# Jonathan J. Helmus, Ph.D.

CONTACT Information Environmental Science Division Argonne National Laboratory 9700 South Cass Ave. Bldg 240 Argonne, IL 60439 Phone (office): (630) 252-1488 Phone (cell): (331) 444-3896 Email: jjhelmus@gmail.com Code: github.com/jjhelmus

**EDUCATION** 

University of Connecticut Health Center, Farmington, Connecticut.

Postdoctoral Fellow, July, 2011-January 2013.

Advisor: Jeffrey Hoch.

The Ohio State University, Columbus, Ohio.

Ph.D., Chemical Physics, GPA 3.90, June 2005-July 2011.

Advisor: Christopher Jaroniec Coe College, Cedar Rapids, Iowa.

NSF Research for Undergraduates (REU) student, Summer 2004.

Michigan Technological University, Houghton, Michigan.

B.S. Chemistry (Chemical Physics), Minor: Mathematics, May 2005.

Honors and Awards Presidential Fellowship from the Ohio State University, 2010-2011.

Phi Delta Gamma Graduate School Scholarship, 2010.

Isotech Experimental NMR Conference (ENC) Travel Scholarship, 2009, 2010.

ORAU sponsored attendee to the 59th Meeting of Nobel Laureates in Lindau, Germany, 2009.

ENC Student Travel Award, 2007, 2009, 2010.

Graduate School Fellowship, Ohio State University, 2005.

Michigan Tech. Physical Chemistry Student of the Year, 2003.

A.C.S. Upper Michigan Junior of the Year Majoring in Chemistry, 2003.

N.S. Mackie Scholarship, 2002.

Deans List, 2001-2005.

Board of Control Scholarship, Michigan Tech., 2001-2005.

Eagle Scout, BSA Troop 275, Kentwood, Michigan, 2001.

Valedictorian of High School Class, 2001

Finalist on National Chemistry Olympiad Test, 2000, 2001.

RESEARCH EXPERIENCE Argonne National Laboratory, Argonne, Illinois

January 2013-present

I am working in the environmental science division at Argonne National Laboratory as a scientist and software engineer for the Atmospheric Radiation Measurement (ARM) Climate Research Facility. I am involved in a number of projects within ARM with other scientists and developers to create and release value added products from data collected by ARMs scanning precipitation and cloud radars. This work is highly collaborative with frequent input and interactions with scientists from universities and research centers across the globe. In addition, I am the lead developer of the Python ARM Radar Toolkit (Py-ART), an open source toolkit for the analysis and manipulation of weather radar data.

UConn Health Center, Farmington, Connecticut

July 2011-January 2013

I completed a postdoctoral position in the lab of Dr. Jeffrey C. Hoch where I worked on a number of projects focusing on using modern signal processing methods to process NMR data. These projects include maintaining and updating the Rowland NMR Toolkit, a software package for processing NMR data written primarily in FORTRAN 77 and C. In addition, I developed the software needed for my research into the effects of deconvolution kernels on NMR spectra processed using Maximum Entropy and  $l_1$ -norm (compressive sensing) reconstruction methods.

#### The Ohio State University, Columbus, Ohio

June 2005-July 2011

While performing research for my doctoral thesis, I worked on a 500 MHz Varian (Agilent) NMR spectrometer equipped with multiple probes for magic angle spinning (MAS) of solid samples. I shared responsibility for the upkeep of the magnet with other graduate students including performing nitrogen and helium cryogen fills and troubleshooting hardware and software problems. I wrote a number of pulse sequences for the spectrometer, as well as numerous scripts and software programs for automated processing and analysis of solid state NMR data which are used by the entire Jaroniec research group. In addition, I designed and wrote the open source software package nmrglue (http://www.nmrglue.com) a Python module for working with NMR data. My major projects as a graduate student included structural and dynamic studies of the Y145Stop variant of the human prion protein and development of methods for using covalently attached paramagnetic spin labeled to probe distances in biological solids.

#### Coe College, Cedar Rapids, Iowa USA

**Summer 2004** 

As a research experience for undergraduates students, I synthesised and characterized alkali vanadate glasses using plate and roller quenching techniques.

### SOFTWARE ENGINEERING

**Programming Languages:** Python, FORTRAN (77 and modern versions), C, and C++. **Python modules:** NumPy, SciPy, matplotlib, Jupyter, Cython, and f2py

Operating Systems: Linux, Windows, and OS X.

