MSN 514 - Computational Methods for Material Science and Complex Systems

Homework 01

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I. INTRODUCTION

This report compares two numerical methods for simulating the motion of a three-mass system connected by springs of different stiffnesses: the velocity Verlet algorithm and the time-evolution operator method. Both methods solve the system's equations of motion but differ in their approach, accuracy, and computational efficiency.

The velocity Verlet algorithm is a widely used symplectic integration method that ensures good energy conservation over long simulations. It updates positions and velocities iteratively using both current and future accelerations. The time-evolution operator method, on the other hand, formulates the system in matrix form and propagates the state vector using matrix exponentiation.

The primary goal of this study is to compare these two approaches and evaluate their strengths and weaknesses in terms of accuracy, computational efficiency, and ease of implementation.

II. RESULTS

A. Mathematical Formulation

The velocity Verlet algorithm updates the position and velocity at each time step as follows:

$$x_i(t+\Delta t) = x_i(t) + v_i(t)\Delta t + \frac{1}{2}a_i(t)\Delta t^2, \tag{1}$$

$$v_i(t+\Delta t) = v_i(t) + \frac{1}{2}\left[a_i(t) + a_i(t+\Delta t)\right]\Delta t. \tag{2}$$

where x_i, v_i, and a_i are the position, velocity, and acceleration of mass i. The accelerations are computed from Newton's second law, considering spring forces.

In the time-evolution operator approach, the system is written in matrix form:

$$\frac{d\mathbf{r}}{dt} = \mathbf{A}\mathbf{r}, \tag{3}$$

where $\mathbf{r} = [u_1, u_2, u_3, v_1, v_2, v_3]^T$ represents the state vector, and $\mathbf{A}$ is the coefficient matrix encoding the system's dynamics. The solution is obtained using the matrix exponential:

$$\mathbf{r}(t + \Delta t) = e^{\mathbf{A}\Delta t}\mathbf{r}(t). \tag{4}$$

B. Comparison of Results

Figures 1 and 2 show the computed trajectories for both methods. The oscillatory motion of the masses is observed, and both methods yield nearly identical results.

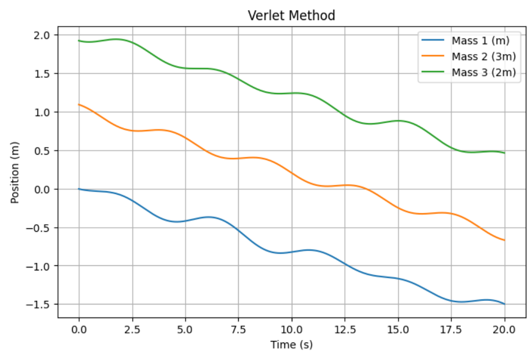

FIG. 1. Positions of the three masses using the velocity Verlet algorithm.

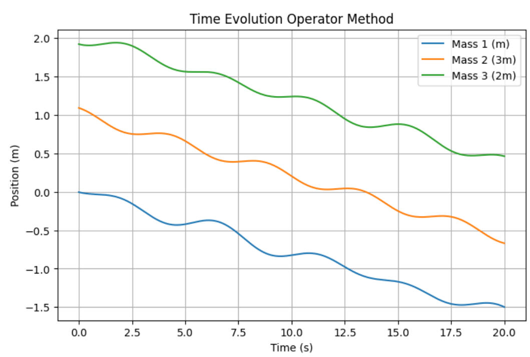

FIG. 2. Positions of the three masses using the time-evolution operator method.

A direct comparison between the two methods is shown in Fig. 3. The results overlap almost perfectly, with only minor numerical differences.

C. Methodological Differences

Although both methods provide accurate solutions, they have key differences:

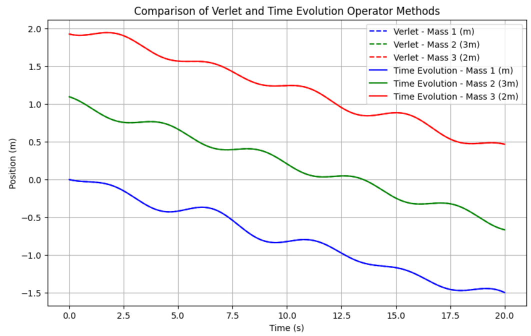

FIG. 3. Comparison of velocity Verlet (dashed) and time-evolution operator (solid).

- **Accuracy:** The velocity Verlet method conserves energy well and is widely used in molecular dynamics. The time-evolution operator is exact for linear systems but requires matrix exponentiation.
- **Computational Efficiency:** Verlet scales linearly with system size, whereas the time-evolution operator involves an expensive matrix exponential computation.
- **Implementation Complexity:** Verlet is straightforward and requires only force evaluations. The time-evolution operator is elegant for linear systems but impractical for nonlinear cases.

III. CONCLUSION

Both methods successfully simulate the motion of the three-mass system. The velocity Verlet algorithm is computationally efficient, simple to implement, and conserves energy over long simulations. It is generally preferred for large-scale or nonlinear systems. The time-evolution operator method, while elegant and exact for linear systems, is computationally expensive due to matrix exponentiation, making it less practical for larger problems.

The choice of method depends on the problem's characteristics. For nonlinear or large-scale simulations, the velocity Verlet algorithm is preferable. When dealing with small systems where exact solutions are possible, the time-evolution operator method can provide an elegant alternative.