SHOAIB AHMAD GORAYA

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RESEARCH SUMMARY

I am interested in developing numerical methods for coupled multiphysics problems. Specifically, I have worked on stabilized finite element methods for variational coupling between Navier-Stokes equations and scalar transport equations. The scalar field is either temperature, concentration of chemical species, or signed-distance field. The fundamental nature of these methods makes them suitable for application in broad areas of smart and sustainable infrastructure, fluid dynamics, precision medicine, and energy efficient engineering systems. The classes of problems involve multiple interacting physical phenomena that span a spectrum of spatial, material, and temporal scales, and thus require simulation tools that are mathematically rigorous and computationally robust. I have developed a computational framework for vascular targeted drug delivery, a stabilized finite element method for multiphase flows, a data-driven variational method for discrepancy modeling of physical systems, and a physics informed neural network for thermofluids. By leveraging high performance computing, these methods are becoming an increasingly important frontier of computational mechanics as the complexity and multi-disciplinary nature of scientific problems grows in future.

EDUCATION

University of Illinois Urbana-Champaign (UIUC) Expected August 2024
Ph.D. in Computational Mechanics
Advisor: Prof. Arif Masud

University of Illinois Urbana-Champaign August 2019
M.Sc. in Civil Engineering
Concentration: Computational Science and Engineering

University of Engineering and Technology (UET) Lahore, Pakistan August 2015
B.Sc. in Civil Engineering

RESEARCH EXPERIENCE

University of Illinois Urbana-Champaign September 2017 - Present
Graduate Research Assistant Urbana, IL

Variational Multiscale Method for Buoyancy-Induced Natural Convection in Thermofluids

- Developed a stabilized numerical method for Navier-Stokes equations coupled with convection-diffusion equation for buoyancy-induced thermal convection.
- The formulation preserves cross-coupling effects of mechanical and thermal fields through a variationally derived stabilization tensor.
- The method yielded optimal mathematical convergence rates across different spatial and temporal discretizations as well as quadratic convergence in the iterative solution of nonlinear coupled system of equations.
- Simulations provided insights into explaining the underlying physical mechanisms observed in the experiments and enhancing the capabilities of the thermal management devices such as heat exchangers.

Computational Framework for Vascular Targeted Drug Delivery

- Developed a stabilized finite element method for targeted drug delivery via nano-carriers in blood vessels.
- Simulated drug transport, adhesion, and retention at the targeted site in patient-specific geometries.
- Investigated effect of circadian rhythm modulated blood flow on drug delivery *in vivo* using shear-rate dependent blood flow model.

Physics Informed Neural Networks for Thermofluids

- Proposed a physics-informed augmentation in neural network for thermally coupled incompressible Navier-Stokes equations that resulted in an order of magnitude increase in the accuracy of pressure field prediction.
- Conducted convergence rate study and computed error estimates for the proposed machine learning model.

Algorithmic Flattening of Virtual Heart Patches for Surgical Patching

- Developed a mechanics-based algorithm for the 2D flattening of a 3D heart patch, which is cut out from a patient-specific model in virtual reality by a surgeon.

- The flattened 2D geometry provides surgeons the precise size and shape of the patch to be replaced with biocompatible material before the surgical procedure, thereby reducing the need for time-consuming trial and error.

Stabilized Finite Element Method for Multiphase Flows

- Developed a novel interface-capturing method for multiphase flows with large-amplitude free-surface motion.
- Employed variational multiscale (VMS) framework to derive interfacial terms by embedding level-set equation in the momentum balance equations via material properties dependency on the signed distance field.
- Simulated free surface flows such as dam break, free-falling water jet, and tank sloshing.

Variational Method for Data Assimilation in Modeling of Physical Systems

- Developed a method that embeds computational intelligence in modeling and analysis of physical systems through data assimilation using finite element variational multiscale discontinuous Galerkin framework.
- First-principle based model is augmented with variational loss function that results in forward simulations of dynamical systems wherein high-fidelity sensor data compensates for discrepancy in model parameters.
- The method was applied to time-dependent solid mechanics problems involving nonlinear elasticity and viscoelasticity.
- The approach effectively addresses modeling uncertainties in underlying physics, material parameters, and boundary conditions by matching model prediction with actual observed behavior of the systems.

