



# Jonathan P. Coles

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Date of Birth: 17. August 1981; Reading, England  
Nationalities: English, USA  
Languages: English (native), German (High-/Swiss-, conversational)  
Family Status: Married 5 years to Swiss citizen; two daughters.  
Employment Status in DE: Permanent resident since 2016.  
Employment Status in CH: B Permit through marriage upon relocation.

## QUALIFICATIONS

- Advanced degrees in Computer Science (B.Sc./M.Sc.) and Theoretical Astrophysics (Ph.D.).
- 16 years experience developing high performance, massively parallel scientific software with MPI/OpenMP.
- 25 years programming experience in multiple languages (C/C++, modern Fortran, Python, Java, CUDA, Matlab)
- 11 years experience building and maintaining HPC computing clusters.
- Highly skilled in communicating between domain scientists and software developers.
- Proven track record of knowledge transfer from Computer Science to Astrophysics to Computational Biophysics.
- Proficient in big data modeling and analysis, particularly with high-dimensional data sets and Bayesian statistics.
- Published in peer-reviewed scientific and computational journals.

## WORK EXPERIENCE

### 2021–Present **HPC Specialist for Astrophysics Applications**

*Computational X Support Group, Leibniz Rechenzentrum der BAdW; Garching, Germany.*  
Support users in running parallel, distributed software on the supercomputing resources of the LRZ. Collaborate with astrophysicists to extend existing code. • Profile and optimize software for current CPU architectures and parallel frameworks such as MPI and OpenMP. • Provide external training in modern HPC tools • Prepare for new exascale computing hardware, including the tight integration of GPU and CPU designs.

#### **Freelance Scientific Computing Consultant**

System administrator at the TU Munich Center for Functional Protein Assemblies. • Provide technical knowledge and support for researchers. • Maintain a computing cluster of 100+ GPUs and 170 TB of storage.

### 2016–2021 **Research associate & System administrator**

*Department of Theoretical Biophysics, Technical University of Munich; Garching, Germany.*  
Developed the molecular dynamics software POLARIS(MD); improved my parallel Fast Multipole Method implementation to support more than 3 million atoms on over 100,000 CPU cores of the LRZ SuperMUC-NG supercomputer. • Investigated the effects of including sophisticated physical models on protein interactions using the molecular dynamics program POLARIS(MD). • Performed molecular dynamics simulations using the GPU accelerated AMBER software. • Applied deep learning methods to protein interface identification. System administrator at the TU Munich molecular dynamics group, upgrading and maintaining a GPU computing cluster. • Assisted in the design and installation of a new high performance computing cluster. • Improved scientific throughput of the cluster using the SLURM queuing system.

### 2013–2016 **Post-doctoral researcher**

*Exascale Computing Research Lab, University of Versailles (UVSQ); Versailles, France.*  
Implemented the Fast Multipole Method (FMM) for computing long-range electrostatic and polarization forces in the molecular dynamics program POLARIS(MD). • Used a hybrid MPI/OpenMP software architecture to run on massively parallel supercomputers using thousands of cores. • Consulted with computer scientists from UVSQ and Intel Corp. on parallel code development. • Performed simulations on Curie, JURECA, and TACC supercomputers. • Applied the FMM algorithm to study ion properties in large water droplets.



**WORK EXPERIENCE (cont.)**

- 2010–2013      **Post-doctoral researcher**  
*Institute for Theoretical Physics, University of Zürich; Zürich, Switzerland.*  
 Wrote the non-parametric gravitational lens modeling software GLASS using Python and C. • Applied GLASS to estimate the age of the Universe and the distribution of dark matter around galaxies. • Developed a new Monte Carlo sampling algorithm for high-dimensional spaces. • Developed a parallel, 6D phase-space clustering algorithm to identify dark matter structures within cosmological simulations. • Assisted in the construction of the zBox4, a custom, in-house computing cluster. • Scientific adviser for a year-long special museum exhibit on the search for life in the Universe.
- 2005–2010      **Ph.D. candidate**  
*Institute for Theoretical Physics, University of Zürich; Zürich, Switzerland.*  
 Improved estimates of the age of the universe via non-parametric Bayesian modeling of gravitationally lensed quasars. • Performed state-of-the-art dark matter simulations on Top 500 supercomputers in the US and Switzerland. • Co-developed a high-precision floating-point math library for the IBM Cell processor. • Collaborated with inorganic chemists to develop an iterative numerical scheme in Matlab for estimating magnesium ion binding affinities with RNA.

