NASA scientists and engineers are increasingly turning to large-scale numerical simulation on supercomputers to advance understanding of Earth and astrophysical systems, as well as to conduct high-fidelity engineering analyses. The goal of this subtopic is to make NASA’s supercomputing systems and associated resources easier to use, thereby broadening NASA’s supercomputing user base and increasing user productivity. Specific objectives are to:

- Reduce the learning curve for using supercomputing resources;
- Minimize total time-to-solution (i.e., time to discovery, understanding, or prediction);
- Increase the scale and complexity of computational analysis and data assimilation;
- Accelerate advancement of system models and designs.

The approach of this subtopic is to develop intuitive, high-level tools, interfaces, and environments for users, and to infuse them into NASA supercomputing operations. Successful technology development efforts under this subtopic would be considered for follow-on funding by, and infusion into either of the NASA high-end computing projects, including the High End Computing Columbia (HECC) project at Ames and the NASA Center for Computational Sciences (NCCS) at Goddard. Research should be conducted to demonstrate technical feasibility during Phase 1 and show a path toward a Phase 2 prototype demonstration. Open Source software and open standards are strongly preferred.

Specific areas of interest include:
Application Development

With the increasing scale and complexity of supercomputers, users must often expend a tremendous effort to translate their physical system model or algorithm into a correct and efficient supercomputer application code. This subtopic element seeks intuitive, high-level application development environments, ideally leveraging high-level programming languages (e.g., parallel Matlab or IDL) to enable rapid supercomputer application development, even for novice users. This environment should dramatically simplify application development activities such as porting, parallelization, debugging, scaling, performance analysis, and optimization.

Results V&V

A primary barrier to effective use of supercomputing by novices is understanding the accuracy of their computational results. Errors in the input data, domain definition, grids, algorithms, and application code can individually or in combination produce non-physical results that a user may not detect. This subtopic element seeks tools and environments to help users with verification and validation (V&V) of simulation results. This could be accomplished by enabling comparison of results from similar applications or with known accurate results, access to results analysis tools and domain experts, or access to error estimation tools and training.

Data Analysis and Visualization

Supercomputing computations almost invariably result in tremendous amounts of data, measuring in the gigabytes or terabytes, and with many dimensions and other complexity aspects. This subtopic element seeks user-friendly tools and environments for analysis and visualization of large-scale, complex data sets typically resulting from supercomputing computations.

Ensemble Management

Conducting and fusing the results from an ensemble of related computations is an increasingly common use of supercomputers. However, ensemble computing and analysis introduces a new set of challenges for deriving full value from using supercomputing. This subtopic element seeks tools and environments for managing and automating ensemble supercomputing-based simulation, analysis, and discovery. Functions could include managing and automating the computations, model or design optimization, interactive computational steering, input and output data handling, data analysis, visualization, progress monitoring, and completion assurance.

Integrated Environments

The user interface to a supercomputer is typically a command line or text window, where users may struggle to
locate or develop applications, understand the job queue structure, develop scripts to submit jobs to the queue, manage input and output files, archive data, monitor resource allocations, and many other essential supercomputing tasks. This subtopic element seeks more intuitive, intelligent, and integrated interfaces to supercomputing resources. This integrated environment could include access to user training (e.g., tutorials, case studies, and experts), application development tools, standard (e.g., production, commercial, and Open Source) supercomputing applications, results V&V tools, computing and storage resources, ensemble management tools, workflow management, data analysis and visualization tools, and remote collaboration.