

Don E. Willcox / Curriculum Vitæ

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Recent Position:

Applied Mathematics and Computational
Research Division

Lawrence Berkeley National Laboratory
1 Cyclotron Road Mailstop 50A3111
Berkeley, CA 94720

2022-2024 *Project Scientist*, Center for Computational Sciences & Engineering, Lawrence
Berkeley National Laboratory

2018-2022 *Postdoctoral Researcher*, Center for Computational Sciences & Engineering, Lawrence
Berkeley National Laboratory

Research Interests:

I am a computational physicist most recently employed as a project scientist in the Applied Mathematics and Computational Research Division at Berkeley Lab. My contractual funding ended in 2024, so I am looking for ways to continue advancing basic and applied research with physics, mathematics, and computation.

I first developed efficient GPU algorithms for implicit time integration to model nucleosynthesis in high-energy astrophysical events. I then collaborated with other scientists to study relativistic magnetic reconnection with WarpX, our electromagnetic Particle-In-Cell (PIC) code. This enabled me to develop Emu, the first open, performance-portable PIC code for solving six-dimensional, three-flavor neutrino quantum kinetics. Most recently, I helped develop the Energy Research and Forecasting code for mesoscale weather modeling to enable optimum wind energy production. I am very interested in developing techniques for multiphysics modeling to answer open science questions.

One of the challenges of modern science is that researchers often discover partial differential equations impossible to solve analytically. I addressed this with other Berkeley Lab researchers by developing symbolic code-generation frameworks for translating partial differential equations into high-performance simulation code. We published our validated techniques for solving respectively the challenging equations of numerical general relativity and neutrino quantum kinetics.

However, sometimes we do not yet know what equations describe nature, so modern data science often searches for patterns using machine learning to assimilate large datasets. Thus, I also led a project at Berkeley Lab to construct machine learning surrogate models from simulated datasets of astrophysical flames. In addition to enabling faster computation, our work provides a starting point for future research analyzing trained models to discover unknown underlying equations.

Education:

- **Stony Brook University** – Stony Brook, NY, USA

Ph.D., Physics, August 2018

- **LeTourneau University** – Longview, TX, USA

B.S., Engineering Physics, May 2011

B.S., Electrical Engineering, May 2011

Minors: Mathematics, Applied Sciences

Fellowships / Awards:

2011-2018 Turner Fellow, Stony Brook University Center for Inclusive Education

2007-2011 Heritage Scholarship, LeTourneau University

Funding Proposals And Status:

2023 (Partially Funded) Principal Investigator, Berkeley Lab FY 2024 Multi-Area LDRD, Co-Investigator: Hector Garcia Martin (LBNL, Biosciences Area), *Bioreactor digital twinning - Accelerating bioprocess scaling by combining computational fluid dynamics with metabolic modeling*

2023 (Not Funded) Principal Investigator, DOE Wind Energy Technologies Office, Co-Investigators: Adam Lavelly (LBNL), Ganesh Vijayakumar (NREL), *Advancing AMR-Wind Turbine Simulations With Machine Learning*

2023 (Not Funded) Principal Investigator, DOE Wind Energy Technologies Office, *Artificial Intelligence for Multiscale Wind Modeling with the ERF Simulation Code*

Large Computer Time Allocations Awarded:

2023 Co-Investigator on an INCITE 2023 award, *Exascale Models of Astrophysical Thermonuclear Explosions* (Awarded: 400 k node-hours on Summit, 300 k node-hours on Frontier, 100 k node-hours on Polaris)

2022 Co-Investigator on an INCITE 2022 award at OLCF, *Approaching Exascale Models of Astrophysical Explosions* (Awarded: 590 k node-hours on Summit)

2021 Senior Investigator on a NERSC 2021 Allocation, *Three-dimensional studies of white dwarfs, massive stars, and neutron star systems* (Awarded: 30 M MPP hours)

2021 Senior Investigator on a NERSC 2021 Allocation, *Neutrino Flavor Transformation in Neutron Star Mergers* (Awarded: 18 M MPP hours)

2021 Senior Investigator on a NERSC 2021 Allocation, *Rotating Superfluids via Complex Langevin* (Awarded: 17 M MPP hours)

