PHYS 760: Extreme-Scale Quantum Simulations (Selected Topics in Computational Physics)
Units: 3
Fall 2024

Time: M W, 12:00-1:20 pm
Location: DMC 202
URL: https://aiichironakano.github.io/phys760.html

Instructor: Aiichiro Nakano
Office: VHE 610
Office Hours: F, 12:00-1:20 pm
Contact Info: anakano@usc.edu, timeline for replying to emails: within 24 hours

Teaching Assistant: TBD
Office:
Office Hours:
Contact Info:

IT Help: Center for Advanced Research Computing (CARC)
Hours of Service: T, 2:30-5:00 pm
Contact Info: https://www.carc.usc.edu/education-and-resources/office-hours

Course Description

Computer simulation of quantum-mechanical dynamics has become an essential enabling technology for physical, chemical and biological sciences and engineering. Quantum-dynamics simulations on extreme-scale parallel supercomputers would provide unprecedented predictive power, but pose enormous challenges as well. This course surveys and projects algorithmic and computing technologies that will make quantum-dynamics simulations metascalable, *i.e.*, "design once, continue to scale on future computer architectures".

The course first covers how the exponential time complexity for solving the quantum *N*-body problem is reduced to (1) $O(N^3)$ within the density functional theory (DFT), for which Walter Kohn received a Nobel chemistry prize in 1998, and (2) $O(N)$ based on physical data-locality principles (*e.g.*, Kohn's quantum nearsightedness principle). The course then introduces key abstractions (*e.g.*, pseudopotentials and exchange-correlation functionals) and representation issues (*e.g.*, planewave basis *vs*. real-space multigrids), which are necessary for efficient implementation of quantum molecular dynamics (QMD) simulations. This is followed by the design of QMD simulation algorithms on massively parallel supercomputers using message passing and multithreading, including our metascalable divide-conquer-recombine (DCR) algorithmic framework, as well as performance optimization on modern many-core processors and accelerators through memory hierarchies and vectorization. Advanced topics to be covered include (1) DCR approaches to excitation dynamics, (2) intersection of machine learning and quantum *N*-body problem, and (3) merger of quantum Monte Carlo (QMC) and QMD methods. The course ends with best software practices for co-developing extreme-scale QMD software for million-way parallelism.

Learning Objectives

Students will learn fundamental knowledge and gain hands-on experience in order to:

1. Reduce the intractable quantum many-body problem to lower-complexity problems, while retaining the essential physics.
2. Design scalable parallel algorithms for linear-scaling quantum-dynamics simulations.
3. Develop metascalable quantum-dynamics software on current and future computer architectures.

Prerequisite(s): (1) CSCI596 or basic experience in parallel computing; and (2) PHYS 516 or basic knowledge of numerical methods in computational sciences.

Co-Requisite(s): None

Concurrent Enrollment: None

Recommended Preparation: Review basic parallel computing and numerical methods.

Course Notes

Grading type: letter grade. All course materials will be provided online on the course Web page.

Technological Proficiency and Hardware/Software Required

Every student will be provided a computing account at the USC Center for Advanced Research Computing (CARC). In addition, students will be given access to the instructor's research-level parallel QMD simulation software for hands-on exercises and assignments.

Required Readings and Supplementary Materials

Required readings will be posted on the course Web page.

Description and Assessment of Assignments

The learning outcome will be assessed through programming assignments and a final project. The programming assignments will provide students with solid understanding and hands-on experience on the basics of QMD simulations, parallelization of QMD codes, and performance tuning of QMD codes on modern computer architectures. In the final project, each student will apply what he/she has learned from the course to a challenging scientific or engineering problem. In addition, every student will present one of the reading materials (which are listed in the course schedule) and leads its discussion in the class.

Grading Breakdown

Assignment	% of grade
Programming #1: basic QMD	20
Programming #2: pseudopotential	20
Programming #3: Nonadiabatic (NA) QMD	20
Programming #4: Parallel NAQMD	20
Paper presentation	10
Final project	10
Total	100

Grading Scale (Example)

Course final grades will be determined using the following scale.

