Ondřej Čertík

Computational Physics and Methods (CCS-2)
Los Alamos National Laboratory
PO Box 1663, MS D413, Los Alamos, NM 87545
(505) 665-2447, certik@lanl.gov

Professional Experience

Jul '14 - pres Los Alamos National Laboratory, CCS-2: Computational Physics and Methods Group, *Scientist 2*

- *Computational Physics*

Apr '13 - Jun '14 Los Alamos National Laboratory, *PostDoc*

- *Implementing real space finite element solver for orbital free molecular dynamics (warm dense matter)*

Jun '12 - Apr '13 Continuum Analytics, *Release Manager*

- *Building Python distribution, Release Manager for NumPy 1.7 release*

Aug '11 - May '12 University of Nevada, Reno, *Teaching Assistant*

- *Supervising and grading physics labs*

Feb-Aug 2011 Lawrence Livermore National Laboratory, *Internship*

- *Development of Schrödinger, Dirac and Kohn-Sham shooting and finite element solvers.*

Jun-Aug 2010 Lawrence Livermore National Laboratory, *Computational Chemistry and Materials Science Summer Institute*

- *High-Order, Adaptive Methods for Atomic Structure Calculations*

Jan '10 - Jan '11 University of Nevada, Reno, *Graduate Research Assistant*

- *Development of hp-FEM methods*

Aug '09 - Jan '10 Desert Research Institute, Reno, NV, *Research Assistant*

- *Development of a sea breeze model*

Jun-Aug 2009 Los Alamos National Laboratory, *Summer Internship*

- *Development of finite element magnetohydrodynamic solver*

Jan-May 2009 University of Nevada, Reno, *Teaching Assistant*

- *Calculus I*

Jun-Aug 2006 The Space Telescope Science Institute, Baltimore, MD, *Summer Internship*

- *MCMC fitting of stellar evolution models to color-magnitude diagrams from M31 galaxy*

Jun-Aug 2005 Portland State University, Portland, OR, *Summer Internship*

- *Helped to develop free-access crystallographic database*

1999 - 2002 Center for Machine Perception (CMP), Department of Cybernetics, Faculty of Electrical Engineering, Czech Technical University, *Scientific assistant*

- *Robot control software (Cartesian to joint coordinates conversion, ...)*

Education

Dec 2012 Ph.D., Chemical Physics, University of Nevada, Reno
Thesis: *Physics in Screening Environments*
Advisor: Dr. Peter Winkler
GPA: 3.91

Sep 2008 Master, Theoretical Physics, Faculty of Mathematics and Physics, Charles University, Czech Republic
Thesis: *Calculation of Electron Structure in the Framework of DFT in Real Space*
Advisor: Dr. Jiří Vackář

Sep 2006 Bachelor, Physics, Faculty of Mathematics and Physics, Charles University, Czech Republic
Thesis: *Numerical solution of the radial Dirac equation in pseudopotential construction*
Advisor: Dr. Jiří Vackář

Jun 2003 High School, Mathematics and Physics, Gymnázium Christiana Dopplera, Czech Republic

Open Source Projects

- SymPy (https://sympy.org/): a Python library for symbolic mathematics; Original author; Over 845 contributors; 89 students as part of Google Summer of Code (GSoC)
- SymEngine (https://github.com/symengine/symengine/): a fast C++ symbolic manipulation library; Original author; 63 contributors

- dftatom (https://github.com/certik/dftatom): A robust and general Schrödinger and Dirac solver for atomic structure calculations (Fortran); Accompanying article published in CPC
- LFortran (https://lfortran.org): Modern interactive LLVM-based Fortran compiler; Original author
- stdlib (https://github.com/fortran-lang/stdlib): Fortran Standard Library; Founding member

More projects available at:

- https://github.com/certik
- https://gitlab.com/certik

Books and Online Resources

- Theoretical Physics Reference (https://theoretical-physics.com): Open source book deriving equations in many areas of theoretical physics, html and pdf (456 pages)
- Modern Fortran webpage (https://fortran90.org/): Showing the best practices in modern Fortran
- Fortran Home (https://fortran-lang.org/): Founding member of the effort to build a Fortran community around the webpage

