James E. McClure

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National Security Institute
1311 Research Center Drive
Virginia Tech
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Google scholar

EDUCATION

Ph.D., Environmental Sciences and Engineering
University of North Carolina at Chapel Hill, Chapel Hill, NC — May 2011
Dissertation: "Microscale Modeling of Fluid Flow in Porous Medium Systems."
Advisor: Cass T. Miller.

B.S.P.H., Environmental Sciences and Engineering
University of North Carolina at Chapel Hill, Chapel Hill, NC — May 2003

PROFESSIONAL EXPERIENCE

National Security Institute, Virginia Tech — 2022-Present
Research Associate Professor

Advanced Research Computing, Virginia Tech — 2012-2022
Computational Scientist

- PI or Co-PI on $4,222,520 in external research funding
- Published more than 50 peer-reviewed journal articles and conference proceedings publications
- Participation in U.S exascale software development through the Summit Early Science Program and Frontier Center for Accelerated Application Readiness (CAAR)
- Provide support for research computing infrastructure used by several hundred Virginia Tech faculty and several thousand students, including two Top 500 supercomputers;
- Manage HelpDesk for Research Computing Support, including staffing, training and day-to-day project management for ticketing systems (JIRA, ServiceNow)
- Supervision of graduate students (15), undergraduate students (2), and post-doctoral scholars (3)
- Coordinated procurement and deployment of a 14-node IBM "Minsky" cluster (Power 8 / NVIDIA P100 / NVLINK) for the Virginia Tech research community
- Developed, organized and taught a variety of workshops in parallel and distributed computing including programming workshops in MPI, OpenMP, CUDA, heterogeneous computing
- Developed, organized and taught workshops in artificial intelligence and machine learning;
- Participation in software development for U.S. exascale computers; developed simulation tools (C/C++ with CUDA and MPI) capable of scaling to thousands of GPU
- Principal Investigator for two Department of Energy INCITE Awards through the Oak Ridge Leadership Computing Foundation (OLCF).
- Develop and promote an investment program to encourage faculty investment in centralized computing resources

Department of Aerospace and Ocean Engineering, Virginia Tech — 2013-2015
Lecturer

- Developed and taught a graduate-level course "Introduction to Parallel Computing Applications" (offered twice as a special topics course)

Environmental Sciences and Engineering, University of North Carolina 2011-2012
Postdoctoral Research Associate

- Multi-scale model development for flow and transport in porous medium systems

Environmental Sciences and Engineering, University of North Carolina 2003–2011
Graduate Research Assistant

- Implementation of lattice Boltzmann methods for two-fluid flows
- Implementation of image analysis techniques for post-processing of 3D images of simulated and experimental systems
- Conducted computed micro-tomography experiments for multiphase porous medium systems using the advanced photon source at Argonne National Lab

PUBLICATIONS

Journal Articles

1. J.E. McClure, Z. Li (2023) Capturing membrane structure and function in lattice Boltzmann models, *Physical Review E* (accepted).
2. Y. da Wang, Q. Meyer , K. Tang , J.E. McClure , R. White, S. Kelly, M. Crawford, F. Iacoviello, D. Brett , P. Shearing , P. Mostaghimi , C. Zhao , R. Armstrong. (2023) Large-scale Modeling of Real Proton Exchange Membrane Fuel Cell with Deep Learned Physically Accurate Digital Twin, *Nature Communications* (accepted).
3. H. Wang, L. Dalton, R. Guo, J. McClure, D. Crandall, C. Chen (2023) Application of unsupervised deep learning to image segmentation and in-situ contact angle measurements in a CO2-water-rock system *Advances in Water Resources* (accepted).
4. F Alzubaidi, P Mostaghimi, Y Niu, RT Armstrong, G Mohammadi, S Berg, J.E. McClure. (2022) Effective permeability of an immiscible fluid in porous media determined from its geometric state, *Physical Review Fluids* (in review).
5. J.E. McClure, M. Fan, S. Berg, R.T. Armstrong, C.F. Berg, Z. Li, T. Ramstad (2022) Relative permeability as a stationary process: energy fluctuations in immiscible displacement, *Physics of Fluids* 34 (9), 092011 (**Feature Article**).
6. X.H. Zhou, J.E. McClure, C. Chen, H. Xiao (2022) Neural network-based pore flow field prediction in porous media using super resolution, *Physical Review Fluids* 7 (7), 074302.
7. H. Wang, L. Dalton, M. Fan, R. Guo, J. McClure, D. Crandall, C. Chen (2022) Deep-learning-based workflow for boundary and small target segmentation in digital rock images using UNet++ and IK-EBM, *Journal of Petroleum Science and Engineering* 215, 110596.
8. K. Tang, Y. Da Wang, J. McClure, C. Chen, P. Mostaghimi, R.T. Armstrong. (2022) Generalizable Framework of Unpaired Domain Transfer and Deep Learning for the Processing of Real-Time Synchrotron-Based X-Ray Microcomputed Tomography Images of Complex Structures, *Physical Review Applied*, 17 (3), 034048.
9. R. Guo, L. Dalton, D. Crandall, J. McClure, H. Wang, Z. Li, C. Chen. (2022) Role of heterogeneous surface wettability on dynamic immiscible displacement, capillary pressure, and relative permeability in a CO2-water-rock system, *Advances in Water Resources*, 104226.
10. J.E. McClure, N. Abaid, (2022) Effect of Topology and Geometric Structure on Collective Motion in the Vicsek Model,Frontiers in Applied Mathematics and Statistics 8, 829005.
11. C. Sun, J.E. McClure, S. Berg, P. Mostaghimi, R.T. Armstrong (2022) Universal description of wetting on multiscale surfaces using integral geometry, *Journal of Colloid and Interface Science* 608, 2330-2338.

