David Roundy
Curriculum Vitae

A. Education and Employment Information

Education

Ph.D. (2001)	in Physics, University of California at Berkeley. Thesis "Mechanical and Superconducting Properties of Materials from First Principles" **Ph.D. Advisor: Marvin L. Cohen**
B.A. (1995)	in Physics and Chemistry, University of California at Berkeley.

Professional Appointments

2014-Present	Associate Professor — Dept. of Physics, Oregon State University
2006-2014	Assistant Professor — Dept. of Physics, Oregon State University
2004-2006	Postdoctoral researcher — Dept. of Physics, Cornell University
2002-2003	Postdoctoral researcher — Dept. of Physics, Massachusetts Institute of Technology
1998-2001	Graduate Research Assistant — Dept. of Physics, University of California at Berkeley
1992-1996	Research Assistant — Dept. of Physics, California State University at Fullerton

B. Teaching, advising and other assignments

Course	**Term**	**Year**	**# students**
PH 631 Electromagnetic Theory	Fall	2006	5
PH 632 Electromagnetic Theory	Winter	2007	5
(teaching release time)	Spring	2007	
(unpaid personal leave)			
PH 265 Scientific Computing	Winter	2009	28
PH 423 Paradigms in Physics: Energy and Entropy	Spring	2009	15
PH 320 Paradigms in Physics: Symmetries and Idealizations	Fall	2009	24
PH 265 Scientific Computing	Winter	2010	26
PH 423 Paradigms in Physics: Energy and Entropy	Spring	2010	18
(2/3 FTE for the year)			
PH 265 Scientific Computing	Winter	2011	22
PH 423 Paradigms in Physics: Energy and Entropy	Spring	2011	25
(returning to 1.0 FTE)			
PH 365X Applications in Computational Physics I	Fall	2011	8
PH 265 Scientific Computing	Winter	2012	22
PH 366X Applications in Computational Physics II	Winter	2012	2
PH 423 Paradigms in Physics: Energy and Entropy	Spring	2012	38
PH 523 Paradigms in Physics: Energy and Entropy	Spring	2012	1

Course	**Term**	**Year**	**# students**
PH 367X Applications in Computational Physics III	Spring	2012	2
PH 320 Paradigms in Physics: Symmetries and Idealizations	Fall	2012	37
PH 365X Applications in Computational Physics I	Fall	2012	9
PH 366X Applications in Computational Physics II	Winter	2013	11
PH 265 Scientific Computing	Spring	2013	11
PH 423 Paradigms in Physics: Energy and Entropy	Spring	2013	28
PH 523 Paradigms in Physics: Energy and Entropy	Spring	2013	1
PH 367X Applications in Computational Physics III	Spring	2013	9
PH 320 Paradigms in Physics: Symmetries and Idealizations	Fall	2013	36
PH 365 Applications in Computational Physics I	Fall	2013	8
PH 223H Recitation for PH 213	Winter	2014	8
PH 366 Applications in Computational Physics II	Winter	2014	10
PH 423 Paradigms in Physics: Energy and Entropy	Spring	2014	35
PH 367 Applications in Computational Physics III	Spring	2014	7
PH 422 Paradigms in Physics: Static Vector Fields	Fall	2014	29
PH 365 Applications in Computational Physics I	Fall	2014	17
PH 366 Applications in Computational Physics II	Winter	2015	17
PH 367 Applications in Computational Physics III	Spring	2015	19
PH 464 Scientific Computing II	Spring	2015	6
(sabbatical leave)			
PH 265 Scientific Computing	Winter	2016	27
PH 366 Applications in Computational Physics II	Winter	2016	19
PH 367 Applications in Computational Physics III	Spring	2016	16
PH 365 Applications in Computational Physics I	Fall	2016	33
PH 642 Statistical Thermophysics	Fall	2016	9
PH 366 Computational Physics Lab I	Winter	2017	25
PH 426 Paradigms in Physics: Periodic Systems	Spring	2017	33
PH 367 Computational Physics Lab III	Spring	2017	24
PH 365 Computational Physics Lab I	Fall	2017	26
PH 366 Computational Physics Lab II	Winter	2018	24
PH 367 Computational Physics Lab III	Spring	2018	23
PH 441 Capstone: Thermal and Statistical Physics	Spring	2018	23
PH 367 Computational Physics Lab I	Fall	2018	44
PH 223H Recitation for PH 213	Winter	2019	23
PH 366 Computational Physics Lab II	Winter	2019	40
PH 441 Capstone: Thermal and Statistical Physics	Spring	2019	20
PH 367 Computational Physics Lab III	Spring	2019	42
Shadowed PH 315 Contemporary Challenges	Fall	2020	
PH 365 Computational Physics Lab I	Winter	2020	41
PH 366 Computational Physics Lab II	Spring	2020	35
PH 441 Capstone: Thermal and Statistical Physics	Spring	2020	36
PH 222H Recitation for PH 212	Fall	2020	8
PH 423 Paradigms in Physics: Energy and Entropy	Fall	2020	38
PH 365 Computational Physics Lab I	Winter	2021	35
PH 315 Physics of Contemporary Challenges	Spring	2021	17
PH 366 Computational Physics Lab II	Spring	2021	35

Curriculum Development

I have engaged in the three major course development projects, and one major curricular reform.

PH 423: *Energy and Entropy* While I was on unpaid leave prior to the winter of 2009, I joined a collaborative effort, funded by the NSF, to develop and test teacher materials for the dissemination of concepts in the *Energy and Entropy* Paradigm. As part of this work, I redesigned the course, developing a series of integrated experiments, and active engagement materials.

PH 265: *Introductory Scientific Computing* Also while I was on unpaid leave prior to the winter of 2009, I developed a new curriculum for PH 265, "Introductory Scientific Computing." I redesigned this course using Visual Python to help students begin using programming to solve physics problems. This resulted in an 88-page text with homework assignments that is available online for students or as a print-on-demand book (C.1.59). This text has since been used by other faculty in our department to teach this course, and has also been adopted at Linn-Benton Community College. This course has since been discontinued as part of the Paradigms 2.0 reform, see below.