- 2021 Senior Investigator on a NERSC 2021 Allocation, *Astrophysics of Supernova Progenitors* (Awarded: 13 M MPP hours)
- 2020 Senior Investigator on a NERSC 2020 Allocation, *Three-dimensional studies of white dwarfs, massive stars, and neutron star systems* (Awarded: 30 M MPP hours)
- 2019-2020 Co-Investigator on an INCITE 2019 award at OLCF, *Approaching Exascale Models of Astrophysical Explosions* (Awarded 2019: 1.5 M node-hours on Titan, 105 k node-hours on Summit; Awarded 2020: 300 k node-hours on Summit)
- 2018 Senior Investigator on a NERSC 2018 Allocation, *Three-dimensional studies of white dwarf and neutron star systems* (Awarded: 20.8 M MPP hours)
- 2018 Co-Investigator on an INCITE 2018 award at OLCF, *Approaching Exascale Models of Astrophysical Explosions* (Awarded: 40 Mh)

Scientific Software Projects:

- ongoing Co-creator of the **Emu** simulation code for astrophysical neutrino quantum kinetics in 6-dimensional phase space. <https://github.com/amrex-astro/Emu>
- ongoing Core developer of the **Castro** simulation code for astrophysical radiation-hydrodynamics on adaptive meshes, <https://github.com/amrex-astro/Castro>
- ongoing Core developer of the **StarKiller Microphysics** code, a collection of publicly-available astrophysical microphysics routines and nuclear reaction network integrators, <https://github.com/starkiller-astro/Microphysics>
- ongoing Co-developer of **pynucastro**, a publicly-available Python interface to the JINA ReacLib nuclear reaction rate database for rate visualization and ODE right hand side code generation in Python and C++, <https://github.com/pynucastro/pynucastro>
- ongoing Co-creator of the **StarSTRUQ** github organization for publicly-available code implementing uncertainty quantification algorithms useful for stellar evolution calculations, <https://github.com/StarSTRUQ>
- ongoing Core developer of the **ERF** simulation code for large-scale (ie. mesoscopic) weather modeling, <https://github.com/erf-model/erf>

Professional Mentoring:

- 2019–2021 *Co-mentor for LBNL intern - Eloise Yang*
- 2020–2021 *Associate mentor for Fall 2020 & Spring 2021 DOE SULI intern at LBNL - Nicole Ford*
- Summer 2021 *Mentor for NSF MSGI intern at LBNL - Chris Degrendele*
- Summer 2020 *Mentor for LBNL summer intern - Chris Degrendele*
- Summer 2020 *Mentor for NSF MSGI intern at LBNL - Ty Frazier*
- Summer 2019 *Co-mentor for LBNL summer interns - Chris Degrendele and Kiran Eiden*

Professional Service:

- ongoing Referee for the *Astrophysical Journal* and *Communications in Applied Mathematics and Computational Science*
- 2021 Organizer for SIAM CSE 2021 Minisymposium MS137, *Machine Learning Approaches in Computational Astrophysics and Cosmology*

Professional Development:

- 2019 Participated in GPU Hackathon organized by NERSC.
- 2018 Participated in GPU Hackathon at Brookhaven National Laboratory.
- 2018 Participated in GPU Hackathon at University of Colorado, Boulder.
- 2018 Achieved Software Carpentry instructor certification
- 2017 Participated in GPU Hackathon at Brookhaven National Laboratory.
- 2016 Participated in GPU Hackathon hosted by the Oak Ridge Leadership Computing Facility.
- 2015 Participated in GPU Hackathon hosted by the Oak Ridge Leadership Computing Facility.
- 2015 Studied at the Argonne Training Program on Extreme-Scale Computing.
- 2014 Studied at the MESA Summer School for simulating massive stars, accreting white dwarfs, stellar mixing processes and more at UC Santa Barbara.
- 2014 Studied at the JINA TALENT Course on Nuclear Theory for Astrophysics at Michigan State University.

