

**Jonathan P. Coles**

Händelstr. 7  
 81675 Munich, Germany  
 +49 170 933 1795  
 jonathan.coles@tum.de  
 www.jpcoles.com

Date of Birth: 17. August 1981; Reading, England  
 Nationality: English  
 Languages: English (native), German (conversational), French (beginner)

**ACADEMIC POSITIONS**

- 2016–Present **Research associate**  
*Department of Theoretical Biophysics, Technical University of Munich; Garching, Germany.*
- 2013–2016 **Post-doctoral researcher**  
*Exascale Computing Research Lab, University of Versailles; Versailles, France.*
- 2010–2013 **Post-doctoral researcher**  
*Institute for Theoretical Physics, University of Zürich; Zürich, Switzerland.*
- 2005–2010 **Ph.D. student**  
*Institute for Theoretical Physics, University of Zürich; Zürich, Switzerland.*

**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
- 2003 **Study abroad, Cognitive Science**  
 University of Osnabrück; Osnabrück, Germany.

**SELECTED PUBLIC OUTREACH**

- 2012 **Volkhochschule Beider Basel**  
 Delivered a public talk (in German) on the search for life and planets 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 Special Exhibit.  
 Scientific advisor for a one-year special exhibit on the scientific search for planets and life in the Universe. Designed and developed several interactive computer stations highlighting cellular automata, the solar system, and the formation of structure in the Universe. Conducted several guided tours and radio interviews in German.
- 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.

## TEACHING ACTIVITIES

- 2016–Present **Mentor**  
Department of Physics, Technical University of Munich  
Currently acting as official mentor for one PhD student.
- 2017 **Supervisor**  
Department of Physics, Technical University of Munich  
Supervised a bachelor's thesis on the topic of simulating Ubiquitin binding proteins with a polarizable force field using the molecular dynamics code Polaris(MD).
- 2018–Present **Journal club organizer**  
Established a weekly journal club.
- 2017–2019 **Co-instructor**  
*Molecular Dynamics Simulations*. Master's level; Technical University of Munich.  
Delivered lectures on Monte-Carlo methods, thermodynamic integration, and advanced numerical methods for molecular dynamics.
- 2016–2019 **Teaching assistant**  
*Continuum Mechanics*. Master's level; Technical University of Munich.  
Conducted tutorial for weekly class assignments.
- 2016 **Guest lecturer**  
*Data Analysis in Python for Biosensors*; Undergraduate level; Paris Descartes University.  
Lectured on data analysis techniques using the Python computer language. The Biosensors project-based course teaches interdisciplinary biology students about biological sensors using electronic sensors.
- 2008 **Teaching assistant**  
*Computational Astrophysics*. Master's level. University of Zurich.  
Assisted students with weekly projects in the computer lab.
- 2000–2002 **Lab instructor**  
*Computer Science*. Undergraduate level. Rochester Institute for Technology.  
Held office hours and assisted students with weekly projects.

## MEMBERSHIP OF SCIENTIFIC SOCIETIES

- 2018 Biophysical Society

## TECHNICAL SKILLS

- 23 years programming experience; Modern Fortran, Python, C/C++, Java, CUDA, shell; Scheme, Haskell, Prolog.
- Distributed, parallel computing. OpenMP with tasks, MPI. 3D visualization.
- Linux configuration and networking. Computing cluster construction, slurm.
- GNU/Intel/Cray compilers and profiling tools, GNU make, etc. Software optimization.
- Source code control (git, Subversion, etc.).

## PUBLICATIONS

h-index: 9      ORCID:0000-0003-4526-5021

18. **J. Coles**. A Scalable Task-based Approach for Hiding Remote Communication in the Distributed Fast Multiple Method. *To be submitted.*, 2019.
17. **J. Coles** & R. Bieri. A Fully Traceless Cartesian Multipole Formulation for the Distributed Fast Multipole Method. *arXiv e-prints*, arXiv:1811.06332, 2018. *Submitted to Computer Physics Communications*.
16. 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. Citations: 1.
15. **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. Citations: 4.
14. 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. Citations: 11.
13. **J. Coles** & M. Masella. The fast multipole method and point dipole moment polarizable force fields. *J. Chem. Phys.*, 142(2):024109, 2015. Citations: 8.
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. Citations: 9.
11. **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. Citations: 9.
10. 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. Citations: 15.
9. 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. Citations: 14.
8. 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. Citations: 17.
7. F. Courbin, V. Chantry, Y. Revaz, D. Sluse, C. Faure, M. Tewes, E. Eulaers, M. Koleva, I. Asfandiyarov, S. Dye, P. Magain, H. van Winckel, **J. Coles**, P. Saha, M. Ibrahimov, & G. Meylan. COSMOGRAIL: the COSmological MONitoring of GRAVItational Lenses IX. Time delays and N-body realisations of the lens in HE 0435-1223. *ArXiv e-prints*, 2010. Citations: 95.
6. **J. Coles**, P. Saha, & H. M. Schmid. Weak microlensing. *Mon. Not. R. Astron. Soc.*, 402:L21–L24, 2010. Citations: 1.
5. **J. Coles**. A New Estimate of the Hubble Time with Improved Modeling of Gravitational Lenses. *Astrophys. J.*, 679:17–24, 2008. Citations: 64.
4. C. Vuissoz, F. Courbin, D. Sluse, G. Meylan, V. Chantry, E. Eulaers, C. Morgan, M. E. Eyler, C. S. Kochanek, **J. Coles**, P. Saha, P. Magain, & E. E. Falco. COSMOGRAIL: the COSmological MONitoring of GRAVItational Lenses. VII. Time delays and the Hubble constant from WFI J2033-4723. *Astron. Astrophys.*, 488:481–490, 2008. Citations: 71.
3. 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. Citations: 83.
2. **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. Citations: 20.
1. H.-P. Bischof & **J. Coles**. A Movie Is Worth More Than a Million Data Points. *Lecture Notes in Computer Science*, 3514:703–710, 2005. Citations: 2.

## ACADEMIC COMMUNICATION

- Website** Polaris(MD) main site ; [biodev.cea.fr/polaris](http://biodev.cea.fr/polaris)
- Invited Talk** T.B.D. *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
- Poster** A Multi-Scale Polarizable Approach for Proteins with Polaris(MD). *BPS 2018*.
- Poster** A Multi-Scale Polarizable Approach for Proteins with Polaris(MD). *WATOC 2017*.
- 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.
- Poster** A Multi-Scale Polarizable Approach for Proteins with Polaris(MD). *CECAM: Intrinsically Disordered Proteins - Bringing together Physics, Computation and Biology*. 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*.
- Talk** A Shared Future for Molecular Dynamics & Astrophysics at Exascale? *AstroSim; Exascale In Astrophysics*. 2013.
- Seminar** Identifying Dark Matter Structure in Phase-Space. *ETHZ CSE Lab*. 2012
- Talk** Estimating a Star's Mass from Weak Microlensing. *Lensing Soiree, UZH*. 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*.
- Poster** Limits of Gravitational Lensing for Determining Mass Profiles of Galaxies and Clusters. *AstroSim; Frontiers in Computational Astrophysics: The Origin of Stars, Planets and Galaxies*. 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.
- Talk** Computing the Vertex Folkman Number  $F_v(2, 2, 3; 4)$ . *MCCCC*. 2004.