Requirements on PDE solver component interfaces for multi-physics simulations

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Background

Motivating Examples

- Overlayed
- FSI

Evaluation Prototype

- Functionality
- Infrastructure

Summary

Background

Different solvers are optimized for different domains.

We want to use solvers as components to enable us to treat multi-component (multi-physics, multi-numerics, multi-domain, multi-cultural...) problems.

We are developing a prototype in order to investigate the requirements on the solver components and their interfaces.

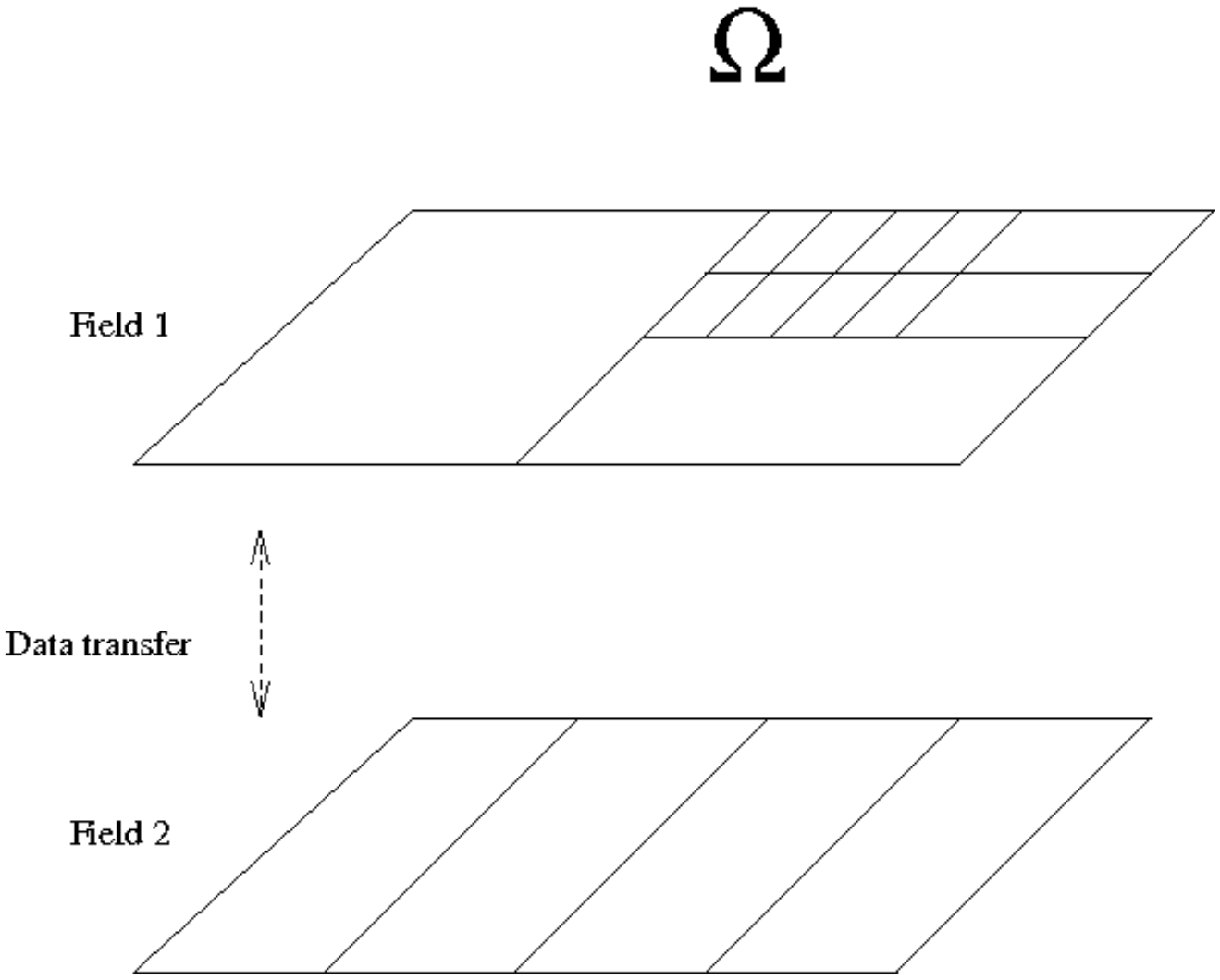
Motivating Examples

- Tsunami

Motivating Examples

- Tsunami
- Heart valve

Overlayed geometries



Also referred to as *field coupling*.

Overlayed geometries

Even with identical geometries for the two solver components, grids may be still non-matching due to e.g.

- adaptive mesh refinement (AMR),
- dynamic load balancing (DLB).

Key issues

Rendezvous algorithm identifies the necessary process communication pattern.

AMR and DLB result in a need for a continuously updated process communication pattern.

Large amounts of transfered data means that point-to-point communication and a shared address space are preferred in order to avoid a communication bottleneck.

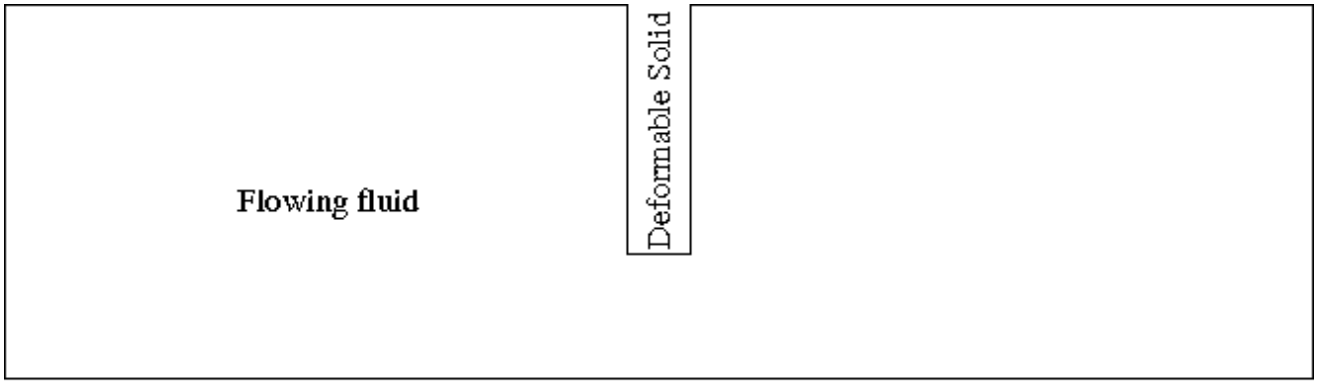
Relevant Projects

Sierra internal project at Sandia National Laboratories, has a well designed rendezvous algorithm. Interfaces a large number (> 10) proprietary Sandia codes.

Common Component Architecture, CCA open project under the auspices of the US, Department of Energy. The CCA goes hand in hand with

Babel with SIDL by CASC at the Lawrence Livermore National Laboratory (LLNL). SIDL is a Scientific Interface Definition Language, and Bable is a multi-language stub generator for it.

Fluid-Structure Interaction



Also referred to as *interface coupling*.
Interface grids are, in the general case,

- moving,
- non-matching.

Key issues

Projection is needed if the two surfaces do not coincide.

Association (neighbor search) identifies the data points that are needed in order to determine a new field value at a specific point.

Interpolation is used to compute new values for the case of non-matching grids. Depending on the type of interpolation it may be necessary to communicate information about element types along with the field values.

Component issues

Dynamic grids are needed if the interface is moving. This is not a communication issue but rather a requirement on the solver components.

Sub-iteration Iteration until convergence at each time step increases accuracy. Not all external modules support this.