Community Outreach:

- 10/20/2020 Panelist at CAUSE Career Panel, University of Minnesota
- 06/18/2019 Public talk at the Berkeley Public Library, Claremont, *How to Simulate a Thermonuclear Supernova*
- 01/2019 Judge for Chambliss poster competition at the 233rd Meeting of the American Astronomical Society.
- 02/21/2018 Public talk at the Astronomical Society of Long Island, Vanderbilt Museum & Planetarium, *Saturn in 13 Years: the Cassini-Huygens Mission*
- 11/03/2017 Public talk in the Astronomy Open Night Series, Stony Brook University, *Saturn in 13 Years: the Cassini-Huygens Mission*

Teaching Experience:

LBNL

2019,2020,2021 *ATPESC Lecturer Support Staff*

Designed and presented hands-on exercises for the AMReX code at the Argonne Training Program on Extreme-Scale Computing.

Stony Brook University

Spring 2017 *WISE Computational Astrophysics*

Co-instructor for a computational astrophysics course for the Women In Science and Engineering program.

Summer 2015 *IACS Computes!*

Teaching assistant for a Python programming workshop for high school students by the Institute for Advanced Computational Sciences.

Spring 2014 *Astronomy*

Teaching assistant for an undergraduate astronomy course.

Spring 2013 *Modern Physics*

Instructor for an undergraduate laboratory on relativity and quantum mechanics.

Summer 2012 *Introduction to Calculus II*

Instructor for a 3-week course on integral calculus for incoming freshman students.

2012 *Introductory Physics*

Instructor for undergraduate laboratory on electricity and magnetism.

LeTourneau University

Fall, 2008-2010 *Electricity and Magnetism*

Recitation instructor for undergraduates taking the physics course on electricity and magnetism.

Spring 2010 *Classical Mechanics*

Recitation instructor for undergraduates taking the physics course on classical mechanics.

Refereed Publications:

26. *ERF: Energy Research and Forecasting Model*
A. Lattanzi, A. Almgren, E. Quon, M. Natarajan, B. Kosovic, J. Mirocha, B. Perry, D. Wiersema, D. Willcox, X. Yuan, W. Zhang
2024, arXiv:2412.04395
doi.org/10.48550/arXiv.2412.04395
25. *Code Generation for AMReX with Applications to Numerical Relativity*
A. J. Peterson, D. Willcox, and P. Moesta
2023, Classical and Quantum Gravity, 40, 245013
doi.org/10.1088/1361-6382/ad0b37
24. *Dimming the Lights: 2D Simulations of Deflagrations of Hybrid C/O/Ne White Dwarfs using FLASH*
C. Feldman, N. Gutierrez, E. Eisenberg, D. E. Willcox, D. M. Townsley, A. C. Calder
2023, Astrophysical Journal, 959, 112
doi.org/10.3847/1538-4357/acf658
23. *ERF: Energy Research and Forecasting*
A. Almgren, A. Lattanzi, R. Haque, P. Jha, B. Kosovic, J. Mirocha, B. Perry, E. Quon, M. Sanders, D. Wiersema, D. Willcox, X. Yuan, W. Zhang
2023, Journal of Open Source Software, 8, 87
doi.org/10.21105/joss.05202
22. *Particle-in-Cell Simulations of Relativistic Magnetic Reconnection with Advanced Maxwell Solver Algorithms*
H. Klion, R. Jambunathan, M. E. Rowan, E. Yang, D. Willcox, J. L. Vay, R. Lehe, A. Myers, A. Huebl, W. Zhang
2023, Astrophysical Journal, 952, 8
doi.org/10.3847/1538-4357/acd75b
21. *pynucastro: A Python Library for Nuclear Astrophysics*
A. Smith Clark, E. T. Johnson, Z. Chen, K. Eiden, D. E. Willcox, B. Boyd, L. Cao, C. J. DeGrendele, M. Zingale
2023, Astrophysical Journal, 947, 65
doi.org/10.3847/1538-4357/acbaff