PH 365, 366 and 367: *Computational Physics Lab* In 2010, I proposed and introduced a new upper-division computational laboratory course, inspired by my experiences developing the lower-division PH 265. The new course uses "pair programming," a known teaching method in Computer Science, with a goal of helping students who are not yet comfortable programming to become comfortable doing so with minimal help from the instructor. This course parallels the *Paradigms in Physics* content, in order to reinforce student learning in these critical middle-division courses, while at the same time reducing the cognitive load as students adapt to using computational methods to solve problems. I also received an NSF grant as sole PI to continue development of this lab.

Paradigms 2.0 In 2016, I was a member of the Paradigms 2.0 committee, which led a department-wide reform of our curriculum for physics majors. This process involved discussing the content of each upper-division class in the physics major, discussing what material should be prioritized and where we could develop synergies between classes, and finally developing a proposal for a revised set of courses that could address some longstanding challenges in our existing courses. After discussing and revising these plans with the department and reaching unanimity, I submitted the courses through the university curriculum proposal system, and the new courses were first taught in the 2016/2017 school year.

In 2019 the Paradigms 2.0 committee reviewed the outcome of this reform effort. After meeting with faculty and further discussion, we proposed a reordering of courses to address several issues that had arisen in the implemention of the Paradigms 2.0 redesign. The faculty again unanimously approved the changes after a few rounds of discussion and revision. The new ordering of courses is being introduced in the 2019/2020 academic year.

Graduate and Undergraduate Student Trainees and Postdoctoral Trainees

Ph.D. thesis advisor for:

		Graduation	Thesis
1. Dennis Jackson	Physics Ph.D.	2011	"An Ising-like model to predict dielectric properties of the relaxor ferroelectric solid solution $BaTiO_3$-$Bi(Zn_{1/2}Ti_{1/2})O_3$"
2. Jeff Schulte	Physics Ph.D.	2015	"Hard spheres within classical density functional theory and Min proteins within *Escherichia Coli*
3. Eric Krebs	Physics Ph.D.	2015	"Theory of inhomogeneous fluids"
4. Jordan Pommerenck	Physics Ph.D.	2020	"Advancing Renewable Gas Storage using Flat-histogram Methods"
5. Kirstie Finster	Physics Ph.D.	expected 2023	*Began in 2017 working on classical density functional theory for the Weeks-Chandler-Anderson fluid.*
6. Nickolas Gantzler	Physics Ph.D.	expected 2023	*Began in 2019 working on metal-organic framework Monte Carlo simulations for gas storage. Co-advised by Cory Simon, Assistant Professor of Chemical Engineering.*
7. Christian Solorio	Physics Ph.D.	expected 2023	*Began in 2019 studying student learning of quantum mechanics in a computational physics lab course.*

Masters thesis advisor for:

		Graduation	Thesis
8. Jason Dagit	Computer Science M.S.	2009	"Type Correct Changes—A Safe Approach to Version Control Implementation"
9. Jessica Hughes	Physics M.S.	2011	"A Classical Density-Functional Theory for Describing Water Interfaces"
10. Zhiyuan Zhang	Physics M.S.	2012	"A Code Generator for Density-Functional Theory in Haskell"
11. Daniel Roth	Physics M.S.	2014	"Applying Renormalization Group Theory to the Square Well Liquid"
12. Ryan Scheirer	Physics M.S.	2016	"Exploring Phase Equilibrium with Statistical non-Associating Fluid Theory: A Generalized Renormalization Group Theory Approach
13. Billy Geerhart III	Physics M.S.	2016	"Finding the arbitrary parameter L in Renormalization Group Theory via fitting Monte Carlo simulations to Statistical Associating Fluid Theory"

Senior project mentor for	Graduation	Thesis
14. Steve Brinkley	2010	"Measuring the Acoustic Response Function with White Noise"
15. Michael Nielson	2010	"Modeling the linear response function for broad frequency sound generation"
16. Murray Wade	2012	"Creating a Thermodynamics Simulation Using the Ising Model: A Microcanonical Monte Carlo Approach"
17. Rene Zeto	2014	"Testing the model for Min D protein oscillations in Escherichia coli"
18. Paho Lurie-Gregg	2014	"The contact value approximation to the pair distribution function for an inhomogeneous hard sphere fluid"
19. Michael Perlin	2015	"Optimizing Monte Carlo simulation of the square-well fluid"
20. Patrick Kreitzberg	2015	"Monte Carlo simulations for a soft sphere fluid"
21. Samuel Loomis	*Left program* 2014	*Studied interaction between spherically symmetric, softly repulsive particles.*
22. Josh Montegna	2015	"Determining the effective entropy of a visual hash system"
23. Austin Valeske	2015	"Determining free energies of hard sphere fluids via Monte Carlo simulation"
24. Brenden Vischer	2016	"The free energy of a liquid"
25. Elliott Capek	2017	"Simulating dynein's powerstroke using Brownian dynamics"
26. Chris May	2018	"Freezing a Softly Repulsive Fluid: Monte Carlo Methods and the Weeks-Chandler-Andersen Potential"
27. Joel Chantland	2018	"Evolving Boltzmann-Gibbs Income Distributions."
28. Tanner Simpson	2018	"Broad Histogram Algorithm Comparison for the Square Well Fluid"
29. Patrick Flynn	2018	*Studied square well fluid using grand canonical Monte Carlo, but did not do his thesis on this project.*
30. Garrett Jepson	*Left group 2018*	*Studied the Weeks-Chandler-Andersen fluid using Monte Carlo methods.*
31. Lahiru Fernando	Fall 2018	"Econophysics: Lagrangian Description of an Economic System"
32. John Waczak	2019	*Studying the dynein motor protein using Brownian dynamics simulation.*
33. Sean Mc Donough	2019	"Calculating Lift and Drag Forces on Surfboards using a Navier-Stokes solver and Momentum Conservation"
34. Cade Trotter	2019	"Multi-Grand, Multi-Canonical, Flat Histogram, Monte Carlo Simulations for the Square Well Fluid"

