Curriculum Vitæ of James Emil Avery

Contact Information

Dr. James Emil Avery
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Date of Birth 13/12/1979

Citizenships Denmark and USA

Education

University of Copenhagen,
Copenhagen, Denmark
Ph.D., Dep. of Computer Science (DIKU), 8th March 2011.
- Thesis: *New Computational Methods in the Quantum Theory of Nano-structures.*
- Advisor: Professor Dr. Techn. Stig Skelboe.

M.Sc., Dep. of Computer Science (DIKU), 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., Mathematics (IMF) and Computer Science (DIKU), 2005

Current position

Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
Assistant Professor **Apr 2017–Apr 2018**

Research Summary: Independent research. *Chemical physics:* Hyperangular methods and generalized Sturmians in electronic structure theory; Fullerenes. Discrete geometry, graph theory, and combinatorial methods in quantum theory. *Mathematics:* Dynamical systems and automaton theory in operator algebra. *Computer science:* Algebraic methods in automatic program analysis. The *Bohrium* automatic parallelization platform for HPC.

Previous Positions

Dep. of Computer Science, University of Copenhagen, Copenhagen, Denmark
Postdoctoral Researcher **Jan 2016–Jan 2017**

Project: Complexity through Logic and Algebra (COLA).

Research Summary: (1) Computing with graph C^*-algebra endomorphisms as dynamical systems. (2) Chains and antichains in transfinite lattices and computable sets. (3) Continued independent lines of research and collaborations. Quantum theory; Fullerenes; Hyperspherical harmonics and hyperangular methods for modeling N-body interaction in higher-dimensional space; Molecular electron repulsion integrals.

Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
Postdoctoral Researcher **July 2012–Jan 2016**

Project: VILLUM FONDEN Experimental Mathematics in Number Theory, Operator Algebras, and Topology.

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. (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 (Permanent research position) **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. (6) Built the shared HPC computing facility for the College of Science.

Uptime Company I/S, Copenhagen, Denmark
Co-founder and software developer **2003–2004**

Summary: Mobile device simulation. Wrote and deployed software for monitoring states of train stations for Storstrøm Traffic Company/Movia. Extended hardware drivers of STS' electronic ticketing systems with encryption for anti-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**

Leadership experience

I worked 4 years as a software developer on wireless devices, protocols, and communications systems. In *Wapmore*, a 12-man software start-up company, I became lead developer and also managed our external dev.-team in in Poznań, Poland. The CTO and I then co-founded *Uptime Company*, a three-man company in which I was in charge of development. Having managed small development teams has been useful in my later scientific work for organizing and keeping projects on course. Lastly, I have led the scientific work in three Ph.D.-projects, detailed below.

Co-supervision of Ph.D. Students

I have overseen day-to-day scientific supervision of the following projects:

Michael Herbst *Finite Element Methods in Quantum Chemistry*, IWR, Heidelberg University. Aug. 2015–present (Advisor: Prof. A. Dreuw)

Lukas Wirz *Topological, graph theoretical, and electronic properties of fullerenes*, Centre for Theoretical Chemistry and Physics, NZIAS, Massey University, Auckland, New Zealand. Apr. 2012–2015. (Advisor: Prof. P. Schwerdtfeger).

Weifeng Liu *Parallel and Scalable Sparse Basic Linear Algebra Subprograms*, E-Science Center, Niels Bohr Institute, U. of Copenhagen. Sep. 2012–2015 (Advisor: Prof. B. Vinter)

Major Collaborations

John Scales Avery, Long standing father-son collaboration on novel computational methods in quantum chemistry and physics. 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. Director of CTCP, NZ Institute for Advanced Study, Massey University, Auckland, New Zealand.

Michael Wormit(†) and Michael Herbst. *MolSturm*: A quantum chemistry platform for experimental methods, built on my methods for 4-centre electron repulsion integrals. 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.

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.

Thomas Seiller and Jakob Grue Simonsen. Graph C^*-algebras and dynamical systems.

Research stays abroad

2016, 2014, 2013 6 months total at Centre for Theoretical Chemistry and Physics, Massey University, Auckland, New Zealand. I am one of four honorary fellows at CTCP.
Ongoing collaboration with Prof. Peter Schwerdfeger on the topology and chemistry of fullerene structures. I developed mathematical methods and open source software for topological analysis of fullerenes and fulleroids, http://tinyurl.com/fullerenes.

