

ORAU Event Sponsorship Program

Report on UNT Hackathon 2018

The event took place in the Denton area from the 13th to the 17th of August 2018. It was composed by two connected events: a four-days long hackathon, followed by a one-day symposium on methods and applications in computational science.

The first four days of the event were organized following the hackathon format: a group of participants with common computational skills and goals joined their efforts in developing and implementing new tools and codes related to quantum chemistry and condensed matter physics.

The final list of the participants to the hackathon part of the event is the following:

- Dr. Oliviero Andreussi (Assistant Professor at UNT, organizer)
- Dr. Marco Buongiorno Nardelli (Full Professor at UNT)
- Dr. Michele Pavanello (Associate Professor at Rutgers Newark)
- Dr. Andrew Baczewski (Permanent Researcher at Sandia National Lab)
- Dr. Davide Ceresoli (Permanent Researcher at CNR Milan, Italy)
- Dr. Francesco Nattino (Postdoc at EPFL, Switzerland)
- Dr. Wenhui Mi (Postdoc at Rutgers Newark)
- Haihang Wang (PhD Student at UNT)
- Frank Cerasoli (PhD Student at UNT)
- Matthew Truscott (PhD Student at UNT)
- Andrew Supka (PhD Student at Central Michigan University)
- Quinn Campbell (PhD Student at Penn State)
- Alina Umerbekova (PhD Student at Rutgers Newark)
- Bojan Ljubovic (ORAU representative)

The above participants, in particular the most experienced ones, have in common a significant development track record in the Quantum ESPRESSO suite of codes for first-principles simulations of condensed matter and materials. The hackathon program, attached to this report, was devised in order to leave most of the time to the participants to code, individually or in small groups. Some specific sessions were devoted to more collective planning and work. In particular, four main projects started during the UNT Hackathon 2018:

1. Quantum RISTRETTO, a refactoring and modularization of a reduced version of Quantum ESPRESSO (Andreussi, Ceresoli, with contributions from most of the participants).
2. Analytical continuum approaches for electrolytes and semiconductors interfaces in the Environ plugin (Andreussi, Nattino, Campbell, Truscott).

3. Ehrenfest dynamics and time-dependent density functional theory through the eQE package (Pavanello, Baczewski, Ceresoli, Mi, Umerbekova)
4. Extending the capabilities of the PAOFLOW post-processing tool and AFLOW-p high-throughput infrastructure (Buongiorno Nardelli, Ceresoli, Wang, Cerasoli, Supka)

Most of the started projects showed significant progresses during the four days of the hackathon, with some projects arriving at a testing stage by the end of the event. The four projects are expected to lead to the release of the corresponding open-source codes in the near future. In addition, several publications are expected to appear related to the developments performed during the event. At this moment, one publication has been submitted for review to the Journal of Chemical Physics ("*Continuum models of the electrochemical diffuse layer in electronic-structure calculations*" F. Nattino, M. Truscott, N. Marzari, and O. Andreussi, submitted the 30th of August 2018).

In addition to these practical outcomes, a significant achievement of the event is represented by the training of the youngest participants, in particular of the PhD students. They represented the largest group of participants, their commitment during the event, their progresses in terms of computational skill and their feedbacks provided a good estimate of the success of the hackathon.

The UNT Hackathon Symposium on methods and applications in computational science was organized in the Department of Physics at UNT, the 17th of August 2018. It included presentations from the participants of the hackathon and from several computational groups from the Dallas – Fort Worth (DFW) area. In addition to UNT, speakers were invited from the University of Texas Arlington (UTA) and from the University of Texas Dallas (UTD). The symposium was interdisciplinary in nature, with participants coming from Physics, Chemistry and Materials Science and Engineering Departments. The list of presenters at the symposium is the following:

- Michael Monticino (Chair of Physics, UNT)
- Oliviero Andreussi (Physics, UNT)
- Srivilliputhur Srinivasan (Materials Science and Engineering, UNT)
- Andrew Baczewski (Sandia National Lab)
- Andres Cisneros (Chemistry, UNT)
- Ilaria Siloi (Physics, UNT)
- Francesco Nattino (Materials Science and Engineering, EPFL, Switzerland)
- Kyeongjae Cho (Materials Science and Engineering, UTD)
- Muhammad Huda (Physics, UTA)
- Qiming Zhang (Physics, UTA)

The program of the symposium is attached to this report. Also attached is the presentation of the main organizer of the event (Dr. Oliviero Andreussi, PI of the ORAU Event Sponsorship

Program), summarizing the progresses obtained during the UNT Hackathon 2018 and its future perspectives.

The final budget of the event included the initial contribution from ORAU (4000\$), the support of the Department of Physics at UNT (1000\$), the support of the College of Science at UNT (1000\$), the support of the Office of Research and Innovation at UNT (1000\$), and part of NSF support to one of the co-organizers (Michele Pavanello, Rutgers Newark, 2400\$).