Senior project mentor for	Graduation	Thesis
35. Jacob Vande Griend	2020	"Simulating Fluids: Testing a New Grand Canonical Histogram Method on the Square-Well Fluid"
36. Jonathan Carney	2021	"Practical Mechanically Interlocked Molecules: A Model of Gaas Adsorption in Metal Organic Frameworks harboring Rotaxane Molecular Shuttles" (Co-advised by Cory Simon)
37. Jin Kiatvongcharoen	2021	"Simulating the Dynein Motor Protein: A Monte Carlo Approach to Achieve Coordinated Stepping"
38. Valerie Aranth	Expected 2022	*Studying histogram Monte Carlo methods.*
39. Nelson Kangethe	Expected 2022	*Using flat histogram Monte Carlo simulation to model the WCA fluid.*
40. Leah Holmes	Expected 2022	*Working on finer-grained analysis of flat-histogram Monte Carlo data.*
41. Henry Sprueill	Expected 2022	*Developed a potential energy function with two local minima for which the density of states is analytically solvable, for testing the convergence of Monte Carlo algorithms on a system with a phase transition.*

Research mentor for	Year	Major	Research topic
42. Lincoln Worley	2018	Mech. E.	*Worked to enable checkpointing in our Monte Carlo code.*
43. Felix Tyson	2018	Math	*Improved code generation in our classical density functional theory code.*
44. Josie O'Harrow	2019-2020	Math	*Used cubic interpolation to improve collection of histogram data.*
45. Noah Bean	2019-2020	Math	*Used 2D histogram methods to study a lattice gas.*

C. Scholarship and Creative Activity

1. Publications

Citation counts in the listing below are based on Google Scholar as of August 2021, which gives an h-index of 26—or 27 if you include one non-peer-reviewed publication, a conference proceedings article on Darcs.

key: my undergraduate student[UG]
my graduate student

Peer-reviewed articles, submitted

1. Jordan K. Pommerenck, Cory Simon, and **David Roundy**. An upper bound to gas delivery via pressure-swing adsorption in nanoporous materials. Submitted to *Materials Advances* (2020).

   This paper introduces a theoretical upper bound to the volumetric storage capacity of rigid porous materials based on the experimentally measured state properties of the gas. This upper bound—which omits any steric hindrance effecs—is very close to the targets set by the DOE for methane and hydrogen. This project was largely my theoretical work, inspired by discussions with Cory, who also was essential in the writing process. Jordan wrote the code that downloaded the experimental data from NIST, performed the unit conversions, compared with experimental results for real porous materials, and generated the figures.

Peer-reviewed articles, published

2. Christian D. Solorio, Elizabeth Gire, and **David Roundy**: Interactive remote interviews during emergency remote teaching. *Phys. Rev. Physics Education Research* **17** 020114 (2021). **0 citations**

   This paper was almost entirely written by my graduate student Christian. My contributions (and those of Prof. Gire) were advice in formulating and writing the paper, and assistance in proof reading and editing the paper, and revising it in response to referee criticism.

3. Melanie Huynh, Nickolas Gantzler, Samuel Hough, **David Roundy** Praveen Thallapally, Cory Simon Adsorbed xenon propellant storage: are nanoporous materials worth the weight? *Materials Advances*, **2**, 4081-4092 (2021). **0 citations**

   My contributions to this paper were relatively small. I assisted in checking the reasoning on the relationship between the yield strength, pressure, and required thickness of the tank walls. I also assisted in the final editing process.

4. Jordan K. Pommerenck, and **David Roundy**. Flat-histogram method comparison on the 2D Ising model. *Phys. Rev. E* **102** (3), 01886 (2020). **1 citations**

   This paper was mostly written by Jordan under my supervision.

5. Jonathan Carney$^{\mathrm{UG}}$, **David Roundy** and Cory M. Simon. Statistical thermodynamic model of gas adsorption in a metal-organic framework harboring a rotaxane molecular shuttle. *Langmuir* (43) 13112-13123 (2019). **3 citations**

   Cory had the original idea for a four-state model for gas adsorption on a metal-organic framework with a rotaxane on an axle. I met weekly with Jonathan and Cory to discuss the results and in particular to develop an explanation of the model's predictions. Cory did the bulk of of the writing, and helped write some sections and edit the paper as a whole.

6. Jordan K. Pommerenck, Tanner T. Simpson$^{\mathrm{UG}}$, Michael A. Perlin$^{\mathrm{UG}}$ and **David Roundy**. Stochastic Approximation Monte Carlo with a Dynamic Update Factor. *Physical Review E* **101** (1), 013301 (2020). **1 citations**

   This paper introduced a new flat histogram Monte Carlo algorithm. Michael originally wrote the Monte Carlo code that we used in this project, but was not part of the project for the finalization of the new algorithm. Jordan and I developed the new algorithm, and Tanner did a lot of running of simulations and wrote code to compare the convergence of a variety of flat histogram algorithms. Jordan and I wrote the paper.

7. Tevian Dray, Elizabeth Gire, Mary Bridget Kustusch, Corinne A Manogue, and **David Roundy**, Interpreting Derivatives, *Problems, Resources, and Issues in Mathematics Undergraduate Studies (PRIMUS)* (2019). **4 citations**

   This paper was written by Tevian, and my contributions were relatively minor, although the ideas in the paper came out of discussions we all had together.

8. **David Roundy**, Tevian Dray, Corinne A. Manogue, Joseph F. Wagner, and Eric Weber, An Extended Theoretical Framework for the Concept of the Derivative, *Proceedings of the 2015 Research in Undergraduate Math Education Conference* (2015). **21 citations**

   This paper was primarily my writing and the work was lead by myself, but involved intense discussions of the authors.

9. **David Roundy**, Eric J. Krebs, Jeff Schulte, and Greg Mulder. Look ma, no templates! Problem-based learning of computational physics for novice programmers, *Frontiers in Education proceedings* (2015).

   This conference paper was written by myself with editing assistance from Jeff and Eric, who helped me analyze the data from my Computational Physics Lab course.

