Interoperable Software Components for CFD

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1 INTRODUCTION

Creating automated, reliable and flexible CFD codes requires the use of advanced techniques in a variety of areas. For example, automatic mesh generation and adaptation contribute significantly to simulation automation and reliability, while robust discretization schemes and error control are central components to solution reliability. As new and better techniques for discretization, flux calculation, turbulence modeling, and multi-disciplinary coupling are developed, existing modules in CFD software must be enhanced or replaced to take advantage of these new tools. Traditionally, four approaches have been used to provide tools and technologies to CFD code developers:

1. Complete *simulation codes* that support the integration of specific user-defined modules (e.g., Fluent [6]) are most useful for enhancing existing physics capabilities of the simulation code.

2. *Simulation frameworks* that support the overall development process (e.g. FEMLab [4]) can be both powerful and flexible, but are aimed primarily at development of new simulation codes, not enhancement of existing codes.

3. *Libraries* that support specific aspects of the simulation process (e.g., LAPACK [9] or PETSc [1] for numerical linear algebra) typically provide important supporting infrastructure for a simulation, with the drawback that different libraries express essentially the same functionality differently at the programming level.

4. *Components* are software objects that encapsulate specific functionalities using a clearly-defined interface. Typically, each interface is supported by multiple implementations which allows code developers to easily experiment with different approaches.

While each of these approaches is useful under some circumstances, this paper will focus on the component approach. The primary difference between a component and a library — and the primary advantage of using components — is that a component has a fixed API, and so applications can use components interchangeably, as opposed to a library, where changing from one to another requires (perhaps significant) re-programming effort. Because components have a specifically prescribed interface and behavior, application-component and component-component interactions are much simpler than in the other cases listed above — replacing one component with another requires no re-writing of existing code. The use of components is ideal in the case where there is already a substantial investment in the simulation code and the developers are interested in incorporating advanced functionality or experimenting with several different, related approaches.

This paper introduces the work of the Terascale Simulation Tools and Technologies (TSTT) consortium to develop components for mesh, geometry, and field functionality, including general relationships between them. In addition to defining interfaces for these components, members of the consortium are adding support for these interfaces to their existing tools. We

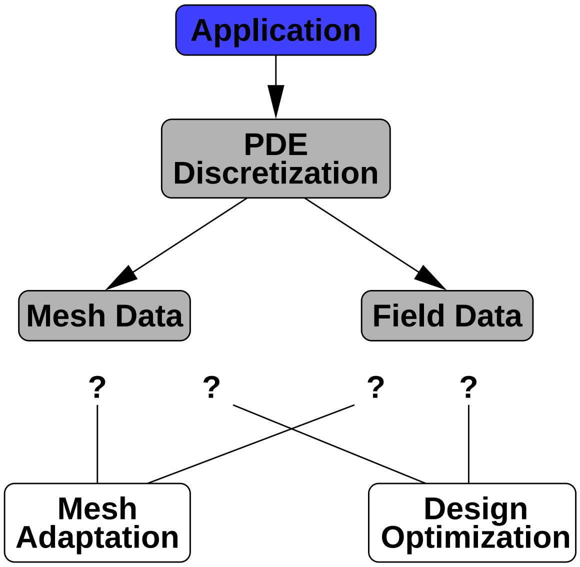


Figure 1: Current typical scenario for interfacing existing code with external services.

