Qiang Liu

Research Scientist | AI for Science / AI4PDE
Male | Age 28 | Born 1 October 1998
TUM | Ph.D. Candidate in Computer Science

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Professional Summary

Ph.D. candidate in Computer Science at the Technical University of Munich, specializing in **scientific foundation models, physics-informed generative models, and differentiable numerical simulation**. Led the development of Tadpole, a foundation model for three-dimensional PDEs; contributed to PDE-Transformer; proposed the ICLR Spotlight method ConFIG; and developed TorchFSM, a PyTorch-based differentiable PDE solver for GPUs. Combines machine learning research with experience in CFD/OpenFOAM, multiphysics solvers, and large-scale three-dimensional training, with the goal of translating scientific machine learning into reliable and efficient engineering simulation tools.

Education

Technical University of Munich *Ph.D. Candidate in Computer Science; Advisor: Prof. Nils Thuerey* *2022 - Present*
Research: AI for Science and PDEs, scientific foundation models, physics-informed generative models, differentiable simulation, and physics-informed neural networks

Harbin Institute of Technology *M.Eng. in Power Engineering and Engineering Thermophysics* *2020 - 2022*
Multiphysics solver development, OpenFOAM simulation and development, and electrohydrodynamics; Outstanding Master's Thesis

Harbin Institute of Technology *B.Eng. in Energy and Power Engineering* *2016 - 2020*
*Fluid mechanics, heat transfer, engineering thermodynamics, and computational fluid dynamics; ranked **3rd out of 146** in the program*

Selected Research and Development Experience

Foundation Models for PDEs

- Contributed to the development of the two-dimensional PDE foundation model PDE-Transformer and led the development of **Tadpole**, a foundation model for three-dimensional PDEs.
- Introduced autoencoder reconstruction as a pretraining objective for PDE foundation models, making Tadpole the first three-dimensional PDE foundation model to support **multiple downstream tasks**.
- Designed an online simulation and training pipeline that completed training on approximately **202 TB** of dynamically generated data **without local data storage**; enabled inference on grids up to 1024^3, corresponding to more than **one billion degrees of freedom**.

Physics-Constrained Generative Models

- Pioneered the use of diffusion-based generative models for **uncertainty quantification** and surrogate modeling in numerical simulation; the resulting paper was among the early works applying diffusion models to flow simulation.
- Proposed the conflict-free multi-task optimization framework **ConFIG** and applied it to physics-constrained generative modeling; subsequently designed ConFIG-based physics-constrained flow matching and a physics-constrained diffusion model for sparse flow reconstruction.
- Extended ConFIG to additional applications, including physics-informed neural networks, multi-objective learning, and federated learning.

TorchFSM: A PyTorch-Based Differentiable PDE Solver for GPUs *https://qiauil.github.io/torchfsm/*

- Developed a Fourier spectral framework for constructing PDE solvers from modular operators such as gradients and advection, with support for **GPU acceleration and batched three-dimensional simulation**.
- Enabled **end-to-end automatic differentiation** and integration with machine learning workflows for online data generation, inverse problems, and the training of physics-informed neural operators.

Selected Publications and Scholarly Work

14 publications, including 5 first-author papers; Google Scholar h-index: 10.

Foundation Models for PDEs

- **Q. Liu**, F. Koehler, B. Holzschuh, N. Thuerey. "Tadpole: Autoencoders as Foundation Models for 3D PDEs with Online Learning," *arXiv*, 2026. Under review at NeurIPS 2026.
- B. Holzschuh, **Q. Liu**, G. Kohl, N. Thuerey. "PDE-Transformer: Efficient and Versatile Transformers for Physics Simulations," *International Conference on Machine Learning (ICML)*, 2025.

Physics-Constrained Generative Models

- **Q. Liu**, M. Chu, N. Thuerey. "ConFIG: Towards Conflict-free Training of Physics Informed Neural Networks," *International Conference on Learning Representations (ICLR)*, 2025. **Spotlight**
- **Q. Liu**, N. Thuerey. "Uncertainty-aware Surrogate Models for Airfoil Flow Simulations with Denoising Diffusion Probabilistic Models," *AIAA Journal*, 2024.
- G. Baldan, **Q. Liu**, A. Guardone, N. Thuerey. "Physics vs Distributions: Pareto Optimal Flow Matching with Physics Constraints," *International Conference on Learning Representations (ICLR)*, 2026.
- M. Amorós-Trepat, L. Medrano-Navarro, **Q. Liu**, L. Guastoni, N. Thuerey. "Guiding diffusion models to reconstruct flow fields from sparse data," *Physics of Fluids*, 2026. The first two authors were master's students supervised by Q. Liu.

