Wenxin Liu

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Education

Imperial College London **Sep. 2024 – Sep. 2025**
Master of Science in Applied Mathematics(Scientific computing and Machine Learning) *First class Distinction*

Xi'an Jiaotong Liverpool University **Sep. 2020 – Jun. 2024**
Bachelor of Science in Applied Mathematics *First class honors*

Highly relevant experiences with numerical analysis and optimization

Research at National supercomputing center **Sep. 2025–Jun. 2026**

- Developed a high-performance Graph Neural Network (GNN) + Advanced MLP fusion model for matrix solver selection. Architected the GNN path using ResidualGCN Blocks (to mitigate over-smoothing) and a Global Attention pooling mechanism, evolving from a standard GCN baseline. Integrated the graph embedding with a gated residual MLP branch and implemented a custom precision-focused loss function. Achieved 80.3% accuracy among 26 combinations of preconditioners and methods for sparse matrix computing, with 3.83× speed-up for matrix solving.
- Developed an intelligent regression framework for **Algebraic Multigrid (AMG)** parameter optimization, enabling automatic tuning of the strong connection threshold θ to improve solver efficiency. Extracted structural features via CNN by separating matrix into $128 * 128$ blocks and global features with MLP, this method achieved 2.86× improvement for matrix solving.

Postgraduate Final Project about Optimal Transport **Jan. 2025–Sep. 2025**

- Conduct symmetric Douglas-Rachford splitting and prime-dual method with proximal operator for solving the dynamic optimal transport problem, compare its performance with the Sinkhorn algorithm.
- Use Schrödinger Bridge to approximate the solution of optimal transport problems in both dynamic way and static way, and implement the algorithm for solving the Schrödinger Bridge problem with Forward and Backward system with proximal recursion.
- Implement the Schrödinger Bridge problem with nonlinear prior drift and reflective boundary conditions, and apply the proximal recursion algorithm and Finite Element Method to solve the problem with prior drift and boundary conditions like obstacles in both 2D and 3D cases.
- Preprint paper coauthor with Dr.Dante Kalise has been submitted to European Control Conference: http://arxiv.org/abs/2511.14355

Computational Partial Difference Equation Project **Jan. 2025 – Apr. 2025**

- Solve second order Nonlinear ODE and nonlinear heat equation with explicit method, lagged approach and implicit Newton linearization, analyze numerical result with physical meaning and theoretical perturbation analysis.
- Develop numerical solutions for elliptic PDEs with non-uniform boundary conditions using structured grid mapping and adaptive mesh refinement (AMR) to enhance accuracy in complex geometries. Implement iterative solvers (Gauss-Seidel, SOR, multigrid) for large sparse linear systems.
- Solve wave equation with Neumann and transparent boundary conditions and perform discrete Fourier analysis to assess numerical dissipation and dispersion. Design a position-dependent Perfectly Matched Layer (PML) to reduce boundary reflections by 85%. Validated accuracy and convergence through analytical Fourier analysis.
- Design an IMEX finite difference framework for coupled wave-heat systems, combining explicit wave solvers and implicit thermal diffusion. Derived stability criteria via Fourier and Jury analysis, and implement efficient solvers using staggered grids. Demonstrated the effect of thermal diffusivity on energy dissipation and wave behavior with vary of variables through numerical experiments.

Finite Element: theory and implementation Project **Jan. 2025 – Apr. 2025**

- Implement an object-oriented finite element framework in Python to solve elliptic PDEs (Helmholtz/Poisson equations), featuring modular classes for Lagrange elements, function spaces, structured meshes (UnitSquareMesh), and Gauss quadrature rules. Engineer a global node numbering system to map local-to-global degrees of freedom, enabling efficient sparse matrix assembly via cell-wise contributions. Utilized einsum-optimized tensor operations to compute stiffness/mass matrices.
- Engineer a mixed finite element solver for Stokes equations ($\mu \Delta \mathbf{u} = \nabla p + \mathbf{f}, \nabla \cdot \mathbf{u} = 0$) with structured 2D meshes. Design vector-valued Lagrange elements with tensor-product basis functions, extending scalar tabulation to handle 2D velocity fields via Vandermonde matrix-based evaluations. Implemented divergence and gradient coupling terms through block matrix assembly ($A = \begin{bmatrix} A_{\mathrm{u}} & B^T \\ B & 0 \end{bmatrix}$) using SciPy's sparse lil_matrix format, and stabilized the saddle-point system via pressure Poisson stabilization (diagonal perturbation). Optimize strain-rate tensor $\left(\epsilon(\mathbf{u}) = \frac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)\right)$ integration using einsum -accelerated operations. Then deploy the solver to simulate incompressible viscous flows ($\mu = 1$) with analytic benchmarks derived from stream functions ($\psi(x, y) = (1 - \cos 2\pi x)(1 - \cos 2\pi y)$).

