Curriculum Vitæ of James Emil Avery

Contact Information

Dr. James Emil Avery
Dep. of Computer Science (DIKU) and
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University of Copenhagen
E-Science Group

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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.
B.Sc., Mathematics (IMF) and Computer Science (DIKU), 2005

Current position

DIKU and NBI, University of Copenhagen
Special Consultant; acting head of e-Science group **Jan 2020–present**

Previous Positions

Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
Associate Professor of Scientific Computing **Jan 2019–Dec 2020**
Teaching: 2/3 of Scientific Computing, course coordinator (∼ 70 MSc-students).
Project: PI on *Folding Carbon: A Calculus of Molecular Origami*, VILLUM Experiment 00023321. I am developing new computational methods to analyse the quantum theory of carbon-systems through non-euclidean manifolds, computing their electronic structure properties by way of combinatorial discrete geometry. At the same time, I am exploring methods to automatically compute planar precursor-molecules for rational synthesis of polyhedral molecules, and simulating their autoassembly.
Other lines of research: Ocean/atmosphere simulations; automatic analysis of climate data; ice core dating; computational medical physics; quantum computing.
Teaching: 2/3 of Scientific Computing, course coordinator (∼ 70 MSc-students).
Supervision: 3 PhD, 13 MSc, 5 BSc (3 PhD, 9 MSc, and 2 BSc ongoing)

Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
Assistant Professor **Apr 2017–Jan 2019**
Research Summary: *Chemical physics:* Hyperangular methods and generalized Sturmians in electronic structure calculations; 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.
Teaching: 1/3 of Scientific Computing course (∼ 30 MSc-students).
Supervision: 2 MSc, co-supervised 1 PhD

Dep. of Computer Science, University of Copenhagen, Copenhagen, Denmark
Postdoc under Prof. J.Grue **Jan 2016–Jan 2017**
Project: DFF 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.
Supervision: 2 BSc

Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
Postdoc under Profs. B. Vinter, S. Eilers, and W. Szymanski **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 own lines of research and collaborations. Quantum theory; hyperangular methods applied to electronic structure theory; Fullerenes. **Supervision**: Co-supervised 2 PhD

Schwerdtfeger group, Centre for Theoretical Chemistry and Physics, NZ Institute for Advanced Study, Massey University, Auckland, New Zealand

Research officer (Permanent research position) **March 2011–July 2012**

Research Summary: (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 train stations with wireless technologies 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**

Teaching

Scientific Computing: 7.5 ECTS, MSc students from Physics, Chemistry, Nanoscience, Math, and Comp Sci: 2017 (1/3, C), 2018 (1/2, B), 2019 (1/2, A), 2020 (2/3, course coordinator, A).

2019: Redesigned the course in preparation for new Computational Physics specialization, as the course doubled in size from 30 to 70 MSc students. Improved evaluation from a C-rating (lowest) to A-rating (highest, "an inspiration for other courses"). 2020: I took over as course-responsible. Despite challenges in changing the course format to conduct it online (in response to COVID-19), we maintained the A-rating and further improved student evaluations.

Completed Supervision

Co-supervisor for **3 completed PhD-theses**: (i) M. Herbst *Finite Element Methods in Quantum Chemistry*, IWR, Heidelberg U., Germany (Main advisor: A. Dreuw) (ii) L. Wirz, *Topological, graph theoretical, and electronic properties of fullerenes*, Massey U., Auckland, New Zealand (Main advisor: P. Schwerdtfeger) (iii) W. Liu, *Parallel and Scalable Sparse Basic Linear Algebra Subprograms*, U. of Copenhagen (Main advisor: B. Vinter). I was main supervisor on **6 completed MSc** theses (among which N. Heim: *Anomaly Detection in Chaotic Time-series* won prize for best Computer Science MSc thesis in Denmark, 2018), and **6 completed BSc**.

Ongoing Supervision

Main supervisor for **7 MSc** theses, **2 BSc**, and **2 PUK**. Co-supervisor for **2 MSc**. Main advisor for **3 PhD** theses (R. Munk, D. Marchant, C. Johnsen), inherited from B. Vinter. In total currently supervising **16 students in total** and **main supervisor for 14**.

Projects are preliminary investigations into my current research ideas, including: new computational methods in quantum theory, automatic analysis of medical tomography, climate simulation analysis, and machine learning methods.

