**Faculty Collaborations/Asya Skyler and Todd Shimoda**

[Astronomy] We have discussed Jorge Moreno’s research and he could run his computation locally (right now he is using a collaborator’s account on a remote cluster at CalTech). <https://www.caltech.edu/content/innovation-speaker-series-talk-7>

[Biology] Dan Martinez is in Vienna on sabbatical, and doing research. We have assisted him with various software installations/configurations which were adapted to run on HPC. His main software is Blast2Go, and likely various other genomics and transcriptomics tools that we did not get a chance to inventory yet.

[Business] We have assisted the business side of Pomona College in speeding up the annuity modeling (100x) by introducing R instead of Excel. We are continuing to work with them to introduce GPUs to provide additional speed improvements.

[Chemistry] We are currently actively working with Dan O’Leary and Maduka Ogba to do a pilot on a VM with Gaussian, Schrodinger software which will be able to scale out to the HPC environment. The two servers they are currently using are rather old and we will assist with migration to VMs/HPC. Maduka is leaving at the end of June for a full-time position so we are trying to document his process. This will be used in SURP. The Gaussian licenses are site licenses (unlimited) purchased by CUC and currently managed by Harvey Mudd. The latest version of Gaussian supports GPUs and the work can be considerably accelerated. There is other software of interest like Schroedinger Maestro (and Desmond can use GPUs), as well as Spartan (no GPUs but we will assist with documenting the software install/configuration process and make it reproducible. They have asked about the assistance with the software licenses for these two ($2,000-$5,000 yearly). <https://www.madukaogba.com/o-maduka-ogba/>

[Computer Science] The recent hire in CS Joe Osborn will be teaching an AI course in 2018/2019 and is very enthusiastic about the DGX workstation we have acquired. There is also strong interest in VR/AR, game design research, and VR/AR applications in higher ed [https://users.soe.ucsc.edu/~jcosborn/](https://users.soe.ucsc.edu/%7Ejcosborn/). We are helping Joe with CI/CD (Continuous Development/Continuous Integration) and self-hosted experimental web sites. We have also had a discussion with David Kauchak regarding various aspects of CS infrastructure support.

[Digital Humanities] Scheduled a meeting with Kevin Mulroy, library reps, the OCAC Director, and members of the Mellon DH award team in August to discuss how we can collaborate.

[Economics] Manisha Goel and Kyle Wilson were the most enthusiastic about the HPC environment. We helped Kyle procure a powerful VM he can use in the meantime. Manisha creates models requiring a lot of RAM. The more the better.

<https://www.pomona.edu/directory/people/manisha-goel>

<https://www.pomona.edu/directory/people/kyle-wilson>

[Environmental Sciences] We have met with Marc Los Huertos and helped streamline some of his R/RStudio related issues. He will likely use the environment once it is available for studying climate in different parts of the world.

[Geology] We have worked with Eric Grosfils to evaluate his current process of teaching with COMSOL. It can use GPUs and this will be one of the first use cases for teaching. He also has a research grant and we could help him build models of volcanic activity using the HPC environment. <https://www.pomona.edu/news/2017/12/19-professor-geology-eric-grosfils-part-research-team-awarded-425000-nasa-grant>

[Linguistics] We have met with Robin Melnick and have started a project migrating his AWS workload locally.

[Mathematics] We have worked with Jo Hardin and helped stabilize the RStudio environment used in class. There was interest in HPC once it is built.

[Molecular Evolution] Andre Cavalcanti is one of the more advanced users and we have met several times. He is using GitHub Classroom, BioPerl, R, various life sciences toolkits that will most definitely run in the HPC environment.

[Physics] We have attended the department meeting and as a result are starting a project with Dwight Whitaker to test moving from ANSYS Fluent to OpenFOAM. The ANSYS license is expensive, OpenFOAM is a good open source/free alternative. We may end up running both but at least a free/open-source alternative is considered. <https://www.pomona.edu/directory/people/dwight-l-whitaker>

[Psychology] We have attended the department meeting and worked with Richard Lewis to help submit a grant for prospective memory research with the use of VR and fNIRS. This is ongoing, we are assisting with consulting regarding VR headsets and eventually there will probably be data to be processed in the HPC environment. This could also be the start of a VR/AR/XR Lab as there is interest in Psychology and CS. We could partner with the library.

[Consortium] We have met with various consortium interested parties that are working on Data Science initiatives. Since data management and processing is one of the aspects of the research computing infrastructure we were able to advise. Specifically, we would like to collaborate with Debra Mashek of HM and Jeanine Finn (contact info below):

Jeanine Finn | CLIR Data Services Postdoctoral Fellow | The Claremont Colleges Library 800 North Dartmouth Ave. | Claremont, CA 91711-5053 Phone (909) 607-7958 | [jeanine.finn@claremont.edu](mailto:jeanine.finn@claremont.edu) Pronouns: she/her

Jeanine comes to our Research Computing Office Hours and can most definitely help us shape the data sharing infrastructure.

There is a proposal that had been submitted by Tanja Srebotnjak titled "Evaluating the GHG and Life Cycle Implications of the Sharing Economy in the Transportation Sector" under the Call for Proposals "Energy, Environment & the Digital Economy." Pomona HPC environment is mentioned in the proposal. Pitzer and Scripps are also involved.

Tanja Srebotnjak, Ph.D. Hixon Assoc. Professor of Sustainable Environmental Design Director, Hixon Center for Sustainable Environmental Design Harvey Mudd College | 301 Platt Blvd. Claremont, CA 91711 Office: Parsons 2363 | Tel: (909)621-8751 | E-mail: [tsrebotnjak@g.hmc.edu](mailto:tsrebotnjak@g.hmc.edu)

The HPC environment could be used for neurosciences, brain imaging, modeling.

We also have a broader interest from Harvey Mudd and Scripps:

Specifically,

* Robert Cave (Chemistry) who is collaborating with Dan O'Leary and they share Gaussian licenses.
* Michael Spezio, Ph.D. Associate Professor of Psychology & Neuroscience Laboratory for Inquiry into Valuation and Emotion (The LIVE Lab) [mspezio@scrippscollege.edu](mailto:mspezio@scrippscollege.edu)

Visiting Researcher Co-PI, Project on Theory of Mind Models in Cooperation Institute for Systems Neuroscience University Medical Center, Hamburg-Eppendorf Hamburg, Germany "

"would be interested to talk with you about HPC resources. I primarily use Matlab, python, and/or R (for Bayesian modeling using Stan), in applications of machine learning, network science, neural models, and cognitive models. So if any of those are of interest to Pomona HPC faculty it would be great to talk about grant opportunities that involve multiple projects or other forms of collaboration"

[Other Colleges]

We have had discussions with Bowdoin, Reed, Dartmouth, Stanford about the possibilty of creating a shared XSEDE-like environment focusing on liberal arts research or cross-discipline studies, especially in such fast growing areas as VR/AR and AI (Virtual Reality/Augmented Reality and Artificial Intelligence)