VIP Project Team: Big Data and Quantum Mechanics

Course Syllabus - Spring 2027

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Office Hours: By Appointment (via email or Slack)

Class Hours: W 2:00-2:50 pm ET

Course Information

Semester: Spring 2027

Academic Year: 2026-2027

This syllabus covers all sections of the VIP Project Team: Big Data and Quantum Mechanics for Spring 2027, listed below.

Course Name	Course Number	Section	CRN
VIP Proj Team: SO I	2601	VVI	25500
VIP Proj Team: JR I	3601	VVI	25501
VIP Proj Team: JR II	3602	VVI	25503
VIP Proj Team: SR I	4601	VVI	25502
VIP Project Team: SR II	4602	VVI	26102
VIP Project Team: SR III	4603	VVI	33950
VIP Proj Team: GR I	6601	VVI	26950
VIP Proj Team: GR II	6602	VVI	26951
VIP Proj Team: GR III	6603	OVI	27408
VIP Proj Team: GR III	6603	VVI	26952

Course Description

About VIP

The Vertically-Integrated Projects (VIP) Program operates in a research and development context. Undergraduate students that join VIP teams earn academic credit for their participation in design/discovery efforts that assist faculty and graduate students with research and development issues in their areas of expertise.

The teams are:

- Multidisciplinary - drawing students from all disciplines on campus;
- Vertically-integrated - maintaining a mix of sophomores through PhD students each semester;
- Long-term - each undergraduate student may participate in a project for up to three years and each graduate student may participate for the duration of their graduate career.

The continuity, technical depth, and disciplinary breadth of these teams are intended to: provide the time and context necessary for students to learn and practice many different professional skills, make substantial technical contributions to the project, and experience many different roles on a large, multidisciplinary design/discovery team. Support long-term interaction between the graduate and undergraduate students on the team. The graduate students mentor the undergraduates as they work on the design/discovery projects embedded in the graduate students' research. Enable the completion of large-scale design/discovery projects that are of significant benefit to faculty members' research programs.

About Big Data and Quantum Mechanics

This course explores projects at the intersection of computational chemistry (quantum mechanics) and data science (big data) within the application domain of surface science and catalysis. The team merges expertise from computational and physical sciences, and students from computer science, electrical engineering, industrial & systems engineering, chemical engineering, chemistry, physics, and materials science. The VIP course consists of sub-teams with research topics developed by graduate students in the Medford group.

Course Objectives / Learning Outcomes

- Generate atomistic simulation and adsorption energy data using density functional theory (DFT)

- Converge numerical calculations with respect to input parameters
- Submit, manage, and analyze high-performance computing jobs
- Utilize machine-learning packages to model and predict the output of atomistic simulations
- Work with a team to solve real-world problems at the intersection of big data and quantum mechanical simulations

Required Course Materials

Training Materials: VIP Training Materials Jupyter Book

No additional textbooks are required. All course materials are provided through the online Jupyter Book and Canvas.

Grading Policy and Weighting

The grade will be assigned based on three categories:

- Documentation: 33.3%
- Personal Accomplishments: 33.4%
- Teamwork and Interactions: 33.3%

A grade of 0-5 will be assigned for each category. A total grade will be computed based on the weighted average of the 3 categories which will be converted to letter grades using the following scale:

- A: > 4
- B: > 3
- C: < 3
- D: < 2

You will receive a grade at the midterm and after the end of the course. Only the final grade will be used to determine your letter grade. The midterm grade is advisory only.

Documentation (33.3%)

The documentation grade will be assessed based on bi-weekly updates submitted via Canvas. Bi-weekly updates will be peer graded on a scale of 0-5. Bi-weekly updates should be compiled into a single document and submitted at the midterm and final. Instructors will review the average score from bi-weekly updates and compare this to the compiled updates to ensure that peer grading is appropriate. Instructors reserve the right to revise the average score up or down if substantial inconsistencies are observed.

Personal Accomplishments (33.4%)

Personal accomplishments will be measured by self-defined goals and assessed by each student's respective sub-team mentor. Each goal should have a deliverable that can be unambiguously evaluated as complete or incomplete. The letter grade will be determined by the sub-team leader based on: (i) ability to plan research and set realistic targets and (ii) ability to achieve goals and deliver on a plan.

Teamwork and Interactions (33.3%)

Teamwork and interaction will be graded based on peer evaluations conducted through the VIP website and participation in peer grading. The grade consists of 3 components:

- 3 points: Reviews from teammates via peer evaluations.
- 1 point: Response rate for peer grading and evaluations.
- 1 point: Regular interactions with classmates and instructors.

Attendance Policy

The course is offered in a primarily virtual format. The main lecture takes place virtually each week. Sub-teams may meet in person and/or use hybrid meetings. Regular attendance and participation in the weekly lecture meeting is expected and will be considered as part of the Teamwork and Interactions grade component. Missing approximately half or more of the lecture meetings without participation on Slack will negatively impact the teamwork grade.

Additional Criteria for Successful Completion

In addition to the grading criteria above, students must:

- Complete all peer evaluations through the VIP website (conducted twice per semester).
- Participate in bi-weekly peer grading of documentation submissions.
- Submit midterm and final achievements documents and presentations by the posted deadlines.
- Maintain regular communication with sub-team mentors and the instructional team via Slack or email.

Academic Integrity

Georgia Tech aims to cultivate a community based on trust, academic integrity, and honor. Students are expected to act according to the highest ethical standards. For

information on Georgia Tech's Academic Honor Code, please visit the Office of the Dean of Students website at the link below.

Georgia Tech Honor Code (Office of Student Integrity)

Any student suspected of cheating or plagiarizing on an assignment, exam, or project will be reported to the Office of Student Integrity, who will investigate the incident and determine appropriate sanctions.

Student-Faculty Expectations Agreement

At Georgia Tech we believe that it is important to strive for an atmosphere of mutual respect, acknowledgment, and responsibility between faculty members and the student body. See the link below for an articulation of some basic expectations that you can have of this course and that we will have of you. In the broadest sense, we will all strive to do our best and treat one another with respect.

Student-Faculty Expectations Agreement (Georgia Tech Catalog)

Accommodations for Students with Disabilities

If you are a student with learning needs that require special accommodation, contact the Office of Disability Services at (404) 894-2563 or visit the website listed below to make an appointment to discuss your special needs and to obtain an accommodations letter. Please also email the instructor as soon as possible in order to set up a time to discuss your learning needs.

Georgia Tech Office of Disability Services

Core IMPACTS Statement

This course is not part of the Core IMPACTS curriculum. Therefore, Core IMPACTS learning outcomes do not apply.

Changes to Syllabus

The schedule and syllabus are subject to change. Given that this is a research course, changes are to be expected; however, we will do our best to notify you of any changes and implement them as fairly as possible.