

James E. McClure

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Interdisciplinary Center for Applied Mathematics
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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

Advanced Research Computing, Virginia Tech 2012-Present
Computational Scientist

- PI or Co-PI on \$4,222,520 in external research funding
- Participation in U.S exascale software development through the Summit Early Science Program and Frontier Center for Accelerated Application Readiness (CAAR)
- Support centralized high-performance research computing services including system design, policy development and documentation, software support and training
- 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 totaling 410,000,000 core hours on Titan through the Oak Ridge Leadership Computing Foundation (OLCF).
- Oversight of graduate and undergraduate students and post-doctoral scholars in both research and service roles
- Provide support for the research computing infrastructure used by hundreds of Virginia Tech faculty and students, including two Top 500 supercomputers
- Developed, organized and taught a variety of workshops in parallel and distributed computing including programming workshops in MPI, OpenMP, CUDA and heterogeneous computing

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

Environmental Sciences and Engineering, University of North Carolina
Undergraduate Research Assistant

2001–2003

- Developed a pore network model for two-phase flow in porous media

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 (1/2020–12/2020) 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: node-hours per year on 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. Best Paper Award, Society of Core Analysts, 2016.
2. Certificate of Reviewing Excellence, Advances in Water Resources, 2014.
3. Outstanding Student Paper Award, "Lattice Boltzmann Simulation of Non-Darcy Flow in Porous Media," American Geophysical Union, 2006.

PUBLICATIONS

Journal Articles

1. J.E. McClure, S. Berg, R.T. Armstrong, Thermodynamics of fluctuations based on time-and-space averages, *Physical Review E* 104, 035106 (2021)
2. J.E. McClure, S. Berg, R.T. Armstrong Capillary fluctuations and energy dynamics for flow in porous media, *Physics of Fluids* 33 (8), 083323 (2021). (Featured Article)

3. Y. Niu, Y. Da Wang, P. Mostaghimi, J.E. McClure, J. Yin, R.T. Armstrong Geometrical-Based Generative Adversarial Network to Enhance Digital Rock Image Quality, *Physical Review Applied* 15 (6), 064033 (2021).
4. R.T. Armstrong, C. Sun, P. Mostaghimi, S. Berg, M. Rücker, P. Luckham, A. Georgiadis, J.E. McClure Multiscale Characterization of Wettability in Porous Media, *Transport in Porous Media* (2021).
5. J.E. McClure, Z. Li, M. Berrill, T. Ramstad The LBPM software package for simulating multiphase flow on digital images of porous rocks *Computational Geosciences* (2021).
6. R. Guo, L.E. Dalton, M. Fan, J. McClure, L. Zeng, D. Crandall, C. Chen 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 (2020).
7. Y. A. Alzahid, H. Aborshaid, M. Asali, J.E. McClure, C. Chen, P. Mostaghimi, Y. Da Wang, C. Sun, R. T. Armstrong Real-time synchrotron-based X-ray computed microtomography during in situ emulsification, *Journal of Petroleum Science and Engineering* 195, 107885 (2020)
8. C. Sun, J.E. McClure, P. Mostaghimi, A.L. Herring, D.E. Meisenheimer, D. Wildenschild, S. Berg, R.T. Armstrong Characterization of wetting using topological principles *Journal of Colloid and Interface Science* 578, 106-115 (2020)
9. M. Fan, J.E. McClure, R.T. Armstrong, M. Shabaninejad, L.E. Dalton D. Crandall, C. Chen Influence of Clay Wettability Alteration on Relative Permeability *Geophysical Research Letters* 47 (18), e2020GL088545 (2020)
10. J.E. McClure, Z. Li, A.P. Sheppard, C.T. Miller An adaptive volumetric flux boundary condition for lattice Boltzmann methods *Computers & Fluids* 210, 104670 (2020).
11. A. Li, J.E. McClure, J. Middleton, T. Varslot, A.P. Sheppard Discretization limits of lattice Boltzmann methods for studying immiscible twophase flow in porous media, *International Journal for Numerical Methods in Fluids* 1-36 (2020).
12. J. E. McClure, J. Yin, R.T. Armstrong, K.C. Maheshwari, S. Wilkinson, L. Vlcek, Y. Da Wang, M.A. Berrill, M. Rivers 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 (2020)
13. J.E. McClure, T. Ramstad, Z. Li, R.T. Armstrong, S. Berg Modeling Geometric State for Fluids in Porous Media: Evolution of the Euler Characteristic *Transport in Porous Media* 133, 229-250 (2020).
14. M. Fan, Y. Han, M. Gu, J. McClure, N. Ripepi, E. Westman, C. Chen Investigation of the conductivity of a proppant mixture using an experiment/simulation-integrated approach, *Journal of Natural Gas Science and Engineering* 78, 103234 (2020)
15. C. Sun, J.E. McClure, P. Mostaghimi, A.L. Herring, S. Berg, R.T. Armstrong Probing effective wetting in subsurface systems *Geophysical Research Letters*, 47 (5) (2020)
16. C Sun, JE McClure, P Mostaghimi, AL Herring, M Shabaninejad, S Berg, et al. Linking continuum-scale state of wetting to pore-scale contact angles in porous media *Journal of Colloid and Interface Science* 561, 173-180 (2020)
17. Y.D. Wang, T. Chung, R.T. Armstrong, J. McClure, T. Ramstad, P. Mostaghimi Accelerated Computation of Relative Permeability by Coupled Morphological and Direct Multiphase Flow Simulation *Journal of Computational Physics* 401, 108966 (2020)
18. DE Meisenheimer, JE McClure, ML Rivers, D Wildenschild Exploring the effect of flow condition on the constitutive relationships for two-phase flow *Advances in Water Resources*, 103506 (2020)
19. 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, 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 (2019).

