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Symplectic and constraint-preserving model order reduction of lattice dynamics

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1. INTRODUCTION & OBJECTIVE

Lattice dynamics is the study of vibrations of atoms in a crystal. Lattice dynamics finds practical applications in the interaction of crystals with sound and light waves [1]. The vibration energy of a crystal lattice can be decomposed into acoustic and optic modes whose propagation through the crystal lattice determines its respective properties and suitability for various applications [2]. In this paper, we reduce and solve high-dimensional parameterized constrained nonlinear differential equations representing such a crystal lattice with structure-preserving algorithms. These algorithms preserve the constrained equation's geometric properties, such as symplecticness and constraints, through model order reduction and numerical integration. We develop a symplectic reduced basis-based approach to reduce the equation and establish well-posedness and geometric properties of the resulting reduced model. We utilize two integrators based on RATTLE [3] to simulate the full and reduced models while preserving their geometric properties. Numerical experiments on the constrained system justify theoretical results and demonstrate advantages of the structure-preserving computational methods for lattice chains.

2. RESULTS & HIGHLIGHTS

Consider a rectangular lattice grid of atoms arranged in two lines in a plane, see Figure 1. The two lines of atoms are separated by a fixed width and the atoms in each line interact with a nearest-neighbor through an inter-atomic potential [4]. There are 2d atoms in the grid, each with three degrees of freedom. Furthermore, the springs, representing inter-atomic potentials, may each have a different spring constant. These characteristics make up the governing Hamiltonian system with holonomic constraints with large configuration and parameter spaces. Model order reduction (MOR) techniques can be used to reduce the system dimension by projecting the original large solution space onto a smaller solution space. MOR is especially useful under repeated simulation scenarios with changing parameter values [5]. In this paper

1. We develop a reduced order model which preserves certain qualitative properties, such as symplecticness and constraints, of the full order model.
2. We also establish the reduced model's well-posedness.
3. We utilize two integrators based on RATTLE to justify preservation of qualitative properties. The numerical results are shown in Figure 2.

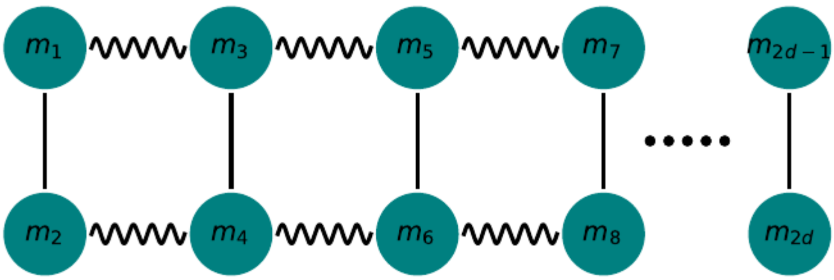

Figure 1: A two-layered lattice structure

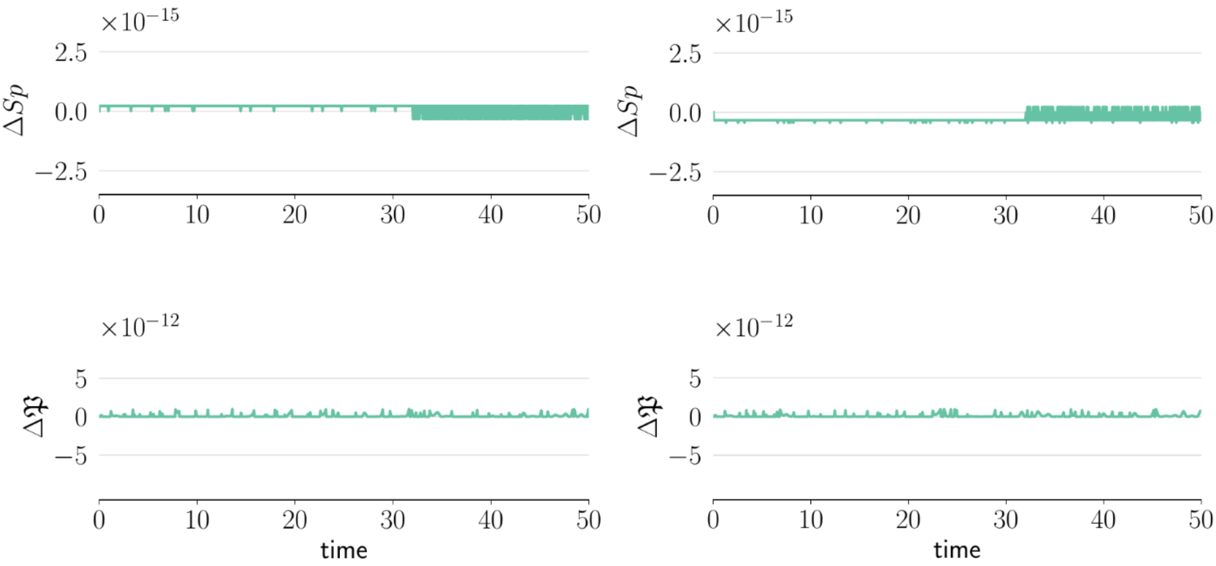

Figure 1: Error in symplecticness (top), and constraints (bottom) by an implicit (left) and an explicit (right) method.

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