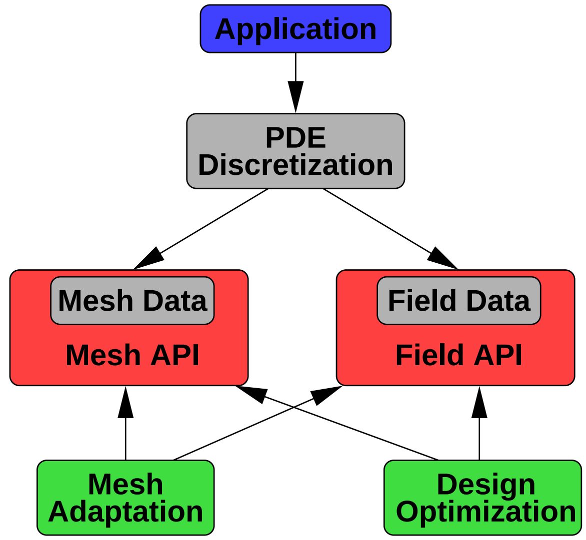


Figure 2: Wrapping existing data in a component API supports use of off-the-shelf services written to use that API.

discuss the component paradigm and its application to CFD simulations in more detail in Section 2.

Essential to the development of any software component is a clear definition of an abstract data model describing the type of data on which the component will operate; the TSTT data model is described in Section 3. The scope of each of the interfaces — mesh, geometry, fields, and relationships — and a summary of the functionality of each is given in Section 4.

2 The Component Paradigm

All CFD application codes, by necessity, store and manipulate both mesh data and solution data discretized on that mesh. Beyond this fundamental similarity, however, lie a dizzying array of ways to represent and retrieve data, each with its advantages for particular scenarios. However, these variations make it essentially impossible to employ software modules written by other developers because of data structure incompatibilities, as suggested in Figure 1.

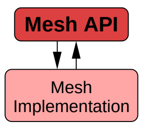
In the component programming paradigm, the data model and application programming interface (API) for a particular set of functionality is standardized as a *component*. In this way, tools like mesh adaptation can exploit the standard functionality of a mesh interface without needing explicit information about how that functionality is implemented. If the code from the previous example were to provide access to its data structures through a component API, adding additional functionality would be trivial, since existing services based on the API could be used for the effort of compiling and linking them, as shown in Figure 2.

The component paradigm supports both horizontal and vertical interoperability. Horizontal interoperability implies that multiple services exist that use the same interface to perform the same task, and an application can choose whichever one best suits its purposes. For instance, two interfaces may be available to query CAD-based geometric data, but one interface might support a CAD file format that the other doesn't. Vertical interoperability implies that services at different levels of complexity can be combined to create a high-level application. For instance, implementations of basic geometry query and mesh query and modification components could be combined with services that perform vertex insertion and topology change to create a mesh generation application.

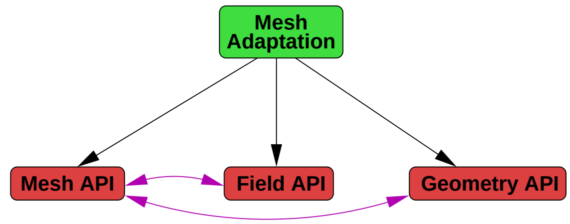
Overall, we envision at least four possible usage modes for our mesh, geometry, and field component interfaces.

1. At the lowest level, we expect to see implementations of the basic interfaces, typically built on existing software infrastructure (mesh databases, geometry modelers, etc; see Figure 3a).

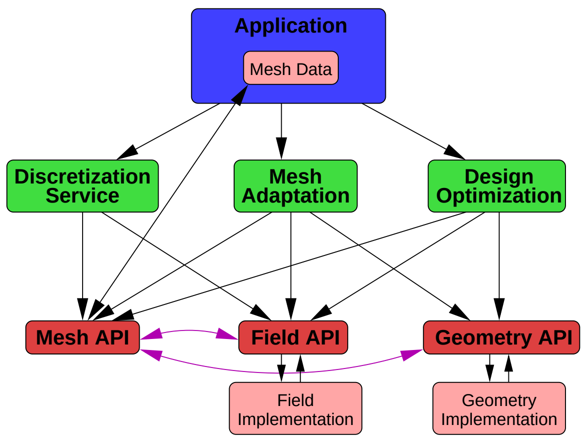
2. Algorithms for common tasks, including mesh manipulation and discretization tasks, can be



