Developing NOAA/National Weather Service's Next Generation Global Prediction System for Future HPC Systems

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NOAA/National Weather Service (NWS) is designing, developing and implementing the Next Generation Global Prediction System (NGGPS), a fully-coupled community modeling system for operational weather and climate prediction to be used and supported by the National Centers for Environmental Prediction (NCEP) over the next two decades. NGGPS includes plans for improved scientific software architecture, performance, scalability and portability.

A central component of NGGPS will be a new global atmospheric model capable of high resolution for explicit simulation of moist convective processes. This will require the ability to take advantage of new processor architectures with very large scale thread concurrency and fine-grain (e.g. vector) parallelism. HPC objectives in the NGGPS Implementation Plan[1] include:

- A software architecture and engineered system that maximizes the benefit from HPC;
- A high-performance, flexible software infrastructure to increase ease-of-use, performance and interoperability;
- Adaptation/optimization of codes for increased performance in multi-cores, participation in co-design to improve suitability of hardware, and exploring new algorithms; and
- Defining model re-architecture requirements for next-generation heterogeneous fine-grain computing platforms.

Within NGGPS, a Software Architecture an Engineering team is developing plans to implementing these objectives, emphasizing HPC architectures with lowest overhead/highest reward path to operations and using standard, mature, widely adopted programming models. Plans will also include monitoring and exploration of developments in other next-generation computing technologies and approaches (e.g. FPGAs and reduced or inexact computing).

Resources related to HPC planning and development include NWS program funds for NGGPS and funds provided under a new Software Architectures for Novel Architectures (SENA) project in the NOAA HPCC under the NOAA Office of the Chief Information Officer.

The remainder of this white paper provides responses to specific topic areas suggested in the HPCOR guidelines:[2]

[1] http://www.nws.noaa.gov/ost/nggps/NGGPS%20Implementation%20Plan%20v1.0.pdf
[2] https://www.orau.gov/hpcor2015/whitepaper.htm

Language: Predominantly Fortran.

Lines of code: The entire operational software suite at NCEP involves pre- and post-processors, data assimilation systems, forecast system and data management scripts and libraries, as well as the computer models themselves. These comprise millions of lines of software. The global forecast model itself involves somewhere between one-half million to a million lines of code, depending on the forecast application and configuration.

Primary methods: Varies depending on software component, but focusing on the forecast model, the current spectral semi-Lagrangian method is giving way to more scalable finite-volume based numerics on cubed-sphere and icosahedral meshes.

Types of problems/domains/science application problems: Operational numerical weather and climate prediction on a spherical global domain, including earth's atmosphere, oceans, land surface and ice caps. Longer-term plans include space weather applications, which involve extending the atmospheric domain upward many hundreds of kilometers into the ionosphere.

Scale of resources used for production runs and Supercomputers Regularly used: The NOAA Weather and Climate Operational Supercomputing System (WCOSS) has been upgraded from 750 TFs (IBM iDataPlex) to 2 PFs with new Cray XC40 systems. NOAA also has several HPC Data Centers for research computing, the newest of which is Theia, a 1.01 PF Cray CS400 cluster. Edison, the NERSC Cray XC30 system, and Stampede at TACC have also been used for NGGPS benchmarks.

Libraries/tools for production science campaigns: MPI, OpenMP, scripting languages (Ksh, python), Intel MKL.

Describe efforts to develop code (application, library, etc.) portable across diverse architectures. The NCAR-supported WRF model used by NWS for hurricane and short term high resolution forecasts, was designed to be performance portable over message-passing, threaded and fine-grain parallel architectures. Similarly, model development at NOAA/ESRL and other Office of Atmospheric Research laboratories has been systematic and proactive in this regard. NWS has been more reactive, relying on the vendor for support porting and tuning to new systems as they are procured. The NOAA Research to Operations Initiative, of which the NGGPS project is a part, includes objectives aimed at a more systematic approach within NWS.

What is your greatest fear going to exascale for application portability and functionality? First, whether operational (real-time) numerical weather prediction as currently formulated will be effective at exascale, given the low computationally intensities, large working sizes, and obstacles to scaling with increased resolution. Secondly, will NOAA and the operational NWP community at large succeed in exploiting future increases in HPC capability to provide continued forecast accuracy improvements that the public expects in return for its investment in its national forecast centers.