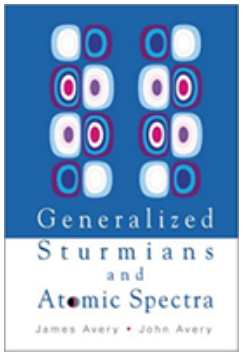
2010 4 months at the Department of Mathematics, Auckland University.
I developed a linear-scaling finite-element version of density functional theory, facilitating calculations that combine classical electrostatic environments with quantum treatment of embedded molecules, scaling to hundreds of atoms. Applied to molecular transistors.

2009, 2007 Two five-week stays at LIPN, Université Paris Nord, collaborating with Dr. Jean-Yves Moyen (LIPN) and Professor Lars Kristiansen (Dep. of Mathematics, U. of Oslo) on a new framework for understanding higher order programing languages through algebraic means, and derived automatic methods for higher order program analysis.

Awards and Distinctions

- Received A-rating in the ERC 2017 Starting Grant call.
- One of four honorary research fellows at the New Zealand Institute for Advanced Study,
- Received Danish Society for Computer Science (Dansk Selskab for Datalogi) thesis award prize for best computer science master's thesis in Denmark, 2008.

Publication summary



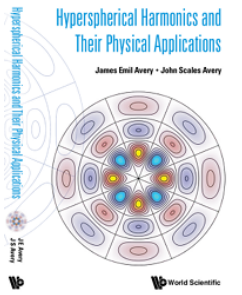
I have published **28 peer reviewed works**, of which **two are scientific textbooks**, and just completed coauthoring a third textbook, *Hyperspherical Harmonics and their Physical Applications*, published late 2017. Contract attached. My *h*-**index** and **i10-index** are both **10**, and the total **number of citations is 330** (Google Scholar), and has **doubled since 2015**. Note that research in mathematical computer science and computational methods has a very different publication and citation culture than that of the applied sciences.
I have had **two cover page features** of articles: The May 2013 issue of Journal of Computational Chemistry, and the January 2014 issue of Journal of Chemical Information and Modeling. The covers (made using my own software) are shown in the left margin. In the electronic version of this document, these images and text in blue link to more information.

Selected results and associated publications

The following results are selected to document the breadth of my work.

- **2015, Interdisciplinary (Math, Chemistry, Computer Science), Fullerene topology**. P. Schwerdtfeger, L. Wirz, and J.E. Avery. **The topology of fullerenes**. *Wiley Interdisciplinary Reviews. Computational Molecular Science* **5**(17), 96–145, Feb. 2015.

  We have developed theory and software for many aspects of mathematical and chemical analysis of fullerenes, published as open source and in use by 400 groups world wide. In the referenced large review paper, I presented some of the fundamental ideas that later led towards the present work. The paper was among the top ten WCMS articles of 2015.

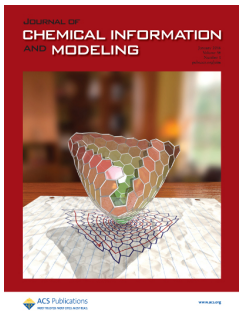


- **2013, Electronic Structure Theory.** J.E. Avery. **Fast electron repulsion integrals for molecular Coulomb Sturmians**. *Advances in Quantum Chemistry*, **67**, 129–151.

  This work presents a breakthrough in solving a long standing open problem in *ab initio* molecular calculations: rapid evaluation of molecular 4-center electron repulsion integrals (ERI) for exponential type orbitals (ETOs). This paper describes the first method able to compute 4-center ERI at practical speeds, achieved through the application of hyperangular theory, multiple coordinate separation, and high levels of off-line precalculation.

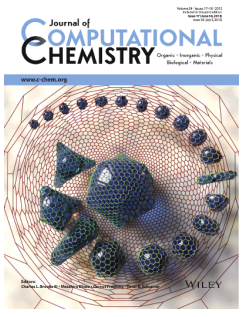
- **2017, Mathematics: Operator algebra and dynamical systems.** J.E. Avery, R. Johansen, and W. Szymanski. **Visualizing automorphisms of graph algebras**. *Proceedings of the Edinburg Mathematical Society, 2017 (In press)*.

