YANFEI TANG

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HIGHLIGHTS

- Five years hands-on modeling experience across molecular dynamics simulation of soft matter, Bayesian inference theory on inverse problems, and quantum model systems.
- Strong coding skills by implementing models with Python or C/C++ with external libraries to solve challenging problems. Great experience to interpret results with visualization tools.
- Three years experience in parallel computing on large computer cluster. Familiar with machine learning analysis tools to deal with data sets.

EDUCATION

Ph.D in Physics August 2012 - December 2018
Virginia Tech, USA

B.S in Physics September 2008 - June 2012
Tongji University, China

SKILLS

Programming language	Python, C/C++, Bash, MATLAB, Java
Programming library	numpy, scipy, matplotlib, pandas, sklearn, Tensorflow, Eigen, OpenMP, MPI
Machine learning algorithms	Linear/Logistic regression, Decision tree, K nearest neighbors, Naive Bayes, Ensemble learning (Random forest, AdaBoost, GBDT, XGBDT), Clustering, Classification (Gaussian mixture, K means, SVM, BIRCH) Deep learning (DNN, CNN, RNN, LSTM)
Software and OS platforms	LAMMPS, macOS, Linux, Windows

KAGGLE PROGRAM

Predict Future Sales

Data dimension(3M $\times$ 6). Given historical time-series dataset consisting of daily sales data, we need to predict total sales for every product and store in the next month. The features contain sales data, item names, item sales per day per store, prices, item category. We first clean and preprocess the data. Then XGBoost is applied to train the data. Result: RMSE = 0.913.

Aerial Cactus Identification

Data dimension(17.5k). It is a binary identification problem. We are tasked with creation of an algorithm to identify a specific type of cactus in an aerial surveillance image. We used a simple convolutional neural network (VGG16) to detect if cactus exist in a 32 $\times$ 32 image Result: AUC = 0.9983.

RESEARCH EXPERIENCE

Research Assistant December 2015 - December 2018
Theoretical and Computational Soft Matter Group, Physics Department, Virginia Tech

• Computational simulation of drying binary colloidal particle suspension

We used Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) to study evaporation of binary colloidal particle suspension on computer clusters. We predicted the "small-on-top" stratification after evaporation through the explicit solvent model. By comparing the simulation results and theoretical state diagram, we pointed

out the drawback of the hydrodynamics screening in the implicit solvent model. The thermal gradient and Soret effect were proposed to control the stratification during the evaporation. A stronger stratification was found in the simulations.
Result: We are the first group to study the binary colloidal particle suspension by explicit solvent model. The results are published in SCI journals.

• Capillary phenomena on a small particle (cylinder) at a liquid-vapor interface

Capillary phenomena on a small particle (cylinder) at a liquid-vapor interface were study by solving Young-Laplace equation and molecular dynamics simulations. The shape of the meniscus and capillary forces were fully explained under the gravity and different length scales. We concluded that the macroscopic theory is still applicable under a few nanometers.
Result: The Joanny-de Gennes spring model is extended under the gravity. The results are published in SCI journals.

Research Assistant January 2015 - November 2015
Computer Science and Mathematics Division, Oak Ridge National Lab

• Extract spectral function from imaginary-time quantum Monte Carlo data
Maximum entropy method and stochastic optimization method were used to extract the spectral function from the imaginary-time quantum Monte Carlo data. Three examples were compared by using these two methods. We concluded that maximum entropy method is applicable in most cases.
Result: The performance of the two methods are compared, the results are published in SCI journals. The script application is used in a collaborated project.

Research Assistant January 2014 - December 2014
Computational Condensed Matter Group, Physics Department, Virginia Tech

• Quantum Monte Carlo (QMC) simulation of bilayer Bose Hubbard model
We studied bilayer Bose Hubbard model on a square lattice by using stochastic series expansion method and Gutzwiller method. The phase diagram was obtained at the finite temperature and zero temperature. The critical exponents from the QMC method were compared to theoretical predication.

PUBLICATIONS

8. **Y. Tang**, G. S. Grest, and S. Cheng, "Stratification of drying particle suspensions: Comparison of implicit and explicit solvent simulations," *J. Chem. Phys.* **150**, 224901 (2019).

7. **Y. Tang**, G. S. Grest, and S. Cheng, "Control stratification in drying particle suspensions via temperature gradients," *Langmuir* **35**, 4296 (2019).

6. **Y. Tang** and S. Cheng, "The meniscus on the outside of a circular cylinder from microscopic to macroscopic scales." *J. Colloid Interface Sci.* **533**, 401 (2019).

5. **Y. Tang** and Shengfeng Cheng, "Capillary forces on a small particle at a liquid-vapor interface: theory and simulation," *Phys. Rev. E* **98**, 032802 (2018).

4. **Y. Tang**, G. S. Grest, and S. Cheng, "Stratification in drying films containing bidisperse mixtures of nanoparticles," *Langmuir* **34**, 7161 (2018).

3. S. Li, **Y.Tang**, T. A. Maier, and S. Johnston, "Phase competition in a one-dimensional three-orbital Hubbard-Holstein model," *Phys. Rev. B* **97**, 195116 (2018).

2. S. Li, N. Kausha, Y. Wang, **Y. Tang**, G. Alvarez, A. Nocera, T. A. Maier, E. Dagotto, and S. Johnston, "Nonlocal correlations in the orbital selective Mott phase of a one-dimensional multiorbital Hubbard model," *Phys. Rev. B* **94**, 235126 (2016).

1. F. Bao, **Y. Tang**, M. Summers, G. Zhang, C. Webster, V. Scarola, and T. A. Maier, "Fast and efficient stochastic optimization for analytic continuation," *Phys. Rev. B* **94**, 125149 (2016).

AWARDS

Outstanding Graduate of Tongji University — June 2012

SELECTED PRESENTATIONS

"Controlling Stratification of Polydisperse Nanoparticles during Solvent Evaporation" 2018 Center for Soft Matter and Biological Physics (CSMBP) Symposium, Blacksburg, Virginia (**Outstanding poster awards**) May 2018

"Theory and Simulation of Capillary Forces on a Nanoparticle at a Liquid-Vapor Interface." APS March Meeting, Los Angeles, California March 2018

"Young-Laplace Equation: Theory and Simulation of Nanoparticles at Liquid-Vapor Interfaces." CSMBP Meeting, Blacksburg, Virginia November 2017

"Stratification in Drying Films Containing Bidisperse Mixtures of Nanoparticles." 5th VSM Workshop, James Madison University, Virginia September 2017

"Solvent Evaporation Induced Assembly in Binary Mixtures of Nanoparticles." APS March Meeting, New Orleans, Louisiana March 2017

"Polyelectrolyte Complexes in Solution: A Molecular Dynamics Study." APS March Meeting, New Orleans, Louisiana March 2017

"Phase diagram of the Bilayer Bose Hubbard Model." APS March Meeting, San Antonio, Texas March 2015

TEACHING

Phys 5564 Polymer physics - TA grading, office hours — Fall 2018

Phys 2305 Fundamentals of physics - TA recitation — Spring 2016

Phys 5705 Statistical mechanics - TA grading, office hours — Spring 2016

Phys 2305 and Phys 2306 - TA coordinate physics labs — 2012, 2013, 2014, 2018

MENTORED STUDENTS

MII REU undergraduate student: Ralph Romero — Summer 2017