DR. SERGEY GALITSKIY

Ph. D, Material Science & Engineering
Current address: Tampa, 33647, FL
Google Scholar; LinkedIn; E-mail: sergeygalitskiy88@gmail.com
Phone: (860) 709-8181

Experienced materials scientist with 10+ years of expertise in multiscale modeling and simulation. Specialized in atomistic modeling to predict microstructural evolution during shock loading, materials processing, performance, and failure. Strong passion for material informatics, including the development and deployment of Machine Learning Interatomic Potentials (MLIPs). Proficient in scientific software development and advanced simulation methods, including Molecular Dynamics (MD), Density Functional Theory (DFT), and Finite Element Modeling (FEM).

EDUCATION

Ph.D. in Materials Science and Engineering; 08/2016 – 10/2021
University of Connecticut, Storrs, CT, US
"Modeling the Laser-Induced Phenomena and Spall Failure of Metal Microstructures at the Atomic Scales and the Mesoscales"

Masters in physics; 09/2009-07/2011
South Federal University, Physics Department, Rostov-on-Don, Russia
"Local selection rules for construction of quasicrystal lattices"

Bachelors in physics; 09/2005-07/2009
South Federal University, Physics Department, Rostov-on-Don, Russia,
“EXAFS spectra of perovskite structures as a function of local atomic arrangement"

WORK EXPERIENCE

Post Doctoral Researcher
University of South Florida, Tampa, Fl, 08/2024- current

- Developed advanced **Machine-Learned Interatomic Potentials (MLIPs):** Trained and optimized SNAP and ACE potentials for accurate atomistic modeling of materials under extreme conditions, enhancing predictive capabilities for diverse material systems.
- Built robust training datasets from atomistic simulations: Generated high-quality datasets from **Molecular Dynamics (MD)** and **Density Functional Theory (DFT) simulations** to support MLIP fitting, property evaluation, and extrapolation stability.
- Designed scalable **HPC workflows** for extreme environments: Implemented automated, high-throughput simulation pipelines to study materials under shock, compression, and high-temperature regimes—relevant to planetary interiors and fusion ignition conditions at NIF.
- Performed large-scale **MD and DFT simulations**: Investigated structural, mechanical, and thermodynamic behavior of advanced materials under dynamic loading, using VASP and LAMMPS on leading HPC platforms.
- **Automated simulation and analysis pipelines**: Streamlined end-to-end workflows using Bash and Python, improving reproducibility, error handling, and data postprocessing across thousands of compute jobs.
- Supported **multi-lab HPC deployment**: Maintained, optimized, and ported codes across national supercomputers (Aurora, Frontier, Perlmutter, Frontera), ensuring performance and compatibility for ML-enhanced simulations.

- **Collaborated with national laboratories**: Worked closely with LLNL and LANL teams on experimental–computational–ML integration projects, connecting atomistic simulations with real-world high-pressure experiments.
- Provided **mentorship and technical training**: Guided graduate and undergraduate students in simulations, Python scripting, HPC usage, and best practices in computational materials science.
- **Published and presented research findings:** Authored peer-reviewed papers and delivered presentations at major conferences, contributing to the broader physics and materials modeling communities.

Material Simulation Scientist II
Stanley, Black & Decker, inc., New Britain, CT, 11/2021 – 02/2024

- **Led an NSF-funded AI-driven sustainability initiative:** Directed a first-of-its-kind project integrating machine learning, polymer science, and manufacturing to advance sustainable polymer recycling; fostered collaboration between industrial and academic partners in materials informatics.
- **Organized internal AI/ML knowledge-sharing:** Organized recurring technical webinars on materials science and ML applications, engaging cross-functional teams across R&D, engineering, manufacturing, and leadership.
- **Applied ML and experimental design for material development:** Managed project budgets and data workflows, utilizing advanced analytics, Design of Experiments (DoE), and ML-based optimization to guide materials selection and processing strategies.
- **Accelerated product development through simulation:** Deployed modeling tools (Ansys, Deform, Forge) to support early-stage prototyping, virtual reliability testing, and design optimization across multiple products
- Delivered high-fidelity **FEM analyses:** Provided robust Finite Element Modeling support for performance prediction under mechanical, modal, acoustic, and thermal loads; authored technical documentation for certification testing and coordinated with external labs.
- Created custom **LS-DYNA simulations using APDL:** Modeled advanced failure mechanisms and nonlinear behavior beyond standard simulation capabilities, enabling deeper insights into component integrity and risk.
- Enhanced reliability via **tribological modeling**: Simulated fatigue, wear, and crack formation to inform design choices that improved long-term durability of mechanical components.
- Integrated **experimental data with simulations**: Combined lab analytics (SEM, EBSD, hardness) and materials property datasets with simulation results to improve R&D decision-making and model validation.
- **Drove IP and material quality improvement:** Collaborated with internal teams, supply chain, and external partners to refine materials and processing methods; contributed to two patent filings