  We uncovered combinatorial structure underlying C^*-algebra automorphisms and constructed a calculus amenable to automatic computation for them. We improved dramatically on the state of the art: one example reproduced in 2.3 seconds automorphism calculations that in prior work took 70 days to complete, a million-fold improvement. A second result, out of reach for existing methods due to estimated runtime of $\sim 10^8$ years, was solved in 10 minutes, an improvement of at least a factor 10^{11}.



- **2006, Computer science: Automatic program analysis, abstract interpretation.** J. E. Avery. **Size-change termination and bound analysis**. In M. Hagiya and P. Wadler, editors, *Functional and Logic Programming*, volume 3945 of *Lecture Notes in Computer Science*, pages 192–207. Springer Berlin Heidelberg.

  I devised an automatic program analysis for size-change termination analysis of C program code by overapproximating reachable program state by convex polyhedra. This is my first single-author result, invented during my master's studies, and it is still being cited 14 years later.



- **2016, Computer science: HPC compiler techniques.** M.R.B. Kristensen, S.A.F. Lund, T. Blum, and J.E. Avery. **Fusion of Parallel Array Operations**. Parallel Architectures and Compilation Techniques, pages 71–85, ACM New York.

  Since 1994, the seminal work of Kennedy (WLF) has been the standard for fusing loops and parallel array operations. We found errors in this method yielding suboptimal data-reuse; designed a new, correct theoretical framework that generalizes WLF and many extensions. I proved correctness, resource use, and approximation properties. Our automatically generated code benchmarked on par with hand coded `C` even when including overhead from analysis and JIT-compilation. Our paper received the ACM PACT *Best artefact* prize.

Full list of peer-reviewed publications

Note: Publications of which I am corresponding author (24 out of 30) are marked with a "⋆" preceding the year.

Books

⋆**2017** **Avery, James Emil**, J. Avery (⋆2017[b]). *Hyperspherical Harmonics and their Physical Applications*. In production. World Scientific Publishing.

⋆**2011** J. S. Avery, S. Rettrup, **Avery, James Emil** (⋆2011). *Symmetry Adapted Basis Sets: Automatic Generation for Problems in Chemistry and Physics*. World Scientific Publishing. ISBN: 978-981-4350-46-4.

⋆**2006** **Avery, James Emil**, J. Avery (⋆2006). *Generalized Sturmians and Atomic Spectra*. 1st ed. World Scientific Publishing. ISBN: 9812568069.

Book Chapters (Peer Reviewed)

⋆**2015** **Avery, James Emil**, J. S. Avery (⋆2015). "Chapter 6: Molecular integrals for exponential-type orbitals using hyperspherical harmonics". In: Advances in Quantum Chemistry. Elsevier Science, pp. 265–324. ISBN: 978-0-12-801891-0.

⋆**2011** **Avery, James Emil**, J. S. Avery (⋆2011). "Chapter 6: The Generalized Sturmian Method". In: *Solving the Schrödinger Equation: Has Everything Been Tried?* Ed. by P. Popelier. Imperial College Press. ISBN: 978-1-84816-724-7.

Journal Articles

⋆**2016** M. R. B. Kristensen, **Avery, James Emil**, T. Blum, S. A. F. Lund, B. Vinter (⋆2016[a]). "Battling Memory Requirements of Array Programming Through Streaming". In: *High Performance Computing: ISC High Performance 2016 International Workshops, P^3MA, Frankfurt, Germany, June 19–23, 2016, Revised Selected Papers*. Ed. by M. Taufer, B. Mohr, and M. J. Kunkel. Springer, pp. 451–469. ISBN: 978-3-319-46079-6.

⋆**2016** M. R. Kristensen, S. A. Lund, T. Blum, **Avery, James Emil** (⋆2016[b]). "Fusion of Parallel Array Operations". In: *Proceedings of the 2016 International Conference on Parallel Architectures and Compilation*. PACT '16. Haifa, Israel: ACM, pp. 71–85. ISBN: 978-1-4503-4121-9.

⋆**2016** **Avery, James Emil**, J. S. Avery (⋆2016). "A chainlike relative coordinate system for few-particle problems". In: *Journal of Mathematical Chemistry*, pp. 1–14. ISSN: 1572-8897.

⋆**2015** J. S. Avery, **Avery, James Emil** (⋆2015). "Rapid evaluation of molecular integrals with ETOs". In: *International Journal of Quantum Chemistry* 115.15, pp. 930–936. ISSN: 0020-7608.

