International Workshop on Mathematical Theory, Methods and Application in Materials Simulation

April 9-11, 2021

上海交通大學 SHANGHAI JIAO TONG UNIVERSITY

自然科学研究院 Institute of Natural Sciences

Contents

1 General Information

Introduction

Materials modeling and simulation is essential in underpinning the discovery and synthesis of new materials and chemicals with novel functionalities in key areas such as energy, information technology and biomedicine. On the other hand, it presents a huge challenge for matheamtics and computational science. This workshop aims to promote academic exchange and collaboration among the researchers in the interdiscipinary field of computaional materials science and mathematics.

Date

April 9-11, 2021

Venue

Room 305, No. 5 Science Building, Minhang Campus, Shanghai Jiao Tong University

Online—Tencent APP

April 10, 2021:
Morning: Conference ID: 355-814-621
Afternoon: Conference ID: 649-902-559

April 11, 2021:
Morning: Conference ID: 335-920-390
Afternoon: Conference ID: 744-532-563

Password: 654321

Organizer

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- Hao Wang,Sichuan University,Chengdu,China
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Sponsor

- Institute of Natural Sciences, Shanghai Jiao Tong University
- Ministry of Education Key Lab in Scientific and Engineering Computing

简介

材料科学中的建模与模拟对新材料的发展和设计具有极其重要的作用，另一方面，它对理论研究人员，尤其是数学和计算科学工作者提出了大量的新问题，新挑战。我们拟于 2021 **年** 4 **月** 9-11 **日（**9 **日报到，**10 **日及** 11 **日开会）在上海交通大学举办“ 材料模拟的数学理论、方法与应用 ”研讨会。**

时间

2021 **年** 4 **月** 9 **日**-4 **月** 11 **日**

地点

上海交通大学闵行校区理科楼群 5 **号楼** 305 **室**

线上会议—腾讯会议

2021 **年** 4 **月** 10 **日**:
上午: **会议** ID: 355-814-621
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会议密码: 654321

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主办单位

- **上海交通大学自然科学研究院**
- **上海交通大学教育部科学工程重点实验室**

2 Schedule

2.1 Day 1, 10 April, Saturday

Time	Speaker	Title
08:00 - 08:20		Registration
08:20 - 08:30		Opening Remarks: Hong Wang, Materials Genome Initiative Center, SJTU
		Morning Session I: Chaired by Shuyang Dai
08:30 - 09:10	Zhijian Yang	Boundary Condition for Dislocation Dynamic Simulation in BCC Crystal
09:10 - 09:50	Guanghui Hu	Towards efficient simulations of KS/TDKS models in a unified framework
09:50 - 10:10		Group Photo & Coffee Break
		Morning Session II: Chaired by Zhijian Yang
10:10 - 10:50	Shuyang Dai	Comparative study of atomistic-based stress evaluation
10:50 - 11:30	Yu Liu	【Online】强关联电子体系第一性原理 DFT+DMFT 计算方法简介
		Afternoon Session I: Chaired by Huajie Chen
13:30 - 14:10	Linfeng Zhang	Efficient sampling of high-dimensional free energy landscapes using adaptive reinforced dynamics
14:10 - 14:50	Xiaoyu Chong	【Online】高通量第一性原理计算耦合相图热力学：模型构建及工程应用
14:50 - 15:30	Chaoyu Quan	A domain decomposition method for the Poisson-Boltzmann solvation model
15:30 - 15:50		Coffee Break
		Afternoon Session II: Chaired by Wei Jiang
15:50 - 16:30	Rui Du	Improved Gauss-Seidel projection methods for micromagnetic simulations
16:30 - 17:10	Qiang Ma	High-order multi-scale asymptotic analysis and computation of axisymmetric piezoelectric problem for composite structures

2.2 Day 2, 11 April, Sunday

Time	Speaker	Title
		Morning Session I: Chaired by Guanghui Hu
08:30 - 09:10	Zhenli Xu	Random-Batch Ewald Algorithm
09:10 - 09:50	Wei Jiang	Phase field approach for simulating solid-state dewetting problems
09:50 - 10:10		Coffee Break
		Morning Session II: Chaired by Lei Zhang
10:10 - 10:50	Kai Jiang	【Online】 Computing Quasiperiodic Systems
10:50 - 11:30	Luchan Zhang	【Online】 Dynamics of Grain Boundaries with Microscopic Constraints
		Afternoon Session: Chaired by Hao Wang
13:30 - 14:10	Zhenlin Guo	A diffuse domain method for solving PDEs in complex domain
14:10 - 14:50	Guisen Liu	Coupled crystal plasticity finite element with phase field method in modeling the plastic deformation of metallic materials
14:50 - 15:10	Mingjie Liao	Adaptive QM/MM Coupling Methods for Crystalline Defects
15:10 - 15:30	Yangshuai Wang	The Applications of Data-Driven Interatomic Potentials to QM/MM Coupling Methods