A	95-100
A-	90-94
B+	87-89
B	83-86
B-	80-82
C+	77-79
C	73-76
C-	70-72
D+	67-69
D	63-66
D-	60-62
F	59 and below

Assignment Submission Policy

Each of the programming assignments is to be submitted in two weeks, as specified in the course schedule.

Grading Timeline

Each assignment is graded and returned with feedback in one week.

Academic Integrity

The University of Southern California is foremost a learning community committed to fostering successful scholars and researchers dedicated to the pursuit of knowledge and the transmission of ideas. Academic misconduct is in contrast to the university's mission to educate students through a broad array of first-rank academic, professional, and extracurricular programs and includes any act of dishonesty in the submission of academic work (either in draft or final form).

This course will follow the expectations for academic integrity as stated in the USC Student Handbook. All students are expected to submit assignments that are original work and prepared specifically for the course/section in this academic term. You may not submit work written by others or "recycle" work prepared for other courses without obtaining written permission from the instructor(s). Students suspected of engaging in academic misconduct will be reported to the Office of Academic Integrity.

Other violations of academic misconduct include, but are not limited to, cheating, plagiarism, fabrication (e.g., falsifying data), knowingly assisting others in acts of academic dishonesty, and any act that gains or is intended to gain an unfair academic advantage.

The impact of academic dishonesty is far-reaching and is considered a serious offense against the university and could result in outcomes such as failure on the assignment, failure in the course, suspension, or even expulsion from the university.

For more information about academic integrity see the student handbook or the Office of Academic Integrity's website, and university policies on Research and Scholarship Misconduct.

Course Schedule: A Weekly Breakdown

Week	Topics/Daily Activities	Readings and Homework	Deliverable/Due Dates
1	**Introduction:** Quantum molecular dynamics (QMD)	"Quantum molecular dynamics in the post-petaflop/s era," Romero *et al*., *IEEE Computer* **48(11)**, 33 ('15); "Iterative minimization techniques for *ab initio* total-energy calculations," Payne *et al.*, *Rev. Mod. Phys*. **64**, 1045 ('92)	Every student will present a reading material of his/her choice according to its scheduled week (see the center column of this table)
2	**Complexity reduction**: Density functional theory (DFT)	"Inhomogeneous electron gas," Hohenberg & Kohn, *Phys. Rev*. **136**, B864 ('64); "Self-consistent equations including exchange and correlation effects," Kohn & Sham, *Phys. Rev*. **140**, A1133 ('65)	
3	**Abstraction**: Pseudopotentials and exchange-correlation functional	"Efficient pseudopotentials for plane-wave calculations," Troullier & Martins, *Phys. Rev. B* **43**, 1993 ('91); "Projector augmented-wave method," Blochl, *Phys. Rev. B* **50**, 17953 ('94); "Generalized gradient approximation made simple," Perdew *et al.*, *Phys. Rev. Lett*. **77**, 3865 ('96) Assignment 1: basic QMD	
4	**Representation**: Plane-wave basis *vs*. real-space multigrids	"Momentum-space formalism for the total energy of solids," Ihm *et al.*, *J. Phys. C* **12**, 4409 ('79); "Real-space multigrid-based approach to large-scale electronic structure calculations," Briggs *et al*., *Phys. Rev. B* **54**, 14362 ('96)	
5	**Linear scaling**: Physical data-locality principles	"Direct calculation of electron-density in density-functional theory," Yang, *Phys. Rev. Lett*. **66**, 1438 ('91); "Linear scaling electronic structure methods," Goedecker, *Rev. Mod. Phys*. **71**, 1085 ('99); "*O*(*N*) methods in electronic structure calculations," Bowler & Miyazaki, *Rep. Prog. Phys*. **75**, 036503 ('12)	Assignment 1 due
6	**Parallelization:** Message passing and multithreading	"A divide-conquer-recombine algorithmic paradigm for multiscale materials modeling," Shimojo *et al.*, *J. Chem. Phys*. **140**, 18A529 ('14); "Exascale computing and big data," Reed & Dongarra, *Commun. ACM* **58(7)**, 56 ('15) Assignment 2: Parallel QMD	
7	**Excitation:** Time-dependent density functional theory (TDDFT)	"Density-functional theory for time-dependent systems," Runge & Gross, *Phys. Rev. Lett*. **52**, 997 ('84); "Time-dependent density functional response theory for	

