Reflective Statement of Cheng-Hau Yang

During my doctoral studies under the supervision of Dr. Baskar Ganapathysubramanian and Dr. Adarsh Krishnamurthy, my research has been predominantly focused on computational engineering. In particular, I have had the chance to work on computational structural dynamics (CSD), computational fluid dynamics (CFD), fluid-structure interaction (FSI), thermofluidic analysis, and non-Newtonian fluid mechanics. My expertise in partial differential equations (PDEs) and numerical methods also earned me the opportunity to work as a PhD resident at **Google X**, focusing on parasitic extraction simulations using PDEs. My doctoral work has spanned three primary avenues:

Solving PDEs on Irregular Geometries

A significant part of my graduate research has focused on solving partial differential equations (PDEs) on irregular domains. In computational mechanics generating boundary-fitted meshes can be labor-intensive. Immersed methods address this issue by placing complex geometries directly into a regular, axis-aligned mesh, thereby avoiding the need for dynamic boundary-conforming mesh generation.

My research covers two principal immersed methods:

- **Finite Cell Method (FCM) or Immersogeometric Analysis (IMGA):** Nitsche-based enforcement of boundary conditions directly on the true geometry.
- **Shifted Boundary Method (SBM):** Weakly enforces Dirichlet conditions on a nearby surrogate boundary, with Taylor expansions accounting for geometric discrepancies.

Finite Cell Method (FCM) Framework

Early in my PhD, I accelerated FCM—an immersed method that uses Nitsche's formulation instead of delta-function forcing. I developed a massively parallel, octree-based FCM solver (hosted on Bitbucket), demonstrating:

- Excellent scalability on multiple processors.
- Precise von Mises stress distributions on complex geometries, closely matching Abaqus.

I presented these results at *USNCCM 2021*.

I also extended Immersogeometric Analysis (IMGA) to fluid-structure interaction, applying it to left ventricles and bioprosthetic heart valves. These simulations showed how reduced bending stiffness induces leaflet flutter, yielding co-authored publications in *Mechanics Research Communications* and *Forces in Mechanics*.

Shifted Boundary Method (SBM) Development

A pivotal milestone in my research was the collaboration with Professor Guglielmo Scovazzi (Duke University), the inventor of SBM. I integrated SBM into an octree-based framework to handle a wide range of PDE problems efficiently. In addition to easing the implementation for complex geometries (closed or open boundaries), I significantly improved the solver's computational efficiency by:

- **Implementing vorticity-based AMR:** Reduced the total mesh node count by a factor of **7**.
- **Developing a linear semi-implicit solver for incompressible flow:** Avoids solving nonlinear Navier-Stokes at every time step, making simulations **2.5× faster**.

Dataset and Open-Source Contributions

The SBM simulation framework I developed produced a dataset of over 10,000 simulations, currently hosted on Hugging Face for the Scientific Machine Learning (SciML) community. A detailed explanation of the dataset and accompanying machine learning results are provided on ArXiv (I am a co-first author), with a journal submission forthcoming.

My key Contributions with SBM

Optimal surrogate boundary selection: Reduced errors by 90%.
First application of Octree-SBM for incompressible flow in a large-scale parallel setting **(video link)**.
First application of Octree-SBM to thermal incompressible flow.
First demonstration of combining SBM with vorticity-based AMR in both incompressible and thermal flows **(video link)**.
First extension to thin-shell geometries (video link) , resolving blockage effects and eliminating the penalty approach in IMGA.
First proof of scalability for SBM on more than 1000 processors.

These results are documented in three first-author papers: one published in *Computer Methods in Applied Mechanics and Engineering (CMAME)* and two on arXiv: *NS* and *NSHT* (both submitted to the *Journal of Computational Physics (JCP)*). I also presented these findings at two prestigious international conferences, *USNCCM2023* and *WCCM2024*, underscoring their importance to the field.