3 Abstracts

3.1 Day 1, 10 April, Saturday

Boundary Condition for Dislocation Dynamic Simulation in BCC Crystal

Zhijian Yang, *Wuhan University*
08:30 - 09:10

The movement of dislocations and the corresponding crystal plastic deformation are highly influenced by the interaction between dislocations and nearby free surfaces. The boundary condition for inclination angle which indicates the relation between a dislocation line and the surface is one of the key ingredients in the dislocation dynamic simulations. In this paper, we first present a systematical study on by molecular static simulations in BCC-irons samples. We also study the inclination angle by using molecular dynamic simulations. A continuum description of inclination angle in both static and dynamic cases is derived based on Onsager ' s variational principle. We show that the results obtained from continuum description are in good agreement with the molecular simulations. These results can serve as boundary conditions for dislocation dynamics simulations.

Towards efficient simulations of KS/TDKS models in a unified framework

Guanghui Hu, *University of Macau*
09:10 - 09:50

In most cases the ground state would be used as an initial state in a dynamic study of a many-body electronic structure. In the numerical study with density functional theory, a complete simulation would consist of obtaining the ground state of the system by solving Kohn-Sham equation and propagating the system by solving time-dependent Kohn-Sham equation. Although there have been many libraries which can handle two processes in a unified framework, the employment of mesh adaptivity towards the efficiency of the simulation would make the realization of the algorithm much more complicated. In this talk, based on our library AFEABIC, a unified realization of the simulation of above process would be introduced. Several mathematical and technical issues, as well as our methods, would be introduced.

Comparative study of atomistic-based stress evaluation

Shuyang Dai, *Wuhan University*
10:10 - 10:50

We present a comparative study on several aspects of atomistic-stress evaluation. Firstly, we derived an Irving-Kirkwood formulation for Cauchy stress evaluation in Eulerian coordinates. Secondly, different from that in the Lagrangian coordinates case, where the time averaging procedure can be performed in a post-processing manner, the stress evaluation in Eulerian system must be evaluated spatially and temporally at the same time. Thirdly, the relation between Cauchy and first Piola-Kirchhoff stress was investigated. At zero temperature, traditional linear relation between these two is satisfied both in Virial and Hardy formulation. While at finite temperature, temporal averaging is required to guarantee this relation for Virial formulation.

For Hardy formulation, Cauchy stress differs from first Piola-Kirchhoff stress, which increases linearly with temperature. Numerical examples were provided to illustrate our investigation.

【Online】强关联电子体系第一性原理 DFT+DMFT 计算方法简介

Yu Liu, Institute of Applied Physics and Computational Mathematics
10:50 - 11:30

强关联电子体系通常是指一类包含部分填充的 d/f 壳层电子的体系。这一类体系对外界的电磁、温度、压力和掺杂等情况极为敏感。拥有反常膨胀、反常熔化等奇特物性的钚材料，连同重要工业领域中某些重要的超导、巨磁阻、光电和高效催化材料均属于该类材料，这使得人们对强关联电子体系的高效、可靠的第一性原理模拟手段有着迫切需求。但是，成熟的密度泛函方法（Density Functional Theory，DFT）由于其单电子特征以及自相互作用误差，使其从原理上无法正确模拟强关联电子体系。目前最为成功的模拟策略之一是将传统的密度泛函方法与求解强关联电子模型的动态平均场近似（Dynamical Mean Field Theory，DMFT）的方法相耦合，常被成为密度泛函 + 动态平均场近似（DFT+DMFT）方法。DFT+DMFT 方法目前已初步成功应用于强关联体系的电子结构和总能量的计算中，然而其较高的算法复杂度与耦合 DFT 造成的收敛问题使得这一方法尚未在实际材料模拟中被大规模使用。

为了降低计算代价，提高方法收敛的稳定性，相关领域的研究人员已做过许多有意义的尝试，如提高 DMFT 解法器的并行效率和内循环收敛性、提高 DFT+DMFT 耦合器的信息处理效率和外循环收敛性。然而，该方法的计算代价仍高出传统密度泛函 34 个数量级，存在较大的改进空间。这里我们将对目前 DFT+DMFT 算法研究的进展进行梳理，针对目前流行的几种解法器与 DFT 耦合方案阐述其原理及影响其效率的关键问题，从而支撑进一步的方法改进。