12. A. L. Herring, C. Sun, R. T. Armstrong, Z. Li1, J. E. McClure, M. Saadatfar (2021) Evolution of Bentheimer Sandstone Wettability During Cyclic scCO2-Brine Injections, *Water Resources Research* 57 (11), e2021WR030891.
13. J.E. McClure, S. Berg, R.T. Armstrong (2021) Thermodynamics of fluctuations based on time-and-space averages, *Physical Review E* 104, 035106.
14. J.E. McClure, S. Berg, R.T. Armstrong (2021) Capillary fluctuations and energy dynamics for flow in porous media, *Physics of Fluids* 33 (8), 083323 (**Feature Article**)
15. Y. Niu, Y. Da Wang, P. Mostaghimi, J.E. McClure, J. Yin, R.T. Armstrong (2021) Geometrical-Based Generative Adversarial Network to Enhance Digital Rock Image Quality, *Physical Review Applied* 15 (6), 064033.
16. R.T. Armstrong, C. Sun, P. Mostaghimi, S. Berg, M. Rücker, P. Luckham, A. Georgiadis, J.E. McClure (2021) Multiscale Characterization of Wettability in Porous Media, *Transport in Porous Media* 140 (1), 215-240.
17. J.E. McClure, Z. Li, M. Berrill, T. Ramstad (2021) The LBPM software package for simulating multiphase flow on digital images of porous rocks *Computational Geosciences* 25 (3), 871-895.
18. R. Guo, L.E. Dalton, M. Fan, J. McClure, L. Zeng, D. Crandall, C. Chen (2020) The role of the spatial heterogeneity and correlation length of surface wettability on two-phase flow in a CO2-water-rock system *Advances in Water Resources* 146, 103763.
19. Y. A. Alzahid, H. Aborshaid, M. Asali, J.E. McClure, C. Chen, P. Mostaghimi, Y. Da Wang, C. Sun, R. T. Armstrong (2020) Real-time synchrotron-based X-ray computed microtomography during in situ emulsification, *Journal of Petroleum Science and Engineering* 195, 107885
20. C. Sun, J.E. McClure, P. Mostaghimi, A.L. Herring, D.E. Meisenheimer, D. Wildenschild, S. Berg, R.T. Armstrong (2020) Characterization of wetting using topological principles *Journal of Colloid and Interface Science* 578, 106-115.
21. M. Fan, J.E. McClure, R.T. Armstrong, M. Shabaninejad, L.E. Dalton D. Crandall, C. Chen (2020) Influence of Clay Wettability Alteration on Relative Permeability *Geophysical Research Letters* 47 (18), e2020GL088545.
22. J.E. McClure, Z. Li, A.P. Sheppard, C.T. Miller (2020) An adaptive volumetric flux boundary condition for lattice Boltzmann methods *Computers & Fluids* 210, 104670.
23. A. Li, J.E. McClure, J. Middleton, T. Varslot, A.P. Sheppard (2020) Discretization limits of lattice Boltzmann methods for studying immiscible twophase flow in porous media, *International Journal for Numerical Methods in Fluids* 1-36.
24. J. E. McClure, J. Yin, R.T. Armstrong, K.C. Maheshwari, S. Wilkinson, L. Vlcek, Y. Da Wang, M.A. Berrill, M. Rivers (2020) Toward Real-Time Analysis of Synchrotron Micro-Tomography Data: Accelerating Experimental Workflows with AI and HPC, *Smoky Mountains Computational Sciences and Engineering Conference*, 226-239.
25. J.E. McClure, T. Ramstad, Z. Li, R.T. Armstrong, S. Berg (2020) Modeling Geometric State for Fluids in Porous Media: Evolution of the Euler Characteristic *Transport in Porous Media* 133, 229-250.
26. M. Fan, Y. Han, M. Gu, J. McClure, N. Ripepi, E. Westman, C. Chen (2020) Investigation of the conductivity of a proppant mixture using an experiment/simulation-integrated approach, *Journal of Natural Gas Science and Engineering* 78, 103234.
27. C. Sun, J.E. McClure, P. Mostaghimi, A.L. Herring, S. Berg, R.T. Armstrong (2020) Probing effective wetting in subsurface systems *Geophysical Research Letters*, 47 (5).
28. C. Sun, J.E. McClure, P. Mostaghimi, A.L. Herring, M. Shabaninejad, S. Berg, R.T. Armstrong (2020) Linking continuum-scale state of wetting to pore-scale contact angles in porous media *Journal of Colloid and Interface Science* 561, 173-180.

29. Y.D. Wang, T. Chung, R.T. Armstrong, J. McClure, T. Ramstad, P. Mostaghimi (2020) Accelerated Computation of Relative Permeability by Coupled Morphological and Direct Multiphase Flow Simulation *Journal of Computational Physics* 401, 108966.

30. DE Meisenheimer, JE McClure, ML Rivers, D Wildenschild (2020) Exploring the effect of flow condition on the constitutive relationships for two-phase flow, *Advances in Water Resources*, 103506.

31. B. Zhao, C. Macminn, B.K. Primkulov, Y. Chen, A.J. Valocchi, J. Zhao, Q. Kang, K. Bruning, J.E. McClure, C.T. Miller, A. Fakhari, D. Bolster, T. Hiller, M. Brinkmann, L. Cueto-Felgueroso, D.A. Cogswell, R. Verma, M. Prodanović, J. Maes, S. Geiger, M. Vassvik, A. Hansen, E. Segre, R. Holtzman, Z. Yang, C. Yuan, B. Chareyre, R. Juanes (2019) Comprehensive comparison of pore-scale models for multiphase flow in porous media, *Proceedings of the National Academy of Sciences of the United States of America* 116 (28), 1379913806.

32. M. Fan, L.E. Dalton, J. McClure, N. Ripepi, E. Westman, D. Crandall, C. Chen (2019) Comprehensive study of the interactions between the critical dimensionless numbers associated with multiphase flow in 3D porous media, *Fuel* **252**, 522-533.

33. C.T. Miller, K. Bruning, C.L. Talbot, J.E. McClure, W.G. Gray (2019) Non-hysteretic capillary pressure in two-fluid porous medium systems: Definition, evaluation, validation, and dynamics, *Water Resources Research* 55 (8), 6825-6849.