Professional Service

Committee

2019 - present	Fortran Standards Committee
2020	Program Committee, SciPy Conference
2020	LANL LDRD ER CNM Committee
2019	LANL LDRD IST ECR Committee
2018	LANL LDRD ER HPF Committee
2017	LANL LDRD IS&T Reserve Proposal Committee
2017	LANL LDRD ER AMQOS Committee
2015 - 2017	Mentor, LANL Computational Physics Summer School
2019	LANL CCS-2 Deputy Group Leader Hiring Committee
2016 - 2017	LANL CCS-2 Scientist Position Hiring Committee

Peer Review

2019 Review of the book Modern Fortran by Milan Curcic for Manning Publications

2014 SciPy Conference Proceedings Reviewer

Software

2007 - present Mentor and Admin, Google Summer of Code (GSoC), SymPy

2012 - 2013 Release Manager, NumPy

Grants

2018 - 2020 LANL LDRD ER, title: Novel Algorithms for Ab-Initio DFT Calculations of Large-Scale Material Systems

Awards and Honors

2020 Spot Award, Los Alamos National Laboratory

2017 Spot Award, Los Alamos National Laboratory

2010 Excellence in Scholarship Award, by the Math/Stat Department, University of Nevada, Reno

2004 4th award at Intel International Science and Engineering Fair, Portland, OR

2004 Honorary sheet from the Minister of Education for the representation of the Czech Republic

2003 Czech Learned Society Award

2003 Minister of Education Award for the representation of the Czech Republic in Physics

Conferences and Presentations

2019 LLVM Developers' Meeting in San Jose, CA

2019 SciPy Conference in Austin, TX. Lightning talk: *LFortran: modern interactive LLVM-based Fortran compiler*

2019 Jupyter Community Workshop, Lawrence Berkeley National Laboratory. Lightning talk: *LFortran: modern interactive LLVM-based Fortran compiler*

2018 13th World Congress in Computational Mechanics (WCCM 2018) in New York City. Talk: *Flat-top Partition of Unity Method for Electronic Structure Calculations*

2017 14th U.S. National Congress on Computational Mechanics (USNCCM14) in Montréal, Canada. Talk: *Direct Energy Deposition Simulation Using Truchas*

2017 EOS Workshop, Laboratory for Laser Energetics (LLE) in Rochester, NY

2016 Transport code comparison workshop, Sandia National Laboratories in Albuquerque, NM. Talk: *Warm Dense Matter Simulations (Orbital-Free Molecular Dynamics)*

2016 SciPy Conference in Austin, TX. Talk: *SymEngine: A Fast Symbolic Manipulation Library*

2014 University of Colorado, Denver. Invited talk: *Real Space Finite Element Methods in Orbital-Free Molecular Dynamics*

2013 SciPy India Conference in Bombay, India. Invited keynote: *Python in Scientific Computing*

2013 U.S. Congress on Computational Mechanics in Raleigh, NC. Invited talk: *Dirac Spectral Finite Element Solver*

2013 SciPy Conference in Austin, TX. Invited tutorial: *Guide to Symbolic Computing with SymPy*

2012 Lawrence Berkeley National Laboratory. Invited talk: *Physics in Screened Environments*

2012 Los Alamos National Laboratory. Invited talk: *Physics in Screened Environments*

2011 APS California-Nevada Section 2011 Annual Meeting, SLAC in Menlo Park, CA. Talk: *Physics in Screened Environments*

2010 Computational Chemistry and Materials Science Summer Institute, Lawrence Livermore National Laboratory. Poster: *High-Order, Adaptive Methods for Atomic Structure Calculations* (http://certik.github.com/ccms-10-poster/)

2009 SIAM Conference on Computational Science and Engineering (CSE09) in Miami, FL. Talk: *FEMhub, distribution for finite element codes with unified Python interface*

2009 Finite Element Methods in Engineering and Science (FEMTEC), Granlibakken Conference Center in Tahoe City, CA. Talk: *SymPy: A Pure Python Symbolic Manipulation System*

2009 SciPy Conference, Caltech in Pasadena, CA. Talk: *SymPy: a library for symbolic mathematics in pure Python*

2008 5th International Workshop on Parallel Matrix Algorithms and Applications (PMAA'08) in Neuchâtel, Switzerland. Talk: *Solving Many-Body Schrödinger Equation Using Density Functional Theory and Finite Elements*