**EDUCATION**

- 2011              **Dr. sc. nat., Theoretical Astrophysics**  
 University of Zürich; Zürich, Switzerland.  
 Thesis: *The Age of the Universe and the Mass of Stars by Gravitational Lensing*  
 Supervisors: George Lake, Prasenjit Saha
- 2005              **M.Sc., Computer Science**  
 Rochester Institute of Technology; Rochester, NY, USA.  
 Thesis: *Algorithms for Bounding Folkman Numbers*  
 Supervisor: Stanisław Radziszowski
- 2005              **B.Sc., Computer Science with Honors** (awarded concurrently with M.Sc.)  
 Rochester Institute of Technology; Rochester, NY, USA.  
 Minors in Mathematics and German Language  
 Study abroad in Cognitive Science (University of Osnabrück; Osnabrück, Germany)
- 1999              **High School Diploma**  
 Sharon High School; Sharon, MA, USA.

**EARLY INDUSTRY EXPERIENCE**

- 2005              **Lead software engineer**  
*Optical Tape Systems, Inc., Shrewsbury, MA, USA.*  
 Developed embedded motor control software for reliable, high speed/acceleration, reel-to-reel streaming of storage tape. • Integrated Altera FPGAs with Maxon Motors hardware controllers.
- 2003–2004      **Assistant system administrator**  
*Rochester Institute of Technology, Rochester, NY, USA.*  
 Co-managed the computer science department labs and servers running Sun Solaris OS.
- 2003              **Software developer**  
*Intevation GmbH, Osnabrück, Germany.*  
 Developed novel user interface components for Thuban, a geographic information systems (GIS) data visualization tool. • Authored the first version of the Thuban user manual.
- 2000,2001,2002 **Software intern**  
*Sun Microsystems, Burlington, MA; Santa Clara, CA, USA.*  
 Implemented the Java debug wire protocol for the K virtual machine, a Java Virtual Machine for low-power devices. Co-developed components for the reference implementation of the Java Mobile Information Device Profile library.
- 1999              **Software intern**  
*Empirix, Waltham, MA, USA.*  
 Designed and developed a network traffic monitoring library for a website stress-testing package.

## ADDITIONAL TECHNICAL SKILLS

- Parallelization strategies, numerical algorithms, domain decomposition, load-balancing (FMM, tree codes).
- Software optimization on modern multi-core CPU architectures (cache efficiency, NUMA).
- Distributed, parallel computing. OpenMP with tasks, MPI, pthreads.
- GPU programming in CUDA. 3D visualization applications for HPC.
- Software engineering practices; Source code control (git, Subversion, CVS, etc.), refactoring, unit testing.
- Data modeling, visualization, and analysis with Python (numpy, scipy, matplotlib, pandas, SQL).
- Knowledge of machine learning and deep learning techniques (PCA, regression, clustering, CNNs)
- GNU/Intel/Cray compilers and profiling tools; OneAPI, Advisor, VTune, GNU make, gdb, autotools, etc.
- Computing cluster construction. Linux configuration and networking (Slurm, DNS, NFS, ZFS, BASH scripting).
- Software package building and deployment (modules, spack, docker, singularity).
- Astrophysics programs: GLASS, PKDGRAV, GASOLINE, RAMSES, PixeLens, TIPSy.
- Molecular dynamics packages: Polaris(MD), Amber, etc.

## PUBLIC OUTREACH

- 2012            **zBox4 construction video and YouTube outreach**  
 Filmed and edited a stop-motion video of the construction of the in-house computing cluster zBox4 in the Institute for Computational Science at the University of Zürich.  
 The video received ~85,000 views worldwide on YouTube.
- 2012            **Volkhochschule Beider Basel**  
 Delivered a public talk (in German) on the search for exo-planets and life in the Universe.
- 2011            ***Extraterrestrials in Science... and Fiction***  
*Scientifica*  
 Co-developed an exhibit showcasing energy use in animals for the Zoology Museum at the joint ETH and University of Zürich scientific open house.
- 2010-2011     ***Keine grünen Männchen!*** — University of Zürich Zoology Museum  
 Scientific advisor for a one-year special exhibit on the scientific search for planets and life in the Universe. Designed and developed interactive computer stations highlighting cellular automata, the solar system, and the formation of structure in the Universe. Conducted several guided tours for children and adults. Interviewed on Swiss radio to promote the exhibit (in German).
- 2010            **Big Bang Street Parade Truck**  
 Co-organized a Zürich Street Parade Truck promoting science at Uni Zürich.
- 2008            **University of Zürich 175th Anniversary**  
 Co-organized the open house exhibit for the Institute for Theoretical Physics.  
 Developed an interactive, 3D computer program for  $N$ -body astrophysical simulations.

