

# Chunyan Li

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## Education

University of South Carolina – Columbia, SC, US

Anticipated Aug. 2023

*Ph.D. in Applied and Computational Mathematics* | Advisor: Professor Qi Wang

Xiangtan University – Xiangtan, Hunan, P. R. China

May 2018

*Bachelor of Science in Mathematics in honors class*

## Research Interests

- Application of data science and machine learning in materials and life science, such as digital twin for health
- Data-driven modeling and computation, such as discovering PDE models and dynamical systems from data using deep neural networks, Neural ODE, and recurrent neural networks (LSTM).
- Application of machine learning to scientific computing and computational science, such as solving PDE models and dynamical system with deep neural networks, and physics-informed learning.
- Dimensionality reduction method for machine learning and Sampling Strategies for class-imbalanced dataset
- High order numerical methods for thermodynamically consistent partial differential equations, such as energy stable numerical schemes, asymptotic preserving numerical schemes, symplectic RK method, invariant energy quadratization approach (IEQ) and scalar auxiliary variable approach (SAV)
- Non-equilibrium theories for thermodynamics, such as Generalized Onsager principle, and thermodynamically consistent dynamic boundary conditions

## Publications

\* means equal contribution

1. Wetthasinghe, Shehani T., **Chunyan Li**, Huina Lin, Tianyu Zhu, Chuanbing Tang, Vitaly Rassolov, Qi Wang, and Sophya Garashchuk. *Correlation between the Stability of Substituted Cobaltocenium and Molecular Descriptors*. The Journal of Physical Chemistry A 126, no. 1 (2022): 80-87. (Impact factor: 2.781).
2. **Li, Chunyan**, Shehani T. Wetthasinghe, Huina Lin, Tianyu Zhu, Chuanbing Tang, Vitaly Rassolov, Qi Wang, and Sophya Garashchuk. *Stability Analysis of Substituted Cobaltocenium [Bis (cyclopentadienyl) cobalt (III)] Employing Chemistry-Informed Neural Networks*. Journal of Chemical Theory and Computation 18, no. 5 (2022): 3099-3110. (Impact factor: 6.006)
3. Hou, Jianguo, Jun Deng, **Chunyan Li**, and Qi Wang. *Tracing and Forecasting Metabolic Indices of Cancer Patients Using Patient-Specific Deep Learning Models*. Journal of Personalized Medicine 12, no. 5 (2022): 742. (Impact factor: 4.453)
4. **Chunyan Li\***, Lu Wang\*, Jianguo Hou, Jun Li, Kexun Li, Hongfei Deng, Yu Wang, Li Chang, Pin Zhou, Jun Zeng, Mingwei Sun, Hua Jiang, and Qi Wang. *Prognosis of Sepsis Built From Small Datasets* (Submitted to Computer Methods and Programs in Biomedicine, impact factor: 7.027)
5. Lu Wang\*, **Chunyan Li\***, Kexun Li, Hongfei Deng, Yu Wang, Li Chang, Ping Zhou, Jun Zeng, Mingwei Sun, Hua Jiang, Qi Wang *Machine-Learning Enabled Prognostic Models for Septic Patients* (Submitted to Critical Care Medicine, impact factor: 9.296)

## Presentations

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1. *Title: An introduction of Principal Component Analysis (PCA)* Oct.15th 2021  
ACM Student Seminar, University of South Carolina, Columbia, SC, US
2. *Title: An introduction of Variational Autoencoder (VAE)* Feb.25th 2021  
ACM Student Seminar, University of South Carolina, Columbia, SC, US
3. *Title: Applications of deep learning in Chemistry and Life Science and the experience of pursuing my Ph.D*  
(invited talk) May 14th 2022  
Department of Mathematics, Xiangtan University, Xiangtan, Hunan, P.R. China
4. *Title: Stability analysis of cobaltocenium employing chemistry-informed neural networks and quadratic neural networks* (poster presentation) Oct.28th 2022  
The 2022 Made in SC Research Fellows and Faculty Conference and Celebration, Greenville, SC, US
5. *Title: Tracing and Forecasting Metabolic Indices of Cancer Patients Using Patient-Specific Deep Learning Models* Nov.12th 2022  
The 40th Southeastern-Atlantic Regional Conference on Differential Equations, Raleigh, NC, US

