Austin R. Dulaney

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OBJECTIVE / QUALIFICATION SUMMARY

Recent Caltech PhD graduate in Chemical Engineering. Expert in computational and theoretical modeling of soft condensed matter systems. Experienced in GPU-accelerated computing and data analysis, machine learning techniques, and analytical modeling. Pursuing a challenging new role in machine learning or data science. Passionate about open-source development, research, and fostering collaboration.

EDUCATION

California Institute of Technology **Pasadena, CA**
PhD, Chemical Engineering; GPA: 3.7/4.0 *Sep 2016 – Dec 2020*
MS, Chemical Engineering; GPA: 3.7/4.0 *Sep 2016 – June 2018*

The University of Texas at Austin **Austin, TX**
BS, Chemical Engineering (with Honors); GPA: 3.8/4.0 *Aug 2012 – May 2016*

SKILLS

- **Programming:**
  - **Proficient Languages:** Python, C++, CUDA, MATLAB
  - **Data Science/Machine Learning:** Pandas, Numpy, scikit-learn, Keras, Tensorflow, Pytorch, XGBoost
  - **Other:** Shell, Git, Linux, LaTeX, SQL
- **Simulations**
  - **Methods:** GPU-accelerated Molecular Dynamics, Brownian Dynamics, and Monte Carlo
  - **Tools:** HOOMD, LAMMPS, Ovito, VMD
- **Computational Techniques:** Finite element methods, High performance computing, Numerical Analysis

EXPERIENCE

PhD Candidate, Caltech – Advisor: John F. Brady **Jan 2017 – Present**

- Built, optimized, and implemented deep learning models in Pytorch and Tensorflow to predict complex phase behavior in active matter systems.
- Utilized dimensionality reduction and random forest techniques to elucidate non-intuitive connections between feature data to improve the interpretability of machine learning results.
- Studied relaxation dynamics and fluctuations in active matter systems through the development of analytic theory, accelerated simulation techniques, and stochastic modeling.
- Generated large datasets to gain meaningful insights into the collective behavior of active matter systems.
- Created an image analysis pipeline in Python to help label training data.
- Developed multiple GPU-accelerated simulation and analysis packages to simulate hard-sphere interactions and perform time-series analysis.

Moncrief Research Fellow, Institute for Computational Engineering and Sciences **May 2015 – June 2016**

- Developed simulations of real-world systems using finite difference and continuum-scale approaches.
- Performed advanced sampling techniques for hyperparameter optimization.
- Presented research findings to collaborators and technical industry experts.

Undergraduate Research Assistant, McKetta Department of Chemical Engineering **Jan 2014 – May 2015**

- Synthesized and patterned nano-scale polymer films for electronic applications.
- Created mathematical models to optimize nanopatterning of finely-tuned thin films.

Chemical Engineering Research Intern, Los Alamos National Laboratories **June 2013 – Aug 2013**

- Characterized and proposed robust, safe disposal methods for "difficult" nuclear waste.
- Modeled and optimized new nuclear waste disposal/containment drums for improved cost and storage efficiency.

RELEVANT COURSEWORK

- Machine Learning & Data Mining
- Methods of Applied Mathematics
- Statistical Thermodynamics
- Introduction to Programming for the Biological Sciences
- Numerical Methods

HONORS AND AWARDS

- Earle C. Anthony Graduate Fellowship (2016)
- Institute for Computational Engineering Sciences Moncrief Fellowship - UT Austin (2015)
- Tau Beta Pi Engineering Honor Society
- Chemical Engineering Honor Society

LEADERSHIP AND MENTORING

Scientific Computing Community (Codecademy Chapter) Founder **July 2019 – Present**

- Created a group to support other computational scientists in the chemical engineering department.
- Developed lessons to teach efficient workflows and advanced computation techniques for scientific computing.
- Organized monthly meetings to empower other members to perform various computational techniques.
- Aided other Codecademy Chapter leaders in designing their chapter charters and growing their local chapters.

Graduate Teaching Assistant **Jan 2018 – June 2018, Sep 2019 – Dec 2019**

Courses: Transport Phenomena (CHE151A/B), Special Topics in Transport Phenomena (CHE174)

- Held office hours and led supplemental lectures on mathematically rigorous topics for 15+ graduate students.
- Facilitated the learning of students through one-on-one tutoring and small focus groups.
- Aided students in developing ideas for final research projects through thoughtful, technical discussion.

