

# WBS 2.3.2 MOLSII and XSEDE Software Discussion 2021-09-10 Meeting

## Dates

10 Sep 2021

## Agenda, Discussion, and Action Items

## Agenda & Discussion

### Goal(s)

Explore opportunities to make MOLSII software more discoverable and available on XSEDE resources.

### Related Information

#### Background material from e-mail

C) Items that we should schedule a meeting to discuss further and explore opportunities

we discussed your suggestion below about your Research Software Portal, but weren't quite sure if you meant the software that MolSSI develops or our community code database at <https://molssi.org/software-search/>. Can you clarify which you meant? As you will see below, we think that getting our software developments (<https://molssi.org/software-projects/>) working well on XSEDE resources and available to the larger community is something that we are quite interested in.

The Research Software Portal may offer useful features both to the software that MolSSI developers and to your community code database. This portal primarily enables research software and digital services discovery, whether that software/services is on XSEDE or not. It aggregates metadata from multiple sources. For example, we could ingest the metadata in the <https://molssi.org/software-search/> catalog making that software discoverable through XSEDE. XSEDE users who discover that software would then be directed to MolSSI's website and catalog to learn more and to use the software.

- We have multiple software projects where connections with XSEDE would be valuable. Among the possibilities here are our: (1) MolSSI Driver Interface, which couples codes together to run simulations like QM/MM and large scale Monte Carlo - often on HPC resources. There are several possibilities here for connections and improvements to performance. (2) Our Machine Learning repository and Portal to access the data. We have an extensive ML database and are looking to increase this. We believe that access to XSEDE resources could be useful here to enable more computation and perhaps help with hosting of data, broader access to the data through a Portal, potential development/expansion of the Portal to enable the use and development of ML models using the data in the Portal. This would also include our QCArchive software. (3) Enabling seamless submission of jobs in our projects onto XSEDE resources. (There are probably other opportunities here, but these are the main ones we discussed.)

we could collaborate on performance of important software on HPC resources.

- We discussed containerization of software, workflows and modular workflows. We do some containerization in our work and we anticipate doing more of this in the future. We will likely focus more on non-HPC resources to start with since our impression is that containerization for each HPC machine can be different and can be very inconsistent between centers. However, this could be an area where we could learn from XSEDE folks.

To address these I recommend we schedule a meeting involving the ECSS and XCI teams to dig a little deeper into software performance, integration, and related activities. In that meeting we will be able to identify and spin off more targeted efforts involving different combinations of MolSSI staff and XSEDE's ECSS and XCI staff.

## Discussion

### MOLSII team shared various software improvement projects

- ECSS could provide assistance if needed through the community codes effort

### Software deployment opportunities

- Between SPs who install codes needed by their users, and uses installing what they need, there are no major MOLSII gaps
- Startup allocations and Community Software Areas might be useful to the SEAMM effort

## Action Items

- Continue discussion in e-mail and maybe followup in a month

## Attendees

- Robert Harrison ✓
- Theresa Windus ✓
- Paul Saxe ✓
- Jonathan Moussa ✓
- Daniel Crawford ✓
- Robert Sinkovits ✓
- JP Navarro ✓
- Shava Smallen ✗