## SELECTED ACADEMIC COMMUNICATION

- Lecturer**    The Roofline Model. *PRACE HPC Code Optimisation Workshop 2021*.
- Invited Talk**    Predictions for Computational Biophysics. *CECAM: Microscopic simulations - forecasting the next two decades*, 2019.
- Invited Talk**    The Future of Exploration: Charting a Path through Statistically Unique System Conformations. *University of Zürich* 2019.
- Invited Talk**    The Fast Multipole Method and Point Dipole Moment Polarizable Force Fields. *PASC 2017*.  
**Talk**            An Efficient, Polarizable, Multi-Scale Molecular Dynamics Approach to Simulating Microscopic Systems. *Computer Simulation and Theory of Macromolecules*, 2017
- Seminar**        The Big Bang Model, The Expansion of the Universe, Dark Energy, and Dark Matter. *iBiTeC, CEA*, 2015.
- Invited Talk**    Molecular Dynamics for the 21st Century. *University of Zürich*, 2015.  
**Talk**            The Future of Molecular Dynamics at Exascale with Polaris(MD). *Exascale and Beyond, Teratec*, 2014.  
**Talk**            Towards Exascale in Molecular Dynamics: Simulating large biomolecular systems with the Fast Multipole Method in Polaris(MD). *EASC 2014*.
- Seminar**        Identifying Dark Matter Structure in Phase-Space. *ETH Zürich CSE Lab*, 2012  
**Talk**            Estimating a Star's Mass from Weak Microlensing. *Lensing Soiree, University of Zürich*, 2010.  
**Talk**            Simple Simplex Sampling: Exploring the Solution Space of Degenerate Problems in High Dimensions. *Swiss Numerical Colloquium*, 2008.
- Seminar**        Free-form Mass Reconstruction of Gravitational Lenses. *Anglo-Australian Observatory*, 2008.  
**Talk**            Lens Reconstruction: Issues for the Next Decade. *OZLens2008*.  
**Talk**            N-Body Simulations as Gravitational Lenses. *N-Body 2008*.  
**Talk**            PixeLens: Lens Modeling Made Easy. *The Dark Matter workshop*, 2007.  
**Talk**            Using 10 time-delay lenses to infer the Hubble time. *Gravitational Lensing. Lorentz Center, University of Leiden*, 2006.

