Muhammad Hassan

Postdoctoral Researcher
Chair of High Performance Numerical Algorithms and Simulations
École Polytechnique Fédérale de Lausanne
MA C1 557, CH-1015 Lausanne

Email: muhammad.hassan@epfl.ch
Webpage: https://prometheus-1757.github.io
Orcid ID: 0000-0002-7582-6670
Cellphone: +41 76 366 89 21

Research Interests

• Numerical methods for electronic structure calculations • Linear and non-linear eigenvalue problems
• Variational quantum eigensolvers • Boundary integral equations • Domain decomposition methods

Academic Appointments

École Polytechnique Fédérale de Lausanne, Switzerland.

- Postdoctoral researcher (October 2023-Present).
- Mentor: Prof. Dr. Laura Grigori.

Laboratoire Jacques-Louis Lions, Sorbonne Université, France.

- Postdoctoral researcher (November 2020-September 2023).
- Research funded by the EMC2 European Research Council Synergy Project.
- Mentor: Prof. Dr. Yvon Maday.

Education

RWTH Aachen University, Germany.

- Dr. rer. nat. in Mathematics (July 2020).
- Dissertation: Mathematical Analysis of Boundary Integral Equations and Domain Decomposition Methods with Applications in Polarisable Electrostatics.
- Advisor: Prof. Dr. Benjamin Stamm.

ETH Zürich, Switzerland.

- Master of Science in Applied Mathematics (April 2016).
- Thesis: Exploring the Carbuncle Phenomenon in Hypersonic Flows using the Framework of Entropy Measure Valued Solutions.
- Advisor: Prof. Dr. Siddhartha Mishra.

Publications and Preprints

13. **Analysis of the Single Reference Coupled Cluster Method for Electronic Structure Calculations: The Discrete Coupled Cluster Equations**
(joint with Y. Maday, and Y. Wang).
Submitted. Preprint

12. **Greedy Gradient-free Adaptive Variational Quantum Algorithms on a Noisy Intermediate Scale Quantum Computer**
(joint with C. Feniou, B. Claudon, A. Courtat, O. Adjoua, Y. Maday, and J.-P. Piquemal).
Submitted. Preprint

11. **Continuity estimates for Riesz potentials on polygonal boundaries**
(joint with X. Claeys and B. Stamm).
Under review. Preprint

10. **Analysis of the Single Reference Coupled Cluster Method for Electronic Structure Calculations: The Full Coupled Cluster Equations**
(joint with Y. Maday, and Y. Wang).
Numerische Mathematik 155 (2023), pp. 121-173. Article

9. **Overlap-ADAPT-VQE: Practical Quantum Chemistry on Quantum Computers via Overlap-Guided Compact Ansätze**
(joint with C. Feniou, D. Traoré, E. Giner, Y. Maday, and J.-P. Piquemal).
Communications Physics 6, 192 (2023). Article, Behind-the-Paper Blog.
Selected as an Editor's Highlights 2023 ($\approx 3\%$ of published articles).

8. **Modified-operator method for the calculation of band diagrams of crystalline materials**
(joint with E. Cancès and L. Vidal).
Mathematics of Computation (2023). Article

7. **Manipulating particle interactions with electric fields and point charges: A general electrostatic many-body framework**
(joint with C. Williamson, J. Baptiste, S. Braun, A. Stace, E. Besley, and B. Stamm).
Journal of Chemical Theory and Computation 18.10 (2022), pp. 6281-6296. Article

6. **The influence of surface charge on the coalescence of ice and dust particles in the mesosphere and lower thermosphere**
(joint with J. Baptiste, C. Williamson, J. Fox, A. Stace, S. Braun, B. Stamm, I. Mann, and E. Besley).
Atmospheric Chemistry and Physics 21 (2021), pp. 8735-8745. Article

5. **A Linear Scaling in Accuracy Numerical Method for Computing the Electrostatic Forces in the N-Body Dielectric Spheres Problem**
(joint with B. Stamm).
Communications in Computational Physics 29 (2021), pp. 319-356. Article

4. **An Integral Equation Formulation of the N-Body Dielectric Spheres Problem. Part II: Complexity Analysis**
(joint with B. Bramas and B. Stamm).
ESAIM: Mathematical Modelling and Numerical Analysis 55 (2021), pp. S625-S651. Article