2008 EuroSciPy Conference in Leipzig, Germany. Talk: *SfePy - Simple Finite Elements in Python*

2007 8th Workshop on the DOE Advanced Computational Software (ACTS) Collection Workshop, Lawrence Berkeley National Laboratory

2007 SciPy Conference, Caltech in Pasadena, CA. Talk: *Using Python for Electronic Structure Calculations, Nonlinear Solvers, FEM and Symbolic Manipulations*

2007 Workshop and Advanced School on Eigenvalue Problems, Software and Applications (EPSA2007) in Porto, Portugal

2006 Comsol Users Conference in Prague, Czechia. Talk: *Modeling of microcrystalline silicon using finite elements*

Publications

[1] O. Čertík, F. Gardini, G. Manzini, G. Vacca: The virtual element method for eigenvalue problems with potential terms on polytopic meshes, Applications of Mathematics, Volume 63, Issue 3, Pages 333-365 (2018)

[2] J. Gaffney, S. Hu, P. Arnault, A. Becker, L. Benedict, T. Boehly, P. Celliers, D. Ceperley, O. Čertík, J. Clérouin, et al.: A Review of Equation-of-State Models for Inertial Confinement Fusion Materials, High Energy Density Physics, Volume 28, Pages 7-24 (2018)

[3] Y. Ding, A. White, S. Hu, O. Certik, L. Collins: Ab Initio Studies on the Stopping Power of Warm Dense Matter with Time-Dependent Orbital-Free Density Functional Theory, Physical review letters, Volume 121, Issue 14, Pages 145001 (2018)

[4] A. J. White, O. Certik, Y. Ding, S. Hu, L. A. Collins: Time-dependent orbital-free density functional theory for electronic stopping power: Comparison to the Mermin-Kohn-Sham theory at high temperatures, Physical Review B, Volume 98, Issue 14, Pages 144302 (2018)

[5] O. Certik, F. Gardini, G. Manzini, L. Mascotto, G. Vacca: The $ p $-and $ hp $-versions of the virtual element method for elliptic eigenvalue problems, arXiv preprint arXiv:1812.09220 (2018)

[6] A. Meurer, C. P. Smith, M. Paprocki, O. Čertík, S. B. Kirpichev, M. Rocklin, A. Kumar, S. Ivanov, J. K. Moore, S. Singh, et al.: SymPy: symbolic computing in Python, PeerJ Computer Science, Volume 3, Pages e103 (2017)

[7] L. X. Benedict, M. P. Surh, L. G. Stanton, C. R. Scullard, A. A. Correa, J. I. Castor, F. R. Graziani, L. A. Collins, O. Čertík, J. D. Kress, et al.: Molecular dynamics studies of electron-ion temperature equilibration in hydrogen plasmas within the coupled-mode regime, Physical Review E, Volume 95, Issue 4, Pages 043202 (2017)

[8] O. Čertík, M. Paprocki, A. Meurer, B. Granger, T. Rathnayake: Symbolic Computing, Encyclopedia of Applied and Computational Mathematics, Pages 1431-1439 (2015)

[9] O. Čertík, J. E. Pask, J. Vackář: dftatom: A robust and general Schrödinger and Dirac solver for atomic structure calculations, Computer Physics Communications, Volume 184, Issue 7, Pages 1777-1791 (2013)

[10] R. Cimrman, M. Tůma, M. Novák, O. Čertík, J. Plešek, J. Vackář: Python-based finite element code used as a universal and modular tool for electronic structure calculation, AIP Conference Proceedings, Volume 1558, Pages 1532 (2013)

[11] O. Čertík, P. Winkler: Computation of screened two-electron matrix elements, International Journal of Quantum Chemistry, Volume 113, Issue 16, Pages 2012-2018 (2013)

[12] P. Solin, O. Certik, L. Korous: Three anisotropic benchmark problems for adaptive finite element methods, Applied Mathematics and Computation, Volume 219, Issue 13, Pages 7286-7295 (2013)

[13] D. Joyner, O. Čertík, A. Meurer, B. E. Granger: Open source computer algebra systems: SymPy, ACM Communications in Computer Algebra, Volume 45, Issue 3/4, Pages 225-234 (2012)