Efficient sampling of high-dimensional free energy landscapes using adaptive reinforced dynamics

Linfeng Zhang, Beijing Institute of Big Data Research
13:30 - 14:10

Enhanced sampling methods have the capability to facilitate crossing large (free) energy barriers. Despite many efforts that have been made in this area, two major difficulties still remain: How to sample high-dimensional free energy landscapes? And how to select the collective variables (CVs) if there is limited prior knowledge of a system? Here we introduce adaptive reinforced dynamics (ARiD), a method to efficiently explore the high-dimensional free energy landscape based on the free energy profile and error indicator estimated by deep neural network models. ARiD is flexible in determining the number of CVs and highly parallel, and it requires little prior knowledge and human intervention. We illustrate this method by studying various representative and challenging examples.

【Online】高通量第一性原理计算耦合相图热力学：模型构建及工程应用

Xiaoyu Chong, Kunming University of Science and Technology
14:10 - 14:50

材料基因工程中高通量计算的目的是实现材料的理性设计，主要有两个关键技术特点：并发式计算、自动流程计算；集成计算 (ICME) 方法，重点突破跨层次/跨尺度材料设计/计算瓶颈。相图热力学模型及数据库是实现跨尺度建模的必要环节，其基础为单相热/动力学数据

与相平衡数据的依赖关系。由于单独依靠 DFT 获取的热力学数据还不足以准确描述相边界，需要同时将实验数据引进到 Calphad 建模中。基于以上思想，我们发展了高通量第一性原理计算提供原数据、通过实验相边界数据和机器学习技术来优化热力学参数，从而建立热力学数据库的方法和标准工作流。通过第一性原理软件包 DFTTK，实现 104 量级晶体结构在有限温度下热力学性质的计算；通过基于马尔科夫链蒙卡的热力学建模程序 ESPEI，实现多元高阶体系多个热力学参数的同时自动优化；通过编写参数传递工具，实现 DFTTK 与 ESPEI 之间热力学数据的自动传递。该工作流及软件克服了传统热力学建模方法的“雪球”效应，尽量减少人的工作量，降低热力学模型优化的门槛，快速建立起用于新材料理性设计的热力学框架。

A domain decomposition method for the Poisson-Boltzmann solvation model

Chaoyu Quan, *Southern University of Science and Technology*
14:50 - 15:30

A domain decomposition method for the Poisson-Boltzmann solvation model that is widely used in computational chemistry is proposed. This method, called ddLPB for short, solves the linear Poisson-Boltzmann equation defined in 3D Euclidean space using the van der Waals cavity as the solute cavity. The Schwarz domain decomposition method is used to formulate local problems by decomposing the cavity into overlapping balls and only solving a set of coupled subequations in balls. A series of numerical experiments is presented to test the robustness and the efficiency of this method including comparisons with some existing methods. We observe exponential convergence of the solvation energy with respect to the number of degrees of freedom which allows this method to reach the required level of accuracy when coupling with quantum mechanical descriptions of the solute.

Improved Gauss-Seidel projection methods for micromagnetic simulations

Rui Du, *Soochow University*
15:50 - 16:30

Micromagnetic simulation is an important tool to study magnetization dynamics in magnetic materials. The underlying model is the Landau-Lifshitz-Gilbert equation, which is solved numerically in general. One of the most popular methods is the Gauss-Seidel projection method developed by Xiao-Ping Wang, Carlos Garcia-Cervera, and Weinan E in 2001. In this talk, we present two improved Gauss-Seidel projection methods with unconditional stability. Compared to the original Gauss-Seidel projection method, which solves heat equations 7 times at each step, saving of these two improved methods are about 2/7 and 4/7, which is verified by both 1D and 3D examples for the same accuracy requirement. Application of both methods to a realistic material is also presented with hysteresis loops and magnetization profiles. We also apply these methods to study the magnetization dynamics in antiferromagnetic and ferrimagnetic materials.