## SELECTED PUBLICATIONS

- [1] **J. Coles**. A Massively Parallel Task-based OpenMP+MPI Implementation of FMM for Sophisticated Polarizable Force Fields. *In prep.*, 2022.
- [2] Valérie Vallet, **J. Coles**, Florent Réal, Céline Houriez, & Michel Masella. NaCl salts in finite aqueous environments at the fine particle marine aerosol scale. *arXiv e-prints*, arXiv:2109.15265, 2021.
- [3] Philipp Denzel, Onur Çatmabacak, **J. Coles**, Claude Cornen, Robert Feldmann, Ignacio Ferreras, Xanthe Gwyn Palmer, Rafael Küng, Dominik Leier, Prasenjit Saha, & Aprajita Verma. The lens SW05 J143454.4+522850: a fossil group at redshift 0.6? *arXiv e-prints*, arXiv:2104.03324, 2021.
- [4] X. Ding, T. Treu, S. Birrer, G. C. F. Chen, **J. Coles**, P. Denzel, M. Frigo, A. Galan, P. J. Marshall, M. Millon, A. More, A. J. Shajib, D. Sluse, H. Tak, D. Xu, M. W. Auger, V. Bonvin, H. Chand, F. Courbin, G. Despali, C. D. Fassnacht, D. Gilman, S. Hilbert, S. R. Kumar, J. Y. Y. Lin, J. W. Park, P. Saha, S. Vegetti, L. Van de Vyvere, & L. L. R. Williams. Time delay lens modelling challenge. *Mon. Not. R. Astron. Soc.*, 503(1):1096–1123, 2021.
- [5] Philipp Denzel, **J. Coles**, Prasenjit Saha, & Liliya L. R. Williams. The Hubble constant from eight time-delay galaxy lenses. *Mon. Not. R. Astron. Soc.*, 501(1):784–801, 2021.
- [6] Philipp Denzel, Sampath Mukherjee, **J. Coles**, & Prasenjit Saha. Lessons from a blind study of simulated lenses: image reconstructions do not always reproduce true convergence. *Mon. Not. R. Astron. Soc.*, 492(3):3885–3903, 2020.
- [7] **J. Coles** & Rebekka Bieri. An optimizing symbolic algebra approach for generating fast multipole method operators. *Computer Physics Communications*, 251:107081, 2020.
- [8] R. Küng, P. Saha, I. Ferreras, E. Baeten, **J. Coles**, C. Cornen, C. Macmillan, P. Marshall, A. More, L. Oswald, A. Verma, & J. K. Wilcox. Models of gravitational lens candidates from space warps cfhtls. *Mon. Not. R. Astron. Soc.*, 474(3):3700–3713, 2018.
- [9] **J. Coles**, C. Houriez, M. Meot-Ner (Mautner), & M. Masella. Extrapolating single organic ion solvation thermochemistry from simulated water nanodroplets. *The Journal of Physical Chemistry B*, 120(35):9402–9409, 2016.
- [10] C. Bruderer, J. I. Read, **J. Coles**, D. Leier, E. E. Falco, I. Ferreras, & P. Saha. Light versus dark in strong-lens galaxies: dark matter haloes that are rounder than their stars. *Mon. Not. R. Astron. Soc.*, 456:870–884, 2016.
- [11] **J. Coles** & M. Masella. The fast multipole method and point dipole moment polarizable force fields. *J. Chem. Phys.*, 142(2):024109, 2015.
- [12] R. Küng, P. Saha, A. More, E. Baeten, **J. Coles**, C. Cornen, C. Macmillan, P. Marshall, S. More, J. Odermatt, A. Verma, & J. K. Wilcox. Gravitational lens modelling in a citizen science context. *Mon. Not. R. Astron. Soc.*, 447:2170–2180, 2015.
- [13] **J. Coles**, J. I. Read, & P. Saha. Gravitational lens recovery with GLASS: measuring the mass profile and shape of a lens. *Mon. Not. R. Astron. Soc.*, 445:2181–2197, 2014.
- [14] M. Lubini, M. Sereno, **J. Coles**, P. Jetzer, & P. Saha. Cosmological parameter determination in free-form strong gravitational lens modelling. *Mon. Not. R. Astron. Soc.*, 437:2461–2470, 2014.
- [15] M. Lubini & **J. Coles**. A sampling strategy for high-dimensional spaces applied to free-form gravitational lensing. *Mon. Not. R. Astron. Soc.*, 425:3077–3084, 2012.
- [16] M.C. Erat, **J. Coles**, C. Finazzo, B. Knobloch, & R.K.O. Sigel. Accurate analysis of  $\text{Mg}^{2+}$  binding to RNA: From classical methods to a novel iterative calculation procedure. *Coordination Chemistry Reviews*, 256:279–288, 2012.
- [17] **J. Coles**, P. Saha, & H. M. Schmid. Weak microlensing. *Mon. Not. R. Astron. Soc.*, 402:L21–L24, 2010.
- [18] **J. Coles**. A New Estimate of the Hubble Time with Improved Modeling of Gravitational Lenses. *Astrophys. J.*, 679:17–24, 2008.
- [19] P. Saha, **J. Coles**, A. V. Macciò, & L. L. R. Williams. The Hubble Time Inferred from 10 Time Delay Lenses. *Astrophys. J., Lett.*, 650:L17–L20, 2006.
- [20] **J. Coles** & S. Radziszowski. Computing the Folkman Number  $F_v(2, 2, 3; 4)$ . *Journal of Combinatorial Mathematics and Combinatorial Computing*, 58:13–22, 2006.
- [21] H.-P. Bischof & **J. Coles**. A Movie Is Worth More Than a Million Data Points. *Lecture Notes in Computer Science*, 3514:703–710, 2005.