20. *Neural Networks for Nuclear Reactions in MAESTROeX*
D. Fan, D. E. Willcox, C. DeGrendele, M. Zingale, A. Nonaka
2022, Astrophysical Journal, 940, 134
doi.org/10.3847/1538-4357/ac9a4b
19. *Dark Matter from Axion Strings with Adaptive Mesh Refinement*
M. Buschmann, J. W. Foster, A. Hook, A. Peterson, D. E. Willcox, W. Zhang, B. R. Safdi
2022, Nature Communications, 13, 1
doi.org/10.1038/s41467-022-28669-y
18. *Neutrino Fast Flavor Instability in Three Dimensions*
S. Richers, D. E. Willcox, N. M. Ford
2021, Physical Review D, 104, 103023
doi.org/10.1103/PhysRevD.104.103023
17. *Practical Effects of Integrating Temperature with Strang Split Reactions*
M. Zingale, M. P. Katz, D. E. Willcox, A. Harpole
2021, Research Notes of the AAS, 5, 71
doi.org/10.3847/2515-5172/abf3cb
16. *Dynamics of Laterally Propagating Flames in X-Ray Bursts. II. Realistic Burning and Rotation*
A. Harpole, N. M. Ford, K. Eiden, M. Zingale, D. E. Willcox, Y. Cavecchi, M. P. Katz
2021, Astrophysical Journal, 912, 36
doi.org/10.3847/1538-4357/abee87
15. *Particle-in-cell Simulation of the Neutrino Fast Flavor Instability*
S. Richers, D. E. Willcox, N. M. Ford, A. Myers
2021, Physical Review D, 103, 083013
doi.org/10.1103/PhysRevD.103.083013
14. *Preparing Nuclear Astrophysics for Exascale*
M. Katz, A. Almgren, M. Barrios Sazo, K. Eiden, K. Gott, A. Harpole, J. Sexton, D. Willcox, W. Zhang, M. Zingale
2020, Supercomputing 20 (SC20)
doi.org/10.1109/SC41405.2020.00095
13. *CASTRO: A Massively Parallel Compressible Astrophysics Simulation Code*
A. Almgren, M. Barrios Sazo, J. Bell, A. Harpole, M. Katz, J. Sexton, D. Willcox, W. Zhang, M. Zingale
2020, Journal of Open Source Software, 5, 54, 2513
doi.org/10.21105/joss.02513

12. *Dynamics of Laterally Propagating Flames in X-Ray Bursts. I. Burning Front Structure*
K. Eiden, M. Zingale, A. Harpole, D. Willcox, Y. Cavecchi, M. P. Katz
2020, Astrophysical Journal, 894, 6
doi.org/10.3847/1538-4357/ab80bc
11. *The Castro AMR Simulation Code: Current and Future Developments*
M. Zingale, A. S. Almgren, M. Barrios Sazo, J. B. Bell, K. Eiden, A. Harpole, M. P. Katz,
A. J. Nonaka, D. E. Willcox, W. Zhang
2020, Journal of Physics: Conference Series, 1623, 012021
doi.org/10.1088/1742-6596/1623/1/012021
10. *Modelling low Mach number stellar hydrodynamics with MAESTROeX*
A. Harpole, D. Fan, M. P. Katz, A. J. Nonaka, D. E. Willcox, M. Zingale
2020, Journal of Physics: Conference Series, 1623, 012015
doi.org/10.1088/1742-6596/1623/1/012015
9. *MAESTROeX: A Massively Parallel Low Mach Number Astrophysical Solver*
D. Fan, A. Nonaka, A. Almgren, D. Willcox, A. Harpole, M. Zingale
2019, Journal of Open Source Software, 4, 43, 1757
doi.org/10.21105/joss.01757
8. *SN Ia Explosions from Hybrid Carbon-Oxygen-Neon White Dwarf Progenitors That Have Mixed During Cooling*
C. N. Augustine, D. E. Willcox, J. Brooks, D. M. Townsley, A. C. Calder
2019, Astrophysical Journal, 887, 188
doi.org/10.3847/1538-4357/ab511a
7. *Toward Resolved Simulations of Burning Fronts in Thermonuclear X-ray Bursts*
M. Zingale, K. Eiden, Y. Cavecchi, A. Harpole, J. B. Bell, M. Chang, I. Hawke, M. P. Katz,
C. M. Malone, A. J. Nonaka, D. E. Willcox, W. Zhang
2019, Journal of Physics: Conference Series, 1225, 012005
doi.org/10.1088/1742-6596/1225/1/012005
6. *Thermonuclear (Type Ia) Supernovae and Progenitor Evolution*
A. C. Calder, D. E. Willcox, C. J. DeGrendele, D. Shangase, M. Zingale, D. M. Townsley
2019, Journal of Physics: Conference Series, 1225, 012002
doi.org/10.1088/1742-6596/1225/1/012002
5. *Quantification of Incertitude in Black Box Simulation Codes*
A. C. Calder, M. M. Hoffman, D. E. Willcox, M. P. Katz, F. D. Swesty, S. Ferson
2018, Journal of Physics: Conference Series, 1031, 012016
doi.org/10.1088/1742-6596/1031/1/012016