34. M. Fan, J. McClure, Y. Han, N. Ripepi, E. Westman, M. Gu, C. Chen (2019) Using an Experiment / Simulation-Integrated Approach To Investigate Fracture-Conductivity Evolution and Non-Darcy Flow in a Proppant-Supported Hydraulic Fracture *SPE Journal*

35. Y. Da Wang, T. Chung, R.T. Armstrong, J.E. McClure, P. Mostaghimi (2019) Computations of permeability of large rock images by dual grid domain decomposition, *Advances in Water Resources* **126**, 1–14.

36. R.T. Armstrong, J.E. McClure, V. Robins, Z. Liu, C.H. Arns, S. Schlüter, S. Berg (2018) Porous Media Characterization Using Minkowski Functionals: Theories, Applications and Future Directions *Transport in Porous Media*, 1–31

37. Z Liu, JE McClure, RT Armstrong (2018) Influence of wettability on phase connectivity and electrical resistivity *Physical Review E* 98 (4), 043102

38. McClure, J.E., Armstrong, R.T., Berrill, M.A. Rücker, M. Schlüter, S. Berg, W.G. Gray and C.T. Miller. (2018) A geometric state function for two-fluid flow in porous media. *Physical Review Fluids* Vol. 3, 084306.

39. Herring, A.L., Gilby, F.J., Li, Z., McClure, J.E., Turner, M., Veldkamp, J.P., Beeching, L., A.P. Sheppard (2018) Observations of nonwetting phase snap-off during drainage. *Advances in Water Resources* Vol. 121, 32–43.

40. Fan, M., McClure, J.E., Han. Y. and C. Cheng (2018) Interaction between Proppant Compaction and Single/Multiphase Flows in a Hydraulic Fracture, *SPE Journal*.

41. Armstrong, R.T., McClure, J.E., Berrill, M.A. Rücker, M. Schlüter, and S. Berg (2017) Flow regimes during immiscible displacement *Petrophysics* Vol. 58, No. 1 pp. 10-18 (**Journal cover**)

42. McClure, J.E. Dye, A.L., Gray, W.G. and C.T. Miller (2017) On the Consistency of Scale Among Experiments, Theory, and Simulation *Hydrology and Earth System Sciences* Vol. 21, pp. 1063-1076.

43. Im, D.K., Choi, S., McClure, J. and S.H. Park (2017) Numerical analysis of synthetic jet flows using a diagonally implicit harmonic balance method with preconditioning. *Computers & Fluids* Vol. 147, pp. 12-24.

44. Armstrong, R.T., McClure, J.E. Berrill, M.A., Rücker M., Schlüter, S. and S. Berg (2016) Beyond Darcy's Law: The Role of Phase Topology and Ganglion Dynamics for Two Fluid Flow. *Physical Review E* Vol. 94, 043113.

45. McClure, J.E., Berrill, M.A., Gray, W.G. and C.T. Miller (2016) Influence of phase connectivity on the relationship among capillary pressure, fluid saturation, and interfacial area in two-fluid-phase porous medium systems. *Physical Review E* Vol. 94, 033102.

46. McClure, J.E., Berrill, M.A., Gray, W.G. and C.T. Miller (2016) Tracking Interface and Common Curve Dynamics for Two-Fluid Flow in Porous Media, *Journal of Fluid Mechanics* Vol. 796, pp. 211-232.
47. Dye, A.L., McClure, J.E., Adalsteinsson, D. and C.T. Miller (2016) An adaptive lattice Boltzmann scheme for modeling two-fluid-phase flow in porous medium systems, *Water Resources Research* Vol. 52, No. 4 pp 2601–2617.
48. Gray, W.G., Dye, A.L., McClure, J.E., Pyrak-Nolte, L.J., and C.T. Miller (2015) On the dynamics and kinematics of two-fluid-phase flow in porous media, *Water Resources Research* Vol. 51, No. 7 pp. 5365-5381.
49. Im, D.K., Choi, S., McClure, J.E. and F. Skies. (2015) A Mapped Chebyshev Pseudospectral Method for Unsteady Flow Analysis, *AIAA Journal*, Vol. 53, No. 12, pp. 3805-3820
50. McClure, J.E., J.F. Prins and C.T. Miller (2014) A Novel Heterogeneous Algorithm to Simulate Multiphase Flow in Porous Media on Multicore CPU-GPU Systems, *Computer Physics Communications*, Vol. 185. pp. 1865–1874.
51. Dye, A.L., J.E. McClure, C.T. Miller and W.G. Gray (2013) Description of Non-Darcy Flows in Porous Medium Systems, *Physical Review E*, Vol. 87, Issue 3, 033012.
52. McClure, J.E., W.G. Gray, and C.T. Miller (2010) Beyond Anisotropy: Examining Non-Darcy Flow in Asymmetric Porous Media, *Transport in Porous Media*, Vol. 84, No. 2, pp. 535-548.
53. McClure, J.E., D. Adalsteinsson, C. Pan, W.G. Gray, and C.T. Miller (2007) Approximation of Interfacial Properties in Multiphase Porous Medium Systems, *Advances in Water Resources*, Vol. 30, No. 3, pp. 354-365.

Book Chapters

1. McClure, J.E., Numerical Solution of Linear Systems of Equation (2018) In: Fundamentals of Finite Element Analysis: Linear Finite Element Analysis, I. Koutromanos, Wiley, Hoboken, United States.
2. Dye, A.L., J.E. McClure, W.G. Gray, and C.T. Miller (2015) Multiscale Modeling of Porous Medium Systems, In: Handbook of Porous Media, Third Edition, K. Vafai (Editor), Taylor and Francis, London, United Kingdom.

