Randy Heiland

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Education

Arizona State University Tempe, AZ
M.A. Mathematics *1992*
Dynamical Systems. Advisor: Prof. Dieter Armbruster
Thesis: *KLTool: A Mathematical Tool to Analyze Spatiotemporal Data*

University of Utah Salt Lake City, UT
M.S. Computer Science *1987*
Computer Graphics, Computer-Aided Geometric Design. Advisor: Prof. Richard Riesenfeld
Thesis: *A Front-End User Interface to a Geometric Modeling System*

Eastern Illinois University Charleston, IL
B.S. Computational Mathematics *1979*

Work Experience

Indiana University *(2003–present)*

- Intelligent Systems Engineering, 2017–present *Research Associate*
- Center for Applied Cybersecurity Research, 2013–2017 *Senior Systems Analyst/Programmer*
- Open Systems Lab (then part of pti.iu.edu; later became CREST), 2007–2012 *Research Associate*
  (∼50% effort in Biocomplexity Institute)
- UITS High Performance Applications Group, 2007 *Acting Manager*
- Scientific Data Analysis Lab, Pervasive Technology Labs, 2003–2007 *Associate Director*

Acquired Science, LLC
President. Scientific software development and consulting. *2005–2010*

NCSA, University of Illinois Urbana, IL
Senior Research Scientist. Scientific visualization and data analysis. *1997–2003*

Pacific Northwest National Lab Richland, WA
Computer Scientist. Computational chemistry, image analysis, visualization. *1993–97*

Los Alamos National Lab Los Alamos, NM
Graduate Research Associate. Visualization and analysis software for the CM5 supercomputer. *1992*

Center for Industrial Research (now SINTEF) Oslo, Norway
Computer Scientist. Computer-aided geometric design software. *1985–87*

Caterpillar Tractor Co. Peoria, IL
Computer Scientist. Data analysis and computer-aided design. *1979–82*

Teaching Experience

Undergraduate research projects Bloomington
Mentor *2017–present*

Science Gateways Bootcamp Indianapolis
Instructor *April 24–28, 2017*

Brief Survey of Calculus (MATH 119) Indiana University
Instructor *Fall 2013*

Tutorial: Multi-cell, Multi-scale Modeling NIMBioS, UT-Knoxville
Instructor *May 18–21, 2011*

Outreach: Squeak and Scratch Modeling Girl Scouts of Central Indiana
Instructor *2007*

Computer Graphics I (CSC 231) Parkland College
Instructor *Fall 2001*

Notable Projects

- **PhysiCell** (physicell.org): Physics-based multicellular modeling software (center-based, off lattice).
- **CTSC** (trustedci.org): The NSF Cybersecurity Center of Excellence.
- **CompuCell3D** (compucell3d.org): Multicellular modeling software (Cellular Potts).
- **EMSL** (emsl.pnnl.gov): Extensible Computational Chemistry Environment.
- **rheiland.github.io**: Variety of past projects.

Publications

Google Scholar: https://scholar.google.com/citations?user=0SeiPdoAAAAJ

Journal Articles (newest first)

1. Y. Wang, J. Metzcar, E. Bucher, H.L. Rocha, V. Jadhao, R. Heiland, H.B. Frieboes, P. Macklin. Drug-loaded nanoparticles for cancer therapy: A high-throughput multicellular agent-based modeling study. *Journal of Theoretical Biology*, 616:112266, 2025. https://doi.org/10.1016/j.jtbi.2025.112266

2. J.A.I. Johnson, D.R. Bergman, H.L. Rocha, D.L. Zhou, E. Cramer, I.C. Mclean, Y.W. Dance, M. Booth, Z. Nicholas, T. Lopez-Vidal, A. Deshpande, R. Heiland, E. Bucher, F. Shojaeian, M. Dunworth, A. Forjaz, M. Getz, I. Godet, F. Kurtoglu, et al., P. Macklin. Human interpretable grammar encodes multicellular systems biology models to democratize virtual cell laboratories. *Cell*, 188(17):4711–4733.e37, 2025. https://doi.org/10.1016/j.cell.2025.06.048

3. D.R. Bergman, J.A.I. Johnson, M. Naji, M. Booth, H.L. Rocha, A. Deshpande, D.N. Sidiropoulos, T. Lopez-Vidal, R. Heiland, L.T. Kagohara, R.A. Anders, L. Zheng, E.M. Jaffee, G.L. Stein-O'Brien,