4. *pynucastro: an interface to nuclear reaction rates and code generator for reaction network equations*
D. E. Willcox, M. Zingale
2018, Journal of Open Source Software, 3(23), 588
doi.org/10.21105/joss.00588
3. *Meeting the Challenges of Modeling Astrophysical Thermonuclear Explosions: Castro, Maestro, and the AMReX Astrophysics Suite*
M. Zingale, A. S. Almgren, M. G. Barrios Sazo, V. E. Beckner, J. B. Bell, B. Friesen, A. M. Jacobs, M. P. Katz, C. M. Malone, A. J. Nonaka, D. E. Willcox, W. Zhang
2018, Journal of Physics: Conference Series, 1031, 012024
doi.org/10.1088/1742-6596/1031/1/012024
2. *Cosmic Chandlery with Thermonuclear Supernovae*
A. C. Calder, B. K. Krueger, A. P. Jackson, D. E. Willcox, B. J. Miles, D. M. Townsley
2017, Journal of Physics: Conference Series, 837, 012005
doi.org/10.1088/1742-6596/837/1/012005
1. *Type Ia Supernova Explosions From Hybrid Carbon-Oxygen-Neon White Dwarf Progenitors*
D. E. Willcox, D. M. Townsley, A. C. Calder, P. Denissenkov, F. Herwig
2016, Astrophysical Journal, 832, 13
doi.org/10.3847/0004-637X/832/1/13

Meeting Talks / Invited Talks / Seminars:

- 07/15/2021 Seminar for the CS Summer Student Seminar Series, Computing Sciences, Lawrence Berkeley National Laboratory, *Supercomputing For Nuclear Astrophysics*
- 04/19/2021 Invited Speaker in APS April Meeting 2021 Session T05, *Neutrino Flavor Transformations with Emu: A New Particle-in-Cell Code for Quantum Kinetics*
- 03/02/2021 Speaker in SIAM CSE 2021 Minisymposium MS137, *Towards Surrogate Models for Nuclear Reactions in Astrophysics*
- 07/09/2020 Seminar for the CS Summer Student Seminar Series, Computing Sciences, Lawrence Berkeley National Laboratory, *Simulating Supernovae with Supercomputers*
- 01/31/2020 Talk at the 1st Annual CS Area Postdoc Symposium, Computing Sciences, Lawrence Berkeley National Laboratory, *Towards ExaScale Supernovae Simulations*
- 11/15/2017 Seminar for the Student Seminar Series, Institute for Advanced Computational Sciences, Stony Brook University, *Stellar Explosion Mechanics: Properties and Physical Processes in White Dwarf Interiors*
- 10/05/2017 Talk at the Interdisciplinary Theoretical and Computational Physical Science meeting, Tokyo Institute of Technology, Japan, *The Dynamics and Origins of Thermonuclear (Type Ia) Supernovae*

- 09/29/2017 Talk at NY Area Computational Hydro Workshop, Flatiron Institute/CCA, *A Brief Tour of the AMReX Astrophysics Suite of Codes*
- 06/28/2017 Seminar for the Research Café Series, Center for Inclusive Education, Stony Brook University, *White Dwarfs as Type Ia Supernovae Progenitors*
- 06/16/2017 Invited talk at Current Challenges in the Physics of White Dwarf Stars, Santa Fe, NM, *Simulations of Various White Dwarf Progenitor Models for Type Ia Supernovae*
- 06/14/2017 Invited astrophysics seminar at Los Alamos National Laboratory, NM, *Status of Recent Work for Type Ia Supernovae Progenitors: Hybrid C-O-Ne White Dwarfs, the Convective Urca Process, and Accelerated Reaction Networks*
- 02/05/2017 Talk at JINA-CEE Frontiers in Nuclear Astrophysics: Junior Researchers Workshop, Michigan State University, *Elucidating the Convective Urca Process in Pre-Supernova White Dwarfs Using Three-Dimensional Simulations*

Conference Posters:

