Justin Gage Lietz, Ph.D. - Curriculum Vitae

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INFORMATION Oak Ridge National Lab

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RESEARCH INTERESTS

Computational Quantum Many-Body Physics: Numerically solving systems of many interacting particles is relevant to a wide range of scientific domains from nuclear and particle physics to quantum chemistry and quantum computing. A key challenge in this field is that these simulations of interacting particles scale exponentially with system size, quickly creating computational bottlenecks for physically relevant systems. To meet these computational challenges, I work on: improving polynomially scaling quantum many-body methods for accurate simulations at a tractible cost, implementing efficient data structures to compress the growing amount of data needed to represent the many-body tensors, and developing massively parallel GPU-based algorithms that target leadership class supercomputers like Summit and Frontier.

CURRENT APPOINTMENT

Oak Ridge Leadership Computing Facility, National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN

September 2021 to present

Performance Engineer - Algorithms and Performance Analysis Group

- Researching nuclear physics applications using machine learning methods and quantum computing.
- Co-author of the Nuclear Tensor Contraction Library (NTCL), a library focusing on performance and portability for computational quantum mechanics.
- Analyzing performance of various mathematical and scientific software running on the Summit and Frontier supercomputers.

PREVIOUS APPOINTMENTS

Oak Ridge Leadership Computing Facility, National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN

September 2019 to August 2021

Postdoctoral Research Associate -

Advanced Computing for Nuclear, Particles, and Astrophysics Group

- Worked in the Center for Accelerated Application Readiness (CAAR) to prepare the nuclear many-body physics code, NUCCOR, for the exascale supercomputer Frontier.
- Extended coupled cluster calculations for nuclear physics, quantum chemistry, and solid state physics to new levels of precision and system size.
- Developed massively parallel data structures and algorithms so that large scale tensor operations can run at the scale of thousands of GPUs.

PREVIOUS EDUCATION

National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI

July 2013 to August 2019

Dual Ph.D. in Physics and Computational Math, Science, and Engineering

- Advisor: Morten Hjorth-Jensen
- Thesis Title: Computational Developments for Ab Initio Many-Body Theory
- Areas of study: Theoretical nuclear physics and computational quantum mechanics

B.S. in Physics and Mathematics

- Senior thesis in theoretical nuclear physics (no-core shell model for halo nuclei).
- Mathematics independent research in random matrix theory.

Vanderbilt University, Nashville, TN

Summers of 2011 and 2012

REU Summer Program

- Compared neutrino experiment data to numerical simulations.
- Investigated of possibility of sterile neutrinos.

PUBLICATIONS

J.G. Lietz, S. Novario, G.R. Jansen, G. Hagen and M. Hjorth-Jensen,

"Computational Nuclear Physics and Post Hartree-Fock Methods"

An advanced course in computational nuclear physics - Bridging the scales from quarks to neutron stars, Eds. M. Hjorth-Jensen, M.P. Lombardo, U. van Kolck, Lecture Notes in Physics **936**, (2017) Pages 293-400

H. Hergert, S.K. Bogner, J.G. Lietz, T.D. Morris, S.J. Novario, N.M. Parzuchowski, and F. Yuan "In-Medium Similarity Renormalization Group Approach to the Nuclear Many-Body Problem" *An advanced course in computational nuclear physics - Bridging the scales from quarks to neutron stars*, Eds. M. Hjorth-Jensen, M.P. Lombardo, U. van Kolck, Lecture Notes in Physics **936**, (2017) Pages 477-570

NTCL: Nuclear Tensor Contraction Library G.R. Jansen, J.G. Lietz and X. Mao (in prep.)

Many-Body Approaches to the Homogeneous Electron Gas in Two and Three Dimensions J.G. Lietz, S.K. Bogner, G.R. Jansen, and M. Hjorth-Jensen (in prep.)

Algorithms and Efficient Data Structures for Ab-Initio Calculations of Infinite Matter J.G. Lietz, G.R. Jansen, and M. Hjorth-Jensen (in prep.)

AWARDS AND TRAINING

2020 - Argonne Training Program on Extreme-Scale Computing (ATPESC) Virtual Program (hosted by Argonne National Laboratory), Summer 2020

2020 - Your Science in a Nutshell lightening talk competition (finalist) Virtual Program (hosted by Oak Ridge National Laboratory), Summer 2020

2017 - DOE SCGSR Award: Office of Science Graduate Student Research Program,
5 Months Funding to work at Oak Ridge National Lab,
Project Title: Ab-Initio Theory for Dense Matter with Three-Body Forces
Advisor: Gustav Jansen, Oak Ridge National Lab, August - December 2017

2016 - OLCF GPU Hackathon Oak Ridge National Lab, October 2016

2016 - Parallel Computing Summer Research Internship (PCSRI), Los Alamos National Lab, June - August 2016 2015 - TALENT Summer School,

Many-Body Methods for Nuclear Physics, June-July 2015

2014 - TALENT Summer School,

Theory for Nuclear Structure Experiments, August 2014

2014 - TALENT Summer School.