Future Directions

Looking ahead, a number of compelling directions merit further exploration:

- **Higher-Order Basis Functions:** Incorporate higher-order polynomial expansions into the finite element basis for greater numerical accuracy.
- **AMR Integration:** Combine the SBM with adaptive mesh refinement (AMR) to address multiphysics problems such as Navier–Stokes–Cahn–Hilliard and Poisson–Nernst–Planck.
- **Adaptive Error Estimation:** Develop a residual-based *a posteriori* error estimator to enable automatic, efficient mesh refinement driven by elementwise error measurements, rather than manually setting vorticity thresholds.
- **Thin-Shell Extensions:** Extend the thin-shell Octree-SBM framework to handle moving and deforming thin-shell geometries (e.g., heart valves, parachutes), and ultimately apply Octree-SBM to fluid–structure interaction (FSI) simulations.

Navier-Stokes and Heat Transfer Coupled Building Simulation

I was also part of the Iowa UrbanFEWS project, a collaborative research effort spanning multiple departments at Iowa State University and beyond. The primary goal is to enhance urban sustainability in rain-fed agricultural regions, like Des Moines, through greater self-reliance in food, water, and energy systems. Traditional building energy simulations (BES) integrate computational fluid dynamics (CFD) to refine heat-consumption estimates, but face three main challenges:

1. Many models overlook the impact of trees on energy usage,
2. Flow and heat effects often remain decoupled,
3. Direct CFD-based calculations in BES are prohibitively time-consuming.

To address these issues, I developed advanced CFD and heat-transfer models that explicitly account for tree placement in front of buildings, including canopy size, wind speed, and ground temperature. By applying linear semi-implicit Navier–Stokes equations, backflow stabilization, and variational multiscale formulations, my approach remains robust under both laminar and turbulent conditions. I also introduced a Bayesian-optimized Nusselt number correlation, significantly reducing runtime by using machine learning surrogates instead of full CFD. Additionally, we adapted this tree-excluded, SBM-excluded framework to study aerosolized particle transmission during COVID-19, with our results published in *Engineering with Computers*.

My Contributions

- **BES Coupling with Thermal Incompressible Flow (NS–HT):** Developed a unified approach that captures both flow and heat transfer beyond purely CFD-based methods.
- **CFD Models for Tree Effects:** Incorporated wind-blocking and evapotranspiration from trees—critical factors often overlooked in prior building simulations.
- **Efficient CFD Corrections in BES:** Established a correction model (trained via CFD) accessible through a lookup table, drastically lowering total simulation time by avoiding repeated, high-cost CFD computations.

Future Directions

Looking ahead, key steps include validating the Nusselt number correlation against experimental data to further refine the simulation models and enhance predictive accuracy in real-world urban settings.

Projection-Based Non-Newtonian Cahn-Hilliard Navier-Stokes Solver

I initially focused on pulsating-jet simulations **(video link)** in two-phase Newtonian flows, which were presented at the 2021 CoMFRE Conference. Building on these results, I explored the largely uncharted territory of extending the Cahn–Hilliard–Navier–Stokes (CHNS) model to non-Newtonian fluids. By training a PyTorch neural network on experimental data from Professor Chabinyc's lab at UCSB, I avoided separate ODE/PDE integrations or cumbersome curve-fitting. The resulting 2D simulations showed strong agreement with experimental observations, validating the effectiveness of this integrated approach.

My Contributions

- **Non-Newtonian CHNS Solver Development:** Extended the CHNS framework to incorporate non-Newtonian effects, rigorously tested through canonical benchmarks.
- **Neural Network Constitutive Modeling:** Employed PyTorch to learn strain-rate and viscosity relationships from UCSB's experimental data, bypassing separate ODE/PDE integrations and complex curve-fitting.
- **High-Fidelity Experimental Matching:** Demonstrated close agreement between numerical predictions and experimental measurements, validating the robustness of the approach.

Future Directions

We aim to expand our non-Newtonian CHNS work into 3D simulations using the constitutive equations developed in PyTorch. This will enable us to perform more detailed and accurate comparisons with experimental data from UCSB.