# DR. SERGEY GALITSKIY

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## Summary

Research engineer with 10+ years in advanced simulation and multiscale modeling. Expertise in developing physics-based models and numerical methods for thermodynamics and fluid dynamics applications. Proficient in Python, HPC, and scientific computing libraries to build high-fidelity simulators. Demonstrated ability to collaborate across disciplines and translate first-principles research into scalable, AI-integrated solutions.

## COMPUTATIONAL METHODS

- **Machine Learning (ML)**: Python, scikit-learn, ML pipelines
- **Molecular Dynamics (MD)**: LAMMPS, GROMACS, custom in-house codes
- **Finite Element Modeling (FEM)**: Ansys Workbench, LS-Dyna
- **CAD Integration**: Catia, SpaceClaim
- **Specialized Simulations**: COMSOL, Forge, Deform
- **Multiscale Methods**: hybrid MD-FEM frameworks, Two-Temperature Model (MD-TTM) simulations
- **Ab Initio / First-Principles Methods**: VASP, Single-Center Method (GAMESS-based)
- **Materials Informatics & Selection**: Ansys Granta, Ansys, nCode DesignLife
- **Programming & Scripting**: Python, Bash, Fortran, C
- **HPC & Parallel Computing**: multiprocessor and GPU environments
- **Workflow & Data Management**: Linux, Windows
- **Simulation Automation**: Ansys Parametric Design Language (APDL)
- **Industrial Integration**: simulation and analysis pipelines
- **Cross-Functional Collaboration**: Cross-Functional Collaboration
- **Research & Communication**: technical writing, scientific literature and patent review, presenting research
- **Teaching & Mentorship**: Physics, Calculus, Thermodynamics, Computational Physics

## WORK EXPERIENCE

**University of South Florida** **Aug 2024**

*Post Doctoral Researcher* *Tampa, Fl*

Developed advanced Machine-Learned Interatomic Potentials (MLIPs) for atomistic modeling by integrating Python-driven simulation automation with HPC-based numerical methods, aligning with first-principles physics models.

- Built robust training datasets from Molecular Dynamics (MD) and Density Functional Theory (DFT) simulations to support model fitting and thermodynamic property evaluation, demonstrating applied engineering in simulation tool development.
- Designed scalable HPC workflows for extreme environments, implementing automated, high-throughput simulation pipelines that solved complex governing equations relevant to high-temperature and fluid dynamic conditions.
- Performed extensive MD and DFT simulations to investigate structural, mechanical, and thermodynamic behavior of materials under dynamic loading, thereby reinforcing foundational principles in fluid mechanics and heat transfer.
- Automated simulation and analysis pipelines using Bash and Python, improving reproducibility, error handling, and numerical postprocessing across thousands of compute jobs to ensure fidelity in simulation outputs.
- Supported multi-lab HPC deployment by maintaining and optimizing simulation codes across national supercomputers, ensuring performance compatibility for research-driven numerical experiments.
- Collaborated with national laboratories to integrate experimental and computational projects, contributing to the development of physics-based models and validating simulation frameworks against real-world data.
- Provided mentorship and technical training to graduate and undergraduate students in simulation methodologies, Python scripting, and HPC usage, while clearly documenting technical findings and simulation procedures.
- Published and presented research findings that contributed to the broader physics and materials modeling communities, showcasing proficiency in reading academic literature and implementing physics models from scratch.

**Stanley, Black & Decker, inc.** **Nov 2021 - Feb 2024**

*Material Simulation Scientist II* *New Britain, CT*

- Directed an NSF-funded AI-driven sustainability initiative that integrated simulation tools with polymer science, fostering collaboration to develop models for material recycling and process optimization.
- Organized internal AI/ML knowledge-sharing sessions to align cross-functional teams, enhancing understanding of simulation techniques and numerical methods in material and thermal analyses.
- Applied machine learning and experimental design for material development, managing advanced analytics and simulation-based optimization to guide materials selection and processing strategies.
- Accelerated product development by deploying modeling tools to perform early-stage simulation for virtual reliability testing, iteratively refining thermal and mechanical performance using established numerical methods.
- Delivered high-fidelity Finite Element Modeling analyses for performance prediction under mechanical, thermal, and acoustic loads, supporting certification testing and ensuring alignment with thermodynamic and fluid dynamic principles.

- Created custom LS-DYNA simulations using APDL to model advanced failure mechanisms and nonlinear behavior, providing deeper insights into component integrity under dynamic loading conditions.
- Enhanced reliability through tribological modeling by simulating fatigue, wear, and crack formation, which informed design choices and contributed to improved long-term durability of systems.
- Integrated experimental data with simulations by combining lab analytics and materials property datasets, thereby validating simulation outputs and ensuring robust model performance in industrial applications.
- Collaborated with internal teams and external partners to drive materials and quality improvements, contributing to patent filings while emphasizing precision in simulation and applied physics evaluations.

