

Curriculum Vitæ of James Emil Avery

CONTACT INFORMATION

Dr. James Emil Avery
Postdoctoral researcher

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BORN

13/12/1979, Albertslund, Denmark.

CITIZENSHIPS

Denmark and USA.

RESEARCH INTERESTS

Chemical Physics

Discrete and differential geometry in molecular and atomic physics. Development of new computational methods for ab initio many body problems. Harmonic analysis and Hyperspherical harmonics. Scalability of computational methods. Combining classical and quantum methods. Finite element DFT.

Computational Mathematics

Experimental mathematics in operator algebra, topology, and number theory. Graph theory, topology, and differential geometry of fullerene structures. Geometry of physical systems.

Theoretical Computer Science

Automatic program analysis and transformation. Abstract interpretation and formal verification. Formal languages. Graph theory and combinatorics in abstract algebra.

EDUCATION

University of Copenhagen, Copenhagen, Denmark

Ph.D., 2006-2011.

- Title: *New Computational Methods in the Quantum Theory of Nano-structures*.
- Advisor: Professor Dr. Techn. Stig Skelboe.

M.Sc., Computer Science, October 2008

- Emphasis: automatic program analysis, abstract interpretation, calculi of formal languages, and on the Sturmian method in quantum theory.
- Thesis: *The Generalized Sturmian Method: Development, Implementation and Applications in Atomic Physics*, supervised by Professor Dr. Techn. Stig Skelboe.

B.Sc., Department of Mathematical Sciences, June 2005

- Emphasis: functional analysis and operator algebras.

B.Sc., Department of Computer Science, June 2005

- Emphasis: algorithms, heuristics for infeasible problems, and scientific computing.

AWARDS

Danish Society for Computer Science (Dansk Selskab for Datalogi) prize for **best computer science master's thesis** in Denmark, 2008, among nominees from 7 Danish universities.

CO-SUPERVISION OF PH.D. STUDENTS

Lukas Wirz *Topological, graph theoretical and electronic properties of fullerenes*, Centre for Theoretical Chemistry and Physics, NZ Institute for Advanced Study, Massey University, Auckland, New Zealand. Apr. 2012–2015. (Main advisor: Prof. Peter Schwerdtfeger).

Weifeng Liu *Sparse matrix and tensor algorithms for GPU*, E-Science Center, Niels Bohr Institute, Copenhagen, Denmark. Sep. 2012–2015 (Main advisor: Prof. Brian Vinter)

Michael Herbst *Finite Element Methods in Quantum Chemistry*, Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, Heidelberg University. Aug. 2015– (Main advisor: Prof. Andreas Dreuw)

PROFESSIONAL
EXPERIENCE

Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark

Postdoctoral Researcher

July 2012–present

Project: Experimental Math. in Operator Algebra, Topology, and Number Theory.

Research Summary: (1) Methods for automatic computation in abstract mathematics. The main task is to uncover structures underlying pure mathematical objects that make them amenable to computerized analysis. Collaborative project between NBI and mathematics departments at Copenhagen University, Lund University, and University of Southern Denmark.

(2) Continued independent lines of research and collaborations. Quantum theory; hyperangular methods applied to electronic structure theory; Fullerenes.

Schwerdtfeger group, CTCP, Massey University, Auckland, New Zealand

Research officer

March 2011–July 2012

Research Summary: Worked on the following research problems: (1) A massively parallel, linear scaling finite element DFT method. (2) Hyperspherical methods for multicenter interelectron repulsion integrals. (3) Graph-theoretical properties of Fullerenes. (4) Automatic generation of symmetry adapted basis sets for atoms and molecules. (5) MCTDH methods for calculations on Bose-Einstein condensates. The QiwiB software for many-body dynamics of cold bosons.

Uptime Company I/S, Copenhagen, Denmark

Co-founder and software developer

2003–2004

Summary: Development of mobile device simulation. Wrote and deployed software for automatic monitoring states of train stations with wireless technologies for Storstrøms Traffic Company (STS). Extended hardware drivers of STS' electronic ticketing systems with encryption for protection against counterfeiting.

Wapmore A/S Copenhagen, Denmark

Software developer

2000–2003

Summary: Designed and implemented a wireless telephone emulator, implemented interpreters for the WAP 1.x-standards and a system for emulating many wireless devices. Managed external programming team in Poznań, Poland.

Dep. of Computational Linguistics, Copenhagen Business School, Denmark

Unix systems administrator and programmer

1999–2000

Summary: Wrote user and course management system. Extended the Linux kernel with a module for realtime patching of NetBIOS protocol packages to allow Windows clients to log on to SMB resources through a NAT. (Previously impossible due to NetBIOS protocol specification). Semi-automatic tagging process for natural language analysis of text corpora. Administration of Unix servers.

LONGER RESEARCH VISITS ABROAD **2014** 1.5 months at Centre for Theoretical Chemistry and Physics, Massey University, Auckland, New Zealand. Ongoing collaboration with Prof. Peter Schwerdtfeger on the topology of fullerene structures.

2013 2 months at Centre for Theoretical Chemistry and Physics, Massey University, Auckland, New Zealand. Developed methods and software for topological analysis of fullerene molecules in collaboration with Prof. Peter Schwerdtfeger.

2010 4 months at the Department of Mathematics, Auckland University. Developed methods and software for finite-element method density functional theory calculations.

2009 1 month at LIPN, Université Paris Nord, collaborating with Dr. Jean-Yves Moyen (LIPN) and Professor Lars Kristiansen (Dep. of Mathematics, University of Oslo) on a new automatic method for higher order program analysis.

2007 1 month at LIPN, Université Paris Nord, collaborating with Dr. Jean-Yves Moyen on a new, general algebraic method for understanding higher order program analysis.

ONGOING
COLLABORATIONS

- John Scales Avery. Father-son collaboration on theory and application of the Generalized Sturmian method; Hyperspherical harmonics. *Dep. of Chemistry (Emeritus)*, University of Copenhagen.
- Peter Schwerdtfeger and group. Topological, graph theoretical and electronic properties of fullerenes and fulleroid structures. *Program Fullerene*. CTCP, NZ Institute for Advanced Study, Massey University, Auckland, New Zealand.
- Gustavo Gasaneo and group. Generalized Sturmians in the quantum theory of reactive scattering. *Universidad Nacional del Sur and National Scientific and Technical Research Council (CONICET)*, Buenos Aires, Argentina.
- Michael Wormit. *MolSturm*: A quantum chemistry platform for experimental methods. Dreuw group at *IWR*, University of Heidelberg, Germany
- Wojciech Szymanski and Rune Johansen. Automorphisms and endomorphisms of graph C^* -algebras; Experimental mathematics in operator algebra; Dynamical systems. *IMDA*, University of Southern Denmark and Department of Mathematics, University of Copenhagen, Denmark.
- Jean-Yves Moyen and Jakob Grue Simonsen. Foundations of computability; Partition lattices and decidability. *LIPN*, Université Paris Nord, France, and Department of Computer Science, University of Copenhagen (DIKU), Denmark.