10. **David Roundy**, Eric Weber, Tevian Dray, Rabindra R. Bajracharya, Allison Dorko, Emily M. Smith, and Corinne A. Manogue, Experts' understanding of partial derivatives using the Partial Derivative Machine, *Physical Review Special Topics: Physics Education Research* **11(2)**, 020126 (2015). **19 citations**

    This paper was a major expansion of the previous conference paper, and was again largely written by myself with contributions from the other authors.

11. Jeff Schulte, Rene Zeto[UG], and **David Roundy**. Theoretical Prediction of Disrupted Min Oscillation in Flattened *Escherichia coli*. *PLoS ONE*, **10(10)**, e0139813 (2015). **2 citations**

    This paper was largely Jeff's idea, and both Jeff and Rene worked on writing the code and running the simulations. Jeff and I did most of the writing of the paper, with editing assistance from Rene.

12. **David Roundy**, Eric Weber, Grant Sherer and Corinne A. Manogue. Experts' Understanding of Partial Derivatives Using the Partial Derivative Machine. *2014 Physics Education Research Conference Proceedings*, 227-230 (2014).

    This paper analyzed interviews of faculty in several fields on their interpretation of partial derivatives in an experimental context. Corinne and I conducted the interviews, and I wrote the bulk of the paper with contributions from the other authors.

13. Paho Lurie-Gregg[UG], Jeff Schulte and **D. Roundy**. Approach to approximating the pair distribution function of the inhomogeneous hard-sphere fluid. *Physical Review E*, **90**, 042130 (2014). **6 citations**

    This paper examines approximations for the average of the pair distribution of a hard-sphere fluid, which is a key input to Statistical Associating Fluid Theory (SAFT). Paho performed Monte Carlo simulations of the pair distribution function for inhomogeneous systems, and Jeff developed a classical density functional theory for the contact density. Each of us contributed similarly in actually writing the paper.

14. Eric Krebs, Jeff Schulte, **David Roundy**. Improved association in a classical density functional theory for water. *Journal of Chemical Physics*, **140**, 124507 (2014). **8 citations**

    This paper describes an extension of our classical density functional for water, which incorporates the approach for correlation from publication C.1.21 below. The paper is written primarily by Eric and myself, and Eric did the bulk of the work that was specific to this paper, while Jeff assisted in editing the paper, and created the functional for correlation that gives the paper its purpose.

15. Mary Bridget Kustusch, **David Roundy**, Tevian Dray, and Corinne Manogue. Partial Derivative Games in Thermodynamics: A Cognitive Task Analysis. *Physical Review Special Topics – Physics Education Research*, 10(1):010101, (2014). **28 citations**

    This paper presents education research done primarily by Dr. Kustusch, who is a postdoc of Prof. Manogue. This research was inspired by an activity I introduced in the *Energy and Entropy* course. It analyzes expert responses in interviews by Dr. Kustusch to a thermodynamics problem that I developed. The paper was primarily written by Dr. Kustusch, with the other authors, including myself, strongly involved in editing and improving the paper.

16. **David Roundy**, Mary Bridget Kustusch, and Corinne Manogue. Name the Experiment! interpreting thermodynamic derivatives as thought experiments *American Journal of Physics*, 82(1):39-46, (2014). **11 citations**

This paper describes a sequence of activities that I developed to help students connect thermodynamic partial derivatives with experimental measurements. The paper was written by myself, with a small portion written by Dr. Kustusch, who is a postdoc of Prof. Corinne Manogue, regarding results of student interviews that she performed.

17. Grant Scherer, Mary Bridget Kustusch, Corinne A. Manogue, and **David Roundy**. The Partial Derivative Machine. *2013 Physics Education Research Conference Proceedings—American Institute of Physics*, pages 341-344, (2013). **6 citations**

    This paper was primarily written by Grant Scherer, who is an undergraduate student working on his senior thesis research under the supervision of Prof. Corinne Manogue. The paper describes the pedagogical use of a device that I developed as a mechanical analogue of a thermodynamic system, for teaching students properties of partial derivatives in a more familiar setting. I was heavily involved in every stage of the writing and editing of this paper.

18. Mary Bridget Kustusch, **David Roundy**, Tevian Dray, and Corinne Manogue. An expert path through a thermo maze. In *2012 Physics Education Research Conference Proceedings—American Institute of Physics*, volume 1513, page 234, (2013). **7 citations**

    The PERC conference proceedings publishes both peer-reviewed and non-peer-reviewed articles. This article is peer-reviewed, while the article on derivatives in thermodynamics (paper #56 below) is *not* peer-reviewed, although it is in the same journal. My contribution to this paper was first in creating the thermodynamics problem that was studied, participating in discussions regarding the research and its understanding and finally in assisting to edit the paper. The research itself was done by Mary Bridget Kustusch, who is a postdoc of Prof. Corinne Manogue.

19. Jessica Hughes, Eric Krebs, **David Roundy**. A classical density-functional theory for describing water interfaces. *The Journal of Chemical Physics* **138**(2), 024509–024509 (2013). **45 citations**

    This paper describes a new classical density functional for water. I developed the functional myself, and wrote the code to implement it. Jessica and Eric wrote code to apply the functional in different scenarios, and ran this code to create the data presented in the paper. Most of the figures in the paper were created by my two graduate students, while I wrote most of the text.

20. **D. Roundy** and M. Rogers. Exploring the thermodynamics of a rubber band. *The American Journal of Physics* **81**, 20 (2013). **30 citations**

    This paper describes an experiment that I developed, which uses a Maxwell relation and measurement of tension as a function of both temperature and length to perform a measurement of changes in entropy, internal energy and free energy. It was based on a much simpler experiment used by Prof. Rogers, who also assisted in editing the paper.

21. Jeff Schulte, Patrick Kreitzburg$^{\mathrm{UG}}$, Chris Haglund$^{\mathrm{UG}}$ and **D. Roundy**. Using Fundamental Measure Theory to Treat the Correlation Function of the Inhomogeneous Hard-Sphere Fluid. *Physical Review E* **86**, 061201 (2012). **11 citations**

    This paper describes a continuum approximation for the correlation of hard spheres at the point of contact. We test this approximation by comparing with a Monte Carlo simulation. The code to do the Monte Carlo simulation was initially written by Chris, and was then extended to different boundary conditions by Patrick with assistance and oversight from Jeff. I developed one continuum approximation before Jeff began working with me, and then Jeff and I together developed a second approximation. With my assistance, Jeff implemented and debugged our continuum approximations. The paper itself was primarily written by myself, with assistance from Jeff in the editing process.