P. Macklin, E.J. Fertig. BIWT: a bioinformatics walkthrough for embedding spatial multiomics in agent-based models for virtual cells. *Bioinformatics*, 41(11), 2025. https://doi.org/10.1093/bioinformatics/btaf571

4. J. Metzcar, B.S. Duggan, B. Fischer, M. Murphy, R. Heiland, P. Macklin. A simple framework for agent-based modeling with extracellular matrix. *Bulletin of Mathematical Biology*, 87(3):43, 2025. https://doi.org/10.1007/s11538-024-01408-8

5. R. Heiland, D. Bergman, B. Lyons, G. Waldow, J. Cass, H. Lima da Rocha, M. Ruscone, V. Noël, P. Macklin. PhysiCell Studio: a graphical tool to make agent-based modeling more accessible. *Gigabyte*, 2024, pp. 1–19. https://doi.org/10.46471/gigabyte.128

6. M. Ruscone, A. Checcoli, R. Heiland, E. Barillot, P. Macklin, L. Calzone, V. Noël. Building multiscale models with PhysiBoSS, an agent-based modeling tool. *Briefings in Bioinformatics*, 25(6), 2024. https://doi.org/10.1093/bib/bbae509

7. G. Letort, A. Montagud, G. Stoll, R. Heiland, E. Barillot, P. Macklin, A. Zinovyev, L. Calzone. PhysiBoSS: a multi-scale agent-based modelling framework integrating physical dimension and cell signalling. *Bioinformatics*, 35(7):1188–1196, 2019. https://doi.org/10.1093/bioinformatics/bty766

8. R. Heiland, D. Mishler, T. Zhang, E. Bower, P. Macklin. xml2jupyter: Mapping parameters between XML and Jupyter widgets. *Journal of Open Source Software*, 4(39):1408, 2019. https://doi.org/10.21105/joss.01408

9. M.P. Snyder, et al. (HuBMAP Consortium, incl. R. Heiland). The human body at cellular resolution: the NIH Human Biomolecular Atlas Program. *Nature*, 574(7777):187–192, 2019. https://doi.org/10.1038/s41586-019-1629-x

10. J. Ozik, N. Collier, R. Heiland, G. An, P. Macklin. Learning-accelerated discovery of immune-tumour interactions. *Molecular Systems Design & Engineering*, 4(4):747–760, 2019. https://doi.org/10.1039/c9me00036d

11. J. Metzcar, Y. Wang, R. Heiland, P. Macklin. A review of cell-based computational modeling in cancer biology. *JCO Clinical Cancer Informatics*, 3:1–13, 2019. https://doi.org/10.1200/CCI.18.00069

12. J. Ozik, N. Collier, J.M. Wozniak, C.M. Macal, C. Cockrell, S.H. Friedman, A. Ghaffarizadeh, R. Heiland, G. An, P. Macklin. High-throughput cancer hypothesis testing with an integrated PhysiCell-EMEWS workflow. *BMC Bioinformatics*, 19(Suppl 18):81–97, 2018. https://doi.org/10.1186/s12859-018-2510-x

13. A. Ghaffarizadeh, R. Heiland, S.H. Friedman, S.M. Mumenthaler, P. Macklin. PhysiCell: An open source physics-based cell simulator for 3-D multicellular systems. *PLoS Computational Biology*, 14(2):e1005991, 2018. https://doi.org/10.1371/journal.pcbi.1005991
(Winner, 2019 PLOS Computational Biology Research Prize for Public Impact)

14. J.P. Sluka, A. Shirinifard, M. Swat, A. Cosmanescu, R. Heiland, J.A. Glazier. The cell behavior ontology: describing the intrinsic biological behaviors of real and model cells seen as active agents. *Bioinformatics*, 30(16):2367–2374, 2014. https://doi.org/10.1093/bioinformatics/btu210

15. S. Ito, M.E. Hansen, R. Heiland, A. Lumsdaine, A.M. Litke, J.M. Beggs. Extending transfer entropy

improves identification of effective connectivity in a spiking cortical network model. *PLoS ONE*, 6(11):e27431, 2011. https://doi.org/10.1371/journal.pone.0027431

16. A. Singh, A. Olowoyeye, P.H. Baenziger, J. Dantzer, M.G. Kann, P. Radivojac, R. Heiland, S.D. Mooney. MutDB: update on development of tools for the biochemical analysis of genetic variation. *Nucleic Acids Research*, 36(Database issue):815–819, 2008. https://doi.org/10.1093/nar/gkm659