3. **An Integral Equation Formulation of the N-Body Dielectric Spheres Problem. Part I: Numerical Analysis**
(joint with B. Stamm).
ESAIM: Mathematical Modelling and Numerical Analysis 55 (2021), pp. S65-S102. Article

2. **On the Scalability of the Schwarz Method**
(joint with G. Ciaramella, and B. Stamm.).
SMAI Journal of Computational Mathematics, 6 (2020), pp. 33-68. Article

1. **On the Scalability of the Parallel Schwarz Method in One Dimension**
(joint with G. Ciaramella, and B. Stamm.).
Domain Decomposition Methods in Science and Engineering XXV (2020), pp. 151-158. Article

Research Talks

28. *The Numerical Analysis of the Coupled Cluster Method for Electronic Structure Calculations.* Symposium on Sparsity and Singular Structures 2024, RWTH Aachen University, Germany, February 2023. **Invited Talk**.

27. *On Plane-wave Discretisations for Band Structure Calculations of Crystalline Materials.* Séminaire Analyse Appliquée (A3) du Laboratoire Amiénois de Mathématique Fondamentale et Appliquée, Université de Picardie Jules Verne, Amiens, France, February 2023. **Invited Talk**.

26. *On the Numerical Analysis of the Coupled Cluster Method in Computational Quantum Chemistry.* Seminar Talk, University of British Columbia, Canada, February 2023. **Invited Talk**.

25. *Numerical Methods for Ground-State Electronic Structure Calculations.* Colloquium Talk, University of British Columbia, Canada, February 2023. **Invited Talk**.

24. *Resource Saving Enhancements for Adaptive Variational Quantum Algorithms.* Annual Meeting of the 'Modelling, Analysis and Simulation of Molecular Systems' GAMM Activity Group, Universität Stuttgart, Germany, November 2023.

23. *Band Structure Calculations for Crystalline Materials using an Operator Modification Approach.* ERC EMC2 Seminar, Laboratoire Jacques-Louis Lions, Sorbonne Université, Paris France, September 2023. **Invited Talk**.

22. *Numerical Analysis of the Operator Modification Approach for the Calculation of Band Diagrams of Crystalline Materials.* Mini-symposium on Eigenvalue Problems in Electronic Structure Calculations, ICIAM 2023, Waseda University, Tokyo, Japan, August 2023. **Invited Talk**.

21. *Numerical Analysis of the Single-Reference Coupled Cluster Method in Quantum Computational Chemistry.* Numerical Analysis in the 21st Century, University of Oxford, United Kingdom, August 2023.

20. *On the Well-Posedness of the Discrete Single-Reference Coupled Cluster Equations.* Gesellschaft für Angewandte Mathematik und Mechanik (GAMM) Annual Meeting 2023, Technische Universität Dresden, Germany, June 2023.

19. *Quantitative Error Estimates for the Single-Reference Coupled Cluster Method in Quantum Computational Chemistry.* Séminaire du Laboratoire, Laboratoire Jacques-Louis Lions, Sorbonne Université, Paris France, March 2023. **Invited Talk**.

18. *Band Structure Calculations for Crystalline Materials using an Operator Modification Approach.* ANCS seminar, Laboratoire de Mathématiques de Besançon, Université Bourgogne Franche-Comté, Besançon, France, February 2023. **Invited Talk**.

17. *A New Well-Posedness Analysis for the Single-Reference Coupled Cluster Equations.* ERC EMC2 Seminar, Laboratoire Jacques-Louis Lions, Sorbonne Université, Paris France, October 2022.

16. *Modified-operator method for the calculation of band diagrams of crystalline materials.* Oberseminar, Institut für Angewandte Analysis und Numerische Simulation, Universität Stuttgart, Germany, October 2022. **Invited Talk**.

15. *Numerical Analysis of Integral Equations for N-body Polarisable Electrostatics.* 20^{th} Söllerhaus workshop on Fast Boundary Element Methods in Industrial Applications 2022, Kleinwalsertal, Austria, October 2022.

14. *Towards the development of a posteriori error analysis for the coupled cluster equations.* Gesellschaft für Angewandte Mathematik und Mechanik (GAMM) Annual Meeting 2022, RWTH Aachen University, Germany, August 2022.