Conference Proceedings Papers

1. B. Barbour, R. Gibbons, S. Kenyon, J. McClure, D. Ridge, J Black. Network Testbed for Small Satellites (NeTSat) - Distributed Space Adaptive Communications and Security for Multi-Constellation Networks, AIAA 2023-1502. AIAA SCITECH 2023 Forum. January 2023.
2. C. Patnayak, J.E. McClure, R.K. Williams, WASP: A Wearable Super-Computing Platform for Distributed Intelligence in Multi-Agent Systems 2021 IEEE High Performance Extreme Computing Conference, HPEC 2021, Waltham, MA, USA, September 22-24, 2021. (accepted)
3. Fowler, C.P., Bowers, C.A., Bruning, K., McClure, J.E., and C.T. Miller. Advancements in Large-Scale Simulation of Microscale Porous Medium Systems Using Lattice Boltzmann Methods. Computational Methods in Water Resources XXII, Saint Maloes, France, 3-7
4. McClure, J.E., Berrill, M.A., Prins, J.F., and Miller, C.T. "Asynchronous *in situ* connected components analysis for complex fluid flows" *ISAV '16* Salt Lake City, UT, USA, 13 Nov. 2016
5. Armstrong, R.T., McClure, J.E. Berrill, M.A., Rücker M. Schlüter, S. and S. Berg "Flow Regimes During Immiscible Displacement" *International Symposium of the Society of Core Analysts* Snow Mass, Colorado, USA, 21-26 August 2016 **Best paper award**

6. Im, D.K., Choi, S., McClure, J.E., Choi, J.Y. and F. Skies (2015) A mapped Chebyshev pseduospectral method for unsteady flow analysis, 22^{nd} *AIAA Computational Fluid Dynamics Conference, Aviation Forum 2015*
7. McClure, J.E., H. Wang, J.F. Prins, C.T. Miller and W. Feng (2014) Petascale Application of a Coupled CPU-GPU Algorithm for Simulation and Analysis of Multiphase Flow Solutions in Porous Medium Systems *28th Annual IEEE International Parallel & Distributed Processing Symposium (IPDPS)* May 19-23 2014, Phoenix, AZ (Featured by InsideHPC.com on May 24, 2014)
8. McClure, J.E., J.F. Prins, and C.T. Miller (2010) Comparison of CPU and GPU Implementations of the Lattice Boltzmann Method, *Proceedings of the* 18^{th} *International Conference on Computational Methods in Water Resources (CMWR XVIII)*, Barcelona, Spain, 21-24 June 2010, Paper 273.
9. Pan, C. J.E. McClure, W.G. Gray, and C.T. Miller (2006) Lattice Boltzmann Simulation of Non-Darcy Flow, *Proceedings of the* 16^{th} *International Conference on Computational Methods in Water Resources (CMWR XVI)*, Copenhagen, Denmark, 19-22 June 2006. http://proceedings.cmwr.xvi.org, Paper 248.
10. McClure J.E., D. Adalsteinsson, D. Wildenschild, W.G. Gray, and C.T. Miller (2006) Computation of Interfacial Areas, Common Curve Lengths, and Interfacial Curvatures from Experimentally Derived Data, *Proceedings of the* 16^{th} *International Conference on Computational Methods in Water Resources (CMWR XVI)*, Copenhagen, Denmark, 19-22 June 2006. http://proceedings.cmwr.xvi.org, Paper 224.
11. McClure, J.E., C. Pan, D. Adalsteinsson, W.G. Gray, and C.T. Miller (2004) Estimating Interfacial Areas Resulting from Lattice-Boltzmann Simulation of Two-Fluid-Phase Flow in a Porous Medium, *Proceedings of the* 15^{th} *International Conference on Computational Methods in Water Resources (CMWR XV)*, 13-17 June 2004, Chapel Hill, North Carolina, Computational Methods in Water Resources, Vol. 1, Developments in Water Science 55, Edited by: C.T. Miller, M.W. Farthing, W.G. Gray and G.F. Pinder, Elsevier Science, Amsterdam, The Netherlands, pp. 23-55.

Published Abstracts and Presentations

1. "Non-equilibrium theory for non-ergodic systems based on time-and-space averaging" J.E. McClure, S. Berg, R. Armstrong Bulletin of the American Physical Society
2. "Super resolution-assisted pore flow field prediction using neural networks" X.H. Zhou, J. McClure, C. Chen, H. Xiao Bulletin of the American Physical Society
3. "Learning from a Big Dataset of Digital Rock Simulations" J.E. Santos, B. Chang, A. Gigliotti, E. Guiltinan, M. Mehana, A. Mohan, J.E. McClure, Q. Kang, H. Viswanathan, N. Lubbers, M. Prodanovic, M. Pyrcz, AGU Fall Meeting Abstracts 2021, H25O-1207
4. "Digital Rocks Portal: connecting data, simulation, machine learning and research community" M. Prodanovic, J. McClure, A. Radhakrishnan, H. Khan, J.E. Santos, A. Singh, AGU Fall Meeting Abstracts 2021, H25O-1203
5. "Capillary Fluctuations and Two-Fluid Flow in Porous Media" James E. McClure, Steffen Berg, Ryan Armstrong, SIAM GS21, MS95 Multiphase Flow in Porous Media from Pore to Darcy Scale, (21-24 June 2021)
6. "The impact of spatial variation and correlation length of wettability on scCO2-brine immiscible displacement in 3D porous media" R. Guo, L. Dalton, M. Fan, J.E. McClure, L. Zeng, D. Crandall, C. Chen, AGU Fall Meeting Abstracts 2020, MR023-0014
7. "Visualization and data reuse via the Digital Rocks Portal" M. Prodanovic, M. Esteva, J.E. McClure AGU Fall Meeting 2019
8. "LBM-based Simulation on Impact of Wettability Heterogeneity on Relative Permeability in Sandstone" R Guo, JE McClure, C Chen, M Fan AGU Fall Meeting 2019