2014 P. Schwerdtfeger, L. Wirz, **Avery, James Emil** (2014). "The topology of fullerenes". In: *Wiley Interdisciplinary Reviews. Computational Molecular Science*. ISSN: 1759-0876.

⋆**2014** **Avery, James Emil**, J. S. Avery (⋆2014). "Molecular Integrals for Slater Type Orbitals Using Coulomb Sturmians". In: *Journal of Mathematical Chemistry* 52.1, pp. 301–312. ISSN: 0259-9791.

2013 L. Wirz, P. Schwerdtfeger, **Avery, James Emil** (2013). "Program Fullerene: a software package for constructing and analyzing structures of regular fullerenes". In: *Journal of Computational Chemistry* 34.17, pp. 1508–1526. ISSN: 0192-8651.

2013 L. Wirz, R. Tonner, **Avery, James Emil**, P. Schwerdtfeger (2013). "Structure and Properties of the Nonface-Spiral Fullerenes T-C_{380}, D_3-C_{384}, D_3-C_{440}, and D_3-C_{672} and Their Halma and Leapfrog Transforms". In: *Journal of Chemical Information and Modeling* 54.1, pp. 121–130. ISSN: 1549-9596.

⋆**2013** **Avery, James Emil** (⋆2013). "Fast Electron Repulsion Integrals for Molecular Coulomb Sturmians". In: *Advances in Quantum Chemistry*. Vol. 67. Advances in Quantum Chemistry, pp. 129–151.

2012 J. S. Avery, **Avery, James Emil** (2012a). "Coulomb Sturmians as a basis for molecular calculations". In: *Molecular Physics* 110.15-16, pp. 1593–1608. ISSN: 0026-8976.

2012 J. S. Avery, **Avery, James Emil** (2012b). "Sturmians and generalized sturmians in quantum theory". In: *Molecular electronic structures of transition metal complexes II*. Ed. by D. Mingos, P. Day, and J. Dahl. Structure and Bonding. Springer, pp. 53–99.

⋆**2009** J. S. Avery, **Avery, James Emil** (⋆2009). "Can Coulomb Sturmians Be Used as a Basis for N-Electron Molecular Calculations?" In: *Journal of Physical Chemistry A* 113.52, 14565–14572. ISSN: 1089-5639.

⋆**2009** **Avery, James Emil**, L. Kristiansen, J.-Y. Moyen (⋆2009). "Static Complexity Analysis of Higher Order Programs". In: *FOPARA 2009*. Ed. by M. van Eekelen and S. Olha, pp. 34–49.

⋆**2008** **Avery, James Emil**, J. S. Avery (⋆2008). "Atomic core-ionization energies; approximately piecewise-linear and linear relationships". In: *Journal of Mathematical Chemistry* 46.1, pp. 164–181. ISSN: 0259-9791.

⋆**2006** **Avery, James Emil** (⋆2006). "Size-change Termination and Bound Analysis". In: *Lecture Notes in Computer Science* 3945, pp. 192–207. ISSN: 0302-9743.

⋆**2005** **Avery, James Emil**, J. S. Avery (⋆2005). "Autoionizing States of Atoms Calculated Using Generalized Sturmians". In: *Advances in Quantum Chemistry*. Ed. by J. Sabin and E. Brandas. Vol. 49. Academic Press, Incorporated, pp. 103–119. ISBN: 0120348497.

2004 J. S. Avery, **Avery, James Emil** (2004). "Generalized Sturmian solutions for many-particle Schrödinger equations". In: *Journal of Physical Chemistry A* 108.41, pp. 8848–8851.

⋆**2004** J. S. Avery, **Avery, James Emil**, V. Aquilanti, A. Caligiana (⋆2004). "Atomic Densities, Polarizabilities, and Natural Orbitals Derived from Generalized Sturmian Calculations". In: *Advances in Quantum Chemistry* 47, pp. 157–176. ISSN: 0065-3276.

⋆**2003** J. S. Avery, **Avery, James Emil** (⋆2003[a]). "Kramers Pairs in Configuration Interaction". In: *Advances in Quantum Chemistry* 43, pp. 103–118. ISSN: 0065-3276.

⋆**2003** J. S. Avery, **Avery, James Emil** (⋆2003[b]). "Natural Orbitals from Generalized Sturmian Calculations". In: *Advances in Quantum Chemistry* 43, pp. 207–216. ISSN: 0065-3276.

