Curriculum Vitae
Muhammad Hassan

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Research Interests

I work on numerical methods for PDEs and integral equations that arise in computational chemistry. As a post-doctoral researcher, I have been working on the analysis of state-of-the-art numerical techniques used in quantum chemistry. During my Ph.D., I worked on the analysis of boundary integral equations and domain decomposition methods with applications in N-body polarisable electrostatics and implicit solvation modelling in theoretical chemistry, and I also continue to work on problems in these fields.

Academic Appointments

Postdoctoral Researcher in Applied Mathematics **Nov. 2020- Present**
EMC2 ERC Synergy Project,
Laboratoire Jacques-Louis Lions, Sorbonne Université, Paris.
Supervisor: Prof. Dr. Yvon Maday.

Education

Dr. rer. nat. in Mathematics **July 2020**
Applied and Computation Mathematics (ACOM),
RWTH Aachen University, Germany.
Supervisor: Prof. Dr. Benjamin Stamm.

Master of Science in Applied Mathematics **April 2016**
Seminar for Applied Mathematics, Mathematics Department,
Swiss Federal Institute of Technology Zurich (ETHZ), Switzerland.
Supervisor: Prof. Dr. Siddhartha Mishra.

Preprints and Publications

† indicates equal contribution

C. Feniou†, M. Hassan†, D. Traoré, E. Giner, Y. Maday, and J.-P. Piquemal. **Overlap-ADAPT-VQE: Practical Quantum Chemistry on Quantum Computers via Overlap-Guided Compact Ansätze**, *submitted*
https://doi.org/10.48550/arXiv.2301.10196

M. Hassan, Y. Maday, and Y. Wang. **Analysis of the Single Reference Coupled Cluster Method for Electronic Structure Calculations: The Full Coupled Cluster Equations**, *submitted*
https://doi.org/10.48550/arXiv.2212.12788

E. Cancès, M. Hassan, and L. Vidal. **Modified-operator method for the calculation of band diagrams of crystalline materials**, *under review.*
https://doi.org/10.48550/arXiv.2210.00442

X. Claeys, M. Hassan, and B. Stamm. **Continuity estimates for Riesz potentials on polygonal boundaries**, *under review.*
https://doi.org/10.48550/arXiv.2107.10713

M. Hassan, C. Williamson, J. Baptiste, S. Braun, A. Stace, E. Besley, and B. Stamm. **Manipulating particle interactions with electric fields and point charges: A general electrostatic many-body framework**, *Journal of Chemical Theory and Computation (2022)*. https://doi.org/10.1021/acs.jctc.2c00008

J. Baptiste, C. Williamson, J. Fox, A. Stace, M. Hassan, S. Braun, B. Stamm, I. Mann, and E. Besley. **The influence of surface charge on the coalescence of ice and dust particles in the mesosphere and lower thermosphere**, *Atmospheric Chemistry and Physics* 21 (2021), pp. 8735-8745. https://doi.org/10.5194/acp-21-8735-2021

M. Hassan and B. Stamm. **A Linear Scaling in Accuracy Numerical Method for Computing the Electrostatic Forces in the N-Body Dielectric Spheres Problem**, *Communications in Computational Physics* 29 (2021), pp. 319-356. https://doi.org/10.4208/cicp.OA-2020-0090

B. Bramas, M. Hassan, and B. Stamm. **An Integral Equation Formulation of the N-Body Dielectric Spheres Problem. Part II: Complexity Analysis**, *ESAIM:M2AN* 55 (2021), pp. S625-S651. https://doi.org/10.1051/m2an/2020055

M. Hassan and B. Stamm. **An Integral Equation Formulation of the N-Body Dielectric Spheres Problem. Part I: Numerical Analysis**, *ESAIM:M2AN* 55 (2021), pp. S65-S102. https://doi.org/10.1051/m2an/2020030

G. Ciaramella, M. Hassan, and B. Stamm. **On the Scalability of the Schwarz Method**, *The SMAI Journal of Computational Mathematics*, 6 (2020), pp. 33-68. https://doi.org/10.5802/smai-jcm.61

G. Ciaramella, M. Hassan, and B. Stamm. **On the Scalability of the Parallel Schwarz Method in One Dimension**, *Domain Decomposition Methods in Science and Engineering XXV* (2020), pp. 151-158. https://doi.org/10.1007/978-3-030-56750-7_16

Presentations

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

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

August 2022 *Towards the development of a posteriori error analysis for the coupled cluster equations*, GAMM Annual Meeting 2022, RWTH Aachen, Germany.

May 2022 *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, UCLA, USA.

April 2022 *On the Approximation of Energy Bands in the Brillouin Zone*, IPAM 2022 Long Program on Quantum Mechanics Seminar series, UCLA, USA.

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

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

September 2019 *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.

July 2019 *On the Scalability of the Schwarz Method*, MathCCES Seminar, RWTH Aachen.

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

February 2019 *Scalability Analysis of an Integral Equation Formulation of the Many-Body Dielectric Problem in Electrostatics*, GAMM Annual Meeting 2019, TU Wien.

October 2018 *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, TU Berlin/ Zuse Institute.

September 2018 *On the Numerical Analysis of the Many-Body Dielectric Problem in Electrostatics*, Universität Konstanz.

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

March 2018 *On the Numerical Analysis of the ddCOSMO Algorithm*, Universität Konstanz.

January 2017 *On the Numerical Analysis of the ddCOSMO Algorithm*, Young Researchers Workshop on Mathematical Methods in Quantum Chemistry, Laboratoire Jacques-Louis Lions, UPMC, Paris.

February 2016 *Exploring the Carbuncle Phenomenon using the Framework of Entropy Measure Valued Solutions*, MathCCES Seminar, RWTH Aachen.

