TRANSPORT COEFFICIENT COMPUTATION BASED ON INPUT/OUTPUT REDUCED ORDER MODELS

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ABSTRACT

The guiding purpose of this thesis is to address the optimal material design problem when the material description is a molecular dynamics model. The end goal is to obtain a simplified and fast model that captures the property of interest such that it can be used in controller design and optimization. The approach is to examine model reduction analysis and methods to capture a specific property of interest, in this case viscosity, or more generally complex modulus or complex viscosity. This property and other transport coefficients are defined by a input/output relationship and this motivates model reduction techniques that are tailored to preserve input/output behavior. In particular Singular Value Decomposition (SVD) based methods are investigated. First simulation methods are identified that are amenable to systems theory analysis. For viscosity, these models are of the Gosling and Lees-Edwards type. They are high order nonlinear Ordinary Differential Equations (ODEs) that employ Periodic Boundary Conditions. Properties can be calculated from the state trajectories of these ODEs.

In this research local linear approximations are rigorously derived and special attention is given to potentials that are evaluated with Periodic Boundary Conditions (PBC). For the Gosling description LTI models are developed from state trajectories but are found to have limited success in capturing the system property, even though it is shown that full order LTI models can be well approximated by reduced order LTI models. For the Lees-Edwards SLLOD type model nonlinear ODEs will be approximated by a Linear Time Varying (LTV) model about some nominal trajectory and both balanced truncation and Proper Orthogonal Decomposition (POD) will be used to asses the plausibility of reduced order models to this system description.

An immediate application of the derived LTV models is Quasilinearization or Waveform Relaxation. Quasilinearization is a Newton's method applied to the ODE operator equation. Its a recursive method that solves nonlinear ODE's by solving a LTV systems at each iteration to obtain a new closer solution. LTV models are derived for both Gosling and Lees-Edwards type models. Particular attention is given to SLLOD Lees-Edwards models because they are in a form most amenable to performing Taylor series expansion, and the most commonly used model to examine viscosity.

With linear models developed a method is presented to calculate viscosity based on LTI Gosling models but is shown to have some limitations. To address these issues LTV SLLOD models are analyzed with both Balanced Truncation and POD and both show that significant order reduction is possible. By examining the singular values of both techniques it is shown that Balanced Truncation has a potential to offer greater reduction, which should be expected as it is based on the input/output mapping instead of just the state information as in POD. Obtaining reduced order systems that capture the property of interest is challenging. For Balanced Truncation reduced order models for 1-D LJ and FENE systems are obtained and are shown to capture the output of interest fairly well. However numerical challenges currently limit this analysis to small order systems. Suggestions are presented to extend this method to larger systems. In addition reduced 2nd order systems are obtained from POD. Here the challenge is extending the solution beyond the original period used for the projection, in particular identifying the manifold the solution travels along. The remaining challenges are presented and discussed.