**Editorial**
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# Editorial Note on High Performance Computing

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## Editorial Note

In computational parts of logical examination (Physics, Chemistry, Philosophy) projects and PCs assume a focal part. The projects utilized can be either privately created code or business programming. The last is frequently utilized as a discovery application. Nonetheless, in any event, when utilizing programming as a discovery instrument, it is imperative to have some information on the constraints and eccentricities of the product utilized. These are obtained in 2 ways: firstly by considering the basic speculations and calculations utilized, and besides by experience. One will frequently find that realizing how a code ought to act, and how it really does, can be very various things.

Likewise with most undertakings in science, additionally computational researchers need to follow the lines of what is conceivable, and if conceivable look past. For computational issues, there are two fundamental computational assets that play a role: (1) time and (2) memory. As the issue size develops, so do these assets. The last is principally cured by utilizing machines with more RAM-memory, the previous can be cured through equal use of numerous CPU's. This is the place where supercomputer foundations become an integral factor. Albeit a work area machine can be helpful for testing purposes, or little issues, a computational researcher likewise should be comfortable with fundamental use of equal codes on a supercomputer. As a matter of fact, even cutting edge individual machines have a multi-centre design making parallelism likewise here a significant idea.

## Supercomputers

Most supercomputers run some version of a unix based OS, with all eccentricities included. The degree of this establishment can change altogether, which will have its impact on the client experience. Realizing how to function in the order line-just climate of a supercomputer is, accordingly, an unquestionable requirement for practically any computational researcher.

Notwithstanding the over, a computational researcher ought to likewise have a decent information on how productive the code has been utilizes is parallelized, which means, we should do scaling tests. Having run VASP on a few supercomputers throughout the long term, I aggregated helpful data on the effectiveness of the VASP code:

- CMS bunch group at University Twente
- The Aster, Teras and Huygens supercomputers at SARA
- The Stevin supercomputers at Ugent. On a few of these machines I functioned as pilot-client.
- The Flemish TIER-1 supercomputer situated at Ugent. On this machine I was one of the pilot clients, and I was allowed estimation time for a few tasks throughout the long term.

## Code development

Density Functional Theory (DFT) utilizes the VASP code. This code is well known for its quality and execution. It ought to, notwithstanding, not be utilized simply as a discovery instrument. On the VASP Info page a few connections are given that will guide you to extra data and instructional exercises.

All outcomes acquired with VASP, or some other general stomach muscle initio code, is given as text-information in at least one yield records. There is no formally included programming to envision information like the Density of State (DOS) or band structure results. For these and different purposes you are required to either compose your own projects or contents, or utilize these composed by outsiders. Because of the intricacy of the conceivable yield it's anything but an inconsequential assignment to compose a content or code that works for all potential settings of the stomach muscle initio code. Over the long time, as I was composing such numerous little projects I began adding them as modules and subroutines to a bigger universally handy program: HIVE (Humble Interface for VASP yield Editing).

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