Conferences, Workshops and Mini-Schools

October 2022 *20^{th} Söllerhaus workshop on Fast Boundary Element Methods in Industrial Applications 2022*, Kleinwalsertal, Austria.

September 2022 *EMC2 ERC Synergy Project Workshop on mathematical aspects of quantum chemistry*, Roscoff, France.

August 2022 *DFTK School 2022: Numerical methods for density-functional theory simulations*, Sorbonne Université, Paris, France.

August 2022 *GAMM Annual Meeting 2022*, RWTH Aachen.

July 2022 *EMC2 ERC Synergy Project Workshop on mathematical aspects of quantum chemistry*, Roscoff, France.

March - June 2022 IPAM Long Program on Advancing Quantum Mechanics with Mathematics and Statistics, UCLA, USA.

July 2021 *EMC2 ERC Synergy Project Workshop on a posteriori estimators for post-Hartree Fock methods*, Roscoff, France.

December 2020 *Congrès d'Analyse Numérique pour les Jeunes - 2020* (Electronic).

August 2020 *EMC2 ERC Synergy Project Workshop on Implicit Solvation Modelling*, Roscoff, France.

September 2019 *Annual Meeting of European SIAM and GAMM Student Chapters*, RWTH Aachen.

June 2019 *MAEFLAP 2019*, Brunel University, London.

February 2019 *GAMM Annual Meeting 2019*, TU Wien.

October 2018 *Annual Meeting of the 'Modelling, Analysis and Simulation of Molecular Systems' GAMM activity Group*, TU Berlin/ Zuse Institute.

April 2018 *2nd Edition of the GDR CORREL Mini-school on Mathematics in Electronic Structure Theory*, Laboratoire Jacques-Louis Lions, UPMC, Paris.

October 2017 *Annual Meeting of the 'Modelling, Analysis and Simulation of Molecular Systems' GAMM activity Group*, RWTH Aachen.

January 2017 *1st GDR CORREL Mini-school on Mathematics in Electronic Structure Theory*, Laboratoire Jacques-Louis Lions, UPMC, Paris.

Teaching and Professional Experience

RWTH Aachen University:
Mathematical Aspects of Computational Chemistry (*SS2016, SS2017, SS2018, SS2019*).
Partial Differential Equations (*WS2018 and WS2019*).
Gewöhnliche Differentialgleichungen (*SS2019*).
Analysis für Informatiker (*WS2017*).
Mathematische Grundlagen II (*SS2016*).
Mathematische Grundlagen I (*WS2016*).

ETH Zürich:
Part-time assistant in charge of typesetting lecture notes for
Topics in Mathematical and Computational Fluid Dynamics (*February-May 2016*).
Computational Methods for Engineering Applications II (*WS2015*).

Additional:
Tutor for the CAMMP Week Pro excursion week event in SS2017, SS2018, and SS2019.

Supervision Experience

The Crystallization Conjecture, **Semester Project of Mario Drevers**, RWTH Aachen, 2020.

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

The Alternating Schwarz Method for solving Eigenvalue Problems by Inverse Power Iteration and Steepest Descent, **Semester Project of Hendrik Borchardt**, RWTH Aachen, 2019.

Continuum Solvation Models, **Semester Project of Lucia Baltz**, RWTH Aachen, 2019.

Variational Markov-Chain Monte-Carlo Methods in the context of Computational Chemistry, **Semester Project of Lucia Baltz**, RWTH Aachen, 2018.

Efficient solvers for computing the scalar magnetic potential for multiple spheres, **MS Thesis of Christian Bauer**- Co-supervised with Prof. Benjamin Stamm, RWTH Aachen, 2017.

Theses and Projects

Mathematical Analysis of Boundary Integral Equations and Domain Decomposition Methods with Applications in Polarisable Electrostatics, **Doctoral dissertation**, RWTH Aachen, 2020.

Exploring the Carbuncle Phenomenon in Hypersonic flows using the Framework of Entropy Measure Valued Solutions, **Master thesis**, ETH Zürich, 2016.

The Girsanov Transformation Theorem Revisited, **Semester Project** in the Numerical Analysis of Stochastic Ordinary Differential Equations, ETH Zürich, 2015.

Entropy Stable Schemes for Hyperbolic Conservations Laws, **Semester Project** in the Numerical Analysis of Hyperbolic Partial Differential Equations, ETH Zürich, 2015.

Minkowski's Theorem and Ideal Class Groups, **Semester Project** in Algebraic Number Theory, LUMS Pakistan, 2012.

Undergraduate Publications

A. Khan, M. Hassan, and M. Imran. **Estimating the basic reproduction number for single-strain dengue fever epidemics.** *Infectious diseases of poverty* 3.1 (2014): 12. https://doi.org/10.1186/2049-9957-3-12

M. Imran, M. Hassan, M. Dur-E-Ahmad, and A. Khan. **A comparison of a deterministic and stochastic model for Hepatitis C with an isolation stage.** *Journal of biological dynamics* 7.1 (2013), pp. 276-301.
`https://doi.org/10.1080/17513758.2013.859856`

Scholarships and Awards

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

Professional Activity

- Co-organiser with Mi-Song Dupuy and Pierre Monmarché of the ERC EMC2 seminar (`https://erc-emc2.eu/`), a joint applied mathematics and computational chemistry seminar of the Laboratoire Jacques-Louis Lions and the Laboratoire de Chimie Théorique at Sorbonne Université;

- Co-organiser 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 scheduled to take place in Amsterdam (February-March 2023).

- Review activity performed for Zeitschrift für angewandte Mathematik und Physik, ESAIM: Mathematical Modelling and Numerical Analysis, Journal of Chemical Theory and Computation, MathSciNet, and zbMATH Open.