Large Eddy Simulations (LES) of Incompressible Turbulent Flows

- Carried out large eddy simulations of isotropic turbulence, stratified turbulence, and separated-reattached turbulent flows using a variationally derived closure model.

TEACHING EXPERIENCE

University of Illinois Urbana-Champaign — August 2019 - May 2022
Graduate Teaching Assistant — Urbana, IL

Delivered class lectures, conducted office hours, designed and graded homeworks as well as exams for the following graduate level courses:

- Spring 2022 CEE 474 Mechanics of Additive Manufacturing (Ranked **Excellent** by students)
- Spring 2021 CSE 553 Computational Inelasticity (Ranked **Excellent** by students)
- Fall 2019 CSE 552 Nonlinear Finite Element Methods

AWARDS AND HONORS

2022	Burton & Erma Lewis Teaching **Fellowship**, UIUC, Urbana IL.
2021, 2022	Teacher Ranked as **Excellent** by Students (Spring 2021, Spring 2022), Center for Innovation in Teaching & Learning, UIUC, Urbana IL.
2021	Mavis Future Faculty **Fellowship**, UIUC, Urbana IL.
2019	Jacob Karol Estate **Fellowship**, UIUC, Urbana IL.
2017	Fulbright **Scholarship**, Department of State, Washington DC.
2016	**LEAD Fellow**, Leadership Development Program on Urban Resilience & Sustainable Cities, Pakistan.
2012-2015	5 **Dean's Honor Rolls**, UET Lahore, Pakistan.
2015	**Best Senior Year Project** Poster (out of 60 projects), UET Lahore, Pakistan.
2011-2015	UET Merit **Scholarship**, UET Lahore, Pakistan.
2011	National Talent **Scholarship**, Pakistan.

TRAVEL AWARDS

2024	United States Association of Computational Mechanics (USACM) Travel Award.
2024	Graduate College Conference Presentation Award, UIUC, Urbana IL.
2020	CEE Structures Student Travel Award, UIUC, Urbana, IL.
2018	13th World Congress on Computational Mechanics (WCCM), July 2018, NYC NY.

TECHNICAL STRENGTHS

Programming	FORTRAN, Python, Bash, C++, MPI, PETSc
Software Tools	Visual Studio Code, Git, MATLAB, PyTorch, FEAP, ParaView, ABAQUS, GNU Debugger, SLURM, PBS, Gmsh, Linux, LaTeX

PUBLICATIONS

[9] **S.A. Goraya**, S. Ding, R.C. Miller, M.K. Arif, H.J. Kong, and A. Masud, "Modeling of spatiotemporal dynamics of ligand-coated particle flow in targeted drug delivery processes", *Proceedings of the National Academy of Sciences*, (In press 2024).

[8] A. Masud and **S.A. Goraya**, "Data-driven variational method for discrepancy modeling: Dynamics with small-strain nonlinear elasticity and viscoelasticity", *International Journal for Numerical Methods in Engineering*, (In press 2024).

[7] **S.A. Goraya**, S. Ding, M.K. Arif, H.J. Kong, and A. Masud, "Effect of circadian rhythm modulated blood flow on nanoparticle-based targeted drug delivery *in vivo*", (*Submitted to Brain Multiphysics, 2024*).

[6] **S.A. Goraya**, N. Sobh, and A. Masud, "Error estimates and physics informed augmentation of neural networks for thermally coupled incompressible Navier Stokes equations", *Computational Mechanics* (2023): 1-23.

[5] A. Masud, S. Nashar, and **S.A. Goraya**, "Physics-constrained data-driven variational method for discrepancy modeling", *Computer Methods in Applied Mechanics and Engineering*, 417 (2023): 116295.

[4] L. Zhu, **S.A. Goraya**, and A. Masud. "A variational multiscale method for natural convection of nanofluids", *Mechanics Research Communications* 127 (2023): 103960.

[3] **S.A. Goraya**, L. Zhu, and A. Masud, "Stabilized finite element method for transient thermal convection of nanofluids: effects of irregular geometries and electromagnetic force field", (*Submitted 2023*).

