CHENG-HAU YANG

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Professional Summary

Computational mechanics researcher at Argonne National Laboratory developing scalable finite-element methods and open-source scientific software. Research focuses on **immersed methods (SBM/SCZM)**, cohesive fracture, and multiphysics simulations, with recent work on **MOOSE–NEML2 integration** and **GPU-accelerated solid mechanics**. Experienced in numerical algorithms, MPI-based HPC, and scientific machine learning.

Employment, Research, and Other Activities

03/10/2025 – Present

Postdoctoral Appointee

Argonne National Laboratory, Applied Materials Division – Lemont, Illinois, USA

- **Shifted Cohesive Zone Method (SCZM):** Developed, validated, and upstreamed cohesive fracture capabilities in MOOSE for non-interface-fitted meshes, including geometric search, fast point classification, and shifted-interface formulations (MOOSE #31938, #33398, #33667).
- **MOOSE–NEML2 Integration:** Collaborated with Idaho National Laboratory researchers on the v3 migration, package/build infrastructure, and boundary/interface execution capabilities (MOOSE #34170, Marlin #198, MOOSE #34422).
- **GPU Computing:** Prototyped and benchmarked solid mechanics and NEML2 material updates with Kokkos/CUDA; enabled Jacobian-based automatic scaling for Kokkos kernels (MOOSE #33867).
- **Interface Robustness:** Improved distributed-mesh and cohesive-interface handling, boundary callbacks, and consistent Jacobians (MOOSE #32309, #33902, #34283).
- **Welding and Additive Manufacturing:** Improved workflows through subdomain restrictions, patch-based variable reinitialization for activated elements, and selective projection (MOOSE #30300, #30630, libMesh #4368, MOOSE #32385).
- **Weld Residual Stress:** Collaborated with INL researchers on crack-propagation simulations, including model setup, verification, and co-authorship of a technical report.

01/30/2025 – 03/09/2025

Independent Academic Activities Following Ph.D. Completion

Iowa State University – Ames, Iowa, USA

- Voluntarily revised manuscripts based on Ph.D. research prior to joining Argonne National Laboratory.

08/21/2023 – 12/28/2023

Ph.D. Resident (Curricular Practical Training)

X (formerly Google X), Google LLC – Mountain View, California, USA

- **Parasitic Extraction (PEX):** Developed parallel PDE solvers using deal.II and MPI. Replaced Gmsh-based meshing with a Protocol Buffers workflow to eliminate redundant meshing and improved code reliability using GoogleTest.
- **Geometry Optimization:** Developed a remeshing-free optimization method, improving scalability and reducing iteration time by **50%**.

01/2021 – 01/2025

Computational Physics Research Assistant – ComPM Lab

Iowa State University – Ames, Iowa, USA

- **SBM – Numerical Methods:** Developed and extended immersed finite element methods for complex geometries without body-fitted meshing. Improved numerical accuracy by **50%** through optimized surrogate boundary selection.
- **SBM – High-Performance Computing:** Scaled simulations to **1,280 MPI processes** and **billions of degrees of freedom**. Accelerated geometric distance calculations by **10×** using k-d trees.
- **SBM – Multiphysics Applications:** Extended SBM to turbulent and thermal flows, adaptive mesh refinement, and thin-shell geometries, expanding its applications to large-scale multiphysics simulations.
- **Finite Cell Method:** Implemented parallel octree-based FEM for linear elasticity using MPI, validating von Mises stress against Abaqus.
- **Non-Newtonian Two-Phase Flow:** Simulated coupled Navier–Stokes/Cahn–Hilliard flows and modeled non-Newtonian viscosity using PyTorch neural networks.
- **Fluid Flow and Heat Transfer:** Investigated vegetation effects on building heat transfer and developed Nusselt number

correlations using Bayesian optimization.
- **Geometry Processing:** Developed an automated Grasshopper framework for molecular geometry generation and van der Waals volume calculations.

08/2019 – 01/2021

Computational Physics Research Assistant – CFSI Lab

Iowa State University – Ames, Iowa, USA

- **Heart Valve FSI:** Simulated bioprosthetic heart valves using FEniCS and extended an in-house IMGA framework for one-way coupled left ventricular simulations.
- **TAVR and Structural Modeling:** Automated mesh generation and refinement, including the connection of 200+ surface patches using Grasshopper.
- **Leaflet Flutter:** Investigated structural effects on leaflet flutter, identifying bending stiffness as a dominant factor.

09/2018 – 08/2019

Research Assistant, Applied Mathematics

National Chiao Tung University – Hsinchu, Taiwan

- **Stokes Flow and FSI:** Implemented finite element solvers for the Stokes equations and one-way coupled fluid–structure interaction (FSI) from scratch in MATLAB.