20. M. Fan, L.E. Dalton, J. McClure, N. Ripepi, E. Westman, D. Crandall, C. Chen, Comprehensive study of the interactions between the critical dimensionless numbers associated with multiphase flow in 3D porous media, *Fuel* **252**, 522-533 (2019).
21. C.T. Miller, K. Bruning, C.L. Talbot, J.E. McClure, W.G. Gray, Non-hysteretic capillary pressure in two-fluid porous medium systems: Definition, evaluation, validation, and dynamics, *Water Resources Research* (2019).
22. M. Fan, J. McClure, Y. Han, N. Ripepi, E. Westman, M. Gu, C. Chen Using an Experiment/Simulation-Integrated Approach To Investigate Fracture-Conductivity Evolution and Non-Darcy Flow in a Proppant-Supported Hydraulic Fracture *SPE Journal* (2019)
23. Y. Da Wang, T. Chung, R.T. Armstrong, J.E. McClure, P. Mostaghimi Computations of permeability of large rock images by dual grid domain decomposition, *Advances in Water Resources* **126**, 1–14 (2019).
24. 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
25. Z Liu, JE McClure, RT Armstrong (2018) Influence of wettability on phase connectivity and electrical resistivity *Physical Review E* 98 (4), 043102
26. 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.
27. 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.
28. 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*.
29. 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**
30. 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
31. 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
32. 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
33. 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
34. 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
35. 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.
36. 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.

37. 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
38. 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.
39. 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.
40. 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.
41. 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. 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)
2. 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
3. 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
4. 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**
5. Im, D.K., Choi, S., McClure, J.E., Choi, J.Y. and F. Skies (2015) A mapped Chebyshev pseudospectral method for unsteady flow analysis, 22nd *AIAA Computational Fluid Dynamics Conference, Aviation Forum 2015*
6. 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)
7. 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 18th International Conference on Computational Methods in Water Resources (CMWR XVIII)*, Barcelona, Spain, 21-24 June 2010, Paper 273.
8. Pan, C. J.E. McClure, W.G. Gray, and C.T. Miller (2006) Lattice Boltzmann Simulation of Non-Darcy Flow, *Proceedings of the 16th International Conference on Computational Methods in Water Resources (CMWR XVI)*, Copenhagen, Denmark, 19-22 June 2006. <http://proceedings.cmwr.xvi.org>, Paper 248.

