Muhammad Hassan

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Research Interests

• Numerical methods for electronic structure calculations • Linear and non-linear eigenvalue problems
• Hybrid quantum/classical algorithms • Domain decomposition methods • Boundary integral equations

Academic Appointments

Technische Universität München, Germany.

- Emmy Noether Junior Research Group Leader (July 2025-Present).

Paul Scherrer Institute, Switzerland.

- Tenure-Track Scientist (December 2024-June 2025).

École Polytechnique Fédérale de Lausanne, Switzerland.

- Postdoctoral researcher (October 2023-November 2024).
- 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

16. **An additive two-level parallel variant of the DMRG algorithm with coarse-space correction**
(joint with L. Grigori).
Under Review. Preprint

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

14. **Trace estimates for harmonic functions along circular arcs with applications to domain decomposition on overlapping disks**
(joint with T. C. Corso, A. Jha, and B. Stamm).
Accepted for publication in the SIAM Journal on Mathematical Analysis (2025). Preprint

13. **On the relation between Galerkin approximations and canonical best-approximations of solutions to some non-linear Schrödinger equations**
(joint with Y. Maday and Y. Wang).
Accepted for publication in the IMA Journal of Numerical Analysis (2025). 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).
Scientific Reports 15, 18689 (2025). Article

11. **Continuity estimates for Riesz potentials on polygonal boundaries**
(joint with X. Claeys and B. Stamm).
Partial Differential Equations and Applications 5, 11 (2024). Article

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 Highlight 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 93, 1203-1245 (2024). 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

37. *On the Analysis of the Coupled Cluster Method in Quantum Chemistry.* Augsburg-Munich Analysis Seminar, Technische Universität München, Germany, July 2025. **Invited Talk**.

36. *The Numerical Analysis of the Coupled Cluster Method for Electronic Structure Calculations.* Seminari di Matematica Applicata, Università di Pavia, Italy, May 2025. **Invited Talk**.

35. *On the relation between Galerkin approximations and canonical best-approximations of solutions to some non-linear Schrödinger equations.* Oberwolfach Workshop on Mathematical Methods in Quantum Chemistry, Oberwolfach, Germany, March 2025. **Invited Talk**.

34. *Investigating the DMRG Algorithm for Optimisation Problems in the Tensor-Train Format.* EPFL MATHICSE Annual Retreat 2025, Leysin, Switzerland, January 2025.

33. *On the Well-Posedness of the Discrete Coupled Cluster Equations.* Mathematical and Numerical Analysis of Electronic Structure Models (MANUEL) 2024, Universität Stuttgart, Germany, September 2024. **Invited Talk**.

32. *Some Recent Mathematical Developments in Eigenvalue Solvers and Band Structure Calculations.* Marvel Junior Retreat 2024, St. Moritz, Switzerland, September 2024. **Invited Talk**.

31. *On the Analysis of the Discrete Coupled Cluster Equations.* EMC2 @ Roscoff Workshop, Roscoff, France, July 2024. **Invited Talk**.

30. *Some Remarks on the Analysis of the Coupled Cluster Equations.* Workshop on Optimization Techniques in Quantum Chemistry, RWTH Aachen University, Germany, June 2024. **Invited Talk**.

29. *Using a posteriori error estimators to construct low-cost solution strategies for the Gross-Pitaevskii equation.* Gesellschaft für Angewandte Mathematik und Mechanik (GAMM) Annual Meeting 2024, Otto von Guericke Universität Magdeburg, Germany, March 2024.

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 2024. **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 2024. **Invited Talk**.

26. *On the Numerical Analysis of the Coupled Cluster Method in Computational Quantum Chemistry.* Seminar Talk, University of British Columbia, Canada, February 2024. **Invited Talk**.

25. *Numerical Methods for Ground-State Electronic Structure Calculations.* Colloquium Talk, University of British Columbia, Canada, February 2024. **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

9. *Time-stepping schemes for tensor trains.* Kressner and Grigori Group Seminar, EPFL, Switzerland, May 2025.

8. *A gentle introduction to density functional theory models for materials modelling.* Annual Laboratory for Simulation and Modelling (LSM) Retreat, Aarau, Switzerland, February 2025.

7. *Using a posteriori error estimators to construct low-cost solution strategies to PDEs in quantum chemistry.* Kressner and Grigori Group Seminar, EPFL, Switzerland, October 2023.

6. *Introduction to Electronic Structure Theory.* Pre-GAMM Scientific Onboarding Event, GAMM Annual Meeting Magdeburg, 2024, March 2024.

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.

Mini-Courses

1. *6 Hours of Lectures on the Mathematical Formulation of Wave-Function Methods.* Mini-school on mathematics for theoretical chemistry and physics, Laboratoire Jacques-Louis Lions, Sorbonne Université, Paris France, May 2024. **Invited Speaker**.

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

Postdoctoral Researchers

- **Alfred Kirsch** (PhD *CERMICS, École des Ponts ParisTech*): October 2025– Present.

Graduate Theses Co-supervision

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

Graduate Semester Project Co-Supervision

- *Axel Caulier*: **The Analysis of an Integral Equation Formulation of the Inhomogeneous N-Body Dielectric Spheres Problem**, EPF Lausanne, 2025.
- *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

- *Bilguun Batbileg*: **Numerical Approaches for Resolving Singularities in Two-Electron Integrals in Quantum Chemistry**, EPF Lausanne, 2024.
- *Pawel Bittner*: **Application of Grassmann Manifold Interpolation and Model Order Reduction to Eigenvalue Problems in Computational Chemistry**, RWTH Aachen University, 2019.

Summer Schools

- Co-supervisor (with Yvon Maday) of two projects at the **2025 CEMRACS Summer School on Quantum Computing** at the Centre International des Rencontres en Mathématiques" (CIRM) in Marseille.

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

- Co-organizer with Benjamin Stamm of the *Modelling, Analysis, and Simulation of Molecular Systems* Section at the 2026 Annual Meeting of the Gesellschaft für angewandte Mathematik und Mechanik (GAMM) at the Universität Suttgart (March 16-20, 2026).
- Co-organizer with Gero Friesecke of the 2025 Annual Meeting of the *Modelling, Analysis, and Simulation of Molecular Systems* GAMM Activity group at the Technische Universität München (November 20-21, 2025).
- 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 (March 11-13, 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- October 2024).
- 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 (Rensselaer Polytechnic Institute, USA) 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, Mathematical Models and Methods in Applied Sciences (M3AS), AMS Mathematical Reviews, and zbMATH Open.

External Referee

Master Theses

- *Viacheslav Karpii*: **On randomized trace estimation for operators**, EPF Lausanne, 2024.
- *Florence Osmont*: **Landscape of the Low-Rank-Tensor Nearness Problems**, EPF Lausanne, 2024.

Grants, Scholarships and Travel Awards

- Emmy Noether Grant of the Deutsche Forschungsgemeinschaft (DFG) to lead an independent Junior Research Group (January 2025).

  (Total Value: €1.39 Million over 3+3 years)

- Workshop organisation grant from the Bernoulli Center for Fundamental Studies in January 2024.

  (Total Value: 10,000 CHF)

- 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)

- Fulbright scholarship in 2013 for graduate studies in the US (declined).