

Addendum to
Response of the Canadian Association of Theoretical Chemists (CATC)
to Compute Canada's Call - SPARC2

The Canadian Association of Theoretical Chemists (CATC) had submitted a response to Compute Canada's original call for whitepapers for Sustainable Planning for Advanced Research Computing (SPARC) – see attached. The CATC believes that the statements provided in this whitepaper submission, regarding the nature of our science and its resource implications, have essentially not changed and can still be assumed to be current and valid.

However, in consulting its membership there were significant concerns raised regarding limited resources being dramatically out paced by growing demand and the resultant impacts, both current and projected, to the community. From data collected through the original SPARC exercise, the theoretical and computational chemistry community projected the largest increase in compute demand (i.e. 12x through to 2020); this community has also represented the largest users of compute resources within Compute Canada. It is then not surprising that this community is already experiencing some dramatic repercussions. Theoretical and computational chemistry has been extremely strong in Canada and has, at least to this point in time, been an international leader. If current trends are not reversed, it will become very difficult for this community to maintain this international status.

If one looks internationally, our current Canadian facilities have already fallen well behind the infrastructure available to researchers in other countries (e.g. TITAN at Oak Ridge National Lab (USA) eclipses the total compute power of the whole Compute Canada infrastructure). Since our current aging infrastructure is not competitive, some leading Canadian research groups are seeing other researchers, using their models and/or methods, out pacing them. Hence, it is already difficult to carry out many leading-edging computational studies on present Compute Canada facilities. It will presumably also become increasingly difficult to attract or retain top international researchers and students in the field.

Faced with the dramatically widening gap between needs and available compute resources (without further injection of significant capital into Compute Canada), researchers within the CATC expressed strong views on the negative impacts the limited availability of resources will continue to have on their research programs and HQP training, captured in comments such as:

“This will make it impossible for me to tackle larger problems”

“My group's needs have increased 50% in the last year, but in following the RAC process (where we asked for only what we need) we obtained essentially the same allocation. Hence some excellent science will simply not get done this year (hence few papers, longer completion times for students, less funding)”

unless we will be somehow fortunate enough to pick up time well above our allocation. And then this only gets (multiplicatively) worse next year."

"this is absolutely a big deal for us at the moment for our work on more complex models (again, with the irony that we're behind other researchers that use the methods we have developed, on applications we would like to pursue)"

To help offset their inability to secure adequate resources on the Compute Canada infrastructure, researchers suggested that they might expect to either:

- (1) Apply for grants for equipment specifically for their research groups or projects (indicating "*this is not an ideal solution but it's better than nothing*"); or
- (2) Apply for compute time elsewhere, e.g. US, Japan, Europe (this may work for some but "*is a bit humiliating*").

Ending with a positive comment, researchers acknowledged the great (local) support they receive.