark Beta methods preserve linear first integrals

Proof.

Let $I(\mathbf{x}, \mathbf{v}) = b^T\mathbf{x} + c^T\mathbf{v}$ be a linear first integral, where b and c are some constant vectors.
We want that $I'(\mathbf{x}, \mathbf{v}) = 0 \ \forall \mathbf{x}, \mathbf{v}$.
But $I'(\mathbf{x}, \mathbf{v}) = b^T\mathbf{v} + c^T\mathbf{a}(\mathbf{x}) \ = 0 \implies b^T = 0$ and $c^T\mathbf{a}(\mathbf{x}) = 0 \, \forall \mathbf{x}$. So, $I(\mathbf{x}, \mathbf{v}) = I(\mathbf{v}) = c^T\mathbf{v}$.

$$
\begin{aligned}
I\left(\mathbf{v}_{i+1}\right) &= c^T\mathbf{v}_{i+1} \\
&= c^T\mathbf{v}_i + h\left[\left(1-\gamma\right)c^T\mathbf{a}(\mathbf{x}_i) + \gamma c^T\mathbf{a}(\mathbf{x}_{i+1})\right] \\
&= c^T\mathbf{v}_i = I\left(\mathbf{v}_i\right)
\end{aligned}
$$

□

Total Angular Momentum

Theorem

Total angular momentum $L = \sum_{i=1}^{N} q_i \times p_i$ *is a first integral.*

Proof.

$$\begin{aligned}
\nabla L &= \sum_{i=1}^{N} (\dot{q}_i \times p_i + q_i \times \dot{p}_i) \\
&= \sum_{i=1}^{N} \left(\frac{1}{m_i} p_i \times p_i \right) + \sum_{i=1}^{N} \sum_{j=1}^{N} (q_i \times \nu_{ij} (q_i - q_j)) \\
&= 0 \qquad \cdots \text{ as } \nu_{ij} = \nu_{ji} \text{ and } p_i \times p_i = 0 \, \forall i, j
\end{aligned}$$

□

Total Angular Momentum

Claim

Angular momentum is preserved $\Leftrightarrow \beta = 0, \gamma = \frac{1}{2}$.

Proof.

$$L_{i+1} - L_i = \sum_{k=1}^{N} (q_{i+1})_k \times (p_{i+1})_k - \sum_{k=1}^{N} (q_i)_k \times (p_i)_k$$

$$= h^2 \left(\gamma - \frac{1}{2}\right) \sum_{k=1}^{N} (\mathbf{a}_i)_k \times (\mathbf{p}_i)_k$$

$$+ h^2 \beta \sum_{k=1}^{N} (\mathbf{a}_{i+1})_k \times (\mathbf{p}_{i+1})_k - (\mathbf{a}_i)_k \times (\mathbf{p}_i)_k.$$

So $L_{i+1} - L_i = 0 \Leftrightarrow \beta = 0, \gamma = \frac{1}{2}$. □

Total Angular Momentum

Iteration	x-component	y-component	z-component
10	493.28	-402.32	1407.30
20	-4.80	-10.18	914.24
30	320.20	-147.35	980.93
40	717.70	-181.21	704.27
50	594.66	152.47	507.19

Table: Total angular momentum of the system with $\beta = 0, \gamma = \frac{1}{2}$ over the first 50 iterations

Total Energy

Theorem

The total energy, or the Hamiltonian, is a first integral.

Proof.

From definitions

$$\frac{dH}{dt} = \begin{pmatrix} -\nabla_q H \\ \nabla_p H \end{pmatrix} and \nabla H = \left(\nabla_p H^T, \nabla_q H^T \right) \text{ and}$$

Then,

$$\nabla H(p,q) \cdot \frac{dH}{dt} = \nabla_p H^T \cdot -\nabla_q H + \nabla_q H^T \cdot \nabla_p H = 0 \quad \square$$

