

# XAB August 2020 Call

## Executive Summary of August 2020 Meeting

8/28 – 2pm ET | 1pm CT | 12pm MT | 11am PT

Attendees:

NAME	PRESENT  
<b>XAB Members</b>	
Lisa Arafune	
Leah Bendavid	
Ken Bloom	
Randy Bryant	
Thomas Cheatham	
Elizabeth Cherry	
Toni Collis	
Peter Couvares	
Rudolph Eigenmann	
Ani Ural	
<b>Service Provider Forum</b>	
Ruth Marinshaw	
<a href="#">Jonathon Anderson</a>	
David Hancock	
<b>User Advisory Committee</b>	
<a href="#">Emre Brookes</a>	
<b>XSEDE Staff</b>	
<a href="#">John Towns</a>	
<a href="#">Tim Boerner</a>	
<a href="#">Robert Sinkovits</a>	
<a href="#">Philip Blood</a>	
<a href="#">Kelly Gaither</a>	
<a href="#">David Lifka</a>	
<a href="#">David Hart</a>	
<a href="#">Gregory Peterson</a>	
<a href="#">Victor Hazlewood</a>	
<a href="#">Ron Payne</a>	
<a href="#">Sergiu Sanielevici</a>	
<a href="#">Linda Akli</a>	
<a href="#">Leslie Froeschl</a>	
<a href="#">Lizanne DeStefano</a>	

## Agenda

Time	Item	Lead	Notes
5 minutes	Welcome June XAB meeting summary	Lisa	XAB Meeting Summary for June: Emre, Rudi: move to approve. Approved unanimously.
	XSEDE involvement in COVID-19 HPC Consortium	John	<p>Good June review. Our response to the report was accepted by NSF &amp; funding for next project year was approved.</p> <ul style="list-style-type: none"> <li>• Response doc will be circulated to the XAB.</li> <li>• No major concerns presented by panel. Some good suggestions that we've addressed. Nothing to change our plans for the coming year.</li> </ul> <p>Supplemental year to XSEDE2 was approved, so new project end date is August 31, 2022 with \$21.8M in funding.</p> <p>No solicitation for what will follow XSEDE2 at this point. Hope to see that solicitation no later than first quarter of next calendar year. If not we will have a similar problem to what we had this year.</p> <ul style="list-style-type: none"> <li>• John has noted to NSF that it is not productive to request us to submit a bridge proposal</li> <li>• Believe XSEDE's response to the Blueprint doc may have made them revisit their thinking re. what will follow XSEDE</li> <li>• 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.</li> </ul> <p>COVID-19 HPC Consortium Update:</p> <ul style="list-style-type: none"> <li>• 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 instance of XTRAS to support 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.</li> <li>• Most proposals around molecular biophysics in various forms. Understanding structure &amp; docking, some on small molecule design.</li> <li>• Less that looks more 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. <ul style="list-style-type: none"> <li>• Reluctance by NSF to go this route.</li> <li>• Incorporating into review more weighting for proposals of this nature.</li> </ul> </li> <li>• Providers come from throughout community including NSF, DOE, Microsoft, AWS, variety of companies like BP. More recently includes some international partners. <ul style="list-style-type: none"> <li>• 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.</li> <li>• Have helped with crises in the past. NSF directly involved in making the decision to commit resources. High level NSF commitment before it came to XSEDE.</li> <li>• 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 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.</li> </ul> </li> </ul>

- Question to XAB: How should XSEDE conduct itself if NSF pushes away from consortium. Should we push back? How hard?
  - Emre: what resources/effort being given by XSEDE?
    - XTRAS is the mechanism that proposals are 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
  - Tom: If competition can help solve COVID problems, it is worth continuing to do. 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 try to limit participation.
  - Lisa: 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 official statement about how they support this consortium, agencies working together for good of the nation. John will ask Amy about this to see if she can push this.
  - Rudi: Would be suprised if NSF isn't having the same discussions. If they pull out, likely because they can't bend the rules.
  - Ruth: Is 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 proposal received are molecular dynamic simulations in one way or other. That is the community that is associated with those involved in the consortium, so not a surprise.
  - John: XTRAS is linchpin to everything running.
  - Rudi: Disease spread types of projects? Just a few
    - Kelly: 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.
  - Ken: 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 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 pandemic is a priority issue. Worried about what will happen in the next couple months with schools back in session. Could see a dramatic spike depending on how it is handled.
  - Rudi: 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 report 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.
    - Peter: Hidden impacts. Some people are well-suited to working at home, but others are dealing with 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 home schooling 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.
  - Emre: support John staying the course. Have contingency plan in case NSF pulls out.
  - Emre: 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 trouble 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 point that transition from TeraGrid to XSEDE was disruptive to the community. Feel that NSF has heard this & appreciates need for overlap, but not clear how it will play out as time goes on. If we're going to do detailed & careful transition, 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.
  - Jonathon: knowing the transition will be a problem, is there a mechanism to have XSEDE not get reawarded from 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 next award. Makes sense in 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.

Close Meeting

Emre, Ruth: Move to end the meeting.

Next meeting: 4 hour webinar: Friday, Oct. 23 9am-1pm ET