22. L. Prisbrey, **D. Roundy**, K. Blank, L.S. Fifield, and E.D. Minot. Electrical Characteristics of Carbon Nanotube Devices Prepared with Single Oxidative Point Defects. *The Journal of Physical Chemistry C* **116**(2), 1961 – 1965 (2012). **14 citations**

All experimental work was performed by L. Prisbey under the supervision of Prof. Minot. I was responsible for numerical modeling of transport properties. Dr. Blank and Dr. Fifield contributed to discussions, editing, and planning experiments.

23. A.F. Oskooi, **D. Roundy**, M. Ibanescu, P. Bermel, J.D. Joannopoulos, and S.G. Johnson. Meep: A flexible free-software package for electromagnetic simulations by the FDTD method. *Computer Physics Communications* **181**(3), 687 – 702 (2010). **2485 citations**

    This paper was primarily written by Ardavan, the first author, and describes Meep, a software package that I created, which has since been improved by a number of collaborators. The majority of the text of this paper describes features that I added to the code, including general principles, such as "pervasive interpolation" to provide the illusion of continuity.

24. Daniel A. Freedman, **D. Roundy**, and T. A. Arias. Elastic effects of vacancies in strontium titanate: Short- and long-range strain fields, elastic dipole tensors, and chemical strain. *Phys. Rev. B* **80**(6), 064108 (2009). **134 citations**

    The research described in this paper took place during my unpaid leave of absence, in the year of 2008. Daniel, the first author, was a graduate student of Tomás Arias, my former postdoctoral advisor. I did a number of calculations using density functional theory that were included in the paper, and was heavily involved in the writing of the paper.

25. Sahak A. Petrosyan, Jean Francois Briere, **David Roundy**, and Tomás A. Arias. Joint density-functional theory for electronic structure of solvated systems. *Phys. Rev. B* **75**(20), 205105 (2007). **56 citations**

    This paper describes research that I did as a postdoc of Tomás Arias at Cornell. I was deeply involved with Sahak in the creation of the theory and proof that lie at the heart of the paper. I also closely adviced Jean Francois, who performed computations to demonstrate our theory, and wrote much of the code that we used to generate the results in the paper.

26. A. Farjadpour, **D. Roundy**, Alejandro Rodriguez, M. Ibanescu, Peter Bermel, J. D. Joannopoulos, Steven G. Johnson, and G. W. Burr. Improving accuracy by subpixel smoothing in the finite-difference time domain. *Optics Letters* **31**(20), 2972–2974 (2006). **559 citations**

    This is a paper describing research that I began as a postdoc with John Joannopoulos at MIT. It was the first paper to result from the development of the Meep code. I had just initiated this subpixel smoothing project when I left for my second postdoc at Cornell, so most of the research presented in the final paper—as well as the majority of writing—was done by other authors.

27. H. Üstünel, **D. Roundy**, and T. A. Arias. Modeling a suspended nanotube oscillator. *Nano Letters* **5**(3), 523–526 (2005). **98 citations**

28. M. Ibanescu, S. G. Johnson, **D. Roundy**, Y. Fink, and J. D. Joannopoulos. Microcavity confinement based on an anomalous zero group-velocity waveguide mode. *Optics Letters* **30**(5), 552–554 (2005). **49 citations**

29. H. Üstünel, **D. Roundy**, and T. A. Arias. *Ab initio* mechanical response: internal friction and structure of divacancies in silicon. *Phys. Rev. Lett.* **94**, 025503 (2005). **7 citations**

30. **D. Roundy**, E. Lidoriki, and J. D. Joannopoulos. Polarization-selective waveguide bends in a photonic crystal with layered square symmetry. *J. Appl. Phys.* **96**(12), 7750–7752 (2004). **8 citations**

31. V. Sazonova, Y. Yaish, H. Üstünel, **D. Roundy**, P. L. McEuen, and T. A. Arias. A tunable carbon nanotube electromechanical oscillator. *Nature* **431**, 284–287 (2004). **1570 citations**

32. M. Ibanescu, S. G. Johnson, **D. Roundy**, C. Luo, Y. Fink, and J. D. Joannopoulos. Anomalous dispersion relations by symmetry breaking in axially uniform waveguides. *Phys. Rev. Lett.* **92**(6), 063903 (2004). **82 citations**

33. **D. Roundy** and John Joannopoulos. Photonic crystal structure with square symmetry within each layer and a three-dimensional band gap. *App. Phys. Lett.* **82**(22), 3835 (2003). **43 citations**

34. Seung-Hoon Jhi, **D. Roundy**, S. G. Louie, and M. L. Cohen. Formation and electronic properties of double-walled boron nitride nanotubes. *Solid State Commun.* **134**, 397–402 (2005). **56 citations**

35. R. E. Kraig, **D. Roundy**, and M. L. Cohen. A study of the mechanical and structural properties of polonium. *Solid State Commun.* **129**(6), 411–413 (2004). **22 citations**

36. Hong Sun, F. J. Ribeiro, Je-Luen Li, **D. Roundy**, M. L. Cohen, and S. G. Louie. *Ab initio* pseudopotential studies of equilibrium lattice structures and phonon modes of bulk BC_3. *Phys. Rev. B* **69**, 024110 (2004). **42 citations**

37. H. J. Choi, **D. Roundy**, H. Sun, M. L. Cohen, and S. G. Louie. Reply to "Comment on 'First-principles calculation of the superconducting transition in MgB_2 within the anisotropic Eliashberg formalism.' " *Phys. Rev. B* **69**(5), 056502 (2004). **18 citations**

38. W. Luo, **D. Roundy**, M. L. Cohen, and J. W. Morris, Jr. Ideal strength of bcc molybdenum and niobium. *Phys. Rev. B* **66**, 094110 (2002). **221 citations**

39. F. J Ribeiro, **D. Roundy**, and M. L. Cohen. Electronic Properties of MoSe nanowires. *Phys. Rev. B* **65**, 153401 (2002). **41 citations**