#### Publications

- 18) H. Guo, W. He, T. Peterka, H. Shen, S. Collis, <u>J. Helmus</u>. Finite-Time Lyapunov Exponents and Lagrangian Coherent Structures in Uncertain Unsteady Flows *IEEE Transactions on Visualization and Computer Graphics* **2016**, 22 (6), 1672-1682.
- 17) M. van Lier-Walqui, A.M. Fridlind, A. S. Ackerman, S. Collis, <u>J. Helmus</u>, D. R. MacGorman, K. North, P. Kollias, D. J. Posselt. On polarimetric radar signatures of deep convection for model evaluation: columns of specific differential phase observed during MC3E, *Monthly Weather Review* **2015**, 144, 737-758.
- 16) M. Heistermann, S. Collis, M.J. Dixon, <u>J.J. Helmus</u>, A. Henja, D.B. Michelson, Thomas Pfaff. An Open Virtual Machine for Cross-Platform Weather Radar Science *Bulletin of the American Meteorological Society* **2015**, 96 (10), 1641-1645.
- 15) M. Heistermann, S. Collis, M.J. Dixon, S. Giangrande, <u>J.J. Helmus</u>, B. Kelley, J. Koistinen, D.B. Michelson, M. Peura, T. Pfaff, D.B. Wolff. The Emergence of Open-Source Software for the Weather Radar Community, *Bulletin of the American Meteorological Society* **2015**, 96 (1), 117-128.
- 14) <u>J.J. Helmus</u>, C.P. Jaroniec. Nmrglue: An open source Python package for the analysis of multidimensional NMR data, *Journal of Biomolecular NMR* **2013**, 55, 355-367.
- 13) I. Sengupta, P.S. Nadaud, <u>J.J. Helmus</u>, C.D. Schwieters, C.P. Jaroniec. Protein fold determined by paramagnetic magic-angle spinning solid-state NMR spectroscopy, *Nature Chemistry* **2012**, 4, 410-417.
- 12) E.M. Jones, B. Wu, K. Surewicz, P.S. Nadaud, <u>J.J. Helmus</u>, S. Chen, C.P. Jarnoniec, W.K. Surewicz. Structural polymorphism in amyloids: New insights from studies with Y145Stop prion protein fibrils. *The Journal of Biological Chemistry* **2011**, 286, 42777-42784.
- 11) <u>J.J. Helmus</u>, K. Surewicz, M.I. Apostol, W.K. Surewicz, C.P. Jaroniec. Intermolecular alignment in Y145Stop human prion protein amyloid fibrils probed by solid-state NMR spectroscopy, *Journal of the American Chemical Society* **2011**, 133, 13934-13937.

- 10) P.S. Nadaud, I. Sengupta, J.J. Helmus, C.P. Jaroniec. Evaluation of the influence of intermolecular electron-nucleus couplings and intrinsic metal binding sites on the measurement of <sup>15</sup>N longitudinal paramagnetic relaxation enhancements in proteins by solid-state NMR. Journal of Biomolecular NMR **2011**, 51, 293-302.
- 9) P.S. Nadaud, J.J. Helmus, I. Sengupta, C.P. Jaroniec. Rapid acquisition of multidimensional solid-state NMR spectra of proteins facilitated by covalently bound paramagnetic tags. Journal of the American Chemical Society 2010, 132, 9561-9563.
- 8) H. Shao, J. Seifert, N.C. Romano, M. Gao, J.J. Helmus, C.P. Jaroniec, D.A. Modarelli, J.R. Parquette. Amphiphilic self-assembly of an n-type nanotube. Angewandte Chemie International Edition 2010, 49, 7688-7691.
- 7) J.J. Helmus, K. Surewicz, W.K. Surewicz, C.P. Jaroniec. Conformational flexibility of Y145Stop human prion protein amyloid fibrils probed by solid-state nuclear magnetic resonance spectroscopy. Journal of the American Chemical Society 2010 132, 2393-2403.
- 6) P.S. Nadaud, J.J. Helmus, S.L. Kall, C.P. Jaroniec. Paramagnetic ions enable tuning of nuclear relaxation rates and provide long-range structural restraints in solid-state NMR of proteins. Journal of the American Chemical Society. 2009, 131, 8108-8120.
- 5) J.J. Helmus, K. Surewicz, P.S. Nadaud, W.K. Surewicz, C.P. Jaroniec. Molecular conformation and dynamics of the Y145Stop variant of human prion protein in amyloid fibrils. Proceedings of the National Academy of Sciences USA, 2008, 105, 6284-6289.
- 4) J.J. Helmus, P.S. Nadaud, N. Höfer, C.P. Jaroniec. Determination of methyl <sup>13</sup>C-<sup>15</sup>N dipolar couplings in peptides and proteins by three-dimensional and four-dimensional magic-angle spinning solid-state NMR spectroscopy. Journal of Chemical Physics, 2008, 128, 052314.
- 3) P.S. Nadaud, J.J. Helmus, C.P. Jaroniec. <sup>13</sup>C and <sup>15</sup>N chemical shift assignments and secondary structure of the B3 immunoglobulin-binding domain of streptococcal protein G by magic-angle spinning solid-state NMR spectroscopy. Biomolecular NMR Assignments, 2007, 1, 117-120.
- 2) P.S. Nadaud, J.J. Helmus, N. Höfer, C.P. Jaroniec. Long-range structural restraints in spinlabeled proteins probed by solid-state nuclear magnetic resonance spectroscopy. Journal American Chemical Society, 2007, 129, 7502-7503.
- 1) S. Giri, C. Gaebler, J. Helmus, M. Affatigato; S. Feller, M. A. Kodama. General study of packing in oxide glass systems containing alkali. Journal of Non-Crystalline Solids, 2004, 347, 87-92.

