FRANCIS G. VANGESSEL

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PROFESSIONAL SUMMARY

Computational Scientist with advanced expertise in scientific computing, physics-informed machine learning, and high-performance computing applications. I develop innovative solutions at the intersection of traditional physics-based modeling and machine learning across materials science, fluid dynamics, and energetics domains. My research has successfully demonstrated computational acceleration of scientific modeling by several orders of magnitude, enabling new capabilities in multiphysics simulation and parameter identification. I have secured over $5M in Department of Defense funding for projects advancing scientific machine learning approaches for computational energetics models. My collaborative research approach bridges disciplinary boundaries, working effectively with engineers, physicists, and chemistry experts to translate theoretical advances into practical applications with measurable impact.

RESEARCH EXPERTISE & TECHNICAL SKILLS

ML/AI Methods:
- Physics-Informed ML • Gaussian Processes • Transfer Learning
- Transformers • Bayesian Optimization • Deep Learning

Scientific Computing:
- Multi-physics Simulation • Numerical Methods • High-Performance Computing
- Parallel Programming • Monte Carlo Methods • Finite Volume Methods

Programming Laguages:
- FORTRAN • C++ • Python • PyTorch • Bash

Application Domains:
- Energetics • Fluid dynamics • Thermal transport • Fluid-Structure Interactions,
- Multiscale Material Science • Molecular Dynamics

EDUCATION

University of Maryland, College Park — College Park, MD
Ph.D., Mechanical Engineering — 2018
Dissertation: Phonon Modeling in Nano-and Micro-scale Crystalline Systems
Center for Engineering Concepts Development Fellow

University of Maryland, College Park — College Park, MD
M.S., Mechanical Engineering — 2016

St. Mary's College of Maryland — St. Mary's City, MD
B.S., Physics — 2013

AWARDS

Center for Engineering Concepts Development Fellow — 2018
University of Maryland, College Park

Computational Physics Student Summer Workshop — 2015
Los Alamos National Laboratory

RESEARCH EXPERIENCE

Assistant Research Professor 2024 - Present
University of Maryland, College Park, MD *Engineering Transfer Learning Lead*

- Lead a multidisciplinary government-academic research initiative comprising 10+ scientists, pioneering scientific machine learning approaches to extract and transfer physics knowledge from large datasets to complex 3D multiphysics design applications
- Direct research activities of 6 scientists, including postdoctoral researchers and graduate students, establishing methodological frameworks for transfer learning across aerodynamic, thermal, and structural domains
- Develop novel computational frameworks that enable rapid translation of machine learning-generated designs to physical prototypes through advanced manufacturing techniques
- Establish strategic research priorities aligned with Department of Defense requirements, ensuring relevance and applicability to defense-critical applications
- Implement comprehensive testing protocols and advanced image processing methodologies for evaluating performance of fabricated micro-air devices
- Present research findings and technical briefings to Department of Defense stakeholders and executive leadership, articulating complex technical concepts for non-specialist audiences

Scientific ML Research Lead(2019-2024) Naval Surface Warfare Center, Indian Head, MD
Research Focus: Development and integration of scientific machine learning approaches with traditional physics-based modeling for DoN lethality and vulnerability analysis

- Pioneered Deep Neural underwater explosion surrogate models achieving high-fidelity predictions >4000x faster than legacy solvers, enabling first-of-kind gradient-based parameter identification for unknown dynamics
- Developed novel ML-physics integration architecture connecting PyTorch with FORTRAN-based fluid solvers for enhanced constitutive and sub-grid modeling
- Created HPC-based automation framework for fluid-structure dynamics data generation, resulting in surrogate models 9 orders of magnitude faster than traditional approaches
- Computational Methods Team Lead of 5-member research team implementing ML optimization frameworks for material model calibration, reducing development timelines from months to days

Energetics LLM Research Technical Lead 2020 - Present
Naval Surface Warfare Center, Indian Head, MD *Machine Learning for Energetics*