**University of Connecticut** **Aug 2016 - Oct 2021**

*Graduate Assistant, Department of Material Science and Engineering* *Storrs, CT*

Led research on dynamic fracture mechanisms in lightweight and refractory metals (Al, Mg, Ta) subjected to extreme loading conditions such as laser irradiation and impact-induced shock. This work revealed critical insights into dislocation dynamics, twinning, void nucleation, and other deformation mechanisms at the atomic scale, contributing to a deeper understanding of material response under high strain rates and pressures.

- Designed and implemented advanced computational frameworks by developing custom Fortran and Python modules for large-scale Molecular Dynamics (MD) simulations, as well as coupling MD with Finite Element Methods (MD+FEM) to capture multi-scale phenomena. These innovations allowed simulation of realistic boundary conditions and stress wave propagation in complex geometries.
- Developed scientific codes for state-of-the-art high-performance MD simulations by significantly extending the capabilities of the MD–Two Temperature Model (MD-TTM) code to account for ultrafast energy exchange between electrons and ions during laser irradiation of metals. This enhancement enabled predictive modeling of non-equilibrium processes relevant to laser-based manufacturing and material processing.
- Collaborated on cross-disciplinary projects involving multi-physics and multi-scale simulations, integrating atomistic insights with continuum-scale understanding to inform the development of new materials and processing techniques.
- Authored and contributed to multiple high-impact journal publications in the fields of materials modeling and shock physics; played a central role in manuscript preparation, data analysis, and peer review coordination.
- Presented research findings at national and international conferences, including TMS, MRS, APS, Mach, Gordon and others, receiving recognition for clarity, depth, and relevance of technical contributions.
- Provided mentorship and technical guidance to junior graduate students and supported instructional efforts in thermodynamics and atomistic modeling courses, earning the 2021 UConn Teaching Excellence Award in recognition of outstanding teaching and student engagement.

**University of Kassel, Germany** **Oct 2013 - Feb 2016**

*Graduate Assistant, Physics Department* *Kassel, Germany*

Simulated biomolecular systems via atomistic MD: Investigated neuron cell behavior by modeling protein-membrane interactions under varying calcium concentrations to understand exocytosis phenomena

- Developed novel ab initio methods for electron dynamics: Modeled excitation, ionization, and relaxation processes including fluorescence and Auger decay, enhancing predictive tools for radiation-matter interactions.
- Published original research in computational spectroscopy: Authored peer-reviewed articles on electron and photon emission spectra from small molecules under single-photon excitation.
- Taught undergraduate mathematical & physics courses: Delivered lectures and provided academic support in analytical methods, helping students strengthen problem-solving foundations.

## EDUCATION

**University of Connecticut, Storrs, CT, US** **Aug 2016 - Oct 2021**

*Ph.D., Materials Science and Engineering*

**South Federal University, Physics Department, Rostov-on-Don, Russia** **Sep 2009 - Jul 2011**

*Masters, physics*

**South Federal University, Physics Department, Rostov-on-Don, Russia** **Sep 2005 - Jul 2009**

*Bachelors, physics*

## LANGUAGES

- Russian (native)
- English (fluent)
- German (intermediate)

## SELECTED PUBLICATIONS

- S. Galitskiy, J. Willman, J. Gonsalez, Ivan Oleynik. Spectral Neighbor Analysis Potential (SNAP) for simulations of Carbon at extreme conditions. PRL (in submission 2025)
- D. Kraus, S. Galitskiy, et all. The tetrahedral structure of liquid carbon elucidated by in-situ X-ray diffraction. Nature 642 (2025)
- S. Galitskiy and A. M. Dongare. Interaction of the Shockwave with Voids in Single-crystal Ta at Mesoscales. Int J Plasticity 164 (2024)
- S. Galitskiy and A. M. Dongare. Modeling the Damage Evolution and Recompression Behavior during Laser Shock Loading of Aluminum Microstructures at the Mesoscales. J Material Science, 56 (2021) [Journal cover article]

- S. Galitskiy, D. Ivanov, and A. M. Dongare. Dynamic Evolution of Microstructure during Laser Shock Loading and Spall Failure of Single-crystal Al at the Atomic Scales. J Applied Physics (2018) [Journal cover article]
- S. Galitskiy, D Ivanov, A Dongare. Atomic Scale Modeling of Laser Shock Induced Spallation of FCC Metals. APS Shock Compression of Condensed Matter (2017)
- S. Galitskiy, A. N. Artemyev, K. Jankälä, B. M. Lagutin, and Ph. V. Demekhin. Hartree-Fock Calculation of the Differential Photoionization Cross-sections of Small Li Clusters. J Chemical Physics, (2015)