9. "Synchrotron-Based X-ray Micro-Computed Tomography for Real Time Investigation of Alkaline Surfactant Flooding" H Aborshaid, Y Alzahid, P Mostaghimi, J McClure, C Chen, C Sun, R.T. Armstrong, M. Asali, Abu Dhabi International Petroleum Exhibition & Conference
10. Combining Discrete Element Method with Lattice Boltzmann Modeling to Advance the Understanding of the Performance of Proppant Mixtures M Fan, Y Han, M Gu, J McClure, N Ripepi, E Westman, C Chen 53rd US Rock Mechanics/Geomechanics Symposium
11. On the interactions between the critical dimensionless numbers associated with multiphase flow in 3D porous media M Fan, L Dalton, JE McClure, N Ripepi, E Westman, D Crandall, C Chen AGU Fall Meeting Abstracts
12. Microscale simulation of three-fluid flow in porous media CP Fowler, JE McClure, CT Miller AGU Fall Meeting Abstracts
13. Lattice Boltzmann Modeling of Gas Adsorption and Desorption in Shale Matrix R Xu, M Prodanovic, CJ Landry, JE McClure AGU Fall Meeting Abstracts
14. Storage, visualization and simulation using data in Digital Rocks Portal M Prodanovic, M Esteva, JE McClure AGU Fall Meeting Abstracts
15. McClure, J.E., R.T. Armstrong, M.A. Berrill, S. Schlüter, S. Berg, W.G. Gray, and C.T. Miller (2017) Digital Rock Physics and Macroscale Models for Two-Fluid Flow, Abstract H11L-05. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11–15 December 2017. (invited)
16. Bowers, C.A., P.B. Schultz, C.P. Fowler, J.E. McClure, and C.T. Miller (2017) Experimental Observation of Dispersion Phenomenon for Non-Newtonian Flow in Porous Media, Abstract H43I-1766. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11–15 December 2017.
17. Fowler, C.P., C.A. Bowers, J.E. McClure, and C.T. Miller (2107) Systems Using the Lattice Boltzmann Method, Abstract H11G-1285. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11–15 December 2017.
18. McClure, J.E., C.L. Talbot, R.T. Armstrong, P. Mostaghimi, Y. Yu, and C.T. Miller (2017) Stochastic Models of Macroscale Quantities for the Prediction of the REV Scale for Multiphase Flow Through Porous Media, Abstract H13A-1348. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11–15 December 2017.
19. Miller, C.T., J.E. McClure, and K. Bruning (2017) Lattice-Boltzmann Modeling of Community Challenge Microfluidic Experiments to Evaluate the Effects of Wettability on Two-Fluid Flow in Porous Media, Abstract H14G-04. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11–15 December 2017.
20. Talbot, C.L., J.E. McClure, R.T. Armstrong, P. Mostaghimi, Y. Yu, and C.T. Miller (2017) Reduced Dynamic Models of Macroscale Quantities for the Prediction of Equilibrium System States for Multiphase Porous Medium Systems, Abstract H21G-1568. American Geophysical Union Fall Meeting, New Orleans, Louisiana, 11–15 December 2017.
21. Miller, C.T., J.E. McClure, and W.G. Gray (2017) Toward the Closure of a New Generation of Multiphase Flow Models, Alliance of Laboratories in Europe for Education, Research and Technology, ALERT Geomaterials Workshop 2017, Aussois, France, 2–4 October 2017.
22. Fan, M., McClure, J., Crandall, D., Dalton, L., Jarvis, K., Chen, C. Combining Pore-scale Simulation Capabilities with NETLs Geoimaging Lab Facilities to Develop Digital Rock Technologies for Geologic Carbon Sequestration and Oil & Gas applications. Mastering the Subsurface Through Technology Innovation, Partnerships & Collaboration: Carbon Storage & Oil & Natural Gas Technologies Review Meeting, Pittsburgh, PA, USA. 1-3 Aug. 2017.
23. McClure, J.E., Armstrong, R.T., Rücker, M. Schlüter, S., Berg, S., Miller, C.T. and W.G. Gray The effect of topology on two-fluid flow in porous media American Geophysical Union Conference, San Francisco, CA, USA. 14-19 Dec. 2016.

24. Fan, M., McClure, J.E., Han, Y., and C. Chen, Interaction between Proppant Packing, Reservoir Depletion, and Fluid Flow in Pore Space American Geophysical Union Conference, San Francisco, CA, USA. 14-19 Dec. 2016.
25. Armstrong, R.T., McClure, J.E., Berrill, M.A., Rücker, M. Schlüter, S. and S. Berg. Beyond Darcy's law: The Role of Phase Topology and Ganglion Dynamics for Two Fluid Flow. Gordon Research Conference on Flow & Transport in Permeable Media, Girona, Spain. 31 July - 5 Aug. 2016.
26. C.T. Miller, W.G. Gray, J.E. McClure, and A.L. Dye A multiscale talk. The XXI International Conference Computational Methods in Water Resources, CMWR 2016. Toronto, Canada, 20-24 June, 2016
27. J.E. McClure. A new class of models for multiphase flow in hydrologic systems. Observations and Modeling Across Scales:Symposium in Honor of Eric Wood. Princeton University, June 2-3, 2016
28. Miller, C.T., Dye, A.L., Weigand, T.M., McClure, J.E. and W.G. Gray Multiscale analysis of two-fluid-phase flow in porous medium systems. 7^{th} International Conference on Porous Media & Annual Meeting, International Society for Porous Media, Padova, Italy. 18-21 May 2015.
29. Miller, C.T., Dye, A.L. McClure, J.E. and W.G. Gray (2015) Simulation of Multiphase Porous Medium Systems ITS Research Computing Symposium, UNC, Chapel Hill, NC. 14 May 2015.
30. McClure, J.E., Miller, C.T., and A.L. Dye (2014) Connecting Pore-Scale Dynamics to Macroscopic Models for Multiphase Flow American Geophysical Union Conference, San Francisco, CA, USA. 14-19 Dec. 2014.
31. Dye, A.L., McClure, J.E., Adalsteinsson, D., Gray, W.G., Miller, C.T. (2014) A Two-Dimensional Lattice Boltzmann Scheme for Analyzing Equilibrium States in a Two-Fluid-Phase Porous Medium System. American Geophysical Union Conference, San Francisco, CA, USA. 14-19 Dec. 2014.
32. Weigand, T. Dye, A.L., McClure, J.E., Farthing, M., Gray, W.G., Miller, C.T. (2014) Simulation of Two-Phase Flow Based on a Thermodynamically Constrained Averaging Theory Flow Model. American Geophysical Union Conference, San Francisco, CA, USA. 14-19 Dec. 2014.
33. McClure, J.E., Dye, A.L., Prins, J.F., Miller, C.T., Gray, W.G. (2014) Pore-Scale Simulation and Analysis of Two-Fluid Flow in Porous Medium Systems Gordon Research Conference on Flow & Transport in Permeable Media, Bates College, Lewiston, ME, USA. 6-11, July 2014.
34. Dye A.L., J.E. McClure, W.G. Gray, C.T. Miller (2014) Interfacial dynamics in a two-fluid-phase porous medium system Computational Methods in Water Resources XX, Stuttgart, Germany 10-13 June 2014.
35. Dye A.L., S.C. Hauswirth, J.E. McClure, L. Pyrak-Nolte, W.G. Gray, C.T. Miller (2014) Analysis of capillary pressure in a two-fluid-phase porous medium system using micro-model experiments and pore-scale modeling Computational Methods in Water Resources XX, Stuttgart, Germany 10-13 June 2014.
36. Weigand, T. A.L. Dye, J.E. McClure, W.G. Gray, C.T. Miller (2014) Simulation of two-phase flow based on a thermodynamically constrained averaging theory flow model Computational Methods in Water Resources XX, Stuttgart, Germany 10-13 June 2014.
37. Dye A.L., J.E. McClure, L.J. Pyrak-Nolte, W.G. Gray and C.T. Miller (2013) Capillary Pressure Dynamics in a Two-Fluid-Phase Porous Medium System, American Geophysical Union Conference, San Francisco, CA, USA 9-13 Dec. 2013.
38. Carter, B., A.L. Dye, S. Hauswirth, J.E. McClure, L.J. Pyrak-Nolte, W.G. Gray and C.T. Miller (2013) Analysis of Capillary Pressure in a Two-Fluid-Phase Porous Medium System Using Micro-Model Experiments and Pore-Scale Modeling, American Geophysical Union Conference, San Francisco, CA, USA 9-13 Dec. 2013.
39. McClure, J.E., A.L Dye, C.T. Miller and W.G. Gray (2012) Description of Non-Darcy Flow in Anisotropic Porous Media, American Geophysical Union Conference, San Francisco, CA, USA 3-7 Dec. 2012.