Education

08/2019 – 01/2025

Ph.D., Mechanical Engineering; Minor in Applied Mathematics

Iowa State University – Ames, Iowa, USA

GPA: 3.93/4.00; Dean Fellowship recipient.

07/2014 – 06/2016

M.S., Mechanical Engineering

National Taiwan University – Taipei, Taiwan

GPA: 3.92/4.30.

09/2010 – 06/2014

B.S., Mechanical Engineering

National Cheng Kung University – Tainan, Taiwan

GPA: 3.80/4.00; ranked 2nd of 59.

Science and Technology Specialties

Core research: **Shifted Boundary Method (SBM)**, **Shifted Cohesive Zone Method (SCZM)**, immersed FEM, fracture/interface mechanics, crystal plasticity, CFD, FSI, and multiphysics modeling.

Computational methods: Adaptive octree meshes, adaptive refinement, numerical PDE solvers, MPI/OpenMP, GPU-accelerated solid mechanics, and NEML2 constitutive integration.

Additional expertise: Thermal/fluid sciences, scientific machine learning, neural networks, Bayesian optimization, and geometric modeling.

Technical Skills

- Programming: C, C++, Fortran, Julia, Python, and MATLAB
- Mesh generation tools: ANSA, Gmsh, Netgen, and DistMesh
- CAD Design Software: AutoCAD, SOLIDWORKS, Rhino, and Grasshopper
- Simulation Software: ANSYS Fluent, COMSOL, and Abaqus
- Visualization tools: Tecplot and ParaView
- Scientific computing and HPC: MOOSE, libMesh, NEML2, PETSc, deal.II, MPI, OpenMP, Kokkos, CUDA, and PyTorch
- Build Systems: CMake and Make
- Containers: Docker and Apptainer (Singularity)
- Version Control: Git, GitHub, and Bitbucket

Honors and Awards

- **Robert J. Melosh Medal for Best Student Paper in Finite Element Analysis**, Duke University, 2025
- Research Excellence Award, Iowa State University 2025
- USACM Travel Award, U.S. Association for Computational Mechanics 2024
- NATPA 2021 Poster Award, North America Taiwanese Professors' Association 2021
- Dean Fellowship (Appointed as a Graduate Dean Scholar), Iowa State University 2019
- Outstanding Student Award for Academic Achievement*2, National Cheng Kung University 2011,2012
- Remarkable Achievement Award for Calculus Contest, National Cheng Kung University 2011
- Taipower Scholarship, Taiwan Power Company 2011-2016

Selected Publications

1. **Yang CH**, Messner MC, Hu T. **A shifted cohesive-zone method for non-interface-fitted meshes with applications to crystal plasticity.** *Computer Methods in Applied Mechanics and Engineering*. 2026;461:119259. doi:10.1016/j.cma.2026.119259.
2. Karki S, Shadkhah M, **Yang CH**, Balu A, Scovazzi G, Krishnamurthy A, Ganapathysubramanian B. Direct flow simulations with implicit neural representation of complex geometry. *Computer Methods in Applied Mechanics and Engineering*. 2025;446:118248. doi:10.1016/j.cma.2025.118248.
3. **Yang CH**, Saurabh K, Scovazzi G, Canuto C, Krishnamurthy A, Ganapathysubramanian B. **Optimal surrogate boundary selection and scalability studies for the shifted boundary method on octree meshes.** Computer Methods in Applied Mechanics and Engineering. 2024 Feb 1;419:116686.
4. **Yang CH**, Scovazzi G, Krishnamurthy A, Ganapathysubramanian B. **Simulating incompressible flows over complex geometries using the shifted boundary method with incomplete adaptive octree meshes.** Journal of Computational Physics. 2025 Sep 8; 114334.
5. **Yang CH**, Scovazzi G, Krishnamurthy A, Ganapathysubramanian B. **A shifted boundary method for thermal flows.** Journal of Computational Physics. 2025 Oct 17;114333.
6. **Yang CH**, Scovazzi G, Krishnamurthy A, Ganapathysubramanian B. Octree-based adaptive mesh refinement and the shifted boundary method for efficient fluid dynamics simulations. Advances in Computational Science and Engineering. 2025;4(0):57–84. doi:10.3934/acse.2025012.
7. Tali R, Rabeh A, **Yang CH** (co-first author), Shadkhah M, Karki S, Upadhyaya A, Dhakshinamoorthy S, Saadati M, Sarkar S, Krishnamurthy A, Hegde C, Balu A, Ganapathysubramanian B. FlowBench: A Large Scale Benchmark for Flow Simulation over Complex Geometries. *Data-centric Machine Learning Research*. 2025. [Project Page] [arXiv]
8. Tan K, Gao B, **Yang CH**, Johnson EL, Hsu MC, Passalacqua A, Krishnamurthy A, Ganapathysubramanian B. A computational framework for transmission risk assessment of aerosolized particles in classrooms. Engineering with Computers. 2024 Feb;40(1):235-56.
9. Johnson EL, Rajanna MR, **Yang CH**, Hsu MC. Effects of membrane and flexural stiffnesses on aortic valve dynamics: identifying the mechanics of leaflet flutter in thinner biological tissues. Forces in mechanics. 2022 Feb 1;6:100053.
10. Xu F, Johnson EL, Wang C, Jafari A, **Yang CH**, Sacks MS, Krishnamurthy A, Hsu MC. Computational investigation of left ventricular hemodynamics following bioprosthetic aortic and mitral valve replacement. Mechanics Research Communications. 2021 Mar 1;112:103604.
11. Heisler E, **Yang CH**, Deshmukh A, Ganapathysubramanian B, Sundar H. Generating Finite Element Codes combining Adaptive Octrees with Complex Geometries. arXiv preprint arXiv:2305.19398. 2023 May 30.
12. Shadkhah M, **Yang CH**, Karki S, Ganapathysubramanian B. Octree-Based Shifted Boundary Method: Evaluating the Impact of Hanging-Node Removal on Convergence and Solver Performance for Linear PDEs. Advances in Computational Science and Engineering, 4, pp.119-141.
13. Shadkhah M, Tali R, Rabeh A, **Yang CH** (co-second author), Herron E, Upadhyaya A, Krishnamurthy A, Hegde C, Balu A, Ganapathysubramanian B. MPF-Bench: A Large Scale Dataset for SciML of Multi-Phase-Flows: Droplet and Bubble Dynamics. *Data-centric Machine Learning Research*. [Project Page]