40. C. R. Krenn, **D. Roundy**, M. L. Cohen, D. C. Chrzan, and J. W. Morris, Jr. Connecting Atomistic and Experimental Estimates of Ideal Strength. *Phys. Rev. B* **65**, 134111 (2002). **143 citations**

41. H. J. Choi, **D. Roundy**, H. Sun, M. L. Cohen, and S. G. Louie. The origin of the anomalous superconducting properties of MgB_2. *Nature* **418**, 758–760 August (2002). **1063 citations**

42. H. J. Choi, **D. Roundy**, H. Sun, M. L. Cohen, and S. G. Louie. First-principles calculation of the superconducting transition in MgB_2 within the anisotropic Eliashberg formalism. *Phys. Rev. B* **66**, 020513 (2002). **377 citations**

43. **D. Roundy** and M. L. Cohen. Ideal strength of diamond, Si and Ge. *Phys. Rev. B* **64**, 212103 (2001). **298 citations**

44. C. R. Krenn, **D. Roundy**, J. W. Morris, Jr., and M. L. Cohen. The Ideal Strengths of BCC Metals. *Mat. Sci. Eng. A* **319**, 111–114 (2001). **115 citations**

45. H. Sun, S. H. Jhi, **D. Roundy**, M. L. Cohen, and S. G. Louie. Structural forms of cubic BC_2N. *Phys. Rev. B* **64**(9), 094108 (2001). **193 citations**

46. J. W. Morris, Jr., C. R. Krenn, **D. Roundy**, and M L Cohen. Deformation at the limit of elastic stability. *Mat. Sci. Eng. A* **309**, 121–124 (2001). **26 citations**

47. C. R. Krenn, **D. Roundy**, J. W. Morris, Jr., and M. L. Cohen. The non-linear elastic behavior and ideal shear strength of Al and Cu. *Mat. Sci. Eng. A* **317**, 44–48 (2001). **43 citations**

48. **D. Roundy**, C. R. Krenn, M. L. Cohen, and J. W. Morris, Jr. The ideal strength of tungsten. *Phil. Mag. A* **81**(7), 1725 (2001). **265 citations**

49. **D. Roundy**, C. R. Krenn, M. L. Cohen, and J. W. Morris, Jr. Ideal shear strengths of fcc Aluminum and Copper. *Phys. Rev. Lett.* **82**(13), 2713 (1999). **454 citations**

50. M. A. Khakoo, **D. Roundy**, C. Hicks, N. Margolis, E. Yeung, A. W. Ross, and T. J. Gay. Monte Carlo studies of Mott scattering asymmetries from gold foils. *Phys. Rev. A* **64**(5), 052713 (2001). **17 citations**

51. F. Rugamas, **D. Roundy**, G. Mikaelian, G. Vitug, M. Rudner, J. Shih, D. Smith, J. Segura, and M. A. Khakoo. Angular profiles of molecular beams from effusive tube sources: I. Experiment. *Measurement Science and Technology* **11**(12), 1750–1765 (2000). **48 citations**

52. M. A. Khakoo, **D. Roundy**, and F. Rugamas. Electron-impact excitation of the ^{1}S$\to^3$1P and ^{1}S$\to$431P transition in Helium. *Phys. Rev. A* **54**(5), 4004–4014 (1996). **12 citations**

53. M. A. Khakoo, **D. Roundy**, and F. Rugamas. Electron-impact excitation of the ^{1}1S$\to^3$1P transition in Helium. *Phys. Rev. Lett.* **75**(1), 41–44 (1995). **7 citations**

Conference Proceedings (not peer-reviewed) and Invited Review Articles

54. **David Roundy**, Ayush Gupta, Joseph F. Wagner, Tevian Dray, Mary Bridget Kustusch, Emily van Zee, and Corinne A. Manogue. From Fear to Fun in Thermodynamics. In *2013 Physics Education Research Conference Proceedings—American Institute of Physics*, 42–45 (2013). **3 citations**

55. Corinne A. Manogue, Elizabeth Gire, and **David Roundy**. Tangible Metaphors. In *2013 Physics Education Research Conference Proceedings—American Institute of Physics*, 27–30 (2013). **7 citations**

56. J.R. Thompson, C.A. Manogue, **D.J. Roundy**, D.B. Mountcastle. Representations of partial derivatives in thermodynamics. In *2011 Physics Education Research Conference Proceedings—American Institute of Physics*, volume 1413, page 85, (2012). **16 citations**

57. D. Roundy. Darcs: distributed version management in Haskell. In *Proceedings of the 2005 ACM SIGPLAN workshop on Haskell*, pages 1–4. ACM, (2005). **62 citations**

Published curricular materials

58. **D. Roundy**, Paradigms website, `http://www.physics.oregonstate.edu/portfolioswiki/topic:thermodynamics`, Energy and Entropy curricular materials, including instructor guides to 17 class activities and 3 integrated laboratory experiments.

59. **D. Roundy**, *Introduction to Computational Physics*. `http://www.lulu.com/shop/david-roundy/introduction-to-computational-physics/paperback/product-15149034.html`

2. Meeting participation

In the list below, in the interest of brevity I have omitted the 12 non-invited talks given before I came to Oregon State University.

1. Physics Education Research Conference (PERC): Co-authored the poster "How Students Organize Quantum Concepts and Representations: A Card Sorting Task" (2021).

2. Physics Education Research Conference (PERC): Presented the poster "The new Paradigms in Physics Curriculum Website" (2021).

3. AAPT Summer meeting: Presented the talk "Introducing the new Paradigms in Physics Curriculum Website" (2021).

4. AAPT Summer meeting: Co-authored the talk "Computation to Support Understanding of Discrete and Continuous Quantum Systems" presented by Christian Solorio (2021).

5. AAPT Summer meeting: Presented the talk "Introducing the new Paradigms in Physics Curriculum Website" (2021).

6. APS March Meeting in Denver: Co-authored the talk "A theoretical upper bound on gas deliverable capacity via pressure-swing adsorption in nanoporous materials" presented by Jordan Pommerenck (2020).