13. *Towards the development of a posteriori error analysis for the coupled cluster equations.* IPAM 2022 Workshop III: Large-Scale Certified Numerical Methods in Quantum Mechanics, University of California, Los Angeles, United States, May 2022. **Invited Talk**. Video Recording

12. *On the Numerical Analysis of a Linear Scaling Method for the N-body Dielectric Spheres Problem.* Congrès d'Analyse Numérique pour les Jeunes, (Electronic), December 2020.

11. *Mathematical Analysis of Boundary Integral Equations with Applications in Polarisable Electrostatics.* Ph.D. Defence Talk, RWTH Aachen University, Germany, June 2020.

10. *Analysis of a Linear Scaling Algorithm for Calculating Electrostatic Interactions in N-body Dielectric Systems.* 2019 Annual Meeting of European SIAM and GAMM Student Chapters, RWTH Aachen University, Germany, September 2019.

9. *On the Scalability of the Schwarz Method.* Centre for Computational Engineering Science (MathCCES) Seminar, RWTH Aachen University, Germany, July 2019.

8. *Scalability Analysis of an Integral Equation Formulation of the Many-Body Dielectric Problem in Electrostatics.* MAFELAP 2019, Brunel University, London, United Kingdom, June 2019.

7. *Scalability Analysis of an Integral Equation Formulation of the Many-Body Dielectric Problem in Electrostatics.* Gesellschaft für Angewandte Mathematik und Mechanik (GAMM) Annual Meeting 2019, Technische Universität, Vienna, February 2019.

6. *Scalability Analysis of an Integral Equation Formulation of the Many-Body Dielectric Problem in Electrostatics.* Annual Meeting of the 'Modelling, Analysis and Simulation of Molecular Systems' GAMM Activity Group, Zuse Institute and Technische Universität Berlin, Germany, October 2018.

5. *On the Numerical Analysis of the Many-Body Dielectric Problem in Electrostatics.* Chair for Numerical Optimization Seminar, Universität Konstanz, Germany, September 2018.

4. *On the Numerical Analysis of the Many-Body Dielectric Problem in Electrostatics.* Franco-German Workshop on Mathematical Aspects of Computational Chemistry, RWTH Aachen University, Germany, September 2018.

3. *On the Numerical Analysis of the ddCOSMO Algorithm.* Chair for Numerical Optimization Seminar, Universität Konstanz, Germany, March 2018.

2. *On the Numerical Analysis of the ddCOSMO Algorithm.* Young Researchers Workshop on Mathematical Methods in Quantum Chemistry, Laboratoire Jacques-Louis Lions, Université Pierre-et-Marie-Curie, Paris, France, January 2017.

1. *Exploring the Carbuncle Phenomenon using the Framework of Entropy Measure Valued Solutions.* Centre for Computational Engineering Science (MathCCES) Seminar, RWTH Aachen University, Germany, February 2016.

Expository and Outreach Talks

5. *Discretisation strategies for band structure calculations.* Kressner and Grigori Group Seminar, EPFL, Switzerland, October 2023.

4. *An Introduction to Variational Quantum Eigensolvers.* EMC2 ERC Synergy Project Workshop on Quantum Computing, Roscoff, France, July 2023.

3. *The Quantum Fourier Transform.* Working group on numerical analysis and quantum computing (NumerIQ) bi-monthly seminar, Laboratoire Jacques-Louis Lions, Sorbonne Université, Paris, France, May 2023.

2. *Theorems, Proofs and Mathematical Beauty.* Research Club Maison de l'Inde, Cité Universitaire, Paris, France, April 2023.

1. *On the Approximation of Energy Bands in the Brillouin Zone.* IPAM 2022 Long Program on Quantum Mechanics seminar series, University of California Los Angeles, USA, April 2022.

Research Stays at External Institutions

5. *IPAM Long Program on Advancing Quantum Mechanics with Mathematics and Statistics.* University of California, Los Angeles, March 2022-June 2022 (3 months).

4. *Institut für Angewandte Analysis und Numerische Simulation.* Universität Stuttgart, Germany, October 2022, Host: Benjamin Stamm (1 week).

3. *Laboratoire Jacques-Louis Lions, Sorbonne Université.* Paris, France, October 2018, Host: Xavier Claeys (2 weeks).

2. *Chair for Numerical Optimization Seminar.* Universität Konstanz, Germany, March 2018 and September 2018, Host: Gabriele Ciaramella (4 days each).

