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TECHNICAL
REPORT

High-Performance Computing Opportunities and Challenges for Army R&D

Robert H. Anderson, Amado Cordova,
Anthony C. Hearn, Rosalind Lewis,
John Matsumura, Isaac R. Porche III,
Randall Steeb

Prepared for the United States Army

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201 North Craig Street, Suite 202, Pittsburgh, PA 15213-1516
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Summary

Members of this project have studied the academic and industrial uses of HPC and have conducted site visits at a number of Army R&D HPC user and provider sites, including the Medical Research and Materiel Command (MRMC), Edgewood Chemical Biological Center (ECBC), the Army Research Lab's Major Shared Resource Center (MSRC), the Developmental Test Command (DTC), Research, Development, and Engineering Command's (RDECOM's) Communications-Electronics Research, Development, and Engineering (RD&E) Center (CERDEC), Scalable Network Technologies, Inc., and the Director for Command, Control, Communication, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR) for Future Combat Systems (FCS) at Boeing, Huntington Beach, California.

Because of the breadth of possible uses of HPC in Army R&D, our client asked us to concentrate on two HPC application areas: biotechnology and biomedicine, and modeling and simulation of the complex battlefield wireless network communication systems. We did so, and concluded that these areas are of great importance and merit focused funding and attention.

Our primary recommendations are these:

- Because both biotech and communications network modeling are important, we believe that incremental HPC R&D funding from the Assistant Secretary of the Army for Acquisition, Logistics, and Technology (ASA(ALT)) should concentrate on developing common tools and techniques valuable in both areas; we provide several examples of HPC tools of relevance to both areas.
- DoD challenge grants work effectively to focus attention and resources on new areas; ASA(ALT) should consider a small challenge grant program tailored to the unique needs of Army R&D.
- There are important uses for additional Army HPC "swat teams," which can provide training, startup aid, and links to High Performance Computing Modernization Office (HPCMO) software toolkits for new users and applications; this is especially needed with the proliferation of HPC to individual labs due to the availability of inexpensive personal computer (PC) clusters acting as supercomputers.
- ASA(ALT) should consider recommending the addition of a "BIO" computational technology area (CTA), and possibly one ("NET") tailored to communication network modeling and simulation, to focus attention on these important HPC applications.

In biotechnology/biomedicine, there are very important R&D application areas specific to Army needs, for example, rapid creation and tailoring of vaccines. The establishment in FY 2004 of a Biotechnology HPC Software Applications Institute at MRMC is an important first step, but many biological R&D topics of vital importance to the Army are not being addressed currently. Indeed, in our study of FY 2004 data, we found that only four of 115 HPC projects were of a biotech nature, and most of those related to dispersion or epidemiological modeling. A number of biotech/biomed applications are of vital interest to the Army but are not being given the attention they deserve.

In C4ISR modeling and simulation, CERDEC has very substantial expertise. It understands the problem well and it has in-house competence and focus on the problem. But battlefield network modeling does not scale well with increasing parallelization of computation, so the problem is currently intractable for analyzing tens of thousands of intercommunicating nodes in a battlefield scenario. Therefore, the Army's FCS is being designed without the benefit of such large-scale *detailed* analyses and simulations; simplifications are being made, of necessity, which may or may not prove realistic.

We find clusters of commercial off-the-shelf PCs (most often with high-speed backplanes) increasingly dominating HPC because of their cost-effectiveness. But vector machines do outperform cluster computing by a substantial amount and will continue to have an important role at the high (and expensive) end of HPC. There is a continuing tension as more R&D centers want to obtain in-house cluster computing to support their local HPC needs, yet that trend tends to scatter and distribute HPC software and operational expertise—perhaps below a critical mass at many locations. Meanwhile, the MSRCs wish to provide centralized HPC services to the Department of Defense (DoD) R&D community, which some users regard as too batch-oriented with delays and too uncertain in terms of security, not allowing them to build sufficient in-house expertise in all aspects of HPC use.

One question this study addressed was: "Is Army HPC R&D getting its fair share of DoD HPC resources?" The short answer is yes—although the Army has a smaller number of HPC projects using shared DoD resources, it gets about a third of the teraflops available.

Throughout this project, we were impressed by the operations and facilities of the DoD HPCMO, and its Common HPC Software Support Initiative (CHSSI) and Programming Environment and Training (PET) initiative. They seem well-respected in the DoD HPC community, although, of course more could be done in all of these areas as cluster computing brings HPC to many more sites and laboratories.

Because resources for new initiatives in Army HPC R&D are limited, we concentrated on describing some tools and techniques that appear to be common across both the biotech and network modeling application areas. These include better tools for multiresolution models that describe hierarchical structures and systems, application of network concepts for analysis of complex biological processes, and the use of some biological concepts within C2 network modeling.

Our primary recommendation is that the set of common tools and techniques spanning both the bio and network modeling application areas be given priority for funding. These include post-processing, visualization, hierarchical decomposition processes, and accelerators for processor-intensive activities such as line-of-sight calculations.

We are very impressed with the ability of the High Performance Computing Modernization Program (HPCMP) challenge grants to focus resources and attention on specific

areas of DoD interest. ASA(ALT) might consider a smaller, even more focused program patterned after the HPCMP one, tailored to specific Army requirements.

We recommend that additional resources be provided to study the concept of an Army-specific HPC "swat team" that can focus on a particular laboratory's interests, provide specialized training and education in HPC, help migrate applications from serial to parallel computing architectures, and adapt and use the software tools and toolkits of the CHSSI program within the HPCMP. After several weeks or months of such intensive support, the team would leave a residual staff behind and tackle the next lab or agency in need of such focused assistance. Such a team should be supplemented by an HPC "help line" for those Army R&D organizations needing other HPC-related assistance. The purpose of this recommendation is to address the growing use of "home-grown" HPC within individual labs (e.g., using small- to medium-sized clusters) and the problem of having less-than-critical-mass expertise in HPC within those separate labs and agencies.

We believe ASA(ALT) should support the use of cluster computing for HPC within individual labs and agencies. These provide valuable hands-on HPC expertise and allow the migration, development, and debugging of HPC-related codes in a more interactive, intensive manner than submitting batch jobs to an MSRC.

A workshop we conducted in November 2004 highlighted what we have called "conceptual, tactical, and cultural problem areas" related to HPC use. End-users or customers of Army R&D have often asked, "Why is HPC needed for this?" "Will the resulting HPC-driven models and simulations replace any field testing?" "What is the business case for using HPC, as opposed to our normal methods?" Someone within the Army lab system should be tasked to compile "lessons learned" and accurate data and logic stating *when* HPC is best used, *how* it will affect outcomes, and *why* it is worthwhile in particular application areas. Analysis based on business cases should be provided to support these lessons learned. These questions are apparently encountered often enough that guidance and support for answering them are needed.

Last, we recommend that the Army request that the HPCMP add one or two CTAs to their existing list (or else recast some existing ones). The purpose is to give prominence and focus to the areas of biotech/biomed R&D and network modeling and simulation (with special attention to large-scale mobile communication networks). At present, these R&D application areas are scattered among a number of CTAs.

The above recommendations constitute a plan for focusing incremental Army R&D HPC activities, in addition to the substantial and important work already under way in more traditional areas such as computational fluid dynamics and projectile/armor impact studies.