		molecules," Casida, in *Recent Advances in Density Functional Methods*, (World Scientific, '95), 155; "A long-range-corrected time-dependent density functional theory," Tawada *et al.*, *J. Chem. Phys*. **120**, 8425 ('04)	
8	**Excitation dynamics:** Nonadiabatic quantum molecular dynamics (NAQMD)	"Molecular dynamics with electronic transitions," Tully, *J. Chem. Phys*. **93**, 1061 ('90); "Time-domain *ab initio* study of charge relaxation and recombination," Duncan *et al*., *J. Am. Chem. Soc*. **129**, 8528 ('07)	Assignment 2 due
9	**New computer architectures:** Many cores and accelerators	"Knights Landing: second-generation Intel Xeon Phi product," Sodani *et al*., *IEEE Micro* **36(2)**, 34 ('16)	
10	**Performance optimization:** Memory hierarchy and vectorization	"Metascalable quantum molecular dynamics simulations of hydrogen-on-demand," Nomura *et al.*, *Proc. Supercomputing, SC14*, 661 (IEEE/ACM, '14) Assignment 3: performance	
11	**Metascalable algorithms:** Divide-conquer-recombine	"A divide-conquer-recombine algorithmic paradigm for multiscale materials modeling," Shimojo *et al.*, *J. Chem. Phys*. **140**, 18A529 ('14); "Maxwell + TDDFT multiscale simulation for laser-matter interactions," Sato & Yabana, *J. Adv. Simulat. Sci. Eng*. **1**, 98 ('14); "Dielectric genome of van der Waals heterostructures," K. Andersen *et al*., *Nano. Lett*. **15**, 4616 ('15); "Efficient method for calculating spatially extended electronic states of large systems with a divide-and-conquer approach," Yamada *et al.*, *Phys. Rev. B* **95**, 045106 ('17)	Assignment 3 due
12	**Quantum learning:** Machine learning for quantum *N*-body problems	"A practical introduction to tensor networks," R. Orus, *Ann. Phys*. **349**, 117 ('14); "Constructing high-dimensional neural network potentials," Behler, *Int. J. Quant. Chem.* **115**, 1032 ('15); "Solving the quantum many-body problem with artificial neural networks," Carlo & Troyer, *Science* **355**, 602 ('17)	
13	**Advanced topics:** Quantum Monte Carlo-based molecular dynamics by Mori-Zwanzig projection	"*Ab initio* molecular dynamics with noisy forces: Validating the quantum Monte Carlo approach with benchmark calculations of molecular vibrational properties,"	

		Luo *et al.*, *J. Chem. Phys.* **141**, 194112 ('14)	
14	**Best software practice:** Collaborative software development	*Effective Computation in Physics*, Scopatz & Huff (O'Reilly, '15), parts III & IV	Assignment 4 due
15	**Project presentations**	Students' presentations on their final projects	
Final			Final-project report due: For the date and time of the final for this class, consult the USC *Schedule of Classes* at www.usc.edu/soc.

Statement on Academic Conduct and Support Systems

Academic Integrity

The University of Southern California is a learning community committed to developing successful scholars and researchers dedicated to the pursuit of knowledge and the dissemination of ideas. Academic misconduct, which includes any act of dishonesty in the production or submission of academic work, compromises the integrity of the person who commits the act and can impugn the perceived integrity of the entire university community. It stands in opposition to the university's mission to research, educate, and contribute productively to our community and the world.

