

Spotlight

Global Arrays Toolkit Version 4.2 Released

Supercomputers allow scientists to study more complex scientific problems with larger and more realistic models, and to achieve results more quickly by scaling computational models to larger numbers of processors. The Department of Energy's EMSL, located at Pacific Northwest National Laboratory, provides production computing hardware and software resources to support world-class research in the biological, chemical, and environmental sciences. Several software programs critical to EMSL user research that run on EMSL platforms were developed using PNNL's Global Arrays (GA). They include:



- **NWChem** – a computational chemistry package that aims to be scalable both in its ability to treat large problems efficiently and in its usage of available parallel computing resources.
- **STOMP** (Subsurface Transport Over Multiple Phases) – a computer model designed to be a general-purpose tool for simulating subsurface flow and transport that complements other analytical capabilities developed by PNNL's Hydrology Group.
- **ScalaBLAST** – a software program that rapidly processes genomic sequences in parallel.
- **Northwest Grid Generation Code** – software that transforms experimental data into computational models.

GA facilitates the writing of computational software that uses a supercomputer's memory, disk, and communication network. GA provides scientists with an efficient and portable shared-memory style parallel programming interface for use with distributed-memory computers. GA was designed to free the programmer from the low-level management of communication and allow them to address their problems at the level at which they were originally formulated. GA has been in the public domain since 1994 and actively supported and employed in several large codes since then.

The latest GA release is GA Toolkit Version 4.2, which includes significant updates to the previous GA version to support users of EMSL who perform large-scale computational research. GA 4.2 lends support for several new platforms including an optimized port for Cray XT5, a petaflop Linux supercomputer and BlueGene/P, the second generation of Blue Gene supercomputer.

The GA toolkit is essential in supporting DOE's missions to promote energy security through reliable, clean, and affordable energy; ensure nuclear safety; strengthen scientific discovery through innovations and technology; and to protect the environment. The GA toolkit helps EMSL users to advance molecular science in areas such as aerosol formation, bioremediation, catalysis, climate change, hydrogen storage, and subsurface science.

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