PUBLICATIONS

Journal publications under review

- 1 Wade, N. & Graham-Brady, L. (2023). "Estimating Microstructural Property Distributions from Image Data Using a Bayesian Framework," submitted.
- 2 Yaghoobi, M., Stopka, K.S., McDowell, D.L., Graham-Brady, L., Teferra, K. (2023). "Effect of sample size on the maximum value distribution of fatigue driving forces in metals and alloys," submitted.
- 3 Gupta, A., Bhaduri, A., Graham-Brady, L. (2023). "Accelerated multiscale mechanics modeling in a deep learning framework," submitted.

Refereed journal publications

- 4 Prameela, S.E., Pollock, T., Raabe, D., Meyers, M.A., Aitkaliyeva, A., Chintersingh, K.L., Cordero, Z., Graham-Brady, L. (2023). "Materials for Extreme Environments," *Nature Reviews Materials*, 8(2): 81-88.
- 5 Maruyama, B., Hattrick-Simpers, J., Musinski, W., Graham-Brady, L., Li, K., Hollenbach, J., Singh, A., Taheri, M.L. (2022). "Al and Materials Research for Coupled Extremes," *MRS Bulletin*, 47(11): 1154-1164.
- 6 Bhaduri, A., Gupta, A., Graham-Brady, L. (2022). "Stress field prediction in fiberreinforced composite materials using a deep learning approach," *Composites Part B*, 238: 109879.
- 7 Bhattacharjee, A., Hurley, R., Graham-Brady, L. (2022). "Fragmentation and granular transition of ceramics for high rate loading," *Journal of the American Ceramics Society*, 105(5):3062-3080. *Selected for Best Paper Award
- 8 Ramesh, K.T., Graham-Brady, L., Goddard, W.A., Hurley, R.C., Robbins, M., Tonge, A.L., Bhattacharjee, A., Clemmer, J.T., Zeng, Q., Li, W., Shen, Y., An, Q., Mitra, N. (2022). "Models for the behavior of boron carbide in extreme dynamic environments," *Journal of the American Ceramic Society*, 105(5):3043-3061.
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- 11 Bhaduri, A., Gupta, A., Olivier, A., Graham-Brady, L. (2021). "An efficient optimization based microstructure reconstruction approach with multiple loss functions," *Computational Materials Science*, 199:110709.
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- 13 Bhaduri, A., Meyer, C.S., Gillespie, J.W., Haque, B.Z., Shields, M.D., Graham-Brady, L. (2021). "A probabilistic modeling framework for composite plate penetration models under projectile impact," *ASCE Journal of Engineering Mechanics*, 147(11): 04021087.

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- 31 Teferra, K. & Graham-Brady, L.L. (2015). "Grain growth tessellation models for polycrystalline microstructures," *Computational Materials Science*, 102: 57-67.
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- 54 Ferrante, F.J. & Graham-Brady, L.L. (2005). "Stochastic simulation of non-Gaussian/non-stationary properties in a functionally graded plate," *Computer Methods in Applied Mechanics and Engineering*, 194(12-16): 1675-1692.
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9

of Engineering Science Annual Technical Meeting (SES2022), October 16-19, 2022, College Station, TX.

D'Elia, M., Deng, H., Fraces, C., Garikipati, K., Graham-Brady, L., Howard, A., Karniadakis, G., Keshavarzzadeh, V., Kirby, R.M., Kutz, N., Li, C., Liu, X., Lu, H., Newell, P., O'Malley, D., Prodanovic, M., Srinivasan, G., Tartakovsky, A., Tartakovsky, D.M., Tchelepi, H. Vazic, B., Viswanathan, H., Yoon, H., Zarzycki, P. (2022). "Machine Learning in Heterogeneous Porous Materials," *Workshop on Machine learning in heterogeneous porous materials*, AmeriMech Symposium series sponsored by the National Academies and USNCTAM, virtually held on October 4-6, 2020 at the University of Utah. arXiv:2202.04137

Gupta, A., Bhaduri, A., Graham-Brady, L. (2021). "2D and 3D Microstructure Reconstruction using a Transfer Learning Approach and Structure-Property Studies (Abstract Only)", *16th US National Congress on Computational Mechanics*, Virtual, July 25-29, 2021.

Bhaduri, A., Ghosal, S., Graham-Brady, L. (2021). "Stress Field Prediction for Composite Materials Using Deep Learning," *4th International Conference on Uncertainty Quantification in Computational Sciences and Engineering*, Virtual, June 27-30, 2021.