Leadership experience

I worked 4 years as software developer on wireless devices, protocols, and communications systems. As lead developer in *Wapmore*, a 12-man software start-up company, I managed our external dev.-team in in Poland. Experience in managing small development teams has been useful in my later scientific work for leading and organizing research projects. I now manage several research projects, currently supervising the work of 16 students working across 6 research projects, as well as leading research conducted with several former students in their new research positions. This requires both orchestrating work within each research project, and coordinating multiple research teams at once. Since Aug. 2020 I have been acting head of NBI's eScience group after its founder B. Vinter's ascension to vice-dean, and have taken over his PhD and MSc students, including a number of advanced HPC, imaging, and machine-learning activities.

Successful Funding

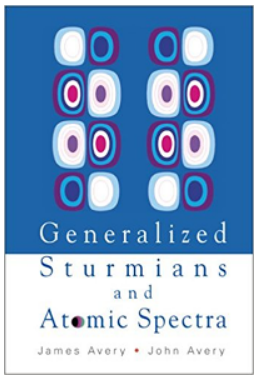
Received VILLUM Experiment grant 2018-2020, 1.7M DKK: *Folding Carbon: A Calculus of Molecular Origami* (00023321)

Applied Funding Awaiting Review

- Novo Nordisk NERD (10M DKK, sole PI): ***Carbon Manifolds****: A Computational Paradigm for Low-dimensional Carbon Nanostructures*
- VILLUM Experiment (1.7M DKK, sole PI): ***OsteoMorph****: Understanding Bone Microphysics through Computational Morphology of SRμCT*
- UCPH Data$^+$ (2M DKK, co-PI) with Peter Ditlevsen (NBI PICE): ***Tipping the climate****: Understanding and predicting rapid climate change from mining the climate model outputs*
- European Synchrotron Radiation Facility (0.8M DKK beam-time, main PI): *Characteristics of Human Mesenchymal Stem Cell mediated new formed bone and periimplant integration*
- UCPH Data$^+$ (2M DKK) with Markus Jochum (NBI Ocean) and Kenneth Skovhede (DIKU) (Co-designed project, but am not co-PI): ***Kexa****: The KU Exascale Datahub for Climate Sciences*

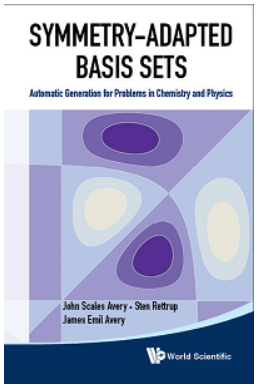
Distinctions

- A-rating in ERC-2017-StG second round; Second round VILLUM-YIP 2017; Second round DFF-SA-StG 2018
- 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.



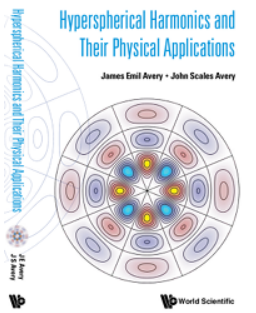
Publication record

I have published **36 peer reviewed works**, of which **three are scientific textbooks** on new computational methods in quantum theory: (*Generalized Sturmians and Atomic Spectra*, 2006; *Symmetry-Adapted Basis Sets; Automatic Calculation for Problems in Chemistry and Physics*, 2012; and *Hyperspherical Harmonics and their Physical Applications*, 2018). My *h*-**index** is 13, **i10-index** is **18**, and the total **number of citations is 644** (Google Scholar). I have been leading research, evidenced by my being **corresponding author of 30 out of 36** publications. The left margin shows journal cover page features of some of these articles, as well as my three books, with hyperlinks to the works in the electronic version of this document.



Monographs

- **2018** J. E. Avery and J. S. Avery ***Hyperspherical Harmonics and their Physical Applications***, World Scientific Publishing, 2017. ISBN: 978-981-3229-29-7. 312 pages.
- **2012** J. S. Avery, S. Rettrup, and J. E. Avery. ***Symmetry Adapted Basis Sets: Automatic Calculation for Problems in Chemistry and Physics***. World Scientific Publishing, 2012, 240 pages. ISBN:978-981-4350-46-4
- **2006** J. E. Avery and J. S. Avery. ***Generalized Sturmians and Atomic Spectra***. World Scientific Publishing, 2006, 256 pages. ISBN:978-981-256-806-9

