

# Executive Summary of XSEDE Advisory Board Meeting, August 28, 2020

Meeting Date: Friday, August 28, 2020

Meeting Place: Teleconference via Zoom

Preface: The main topic of this call was a recap of the NSF Review

Next Call: October 23, 2020

## Approval of June Meeting Minutes

- Approved.

## Recap of NSF June Review

Good June review. Our response to the report was accepted by NSF & funding for next project year was approved.

- Response doc will be circulated to the XAB.
- No major concerns presented by panel. Some good suggestions that we've addressed. Nothing to change our plans for the coming year.

Supplemental year to XSEDE2 was approved, so the new project end date is August 31, 2022 with \$21.8M in funding.

No solicitation for what will follow XSEDE2 at this point. Hope to see that solicitation no later than the first quarter of next calendar year. If not, we will have a similar problem to what we had this year.

- John has noted to NSF that it is not productive to request us to submit a bridge proposal
- Believe XSEDE's response to the Blueprint doc may have made them revisit their thinking re. what will follow XSEDE
- NSF leadership hasn't said much other than that they are actively working on the issue. Hope that means they are writing the solicitation, but can't say for sure.

## COVID-19 HPC Consortium Update

- In March, XSEDE was approached by OSTP to see if we can manage how the collective consortium resources can be allocated to the community. Quickly stood up an instance of XRAS to support the consortium and conducted reviews similar as we would in our XAC process. Have ~170 proposals submitted. ~20 returned because of incomplete submissions. ~150 reviewed with ~90 approved. About 1/3 are on XSEDE allocated resources. Others on resources contributed by other consortium members. Starting to see some results.
- Most proposals around molecular biophysics in various forms. Understanding structure & docking, some on small molecule design.
- Fewer proposals that look at drug design, therapeutics, patient care. Consortium leadership has a strong desire to see more work in that space to have more direct impact on the pandemic. This gets a bit sticky as NSF typically doesn't get involved in this kind of work. Have not received guidance from NSF on whether these changes would impact XSEDE's involvement.
  - Reluctance by NSF to go this route.
  - Incorporating into review more weighting for proposals of this nature.
- Providers come from throughout the community including NSF, DOE, Microsoft, AWS, and a variety of companies like BP. More recently includes some international partners.
  - Q: What NSF resources? All XSEDE Allocated resources that can be requested, Frontera, Cheyenne, Chameleon. Decisions are made on the PI's part about whether to participate.
  - Have helped with crises in the past. NSF is directly involved in making the decision to commit resources. There was high level NSF commitment before it came to XSEDE.
  - The Executive Board observes, manages bringing in major partners including OSTP. They are concerned about aspects of the pandemic that aren't being addressed by the consortium. Feel there should be a better balance of projects with more therapeutics, patient-oriented work. NSF is nervous but hasn't said we aren't going there. NASA is hesitant as well, but they aren't contributing resources.
- Question to XAB: How should XSEDE conduct itself if NSF pushes away from the consortium? Should we push back? How hard?
  - Q: what resources/effort is being given by XSEDE?
    - XRAS is the mechanism that allows proposals to be submitted/reviewed/allocated.

