Quantum Monte Carlo and Density Functional Theory of Superfluid Systems

nuclei, nuclear matter, unitary Femi gas – UW centered group

Major problems addressed and to be addressed:

- Structure of ground and excited states of nucleons and strongly interacting Fermi gases using realistic interactions
- Dynamics of strongly interacting superfluid fermion systems within DFT: nuclear fission, fission fragments distributions (mass, charge, excitation energy sharing, fragment angular momentum, total kinetic energy), low-energy nuclear reactions (pre-equilibrium)
- Neutron star crust structure and dynamics, vortex pinning mechanism and vortex dynamics
- Quantum turbulence in cold gases, neutron stars, great opportunity for the first time to confront in detail a microscopic quantum approach for dynamics of superfluids vs experiment (relevant across all fields of physics)

Major achievements so far since 2007:

- Developed the theory and implemented it on leadership class computers, validated, verified for the first time-dependent DFT for superfluid fermion systems, predicted phenomena and properties (in advance of experiment), lots of firsts!
- Developed and implemented QMC for Fermi gases and neutron matter, now extended to nuclear systems
- Pushed Jaguar and Titan to their limits, runs of full machine, excellent scaling, and impressive speedups using the hybrid architecture (CPU with MPI and GPU with CUDA)
- Educated a large number of young researchers: 4 PhDs, 2 REU students, 5 asst. prof./staff
- 1 Science, 17 Phys. Rev. Lett., 16 Rapid Communications

- Graduate Students:
  - *Joaquín E. Drut*, PhD (2008), winner of Henderson prize (2009) and Kummer international award (2011), now Melchor fellow and Assistant Professor, U of North Carolina
  - *Sukjin Yoon*, PhD (2010), now at APCTP, S. Korea
  - *Gabriel Wlazłowski*, PhD (2010), now Assistant Professor, Warsaw U. of Technology and visiting Assistant Professor, U. Washington (2011-2014)
  - *Yuan-Lung Luo*, PhD (2013), winner of Henderson prize (2014), Graduate Medal of College of A&S (2013), and Karrer prize (2010), now at a start-up in Silicon Valley
  - *Adam Richie-Halford*, current, U. Washington, DOE Computational Science Graduate Fellow
  - *Shi Jin*, current, U. Washington
  - *Ethan Crowell*, current, Washington SU
  - *Maren Mossman*, current, Washington SU
- Undergraduate students:
  - *Michelle M. Kelley*, REU student (2013) from U. of Illinois, Urbana-Champaign
    Gates Cambridge scholarship for scientific computing (2013) and NSF graduate research fellowship (2013)
  - *Wei Quan*, BS, current, U. Washington (2014)
  - *Marie Kirkegaard*, REU student (2014) from Harvey Mudd College
- Junior collaborators:
  - *Ionel Stetcu* (UW 2009-2011), currently staff at LANL, LANL Early Career Award (2014)
  - *Michael M. Forbes* (UW 2005-2008, 2010-2013), now Assistant Professor Washington SU and Affiliate Assistant Professor U. Washington
  - *Gabriel Walzłowski*, Assistant Professor Warsaw U. of Technology and visiting Asst. Prof. UW (2011-2014)
  - *Jeremy W. Holt* (UW 2012-present), postdoc to become Research Assistant Professor 9/2014
  - *Sergej Moroz* (UW 2011-2014), postdoc
- Senior collaborators
  - *Kenneth J. Roche*, Staff PNNL and Affiliate Associate Professor, U. Washington
  - *Piotr Magierski*, Professor, Warsaw U. of Technology and Affiliate Professor U. Washington
  - *Yongle Yu*, (PhD 2003, UW, winner Henderson prize (2004), professor, Chinese Academy of Sciences, Wuhan
  - *Carlos Bertulani*, Professor, Texas A&M, Commerce (his large number of students and postdocs not included here)
- Main publications since 2007 (UNEDF SciDAC and other DOE support):
  1 Science, 17 Phys. Rev. Lett., 16 Rapid Communications, several invited reviews, many invited talks

Evolution of the QMC codes since 2007:

- QMC for canonical unitary Femi gas (started in 2005)
- Implemented extraction of EoS, shear viscosity, spin susceptibility, spin drag, and other transport coefficients
- Started with Fortran serial codes, subsequently converted to C w/ MPI
- Now implementing CPU and GPU version in C w/ MPI and CUDA, preliminary results point to incredible speedups
- Extended to neutron matter (microcanonical), currently implementing finite nuclei (even-even N=Z)

Most of these results were obtained with no SciDAC support!