- 13. *SedonaEx: A Monte Carlo Radiation Transfer Code for Astrophysical Events*,
D. E. Willcox, A. S. Almgren, D. Kasen, A. Myers, & W. Zhang
SIAM CSE 2019 Meeting, Spokane, WA (Best Poster Prize)
- 12. *Visualizing Nuclear Reaction Rates and Constructing Networks with pynucastro*
D. E. Willcox, A. Jacobs, X. Li, & M. Zingale
2019, American Astronomical Society Meeting 233, 457.05
- 11. *Computational Astrophysics and Cosmology*
D. Fan, J. Sexton, & D. Willcox
2019, Computational Research Division Capability Review, Lawrence Berkeley National Laboratory
- 10. *pynucastro: Code Generation and Visualization for Nuclear Reaction Networks*,
D. E. Willcox, A. Jacobs, X. Li, & M. Zingale
Bay Area Scientific Computing Day 2018, Sandia National Laboratories, Livermore, CA, December 7, 2018.
- 9. *Three Dimensional Simulations of the Convective Urca Process in White Dwarf Progenitors of Type Ia Supernovae*,
D. E. Willcox, D. M. Townsley, M. Zingale, & A. C. Calder
2017, Current Challenges in the Physics of White Dwarf Stars, Santa Fe, NM, June 12-16, 2017.
- 8. *Elucidating the Convective Urca Process in Pre-Supernova White Dwarfs Using Three-Dimensional Simulations*,
D. E. Willcox, D. M. Townsley, M. Zingale, & A. C. Calder
2017, JINA-CEE Frontiers in Nuclear Astrophysics Meeting, February 7-9, 2017.

7. *Three-Dimensional Simulations of the Convective Urca Process in Pre-Supernova White Dwarfs*,
D. E. Willcox, D. M. Townsley, M. Zingale, & A. C. Calder
2017, American Astronomical Society Meeting 229, 244.05
6. *On the Quantification of Incertitude in Astrophysical Simulation Codes*,
M. M. Hoffman, M. P. Katz, D. E. Willcox, S. Ferson, F. D. Swesty, & A. C. Calder
2017, American Astronomical Society Meeting 229, 154.27
5. *Thermonuclear Supernova Explosions From Hybrid White Dwarf Progenitors*,
D. E. Willcox, D. M. Townsley, A. C. Calder, P. Denissenkov, & F. Herwig
2016, American Astronomical Society Meeting 227, 237.17
4. *A Comparison of Type Ia Supernovae with C-O and Hybrid C-O-Ne White Dwarf Progenitors*,
D. E. Willcox, D. M. Townsley, A. C. Calder, P. Denissenkov, & F. Herwig
2015, F.O.E. Fifty-One Erg International Workshop, North Carolina State University, NC.
3. *A Study of Steady-State Detonation Structures for Hybrid C, O, Ne White Dwarf Models*,
D. E. Willcox, D. M. Townsley, & A. C. Calder
2014, International Conference: "Type Ia Supernovae: Progenitors, Explosions, and Cosmology," University of Chicago, IL.
2. *Imaging Molecular Structure With High Harmonics*,
D. E. Willcox, M. A. Reber, Y. Chen, K. Halder, & T. Allison
2013, Chemistry Research Day, Stony Brook University, NY.
1. *Cavity-Enhanced Transient Absorption Spectroscopy*,
M. A. Reber, Y. Chen, D. E. Willcox, & T. Allison
2013, Chemistry Research Day, Stony Brook University, NY.

Non-Refereed Conference Proceedings:

3. *Implementation of Digital Radio Mondiale receiver - Part II*,
D. E. Willcox, J. Kim, & J. Wineman
2011, IEEE 43rd Southeastern Symposium on System Theory, Auburn, AL, March 2011.
2. *Implementation of Digital Radio Mondiale Receiver - Part I*,
D. E. Willcox, J. Kim, C. Loewen, & J. Wineman
2010, IEEE 42nd Southeastern Symposium on System Theory, Tyler, TX, March 2010.
1. *Diversity Receiver for Digital Radio Mondiale - a multi-year design project*,
P. Leiffer, J. Kim, R. W. Graff, & D. E. Willcox
2010, ASEE 2010 Annual Conference & Exposition, Louisville, KY, June 2010.