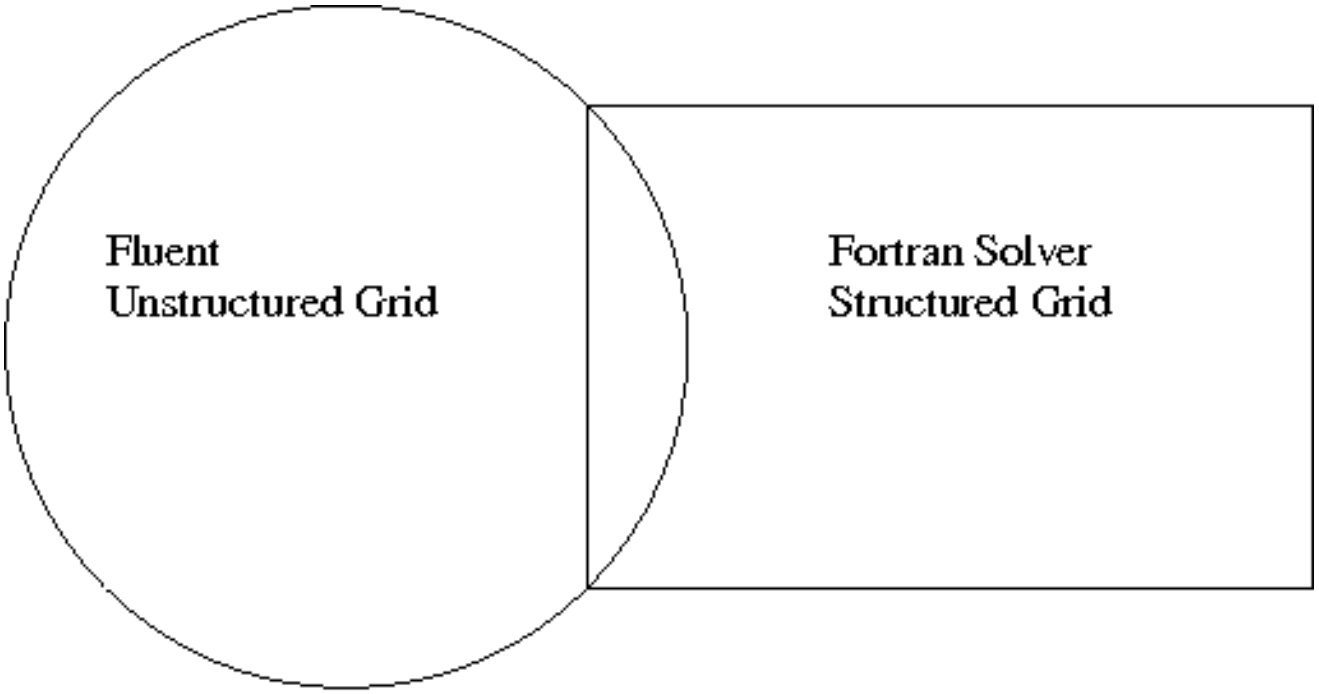
Independent Parallelization The two physics modules may both require control of the MPI address space, which means that their two MPI worlds, i.e. address spaces, need to be separated.

Relevant Projects

MpCCI Commercial project from Fraunhofer-SCAI in Germany. Focuses on FSI, and hence lacks a good rendezvous algorithm. Interfaces a large number (> 10) commercial codes. Has a well documented and general strategy for how to integrate new external modules.

Babel RMI by CASC at LLNL. This is a new prototype implementation of an extended Babel with support for Remote Method Invocation. This means that components can live in separate address spaces.

