John Gounley

CONTACT INFORMATION

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EDUCATION

Old Dominion University, Norfolk, VA

PhD	Computational & Applied Mathematics	2014
MS	Computational & Applied Mathematics	2011

Thomas Aquinas College, Santa Paula, CA

BA	Liberal Arts	2008

EXPERIENCE

Oak Ridge National Laboratory, Oak Ridge, TN — 2018 – present

Computational Sciences and Engineering Division

Group Leader (2023 – present)
Computational Scientist (2018 – present)

Duke University, Durham, NC — 2015 – 2018

Department of Biomedical Engineering
Postdoctoral Scholar

Durham VA Medical Center, Durham, NC — 2016 – 2017

Hematology-Oncology
Postdoctoral Fellow

École Centrale de Marseille, Marseille, France — 2014 – 2015

Laboratoire de Mécanique, Modélisation et Procédés Propres (M2P2)
Postdoctoral Researcher

PUBLICATIONS

1. M. Chandra Shekar, I. Lyngaas, H.A. Hanson, S. Gao, X.-C. Wu, **J. Gounley**. PathBigBird: an AI driven transformer approach to classification of cancer pathology reports. Accepted by *JCO Clinical Cancer Informatics*.
2. P. Zhang, L. Kearney, D. Bhowmik, Z. Fox, A. Naskar, **J. Gounley**. Transferring a molecular foundation model for polymer property predictions. *Journal of Chemical Information and Modeling* (2023)
3. P. Valero-Lara, J. Vetter, **J. Gounley**, A. Randles. Moment representation of regularized lattice Boltzmann methods on Nvidia and AMD GPUs. In *Proceedings of the SC'23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*, 1697-1704 (2023)
4. A. Martin, G. Liu, W. Ladd, S. Lee, **J. Gounley**, J. Vetter, S. Patel, S. Rizzi, V. Mateevitsi, J. Insley, A. Randles. Performance evaluation of heterogeneous GPU programming frameworks for hemodynamic simulations. In *Proceedings of the SC'23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*, 1126-1137 (2023)
5. S. Roychowdhury, S.T. Mahmud, A. Martin, P. Balogh, D.F. Puleri, **J. Gounley**, E.W. Draeger, A. Randles. Enhancing adaptive physics refinement simulations through

the addition of realistic red blood cell counts. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC)*, 1-13 (2023)