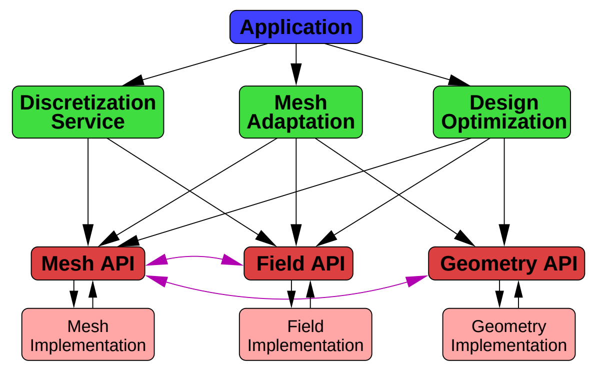
(a) Component interface wrapper for an existing implementation.



(b) Service built on component API's.



(c) Application using builtin API for internal data and external implementations of other components.



(d) Application constructed from high-level services using external implementations for all low-level components.

Figure 3: Possible usage modes for mesh, geometry, and field components.

written as services that use the TSTT interface, and are then interoperable between implementations of the interface (Figure 3b).

3. Applications that already have infrastructure can take advantage of TSTT-based services by providing access to their internal data structures through TSTT interfaces (Figure 3c).

4. Applications can be largely assembled from existing implementations and services, in much the same way that simulation frameworks are currently used (Figure 3d).

3 TSTT DATA MODEL

The TSTT data model partitions the data required by a simulation into three *core data types*: the geometric data, the mesh data, and the field data. Interfaces to the data represented by these abstractions channel the flow of information throughout the simulation. For example, TSTT adaptive mesh refinement services access solution information for error estimation via the field interface; modify the mesh using the mesh interface; and query the geometry interface when creating mesh entities on domain boundaries. These core data types are associated with each other through *data relation managers*. The data relation managers control the relationships among two or more of the core data types, resolve cross references between entities in different groups, and can provide additional functionality that depends on multiple core data types.

A key aspect of the TSTT approach is that we do not enforce any particular data structure or implementation with our interfaces, requiring only that certain questions about the geometry, mesh, or field data can be answered through calls to the interface. To encourage adoption of the interface, we aim to create a small set of interfaces that existing mesh and geometry packages can support. The latter point is critical: hundreds of person-years have been invested in the development of a wide variety of geometry, mesh generation and mesh management toolkits. These software packages will not be rewritten from scratch to conform to a common API; rather the API must be data structure neutral and allow for a broad range of underlying mesh, geometry, and field representations. However, only a small set of functionalities can be covered by a ’core’ set of interface functions. To increase the functionality of the TSTT interface, we define additional, optional, interfaces for which we will provide reference implementations based on the core interface methods. Developers can incrementally adopt the interface by implementing the optional functions on their own mesh database as needed.

The TSTT data models for mesh, geometry and fields all make use of the concepts of *entities*, *entity sets*, and *tags*, and we describe these now in some detail.

3.1 Entities

TSTT *entities* are used to represent atomic pieces of information such as a vertices in a mesh or edges in a geometric model. To allow the interface to remain data structure neutral, entities (as well as entity sets and tags) are uniquely represented by opaque handles. Unless entities are added or removed, these handles must be invariant through different calls to the interface in the lifetime of the TSTT interface, in the sense that a given entity will always have the same handle. Access to entities and their data is provided through the mesh, geometry or field interfaces, which we describe in detail in the sections that follow.

Entity adjacency relationships define how the entities connect to each other and both first-order and second-order adjacencies are supported for the mesh and geometry interfaces.

- *First-order adjacencies*: For an entity of dimension d, first-order adjacencies return all of the entities of dimension q, which are either on the closure of the entity ($d > q$, downward adjacency), or which it is on the closure of ($d < q$, upward adjacency).