7. Undergraduate Research Symposium at Oregon State University: Co-authored the poster “Simulating the walk of the dynein motor protein” presented by Jin Kiatvongcharoen (2019).
8. Celebrating Undergraduate Excellence at Oregon State University: Co-authored the poster “Simulating Dynein’s Walk Using Monte Carlo Methods” presented by Jin Kiatvongcharoen (2019).
9. Annual Meeting of the APS Northwest Section: Co-authored the poster “Multi-Grand, Multi-Canonical, Flat Histogram, Monte Carlo Simulations for the Square Well Fluid” presented by Cade Trotter (2019).
10. Annual Meeting of the APS Northwest Section: Co-authored the talk “An upper bound to gas delivery via pressure-swing adsorption in nanoporous materials” presented by Jordan Pommerenck (2019).
11. Teaching T.A.L.K.S. IV in Corvallis, which is a conference on assessment: Participated (2018).
12. Conference on Research in Undergraduate Mathematics Education (RUME) in San Diego: Co-organized the working group “Education Research at the interface of Mathematics and Physics: ‘Thick’ Derivatives” (2018).
13. AAPT Winter Meeting in San Diego: Presented the talk “Name the Experiment! Relating Thermal Derivatives with the Real World” (2018).
14. Undergraduate Research Symposium at Oregon State University: Co-authored the talk “Broad histogram algorithm comparison for the square well fluid” presented by Tanner Simpson (2017).
15. Physics Education Research Conference (PERC): Presented the poster “Paradigms in Physics 2.0” (2017).
16. 18th Annual Meeting of the APS Northwest Section: Co-authored the talk “Simulating dynein’s powerstroke using Brownian dynamics” presented by Elliott Capek (2017).
17. Undergraduate Research Symposium at Oregon State University: Co-authored the talk “Using Brownian Dynamics to simulate the dynein motor protein” presented by Elliott Capek (2016).
18. Foundations and Frontiers of Physics Education Research: Puget Sound 2016 in Diablo, WA: Presented the poster “Calculus learning goals for thermodynamics and the Partial Derivative Machine” (2016).
19. Frontiers in Educatin (FIE) 2015 in El Paso: Presented the talk “Look ma, no templates! Problem-based learning of computational physics for novice programmers” (2015).
20. **(invited)** Northwest Section Meeting of the APS: Presented the talk “Making calculus tangible” (2015) (actually presented by student MacKenzie Lenz, due to family illness).
21. Research in Undergraduate Math Education Conference (RUME) in Pittsburgh: Presented the talk “An Extended Theoretical Framework for the Concept of Derivative” (2015).
22. Physics Education Research Conference (PERC) in Minneapolis: Presented the poster “Experts’ understanding of partial derivatives using the Partial Derivative Machine” (2014).
23. AAPT Summer Meeting in Minneapolis: Presented the talk “Integration in Electrostatics with a Computational Perspective” (2014).
24. Workshop on the Status of the Upper-Division Physics Curriculum: Presented the talk “Connecting math with experiment in thermal physics” (2014).
25. AAPT Summer Meeting in Portland: Presented the talk “Learning through Computation in Upper-Division Physics” (2013).

26. Physics Education Research Conference (PERC) in Portland: Co-organized the workshop "From Fear to Fun in Thermodynamics: Multiple Research Perspectives for Assessing Learning during a Curricular Sequence" that showcased curricular materials that I developed (2013).

27. Physics Education Research Conference (PERC) in Portland: Co-authored the poster "The Partial Derivative Machine," presented by undergraduate student Grant Scherer (2013).

28. **(invited poster)** Physics Education Research Conference (PERC) in Portland: Co-authored the poster "Tangible Metaphors," presented by Corinne Manogue (2013).

29. APS March Meeting in Baltimore: Co-authored the talk "Testing 'Soft' Fundamental Measure Theory for not-so-hard-sphere fluids" presented by my student Eric Krebs (2013).

30. APS March Meeting in Baltimore: Co-authored the talk "Using fundamental measure theory to treat the correlation function of the inhomogeneous hard-sphere fluid" presented by my student Jeff Schulte (2013).

31. NSF TUES Principal Investigators Conference in Washington, DC: Presented the poster "An Expert Path Through a Thermo Maze" (2013).

32. APS March Meeting in Boston: presented the talk "A SAFT-based classical density functional for water" (2012).

33. Physics Education Research Conference (PERC) in Philadelphia: Co-authored the poster "An Expert Path Through a Thermo Maze," presented by postdoc Mary Bridget Kustusch (2012).

34. **(invited poster)** Physics Education Research Conference (PERC) in Omaha: Co-authored the poster "Representations of Partial Derivatives in Thermodynamics," presented by collaborator John R. Thompson (2011).

35. NSF CCLI/TUES Principal Investigators Conference in Washington, DC: Presented the poster "Energy and Entropy in the Paradigms Curriculum" (2011).

36. APS March Meeting in Portland: Co-authored the talk "Dielectric properties of the $BaTiO_3$–$Bi(Zn_{\frac{1}{2}}Ti_{\frac{1}{2}})0_3$ solid solution from density-functional theory," presented by my student Dennis Jackson (2010).

37. AAPT Summer Meeting in Portland: Presented the talk "Energy and Entropy and More" (2010).

38. APS March Meeting in Pittsburgh: Co-authored the talk "Density-functional study of the of the $Ba_xBi_{(1-x)}(M_{(1-x)/2})Ti_{(1+x)/2}O_3$ perovskite solid solution," presented by my student Dennis Jackson (2009).

39. **(invited)** Oregon AAPT: Presented the talk "A first course in Computational Physics using visual python" (Sept. 2008).

40. APS March Meeting in New Orleans: Presented the talk "A classical density functional for water," presented by my student Dennis Jackson (2008).

41. **(invited)** APS March Meeting in Baltimore: I presented the talk "Losses due to phonon-phonon interactions in nanotube oscillators: from classical potentials through one-dimensional elasticity and many-body perturbation theory" (2006).

42. **(invited)** Free and Open source Software Developers' European Meeting (FOSDEM) in Brussels: I presented the talk "The Darcs Patch Formalism" (2006).