All students are expected to submit assignments that represent their own original work, and that have been prepared specifically for the course or section for which they have been submitted. You may not submit work written by others or "recycle" work prepared for other courses without obtaining written permission from the instructor(s).

Other violations of academic integrity include, but are not limited to, cheating, plagiarism, fabrication (e.g., falsifying data), collusion, knowingly assisting others in acts of academic dishonesty, and any act that gains or is intended to gain an unfair academic advantage.

The impact of academic dishonesty is far-reaching and is considered a serious offense against the university. All incidences of academic misconduct will be reported to the Office of Academic Integrity and could result in outcomes such as failure on the assignment, failure in the course, suspension, or even expulsion from the university.

For more information about academic integrity see the student handbook or the Office of Academic Integrity's website, and university policies on Research and Scholarship Misconduct.

Please ask your instructor if you are unsure what constitutes unauthorized assistance on an exam or assignment, or what information requires citation and/or attribution.

Students and Disability Accommodations:

USC welcomes students with disabilities into all of the University's educational programs. The Office of Student Accessibility Services (OSAS) is responsible for the determination of appropriate accommodations for students who encounter disability-related barriers. Once a student has completed the OSAS process (registration, initial appointment, and submitted documentation) and accommodations are determined to be reasonable and appropriate, a Letter of Accommodation (LOA) will be available to generate for each course. The LOA must be given to each course instructor by the student and followed up with a discussion. This should be done as early in the semester as possible as accommodations are not retroactive. More information can be found at osas.usc.edu. You may contact OSAS at (213) 740-0776 or via email at osasfrontdesk@usc.edu.

Support Systems

Counseling and Mental Health - (213) 740-9355 – 24/7 on call

Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

988 Suicide and Crisis Lifeline - 988 for both calls and text messages – 24/7 on call

The 988 Suicide and Crisis Lifeline (formerly known as the National Suicide Prevention Lifeline) provides free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week, across the United States. The Lifeline is comprised of a national network of over 200 local crisis centers, combining custom local care and resources with national standards and best practices. The new, shorter phone number makes it easier for people to remember and access mental health crisis services (though the previous 1 (800) 273-8255 number will continue to function indefinitely) and represents a continued commitment to those in crisis.

Relationship and Sexual Violence Prevention Services (RSVP) - (213) 740-9355(WELL) – 24/7 on call

Free and confidential therapy services, workshops, and training for situations related to gender- and power-based harm (including sexual assault, intimate partner violence, and stalking).

Office for Equity, Equal Opportunity, and Title IX (EEO-TIX) - (213) 740-5086

Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants.

Reporting Incidents of Bias or Harassment - (213) 740-5086 or (213) 821-8298

Avenue to report incidents of bias, hate crimes, and microaggressions to the Office for Equity, Equal Opportunity, and Title for appropriate investigation, supportive measures, and response.

The Office of Student Accessibility Services (OSAS) - (213) 740-0776

OSAS ensures equal access for students with disabilities through providing academic accommodations and auxiliary aids in accordance with federal laws and university policy.

USC Campus Support and Intervention - (213) 740-0411

Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity, Equity and Inclusion - (213) 740-2101

Information on events, programs and training, the Provost's Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

USC Emergency - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call

Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

USC Department of Public Safety - UPC: (213) 740-6000, HSC: (323) 442-1200 – 24/7 on call

Non-emergency assistance or information.

Office of the Ombuds - (213) 821-9556 (UPC) / (323-442-0382 (HSC)

A safe and confidential place to share your USC-related issues with a University Ombuds who will work with you to explore options or paths to manage your concern.

Occupational Therapy Faculty Practice - (323) 442-2850 or otfp@med.usc.edu

Confidential Lifestyle Redesign services for USC students to support health promoting habits and routines that enhance quality of life and academic performance.