Gupta, A., Bhaduri, A., Graham-Brady, L. (2021). "A transfer learning based 2D and 3D microstructure reconstruction approach using multiple loss functions," *4th International Conference on Uncertainty Quantification in Computational Sciences and Engineering*, Virtual, June 27-30, 2021.

Bhattacharjee, A., Bhaduri, A., Hurley, R., Graham-Brady, L. (2021). "Morphological implications on microstructure of armor ceramics to enhance ballistic performance (Abstract Only)," *Biot-Bažant Conference on Engineering Mechanics and Physics of Porous Materials*, Virtual, June 1-3, 2021.

Gupta, A., Bhaduri, A., Graham-Brady, L. (2021). "Microstructure reconstruction using a transfer learning approach and structure-property studies with applications to porous materials (Abstract Only)," *Biot-Bažant Conference on Engineering Mechanics and Physics of Porous Materials*, Virtual, June 1-3, 2021.

Bhattacharjee, A., Bhaduri, A., Hurley, R., Graham-Brady, L. (2021). "Sensitivity analysis of armor ceramics and the influence of microstructure on fragmentation and impact performance (Abstract Only)," *ASCE EMI Conference (EMI 2020)*, Virtual, May 27-29, 2021.

Gupta, A., Bhaduri, A., Graham-Brady, L. (2021). "Reconstruction of 2D and 3D Random Heterogeneous Media using Transfer Learning Approach (Abstract Only)," *ASCE EMI Conference (EMI 2020)*, Virtual, May 27-29, 2021.

Zare, A., Bhattacharjee, A., Yang, Q., Christian, K., Haber, R.A., Graham-Brady, L. Shaeffer, M., Ramesh, K.T. (2021). "Effects of Microstructure on Dynamic Compressive Response of Hot-pressed Boron Carbide (Abstract Only)," 8th Annual Mach Conference, Virtual, April 7-9, 2021.

Bhattacharjee, A., Bhaduri, A., Hurley, R., Graham-Brady, L. (2021). "Impact behavior of armor ceramics: sensitivity analysis (Abstract Only)," 8th Annual Mach Conference, Virtual, April 7-9, 2021.

Gupta, A., Bhaduri, A., Graham-Brady, L. (2021). "Reconstruction of 2D and 3D microstructures using transfer learning with applications to porous materials (Abstract Only)," 8th Annual Mach Conference, Virtual, April 7-9, 2021.

Bhattacharjee, A., Bhaduri, A., Hurley, R. & Graham-Brady, L. (2021). "Sensitivity analysis of armor ceramics: Sphere indentation simulations (Abstract Only)," *45th International Conference and Exposition on Advanced Ceramics conference (ICACC 2021*), virtual, February 8 - 12, 2021.

Gupta, A., Bhaduri, A., Olivier, A. & Graham-Brady, L. (2020). "A transfer learning based microstructure reconstruction approach using microstructural correlation functions (Abstract Only)," *Society of Engineering Science Virtual Technical Meeting*, virtual, September 29-October 1, 2020.

Graham-Brady, L. & Wade, N. (2020). "Methods for the correction of epistemic resolution error through data collection process simulations (Abstract Only)," *TMS 2020: 149th Annual Meeting and Exhibition*, San Diego, CA, February 23-27, 2020.

Graham-Brady, L., Bhattacharjee, A., Cil, M. (2020). "Impact models for ceramics incorporating fragmentation and subsequent breakage (Abstract Only)," *44th Annual International Conference and Exposition on Advanced Ceramics and Composites*, Daytona Beach, FL, January 28-31, 2020.

Graham-Brady, L. & Bhattacharjee, A. (2019). "Fragment size characterization for granular flow in highly damaged ceramics (Abstract Only)," *ECCOMAS Conference of Computational Methods in Multi-scale, Multi-uncertainty and Multi-physics Problems*, Porto, Portugal, July 16-18, 2019.

Bhaduri, A., Graham-Brady, L., Shields, M. (2019). "Efficient surrogate modeling using gradient information (Abstract Only)," *3rd International Conference on Uncertainty Quantification in Computational Sciences and Engineering*, Crete, Greece, June 24-26, 2019.

Bhattacharjee, A. & Graham-Brady, L. (2019). "Predicting initial fragment sizes for granular flow under dynamic fragmentation of ceramics (Abstract Only)," *ASCE EMI Conference (EMI 2019)*, Pasadena, CA, June 18-21, 2019.