6. D.J. Hsu, H. Lu, A. Kashi, M. Matheson, **J. Gounley**, F. Wang, W. Joubert, J. Glaser. TwoFold: highly accurate structure and affinity prediction for protein ligand complexes from sequences. *International Journal of High Performance Computing Applications* (2023)
7. A. Spannaus, **J. Gounley**, M. Chandra Shekar, Z.R. Fox, J. Mohd-Yusof, N. Schaefferkoetter, H.A. Hanson. FrESCO: framework for exploring scalable computational oncology. Journal of Open Source Software, 8(89):5345 (2023)
8. J. Yin, S. Dash, **J. Gounley**, F. Wang, G. Tourassi. Evaluation of pre-training large language models on leadership-class supercomputers. *The Journal of Supercomputing* (2023)
9. A.E Blanchard, D. Bhowmik, Z. Fox, **J. Gounley**, J. Glaser, B.S. Akpa, S. Irle. Adaptive language model training for molecular design. *Journal of Cheminformatics*, 15(59):1-12 (2023)
10. M. Pepona, **J. Gounley**, A. Randles. Effect of constitutive law on the response of the erythrocyte membrane to large strains. *Computers and Mathematics with Applications*, 132:145-160 (2023)
11. A.E. Blanchard, P. Zhang, D. Bhowmik, K. Mehta, **J. Gounley**, S.T. Reeve, S. Irle, M. Lupo Pasini. Computational workflow for accelerated molecular design using quantum chemical simulations and deep learning models. *22nd Smoky Mountains Computational Sciences and Engineering Conference (SMC 2022)*, 3-19 (2023)
12. M. Vardhan, S.J. Chen, **J. Gounley**, P. Nair, W. Wei, L. Hegele, J. Kusner, A. Kahn, D. Frakes, J.A. Leopold, A. Randles. Evaluation of intracoronary hemodynamics identifies perturbations in vorticity. *Frontiers in Systems Biology*, 36(930396): 1-12 (2022)
13. D.F. Puleri, S. Roychowdhury, P. Balogh, **J. Gounley**, E.W. Draeger, J. Ames, A. Adebayi, S. Chidyagwai, B. Hernández, S. Lee, S. Moore, J.S. Vetter, A. Randles. High performance adaptive physics refinement to enable large-scale tracking of cancer cell trajectory. In *2022 IEEE International Conference on Cluster Computing (CLUSTER)*, IEEE (2022)
14. A.E. Blanchard, **J. Gounley**, D. Bhowmik, M. Chandra Shekar, I. Lyngaas, S. Gao, J. Yin, A. Tsaris, F. Wang, J. Glaser. Language models for the prediction of SARS-CoV-2 inhibitors. *International Journal of High Performance Computing Applications* (2022)
15. I. Jarrah, M.-O.G. Delchini, V. Badalassi, P.K. Jain, **J. Gounley**. Implementation of the energy equation solver to the lattice Boltzmann method-based code PRATHAM. Proceedings of *19th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-19)*, ANS (2022)
16. A.E Blanchard, M. Chandra Shekar, S. Gao, **J. Gounley**, I. Lyngaas, J. Glaser, D. Bhowmik. Automating genetic algorithm mutations for molecules using a masked language model. *IEEE Transactions on Evolutionary Computation*, 26(4): 793-799 (2022)
17. S.H. Chen, M.T. Young, **J. Gounley**, C. Stanley, D. Bhowmik. Distinct structural flexibility within SARS-CoV-2 spike protein reveals potential therapeutic targets. *2021 IEEE International Conference on Big Data (Big Data)*, 4333-4341 (2021)
18. **J. Gounley**, M. Vardhan, E.W. Draeger, P. Valero-Lara, S.V. Moore, A. Randles. Propagation pattern for a moment representation of the regularized lattice Boltzmann method. *IEEE Transactions on Parallel and Distributed Systems*, 33(3):642-653 (2021)