40. Dye, A.L., J.E. McClure, E. Schaberg, M. Talley, W.G.Gray and C.T. Miller (2012) Pore-scale Analysis of Capillary Pressure at Equilibrium in a Two-Fluid-Phase Porous Medium System, American Geophysical Union Conference, San Francisco, CA, USA 3-7 Dec. 2012.
41. Dye, A.L., J.E. McClure, L. Pyrak-Nolte, D.A. Adalsteinsson and W.G.Gray (2012) Analysis of Capillary Pressure in a Two-Fluid-Phase Porous Medium System, Computational Methods in Water Resources XIX, Champaign, IL, USA 17-21 June 2012.
42. McClure J.E., C.T. Miller, and W.G. Gray (2011) Thermodynamic Equilibrium in Multiphase Porous Media: Examining Equilibria Across Spatial Scales, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Long Beach, California, 19-22 March 2011.
43. McClure J.E., J.F. Prins, and C.T. Miller (2010) Comparison of CPU and GPU Implementations of the Lattice Boltzmann Method, Computational Methods in Water Resources XVIII, Barcelona, Spain, 21-24 June 2010.
44. McClure J.E., J.F. Prins, and C.T. Miller (2009) High Performance Implementation of the Lattice Boltzmann Method, Sponsored by US Army Corps of Engineers Engineer Research and Development Center, University of North Carolina, Chapel Hill, North Carolina, 6-7 April 2009.
45. Johnson-Wright, D.N., P.S. Birak, J.A. Pedit, J.E. McClure and C.T. Miller (2007) Multiscale Reductions in Mass Flux as a Function of Residual Saturation, EOS Transactions, American Geophysical Union, Vol. 88, No. 52, Fall Meeting Supplement, Abstract H–. American Geophysical Union Fall Meeting, San Francisco, California, 10-14 December 2007.
46. McClure, J.E., A.B. Sallerson, W.G. Gray, and C.T. Miller (2007) Lattice Boltzmann Modeling and Image Analysis for Multiphase Porous Medium Systems, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Santa Fe, New Mexico, 19-22 March 2007.
47. Sallerson, A.B., W.G. Gray, C.T. Miller, J.E. McClure (2007) Thermodynamically Constrained Averaging Theory Formulation for Two-Phase Flow in Porous Medium Systems, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Santa Fe, New Mexico, 19-22 March 2007.
48. Sallerson, A.B., J.E. McClure, C. Pan, and C.T. Miller (2006) Pore-Scale Simulation of NAPL Dissolution, EOS Transactions, American Geophysical Union, Vol. 87 No. 52, Fall Meeting Supplement, Abstract H11C-1266. American Geophysical Union Fall Meeting, San Francisco, California, 11-15 December 2006.
49. McClure, J.E., C. Pan, W.G. Gray, and C.T. Miller (2006) Lattice Boltzmann Simulation of Non-Darcy Flow in Porous Media, EOS Transactions, American Geophysical Union, Vol. 87, No.52, Fall Meeting Supplement, Abstract H53G-07. American Geophysical Union Fall Meeting, San Francisco, California, 11-15 December 2006.
50. McClure, J.E., D.Adalsteinsson, C. Pan, W.G. Gray, and C.T. Miller (2005) Resolution of Interfaces, Curvatures, and Common Lines in General Porous Media. EOS Transactions, American Geophysical Union, Vol. 86, No. 52, Fall Meeting Supplement, Abstract H33A-1366. American Geophysical Union Fall Meeting, San Francisco, California, 5-9 December 2005
51. McClure, J.E., C. Pan, D. Adalsteinsson, C.T. Miller and W.G. Gray (2004) A Modified Marching Cubes Algorithm for Application to LBM Porous Media Simulations, Computational Methods in Water Resources XV, Chapel Hill, North Carolina, 13-17 June, 2004.