Summer Undergraduate Research Fellow Program Mentor **Jun 2019 – Sep 2019**

- Designed and guided an undergraduate researcher through a realistic research project in the field of soft matter physics.
- Taught student how to think critically and break down complex problems into manageable tasks.
- Engaged in daily meetings to discuss project goals, lessons from the previous day, and academic coaching.

Brady Group Computational Resource Manager **Jun 2018 – Present**

- Built and maintained multiple CPU and GPU clusters.
- Provided computer simulation and data visualization support to other group members.
- Aided in the smooth transition to remote work during the onset of COVID.

CONFERENCES AND INVITED PRESENTATIONS

5. **A.R. Dulaney**, S.A. Mallory, and J.F. Brady, The "isothermal" compressibility of active matter. American Institute of Chemical Engineers–Virtual, **2020** [Link]
4. **A.R. Dulaney** and J.F. Brady, The Wavelike Character of Active Brownian Particles. Annual Southern California Flow Physics Symposium–Los Angeles, CA, **2018**
3. **A.R. Dulaney** and J.F. Brady, The dynamic structure factor of active Brownian particles. APS March Meeting–Los Angeles, CA, **2018**
2. **A.R. Dulaney** and J.F. Brady, The dynamic structure factor of active Brownian particles. Annual Southern California Flow Physics Symposium–San Diego, CA, **2017**
1. **A.R. Dulaney**, C.B. Kim and C.J. Ellison, Bidirectional Control of Marangoni Flow. American Institute of Chemical Engineers Southwest Regional Conference–Austin, TX, **2015**

SELECTED PUBLICATIONS

10. **A.R. Dulaney**, J.F. Brady, "Machine Learning for Phase Behavior in Active Matter." *Soft Matter*. Submitted (2020). (available on arXiv as arxiv:2011.09458)
9. **A.R. Dulaney**, S.A. Mallory, J.F. Brady, "The 'isothermal' compressibility of active matter," *J. Chem. Phys.* 154, 014902 (2021). [Link]
8. **A.R. Dulaney**, J.F. Brady, "Waves in Active Matter: The transition from ballistic to diffusive behavior," *Phys. Rev. E.* 101, 052609 (2020).
7. R. Katsumata, **A. Dulaney**, C.B. Kim, C. Ellison, "Glass transition and self-diffusion of unentangled polymer melts nanoconfined by different interfaces," *Macromolecules*. 51 (19), 7509-7517 (2018).
6. V.R. Heng, H.S. Ganesh, **A.R. Dulaney**, A. Kurzawski, M. Baldea, O.A. Ezekoye, T.F. Edgar, "Energy-Oriented Modeling and Optimization of a Heat Treating Furnace," *Journal of Dynamic Systems, Measurement, and Control*. 139 (6), 061014 (2017).

5. K. Geng, R. Katsumata, X. Yu, H. Ha, **A. Dulaney**, C. Ellison, O.K.C. Tsui, "Conflicting Confinement Effects on the Tg, Diffusivity and Effective Viscosity of Polymer Films: A Case Study with Poly(isobutyl methacrylate) on Silica and Possible Resolution," *Macromolecules.* 50 (2), 609-617 (2017).
4. Y. Fang, **A.R. Dulaney**, J. Gadly, J. Maia, C.J. Ellison, "A comparative parameter study: Controlling fiber diameter and diameter distribution in centrifugal spinning of photocurable monomers," *Polymer.* 88, 102-111 (2016).
3. J.H. Cho, R. Katsumata, S.X. Zhou, C.B. Kim, **A.R. Dulaney**, D.W. Janes and C.J. Ellison, "Ultrasmooth, Polydopamine Modified Surfaces for Block Copolymer Nanopatterning on Inert and Flexible Substrates," *Advanced Materials Interfaces.* 8(11), 7456-7463 (2016).
2. Y. Fang, **A.R. Dulaney**, J.M. Maia and C.J. Ellison, "Manipulating characteristic timescales and fiber morphology in simultaneous centrifugal spinning and photopolymerization," *Polymer.* 73, 42-51 (2015).
1. C.B. Kim, D.W. Janes, S.X. Zhou, **A.R. Dulaney** and C.J. Ellison, "Bidirectional Control of Flow in Thin Polymer Films by Photochemically Manipulating Surface Tension," *Chem. Mater.* 27(13), 4538-4545 (2015).