17. A.J. Moad, C.W. Moad, J.M. Perry, R.D. Wampler, G.S. Goeken, N.J. Begue, T. Shen, R. Heiland, G.J. Simpson. NLOPredict: Visualization and data analysis software for nonlinear optics. *Journal of Computational Chemistry*, 28(12):1996–2002, 2007. https://doi.org/10.1002/jcc.20706

18. X. Dong, K.E. Gilbert, R. Guha, R.W. Heiland, J. Kim, M.E. Pierce, G.C. Fox, D.J. Wild. Web Service Infrastructure for Chemoinformatics. *Journal of Chemical Information and Modeling*, 47(4):1303–1307, 2007. https://doi.org/10.1021/ci6004349

19. J. Dantzer, C.W. Moad, R. Heiland, S.D. Mooney. MutDB services: interactive structural analysis of mutation data. *Nucleic Acids Research*, 33(Web Server issue):W311–W314, 2005. https://doi.org/10.1093/nar/gki404

20. D. Armbruster, R. Heiland, E.J. Kostelich. kltool: A tool to analyze spatiotemporal complexity. *Chaos*, 4(2):421–424, 1994. https://doi.org/10.1063/1.166020

21. D. Armbruster, R. Heiland, E.J. Kostelich, B. Nicolaenko. Phase-space analysis of bursting behavior in Kolmogorov flow. *Physica D: Nonlinear Phenomena*, 58(1–4):392–401, 1992. https://doi.org/10.1016/0167-2789(92)90125-7

Book Chapters

1. R.J. Littlefield, R.W. Heiland, C.R. Macedonia. Virtual Reality Volumetric Display Techniques for Three-Dimensional Medical Ultrasound. In *Medicine Meets Virtual Reality 4: Health Care in the Information Age*, Studies in Health Technology and Informatics, vol. 29, pp. 498–506. IOS Press, San Diego, CA, January 1996. https://doi.org/10.3233/978-1-60750-873-1-498

2. D. Armbruster, E. Stone, R. Heiland. Towards analyzing the dynamics of flames. In *Pattern Formation: Symmetry Methods and Applications*, Fields Institute Communications, vol. 5, pp. 1–17. American Mathematical Society, 1996. https://doi.org/10.1090/fic/005

Conference and Workshop Papers (newest first)

1. A. Madamanchi, R. Heiland, P. Macklin, A.J. Magana. Students' Use of Metacognitive Skills in Undergraduate Research Experiences in Computational Modeling. *IEEE Frontiers in Education (FIE)*, 2019, pp. 1–5. https://doi.org/10.1109/FIE43999.2019.9028386

2. M. Rynge, K. Vahi, E. Deelman, A. Mandal, I. Baldin, O. Bhide, R. Heiland, V. Welch, R. Hill, W.L. Poehlman, F.A. Feltus. Integrity Protection for Scientific Workflow Data: Motivation and Initial Experiences. *PEARC*, 2019, pp. 17:1–17:8. https://doi.org/10.1145/3332186.3332222

3. S. Gesing, M.G. Zentner, J. Casavan, B. Hillery, M. Vorvoreanu, R. Heiland, S. Marru, M.E. Pierce, N. Mullinix, N. Maron. Science Gateways Incubator: Software Sustainability Meets Community Needs. *eScience*, 2017, pp. 477–485. https://doi.org/10.1109/eScience.2017.77

4. R.W. Heiland, S. Koranda, S. Marru, M.E. Pierce, V. Welch. Authentication and Authorization Considerations for a Multi-tenant Service. *SCREAM@HPDC*, 2015, pp. 29–35. https://doi.org/

10.1145/2753524.2753534

5. R. Heiland, A. Shirinifard, M. Swat, G.L. Thomas, J.P. Sluka, A. Lumsdaine, B. Zaitlen, J.A. Glazier. Visualizing cells and their connectivity graphs for CompuCell3D. *IEEE Symposium on Biological Data Visualization (BioVis)*, 2012, pp. 85–90. https://doi.org/10.1109/BioVis.2012.6378597

6. R. Heiland, M. Swat, B. Zaitlen, J.A. Glazier, et al. Workflows for parameter studies of multi-cell modeling. *Proceedings of the 2010 Spring Simulation Multiconference (SpringSim)*, 2010.

7. R.W. Heiland, M.P. Baker. A Survey of Visualization Tools for High Performance Computing. *Proceedings of the Ninth SIAM Conference on Parallel Processing for Scientific Computing (PPSC)*, San Antonio, TX, March 1999.

