ADJOINT SENSITIVITY ANALYSIS OF CONSTANT TEMPERATURE MOLECULAR DYNAMICS

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ABSTRACT

In this research, we proposed an efficient design sensitivity analysis (DSA) method of constant temperature molecular dynamics (MD). A Nose-Hoover thermostat is utilized to represent the possible state of a system that is in thermal equilibrium with a heat bath so that the resulting temperature is constant. The design sensitivity of general performance measures for the constant temperature MD with the Nose-Hoover thermostat is derived using an adjoint variable method (AVM). Since the adjoint system is path-dependent and derived in the form of a terminal value problem, the path of MD analysis is kept and the time reversibility of the MD system with Nose-Hoover thermostat is investigated. The accuracy and efficiency of the developed adjoint DSA method are verified through demonstrative numerical examples.

Keywords: molecular dynamics, canonical ensemble, adjoint variable method, transient dynamic sensitivity, Nose-Hoover thermostat.

INTRODUCTION

Recently, the necessity of design optimization at atomic level is naturally increasing for the development of new materials and the breaking through the limitations in continuum-based analysis. For the atomic level analysis, an MD simulation is widely used but a huge amount of computation is usually required due to transient dynamic analysis. Furthermore, for the DSA of MD systems that have many design variables, the computational cost is very expensive. Also, the MD simulations could include highly nonlinear design parameters.

From the engineering and practical point of view, thermal effects are very important for the atomic level simulations. To make it realistic, we need to consider a statistical approach to deal with macroscopic behaviour due to the variations of microscopic variables since there are numerous cases in microscopic states that can represent identical macroscopic properties (Frenkel and Smit, 2001). In this paper, we developed an adjoint DSA method for the constant temperature MD simulations. The Nose-Hoover thermostat (Nose, 1984a, Nose, 1984b, Hoover, 1985) is utilized to maintain the desired temperature of a given system. The adjoint system of NVT ensemble is inherently path-dependent due to the additional degrees of freedom corresponding to the heat bath which acts as a damping term.

RESULTS AND CONCLUSIONS

To verify the accuracy of the adjoint sensitivity, we applied the developed method to the tensile test of Cu nanowire. The Cu nanowire of 3.615 nm is constructed by $5 \times 5 \times 10$ unit cells and the total number of atoms is 1,270 as shown in Figure 1. The EAM potential is utilized to consider the bond between Cu atoms.
The Young’s modulus of Cu nanowire and temperature are selected as a performance measure and a design variable, respectively. As varying the strain rates for the loading condition, the results of adjoint design sensitivity are compared with those obtained from both the finite difference method (FDM) and the direct differentiation method (DDM) in Table 1, where the agreements between FDM, DDM and AVM are very good. It turns out that the developed AVM gives accurate sensitivity results for all the given strain rates.

### Table 1 - Verification of sensitivity results for various strain-rates

<table>
<thead>
<tr>
<th>Strain rate</th>
<th>(a) FDM $\Delta \psi / \Delta T$</th>
<th>(b) DDM $\psi'_{DDM}$</th>
<th>(c) AVM $\psi'_{AVM}$</th>
<th>(b)/(a) (%)</th>
<th>(c)/(a) (%)</th>
</tr>
</thead>
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<tr>
<td>$3 \times 10^{10}$</td>
<td>-1.4001E+00</td>
<td>-1.4103E+00</td>
<td>-1.4130E+00</td>
<td>100.73</td>
<td>100.92</td>
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<tr>
<td>$1.5 \times 10^{10}$</td>
<td>-2.0900E+00</td>
<td>-2.1091E+00</td>
<td>-2.1087E+00</td>
<td>100.92</td>
<td>100.90</td>
</tr>
<tr>
<td>$6 \times 10^{9}$</td>
<td>-7.9993E-01</td>
<td>-8.2211E-01</td>
<td>-8.4027E-01</td>
<td>102.77</td>
<td>105.04</td>
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<tr>
<td>$3 \times 10^{9}$</td>
<td>-2.9399E+00</td>
<td>-2.9151E+00</td>
<td>-3.0615E+00</td>
<td>99.15</td>
<td>104.13</td>
</tr>
</tbody>
</table>

### ACKNOWLEDGMENTS

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### REFERENCES