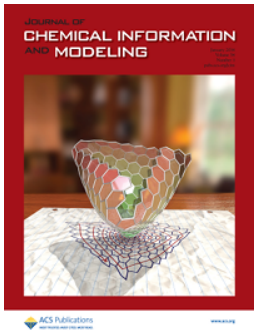


Five selected results and associated publications

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

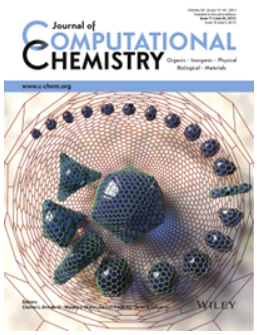
- **2016, Computer science: HPC compiler techniques.**
  M.R.B. Kristensen, S.A.F. Lund, T. Blum, and J.E. Avery. **Fusion of Parallel Array Operations**. Parallel Architectures and Compilation Techniques, pages 71–85, ACM New York.

  For over two decades, the seminal work of Kennedy et al. (WLF) has been the standard for fusing loops and parallel array operations. We found errors in this method yielding suboptimal data-reuse, discovered while designing the JIT-compilation scheme for the automatic parallelization framework Bohrium. Kristensen and I designed a new, correct theoretical framework that generalizes WLF and many subsequent extensions in a way that is both theoretically well-founded and applicable in practice. I proved correctness, resource use, and approximation properties, and our suite of benchmarks showed our automatically generated code to be on par with hand coded `C` even when including overhead from analysis and JIT-compilation. Our results were reproduced by four external reviewers and the paper received the ACM PACT *Best artefact* prize.



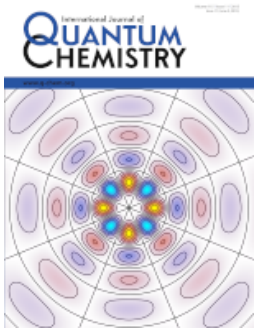
- **2017, Mathematics: Operator algebra and dynamical systems.**
  J.E. Avery, R. Johansen, and W. Szymanski. **Visualizing automorphisms of graph algebras**. *Proceedings of the Edinburg Mathematical Society, 2017 (In press).*

  We uncovered underlying combinatorial structure and constructed a calculus for graph C^*-algebra automorphisms, amenable to automatic computation. Our new methods improved dramatically on the state of the art: one example reproduced in 2.3 seconds an exhaustive calculation of automorphisms that in previous work took 70 days to complete, a million-fold improvement. A second result, far out of reach with existing methods due to an estimated runtime of at least 10^8 years, was reduced to ∼10 minutes of computation, an improvement of at least a factor 10^{11}.



- **2015, Interdisciplinary (Math, Chemistry, Comp. Sci.), 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 (Wirz, Schwerdtfeger, and **Avery, J. E.** 2013). 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, Physics: 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). It has proved so difficult that the much less physically accurate Gaussian type orbitals (GTOs) are nearly ubiquitously used, because inter-electron repulsion calculation dominates computation times, and because these integrals can be evaluated many orders of magnitude faster for GTOs. This paper describes the first method that is able to compute 4-center ERI at speeds comparable to those for GTOs, achieved through the application of hyperangular theory, multiple coordinate separation, and high levels of off-line precalculation.

Full list of peer-reviewed publications

Monographs

2017 **Avery, J. E.** and J. S. Avery (2017). *Hyperspherical Harmonics and their Physical Applications*. World Scientific Publishing. ISBN: 978-981-3229-29-7.

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

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

Book Chapters (Peer Reviewed)

2018 **Avery, J. E.** and J. S. Avery (2018). "Chapter 7: 4-Center STO Interelectron Repulsion Integrals With Coulomb Sturmians". In: *Novel Electronic Structure Theory: General Innovations and Strongly Correlated Systems*. Ed. by P. E. Hoggan. Vol. 76. Advances in Quantum Chemistry. Academic Press, pp. 133–146.

2015 **Avery, J. E.** and 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, J. E.** and 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

2021 Heuser, B., K. V. Mikkelsen, and **Avery, J. E.** (2021). "Simulating fullerene polyhedral formation from planar precursors". In: *Phys. Chem. Chem. Phys.*, pp. –.

2021 Wirz, L. N., P. Schwerdtfeger, and **Avery, J. E.** (2021). "Calculating the number of Hamilton cycles in layered polyhedral graphs". In: *Computational and Mathematical Methods*, e1142.

