Special Report for NASA

Exploring Options for a Bespoke Supercomputer Targeted for Weather and Climate Workloads

Bob Sorensen
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EXECUTIVE SUMMARY

The primary focus of this study was to gather key insights, through a series of surveys within the weather and climate research community along with potential HPC suppliers, on options available to NASA, and others, to develop a bespoke HPC system specifically targeted for weather/climate research.

The study was divided into two major phases:

- The first phase centered on a series of interviews held with a wide range of expert researchers and users in the HPC-based climate and weather community to gather their thoughts and perceptions on current and future operational requirements as well any specific HPC hardware, software, and architectures needed to meet those workloads.
  - For phase one, 15 different weather/climate organizations in the US and overseas were surveyed including ECMWF, LANL, NOAA, ORNL, UCAR, and the University of Delaware.
- Phase two consisted of taking the results of phase one as the basis of a second survey of HPC suppliers and independent HPC designers to assess the challenges and opportunities of developing a bespoke HPC to meet the phase one requirements.
  - For phase two, HPC suppliers providing input included Cray Inc, Dell EMC, HPE, and IBM.

Weather and climate user-base respondents had a broad list of limitations with current HPCs as well as for prospects for future commercial HPC offerings. Key concerns centered on limitations in memory and storage latency and bandwidth, the lack of diversity in processor option/designs, the current reliance on GPUs in the HPC sector writ large that are not well suited to current weather/climate community workloads, and the trend towards HPC vendor-specific interconnect options.

These user-base respondents also provided a number of recommendations for future HPC developments, noting that any project to build such a system would need to be a community effort. The system should not be a one off “science fair project” but instead come from a robust architectural roadmap that would continue for at least 2-3 system generations, and it would need significant demonstrated performance improvements over existing and planned commercial HPCs. Finally, there was mention of the need for bringing AI, particularity machine learning capabilities, into the programming mix, but that opinion was not universally supported.

For phase two of the project, all of the HPC-supplier respondents indicated that they would be interested in exploring the development of a bespoke HPC for NASA. However, the level of commitment and the degree to which a system would use special-purpose or customized hardware and software varied greatly. Indeed, most indicated that the option for building a special-purpose

system, or even a series of systems over time, could not be economically justified regardless of the amount of NRE available unless that system design had value within the wider weather community or across a number of complementary HPC-dependent verticals.

The major concern of HPC supplier respondents centered on NASA's need to modernize and refactor their codes to better capture advances in existing and emerging HPC hardware and software, although the HPC suppliers acknowledged that such a task would be complex and costly.

- Most agreed that any available NRE for such a bespoke system should be committed to code optimization, noting that in two or three years there likely will be a range of interesting architectures suitable for NASA's workloads, but there would still be a significant gap in software capability.
- HPC vendor respondents also indicated that absent any major software upgrades, there will only be escalating costs to support NASA's increasingly obsolete programming paradigm, and the first step to addressing that reality is to 'bite the bullet' and embrace a comprehensive software rewrite plan.
- Cloud service providers were cited as leading the way in driving continual code refactoring as they provide new software releases on a regular basis while allowing for the quick harnessing of any new technology gains and that NASA could learn much from their processes.

HPC providers also indicated that determining exactly what such a bespoke system would look like could be challenging and that improved benchmarking efforts are vital.

- HPC vendors stressed that NASA has a wide and varied range of workloads that needs to be more accurately characterized before they can be turned into a comprehensive set of hardware and software requirements.

Finally, almost all respondents stressed the need for further exploration into the use of GPUs and other accelerators. Their potential for significant performance gains in traditional modeling and simulation jobs, as well as the promise of bringing AI techniques into a range of NASA jobs, was seen as simply too great not to be considered.

Recommendations for next steps included a NASA initiative to more accurately assess the range of existing and planned climate/weather workloads to better define specific hardware and software requirements, compose benchmarks of mini application suites, testcases, or even full applications to help determine the various strengths and opportunities of any potential HPC design, and organize a pre-competitive codesign conference, or series of conferences, to bring together interested commercial vendors to discuss options and opportunities. Topics for discussion could include:

- Generating relevant projections of advances in future HPC hardware and software from a wide base of HPC vendors and users that will better align with NASA requirements but that are in keeping with larger commercial trends.
- Exploring opportunities to leverage potential NASA hardware or software developments into the larger weather/climate HPC ecosystem or even other HPC verticals to help vendors justify the development of non-COTS hardware or software for a NASA system.
- Enlisting HPC vendors, USG organizations, or foreign climate/weather centers on the best ways for NASA to begin refactoring and modernizing their current software base to take advantage of existing and planned commercial technology and HPC product advances.

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Headquarters

365 Summit Avenue
St. Paul, MN 55102
USA
612.812.5798
www.HyperionResearch.com and www.hpcuserforum.com