Olivier, A., Shields, M., Graham-Brady, L. (2019). "Uncovering exploitable insights from microstructures using machine learning algorithms (Abstract Only)," *ASCE EMI Conference (EMI 2019)*, Pasadena, CA, June 18-21, 2019.

Bhaduri, A., Graham-Brady, L., Shields, M., Meyer, C., Haque, B., Gillespie, J. (2019). "Predicting probability of penetration for continuum plain-weave composite plate model under projectile impact (Abstract Only)," *ASCE EMI Conference (EMI 2019)*, Pasadena, CA, June 18-21, 2019.

Cil, M., Hurley, R., Graham-Brady, L. (2019). "Dynamic behavior of granulated boron carbide (Abstract Only)," 7th Annual Mach Conference, Annapolis, MD, April 3-5, 2019.

Bhattacharjee, A. & Graham-Brady, L. (2019). "Fragmentation and granular phase transition in brittle ceramics (Abstract Only)," *43rd Annual International Conference and Exposition on Advanced Ceramics and Composites*, Daytona Beach, FL, January 27-February 1, 2019.

Cil, M., Hurley, R., Graham-Brady, L. (2019). "A constitutive model for granulated ceramics based on breakage mechanics (Abstract Only)," *43rd Annual International Conference and Exposition on Advanced Ceramics and Composites*, Daytona Beach, FL, January 27-February 1, 2019.

Graham-Brady, L. & Wade N. (2018). "Uncertainty propagation from materials characterization to modeling (Abstract Only)," *EMI International Conference*, Shanghai, China, November 2-4, 2018.

Wade, N. & Graham-Brady, L. (2018). "Uncertainty quantification of data collection and data processing in materials characterization (Abstract Only)," *World Congress on Computational Mechanics*, New York, NY, July 22-27, 2018.

Cereceda, D., Arora, R., Krogstad, J.A., Jiménez, F.L., Shields, M.D., Graham-Brady, L. (2018). "Unraveling the structure-property relationships in fiber-composite materials using machine learning and global sensitivity analysis (Abstract Only)," *World Congress on Computational Mechanics*, New York, NY, July 22-27, 2018.

Bhaduri, A., Graham-Brady, L., Abrams, C. (2018). "Development of an efficient surrogate based sampling algorithm using gradient information (Abstract Only)," *ASCE EMI Conference*, Boston, MA, May 29-June 1, 2018.

Bhattacharjee, A. & Graham-Brady, L. (2018). "Analytical model of the transition of a comminuted material to granular phase and evolution of void ratio at transition (Abstract Only)," *ASCE EMI Conference*, Boston, MA, May 29-June 1, 2018.

Cil, M., Hurley, R., Graham-Brady, L. (2018). "Continuum modeling of deformation and comminution in granular ceramics under high strain rate loading (Abstract Only)," *ASCE EMI Conference*, Boston, MA, May 29-June 1, 2018.

PRESENTATIONS

Plenary/keynote lectures

"Lessons from a Successful Large DoD Center in the time of Covid," *National Academies'* Defense Materials, Manufacturing and its Infrastructure Standing Committee (DMMI) Workshop on Materials Science and Engineering in A Post-Pandemic World, December 7-9, 2020.

"Methods for the correction of epistemic resolution error through data collection process simulations," *TMS 2020: 149th Annual Meeting and Exhibition*, San Diego, CA, February 23-27, 2020.

"Uncertainty propagation from materials characterization to modeling," *EMI International Conference*, Shanghai, China, November 2-4, 2018.

