Software platform INMOST for distributed mathematical modeling*

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The solution of industrial boundary-value problems requires high quality approximation and discretization of the problem. In addition to the high accuracy discretization it is necessary to use the general unstructured meshes that fit the problem geometry. On the other hand, to increase the approximation accuracy the usage of very large dimension meshes is required. It results in exploiting of the distributed computations on a modern parallel computers. A developer requires a tool that helps operating with distributed mesh data.

In general, the boundary-value problems solution consist of the following stages: mesh generation, distribution of mesh data to processors, problem discretization, assembling linear system, solution of linear system, as well as visualization of initial data and solution results.

INMOST (Integrated Numerical Modelling and Object-oriented Supercomputing Technologies) software platform [1–3] is designed to help a user in operating with all of this stages. INMOST is a tool for supercomputer simulations characterized by a maximum generality of supported computational meshes, distributed data structure flexibility and cost-effectiveness, as well as crossplatform portability. INMOST is a software platform for developing parallel numerical models on general meshes. User guides, online documentation, and the open-source code of the library is available at `http://www.inmost.org`.

The mesh generation stage is based on the hierarchy of the mesh elements such as vertex, edge, face (polygon in general case), and cell (polyhedron in general case), see Fig. 1a. Some sparse or dense data can be associated of binary, integer, real or reference types as well as value with the derivative can be associated with each element, see Fig. 1b.

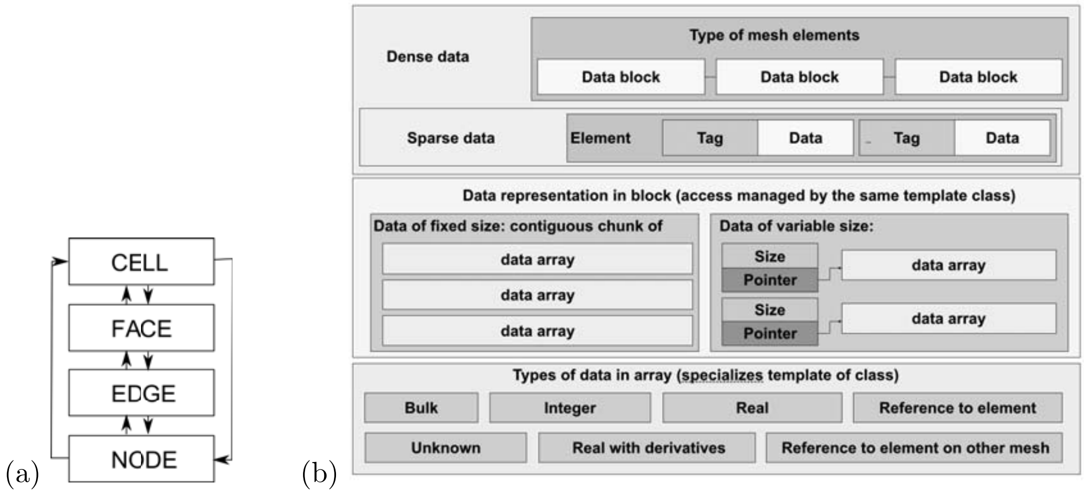

Figure 1. Mesh elements (a) and the INMOST data structure (b).

Except for the main function to operate with the mesh hierarchy, a user can require the following operations to handle distributed mesh data: distribute mesh between processors, specify ghost elements, store data for elements in tags, and exchange tag data for ghost elements. In

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addition, INMOST supports the refinement and coarsening of the mesh as well as the dynamic meshes, including automatic mesh balancing.

The next important stage is the problem discretization for the specified distributed mesh. It can be done both by low level function by filling each nonzero matrix element and by automatic differentiation. The basis for the above module are: a C++ class ‘variable’ representing a value of function with its first order partial derivatives, expression templates, a C++ class ‘variable_expression’, and a dense linked-list structure ‘Sparse::RowMerger’ which is used for fast addition of sparse vectors, corresponding to the partial derivatives. With these functionality the sparse matrix and the residual vector (classes ‘Sparse::Matrix’ and ‘Sparse::Vector’, respectively) can be constructed.

The assembled linear system can be solved by one of the open-source solver libraries such as Trilinos, PETSc, SuperLU or by some of internal linear solvers based on dual threshold triangular factorization.

At present, INMOST contains trial implementation of the multi-physics module. The idea of the module is to provide basic functionality that allows one to split the problem into physical processes. Each physical process is responsible for a subset of unknowns and assembly of equations corresponding to these unknowns. Coupling between two physical processes introduces coupling terms into equations involving unknowns of both processes. This requires access to unknowns and equations of both processes.

At the final stage of modeling INMOST provides a set of functions to visualize the mesh and the associated solution.

INMOST is intensively used for scientific and industrial applications (see, e.g., [4, 5]). The results of the numerical experiments of real-life problems on parallel computers are presented. It includes the following models: incompressible fluid; simulation of blood clotting with thrombus formation; free surface fluid; disaster simulation; black-oil modeling; mechanics of deformable bodies; contact mechanics; fracture mechanics; geomechanics; wrapping the oil rig in the ocean; underground water flow; nuclear waste disposal.

References

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