[14] J. Vackář, O. Čertík, R. Cimrman, M. Novák, O. Šipr, J. Plešek: Finite Element Method in Density Functional Theory Electronic Structure Calculations, Advances in the Theory of Quantum Systems in Chemistry and Physics, Pages 199-217 (2012)

[15] O. Certik, P. Winkler: Physics in Screening Environments, Bulletin of the American Physical Society, Volume 56 (2011)

[16] A. Fejfar, A. Vetushka, V. Kalusová, O. Čertík, M. Ledinský, B. Rezek, J. Stuchlík, J. Kočka: Relation of nanoscale and macroscopic properties of mixed-phase silicon thin films, physica status solidi (a), Volume 207, Issue 3, Pages 582-586 (2010)

[17] P. Solin, O. Certik, S. Regmi: The FEMhub Project and Classroom Teaching of Numerical Methods, Proc. of the 8th SciPy Conference, Pasadena, CA, August 18-23, 2009 (2009)

[18] O. Certík, J. Vackár, J. Plesek: Density Functional Theory Calculations Using the Finite Element Method, Proceedings of the Estonian Academy of Sciences, Pages 155-178 (2008)

[19] K. Výborný, O. Čertík, D. Pfannkuche, D. Wodziński, A. Wójs, J. J. Quinn: Integral and fractional quantum Hall Ising ferromagnets, Physical Review B, Volume 75, Issue 4, Pages 045434 (2007)

[20] O. Certik: Simple derivation of the special theory of relativity without the speed of light axiom, arXiv preprint arXiv:0710.3398 (2007)

[21] O. Certik: Numerical solution of the radial Dirac equation in pseudopotential construction, arXiv preprint arXiv:0710.3408 (2007)

[22] A. F. Dethlefsen, R. J. Haug, K. Výborný, O. Čertík, A. Wójs: Transport gap in a $\ nu$= 1/ 3 quantum Hall system: A probe for skyrmions, Physical Review B, Volume 74, Issue 19, Pages 195324 (2006)

[23] P. Moeck, O. Čertík, G. Upreti, W. Garrick, P. Fraundorf: Crystal structure visualizations in three dimensions with database support, MATERIALS RESEARCH SOCIETY SYMPOSIUM PROCEEDINGS, Volume 909, Pages 61 (2006)

[24] P. Moeck, O. Certik, G. Upreti, B. Seipel, M. Harvey, W. Garrick, P. Fraundorf: Crystal structure visualizations in three dimensions with support from the open access Nano-Crystallography Database, JOURNAL OF MATERIALS EDUCATION, Volume 28, Issue 1/2, Pages 83 (2006)

[25] A. Havránek, O. Čertík: Pružné kyvadlo, Pokroky matematiky, fyziky a astronomie, Volume 51, Issue 3, Pages 198-216 (2006)

[26] K. Výborný, O. Certík, D. Pfannkuche, D. Wodzinski, A. Wójs, J. Quinn: Ising ferromagnetism of composite fermions, Acta Physica Polonica A, Volume 110, Issue 3, Pages 409-415 (2006)

[27] P. Moeck, B. Seipel, G. Upreti, R. Bjorge, L. Noice, O. Certik, E. Mandell, P. Fraundorf: Crystallographic nanometrology in two and three dimensions with on-line database support, Proc. Micro Nano Breakthrough Conference, Pages 44 (2006)

[28] P. Moeck, O. Čertik, B. Seipel, R. Groebner, L. Noice, G. Upreti, P. Fraundorf, R. Erni, N. D. Browning, A. Kiesow, et al.: Identifying unknown nanocrystals by fringe fingerprinting in two dimensions and free-access crystallographic databases, Proceedings of SPIE, Volume 6000, Pages 60000M (2005)

[29] A. Fejfar, T. Mates, O. Čertík, B. Rezek, J. Stuchlík, I. Pelant, J. Kočka: Model of electronic transport in microcrystalline silicon and its use for prediction of device performance, Journal of non-crystalline solids, Volume 338, Pages 303-309 (2004)

[30] O. Certik, A. Havranek: Elastic pendulum, Matematika - fyzika - informatika, Volume 12, Issue 10, Pages 607-611 (2003)