- *Second-order adjacencies*: Many applications require not only information about first-order adjacencies, but also about the next level of neighbors. Although such information can always be determined from the appropriate first-order adjacencies, their application is common enough that supporting a second-order adjacency function is useful. A second-order adjacency determines the set of topological entities of a given type adjacent to entities that share common boundary entities of the specified type. An example would be the set of regions that share a bounding edge with the given region.

3.2 Entity Sets

A TSTT *entity set* is an arbitrary collection of TSTT entities that have uniquely defined entity handles. Each entity set may be an unordered set or it may be a (possibly non-unique) ordered list of entities. When a TSTT mesh, geometry or field object is first created in a simulation, a *root set* is created and can be populated by using the load functionality of the object.

Two primary relationships among entity sets are supported:

- Entity sets may *contain* one or more entity sets. An entity set contained in another may be either a subset or an element of that entity set. The choice between these two interpretations is left to the application; TSTT supports both interpretations. If entity set A is contained in entity set B, a request for the contents of B will include the entities in A and the entities in sets contained in A if the application requests the contents recursively. We note that the *root set* cannot be contained in another entity set.

- *Parent/child relationships* between entity sets are used to represent relations between sets, much like directed edges connecting nodes in a graph. This relationship can be used to indicate that two meshes have a logical relationship to each other, including multigrid and adaptive mesh sequences. Because we distinguish between parent and child links, this is a directed graph. Also, the meaning of cyclic parent/child relationships is dubious, at best, so graphs must be acyclic. No other assumptions are made about the graph.

Users are able to query entity sets for their entities and entity adjacency relationships. Both array- and iterator-based access patterns are supported. In addition, entity sets also have "set operation" capabilities; in particular, existing TSTT entities may be added to or removed from the entity set, and sets may be subtracted, intersected, or united.

3.3 Tags

TSTT *tags* are used as containers for user-defined opaque data that can be attached to TSTT entities and entity sets. Tags can be multi-valued which implies that a given tag handle can be associated with many different entities. In the general case, TSTT tags do not have a predefined type and allow the user to attach any opaque data to TSTT entities. To improve ease of use and performance, we support three specialized tag types: integers, doubles, and entity handles. Tags have and can return their name (as a string), size, handle and data. Tag data can be retrieved from TSTT entities by handle in an agglomerated or individual manner. The TSTT implementation is expected to allocate the memory as needed to store the tag data.

4 THE TSTT INTERFACES

4.1 The Mesh Interface

TSTT *mesh entities* are the fundamental building blocks of the TSTT mesh interface and correspond to the individual pieces of the domain decomposition (mesh). Specific examples of mesh entities include, for example, a hexahedron, tetrahedron, edge, triangle and vertex. Mesh entities are classified by their entity type (topological dimension) and entity topology (shape). Allowable mesh entity types are vertex (0D), edge (1D), face (2D), and region (3D). Allowable entity topologies are point (0D); line segment (1D); triangle, quadrilateral, and polygon (2D); and tetrahedron, pyramid, prism, hexahedron, septahedron, and polyhedron (3D); each of these topologies has a unique entity type associated with it. Mesh entity geometry and shape information is associated with the individual mesh entities. For example, the vertices will have coordinates associated with them. Higher-dimensional mesh entities can also have shape information associated with them. For example the coordinates of higher-order finite-element nodes can be associated with mesh edges, faces, and regions.

Higher-dimensional entities are defined in terms of the lower-dimensional entities on their closure (for instance, a triangle could be defined by a list of edges or by a list of vertices) with shape and orientation determined using canonical ordering relationships. Because not all implementations support all possible adjacency relationships, an application can request an *adjacency table* by using a query through the interface. The adjacency table reports, for each possible upward and downward adjacency, whether that adjacency information is always, sometimes, or never available; and to be available at a cost that is constant, logarithmic (i.e., tree search), or linear (i.e., search over all entities) in the size of the mesh. If adjacency information exists, entities must be able to return information in the canonical ordering using both individual and agglomerated request mechanisms.

