

# Introduction To Molecular Dynamics Simulations Using LAMMPS

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## **LAMMPS Documentation " LAMMPS documentation**

February 17th, 2019 - 8 Feb 2019 version What is a LAMMPS version LAMMPS stands for Large scale Atomic Molecular Massively Parallel Simulator LAMMPS is a classical molecular dynamics simulation code with a focus on materials modeling

## **Computational Materials Science An Introduction 1 June**

January 16th, 2019 - Computational Materials Science An Introduction covers the essentials of computational science and explains how computational tools and techniques work to help solve materials science problems The book focuses on two levels of a materials system the electronic structure level of nuclei and electrons and the atomistic molecular level

## **General purpose computing on graphics processing units**

February 18th, 2019 - General purpose computing on graphics processing units GPGPU rarely GPGP is the use of a graphics processing unit GPU which typically handles computation only for computer graphics to perform computation in applications traditionally handled by the central processing unit CPU The use of multiple video cards in one computer or large numbers of graphics chips further parallelizes the

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