43. **(invited)** Haskell Workshop at the International Conference on Functional Programming in Estonia: I presented the talk "Darcs: Distributed Version Management in Haskell" (2005).

44. **(invited)** Commercial Users of Functional Programming, at the International Conference on Functional Programming in Estonia: I presented the talk "The Myth and Reality of using Haskell in the Real World" (2005).

45. **(invited)** Electronic Structure conference at Cornell: I presented the talk "Internal Friction and the Silicon Divacancy" (2005).

46. **(invited)** MRS Fall Meeting in Boston: I presented the talk "Computation of the ideal strength" (2000).

3. Funding

Pending grants

PIs: Minot, **Roundy** 1/1/2022 – 9/31/2023
Oregon State University Open Educational Resources $8,000
A proposal to create an open textbook for The Physics of Contemporary Challenges.
PI: **Roundy** co-PIs: Simon 6/1/2022 – 6/1/2025
National Science Foundation $494,314
Efficient Molecular Simulation at all Temperatures and Chemical Potentials

Current/Past awarded grants

PI: **Roundy** co-PIs: Dray, Gire, and Manogue 01/01/2018 – 12/31/2022
National Science Foundation $298,948
Paradigms in Physics: Second-Generation Dissemination Strategies

PI: Gire co-PIs: Dray, **Roundy**, and Manogue 01/01/2018 – 12/31/2022
National Science Foundation $299,282
Paradigms in Physics: Representations in Quantum Mechanics

PI: **Roundy** 1/30/2020 – 2/1/2021
College of Science Research and Innovation Seed Program $10,000
Developing new molecular simulation techniques to discover materials for clean energy applications

PI: Hjorth-Jensen, participants: Malthe-Sørenssen, Caballero, Mørken, Wahlstrøm Tellefsen, Henriksen, Sawtelle, O'Shea, Lockwood, **Roundy**, and Gire 1/1/2019 – 12/31/2021
Research Council of Norway, INTPART programme ∼\$660,000
International Partnership for Computing in Science Education (OSU component \$0)

This Norwegian grant supports travel for collaboration on the development of curricular materials for computational science education.

PI: Manogue, co-PIs: Weber, **Roundy**, Dray, van Zee 09/01/2013 – 08/31/2016
National Science Foundation $599,487
Paradigms in Physics: Representations of Partial Derivatives

PI: Roundy 06/01/2012 – 05/30/2014
National Science Foundation $124,236
Developing a computational physics lab integrated with upper-division physics content

PI: Roundy, co-PI: C.A. Manogue, collaborative PIs: M. Rogers, J.R. Thompson 2/15/09 – 2/14/13
National Science Foundation $149,998
Collaborative Research: Paradigms in Physics: Creating and Testing Materials to Facilitate Dissemination of the Energy and Entropy Module (OSU component $44,563)

PI: Minot, co-PIs: Schneider, **Roundy**, Fifield, Chapman 1/1/09 – 12/31/09
Office of Naval Research $230,000
ONAMI: Electronic detection of single molecule dynamics
(Roundy component $3,600)

Student awards

Award	Student	Year	Amount
URSA Engage	Elliott Capek	2014	$1,500
URSA Engage	Felix Tyson	2018	$1,000
URSA Engage	Jin Kiatvongcharoen	2019	$1,000
SURE Science	Jin Kiatvongcharoen	2019	$5,500
URSA Engage	Nelson Kangethe	2020	$1,000
URSA Engage	Leah Holmes	2021	$1,000

4. Other

Invited colloquia and seminars

October 2015 University of Texas, El Paso, Physics Seminar:
"Making Calculus Tangible to Physics Majors"

September 2014 Presented at "Global Physics Department":
"Making Calculus tangible to Physics majors"

September 2014 Presented at "Global Physics Department":
"Using the Partial Derivative Machine"

November 2013 Reed College, Physics Seminar:
"A tale of two E's: Energy and entropy in aqueous interfaces"

November 2013 Lewis and Clark College, Physics Colloquium:
"A tale of two E's: Energy and entropy in aqueous interfaces"

October 2013 Oregon State University, Physics Colloquium:
"Equipping students to connect multivariable calculus with the physical world"

October 2013 Willamette University, Physics Seminar:
"A tale of two E's: Energy and entropy in aqueous interfaces"

September 2013 Texas A & M, Physics Colloquium:
"Active learning in upper-division physics: lessons from the Paradigms"

September 2013 Purdue, Physics Education Seminar:
"Active learning in upper-division physics: lessons from the Paradigms"

September 2013 Purdue, Condensed Matter Seminar:
"A tale of two E's: Energy and entropy in aqueous interfaces"

April 2013 University of Oregon, Physics Colloquium:
"A tale of two E's: Energy and entropy in aqueous interfaces"

October 2012 Oregon State University, Physics Colloquium:
"A tale of two E's: Energy and entropy in aqueous interfaces"

November 2006 Oregon State University, Computer Science Colloquium:
"Verifying the darcs patch code"

October 2006 Oregon State University, Physics Colloquium:
"Classical density functional theory for water"

D. Service

1. Diversity

Faculty-Student Mentor Program (2018) In this program I met every other week with two first-generation or underrepresented minority college students who just started at Oregon State University. We discussed the "hidden curriculum," where they came from, and what they needed to do to succeed in the university.

Bias intervention training (2020) I attended a two-hour workshop by the Office of Insitutional Diversity to build skill in responding to bias incidents and microaggessions as they arise.

White Men Engaging in Anti-Racism (2020) Participated in a seven hour workshop on anti-racism facilitated by Oni Marchbanks and Anakha Coman.

Physicists for Inclusion in Science (PhIS) coffee break (2018-2020) I met with students interested in talking with a faculty member about Physics and our department. This program is an excellent way to help new students to feel connected with the department.

Search advocate workshop (2021) Attended the Search Advocate Workshop, a training program covering issues of implicit bias and inclusive hiring practices.

E. Awards

1. National and International

1. 1997 NSF Graduate Fellowship Honorable Mention
2. 1995 Phi Beta Kappa Inductee

2. University and Community

1. 1995 Merck Index Award