Density Functional Theory and Self-Consistent Methods, July 2014

2014 - TALENT Summer School,

Nuclear Theory for Astrophysics, June 2014

TALKS

 $2021\,$ - J.G. Lietz, "NTCL: The Nuclear Tensor Contraction Library",

APS April Meeting, April 20, 2021

2019 - J.G. Lietz, "Computational Developments for Ab Initio Many-Body Physics",

PhD Defense, June 28, 2019

2018 - J.G. Lietz, "Computational Developments for Coupled Cluster Theory With Triples and

Three-Body Forces",

APS April Meeting, April 17, 2018

2017 - J.G. Lietz, "Many-Body Physics on Many Computers",

Physics Graduate Organization, March 16, 2017

2016 - J.G. Lietz, "Neutron Stars From Nucleons",

NSCL Graduate Seminar, March 28, 2016

2015 - J.G. Lietz, "Run Diffusion Monte Carlo",

Physics Graduate Organization, February 27, 2015

POSTER PRESENTATIONS

2021 - J.G. Lietz, X. Mao, G.R. Jansen, "Nuclear Tensor Contraction Library (NTCL) with

Simple Fortran Interfaces", ORNL Software and Data Expo, May 19 2021

2016 - J.G. Lietz, Stephanie Lauber, Peter Ahrens, "Distributed Memory Implementation of

Coupled Cluster", Los Alamos National Lab Summer Student Symposium, August 2016

SOFTWARE SKILLS Computer Programming:

• C, C++, Fortran, Python, UNIX shell scripting, GNU make, Java

Parallel Computing:

• MPI, OpenMP, CUDA, HIP

Performance Analysis:

• NVIDIA Nsight, ARM MAP

Productivity:

• Git, Make, gdb, valgrind, Vim

TEACHING EXPERIENCE Summer 2017 - Nuclear Science Summer School, Guest Lecturer

Fall 2014 - Graduate Quantum Mechanics, Teaching Assistant

Spring 2014 - Physics Mechanics Lab, Teaching Assistant

Fall 2013 - Physics Mechanics Lab, Teaching Assistant

SERVICE

2021 - October OLCF GPU Hackathon mentor.

2015, 2016, 2017 - Women and Minorities in the Physical Sciences (WaMPS) Treasurer:

My responsibilities in this position were to help plan the yearly budget for the WaMPS student organization, and to frequently check in that we were spending at the proper rate to fall within our budget by the end of the fiscal year. I also acted as a bridge between the graduate students and the fiscal department of the university to handle reimbursements. Along with being treasurer for two terms, I attended the monthly WaMPS meetings, and went on several public outreach trips with the group each year.

2014, 2015, 2016 - Physics Graduate Organization (PGO) Vice President:

My responsibilities centered around representing the graduate student body to the department, and having quarterly discussions with the department chair about pushing forward changes to better the graduate student experience at MSU.

SELECTED COURSES

2013 - 2015 I Completed all standard graduate physics courses with a focus on nuclear theory 2015 - 2017 Once the Computational Math, Science and Engineering (CMSE) department is founded at MSU, I decided to enroll in a dual Ph.D. and took additional courses such as:

Designing and Building Applications for Extreme Scale Systems:

Focused on learning MPI to leverage the power of the Blue Waters supercomputer at the University of Illinois.

Programming for Multi-Core Architectures:

Learned many classic linear algebra algorithms to target GPUs using CUDA.

Mathematical Foundations of Data Science:

Proof based course that went over several key theorems at the backbone of data science and machine learning.

REFERENCES AVAILABLE TO CONTACT

Dr. Philip Roth (email: rothpc@ornl.gov)

- Group Leader: Algorithms and Performance Analysis, Oak Ridge National Laboratory
- ★ Dr. Roth is my group leader.

Dr. Gustav Jansen (email: jansengr@ornl.gov)

- Computational Scientist Nuclear Physics, National Center for Computational Sciences, Oak Ridge National Laboratory
- * Dr. Jansen is a close research collaborator.

Dr. Morten Hjorth-Jensen (email: hjensen@nscl.msu.edu)

- Professor of Physics,
 National Superconducting Cyclotron Laboratory,
 Michigan State University
- * Dr. Hjorth-Jensen was my Ph.D. supervisor
- * Dr. Hjorth-Jensen is also the PI for the NUCCOR INCITE project

Dr. Scott Bogner (email: bogner@nscl.msu.edu)

- Professor of Physics,
 National Superconducting Cyclotron Laboratory,
 Michigan State University
- * Dr. Bogner was my Ph.D. co-supervisor.