TSTT *mesh entity sets* are extensively used to group mesh entities in meaningful ways, for example, to represent the set of all faces classified on a geometric face, or the set of regions in a partition for parallel computing. For some computational applications, it is useful for entity sets to comprise a valid computational mesh. The simplest example of this is a non-overlapping, connected set of TSTT region entities, such as the structured and unstructured meshes commonly used in CFD simulations. Collections of entity sets can compose, for example, overlapping and multi-block meshes. In both of these examples, supplemental information on the interactions of the mesh sets will be defined and maintained by the application. Smooth particle hydrodynamic (SPH) meshes can consist of a collection of TSTT vertices with no connectivity or adjacency information.

The mesh interface also includes modification operators that change the geometry and topology. Capabilities include changing vertex coordinates and adding or deleting entities. No validity checks are provided with this basic interface so that care must be taken when using these interfaces. These interfaces are intended to support higher-level functionality such as mesh quality improvement, adaptive schemes, front tracking procedures, and basic mesh generation capabilities, all of which would provide validity checking. Modifiable meshes require interactions with the underlying geometric model including classifying entities.

4.2 The Geometry Interface

The geometry interface provides access to the topology and shape of a geometric model, including the ability to modify the topology and shape as required by optimization and moving body problems. The interface is defined with the intent of supporting both commercial modelers (which often have an underlying parametric surface representation) and models constructed from an input mesh (which typically are not parametric). In the latter case, some algorithm (for example, [8, 13, 20]) must be used to combine appropriate mesh entities into geometric entities.

Most geometry queries in mesh-based simulations are requests for information from a particular geometric entity: a region, a face, an edge, or a vertex. A few situations, particularly those dealing with evolving geometry, will have need for the additional topological constructs of loops and shells (represented in TSTT as sets of faces and edges, respectively). Typical geometric shape queries can be expressed either in physical coordinates or in parametric coordinate. The latter are much more efficient — as much as two orders of magnitude — but are not always available. To maximize efficiency while still providing general functionality regardless of the underlying shape representation, the TSTT geometry interface provides both parametric and non-parametric versions of all shape queries.

The geometric interface functions are grouped by the level of geometric model information needed to support them and the type of information they provide.The base level includes:

Model loading. This includes not only reading the model data, but also initiating any supporting processes (such as a CAD engine) and preprocessing the data as required (for example, producing a piecewise spline surface from mesh data).

Adjacency queries for regions, faces, edges, and vertices in the geometric model.

Iterators over regions, faces, edges, and vertices.

Geometric shape interrogations. Typical functions include returning the closest point on a model entity, getting coordinates, normals, tangents and curvatures, and requesting bounding boxes of entities.

Tag functionality, to associate user-defined information with entities.

Other groups of functions increase the functionality and/or the efficiency of the interface. Functions of this type that have been defined for the geometry interface include:

Geometric sense information indicating how face normals and edge tangents are oriented.

Parametric coordinates for edges and faces. The functions in this group include conversion between global and parametric coordinates, conversion between parametric coordinates of points on the closure of multiple entities, and the full set of pointwise geometric interrogations for a point given its parametric coordinates on a particular geometric entity.

Tolerance information. These functions provide access to the geometric modeling tolerances used by the modeling system in the determination of how closely adjacent entities must be matched. This information is essential, for instance, when constructing viscous meshes near the intersection of two surfaces.

Additional functions of value to specific mesh-based applications that have not yet been defined include:

General topology. The functions described above do not directly support shells and loops, and do not support non-manifold geometries at all.

Model modification, both topological and geometric.