[2] A. Masud and **S.A. Goraya**, "Variational embedding of measured data in physics-constrained data-driven modeling", *Journal of Applied Mechanics* 89, no. 11 (2022): 111001. [**Nominated for best JAM paper between 2021 and 2023**].

[1] L. Zhu, **S.A. Goraya**, and A. Masud, "Interface-capturing method for free-surface plunging and breaking waves", *Journal of Engineering Mechanics* 145, no. 11 (2019): 04019088.

PUBLICATIONS IN PROGRESS

[3] **S.A. Goraya**, S. Ding, H.J. Kong, and A. Masud, "Using deep learning and mixture theory to predict drug profusion and tissue growth in targeted drug delivery processes".

[2] **S.A. Goraya** and A. Masud, "Variational multiscale method for void evolution and transport in process modeling of polymer materials".

[1] **S.A. Goraya** and A. Masud, "Large eddy simulations of turbulent-laminar transition flows using a variationally derived closure model".

CONFERENCE PRESENTATIONS

[8] **S.A. Goraya** and A. Masud, "Variational multiscale method for void evolution and transport in process modeling of polymer materials", 16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics (WCCM-PANACM), Vancouver, July 2024.

[7] **S.A. Goraya**, S. Ding, R.C. Miller. M.K. Arif, H.J. Kong, and A. Masud, "Effect of circadian rhythm modulated blood flow on nanoparticle based targeted drug delivery *in vivo*", Engineering Mechanics Institute (EMI) Conference, Chicago, May 2024.

[6] **S.A. Goraya**, S. Ding, R.C. Miller. M.K. Arif, H.J. Kong, and A. Masud, "A unified computational framework for predictive multiscale modeling in targeted drug delivery and tissue growth", Society of Engineering Science (SES), Minneapolis, October 2023.

[5] **S.A. Goraya**, N. Sobh, and A. Masud, "Physics informed augmentation of neural networks for thermally coupled incompressible Navier Stokes Equations", SES – Frontiers Matter, October 2021.

[4] **S.A. Goraya**, N. Sobh, and A. Masud, "BeltramiNet: A deep forward neural network for predicting the solution of thermally coupled steady state incompressible Navier Stokes equations", 16th U.S. National Congress on Computational Mechanics (USNCCM), July 2021.

[3] **S.A. Goraya**, M. Bramlet, B.P. Sutton, and A. Masud, "Algorithmic flattening of virtual heart patch for surgical patching", 7th Healthcare Engineering Systems Symposium, October 2020.

[2] **S.A. Goraya**, L. Zhu, and A. Masud, "Residual-based turbulence for large amplitude free-surface waves", Illinois Structural Engineering Conference, Champaign, April 2019.

[1] **S.A. Goraya**, K.R. Usman, and R. Hameed, "Shear damage modeling of RC Beams using a simplified approach to model steel-concrete interface", 9th International Conference on Fracture Mechanics of Concrete and Concrete Structures (FraMCos-9), Berkeley, June 2016.

SERVICE

Mentoring & Advising

- Sharbel Nashar (PhD student, UIUC)
- Sitanan Tainpakdipat (MS student, UIUC)

Journal Referee

- International Journal for Multiscale Computational Engineering

Scientific Events

- Technical Coordinator for 16th US National Congress on Computational Mechanics (USNCCM), July 2021

Outreach

- SEGSO Buddy Program: Guided incoming graduate students to CEE UIUC, Fall 2021
- Math tutor at SOS Children's Villages Pakistan, May-August 2014

GRANT PROPOSALS

Contributed to the following technical proposals for computational resources on high-performance computing platforms:

2023 **NSF TG-DMS100004:** Immersed Boundary Methods for Modeling of Complex Geometry - Data-Driven Modeling of Subgrid Scale Physics in Variational Multiscale based Large Eddy Simulations. [$40,000]

2023 **ACCESS EES230063:** Advanced Open Boundary Conditions, Coupled Multi-Model Method, and PINNs, for Application in Climate Modeling and Simulation.

2022 **NSF TG-DMS100004:** Physics- and Data-Driven Modeling of Blood-Artery Interaction: Aortic Dissection and Brain Hemorrhage [$35,000]

REFERENCES

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