8. R.W. Heiland, M.P. Baker, D.K. Tafti. VisBench: A Framework for Remote Data Visualization and Analysis. *International Conference on Computational Science (ICCS)*, Part II, 2001, pp. 718–727. https://doi.org/10.1007/3-540-45718-6_78

9. G.M. Nielson, R.W. Heiland. Animated rotations using quaternions and splines on a 4D sphere. *Programming and Computer Software*, 18(4):145–154, 1992.

Preprints (bioRxiv)

1. E.M. Cramer, R. Heiland, H. Lima da Rocha, D.R. Bergman, J.W. Gray, G.B. Mills, E.J. Fertig, P. Macklin, L.M. Heiser, Y.H. Chang. Tumor-immune trajectory context connects static tissue architecture to clinical outcomes. *bioRxiv*, 2026.03.26.714521. https://doi.org/10.64898/2026.03.26.714521

2. A. Bertin, E. Bucher, O. Griere, M. Hurtado, H. Rocha, R. Heiland, A. Sundus, P. Macklin, V. François-Lavet, E. Rachelson, V. Pancaldi. PhysiGym: bridging the gap between the Gymnasium reinforcement learning application interface and the PhysiCell agent-based model software. *bioRxiv*, 2025.09.18.677030. https://doi.org/10.1101/2025.09.18.677030

3. T. Ntiniakou, J. Osborne, J. Zhao, J. Dichamp, N. Cogno, R. Heiland, et al., P. Macklin, et al. Open Benchmarking for Cell-Based Multiscale Models: Lessons from a Community Initiative. *bioRxiv*, 2025.07.16.664358. https://doi.org/10.1101/2025.07.16.664358

4. M. Getz, Y. Wang, G. An, M. Asthana, A. Becker, C. Cockrell, N. Collier, M. Craig, C.L. Davis, J.R. Faeder, A.N. Ford Versypt, T. Mapder, J.F. Gianlupi, J.A. Glazier, S. Hamis, R. Heiland, T. Hillen, D. Hou, M.A. Islam, A.L. Jenner, F. Kurtoglu, C.I. Larkin, B. Liu, F. Macfarlane, P. Maygrundter, P.A. Morel, A. Narayanan, J. Ozik, E. Pienaar, P. Rangamani, A.S. Saglam, J.E. Shoemaker, A.M. Smith, J.J.A. Weaver, P. Macklin. Iterative community-driven development of a SARS-CoV-2 tissue simulator. *bioRxiv*, 2020.04.02.019075 (v5, 2021). https://doi.org/10.1101/2020.04.02.019075

5. A. Sundus, F. Kurtoglu, K. Konstantinopoulos, M. Chen, D. Willis, R. Heiland, P. Macklin. PhysiCell training apps: A case study for creating interactive training materials for scientific software packages. *bioRxiv*, 2022.06.24.497566. https://doi.org/10.1101/2022.06.24.497566

Preprints (arXiv)

1. V. Noël, M. Ruscone, R. Heiland, A. Montagud, A. Valencia, E. Barillot, P. Macklin, L. Calzone. PhysiBoSS-Models: A database for multiscale models. *arXiv*, 2508.05550, 2025. https://arxiv.org/abs/2508.05550

Reports and Presentations

1. R. Heiland. Cybersecurity for Science Gateways. SGCI Bootcamp. Indianapolis, IN. April 24–28, 2017. http://hdl.handle.net/2022/21367

2. R. Heiland and V. Welch. Center for Trustworthy Scientific Cyberinfrastructure: The NSF Cybersecurity Center of Excellence. NSF SI2 PI Meeting: Poster session. Arlington, VA. Feb 21–22, 2017. http://hdl.handle.net/2022/21258

3. V. Welch, et al. Center for Trustworthy Scientific Cyberinfrastructure – The NSF Cybersecurity Center of Excellence: Year One Report. Technical Report, Indiana University, December 2016. http://hdl.handle.net/2022/21163

4. R. Heiland, W.C. Garrison III, Y. Qiao, A.J. Lee, V. Welch. The Web's PKI: An Expository Review and Certificate Validation Cost Simulation. Technical Report, Indiana University, September 2016. http://hdl.handle.net/2022/21038

5. R. Heiland, S. Sons. Secure Software Engineering Best Practices. Presentation at the NSF Cybersecurity Summit. August 16, 2016. http://hdl.handle.net/2022/21322

6. R. Heiland, S. Koranda, V. Welch. SciGaP-CTSC Engagement Summary. Technical Report, Indiana University, May 2016. http://hdl.handle.net/2022/20926

7. R. Heiland, S. Koranda, V. Welch. SciGaP-CTSC Engagement: Final Technical Recommendations. Technical Report, Indiana University, April 2016. http://hdl.handle.net/2022/20927