Technical Reports

1. **Yang CH**, Messner MC, Hu T. Non-conformal interface-cohesive modeling with the shifted boundary method. Argonne National Laboratory, ANL-26/22, 2026. doi:10.2172/3422582.
2. Munday LB, Spencer BW, Hu T, Barua B, **Yang CH**. Integrated Simulation of Weld Residual Stress Evolution and Crack Propagation Using XFEM. Idaho National Laboratory, INL/RPT-26-93507, 2026. doi:10.2172/3391368.
3. **Yang CH**, Messner MC, Hu T. Improved Weld Residual Stress Modeling System in BlackBear. Argonne National Laboratory, ANL-25/23, 2025. OSTI:2583685.

Selected Presentations

1. **Yang CH**. From Geometry to Physics without Boundary-Fitted Meshing: Multiphysics Simulation on Complex Domains. *Invited seminar*, USACM Student Chapter Seminar Series, May 19, 2026. Seminar announcement.
2. **Yang CH**. Shifted Cohesive-Zone Method with Applications to Crystal Plasticity and Thermal Contact. *Contributed presentation*, 20th U.S. National Congress on Theoretical and Applied Mechanics (USNCTAM 2026), Pasadena, California, June 2026. Presentation post.
3. **Yang CH**. Multiphysics Simulations of Flow Over Complex Geometries Using an Octree-based Shifted Boundary Method. Robert J. Melosh Medal Competition for the best student paper on Finite Element Analysis, 2025.
4. **Yang CH**, Scovazzi G, Krishnamurthy A, Ganapathysubramanian B. Shifted Boundary Method for flow simulations over complex objects, World Congress on Computational Mechanics, 2024.
5. **Yang CH**, Saurabh K, Scovazzi G, Krishnamurthy A, Ganapathysubramanian B. Optimal surrogate boundary of complex CAD models for solving PDEs using the shifted boundary method, US National Congress on Computational Mechanics, Page 1090, 2023.
6. **Yang CH**, Saurabh K, Sundar H, Krishnamurthy A, Ganapathysubramanian B. Massively parallel implementation of the finite cell method on incomplete octrees, US National Congress on Computational Mechanics, Page 785, 2021.
7. **Yang CH**, Khanwale M, Saurabh K, Sundar H, Krishnamurthy A, Ganapathysubramanian B. Two-phase simulation of 3D pulsating jet breakup using the scalable adaptive finite element method, CoMFRE conference, 2021.

Professional Service

Peer Reviewer, Scientific Journals: *ACM Computing Surveys*; *Journal of Computational Physics*; *Computational Mechanics*; *Archives of Computational Methods in Engineering*; *Engineering with Computers*; *Journal of Mechanics*; *Advances in Computational Science and Engineering*; *Applied Mathematical Modelling*; and *Computer Physics Communications*. ORCID review record.