Professional

2015 ARM/ASR Joint User Facility PI Meeting, Vienna, VA (March 16-12)

MEETING - POSTER SciPy 2014 Conference, Austin, TX (July 6-12, 2014)

Presentations

36th Conference on Radar Meteorology, Breckenridge, CO, (September 16-20, 2013)

SciPy 2013 Conference, Austin, TX (June 24-29, 2013)

2013 ASR Science Team Meeting, Potomac, MD (March 18-21, 2013)

52nd Experimental NMR Conference, Pacific Grove, CA (April 10-15, 2011)

51st Experimental NMR Conference, Daytona Beach, FL (April 18-23, 2010)

50th Experimental NMR Conference, Pacific Grove, CA (March 29-April 3, 2009)

50th Rocky Mountain Conference for Analytical Chemistry, Breckenridge, CO (July 27-31, 2008)

ACS 39th Central Regional Meeting, Columbus, OH (June 10-14, 2008)

Pittsburgh NMR Symposium, Pittsburgh, PA (April 29-30, 2008)

49th Experimental NMR Conference, Pacific Grove, CA (March 9-14, 2008)

48th Experimental NMR Conference, Daytona Beach, FL (April 22-27, 2007)

Research Coordination Network Workshop, Bethesda, MD (January 12-13, 2007)

## Courses and Tutorials

Open Source Radar Short Course, 37th Conference on Radar Meteorology, Norman, Oklahoma, September 13, 2015.

PyART, Python ARM Radar Toolkit, 2015 ARM/ASR Joint User Facility PI Meeting, Vienna, Virgina, March 18, 2015.

Open Source Radar Short Course, 8th European Conference on Radar Meteorology and Hydrology, Garmisch-Partenkirchen, Germany, August 31, 2014.

### Oral Presentations

Building and Distributing Python Software with Conda, DePy 2016, Chicago, IL, May 7, 2016

The Language, Libraries and Culture of Python in Meteorology, 96th AMS Annual Meeting, New Orleans, Louisiana, January 10-14, 2016.

Keep calm and conda install, ChiPy Monthy Meeting, Chicago, IL, August 13, 2015.

Exploring Open Access Weather Radar with the Python ARM Toolkit, Scipy 2015 Conference, Austin, TX, July, 10, 2015.

Speeding Up Python Data Analysis Using Cython, DePy 2015, Chicago, IL, May 29, 2015.

Profiling Python code to improve memory usage and execution time, 2015 SEA Software Enginnering Conference. Boulder, CO, April 14, 2015.

Designing and implementing radar algorithms in Python, 95th AMS Annual Meeting, Phoenix, AZ, January 5, 2014.

New Doppler Spectral Processing Technique for Identifying Atmospheric Signals from Radar Wind Profilers, 8th European Conference on Radar in Meteorology and Hydrology, Garmisch-Partenkirchen, Germany, September 4, 2014.

Tools and Techniques for Developing Atmospheric Python Software: Insight from the Python ARM Radar Toolkit, 94th AMS Annual Meeting, Atlanta, GA, February 3, 2014.

The Development and Use of a Python Data Analysis Package: Nmrglue, Argonne National Laboratory, Argonne, IL, October 15, 2012.

nmrglue: a Python Module for Working with NMR Data, Scipy 2012 Conference, Austin, TX, July, 19, 2012.

Rapid Acquisition of Multidimensional Solid State NMR Spectra for the Study of Proteins, Physical Chemistry Student Lecture Series, The Ohio State University, Columbus, OH, Jan. 12, 2010.

Structure and Dynamics of Proteins using Solid State Nuclear Magnetic Resonance Spectroscopy, Physical Chemistry Student Lecture Series, The Ohio State University, Columbus, OH, Nov. 6, 2007.