8. R. Heiland, A. Adams, E. Heymann. perfSONAR-CTSC Code Review Engagement Final Report. Technical Report, Indiana University, January 2016. http://hdl.handle.net/2022/20596

9. V. Welch, et al. Year Three Report: Center for Trustworthy Scientific Cyberinfrastructure. Technical Report, Indiana University, Oct 2015. http://hdl.handle.net/2022/20401

10. R. Heiland and V. Welch. Analysis of authentication events and graphs using Python. SIAM Workshop on Network Science: Poster session. Snowbird, UT. May 2015. https://github.com/rheiland/authpy

11. V. Welch, et al. Year Two Report: Center for Trustworthy Scientific Cyberinfrastructure. Technical Report, Indiana University, Sept 2014. http://hdl.handle.net/2022/20030

12. J. Marsteller and R. Heiland. IceCube Cybersecurity Improvement Plan. Technical Report, Indiana University, 2014. http://hdl.handle.net/2022/17364

13. R. Heiland, S. Koranda, V. Welch. Globus Data Sharing: Security Assessment. Technical Report, Indiana University, 2014. http://hdl.handle.net/2022/19165

14. R. Heiland and O. Sporns. Comparing Functional Networks of the Brain: An Introductory Tutorial using Python. BioVis 2014 Data Contest, Boston, MA, July 2014. https://github.com/rheiland/biovis2014

15. R. Heiland, S. Marru, M. Pierce, V. Welch. CTSC Recommended Security Practices for Thrift Clients: Case Study – Evernote. Technical Report, Indiana University, May 2014. http://hdl.handle.net/2022/20620

16. V. Welch, et al. Year 1 Report: Center for Trustworthy Scientific Cyberinfrastructure. Technical Report, Indiana University, 2013. http://hdl.handle.net/2022/17205

17. R. Heiland, B. Thomas, V. Welch, C. Jackson. Toward a Research Software Security Maturity Model. Workshop on Sustainable Software for Science, Nov 2013. https://arxiv.org/pdf/1309.1677

18. R. Heiland, S. Koranda, V. Welch. Pegasus-CTSC Engagement Final Report. Technical Report, Indiana University, 2013. http://hdl.handle.net/2022/15562

19. R. Heiland, J. Champlin, S. Ito, A. Litke, A. Lumsdaine, and J. Beggs. Introduction to Modeling and Computational Neuroscience using Python. Presentation at Society for Mathematical Biology (SMB) Annual Meeting and Conference, July 2012.

20. R. Heiland, C. Perry, B. Ream, A. Lumsdaine. Sculpture, Geometry, and Computer Science. Presentation at SIAM Conference on Computational Science and Engineering, Feb 2011. https://obamawhitehouse.archives.gov/blog/2010/12/10/celebrating-computer-science

21. R. Heiland. Squeak: A Free Computer Application to Enhance Math and Science Learning. Presentation, HASTI Conference, Indianapolis, Feb 10, 2006.

22. R. Heiland. XML for Bioinformatics. Book Review, Briefings in Bioinformatics, Feb 2006. https://doi.org/10.1093/bib/bbk013

23. R. Heiland, M. P. Baker, and B. D. Semeraro. A Survey of Visualization Tools for High Performance Computing. Poster presentation at SIAM Parallel Processing for Scientific Computing, 1999. (Abstract)

24. P. Baker, D. Bock, R. Heiland, and M. Stephens. Visualization of Damaged Structures. CEWES MSRC PET Annual Technical Report: Year 2. March 1998.

25. R.W. Heiland. Object-oriented parallel polygon rendering. Technical Report PNL-SA–25031; CONF-9409278–3, Pacific Northwest Lab., Richland, WA (United States), 1 September 1994.

Software Skills

Good level: C/C++, Python (+numerous pkgs), OpenGL, Jupyter/IPython Notebooks, VTK, CMake, ParaView, MATLAB, git, LaTeX, ImageMagick, gdb, Linux, OSX

Intermediate: Docker, Galaxy, Fortran, Java, R, Qt, OpenMP, ITK, HTML, Bash, Valgrind, OpenCV

Basic level: JavaScript, MySQL, MPI, Boost, Pegasus, CUDA, OpenCL, Django, Mathematica, Maple, Blender, Windows

Professional Society Memberships

Society for Mathematical Biology (SMB)
Society for Industrial and Applied Mathematics (SIAM)
Mathematical Association of America (MAA)

References

Available upon request.