2019 Herbst, M. F., **Avery, J. E.**, and A. Dreuw (2019). "Quantum chemistry with Coulomb Sturmians: Construction and convergence of Coulomb Sturmian basis sets at the Hartree-Fock level". In: *Phys. Rev. A* 99 (1), p. 012512.

2019 Kristensen, M. R. B. and **Avery, J. E.** (2019). "Lossy Channels in Bohrium". In: *Communicating Process Architectures 2017 & 2018*. Ed. by J. P. et al. Vol. 70. IOS Press, pp. 347–360.

2018 Herbst, M. F., A. Dreuw, and **Avery, J. E.** (2018). "Toward quantum-chemical method development for arbitrary basis functions". In: *The Journal of Chemical Physics* 149.8, p. 084106.

2018 Kristensen, M. R. B. and **Avery, J. E.** (2018). "Array Streaming for Array Programming". In: *Int. J. of Computational Science and Engineering* 17.3.

2018 **Avery, J. E.** (2018). "Wave equations without coordinates I: fullerenes". In: *Rendiconti Lincei. Scienze Fisiche e Naturali* 29, pp. 609–621.

2018 **Avery, J. E.**, R. Johansen, and W. Szymanski (2018). "Visualizing automorphisms of graph algebras". In: *Proceedings of the Edinburgh Mathematical Society* 61.2. arXiv preprint at arXiv:1401.4274.

2018 **Avery, J. E.**, J.-Y. Moyen, P. Růžička, and J. G. Simonsen (2018). "Chains, Antichains, and Complements in Infinite Partition Lattices". In: *Algebra Universalis* 79. arXiv preprint at arXiv:1501.05284.

2016 Kristensen, M. R. B., **Avery, J. E.**, T. Blum, S. A. F. Lund, and B. Vinter (2016a). "Battling Memory Requirements of Array Programming Through Streaming". In: *High Performance Computing: ISC High Performance 2016 International Workshops, P^{3}MA, 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 Kristensen, M. R., S. A. Lund, T. Blum, and **Avery, J. E.** (2016b). "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, J. E.** and 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 Avery, J. S. and **Avery, J. E.** (2015). "Rapid evaluation of molecular integrals with ETOs". In: *International Journal of Quantum Chemistry* 115.15, pp. 930–936. ISSN: 0020-7608.

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

2014 **Avery, J. E.** and 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 Wirz, L., P. Schwerdtfeger, and **Avery, J. E.** (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 Wirz, L., R. Tonner, **Avery, J. E.**, and 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, J. E.** (2013). "Fast Electron Repulsion Integrals for Molecular Coulomb Sturmians". In: *Advances in Quantum Chemistry*. Vol. 67. Advances in Quantum Chemistry, pp. 129–151.

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

2012 Avery, J. S. and **Avery, J. E.** (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 Avery, J. S. and **Avery, J. E.** (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, J. E.**, L. Kristiansen, and 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, J. E.** and 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, J. E.** (2006). "Size-change Termination and Bound Analysis". In: *Lecture Notes in Computer Science* 3945, pp. 192–207. ISSN: 0302-9743.

2005 **Avery, J. E.** and 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 Avery, J. S. and **Avery, J. E.** (2004). "Generalized Sturmian solutions for many-particle Schrödinger equations". In: *Journal of Physical Chemistry A* 108.41, pp. 8848–8851.

2004 Avery, J. S., **Avery, J. E.**, V. Aquilanti, and 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 Avery, J. S. and **Avery, J. E.** (2003a). "Kramers Pairs in Configuration Interaction". In: *Advances in Quantum Chemistry* 43, pp. 103–118. ISSN: 0065-3276.

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

2003 **Avery, J. E.** and 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.

UNDER REVIEW

2021 Heim, N. and **Avery, J. E.** (2021). "Adaptive Anomaly Detection in Chaotic Time Series with a Spatially Aware Echo State Network". In: *Journal of Machine Learning Reasoning*. https://arxiv.org/abs/1909.01709v1.

PH.D. THESIS

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

Selected Presentations

I have given 23 lectures at international conferences and workshops, of which 12 were invited talks:

- 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.*
- Aug **2016 Invited speaker** at Bornö Workshop 2016, Sweden: Identifying Dansgaard–Oeschger events in ice cores and sediment data series. Lecture: *Discretizing Differential Equations*
- 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.*