- Technical lead for ONR funded (1.3 M) government-academic collaborative effort (Automated Global Energetics), utilizing machine learning and natural language models to accelerate the research and development of novel explosive materials
- Oversaw and directed team of 5 government researchers in areas of data wrangling, model development, and analysis
- Trained unsupervised NLP models (topic model, word2vec, transformer) to extract concepts germane to explosives research, developed first energetics domain finetuned transformer model
- Developed ML classification pipeline to ingest, clean, and classify explosives literature, implemented model improvements boosting baseline classification accuracy by 33%

Government Research Scientist 2019 - Present
Naval Surface Warfare Center, Indian Head, MD *Computational Methods Team Lead*

- Directed team of 5 engineers in development of machine learning optimization framework leveraging high-performance computing resources

- Applied Bayesian Optimization and Genetic Algorithm frameworks to enhanced accuracy material models critical to analysis underwater explosion scenarios, ML-based optimization framework generates calibrated models in days compared to months for the legacy calibration approach
- Extended modeling and simulation capabilities to wider array of weapon effects and structural response scenarios strengthening DoN threat assesment capabilities

University of Maryland, College Park College Park, MD
Graduate Research Assistant *2013 - 2018*

- Developed numerical method for modeling thermal transport in nano- and micro-scale structures. Solver was implemented using in FORTRAN90 code run on HPC resources
- Wrote parallelized FORTRAN90 numerical solver for solving the full Brillouin zone three dimensional Phonon Boltzmann Transport Equation
- Investigated effect of nanowire geometry for engineering reductions in microscale thermal transport
- Applied phonon modeling to complex molecular crystals, elucidating initiation mechanisms in energetic materials

Los Alamos National Laboratory Los Alamos, NM
Fellow in Computational Physics Student Summer Workshop *2015*

- Collaborated with fellows and laboratory scientists in the development of Monte Carlo code (C++) for simulation of radiative transport
- Demonstrated proof of concept for simulating diffusion dominated radiative transport on triangular meshes

FUNDING AND GRANTS

Center for Energetics Concept Development | Trailblazers Seed Program 4/25-7/26
Title: Tunable Energetics – Engineering Explosive Output Through Material-Performance Linkages
Total Award Amount: 66K$ / Total Share to Dr. VanGessel 66K$
Role: PI

Office of the Under Secretary of Defense (R&E) 4/23-4/24
Title: Automated Lethality
Total Award Amount: 2.0M$ / Total Share to Dr. VanGessel 1.0M$
Role: PI

Office of the Under Secretary of Defense (R&E) 4/22-4/24
Title: Machine Learning-Enhanced Energetics
Total Award Amount: 1.5M$ / Total Share to Dr. VanGessel 1.5M$
Role: PI

Naval Innovative Science & Engineering (NISE/ Sec 219) 4/22-4/23
Title: Automated Lethality Analysis
Total Award Amount: 300K$ / Total Share to Dr. VanGessel 300K$
Role: PI

Office of Naval Research 4/20-4/23
Title: Automated Global Energetics
Total Award Amount: 1.3M$ / Total Share to Dr. VanGessel 1.3M$
Role: Technical Lead

LEADERSHIP ROLES

DoD Artificial Intelligence for Energetics (AI4E) Workshop Organizer Spring 2024
Academia/DoD/DoE

· Co-organized the inaugural DoD Artificial Intelligence for Energetics (AI4E) Workshop
· Hybrid event brought together >150 scientist, engineers, and program managers to review opportunities and challenges in applying AI/ML to DoD's energetics challenges

Adjunct Professor Summer 2022 – Present
University of Maryland *Lecturer*

· Taught Applied Finite Element Methods (ENPM652) as adjunct faculty member of the Univ. of MD. Applied Graduate Engineering Department (MAGE)
· Updated course material (lectures, software examples, homework, & projects), presented weekly lectures, and held weekly office hours for class

Computational Methods Team Lead Fall 2021 - Spring 2024
Naval Surface Warfare Center, Indian Head, MD

· Coordinate and facilitate energetics research and software development efforts for team of 5 code developers

