

# 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
<i>(teaching release time)</i>	Spring	2007	
<i>(unpaid personal leave)</i>			
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
<i>(2/3 FTE for the year)</i>			
PH 265 Scientific Computing	Winter	2011	22
PH 423 Paradigms in Physics: Energy and Entropy	Spring	2011	25
<i>(returning to 1.0 FTE)</i>			
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
<i>(sabbatical leave)</i>			
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

## 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.1.56). 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 implementation 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 $\text{BaTiO}_3\text{-Bi}(\text{Zn}_{1/2}\text{Ti}_{1/2})\text{O}_3$ ”
2. Jeff Schulte	Physics Ph.D.	2015	“Hard spheres within classical density functional theory and Min proteins within <i>Escherichia Coli</i> ”
3. Eric Krebs	Physics Ph.D.	2015	“Theory of inhomogeneous fluids”
4. Jordan Pommerenck	Physics Ph.D.	<i>expected 2020</i>	<i>Began in 2017 using Monte Carlo simulations to study the phase diagram of the square well fluid.</i>
5. Kirstie Finster	Physics Ph.D.	expected 2022	<i>Began in 2017 working on classical density functional theory for the Weeks-Chandler-Anderson fluid.</i>
6. Nickolas Gantzer	Physics Ph.D.	expected 2023	<i>Began in 2019 working on metal-organic framework Monte Carlo simulations for gas storage. Co-advised by Cory Simon, Assistant Professor of Chemical Engineering.</i>
7. Christian Solorio	Physics Ph.D.	expected 2023	<i>Began in 2019 studying student learning of quantum mechanics in a computational physics lab course.</i>

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	<i>Left program 2014</i>	<i>Studied interaction between spherically symmetric, softly repulsive particles.</i>
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	<i>Studied square well fluid using grand canonical Monte Carlo, but did not do his thesis on this project.</i>
30. Garrett Jepson	<i>Left group 2018</i>	<i>Studied the Weeks-Chandler-Andersen fluid using Monte Carlo methods.</i>
31. Lahiru Fernando	Fall 2018	“Econophysics: Lagrangian Description of an Economic System”
32. John Waczak	2019	<i>Studying the dynein motor protein using Brownian dynamics simulation.</i>
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	Expected 2020	<i>Currently developing a way to plot and compare two color plots on the same axes (which will be useful for the dynein project).</i>
36. Jin Kiatvongcharoen	Expected 2021	<i>Studying the dynein motor protein using Monte Carlo simulation.</i>
37. Valerie Aranth	Expected 2021	<i>Studying histogram Monte Carlo methods.</i>
38. Nelson Kangethe	Expected 2022	<i>Using flat histogram Monte Carlo simulation to model the WCA fluid.</i>

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

## C. Scholarship and Creative Activity

---

### 1. Publications

---

Citation counts in the listing below are based on Google Scholar as of October 2019, which gives an h-index of 26—which does include one non-peer-reviewed publication, a conference proceeding on Darcs.

key: my undergraduate student<sup>UG</sup>  
my graduate student

#### Peer-reviewed articles, in preparation

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

#### Peer-reviewed articles, submitted

2. Jonathan Carney<sup>UG</sup>, **David Roundy** and Cory M. Simon. Statistical thermodynamic model of gas adsorption in a metal-organic framework harboring a rotaxane molecular shuttle. Submitted to *Langmuir* (2019).

#### Peer-reviewed articles, published

3. Jordan K. Pommerenck, Tanner T. Simpson<sup>UG</sup>, Michael A. Perlin<sup>UG</sup> and **David Roundy**. Stochastic Approximation Monte Carlo with a Dynamic Update Factor. *Physical Review E* (2020).
4. Tevian Dray, Elizabeth Gire, Mary Bridget Kustusich, Corinne A Manogue, and **David Roundy**, Interpreting Derivatives, *Problems, Resources, and Issues in Mathematics Undergraduate Studies (PRIMUS)* (2019). **2 citations**
5. **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). **12 citations**

6. **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).
7. **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). **11 citations**
8. [Jeff Schulte](#), [Rene Zeto](#)<sup>UG</sup>, and **David Roundy**. Theoretical Prediction of Disrupted Min Oscillation in Flattened *Escherichia coli*. *PLoS ONE*, **10(10)**, e0139813 (2015). **1 citations**
9. **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).
10. Paho Lurie-Gregg<sup>UG</sup>, [Jeff Schulte](#) and **D. Roundy**. Approach to approximating the pair distribution function of the inhomogeneous hard-sphere fluid. *Physical Review E*, **90**, 042130 (2014). **4 citations**
11. [Eric Krebs](#), [Jeff Schulte](#), **David Roundy**. Improved association in a classical density functional theory for water. *Journal of Chemical Physics*, **140**, 124507 (2014). **6 citations**
12. 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). **22 citations**
13. **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**
14. 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). **5 citations**
15. 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). **6 citations**
16. [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). **37 citations**
17. **D. Roundy** and M. Rogers. Exploring the thermodynamics of a rubber band. *The American Journal of Physics* **81**, 20 (2013). **22 citations**
18. [Jeff Schulte](#), [Patrick Kreitzburg](#)<sup>UG</sup>, [Chris Haglund](#)<sup>UG</sup> 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**
19. 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**
20. 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). **2093 citations**

