Chunyan Li

Contact and Personal Information

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Emplement

The Pennsylvania State University – University Park, PA, US　　　　Jan. 2024-now
Postdoc researcher | Mentor: Professor Wenrui Hao

Education

University of South Carolina – Columbia, SC, US　　　　Aug. 2018-Dec. 2023
Ph.D. in Applied and Computational Mathematics | Advisor: Professor Qi Wang

Xiangtan University – Xiangtan, Hunan, P. R. China　　　　Sept. 2014-June 2018
Bachelor of Science in Mathematics in honors class

Research Interests

General interests: Numerical Methods for Partial Differential Equations, Machine Learning, Deep Learning

- Data-driven modeling and computation, such as discovering PDE models and dynamical systems from data using deep neural networks (eg. multi-scale neural networks), Neural ODE, and recurrent neural networks (LSTM), etc..
- Application of machine learning to scientific computing and computational science, such as solving PDE models and dynamical system with deep neural networks (eg. structure-preserving and multi-scale neural networks), and physics-informed learning.
- Application of data science and machine learning in materials and life science, such as digital twin for health.
- 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*, Kexun Li, Hongfei Deng, Yu Wang, Li Chang, Ping Zhou, Jun Zeng, Mingwei Sun, Hua Jiang, and Qi Wang. *Prognostic Models for Sepsis Built on Small Datasets.* (Submitted)

5. Lu Wang*, **Chunyan Li***, Kexun Li, Hongfei Deng, Yu Wang, Li Chang, Ping Zhou, Jun Zeng, Mingwei Sun, Hua Jiang, Qi Wang. *Prognostic Models for Sepsis Based on Limited Data.* (Submitted)

6. **Chunyan Li**, Qi Wang. *Learning Dynamic Boundary Conditions Effects: A Dynamic Physics-Informed Neural Network Approach for Thermodynamically Consistent Phase Field Models in Arbitrary Domains* (To be submitted, 2024)

Presentations and Posters

1. *Title: Energy dissipation rate based adaptive dynamic PINN for solving thermodynamically consistent phase field models with thermodynamically consistent dynamic boundary conditions in arbitrary domains*
   Symposium on computational mathematics for engineering and sciences, State College, PA, US   Nov. 2023

2. *Title: Tracing and Forecasting Metabolic Indices of Cancer Patients Using Patient-Specific Deep Learning Models*   June 2023

3. *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

4. *Title: Stability analysis of cobaltcocenium employing chimstry-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: Applications of deep learning in Chemistry and Life Science and the experience of pursuing my Ph.D* (invited talk & online)   May 14th 2022
   Department of Mathematics, Xiangtan University, Xiangtan, Hunan, P.R. China

6. *Title: An introduction of Variational Autoencoder (VAE)*   Feb.25th 2022
   ACM Student Seminar, University of South Carolina, Columbia, SC, US

7. *Title: An introduction of Principal Component Analysis (PCA)*   Oct.15th 2021
   ACM Student Seminar, University of South Carolina, Columbia, SC, US

Awards and Honors

1. **Travel Award by the ICERMS at Brown University**   June 12th-16th 2023
2. **Travel Award by the ICERMS at Brown University**   June 5th-9th 2023
3. **Travel Award by the University of South Carolina**   2023
4. **SPARC Graduate Research Grant** $5,000$ May 1, 2023 - Aug. 15th, 2024
   The Office of the Vice Presidunt for Research, University of South Carolina
   Only 49 Recipients among all graduate students are selected in the university
5. **Travel Award by the 40th SEARCDE Conference** 500 Nov.12th-13th 2022

Awards and Honors

1. **Graduate International Student Achievement Award**   Fall 2023
   ISAA is awarded each semester to TWO international students, one at the graduate level and one at the undergraduate level
2. **SEC Emerging Scholars Fellowship** (UofSC)   2022 – 2023 AY
   Only 5 Recipients among all graduate and postdoctoral students are selected in the university
3. **George W.Johnson Graduate Fellowship in Applied Mathematics** (UofSC)   May 2022

4. **C.C. Royal Fellowship** (UofSC)   Apr. 2022
   Only one student is annually awarded to full-time graduate students who exhibit excellence in graduate study, research and scholarship by the Graduate School.
5. **George W.Johnson Graduate Fellowship in Applied Mathematics** (UofSC)   Apr. 2020
   One graduate student is awarded annually by the Department of Mathematics.
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-June 2018
9. National Encouragement Scholarship (1/19, XTU)   Nov 2016
10. Second class scholarship (2/19, XTU)   May 2015

Professional Services

Reviewers for
- Mathematical Methods in the Applied Sciences

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

Teaching

University of South Carolina – Columbia, SC, US
Math 141 Calculus I (TA), Recitations and laboratory work, about 32 students   Spring 2019
Math 142 Calculus II (TA), Recitations and laboratory work, about 45 students   Fall 2019
Math 115 PreCalculus (Instructor), lectures and recitation, about 28 students   Spring 2020
Math 141 Calculus I (TA and online), Recitations and laboratory work, about 58 students   Fall 2020
Math 528 Mathematical Foundation of Data Science and Machine Learning (TA)   Fall 2021
Lectures on PyTorch and scikit-learn programming for a week

Mentor Experience

University of South Carolina – Columbia, SC, US
Mentor in REU Summer School   June 6th – July 15th 2022
- Lectures on PyTorch and scikit-learn programming.
- Meet with students for at least 2 hours every day to update the research projects for each group (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

Membership

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

Relevant Skills

Lagrange: Chinese, English
Technical skills: Matlab, Python, PyTorch, LaTeX, Neural ODE, Markdown.

References

Qi Wang   qwang@math.sc.edu
Professor, Department of Mathematics, University of South Carolina

Changhui Tan   tan@math.sc.edu
Associate Professor, Department of Mathematics, University of South Carolina

Yi Sun   yisun@math.sc.edu
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Hong Wang   hwang@math.sc.edu
Graduate Director and Professor, Department of Mathematics, University of South Carolina