1. *Laboratoire Jacques-Louis Lions, Sorbonne Université.* Paris, France, December 2017, Host: Yvon Maday (2 weeks).

Teaching Experience

EPF Lausanne

- Teaching Assistant, Analysis IV Math 207-(c) (Spring Semester 2024).

RWTH Aachen University

- Teaching Assistant, Mathematical Aspects of Computational Chemistry (Summer Semester 2016, 2017, 2018, 2019).
- Teaching Assistant, Partial Differential Equations (Winter Semester 2018, 2019).
- Teaching Assistant, Ordinary Differential Equations (Summer Semester 2019).
- Teaching Assistant, Analysis for Computer Science (Winter Semester 2017, **approx. 900 students**).
- Teaching Assistant, Mathematical Foundations II (Summer Semester 2016).
- Teaching Assistant, Mathematical Foundations I (Winter Semester 2016).

Supervision Experience

Graduate Thesis Co-supervision

- *Christian Bauer*: **Efficient solvers for computing the scalar magnetic potential for multiple spheres** RWTH Aachen University, 2017.

Graduate Semester Project Co-Supervision

- *Maddalena Detti*: **Factorized structure of the short-range two-electron integral tensor in quantum chemistry**, EPF Lausanne, 2024
- *Mario Drevers*: **The Crystallization Conjecture**, RWTH Aachen University, 2020
- *Hendrik Borchardt*: **Alternating Schwarz Method for solving Eigenvalue Problems by Inverse Power Iteration and Steepest Descent**, RWTH Aachen University, 2019

- *Lucia Baltz*: **Continuum Solvation Models**, RWTH Aachen University, 2019.
- *Lucia Baltz*: **Variational Markov-Chain Monte-Carlo Methods in the context of Computational Chemistry**, RWTH Aachen University, 2018.

Undergraduate Thesis Co-supervision

- *Pawel Bittner*: **Application of Grassmann Manifold Interpolation and Model Order Reduction to Eigenvalue Problems in Computational Chemistry**, RWTH Aachen University, 2019.

Additional

- Tutor for the annual CAMMP Week Pro mathematical modelling retreat in summer semesters 2017, 2018, and 2019 (RWTH Aachen University).

Organization and Service

Seminars, Mini-Symposia, Workshops and Reading Groups

- Organizer of a 3-day workshop on "Many-body methods for electronic structure calculations in solids" at the Bernoulli Center for Fundamental Sciences at EPF Lausanne (Scheduled for March 2024).
- Co-organizer with Michael Herbst of a reading group on electronic structure theory, a joint initiative of the Institute of Mathematics and the Institute of Materials at EPF Lausanne (January 2024- present).
- Co-organizer with Mi-Song Dupuy and Pierre Monmarché of the ERC Extreme-scale mathematically-based computational chemistry seminar (EMC2), a joint applied mathematics and computational chemistry seminar of the Laboratoire Jacques-Louis Lions and the Laboratoire de Chimie Théorique at Sorbonne Université (September 2022- August 2023).
- Co-organizer with Fabian Faulstich (UC Berkeley) of a mini-symposium on 'Recent advances in numerical methods for electronic structure calculations' at the 2023 SIAM Conference on Computational Science and Engineering in Amsterdam (February-March 2023).

Peer Review

- Reviewer for Zeitschrift für angewandte Mathematik und Physik (ZAMP), ESAIM: Mathematical Modelling and Numerical Analysis (M2AN), Electronic Transactions on Numerical Analysis (ETNA), Journal of Chemical Theory and Computation (JCTC), Journal of Computational Physics (JCOMP), SIAM Journal on Scientific Computing (SISC), Journal of Scientific Computing, AMS Mathematical Reviews, and zbMATH Open.

Grants, Scholarships and Travel Awards

- Awarded workshop organisation grant from the Bernoulli Center for Fundamental Studies in January 2024 (Total value: 10,000 CHF).
- Awarded full financial support to attend the IPAM long program on 'advancing quantum mechanics with mathematics and statistics' at UCLA from March 7th to June 12th, 2022 (Total value: $8700).
- Young Researcher Travel Grant for attending the annual meeting of the 'Modelling, Analysis and Simulation of Molecular Systems' GAMM Activity Group at the Zuse Institute and Technische Universität Berlin, Germany in October 2018.
- Awarded Fulbright scholarship in 2013 for graduate studies in the US (declined).