21. 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). **111 citations**
22. 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). **43 citations**
23. 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). **512 citations**
24. H. Üstünel, **D. Roundy**, and T. A. Arias. Modeling a suspended nanotube oscillator. *Nano Letters* **5**(3), 523–526 (2005). **91 citations**
25. 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). **47 citations**
26. 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). **6 citations**
27. **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**
28. 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). **1446 citations**
29. 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). **73 citations**
30. **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). **38 citations**
31. 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). **52 citations**
32. 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). **19 citations**
33. 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<sub>3</sub>. *Phys. Rev. B* **69**, 024110 (2004). **40 citations**
34. 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<sub>2</sub> within the anisotropic Eliashberg formalism.’ ” *Phys. Rev. B* **69**(5), 056502 (2004). **18 citations**
35. 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). **186 citations**
36. F. J. Ribeiro, **D. Roundy**, and M. L. Cohen. Electronic Properties of MoSe nanowires. *Phys. Rev. B* **65**, 153401 (2002). **37 citations**
37. 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). **129 citations**



38. H. J. Choi, **D. Roundy**, H. Sun, M. L. Cohen, and S. G. Louie. The origin of the anomalous superconducting properties of MgB<sub>2</sub>. *Nature* **418**, 758–760 August (2002). **969 citations**
39. H. J. Choi, **D. Roundy**, H. Sun, M. L. Cohen, and S. G. Louie. First-principles calculation of the superconducting transition in MgB<sub>2</sub> within the anisotropic Eliashberg formalism. *Phys. Rev. B* **66**, 020513 (2002). **353 citations**
40. **D. Roundy** and M. L. Cohen. Ideal strength of diamond, Si and Ge. *Phys. Rev. B* **64**, 212103 (2001). **258 citations**
41. 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). **100 citations**
42. H. Sun, S. H. Jhi, **D. Roundy**, M. L. Cohen, and S. G. Louie. Structural forms of cubic BC<sub>2</sub>N. *Phys. Rev. B* **64**(9), 094108 (2001). **177 citations**
43. 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). **11 citations**
44. C. R. Krenn, **D. Roundy**, J. W. Morris, Jr., and M. L. Cohen. The nonlinear elastic behavior and ideal shear strength of Al and Cu. *Mat. Sci. Eng. A* **317**, 44–48 (2001). **41 citations**
45. **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). **241 citations**
46. **D. Roundy**, C. R. Krenn, M. L. Cohen, and J. W. Morris, Jr. Ideal shear strengths of Aluminum and Copper. *Phys. Rev. Lett.* **82**(13), 2713 (1999). **384 citations**
47. 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). **14 citations**
48. 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). **47 citations**
49. M. A. Khakoo, **D. Roundy**, and F. Rugamas. Electron-impact excitation of the <sup>1</sup>S→<sup>3</sup>P and <sup>1</sup>S→<sup>4</sup>3P transition in Helium. *Phys. Rev. A* **54**(5), 4004–4014 (1996). **8 citations**
50. M. A. Khakoo, **D. Roundy**, and F. Rugamas. Electron-impact excitation of the <sup>1</sup>S→<sup>3</sup>P transition in Helium. *Phys. Rev. Lett.* **75**(1), 41–44 (1995). **5 citations**

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

51. **David Roundy**, Ayush Gupta, Joseph F. Wagner, Tevian Dray, Mary Bridget Kustus, 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). **2 citations**
52. Corinne A. Manogue, Elizabeth Gire, and **David Roundy**. Tangible Metaphors. In *2013 Physics Education Research Conference Proceedings—American Institute of Physics*, 27–30 (2013). **5 citations**
53. 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). **12 citations**
54. D. Roundy. Darcs: distributed version management in Haskell. In *Proceedings of the 2005 ACM SIGPLAN workshop on Haskell*, pages 1–4. ACM, (2005). **56 citations**

## Published curricular materials

55. **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.
56. **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. 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 my student Jordan Pommerenck (2020).
2. Undergraduate Research Symposium at Oregon State University: Co-authored the poster “Simulating the walk of the dynein motor protein” presented by Jin Kiatvongcharoen (2019).
3. Celebrating Undergraduate Excellence at Oregon State University: Co-authored the poster “Simulating Dynein’s Walk Using Monte Carlo Methods” presented by Jin Kiatvongcharoen (2019).
4. 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).
5. 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).
6. Teaching T.A.L.K.S. IV in Corvallis, which is a conference on assessment: Participated (2018).
7. 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).
8. AAPT Winter Meeting in San Diego: Presented the talk “Name the Experiment! Relating Thermal Derivatives with the Real World” (2018).
9. 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).
10. Physics Education Research Conference (PERC): Presented the poster “Paradigms in Physics 2.0” (2017).
11. 18th Annual Meeting of the APS Northwest Section: Co-authored the talk “Simulating dynein’s powerstroke using Brownian dynamics” presented by Elliott Capek (2017).
12. 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).
13. 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).
14. Frontiers in Education (FIE) 2015 in El Paso: Presented the talk “Look ma, no templates! Problem-based learning of computational physics for novice programmers” (2015).