- Receiving funding from the community for their use of XTRAS (NCAR, PSC, Frontera, NCSA). Offering this at no cost to the consortium.
- If NSF chooses to separate from consortium, could be treated as an XTRAS usage that would need to be paid for in some way.
- XSEDE allocated resources: Stampede2, Comet, Bridges. ECSS staff assigned as well
  - SP awards have some discretionary cycles they can allocate as they like
- Q: If competition can help solve COVID problems, it is worth continuing to do so. Suggest pushing NSF to continue.
  - John & Ken's time towards this effort could become problematic.
  - NSF charter: The National Science Foundation (NSF) is an independent federal agency created by Congress in 1950 "to promote the progress of science; to advance the national health, prosperity, and welfare; to secure the national defense... Used this previously when they tried to limit participation.
- Q: Has NSF said anything about their role?
  - Early press releases that recognized participation. Not a delineation of roles.
  - Possibility to get someone to go up through the chain to get an official statement about how they support this consortium, agencies working together for the good of the nation. John will ask Amy about this to see if she can push this.
- Q: Would be surprised if NSF isn't having the same discussions. If they pull out, likely because they can't bend the rules.
- Q: Is the governing committee thinking about completely pivoting focus or just emphasizing other areas more?
  - Won't exclude other work, but will be weighted higher for these healthcare areas
  - Good chunk of the proposals received are molecular dynamic simulations in one way or another. That is the community that is associated with those involved in the consortium, so not a surprise.
- John: XTRAS is the linchpin to everything running.
- Q: Disease spread types of projects? Just a few.

- Q: MD better prepared for parallel/HPC environment. Lauren Myers' lab: works with MatLab or R. Period of transitioning them to a large scale environment. Their use of machines is not sophisticated.
  - JT: not a significant use of these resources in that community. Many haven't had large enough data sets for it to matter, but have larger data sets now.
- Q: Any evaluation of scientific efficacy of what has been done so far?
  - Not a lot yet. People are asking this. Asking PIs to provide biweekly updates & have been getting some good info. Just starting to see results from most of the projects. Consortium is trying to share highlights of results of time & effort that's gone into it. Interesting results thus far have not been articulated well on the website. Webinar this week with a researcher presenting their work. Hard to do an assessment quite yet.
- Overall response from the board: Keep proceeding as you are. Push back at NSF if they try to curb XSEDE's participation.
- John: concerns that other work is being impeded by COVID work, but feel addressing the pandemic is a priority issue. Worried about what will happen in the next couple of months with schools back in session. Could see a dramatic spike depending on how it is handled.
- Q: how has this pandemic impacted the project?
  - Already distributed project.
  - Putting aside consortium work, the impact has been nominal. Have worked effectively as a distributed project for a long time. Not much of a change from an operational perspective.
  - Provide NSF with reports on financial impacts in terms of staff time spent on pandemic. Report weekly to NSF on consortium related work. Part of that is an accounting for time on systems used.
  - Q: Hidden impacts. Some people are well-suited to working at home, but others are dealing with a drop in productivity or personal problems. Not sure we've done a good job of thinking about the long term effects of this. **RECOMMENDATION:** XSEDE should consider long-term effects of this nature on people.
    - JT: we are trying to accommodate people homeschooling or with kids at home doing virtual learning. Groups of people with different tolerance levels. Hard to characterize well, but

it is a concern. At institutional level trying to help staff work through issues.

- Q: support John staying the course. Have a contingency plan in case NSF pulls out.
- Q: worried about what will come after XSEDE. Took a long time for XSEDE to become the well-oiled machine that it is. Community can expect several years (3-4?) of disruption if there is a cold turkey replacement.
  - Was difficult to get the project to where it is today.
  - Overlap on training new teams? Many discussions around continuity/overlap. John has repeatedly made the point that transition from TeraGrid to XSEDE was disruptive to the community. Feel that NSF has heard this & appreciates the need for overlap, but not clear how it will play out as time goes on. If we're going to do a detailed & careful transition, we will need overlap time. Too complex to just turn off and then turn back on. Hope that we'll see a solicitation by the end of the year.
  - Q: knowing the transition will be a problem, is there a mechanism to have XSEDE not get re-awarded from the ground up every 5 years? Persist as a living organism.
    - NSF has a mechanism such as this, but many are reluctant to go that route.
    - The funds have a limit on award length. Incumbent may or may not win the next award. Makes sense in the research base, but much of what we do is infrastructure.
    - MRSEC process doesn't exactly fit, but could be modified. How does NSF provide CI services to awardees in a more holistic way. Looking at it now more narrow. Difficult path for NSF as it would mean a lot of change for the way things are done.

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