Book

- N. Thuerey, B. Holzschuh, P. Holl, G. Kohl, M. Lino, **Q. Liu**, P. Schnell, F. Trost. "Physics-based Deep Learning," Chapter 5: Probabilistic Learning. https://physicsbaseddeeplearning.org/

刘　强

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期望工作起始日期: 2027 年 3 月

专业概述

慕尼黑工业大学计算机科学博士，研究聚焦**科学基础模型、物理生成模型与可微数值模拟**。主导三维 PDE 基础模型 Tadpole，参与 PDE-Transformer，提出 ICLR Spotlight 工作 ConFIG，并开发基于 PyTorch 的 GPU 可微 PDE 求解器 TorchFSM。兼具机器学习研究、CFD/OpenFOAM、多物理场求解器和大规模三维训练经验，致力于将科学机器学习转化为可信、高效的工程仿真能力。

核心能力

科学机器学习： PDE 基础模型、神经算子、物理信息神经网络、代理模型、多目标优化
生成式物理建模： 扩散模型、流匹配、物理约束生成、超分辨率、不确定性建模
数值模拟与工程： CFD、OpenFOAM、多物理场求解器、傅里叶谱方法、可微 PDE 求解、反问题
训练与工程： PyTorch、PyTorch Lightning、DDP/FSDP、Slurm、Linux、Git、在线数据生成

教育背景

慕尼黑工业大学 计算机科学，理学博士；导师：*Nils Thuerey* *2022 - 至今*
研究方向：*AI for PDEs/Science*、物理基础模型、物理生成模型、可微物理模拟、物理信息神经网络

哈尔滨工业大学 动力工程及工程热物理，工学硕士 *2020 - 2022*
多物理场数值求解器开发、*OpenFOAM* 数值模拟与开发、电流体动力学；获优秀硕士论文

哈尔滨工业大学 能源与动力工程，工学学士 *2016 - 2020*
流体力学、传热学、工程热力学、计算流体力学；专业排名 ***3/146***

代表性研究与研发经历

PDE 基础模型

- 参与开发二维 PDE 基础模型 PDE Transformer, 并主导三维 PDE 基础模型**Tadpole**开发。
- 首次提出以自编码重构作为 PDE 基础模型的预训练目标，使得 Tadpole 成为首个支持**多种下游任务**的三维 PDE 基础模型。
- 设计在线仿真训练框架，在**无本地数据存储**的情况下实现约 **202 TB** 数据训练，支持高达 1024^3 网格推理（超过 **10 亿**自由度）。

物理约束的生成模型

- 首次提出将扩散式生成模型用于数值模拟的**不确定性量化**与代理建模，相关论文是将扩散模型应用于流动模拟的先驱工作之一。
- 提出冲突消解多任务优化框架 **ConFIG**，并将其应用于物理约束的生成模型建模。提出并设计基于 ConFIG 方法的物理约束流匹配和用于流场稀疏重建的物理约束扩散模型。
- 将 ConFIG 方法进一步拓展至其它应用，如物理信息神经网络，多目标学习及联邦学习。

TorchFSM：基于 PyTorch 的 GPU 可微 PDE 求解器 *https://qiauil.github.io/torchfsm/*

- 基于傅里叶谱方法，支持从梯度、对流等模块化算子构建 PDE 求解器，支持 **GPU 加速、三维批量仿真**。
- 支持**全流程自动微分**，易于接入机器学习框架用于在线数据生成、反问题和物理信息神经算子训练。

代表性学术成果

共 14 篇论文，其中 5 篇第一作者；Google Scholar h-index 10。

PDE 基础模型：

- **Q. Liu**, F. Koehler, B. Holzschuh, N. Thuerey. “Tadpole: Autoencoders as Foundation Models for 3D PDEs with Online Learning,” arXiv, 2026.（NeurIPS2026 在审）
- B. Holzschuh, **Q. Liu**, G. Kohl, N. Thuerey. “PDE-Transformer: Efficient and Versatile Transformers for Physics Simulations,” *ICML*, 2025.

物理约束的生成模型：

- **Q. Liu**, M. Chu, N. Thuerey. “ConFIG: Towards Conflict-free Training of Physics Informed Neural Networks,” *ICLR*, 2025. **Spotlight**
- **Q. Liu**, N. Thuerey. “Uncertainty-aware Surrogate Models for Airfoil Flow Simulations with Denoising Diffusion Probabilistic Models,” *AIAA Journal*, 2024.
- G. Baldan, **Q. Liu**, A. Guardone, N. Thuerey. “Physics vs Distributions: Pareto Optimal Flow Matching with Physics Constraints,” *ICLR*, 2026.
- M. Amorós-Trepat, L. Medrano-Navarro, **Q. Liu**, Luca Guastoni, N. Thuerey. “Guiding diffusion models to reconstruct flow fields from sparse data,” *Physics of Fluids*, 2026.（一二作均为所指导的硕士生）

专著：

- N. Thuerey, B. Holzschuh, P. Holl, G. Kohl, M. Lino, **Q. Liu**, P. Schnell, F. Trost. ”Physics-based Deep Learning,” Chapter 5: Probabilistic Learning, https://physicsbaseddeeplearning.org/.

主要荣誉

优秀硕士论文（2022）；国家奖学金（2021、2018）；全国流体力学学术会议青年优秀论文（2020）；优秀推免生专项一等奖学金（2020）；哈尔滨工业大学优秀毕业生（2020）；黑龙江省三好学生（2018）