This document provides a summary of the agreed-upon protocols by which the courses associated with the pan-Canadian Computation Chemistry program will be operationalized for September 2024 delivery. Also provided are general updates on the status of modules and other elements of the PC₃ program.

1- Guidelines for PC₃ participants

1. Participating faculty members (i.e. those that have students from their institutions in the courses) will serve as the local instructor-on-record for all PC₃ courses.
2. Local instructors-on-record have the following responsibilities:
   a. Register PC₃ courses at their university. This may be done at some institutions using existing graduate course codes.
   b. Ensure that PC₃ courses are scheduled at their institutions according to the delivery schedule agreed upon by the PC₃ working group.
   c. Provide the names and email addresses of those graduate students from their institution that are participating in PC₃ courses to the appropriate PC₃ instructors (see course outlines) and to [Alireza Sadeghifar](#) (PC₃ coordinator).
   d. Facilitate student access to DRAC/Cedar computing resources.
   e. Engage in mark reviews in the event that students from their institution make a grade appeal.
3. PC₃ course instructors have the following responsibilities:
   a. For PC₃ courses involving multiple instructors, it is recommended that one instructor be identified as the course lead and take responsibility for assembling and submitting final course marks. Note that for courses with six-week modules, some institutions may require marks for two such courses.
   b. Develop course syllabi, lectures, and assignments for portions of their course/module. All material related to the PC₃ modules will be shared with local instructors-on-record and with the PC₃ community.
   c. Deliver courses over Zoom at the scheduled time to all students registered in their course.
   d. Answer student questions on lecture and assignment material outside of class hours.
   e. Mark all assigned work. Marked assignments and tests should be returned to students ideally within one week of the due date.
   f. Provide final marks for the course module at least five working days before the end of the semester during which the course is offered.

2- Computing resources and software for course work

Students must have access to the Cedar or Graham clusters (Digital Resource Alliance of Canada (DRAC): https://docs.alliancecan.ca/wiki/Cedar and https://docs.alliancecan.ca/wiki/Graham). We are asking the local instructor-on-record to have students from their institution use their own DRAC allocation (preferably priority queues (i.e. "rrg") allocations so as to minimize queue wait times for students) for the assignments associated with PC₃ courses. The assignments are relatively

low-demand, and instructors-on-record should not see a significant drain on their allocations.[1] ***Course instructors are asked to reinforce to students that the PC₃ queue is to be used only for PC₃ course-related activities.***

Course instructors should provide information in their course syllabi on how to obtain access to DRAC/Cedar and ensure that the software required for the assignments related to their course are either available on Cedar or can be installed by students on their local computers. Students should be provided with instructions if they are required to install software.

Visit DRAC User Roles to Access Resources for information about access to resources based on role (Faculty, grad students, etc.). To apply for an account, see here. Also, see the DRAC Account Management Policies and DRAC (/Compute Canada) Account Renewals FAQ. For the available resources (including Cedar), technical documentation, and also how to request resources in the online application form visit the followings: for available software see here, for technical support see here, and for consultation and other inquiries see here.

3- Course times and duration

1. The PC₃ group agreed that courses will be delivered by Zoom as two 1.5-hour classes per week. The following schedules have been established:

    Introductory Module – 3 credits (at UBC)
    Mode of delivery: Synchronous Zoom
    Instructors: Richard Bowles, Joshua Hollett, and Robert Szilagyi
    First class: September 4, 2024
    Last class: December 4, 2024
    Schedule: Monday/Wednesday 11:00 AM – 12:30 PM Pacific Time
    Final mark submission to institution leads: Friday, December 13, 2024.
    No classes on Truth and Reconciliation Day, Thanksgiving Day, and Remembrance Day

    Advanced Module I – 1.5 credits (at UBC)
    Mode of delivery: Synchronous Zoom
    Instructors: Erin Johnson, Georg Schreckenbach, and Tom Woo
    First class: January 6, 2025
    End of class: February 13, 2025
    Schedule: Monday/Thursday 12:00 PM - 1:30 PM Pacific Time
    Final mark submission to institution leads: Feb 24, 2025.

    Advanced Module II – 1.5 credits (at UBC)

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[1] Last year, the program used a special queue allocation to Gino's contributed system in Cedar. That contributed system has been taken down and there is no replacement as yet. As a stop gap measure, we are proposing the approach indicated above. We continue to work with DRAC on a more robust solution.

Mode of delivery: Synchronous Zoom
Instructors: Alberto Otero de la Roza, Gino DiLabio
First class: January 24, 2025
End of class: April 3, 2025
Schedule: Monday/Thursday 12:00 PM - 1:30 PM Pacific
Final mark submission to institution leads: April 10, 2025.

2. Course instructors may wish to provide student support through the following mechanisms:
   a. PC₃ course Discord Channel. Discord access can be provided to students by the PC₃ administrators (i.e., Alireza[2]/Gino[3]). This is the preferred approach since it helps to build a community of practice amongst participating students. New channels will be created for students participating in PC₃ courses in 2024-2025.
   b. E-mail.
   c. Extra (Zoom) sessions are not recommended but students may be encouraged to self-organize discussion sessions.

4- Course/Module Offerings in 2024-2025

The Intro module[4] will be offered during the September to December 2024 semester and is the UBC equivalent of a 3-credit course. Advanced Module I (AMI),[5] and Advanced Module II (AMII)[6,7] are each half semester courses that will be offered during the January to April 2025 semester.

The modules will be co-taught; it is envisioned that the modules instruction for PC₃ will result in an overall lower teaching load on participants as compared to graduate teaching they may be currently doing in their own institutions.

Whether or not a PC₃ participant is teaching a PC₃ course this September, you are encouraged to participate as a local instructor-on-record (see above). Please also let students in your graduate program know about PC₃ courses.

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[2] alireza.sadeghifar@ubc.ca
[3] Gino.DiLabio@ubc.ca
[4] The Intro Module covers the introductory topics in computational chemistry. Additional information is provided in the course outlines.
[5] AMI covers the fundamentals of density functional theory, planewave modeling, and relativistic effects in chemistry.
[6] AMII provides an overview of thermodynamics and kinetics in chemical applications.
[7] Note that AMI and AMII modules are six-week modules that are offered in one semester, with the first half of the semester covering the topics in AMI and second half covering the topics of AMII.