Computing Work Group

Since many of the groups in CTBP rely heavily the development and application of novel computing tools, we have established a Computing Working Group. This group involves CTBP graduate students, postdocs and faculty, as well as collaborators. The idea is that pooling our collective knowledge can lower technical barriers, which will facilitate more exciting scientific progress. Since many groups are working with openMM, we are beginning with discussions that focus on this particular tool. However, we plan to expand the scope of this working group, as needed.

If you are interested in participating in this working group, please sign up for the listserve HERE

Tech Talks are back for Fall 2023!

If you want to participate, please **SIGN UP**. Tech talks are in a hybrid format and they are open to the broader research community. But, you must sign up. Talks will be Wednesdays from 11-12:30 central time. Below is the schedule for upcoming talks.

Each talk will have files made available for participants. **See our Github repo for all supporting documents**.

- **October 4** Advanced visualization with VMD, Esteban Dodero-Rojas (Rice Univ)
- **October 11** Introduction to using and creating containers for Docker and Singularity, Prof. Paul Whitford (Northeastern U)
- **October 18** Becoming a pro beginner with Git, Dr. Antonio Oliveira (Rice U)
- **October 25** Becoming competent with Git, Dr. Antonio Oliveira (Rice U)
- **November 1** HPC and cluster computing best practices, Dr. Vinicius Contessoto (Rice U)
- **November 8** Thread-based parallelism with OpenMP, Prof. Paul Whitford (Northeastern U)
- **November 15** MPI-based parallelism, Prof. Paul Whitford (Northeastern U)
- **November 29** Parallel computing with Python, Dr. Vinicius Contessoto (Rice U)
- **December 6** Introduction to Structure-based models, SMOG 2 and OpenSMOG, Prof. Ronaldo Oliveira (Rice U)
- **December 13** Advanced techniques with SMOG models, Esteban Dodero-Rojas (Rice U)

Presentations from 2021 Tech Talk Series

April 21, 2021 - Wei Lu - Building a coarse-grained force field with openMM

May 5, 2021 - Carlos Bueno

May 19, 2021 - Vinicius Contessoto and Antonio Junior

June 2, 2021 - Iryna Zaporozhets - Parameterization of coarse-grained protein models based on experimental data

June 16, 2021 - Paul Whitford - Basic HPC Considerations

September 22, 2021 - Paul Whitford - Visualization Tips