USC Viterbi
School of Engineering
Department of Computer Science

CSCI 699: Extreme-Scale Quantum Simulations

Units: 4
Spring 2018

Time: M W, 5:00-6:50 pm
Location: GFS 223
URL: http://cacs.usc.edu/education/cs699.html

Instructor: Aiichiro Nakano
Office: VHE 610
Office Hours: F, 5:00-5:50 pm
Contact Info: anakano@usc.edu

IT Help: Erin Shaw
Location: LVL 3M
Hours of Service: T, 2:30-5:00 pm
Contact Info: erinshaw@usc.edu

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 High Performance Computing (HPC). 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: parallel QMD	20
Programming #3: performance tuning	20
Paper presentation	20
Final project	20
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.

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)	
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)	Assignment 3 due
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	
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 Conduct

Plagiarism — presenting someone else's ideas as your own, either verbatim or recast in your own words — is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in *SCampus* in Part B, Section 11, "Behavior Violating University Standards" https://policy.usc.edu/student/scampus/part-b. Other forms of academic dishonesty are equally unacceptable. See additional information in *SCampus* and university policies on scientific misconduct, http://policy.usc.edu/scientific-misconduct.

Discrimination, sexual assault, intimate partner violence, stalking, and harassment are prohibited by the university. You are encouraged to report all incidents to the *Office of Equity and Diversity*/*Title IX Office* http://equity.usc.edu and/or to the *Department of Public Safety* http://dps.usc.edu. This is important for the health and safety of the whole USC community. Faculty and staff must report any information regarding an incident to the Title IX Coordinator who will provide outreach and information to the affected party. The sexual assault resource center webpage http://sarc.usc.edu fully describes reporting options. Relationship and Sexual Violence Services https://engemannshc.usc.edu/rsvp provides 24/7 confidential support.

Support Systems

A number of USC's schools provide support for students who need help with scholarly writing. Check with your advisor or program staff to find out more. Students whose primary language is not English should check with the *American Language Institute* http://ali.usc.edu, which sponsors courses and workshops specifically for international graduate students. *The Office of Disability Services and Programs* http://dsp.usc.edu provides certification for students with disabilities and helps arrange the relevant accommodations. If an officially declared emergency makes travel to campus infeasible, *USC Emergency Information* http://emergency.usc.edu will provide safety and other updates, including ways in which instruction will be continued by means of Blackboard, teleconferencing, and other technology.