## Awards and Honors

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1. Travel Award by the 40th SEARCDE Conference \$500 Nov.12th-13th 2022
2. **SEC Emerging Scholars Fellowship** (UofSC) 2022 – 2023 AY  
Assistantship stipend up to \$35,000 and extra \$3000 for professional development
3. **George W.Johnson Graduate Fellowship** \$2000 (UofSC) May 2022  
*Given annually by the Department of Mathematics at the University of South Carolina.*
4. **C.C. Royal Fellowship** \$2000 (UofSC) Apr. 2022  
*C.C. Royal Fellowship is one of the Trustee Fellowships that are awarded to full-time graduate students who exhibit excellence in graduate study, research and scholarship. Given annually by the Graduate school at the University of South Carolina.*
5. **George W.Johnson Graduate Fellowship** \$2000 (UofSC) Apr. 2020
6. **Outstanding First-Year ACM Student** (UofSC) Apr. 2019  
*Given annually by the Department of Mathematics at the University of South Carolina*
7. Xiangjiang Scholarships for excellent students (XTU) Dec 2017
8. Scholarships for excellent students in honors class, 4-year tuition fellowship (XTU) Sept. 2014-Jun 2018
9. National Encouragement Scholarship (XTU) Nov 2016
10. Second class scholarship (Top 2/19) (XTU) May 2015

## Teaching

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### University of South Carolina – Columbia, SC, US

- Math 141 Calculus I (TA) Spring 2019
- Conducted recitation sessions and demonstrated how to use Maple to solve mathematical problems for undergraduate.
  - Math Tutor for undergraduate in Math Tutoring Center
- Math 142 Calculus II (TA) Fall 2019
- Math 115 PreCalculus (Instructor of Record) Spring 2020
- Compositions of Functions, Inverse Functions, Trigonometric Functions in a Right Triangle, Using Inverse Trigonometric Functions, Solving Trigonometric Equations, Using Trigonometric identities, Graphing Elementary Functions
- Math 141 Calculus I (TA and online) Fall 2020
- Math 528 Mathematical Foundation of Data Science and Machine Learning (TA) Fall 2021
- Lectures on PyTorch and scikit-learn programming.

## Mentor Experience

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### University of South Carolina – Columbia, SC, US

#### Mentor in REU Summer School

Jun.6th – Jul.15th 2022

*Research Experience for Undergraduates (REU): Summer School on Mathematical Foundation of Data Science 2022 is supported by the NSF RTG grant at the University of South Carolina*

- Lectures on PyTorch and scikit-learn programming.
- Meet at least 2 hours every day to update the research projects for each groups (5 undergraduate students in 2 groups).
- Help 3 students in group I understand Neural Ordinary Differential Equation (NODE) and how to program using its package, and guide students to do research on “predicting biomarkers of cancer patients using NODE”.
- Help 2 students in group II understand Physics Informed Neural Network (PINN) and how to program using DeepXDE package and guide students to do research on ”solving a Partial Differential Equation using PINN”.

### Xiangtan University – Xiangtan Hunan, P.R. China

Mentor for class 2 in Department of Mathematics

Fall 2016

Mentor for Honor class in Business School

Spring 2017

## Service

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Organizer of the ACM Student Seminar in UofSC

Sept. 2021 – Present

- Organize the applied and computational mathematics seminar with McKenzie Black, Thomas Hamori.
- Invite Professors and Graduate students especially, underrepresented groups to give talks.

Vice president at SIAM student chapter of UofSC

Sept.2020 – Sept.2022

Proctor for the annual UofSC High School Math Contest

2019 – 2020

## Membership

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- Society for Industrial and Applied Mathematics (SIAM)
- American Mathematical Society (AMS)
- Association for Women in Mathematics (AWM)

## Skills

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### Programming

- Proficient in Matlab, Python (PyTorch), DeepXDE, Neural ODE,,  $\text{\LaTeX}$ , Markdown.
- Experience with HTML.