4.3 The Field Interface

The TSTT field interface is intended to provide solution data in a form that supports queries and other operations by external software. Two common situations in which fields are a useful construct are multiphysics analysis, where the solution (or some derived quantity) from one physical problem provides a boundary condition or forcing function for another; and the implementation of mesh adaptation services, where solution fields are used to estimate error and hence the new mesh size and shape distribution. In each of these cases, the use of a field interface hides the way that solution data is treated by the underlying implementation, enabling interchange of physics modules or of adaptation drivers without changing how data is accessed.

Physical information about the dependent flow variables in a CFD simulation can be represented by using tensor quantities, including density (rank 0), velocity (rank 1), and viscous stress (rank 2). While physically these variables are defined at all points in the flow, a field contains only a discrete representation of the variable, stored as a collection of discrete values called degrees of freedom. Each field representation has a method for using this discrete data to compute variable values at all locations; regardless of the underlying discretization scheme, this conversion from discrete to piecewise continuous data is primarily a geometric operation. For example, finite element and discontinuous Galerkin methods use shape functions to compute data at arbitrary locations, while unstructured finite volume methods use reconstruction.

A complex simulation process can involve a number of fields defined over various portions of the domain of the simulation. A single field can be used by a number of different analysis routines that interact, and the field may be associated with multiple meshes and have a different relationship with each one. In addition, different distributions can be used by a field to discretize its associated tensor. The ability to have a specific tensor defined over multiple meshes and/or discretized in terms of multiple distributions is handled by supporting multiple instances. A field instance has a single set of distributions over a given mesh.

The TSTT consortium is currently defining interoperable functions for field I/O, interrogation, coordinate transforms, and transfer between field instances. The latter capability is useful, for instance in projecting a discontinuous stress field onto a set of continuous shape functions or transferring pressure data from a finite volume flow solution to a finite element solid mechanics solver.

4.4 Relationships Between Data in Different Interfaces

In addition to functions that operate only on mesh data or only on geometric, the TSTT interface contains functions to relate mesh, geometry, and field data. For instance, *classification* of mesh faces onto faces of a geometric model is accomplished through the relations interface. In addition to simple set and query functions for one-to-one and one-to-many relationships, the relations interface contains advanced functionality to support deduction of relationships among data of different data. For instance, a mesh file may contain tags that indicate classification of mesh entities onto a geometric model; the relations interface essentially prompts the mesh implementation to convert that tag data into relationships between mesh and geometry entities, which can then be accessed in a standard way through the relations interface.

5 Current Status and Future Plans

5.1 Implementation of the Interfaces

The mesh interface definition effort is complete, and several implementations are also nearly complete, which are built on existing mesh management toolkits: FMDB (RPI) [14], GRUMMP (UBC) [12], MOAB (SNL) [18, 17], NWGrid (PNNL) [19], and Overture (LLNL) [7, 3]. The geometry interface is essentially complete, and implementation efforts are underway, based on the CGM (SNL) [15, 16] geometry toolkit. The field interface definition is not yet complete, and so no implementations that support it directly exist at present.

5.2 Services Built on the Interfaces

Several services have been built on top of the current interfaces. Strictly speaking, these services are themselves components, with their own interfaces. Unlike the mesh, geometry, and field interfaces, which encapsulate data and data access, the services encapsulate *algorithms*. Because the mesh interface and its implementations are the most mature, most current services are built on the mesh interface. These include mesh swapping [11], smoothing [2], and adaptation [10]; these services also require at least some access to mesh geometry information. Other services currently under development include front-tracking (based on FronTier [5]) and general mesh and geometry access (based on MOAB [18, 17] and CGM [15, 16]).

5.3 Future Plans

One of the main short-term technical goals of the TSTT consortium is to complete the definition of the fields interface and implement it. This will open up a new range of possible services, including mesh-to-mesh solution transfer, a general AMR service, and discretization support services. Also planned for the short-term, in conjunction with applications projects, are a shape optimization service and services to generate and manipulate meshes in parallel.

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