19. P. Balogh, **J. Gounley**, S. Roychowdhury, A. Randles. A data-driven approach to modeling cancer cell mechanics during microcirculatory flow transport. *Scientific Reports*, 11(1):1-18 (2021)
20. M. Vardhan, **J. Gounley**, S.J. Chen, E.C. Chi, A. Kahn, J.A. Leopold, A. Randles. Non-invasive characterization of complex coronary lesions. *Scientific Reports*, 11:8415 (2021)
21. S. Gao, M. Alawad, M.T. Young, **J. Gounley**, N. Schaefferkoetter, H.-J. Yoon, X.-C. Wu, E.B. Durbin, J. Doherty, A. Stroup, L. Coyle, L. Penberthy, G. Tourassi. Limitations of Transformers on clinical document classification. *IEEE Journal of Biomedical and Health Informatics* (2021)
22. H.-J. Yoon, H. Klasky, **J. Gounley**, M. Alawad, S. Gao, E. Durbin, X.-C. Wu, A. Stroup, J. Doherty, L. Coyle, L. Penberthy, B. Christian, G. Tourassi. Accelerated training of bootstrap aggregation-based deep information extraction systems from cancer pathology reports. *Journal of Biomedical Informatics*, 110:103564 (2020)
23. S. Roychowdhury, **J. Gounley**, A. Randles. Evaluating the influence of hemorheological parameters on circulating tumor cell trajectory and simulation time. In *Proceedings of the Platform for Advanced Scientific Computing Conference (PASC)*, ACM (2020)
24. J. Ames, D.F. Puleri, P. Balogh, **J. Gounley**, E.W. Draeger, A. Randles. Multi-GPU immersed boundary method hemodynamics simulations. *Journal of Computational Science*, 44:101153 (2020)
25. B. Feiger, **J. Gounley**, D. Adler, J.A. Leopold, E.W. Draeger, R. Chaudhury, J. Ryan, G. Pathangey, K. Winarta, D. Frakes, F. Michor, A. Randles. Accelerating massively parallel hemodynamic models of coarctation of the aorta using neural networks. *Scientific Reports*, 10:9508 (2020)
26. B. Feiger, A. Kochar, **J. Gounley**, D. Bonadonna, M. Daneshmand, A. Randles. Determining the impacts of VA-ECMO parameters on blood oxygenation using a 1D blood flow simulator. *Journal of Biomechanics*, 104:1-12 (2020)
27. M. Dabagh, **J. Gounley**, A. Randles. Localization of rolling and firm-adhesive interactions between circulating tumor cells and the microvasculature wall. *Cellular and Molecular Bioengineering*, 1-14 (2020)
28. H.-J. Yoon, **J. Gounley**, M.T. Young, G. Tourassi. Information extraction from cancer pathology reports with graph convolution networks for natural language texts. In *2019 IEEE International Conference on Big Data (Big Data)*, IEEE (2019)
29. G.J. Herschlag, **J. Gounley**, S. Roychowdhury, E.W. Draeger, A. Randles. Multiphysics simulations of particle tracking in arterial geometries with a scalable moving window algorithm. In *2019 IEEE International Conference on Cluster Computing (CLUSTER)*, IEEE (2019)
30. M. Vardhan, **J. Gounley**, L.A. Hegele, E.W. Draeger, A. Randles. Moment representation in lattice Boltzmann method on massively parallel hardware. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC)*, ACM (2019)
31. M. Vardhan, H. Shi, **J. Gounley**, S.J. Chen, A. Khan, J.A. Leopold, A. Randles. Investigating the role of VR in a simulation-based medical planning system for coronary interventions. In *Medical Image Computing and Computer Assisted Intervention (MICCAI)*, 366-374 (2019)
32. H.-J. Yoon, **J. Gounley**, S. Gao, M. Alawad, A. Ramanathan, G. Tourassi. Model-based hyperparameter optimization of convolutional neural networks for information extraction from cancer pathology reports on HPC. In *2019 IEEE EMBS International Conference on Biomedical & Health Informatics (BHI)*, IEEE (2019)

33. M. Dabagh, P. Nair, **J. Gounley**, D. Frakes, F. Gonzalez, A. Randles. Hemodynamic and morphological characteristics of a growing cerebral aneurysm. *Neurosurgical Focus*, 47:1-10 (2019)

34. M. Vardhan, **J. Gounley**, S.J. Chen, A. Kahn, J.A. Leopold, A. Randles. The importance of side branches in modeling 3D hemodynamics from angiograms for patients with coronary artery disease. *Scientific Reports*, 9:8854 (2019)

35. **J. Gounley**, E.W. Draeger, A. Randles. Immersed boundary method halo exchange in a hemodynamics application. In *International Conference on Computational Science (ICCS)*, 441-455 (2019)

36. B. Grigoryan, S.J. Paulsen, D.C. Corbett, D.W. Sazer, C.L. Fortin, A.J. Zaita, P.T. Greenfield, N.J. Calafat, **J.P. Gounley**, A.H. Ta, A. Randles, J.E. Rosenkrantz, J.D. Louis-Rosenberg, P.A. Galie, K.R. Stevens, J.S. Miller. Multivascular networks and functional intravascular topologies within biocompatible hydrogels. *Science*, 364:458-464 (2019) (Selected for cover image)

37. B. Feiger, M. Vardhan, **J. Gounley**, M. Mortensen, P. Nair, R. Chaudhury, D. Frakes, A. Randles. Suitability of lattice Boltzmann inlet and outlet boundary conditions for simulating flow in image-derived vasculature. *International Journal for Numerical Methods in Biomedical Engineering*, 35(6):e3198 (2019) (Selected for cover image)

38. **J. Gounley**, E.W. Draeger, T. Oppelstrup, W.D. Krauss, J.A. Gunnels, R. Chaudhury, P. Nair, D. Frakes, J.A. Leopold, A. Randles. Computing the ankle-brachial index with parallel computational fluid dynamics. *Journal of Biomechanics*, 82:28-37 (2019)