High-order multi-scale asymptotic analysis and computation of axisymmetric piezoelectric problem for composite structures

Qiang Ma, *Sichuan Univesity*
16:30 - 17:10

A second-order two-scale(SOTS) asymptotic coupled piezoelectric models are developed for the axisymmetric composites. The governing piezoelectric equations are compactly formulated in cylindrical coordinates, and the composite domains are assumed to be periodically occupied by the representative cells. The multi-scale asymptotic expansions for the displacement and the electric potential are formally defined and the effective elastic, piezoelectric, and dielectric coefficients are expressed in terms of the microscopic functions defined on the cell domain. The corresponding SOTS finite element procedure is proposed, in which the Newmark algorithm is applied to construct the computational scheme in the temporal domain. Numerical experiments are carried out to simulate both the static and dynamic asymptotic behavior of the space axisymmetric and the one-dimensional plane axisymmetric structures. It is validated from the numerical examples that the asymptotic models are effective to capture the macroscopic performance of the piezoelectric structures and the second-order expansions of the solutions is essential for obtaining the correct distributions of the stress and electric displacement.

3.2 Day 2, 11 April, Sunday

Random-Batch Ewald Algorithm

Zhenli Xu, *Shanghai Jiao Tong University*
08:30 - 09:10

The development of efficient methods for long-range systems plays important role in all-atom simulations of soft materials, biomolecules and drug design. We present a random-batch Ewald (RBE) method for molecular dynamics simulations of particle systems with long-range Coulomb interactions. The RBE takes advantage of the random minibatch strategy for the force calculation between particles, leading to an order N algorithm. It is based on the Ewald splitting of the Coulomb kernel and the random importance sampling is employed in the Fourier part such that the force variance can be reduced. This new simulation method avoids the use of the FFT and greatly improves the scalability of the molecular simulations. We present numerical results to show the nice features of the algorithm. We will also introduce the algorithm for short-range interactions in this talk.

Phase field approach for simulating solid-state dewetting problems

Wei Jiang, *Wuhan University*
09:10 - 09:50

Thin Solid films are usually thermodynamically unstable in the as-deposited state. Heating can lead to fragmentation (or pinch-off) of a thin film and the formation of micro-/nano- solid particles. This process is well-known as solid-state dewetting in materials science, and it is often driven by the minimization of the total interfacial energy of the system. In this talk, we propose a phase field approach for simulating solid-state dewetting and the morphological evolution of patterned islands on a substrate. The evolution is governed by the Cahn–Hilliard equation with degenerate mobilities coupled with contact line boundary conditions. The proposed approach can include the surface energy anisotropy into the models. Several important features observed in experiments can be reproduced by numerically solving the proposed models.

【Online】Computing Quasiperiodic Systems

Kai Jiang, *Xiangtan University*
10:10 - 10:50

Quasiperiodic structures, related to irrational numbers, are a class of important and widely existing systems. Typical examples include quasicrystals, incommensurate systems, defects, interfacial problems. Due to the irrational numbers, the quasiperiodic system is a space-filling structure without decay, which results in difficulty in numerical computation. A traditional method is using a periodic system to approximate the quasiperiodic system. It produces a Diophantine approximation error. In this talk, we will propose an efficient method to avoid the Diophantine approximation and obtain high accurate quasiperiodic solutions. We also apply the novel method to material computation, including soft quasicrystals, quasiperiodic quantum systems, and interfacial problems.

【Online】Dynamics of Grain Boundaries with Microscopic Constraints

Luchan Zhang, *The Hong Kong University of Science and Technology*
10:50 - 11:30

Dynamic properties of grain boundaries play vital roles in the mechanical and plastic behaviors of polycrystalline materials. The properties of grain boundaries strongly depend on their microscopic structures. We present continuum models for the dynamics of grain boundaries based on the continuum distribution of the line defects (dislocations or disconnections) and the constraints associated them. The long-range elastic interaction between the line defects is included in the continuum models to maintain stable microstructure on grain boundaries during the evolution. However, the calculation of the long-range force is quite time-consuming due to its form of integrals over all the grain boundaries. This limitation can be addressed by replacing with constraints that governs the stable dislocation structure during the evolution. In the other hand, in polycrystalline materials, the motion of grain boundaries is inevitably constrained by other grains and triple junctions, and this essentially influences the materials properties. We incorporate these important microscopic constraints to continuum dynamics models of high-angle grain boundaries whose dynamics are controlled by motion of disconnections.

A diffuse domain method for solving PDEs in complex domain

Zhenlin Guo, *Beijing Computational Science Research Center*
13:30 - 14:10

We will present a diffuse domain approach for solving PDEs in complex, involving domain. The approach extends the original complex domain into a larger and regular domain, where the original PDEs are extended and solved. The original boundary conditions are absorbed as a source term into the reformulated equations. Several numerical examples including multiphase flows, the epitaxial growth of two-dimensional material with anisotropy are shown to illustrate the approach.