Data Science Project **Jan. 2025 – Apr. 2025**

- Develop multi-class classifiers (Decision Trees, Random Forests) and Huberised SVM models for airfield weather condition prediction. Optimized Random Forests via Gini importance-based feature selection. Stabilized SVM training with modified Huber loss and mini-batch SGD, achieving 94.1% test accuracy.
- Design a compound loss MLP for joint runway temperature prediction with physical constraints. Implemented transfer learning by freezing pretrained MLP hidden layers and fine-tuning sigmoid output layers for binary classification, achieving accuracy to 99.8% versus 97% for non-transferred models.
- Design a U-Net convolutional neural network in PyTorch for joint dimensionality reduction and gene expression regression. Achieved $R^2 = 0.69$ on regression with early stopping and dropout.
- Construct a spectral layout using normalized Laplacian eigenvectors for data analysis and clustering, conducting analysis for degree centrality via bipartite histograms.

Computational Linear Algebra Project **Sep. 2024–Jan. 2025**

- Develope QR-based solvers for least squares problems (over/underdetermined systems), implementing 4 algorithms: Normal Equations, Classical/Modified Gram-Schmidt, and Householder (Python/Numpy). Design regularization method for ill-posed least-square problems using augmented QR factorization, reducing condition number by 5 orders of magnitude with $\lambda = 1e - 6$ penalty.
- Implement and analyze the practical QR algorithm for computing eigenvalues of real symmetric matrices, including enhancements such as Wilkinson shift and deflation. Demonstrate the efficiency of Wilkinson shift in accelerating convergence through comparative experiments across varying matrix sizes, and verify eigenvalue accuracy via inverse iteration.
- Extend the GMRES algorithm by implementing Jacobi and Gauss-Seidel preconditioners to improve convergence on ill-conditioned systems. Conduct a comparative analysis of residual decay and convergence rates for varying ϵ values, showing that preconditioning significantly improves performance, especially with Gauss-Seidel under increasing ill-conditioning.

Scientific computing Project **Sep. 2024 – Jan. 2025**

- Implement and analyze linear search, merge sort with binary search method ($O((m+n)\log n)$) for searching and pattern matching in large datasets. Apply the Rabin-Karp algorithm for pattern matching in amino acid sequences, utilizing optimized hash calculations for fast sequence comparison.
- Develop and analyze numerical solutions for a nonlinear dynamical system of ODEs. Implemented tests comparing perturbation energy calculations with simulations, showing consistency and accuracy. Analyzed periodic, aperiodic, and chaotic behaviors for different system sizes, using Principal Component Analysis (PCA) and correlation dimension analysis to identify chaotic dynamics.
- Implement the extended Kalman filter for Lorenz system, analyze the computational cost of one step of the extended Kalman filter. Focused on identifying the most computationally expensive portions of the method and explored trends in wall time with varying problem sizes.

Undergraduate Final Project about Numerical Optimization **Sep. 2023–Jun. 2024**

- Apply the interior point method by transforming inequality-constrained problems into equality-constrained forms using indicator functions, enabling the use of barrier methods for numerical solution approximation, and implement the algorithm for linear programming solvers.
- Implemented Newton's method as the core iterative approach, deriving iterative equations from the KKT conditions. Extended the framework to a primal-dual approach by reformulating the KKT conditions into residual functions.

Teaching Assistant for School Numerical Analysis course **Feb. 2024–Jun. 2024**

- Assistant for lab course and teach basic skills with Matlab.

Honors/Awards

School Operational Research Festival | *Competition* **May 2023**

- Serve as the captain in a team competition at the School of Operational Research, leading a group in the study of integer programming to solve the Traveling Salesman problem. Dive into the intricacies of integer programming models pertaining to scheduling and activity table arrangements. As a result of our diligent research efforts, we secured first place in the inter-school festival competition.

Honor in Mathematic Competition in Modeling(MCM) **Jan. 2021**

- A multi-day mathematical modeling competition is held annually in the US. Awarded to top 15% teams based on an outstanding competition record and unusual potential for math modeling.

Technical Skills

Computer Languages: Python, Java, Matlab, R, Lingo, Linux, C++
Developing Tools: NumPy, Scipy, Pandas, PyTorch