The Damsel Project

A Data Model Storage Library for Exascale Science

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Overview

Computational science applications are steadily increasing the complexity of grids, solution methods on those grids, and data that link the two together on modern petascale computers. Several common motifs can be described, having distinct grid types and computation/communication patterns; examples include structured AMR, unstructured finite element/volume, and spectral elements. From a storage and I/O perspective, these applications exhibit distinct data organization and access patterns during simulation, analysis, and visualization. However, these codes continue to interact with I/O data libraries much the same as they have since the 1990s, in terms of relatively low-level data structures like vertex positions, connectivity arrays, and multi-dimensional solution data arrays. Although these high-level I/O libraries have had a beneficial impact on parallel applications in terms of read/write performance, the impedance mismatch with application data models is growing as applications go to more complex data models and interactions. This mismatch is making it more difficult to achieve I/O performance close to system peak capabilities, while also not supporting the full range capabilities in today's computational science data models.

A different approach is needed, that leverages performance improvements and best practices learned from previous approaches, while raising the level of interaction with application data models and access patterns. As the International Exascale Software Project (IESP) report observes, "[...] The purpose of I/O by an application can be a very important source of information that can help scalable I/O performance when hundreds of thousands (to millions) of cores simultaneously access the I/O system [...]" In other words, the high-level view of the *data model* is overlooked rather than exploited. Also, the *data layout* used in these codes and how that layout interacts with I/O software used to save the data to or read the data from storage systems are highly relevant. Increasing the complexity with which applications can interact with I/O libraries will reduce the impedance mismatch between the two, while also streamlining the I/O process by reducing unnecessary data copying between applications and I/O libraries. This process will be simplified further by developing customized interfaces and formats, or "verticals", for the data model motifs used in today's petascale applications. This model represents the underlying approach of our project.

The goal for Damsel is to enable Exascale computational science applications to interact conveniently and efficiently with storage through abstractions that match their data models. We are pursuing four major activities: (1) constructing a unified, high-level data model that maps naturally onto a set of data model motifs used in a representative set of high-performing computational science applications; (2) developing a data model storage library, called *Damsel*, that supports the unified data model, provides efficient storage data layouts, incorporates optimizations to enable exascale operation, and is tolerant to failures; (3) assessing the performance of this approach through the construction of new I/O benchmarks or the use of existing I/O benchmarks for each of the data model motifs; and (4) productizing Damsel and working with computational scientists to encourage adoption of this library by the scientific community.

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Current Activities

Building on previous work in the SciDAC ITAPS project, we are building the Damsel data model, which extends beyond the traditional multi-dimensional array model used with today's high-level I/O libraries. The Damsel data model, inspired by the data model in the ITAPS MOAB library, supports both structured and unstructured meshes, annotations and solution data on those meshes, as well as a variety of meta-data commonly applied to these models. This data model strikes a careful balance between abstractness, which is crucial for extensibility, as well as concreteness, which is important for usability. The API for this data model will be designed to support more direct data exchange from application data structures, eliminating the need for data copies; this will be crucial for supporting future architectures, where memory is expected to be even more limited than it is in current machines.

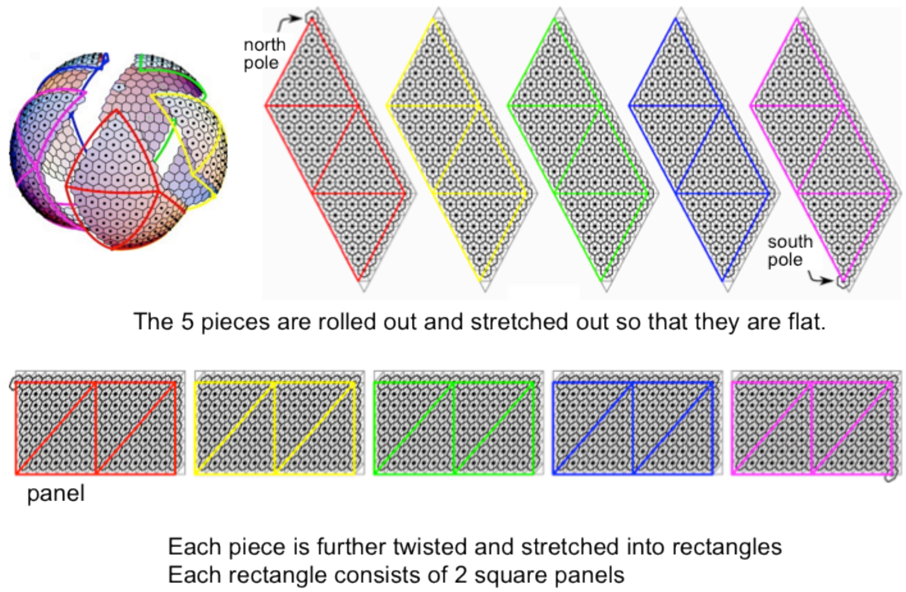

Image courtesy Dave Randall, Bruce Palmer, Karen Schuchardt, PNNL .

One example of the kind of complex data models applications now use is the geodesic grid used in some climate codes, shown here. Vertices represent the centers of either hexagonal or pentagonal grid cells, derived by successive refinement of a triangular mesh. Currently, storage of these structures into a NetCDF format requires a clever transformation into 2D, which does not retain the relation between hexagonal cells and the original coarse grid cells. Damsel will support specification of these geodesic grids natively, as collections of polygons associated with the original coarse grid triangles. Other application data, like Morton ordering for preserving locality, also fits naturally in this data model. Communicating these constructs in terms of higher-level grid objects allows I/O directly to/from application storage, eliminating the need for data copies.

These and other use cases from a variety of computational science problems are being developed, to further refine the data model and in preparation for developing I/O benchmarks for these codes. These use cases and benchmarks will serve both to assess Damsel performance, and as a means of communicating with other applications how best to use Damsel.

Impact

Damsel advances the goals of the ASCR mission through development of core I/O software for Exascale applications and deployment of that framework on DOE capability computing resources. Damsel will improve the productivity of application developers and the performance of their codes, enabling scientific applications of interest to the Department of Energy to more efficiently use future Exascale systems and advance scientific discovery.

Contact

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