Coupled crystal plasticity finite element with phase field method in modeling the plastic deformation of metallic materials

Guisen Liu, *Shanghai Jiao Tong University*
14:10 - 14:50

金属材料的塑性变形主要通过错滑移实现，此外还有孪生和相变诱发塑性，和晶体结构、变形温度和应变速率等因素相关。晶体塑性有限元方法 (Crystal plasticity finite element method, CPFEM) 是根据晶体塑性理论，通过用户自定义子程序建立材料的单晶或多晶弹性塑性本构模型，利用有限元软件求解在任意边界条件下，满足位移连续和应变协调，及弱形式的应力平衡的材料内部各物质点的弹塑性应力应变。但 CPFEM 的塑性本构仅考虑位错滑移对塑性变形的贡献，忽略了孪生变形的贡献，这主要是因为 CPFEM 难以准确描述界面的演化。相场方法 (Phase field method, PFM) 引入序参量描述新相和母相之间的界面，通过求解序参量演化获得界面随时间和空间的演化。采用 CPFEM 与 PFM 相耦合的方法可同时模拟位错滑移和孪生变形对塑性变形的贡献。其中 CPFEM 传递应力场给 PFM，用于计算孪生变形的弹性能驱动力；PFM 根据总自由能降低求解孪生相结构演化及孪晶演化率，并将孪晶演化率传递给 CPFEM，用于计算孪生对塑性应变率的贡献。

CPFEM 与 PFM 相耦合的难点在于界面的处理。CPFEM 为了保证积分点信息能充分反应材料物质点的物理性质，节点位移和积分点应力等信息都定义在和晶粒尺寸接近的稀疏网格上（微米级）。如果 PFM 采用和 CPFEM 相同的稀疏网格，序参量在有限厚度的界面区变化太陡变，造成孪晶形貌不规则。为了获得平滑界面和规则孪晶形貌，PFM 通常采用远小于晶粒尺寸的细密网格（纳米级），通过梯度能控制序参量在界面区平滑地变化。而这会增加二者在实时耦合传递积分点应力场和孪晶演化率信息的难度。我们采用两种方法解决该问题：1. 对 CPFEM 的稀疏网格信息进行插值获得 PFM 需要的细密网格上的相关信息；2. 根据 CPFEM 稀疏网格的节点位移信息自定义单元描述 PFM 细密网格上的孪晶形貌演化。报告最后应用 CPFE-PFM 研究了镁晶体变形中的孪晶形貌演化、介观应力应变分布特征，以及位错与孪晶的耦合作用对这些物理量及宏观流变行为的影响。

Adaptive QM/MM Coupling Methods for Crystalline Defects

Mingjie Liao, *Shanghai Jiao Tong University*
14:50 - 15:10

Hybrid quantum/molecular mechanics models (QM/MM methods) are widely used in material and molecular simulations when MM models do not provide sufficient accuracy but pure QM models are computationally prohibitive. Adaptive QM/MM coupling methods feature on-the-fly classification of atoms during the simulation, allowing the QM and MM subsystems to be updated as needed. We propose such an adaptive QM/MM method for material defect simulations based on a new residual based a posteriori error estimator, which provides both lower and upper bounds for the true error. We compare this new estimator with that of the Atomistic/Continuum (A/C) coupling methods. Based on this new estimator, we propose an inner-outer adaptive strategy, which includes an outer adaptive algorithm to select the QM and MM regions, and an inner adaptive algorithm to compute the approximate estimator for the selection up to a given accuracy. We validate the analysis and illustrate the effectiveness of the new scheme on numerical simulations for material defects.

The Applications of Data-Driven Interatomic Potentials to QM/MM Coupling Methods

Yangshuai Wang, Shanghai Jiao Tong University
15:10 - 15:30

A fundamental input for atomistic simulations of materials is the description of the potential energy surface (PES) as a function of atomic positions. Except for first principle-based models and empirical potentials, a modern alternative has emerged in recent years in the form of machine-learned interatomic potentials, or the so-called " data-driven "models, where the PES is described as a function of local environment descriptors that are invariant to translation, rotation and permutation. We develop and analyze a framework for QM/MM (quantum/classic) hybrid methods for crystalline defects, which admits general atomistic models including the traditional " off-the-shell "interatomic potentials and the state-of-the-art " data-driven "models. The results in this work can (i) establish an a priori error estimate for the QM/MM approximations in terms of the sizes of QM regions and how well the MM models are coupling with the QM model, and (ii) provide a guidance on how to construct the database to train the " data-driven " interatomic potentials or force fields for simulations of crystalline defects.