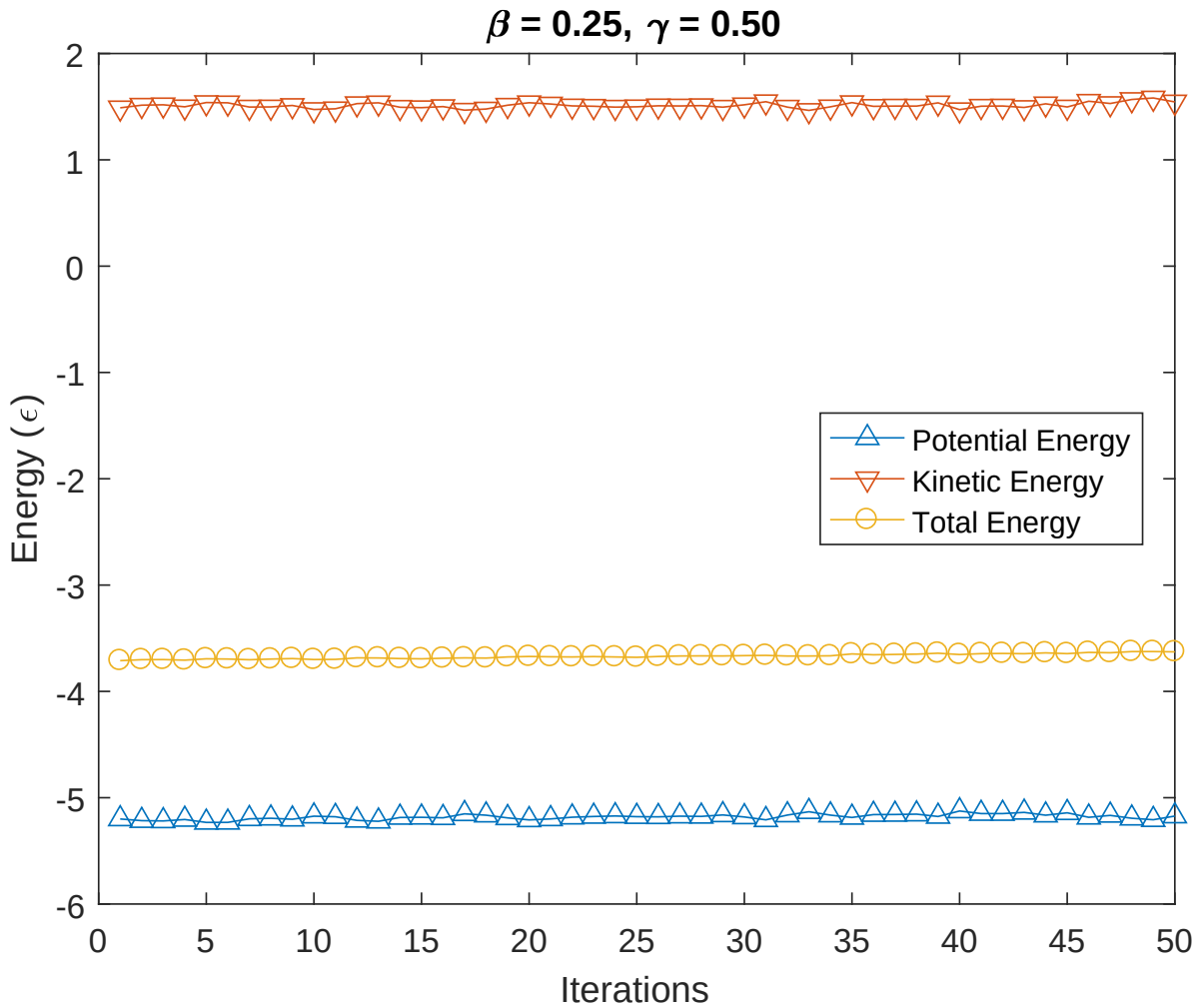
Recap: Physical Interpretation of γ

- γ plays the role of a damping factor in the energy of the system.
- The energy of the system is damped by a factor of $\gamma - \frac{1}{2}$.
- If $\gamma > \frac{1}{2}$, the energy is damped.
- If $\gamma < \frac{1}{2}$, the energy grows.