39. **J. Gounley**, M. Vardhan, A. Randles. A framework for comparing vascular hemodynamics at different points in time. *Computer Physics Communications*, 235:1-8 (2019)

40. S. Lee, **J. Gounley**, A. Randles, J.S. Vetter. Performance portability study for massively parallel computational fluid dynamics application on scalable heterogeneous architectures. *Journal of Parallel and Distributed Computing*, 129:1-13 (2019)

41. M. Vardhan, A. Das, **J. Gounley**, A. Randles. Computational fluid modeling to understand the role of anatomy in bifurcation lesion disease. In *25th IEEE International Conference on High Performance Computing Workshops (HiPCW)*, IEEE (2018)

42. L.A. Hegele, A. Scagliarini, M. Sbragaglia, K. K. Mattila, P. C. Philippi, D. F. Puleri, **J. Gounley**, A. Randles. High Reynolds number turbulent cavity flow using the lattice Boltzmann method. *Physical Review E*, 98(4):043302 (2018)

43. **J. Gounley**, M. Vardhan, A. Randles. A computational framework to assess the influence of changes in vascular geometry on blood flow. In *Proceedings of the Platform for Advanced Scientific Computing Conference (PASC)*, ACM (2017)

44. **J. Gounley**, E.W. Draeger, A. Randles. Numerical simulation of a compound capsule in a constricted microchannel. *Procedia Computer Science, International Conference on Computational Science*, 108C:175-184 (2017)

45. T. Laurence, S. Ly, E. Fong, M. Shusteff, A. Randles, **J. Gounley**, E.W. Draeger. Using stroboscopic flow imaging to validate large-scale computational fluid dynamics simulations. In *Proc. SPIE 10076: High-Speed Biomedical Imaging and Spectroscopy*, SPIE (2017)

46. **J. Gounley**, R. Chaudhury, M. Vardhan, M. Driscoll, G. Pathangey, K. Winarta, J. Ryan, D. Frakes, A. Randles. Does the degree of coarctation of the aorta influence wall shear stress focal heterogeneity? In *2016 38th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC)*, IEEE (2016)

47. **J. Gounley**, G. Boedec, M. Jaeger, M. Leonetti. Influence of surface viscosity on droplet dynamics. *Journal of Fluid Mechanics*, 791:464-494 (2016)

48. **J. Gounley**, G. Boedec, M. Jaeger, M. Leonetti. Influence de la viscosité interfaciale sur la dynamique de gouttes visqueuses en écoulement cisaillé. In *2015 Congrès Français de Mécanique*, Association Française de Mécanique (2015)
49. **J. Gounley**, Y. Peng. Response and recovery times of elastic and viscoelastic capsules in shear flow. *Communications in Computational Physics*, 17(5):1151-1168 (2015)
50. **J. Gounley**, Y. Peng. Computational modeling of membrane viscosity of red blood cells. *Communications in Computational Physics*, 17(4):1073-1087 (2015)
51. **J. Gounley**, Y. Peng. Shape recovery of elastic capsules from shear flow induced deformation. *Communications in Computational Physics*, 16(1):56-74 (2014)

Open Source Software

1. A. Spannaus, **J. Gounley**, H. Hanson, M. Chandra Shekar, N. Schaefferkoetter, J. Mohd-Yusof, Z. Fox. FrESCO: Framework for Exploring Scalable Computational Oncology. https://github.com/DOE-NCI-MOSSAIC/FrESCO (2023)
2. A.E. Blanchard, **J. Gounley**, D. Bhowmik, I. Lyngaas, M. Chandra Shekar, S. Gao, J. Yin, A. Tsaris, F. Wang, J. Glaser. Masked Language Molecules. https://code.ornl.gov/candle/mlmol (2022)