Invited Talks

1. "Mesoscopic modeling for biological membranes" Biological Engineering and Mechanics Fall Colloquium, (Wednesday, September 7, 2022)
2. "Quantum Software Co-Design" Virginia Tech - HBCU Quantum Partnering Workshop (Tuesday, August 9, 2022)
3. "Mesoscopic modeling for biological membranes" Center for Soft Matter and Biological Physics 2022 Annual Symposium (Wednesday, May 18, 2022)

4. "Fluctuations and energy dynamics in complex fluid flows" School Colloquium, Department of Electronic Materials Engineering, Research School of Physics, Australian National University. April 21, 2022. (online)
5. "Large-Scale Digital Rock Physics Simulations with LBPM" SEG Conference for High Performance Computing for Exploration and Reservoir Development December 7, 2021. (online)
6. "LBPM: Massively parallel lattice Boltzmann Simulator for Porous Media" SPE Virtual Workshop: Open Subsurface 20 May 2021 (online).
7. "Modeling multi-phase flow and anomalous diffusion with mesoscopic methods" Joint Condensed Matter and Center for Soft Matter and Biological Physics Seminar. Virginia Tech, Nov. 16 2020. (online)
8. "Topology and its effects on fluid flow" Interpore 2020, Qindao, China. (online)
9. "Modeling wetting phenomena with lattice Boltzmann methods" Shell Pore Scale Physics Seminar, 26 February 2019
10. "GPU-Accelerated Digital Rock Physics Workflows for Titan and Summit" OLCF User Meeting, Oak Ridge National Lab, May 2017
11. "Opportunities for fluid flow simulation and fast-micro tomography" High Resolution 2D & 3D imaging in Geoscience, Virginia Tech, 6 April 2017, Blacksburg, VA, USA.
12. "Embracing Heterogeneous Simulation of Complex Fluid Flows" NVIDIA GPU Technology Theatre, SC15, November 18, 2015 Austin, TX, USA.
13. "The Role of Simulation in Digital Rock Physics for Two-Fluid Flow," Workshop on 3D Printing and Digital Rock Physics, Drury Plaza Hotel / Sandia National Lab, August 2015.
14. "Optimizing Rosetta for the Intel Xeon Phi" XSEDE Conference, July 2014
15. "Principles of Multithreading and Auto-Vectorization" Rosetta MiniCon, February 2014
16. "Advancing Models for Multiphase Flow and Transport in Porous Medium Systems" Oak Ridge National Lab, January 2014
17. "Introduction to XSEDE Resources", SSI Summer School REU, Virginia Tech, July 2013
18. "Microscale Analysis of Porous Medium Flows," Envr 400: Seminar Series, University of North Carolina at Chapel Hill, November 2006.
19. "Introduction to Level Sets for Image Analysis," Summer School in Geophysical Porous Media: Multidisciplinary Science from Nano- to Global-Scale," Purdue University, July 2006.

COMPUTER EXPERTISE

- Participation in Frontier Center for Accelerated Application Readiness (CAAR) performing software optimization for U.S. exascale super-computing systems
- Developed a wearable supercomputer to support multi-UAV teams in remote field settings (NVIDIA Xavier embedded processors, ethernet & wireless, running Kubernetes)
- Test-driven development of scientific software targeted for large-scale parallel computing
- Extensive programming experience in C/C++, R and python and linux shell scripting
- Parallel programming expertise using CUDA, HIP OpenMP and MPI
- Analysis and visualization of scientific data using R and python
- Construction of analysis and data management tools to streamline data acquisition, curation and exploitation and design of hardware infrastructure to support data intensive research
- Experience with cluster management software including schedulers (Moab, Slurm, LSF) and the management of complex HPC software environments

- Support for HPC software packages targeting computational fluid dynamics, machine learning and artificial intelligence, molecular dynamics, bioinformatics, image processing and others in a research-oriented environment
- Familiar with parallel visualization tools including ParaView and VisIt
- Design and implementation of high-performance scientific libraries
- Familiar with parallel debugging and profiling tools
- Certified Software Carpentries Instructor (bash, git, python, R)

GRANTS AND CONTRACTS

1. Assessing biochar feedstocks and preparation methods on soil health in diverse managed ecosystems, Sponsor: USDA, Award Amount: $719,047 (4/01/2022-3/31/2025). Co-PI with John E. Barrett (PI) and Cheng Cheng
2. Balancing Collaboration and Autonomy for Multi-Robot Multi-Human Search and Rescue, Sponsor: NSF NRI (award 1830414) Award Amount: $1,474,719.00 (9/30/18-9/29/22). Co-principal investigator with Ryan Williams, Nathan Lau and Nicole Abaid
3. Digital Rock Physics with LBPM in the Open Porous Media Project, Sponsor: Equinor Energy AS Amount: $439,659.00 (5/1/2019–4/30/2021) Principle Investigator.
4. Electrochemistry capabilities for multiphase flow simulation Sponsor: Shell Amount: $ 100,000 (1/2020–7/2021) Principle Investigator
5. A Physics-Based, Data-Driven Framework for Reducing Uncertainties Associated with Carbon Storage Sponsor: NETL Amount: $480,000 (11/2019–10/2021) Co-principal investigator with Cheng Chen (PI), Heng Xiao and Nino Ripepi
6. Air Quality Modeling and System Services (AQMSS) for Virginia Department of Environmental Air Quality's Air Quality Assessments Group. Sponsor: Virginia Department of Environmental Quality (10/29/20-10/28/23). Award Amount: $243,099 Co-principal investigator with Hosein Foroutan and Matthew Brown
7. Simulating Two-Fluid Flow in Porous Media at the Laboratory Scale, Sponsor: Oak Ridge Leadership Computing Facility, U.S. Department of Energy, Summit Early Science Program (2019). Principal Investigator. Award: Early access to Summit at Oak Ridge National Laboratory.
8. Geometric Sate Function For Multiphase Flow in Porous Systems. Synchrotron Beam Time, June 5 (9am) June 8 (8am), 2018 Co-Principle Investigator with Ryan Armstrong and Cheng Chen. Sponsor: Advanced Photon Source, GSECARS, Sector 13, Argonne National Laboratory
9. Air Quality Modeling and System Services (AQMSS) for Virginia Department of Environmental Air Quality's Air Quality Assessments Group. Co-principal investigator with Linsey Marr, Virginia Tech Sponsor: Virginia Department of Environmental Quality (10/29/16-10/28/19). Award Amount: $243,065
10. Advancing Models for Multiphase Flow and Transport in Porous Medium Systems. Sponsor: Oak Ridge Leadership Computing Facility, U.S. Department of Energy, INCITE Program (1/1/17-12/31/18). Principal Investigator. Award: 115,000,000 core-hours per year on Titan (Cray XK7) at Oak Ridge National Laboratory.
11. Thermodynamically Constrained Averaging Theory for Multiscale Systems. Sponsor: Army Research Office (5/16/14-5/15/18). Co-principal Investigator with Cass T. Miller, University of North Carolina at Chapel Hill. Award Amount: $100,000 from a total award of $693,793.
12. NVIDIA Academic Hardware Donation Program. Sponsor: NVIDIA (6/27/14). Award Amount: One NVIDIA Jetson TK1 embedded processing board.