Total Energy - Implicit Methods

We start by quoting Simo, Tarnow, and Wong:
"*What may seem surprising is that all of the implicit members of the Newmark family, perhaps the most widely used time-stepping algorithms in nonlinear structural dynamics, are not designed to conserve energy and also fail to conserve momentum.*"

Total Energy - Implicit Methods



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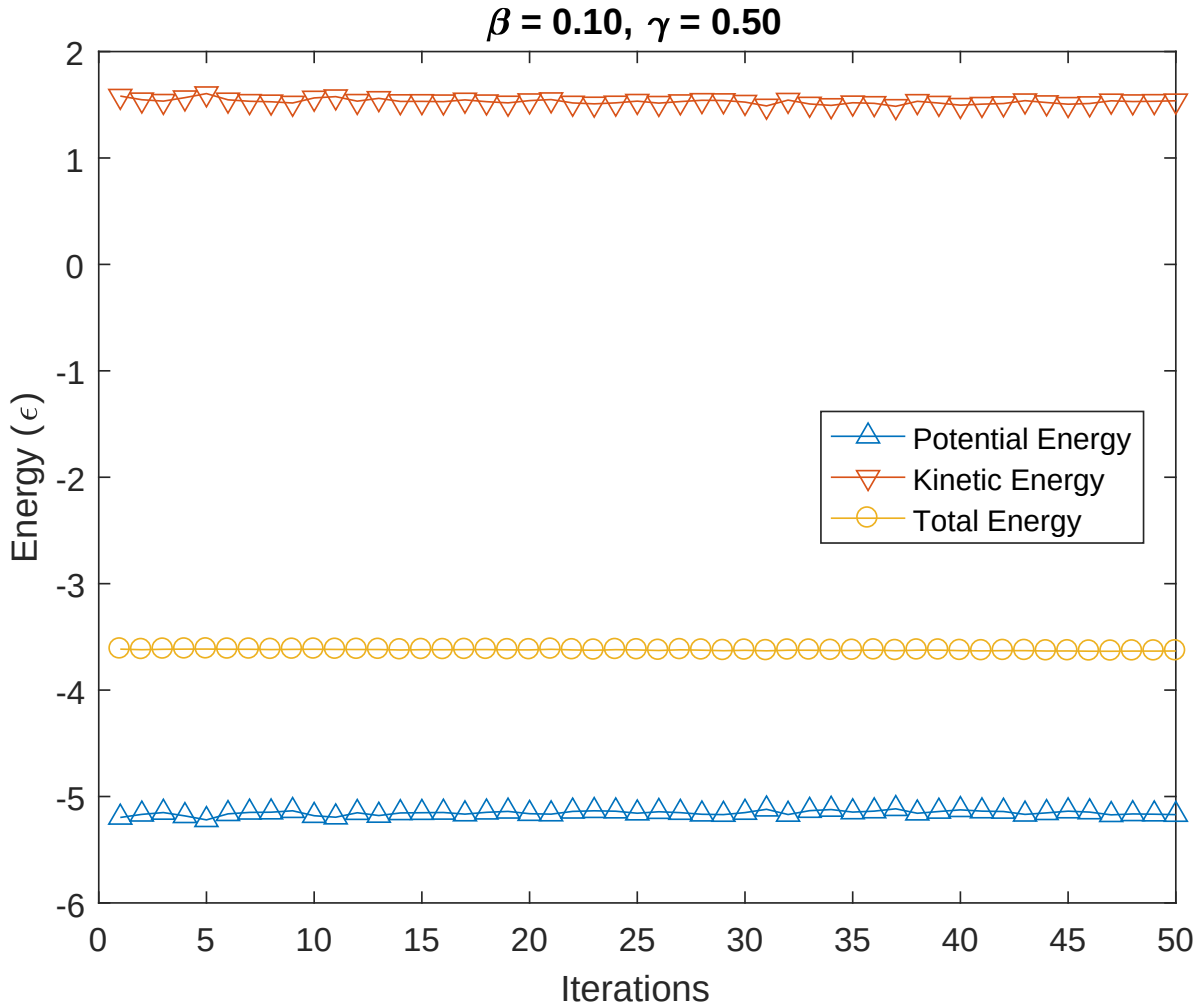
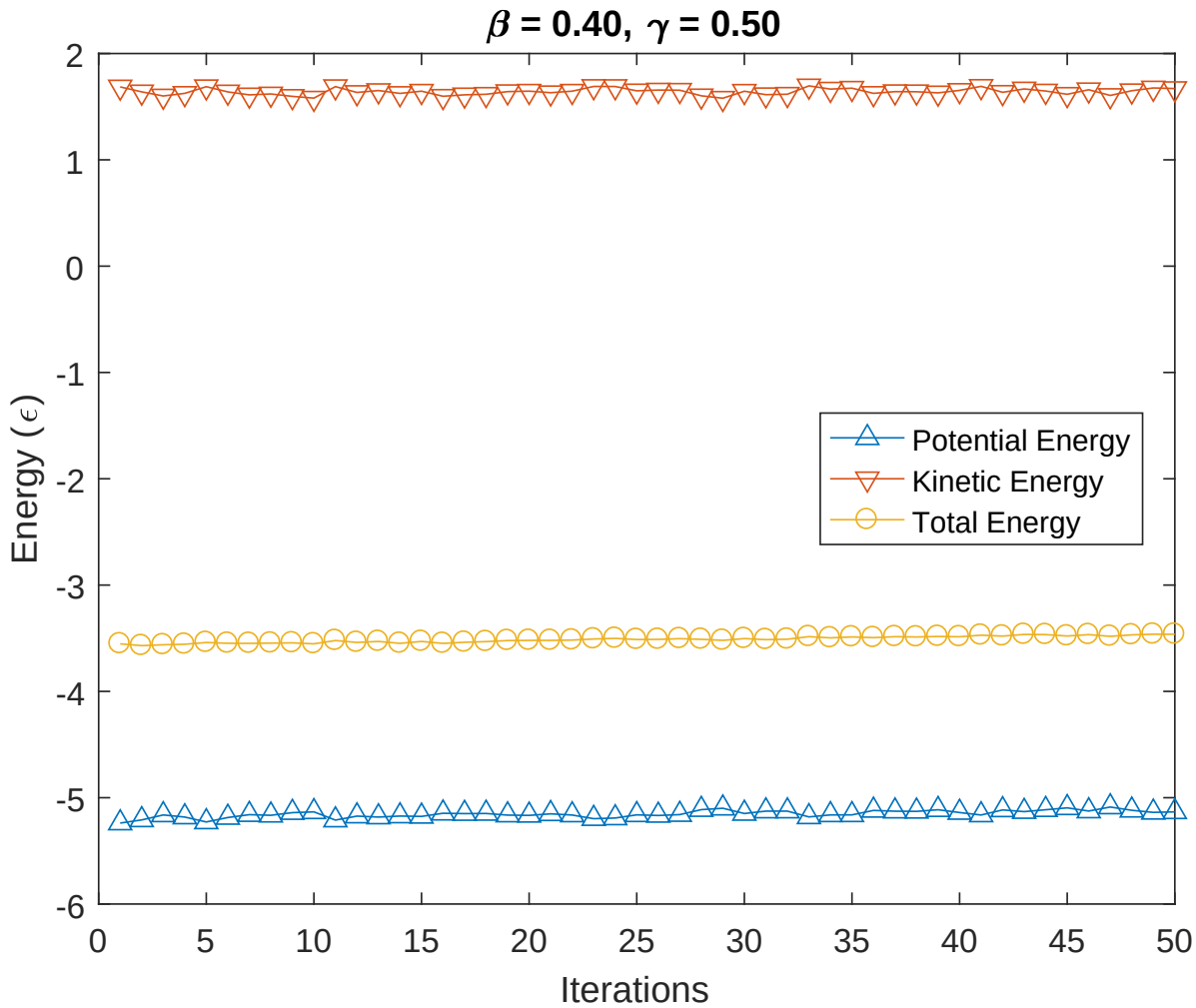


Total Energy - Implicit Methods



Conclusion

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