Graduate Assistant, Department of Material Science and Engineering
University of Connecticut, Storrs, CT, 08/2016 – 10/2021

- **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.

Graduate Assistant, Physics Department
University of Kassel, Germany, Kassel, 10/2013- 02/2016

- 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.

COMPUTATIONAL METHODS

- **Machine Learning (ML):** Applied ML techniques (Python, scikit-learn) to analyze and predict material properties, structure–property relationships, and optimize design workflows in materials science and MLIP development (ACE and SNAP)
- **Molecular Dynamics (MD):** Performed atomistic simulations of biosystems, Carbon, and metallic systems using LAMMPS, GROMACS, and custom in-house codes to study fundamental deformation, fracture, phase transformations, shock, etc.
- **Finite Element Modeling (FEM):** Conducted structural, thermal, and failure analyses using Ansys Workbench and LS-Dyna. Specialized in tribological simulations, vibration studies, and fatigue prediction.
— **CAD Integration:** Utilized Catia and SpaceClaim for pre-processing and geometric modeling.
— **Specialized Simulations:** Hall-effect-based non-destructive defect analysis in COMSOL; heat treatment and forging processes in Forge and Deform to predict microstructure evolution and hardness.
- **Multiscale Methods:** Developed hybrid MD–FEM frameworks, including Two-Temperature Model (MD-TTM) simulations, to investigate ultrafast laser–matter interactions at nano-to-meso scales.
- **Ab Initio / First-Principles Methods:**
— Used **VASP** for DFT-based calculations of condensed-phase systems.
— Developed and applied **Single-Center Method** (GAMESS-based) for electronic structure analysis and photoelectron spectra of molecules, including ionization and excitation cross-section prediction.
- **Materials Informatics & Selection:** Applied Ansys Granta for data-drivenmaterial selection and optimization; performed fatigue analysis using Ansys and nCode DesignLife.

PROGRAMMING & OTHER SKILLS

- **Programming & Scripting:** Proficient in Python, Bash, and Fortran for scientific computing, simulation workflows, and data analysis; Experience in C.
- **Machine Learning (ML):** Designed and implemented ML pipelines for predicting material properties and accelerating materials discovery.
- **HPC & Parallel Computing:** Developed and optimized atomistic modeling codes using multiprocessor and GPU environments; reduced computational overhead through algorithmic and memory optimizations.
- **Workflow & Data Management:** Managed large-scale simulation datasets and workflows on HPC systems (Linux and Windows environments).
- **Simulation Automation:** Developed custom simulation tools and batch automation using Ansys Parametric Design Language (APDL).
- **Industrial Integration:** Optimized simulation and analysis pipelines for materials workflows in manufacturing settings, enabling efficient decision-making across R&D and production.
- **Cross-Functional Collaboration:** Coordinated with R&D, engineering, business, and manufacturing teams to align technical innovations with product development goals.
- **Research & Communication:** Experienced in technical writing, scientific literature and patent review, and presenting research at conferences and internal seminars.
- **Teaching & Mentorship:** Instructed undergraduate and graduate courses in Physics, Calculus, Thermodynamics, and Computational 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. J¨ank¨al¨a, B. M. Lagutin, and Ph. V. Demekhin, "Hartree-Fock Calculation of the Differential Photoionization Cross-sections of Small Li Clusters," J Chemical Physics, (2015)