Teaching Assistant, Finite Element Methods January 2018 - May 2018
University of Maryland, College Park, MD

· Facilitated weekly office hours, graded problem sets and provided feedback, organized and lead recitations

Undergraduate Mentor June - August 2016/2017
University of Maryland, College Park, MD

· Managed two undergraduate students, coordinating the direction and scope undergraduate summer research projects. Results and visualizations of project appeared in peer-reviewed publication

PEER REVIEWED PUBLICATIONS

VanGessel, F. G., & Pandya, M. (2025) *Deep Learning Based Prediction of High Explosive Induced Fluid Dynamics.* Physics of Fluids *Accepted Pending Revision.*

O'Ryan, C., Hayes, K. D., **VanGessel, F. G.**, Doherty, R. M., Wilson, W., Fischer, J., Boukavalas, Z., & Chung, P. (2025) *An Automated Approach for Domain-Specific Knowledge Graph Generation-Graph Measures and Characterization.* Journal of Chemical Information and Modeling 65(3).

VanGessel, F. G., Efrem, P., Mohan, S., Barham, O. M., & Cavolowsky, M. (2023) *Natural language processing for knowledge discovery and information extraction from energetics corpora.* Propellants, Explosives, Pyrotechnics 48(11): e202300109.

Balakrishnan, S., **VanGessel, F. G.**, Barnes, B. C., Doherty, R. M., Wilson, W. H., Boukouvalas, Z., Fuge, M., Chung, P. W. (2023). *Machine Learning for Shock Compression of Solids Using Scarce Data.* Journal of Applied Physics, 133(15).

VanGessel, F. G. & McGrath, T. P. (2022). *An Improved Water Equation of State for Underwater Explosion Simulations.* Journal of DoD Research and Engineering, 4(4), 16-27.

Kumar, G., **VanGessel, F. G.**, Munday, L. B., & Chung, P. W. (2021). *3-phonon Scattering Pathways for Vibrational Energy Transfer in Crystalline RDX*. The Journal of Physical Chemistry A, 125(35), 7723-7734.

Balakrishnan, S., **VanGessel, F. G.**, Boukouvalas, Z., Barnes, B. C., Fuge, M. D., & Chung, P. W. (2021). *Locally Optimizable Joint Embedding Framework to Design Nitrogen-rich Molecules that are Similar but Improved*. Molecular Informatics, 40(7), 2100011.

Kumar, G., **VanGessel, F. G.**, & Chung, P. W. (2020). *Bond Strain and Rotation Behaviors of Anharmonic Thermal Carriers in-RDX*. Propellants, Explosives, Pyrotechnics, 45(2), 169-176.

VanGessel, F. G., & Chung, P. W. (2019). *Phonon backscatter, trapping, and misalignment effects on microscale thermal conductance below the Casimir limit*. International Journal of Heat and Mass Transfer, 128, 807-816.

Kumar, G., **VanGessel, F. G.**, Elton, D. C., & Chung, P. W. (2019). *Phonon lifetimes and thermal conductivity of the molecular crystal α-RDX*. MRS Advances, 4(40), 2191-2199.

VanGessel, F. G., Kumar, G., Elton, D. C., & Chung, P. W. (2018). *A Phonon Boltzmann Study of Microscale Thermal Transport in α-RDX Cook-Off*. arXiv preprint arXiv:1808.08295.

VanGessel, F. G., Peng, J., & Chung, P. W. (2018). *A review of computational phononics: the bulk, interfaces, and surfaces*. Journal of materials science, 53, 5641-5683.

VanGessel, F. G., & Chung, P. W. (2017). *An anisotropic full Brillouin zone model for the three dimensional phonon Boltzmann transport equation*. Computer Methods in Applied Mechanics and Engineering, 317, 1012-1036.

INVITED TALKS

VanGessel, F. G.. "Integrating Machine Learning with Physics-Based Computation for Enhanced Modeling of Underwater Explosive Effects" *Energetic Materials Gordon Research Conference 2024*.