13. Advancing Models for Multiphase Flow and Transport in Porous Medium Systems. Sponsor: Oak Ridge Leadership Computing Facility, U.S. Department of Energy, INCITE Program (1/1/14-12/31/16). Principal Investigator. Award: 60,000,000 core-hours per year on Titan (Cray XK7) at Oak Ridge National Laboratory.
14. Air Quality Modeling and System Services (AQMSS) for Virginia Department of Environmental Air Quality's Air Quality Assessments Group. Co-principal investigator with Linsey Marr, Virginia Tech Sponsor: Virginia Department of Environmental Quality (10/29/13-10/28/16). Award Amount: $391,715
15. NVIDIA Academic Hardware Donation Program. Sponsor: NVIDIA (11/1/12). Award Amount: One M2075 graphics processing unit (GPU).
16. Campus Champion Fellows Program. Sponsor: NSF/XSEDE (7/17/2013-7/16/2014). Award Amount: $31,216
17. Summer Undergraduate Research Fellowship (SURF), Sponsor: Office for Undergraduate Research at the University of North Carolina at Chapel Hill (5/15/02-8/15/02). Award Amount: $2,000.

AWARDS

1. TechConnect Innovation Award, "A wearable computing cluster and platform for multi-agent cyber-physical systems," 2022.
2. Best Paper Award, Society of Core Analysts, 2016.
3. Certificate of Reviewing Excellence, Advances in Water Resources, 2014.
4. Outstanding Student Paper Award, "Lattice Boltzmann Simulation of Non-Darcy Flow in Porous Media," American Geophysical Union, 2006.

PROFESSIONAL SERVICE

- Search Committee for Associate Vice President for Research Computing, Virginia Tech (2022).
- Special Topics Lead Editor, Pore-scale Microstructure, Mechanisms, and Models for Subsurface Flow and Transport, Frontiers in Water (2021).
- Mini-symposium co-organizer, MS6. Interpore Conference (2021).
- "Porous media visualization and data reuse challenge", Digital Rocks Portal, Co-organizer with Masa Prodanovic (November 2020).
- Mini-symposium co-organizer, MS9. Pore-scale modeling. Interpore Conference (2020).
- Peer Reviewer for American Chemical Society, Petroleum Research Fund (2018, 2020).
- OLCF User Group Executive Board, June 2017 - May 2020.
- NVIDIA HPC Containers Advisory Board (2018).
- Program Committee, 3rd Annual Workshop on Reproducibility in Parallel Computing (REPPAR) in conjunction with Euro-Par 2016, (Aug 22-26) Grenoble, France.
- Mini-symposium co-organizer "MS3.3 - Microscale approaches to close, evaluate, and validate emerging multiscale theories" 9^{th} International Conference on Porous Media and Annual Meeting, 2016, May 9-12, Cincinatti, OH, USA.
- Mini-symposium co-organizer "Combining experiment, theory and computation to improve multiscale understanding of porous medium systems," SIAM Conference on Mathematical & Computational Issues in the Geosciences, 2015.
- Chair of hiring committee for two Computational Science Specialist positions at Advanced Research Computing, Virginia Tech.
- Scientific Peer Reviewer for the Swiss National Supercomputing Centre (CSCS), 2014.
- XSEDE Campus Champion for Virginia Tech (2013-2017)

- Judge for Hydrology Section Outstanding Student Paper Award (OSPA) American Geophysical Union Fall Meeting 2012-2017
- Mini-symposium Co-organizer, "Advances in Physical and Numerical Descriptions of Multiphase Systems," SIAM Conference on Mathematical & Computational Issues in the Geosciences, 2011.
- Peer Reviewer, Cambridge, *Journal of Fluid Mechanics*
- Peer Reviewer, American Chemical Society, *Langmuir*
- Peer Reviewer, Nature, *Scientific Reports*
- Peer Reviewer, Elsevier, *Physica A*
- Peer Reviewer, American Physical Society *Physical Review E*
- Peer Reviewer, American Geophysical Union, *Geophysical Research Letters.*
- Peer Reviewer, Elsevier *Journal of Computational Physics*
- Peer Reviewer, American Geophysical Union, *Water Resources Research*
- Peer Reviewer, Elsevier, *Advances in Water Resources*
- Peer Reviewer, Elsevier, *Computers and Mathematics with Applications*
- Peer Reviewer, Elsevier, *International Journal of Multiphase Flow*
- Peer Reviewer, Elsevier, *Journal of Contaminant Hydrology*
- Peer Reviewer, MDPI, *Energies*
- Peer Reviewer, Society of Petroleum Engineers, *SPE Journal*
- Peer Reviewer, Springer, *Hydrogeology Journal.*
- Peer Reviewer, Springer, *Transport in Porous Media*
- Peer Reviewer, Wiley, *AIChE Journal*
- Peer Reviewer, Elsevier, *Earth Science Reviews*
- Peer Reviewer, Elsevier, *Journal of Membrane Science*
- Peer Reviewer, Springer, *European Physical Journal B*
- Peer Reviewer, American Institute of Physics, *Physics of Fluids*
- Peer Reviewer, American Physical Society, *Physical Review Letters*

PROFESSIONAL MEMBERSHIPS

- American Physical Society (APS)
- Institute of Electrical and Electronics Engineers (IEEE)
- Society for Industrial and Applied Mathematics (SIAM)
- American Geophysical Union (AGU)