Prototype Functionality

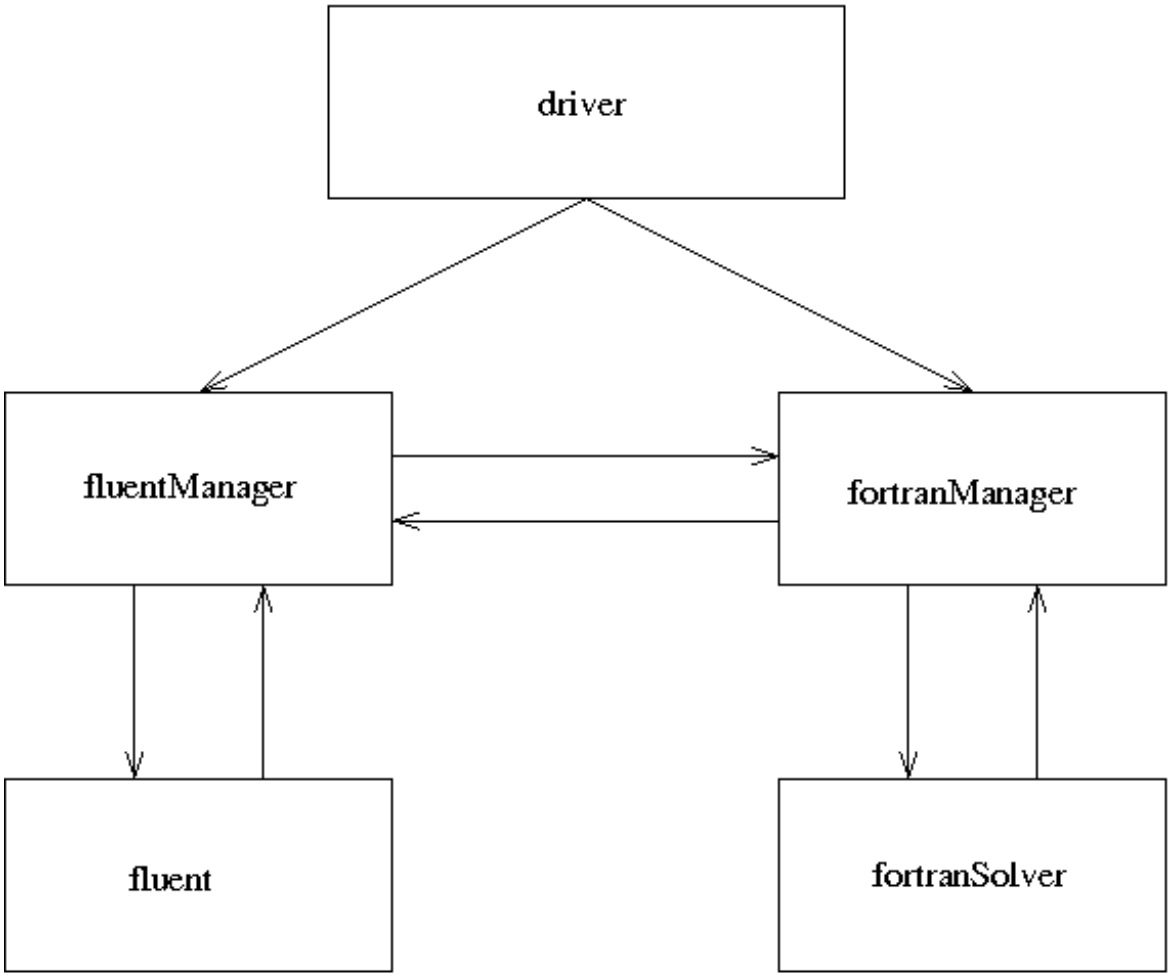


Two component heat solver using Fluent for one component and a small Fortran solver for the other.

Prototype Functionality, cont.

- SIDL/Bable interface definitions
- interface coupling
- radial basis function interpolation
- moving grid

Prototype Infrastructure



Summary

A component architecture is a flexible foundation for developing multi-physics solvers.

Requirements on the component interfaces depend on the type of application as well as on component abilities.

We are developing a multi-physics solver prototype in order to investigate the tradeoffs for different solutions to different problem configurations.