Evolution of the DFT codes for the superfluid fermion systems since 2007

- Developed and implemented new numerical algorithms
- AB started with Y. Yu with a Fortran serial code in 2006 for the time-dependent problem in 3D
- In 2007 KJ Roche parallelized w/ MPI during UNEDF- SciDAC for leadership systems
- Developed MPI codes in Fortran 90 for both static and time-dependent problems
- In 2010 KJ Roche and YL Luo converted codes to C w/ MPI
- Since 2013, Roche, Wlazłowski, and Stetcu extended codes to C w/ MPI and CUDA, for use on hybrid architectures

Without the use of GPUs Titan (27 PFlops) is downgraded to Jaguar (2.6 Pflops)!

- Time-dependent codes exists in several incarnations: split operator (accuracy $O(h^3)$) and Adams-Bashforth-Milne (accuracy $O(h^5)$) time-solvers with 2-components (no spin-orbit) and 4-components quasiparticle wave functions for unitary Fermi gases and nuclear systems
- Our codes fully exploit all aspects of advanced computing from advanced algorithms and math to the use of the most current programming trends
- We employ specialized, scalable high performance I/O for our advanced checkpoint/restarts (libLUT over Lustre) and reached over 10GB/sec, Lustre - sizes vary from 8TB to > 60TB

With no SciDAC support!

- We reduce large time-dependent density-based data to a couple of MBs through advanced visualization analysis techniques (primarily VisIt), results often presented as movies
- Complete transition to hybrid CPU-GPU (most computing punch from GPUs, 24 of 27 Pflops)

With no SciDAC support!

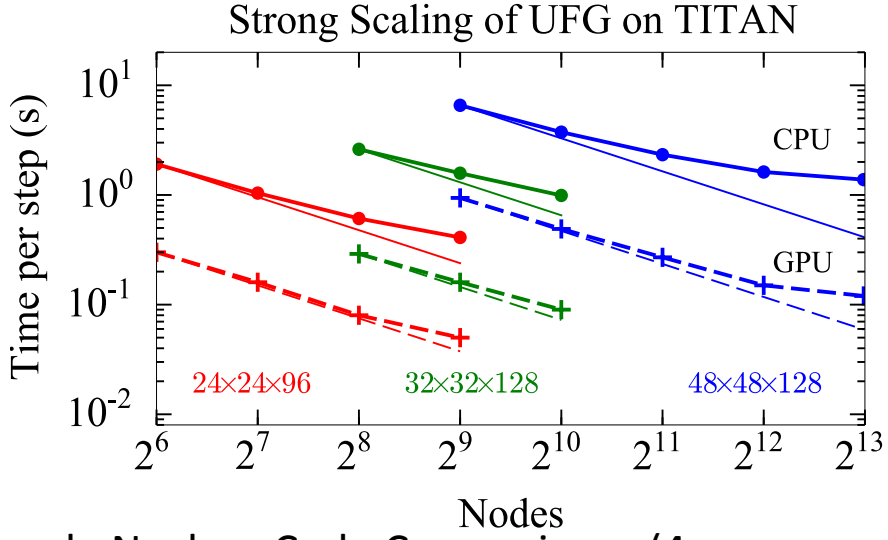
- For the largest problems we obtained speedups of over 25x with the hybrid CPU-GPU codes over the CPU code
- Essentially perfect strong scaling trends on GPUs (coarse-grained scaling model assigns disjoint sets of wave functions to distinct computing elements) to full machine scale

With no SciDAC support!

- Excellent weak scaling (though we care more about strong scaling) to full machine scale

With no SciDAC support!

- Over 140M core hours on Titan, Jaguar, Franklin, Hopper, Edison



FUTURE NEEDS:

- Until now: 30-40M cores hours/year
- Next 5 years: 120-150M core hours/year
- Most time consuming project: TDDFT
- People support needs:
  - 2-3 grad students
  - 1-2 postdocs
  - 2 international collaborators
  - 2-3 senior people

Sample Nuclear Code Comparisons (4-component qwfs)

$N_xN_yN_z$	N_{wf}	memory	CPU comp. + comm.	CPU comp.	GPU comp. + comm.	GPU comp.	# of GPUs	speedup
48^3	110592	10 TB	3.9s	2.4s	0.39s	0.023s	6912	10
64^3	262144	56 TB	20s	9.1s	0.80s	0.48s	16384	25

Over 1 million time-dependent 3D nonlinear complex coupled PDEs

These results were obtained without any SciDAC support!

$N_x \times N_y \times N_z$	N_{wf}	memory	GPUs	time/step	walltime	cost (core hours)
$40 \times 40 \times 60$	100148	0.28 TB	256	0.92s	202h	1.5 million
			512	0.49s	107h	1.6 million
			1024	0.28s	62h	1.9 million
$64 \times 64 \times 64$	274124	2.1 TB	1024	1.06s	235h	7.2 million
			2048	0.68s	151h	9.2 million
			4096	0.42s	92h	11 million

Computational cost of a 10^{-19} sec long trajectory (2-component code), about 750,00 time steps