- "Uncertainty in the Context of Materials by Design: Key Roles for Stochastic Mechanics," *EMI2017: ASCE Engineering Mechanics Institute Conference*, San Diego, CA, June 7, 2017.
- "The role of stochastic simulation in mechanics of materials at multiple scales," *FrontUQ: Frontiers of Uncertainty Quantification Workshop*, Munich, Germany, September 7, 2017.
- "Recent developments on a multi-mechanism model of brittle dynamic failure," 10th *ICACM US-France Symposium: Dynamic Damage & Fragmentation*, Shalimar, FL, May 17-19, 2017.
- "Stochastic simulation as a basis for optimizing microstructural characterization protocols," *Predictive Multiscale Materials Modelling workshop*, Isaac Newton Institute, Cambridge, UK, December 1-4, 2015.
- "Upscaling crack propagation and random interactions in brittle materials under dynamic loading," *IUTAM Symposium on Multiscale Problems in Stochastic Mechanics*, Karlsruhe, Germany, June 26, 2012.
- "Computational simulation of composite materials with random microstructure," workshop on *Validating Damage Evolution Models for Composite Materials*, Los Alamos National Laboratory, Los Alamos, NM, August 14-16, 2007.
- "Microstructural simulation for random composite materials: an overview," *NSF International Workshop: Microstructure and Micromechanics of Stone Based Infrastructure Materials*, Blacksburg, VA, October 5, 2006.
- "Microstructural stochastic simulation," *NSF-FHWA Workshop on Imaging and Simulation of Concrete Microstructure (Nano to Mesoscale)*, Northwestern University, Evanston, IL, July 28, 2003.
- "Moving-window representation of interfacial debonding in concrete," 1st International Symposium on Nanotechnology in Construction, Glasgow, Scotland, June 24, 2003.
- "Stochastic finite element analysis using variability response functions," U.S.-Japan Workshop/Seminar on Stochastic Simulation for Civil Infrastructural Systems, Kyoto, Japan, November, 1997.

Invited seminars

- "Accelerated materials design for extreme environments using high-throughput and Aldriven approaches," Materials Science and Engineering, University of Connecticut, February 17, 2023.
- "Surrogate models as a backbone for Al-driven materials design," Department of Materials Science, New Jersey Institute of Technology, April 11, 2022.
- "Machine Learning and Other Surrogate Models for Solid Mechanics," Department of Mechanical Engineering Seminar, University of Utah, February 25, 2022.
- "ML-enhanced approaches to the mechanics of multi-phase materials," Seminaire du Laboratoire PIMM, CNAM Paris, June 24, 2021.

- "Surrogate modeling approaches to enable uncertainty quantification in mechanics applications," Structures Seminar, Department of Civil & Environmental Engineering, University of Illinois at Urbana-Champaign, September 23, 2019.
- "Efficient uncertainty quantification and sensitivity analysis using surrogate models, with applications to mechanics," Center for Informatics & Computationals Science Seminar Series, Notre Dame University, September 25, 2019.
- "Uncertainty propagation in mechanics and materials by design based on surrogate model development," Department of Applied Mathematics and Statistics Seminar Series, Johns Hopkins University, April 18, 2019.
- "Efficient representation and analysis of structural materials through surrogate modeling," Department of Civil Engineering Seminar Series, Tongji University, November 5, 2018.
- "Surrogate models: a potential foundation for simultaneous structures/materials design," Department of Civil & Environmental Engineering Seminar Series, Carnegie Mellon University, October 12, 2018.
- "Breaking down language barriers in materials-by-design: a framework to enable uncertainty quantification," Department of Civil & Environmental Engineering Seminar Series, University of Virginia, March 16, 2018.
- "Stochastic mechanics: further empowerment for materials-by-design," Department of Civil & Environmental Engineering Seminar Series, Northwestern University, November 29, 2017.
- "Probabilistic Multi-Scaling as a way to Capture Key Localizations in Material Performance," Department of Mechanical & Aerospace Engineering Seminar Series, Arizona State University, March 24, 2017.
- "From micro-scale variations to structural failure using stochastic mechanics," Department of Civil Engineering and Engineering Mechanics Seminar Series, Columbia University, October 4, 2016.
- "What we don't know can hurt us: the case for stochastic mechanics," Department of Civil Engineering Seminar Series, Northeastern University, February 29, 2016.
- "Failure starts small: the role of stochastic mechanics in multi-scale modeling," Warren Lecture Series, University of Minnesota, March 13, 2015.
- "Breaking Up Fast: Failure of Brittle Materials at High Strain Rates," Civil Engineering Seminar, University of Pittsburgh, March 8, 2014.
- "Cracking Up: Micromechanical & Probabilistic Modeling of Dynamic Failure in Brittle Materials from Concrete to Ceramics," Structural Mechanics Seminar Series, Georgia Institute of Technology, Atlanta, GA, April 19, 2013.
- "Probabilistic Modeling of Dynamic Failure in Cementitious Materials," Civil Engineering Seminar Series, Northwestern University, Evanston, IL, April 23, 2013.
- "Probabilistic characterization of material microstructure," Mechanical Engineering seminar, Johns Hopkins University, Baltimore, MD, September 25, 2008.