Grants & allocations

1. ORNL Laboratory Directed Research and Development (LDRD) Grant, "Multiscale foundation models for physical systems." $250,000 total costs. Role: Co-I (2023-2024)
2. ASCR Leadership Computing Challenge (ALCC) Award, "Privacy enabled tumor classification for near real time population health analytics." 140,000 node hours on OLCF Frontier. Role: Co-PI (2023-2024)
3. ASCR Leadership Computing Challenge (ALCC) Award, "Privacy-preserving Transformer models for clinical natural language processing." 150,000 node hours on OLCF Summit and 50,000 node hours on OLCF Frontier. Role: Co-PI (2022-2023)
4. ASCR INCITE Program Award, "Scalable Transformer language models for drug discovery." 390,000 node hours on OLCF Summit. Role: Co-PI (2022)
5. ASCR Leadership Computing Challenge (ALCC) Award, "Next-generation scalable deep learning for medical natural language processing." 130,000 node hours on OLCF Summit. Role: PI (2021-2022)
6. OLCF Director's Discretion (DD) Allocation, "Next-generation scalable deep learning for medical NLP." 10,000 node hours on OLCF Summit. Role: PI (2020-2021)
7. ORNL Laboratory Directed Research and Development (LDRD) Grant, "Performant high-order lattice Boltzmann for exascale applications." $815,000 total costs and 15,000 node hours on OLCF Summit. Role: PI (2019-2021)
8. ASCR Leadership Computing Challenge (ALCC) Award, "AI-enabled computational cancer phenotyping for precision oncology." 200,000 node hours on OLCF Summit. Role: Co-PI (2019-2020)
9. Hartwell Foundation Biomedical Research Fellowship, "Predictive computational modeling of the Norwood procedure." $50,000 direct costs. Role: PI (2017-2018).
10. LLNL Computing Grand Challenge Award, "Boosting the effectiveness of neonatal surgery through simulation." Allocation on LLNL Vulcan and Quartz. Role: Co-PI (2017-2018)
11. LLNL Computing Grand Challenge Award, "Assessing peripheral artery disease with hæmodynamic simulations." Allocation on LLNL Vulcan. Role: Co-PI (2016-2017)

Awards & Honors

1. R&D100 Award for CANDLE: CANcer Distributed Learning Environment (2023)
2. Team finalist for ACM Gordon Bell Special Prize for High Performance Computing-Based COVID-19 Research (2021, 2022)
3. Distinguished Team Technical Contribution award from Computational Sciences and Engineering Division at Oak Ridge National Laboratory (2021)
4. Nominee for Outstanding Postdoc at Duke University (2016, 2017, 2018)
5. Big Data Scientist Training Enhancement Program Fellowship (BD-STEP) from Department of Veterans Affairs and National Cancer Institute (2016-2017)
6. Best poster award at Duke Research Computing Symposium (2016)
7. Modeling and Simulation Scholarship from Old Dominion University (2011-2014)
8. Philip R. Wohl Award from Department of Mathematics & Statistics at Old Dominion University (2011)

Professional Service

Journal reviews:
Biomechanics and Modeling in Mechanobiology
Cardiovascular Engineering and Technology
Communications in Computational Physics
Computer Methods in Biomechanics and Biomedical Engineering
Computers and Fluids
Computers and Mathematics with Applications
Interdisciplinary Neurosurgery
Journal of Computational Physics
Physica A
Scientific Reports
Journal of Parallel and Distributed Computing

Conference reviews:
International Conference on Parallel Processing (ICPP19, ICPP22, ICPP23)
Supercomputing (SC20, SC21)

Minisymposium organizer:
SIAM CSE21 (with Sam Erwin): Computational Modeling for the COVID-19 Pandemic

Birds-of-a-Feather organizer:
SC22 (with Tom Brettin and Adam Moody): Transformers for Science at Scale

Tutorial organizer:
IEEE QCE23 (with Eduardo Coello Perez, Prasanna Date, Mayanka Chandra Shekar, Kathleen Hamilton, Francisco Rios, In-Saeng Suh, and Georgia Tourassi): Quantum plus High-Performance Computing for Natural Language Processing

Professional Organizations

Member:
Society for Industrial and Applied Mathematics 2009 – present