9. 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 16th International Conference on Computational Methods in Water Resources (CMWR XVI)*, Copenhagen, Denmark, 19-22 June 2006. <http://proceedings.cmwr.xvi.org>, Paper 224.
10. 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 15th 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. “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)
2. 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, JE McClure, L Zeng, D Crandall, C Chen AGU Fall Meeting Abstracts 2020, MR023-0014
3. Visualization and data reuse via the Digital Rocks Portal M Prodanovic, M Esteva, JE McClure AGU Fall Meeting 2019
4. 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
5. 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, ... Abu Dhabi International Petroleum Exhibition & Conference
6. 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
7. 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
8. Microscale simulation of three-fluid flow in porous media CP Fowler, JE McClure, CT Miller AGU Fall Meeting Abstracts
9. Lattice Boltzmann Modeling of Gas Adsorption and Desorption in Shale Matrix R Xu, M Prodanovic, CJ Landry, JE McClure AGU Fall Meeting Abstracts
10. Storage, visualization and simulation using data in Digital Rocks Portal M Prodanovic, M Esteva, JE McClure AGU Fall Meeting Abstracts
11. 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)
12. 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.
13. 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.

14. 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.
15. 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.
16. 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.
17. 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.
18. 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.
19. 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.
20. 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.
21. 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.
22. 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
23. 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
24. 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. 7th International Conference on Porous Media & Annual Meeting, International Society for Porous Media, Padova, Italy. 18-21 May 2015.
25. 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.
26. 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.
27. 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.
28. 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.

29. 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.
30. 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.
31. 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.
32. 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.
33. 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.
34. 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.
35. 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.
36. 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.
37. 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.
38. 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.
39. 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.
40. 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.
41. 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.
42. 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.
43. 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.

44. 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.
45. 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.
46. 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
47. 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. "LBPM: Massively parallel lattice Boltzmann Simulator for Porous Media" SPE Virtual Workshop: Open Subsurface 20 May 2021 (online).
2. "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
3. "Topology and its effects on fluid flow" Interpore 2020, Qindao, China,
4. "Modeling wetting phenomena with lattice Boltzmann methods" Shell Pore Scale Physics Seminar, 26 February 2019
5. "GPU-Accelerated Digital Rock Physics Workflows for Titan and Summit" OLCF User Meeting, Oak Ridge National Lab, May 2017
6. "Opportunities for fluid flow simulation and fast-micro tomography" High Resolution 2D & 3D imaging in Geoscience, Virginia Tech, 6 April 2017, Blacksburg, VA, USA.
7. "Embracing Heterogeneous Simulation of Complex Fluid Flows" NVIDIA GPU Technology Theatre, SC15, November 18, 2015 Austin, TX, USA.
8. "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.
9. "Optimizing Rosetta for the Intel Xeon Phi" XSEDE Conference, July 2014
10. "Principles of Multithreading and Auto-Vectorization" Rosetta MiniCon, February 2014
11. "Advancing Models for Multiphase Flow and Transport in Porous Medium Systems" Oak Ridge National Lab, January 2014
12. "Introduction to XSEDE Resources", SSI Summer School REU, Virginia Tech, July 2013
13. "Microscale Analysis of Porous Medium Flows," Envr 400: Seminar Series, University of North Carolina at Chapel Hill, November 2006.
14. "Introduction to Level Sets for Image Analysis," Summer School in Geophysical Porous Media: Multidisciplinary Science from Nano- to Global-Scale," Purdue University, July 2006.

PROFESSIONAL SERVICE

- 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” 9th International Conference on Porous Media and Annual Meeting, 2016, May 9-12, Cincinnati, 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*

PROFESSIONAL MEMBERSHIPS

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