- "Material property simulation based on probabilistic characterization of random microstructure," Civil Engineering seminar, Cornell University, Ithaca, NY, March 4, 2008.
- "Computational modeling of composite materials with random microstructure," part of the UCSD Structural Engineering Distinguished Lecture Series, University of California at San Diego, San Diego, CA, November 18, 2005.
- "Simulation and characterization of composite materials with random microstructure," JHU Applied Mathematics and Statistics Department Seminar, Johns Hopkins University, December 14, 2005.
- "Simulation techniques for random material microstructures," Department of Civil and Environmental Engineering seminar, Columbia University, New York, NY, November 4, 2004.
- "Analysis of materials with random microstructure," GWISE funded lecture to the Department of Civil Engineering, University of Michigan, Ann Arbor, MI, February 20, 2004.
- "Stochastic simulation of materials with random microstructure," Department of Civil Engineering seminar, Purdue University, W. Lafayette, IN, February 11, 2003.
- "Stochastic simulation of random material microstructure," Civil Engineering Department seminar, Northwestern University, Evanston, IL, November 8, 2002.
- "Computational analysis of random material microstructures via stochastic simulation," Sandia National Labs, Albuquerque, NM, December 13, 2001.
- "Micromechanics of random composite materials," Mechanical Engineering Department seminar, Johns Hopkins University, Baltimore, MD, March 3, 2001.
- "Stochastic finite element methods," Engineering Physics seminar, Washington & Lee University, Lexington, VA, March 9, 2000.
- "Stochastic finite element analysis in structural engineering," Department of Civil Engineering seminar, University of Maryland, College Park, MD, November 17, 1997.
- "Introduction of multimedia instruction in ENGR 205: Statics", UVA Teaching Resource Center workshop, November 4, 1998.

Presentations at conferences, workshops, program reviews (last 5 years)

- "ML-driven multi-scale models," Fall Meeting of the ARL-funded HTMDEC program, College Station, TX, November 17, 2022.
- "A Deep Learning Approach to Model the Microstructure-induced Uncertainty in Multiscale Modeling," *Society of Engineering Science Annual Technical Meeting (SES2022)*, College Station, TX, October 16-19, 2022.
- "MEDE Capstone: Overview of the Ten-Year Program", Capstone presentation of the ARL-funded MEDE Center, Baltimore, MD, January 20, 2022.

- "Developing a vision for proposals," Joint USACM Large-Scale TTA EMI CMC Career Path Panel at EMI 2023, Baltimore, MD, May 31, 2022.
- "Fragmentation and granular transition of ceramics for high rate loading," *Symposium for Best Paper Awardees in the Journal of the American Ceramics Society*, MS&T Conference, Pittsburgh, PA, October 11, 2022.
- "MEDE Overview: the last 10 years", Fall Meeting of the ARL-funded MEDE Center, Baltimore, MD, November 20, 2021.
- "Impact models for ceramics incorporating fragmentation and subsequent breakage," *44th Annual International Conference and Exposition on Advanced Ceramics and Composites*, Daytona Beach, FL, January 28-31, 2020.
- "Fragment size characterization for granular flow in highly damaged ceramics," *ECCOMAS Conference of Computational Methods in Multi-scale, Multi-uncertainty and Multi-physics Problems*, Porto, Portugal, July 16-18, 2019.
- "Predicting probability of penetration for continuum plain-weave composite plate model under projectile impact," *ASCE EMI Conference (EMI 2019)*, Pasadena, CA, June 18-21, 2019.
- "Surrogate modeling and model selection in irreducible high dimensions with small sample size," *13th International Conference on Applications of Statistics and Probability in Civil Engineering*, Seoul, Korea, May 26-30, 2019.
- "Uncertainty propagation of composite models using an efficient response surface algorithm," 8th Conference on Computational Stochastic Mechanics, Paros, Greece, June 10-13, 2018.
- "Uncertainty propagation in materials characterization," AFRL CEIMM Final Review Meeting, Baltimore, MD, April 30, 2018.
- "A micro-mechanical modeling approach for dynamic fragmentation in brittle multi-phase materials," *EMI 2017: ASCE Engineering Mechanics Institute Conference*, San Diego, CA, June 4-7, 2017.
- "FEM based uncertainty quantification for computational models of fiber-reinforced composite materials," *12th International Conference on Structural Safety and Reliability*, Vienna, Austria, August 6-10, 2017.
- "Quantification of Error and Uncertainty in Materials Characterization," AFRL CEIMM Annual Review Meeting, Dayton, OH, May 8, 2017.