⋆**2003** **Avery, James Emil**, J. S. Avery (⋆2003). "The generalized Sturmian method for calculating spectra of atoms and ions". In: *Journal of Mathematical Chemistry* 33, pp. 145–162. ISSN: 0259-9791.

Accepted Articles

⋆**2017** M. R. B. Kristensen, **Avery, James Emil** (⋆2017). "Array Streaming for Array Programming". In: *Int. J. of Computational Science and Engineering*.

⋆**2017** L. Wirz, P. Schwerdtfeger, **Avery, James Emil** (⋆2017). "Naming Polyhedra by General Face-Spirals: Theory and Applications to Fullerenes and other Polyhedral Molecules". In: *Fullerenes, Nanotubes and Carbon Nanostructures*.

⋆**2017** **Avery, James Emil**, J. S. Avery (⋆2017[a]). "4-Center STO Interelectron Repulsion Integrals with Coulomb Sturmians". In: *Advances in Quantum Chemistry* 76.

⋆**2016** **Avery, James Emil**, R. Johansen, W. Szymanski (⋆2016). "Visualizing automorphisms of graph algebras". In: *Proceedings of the Edinburgh Mathematical Society*. arXiv preprint arXiv:1401.4274.

⋆**2016** **Avery, James Emil**, J.-Y. Moyen, P. Růžička, J. G. Simonsen (⋆2016). "Chains, Antichains, and Complements in Infinite Partition Lattices". In: *Algebra Universalis*. arXiv preprint arXiv:1501.05284.

Ph.D. Thesis

(Included for completeness, not counted in the publication tally)

2011 **Avery, James Emil** (2011). "New Computational Methods in the Quantum Theory of Nano-Structures". PhD thesis.

Selected Presentations

I have given 22 lectures at international conferences and workshops, of which 12 were invited:

- Jul **2017, Invited speaker** at CMMSE'17 (Comput. and Math. Methods in Science and Engineering) in Cadiz, Spain. Lecture: *Solving Wave Equations on Fullerene Surfaces.*
- Apr **2017, Invited speaker** at *The Quantum World of Molecules: from Orbitals to Spin Networks*, conference at L'Accademia Nazionale dei Lincei in Rome, Italy. Lecture: *Wave Equations on Discrete Non-Euclidean Surfaces.*
- Sep **2016, Invited speaker** at MESBA 2016 (Molecular Electronic Structure) in Buenos Aries, Argentina. Lecture: *Intrinsic Fullerene Geometry.*
- May **2016, Invited seminar** at HGS Mathematical and Computational Methods for the Sciences at HGS, Heidelberg University. Lecture: *The Intrinsic Shapes of Fullerenes.*
- Feb **2016, Invited speaker**, Intl. Conference in honor of Peter Schwerdtfeger's 60th birthday, Auckland, New Zealand. Lecture: *The Shapes of Fullerenes.*
- Jun **2015, Invited speaker** at CMMSE'15 (Comput. and Math. Methods in Science and Engineering) in Cadiz, Spain. Lecture: *Fullerene surfaces and their embeddings in space.*
- Nov **2014, Invited speaker** for the IWR Colloquium on Computational Methods in Sciences at IWR, Heidelberg University. Lecture: *Hyperspherical Harmonics and Molecular Integrals.*
- Feb **2014, Invited seminar** at Laboratoire Structure et Réactivité des Systèmes Moléculaires Complexes (SRSMC) at Université de Lorraine. Lecture: *Fast Multi-Centre Electron Repulsion Integrals for Exponential Orbitals.*
- Sep **2014, Invited speaker** at Molecular Electronic Structure in Amasya (MES 2014), Amasya, Turkey. Lecture: *Practical ETO Molecular Integrals using Hyperspherical Harmonics.*
- Sep **2012, Invited speaker** at Molecular Electronic Structure in Troy (MEST), Canakkale, Turkey. Lecture: *Efficient Multi-Center Electron Repulsion Integrals for Exponential Type Orbitals: Two New Methods.*
- Dec **2010,** APCTCC 5 (Fifth Asian-Pacific Conference on Theor. and Comput. Chemistry), Rotorua, New Zealand. Lecture: *A Linearly Scaling Parallel Finite Element DFT.*