15. **(invited)** Northwest Section Meeting of the APS: Presented the talk “Making calculus tangible” (2015) (actually presented by student MacKenzie Lenz, due to family illness).
16. Research in Undergraduate Math Education Conference (RUME) in Pittsburgh: Presented the talk “An Extended Theoretical Framework for the Concept of Derivative” (2015).
17. Physics Education Research Conference (PERC) in Minneapolis: Presented the poster “Experts’ understanding of partial derivatives using the Partial Derivative Machine” (2014).
18. AAPT Summer Meeting in Minneapolis: Presented the talk “Integration in Electrostatics with a Computational Perspective” (2014).
19. Workshop on the Status of the Upper-Division Physics Curriculum: Presented the talk “Connecting math with experiment in thermal physics” (2014).
20. AAPT Summer Meeting in Portland: Presented the talk “Learning through Computation in Upper-Division Physics” (2013).
21. 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).
22. Physics Education Research Conference (PERC) in Portland: Co-authored the poster “The Partial Derivative Machine,” presented by undergraduate student Grant Scherer (2013).
23. **(invited poster)** Physics Education Research Conference (PERC) in Portland: Co-authored the poster “Tangible Metaphors,” presented by Corinne Manogue (2013).
24. 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).
25. 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).
26. NSF TUES Principal Investigators Conference in Washington, DC: Presented the poster “An Expert Path Through a Thermo Maze” (2013).
27. APS March Meeting in Boston: presented the talk “A SAFT-based classical density functional for water” (2012).
28. 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).
29. **(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).
30. NSF CCLI/TUES Principal Investigators Conference in Washington, DC: Presented the poster “Energy and Entropy in the Paradigms Curriculum” (2011).
31. APS March Meeting in Portland: Co-authored the talk “Dielectric properties of the  $\text{BaTiO}_3\text{-Bi}(\text{Zn}_{\frac{1}{2}}\text{Ti}_{\frac{1}{2}})\text{O}_3$  solid solution from density-functional theory,” presented by my student Dennis Jackson (2010).
32. AAPT Summer Meeting in Portland: Presented the talk “Energy and Entropy and More” (2010).
33. APS March Meeting in Pittsburgh: Co-authored the talk “Density-functional study of the of the  $\text{Ba}_x\text{Bi}_{(1-x)}(\text{M}_{(1-x)/2})\text{Ti}_{(1+x)/2}\text{O}_3$  perovskite solid solution,” presented by my student Dennis Jackson (2009).

34. **(invited)** Oregon AAPT: Presented the talk “A first course in Computational Physics using visual python” (Sept. 2008).
35. APS March Meeting in New Orleans: Presented the talk “A classical density functional for water,” presented by my student Dennis Jackson (2008).
36. **(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).
37. **(invited)** Free and Open source Software Developers’ European Meeting (FOSDEM) in Brussels: I presented the talk “The Darcs Patch Formalism” (2006).
38. **(invited)** Haskell Workshop at the International Conference on Functional Programming in Estonia: I presented the talk “Darcs: Distributed Version Management in Haskell” (2005).
39. **(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).
40. **(invited)** Electronic Structure conference at Cornell: I presented the talk “Internal Friction and the Silicon Divacancy” (2005).
41. **(invited)** MRS Fall Meeting in Boston: I presented the talk “Computation of the ideal strength” (2000).

### 3. Funding

---

#### Current/Past awarded grants

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

Participants: Hjorth-Jensen, Malthe-Sørenssen, Caballero, Mørken, Wahlstrøm Tellefsen, Henriksen, Sawtelle, O’Shea, Lockwood, **Roundy**, Gire 2019 – 2021  
 Research Council of Norway, INTPART programme  
 International Partnership for Computing in Science Education

*This international grant supports travel for collaboration on the development of computational science education.*

PI: **Roundy** co-PIs: Dray, Gire, and Manogue 01/01/2018 – 12/31/2020  
 National Science Foundation \$298,948  
 Paradigms in Physics: Second-Generation Dissemination Strategies

PI: Gire co-PIs: Dray, **Roundy**, and Manogue 01/01/2018 – 12/31/2020  
 National Science Foundation \$299,282  
 Paradigms in Physics: Representations in Quantum Mechanics

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

#### 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 Institutional Diversity to build skill in responding to bias incidents and microaggressions as they arise.

**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.

## 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