

## Simulation of a Conjugate Heat Transfer using a preCICE Coupling Library

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### 1. Introduction

Severe accident may accompany complicated thermo-fluid phenomena including water vaporization, vapor condensation and hydrogen combustion. To mitigate severe accident scenarios, those complicated physics need to be understood in detail. Wall condensation would be accurately resolved when conjugate heat transfer (CHT) including heat conduction through the containment wall is reflected. Fluid-structure interaction could be important to assess structural integrity if a hydrogen detonation propagates.

Multi-scale and multi-physics phenomena can be simulated by an integrated program having several solvers as modules. On the other hand, independent solvers can be coupled via a coupling library. Two approaches have its own pros and cons, but if flexible selection of solvers is preferred, the latter option could be better than the former.

Coupled simulation between different solvers such as flow solver, structural solver, 1D system solver, and so on requires robust treatment at the interfaces between solvers because conservation and stability issues may arise due to coupling. A preCICE library has been developed to couple various solvers [1]. It provides robust coupling capability. In this work, a CHT problem was simulated to study feasibility of the coupling library.

### 2. Methods and Results

To solve a CHT problem, OpenFOAM solvers were applied. *chtMultiRegionSimpleFoam* is an integrated solver tightly coupling *buoyantSimpleFoam* solver and *laplacianFoam* solver. Two solvers can be also coupled via the preCICE library. In this section, governing equations of two solvers are described.

#### 2.1 *buoyantSimpleFoam* solver

Continuity, momentum and energy equations for the *buoyantSimpleFoam* are written as below [2].

##### Continuity equation

$$\nabla \cdot (\rho \mathbf{u}) = 0, \quad (1)$$

where,  $\mathbf{u}, \rho$  are velocity vector and density, respectively.

##### Momentum equations

$$\nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \rho \mathbf{g} + \nabla \cdot (2\mu_{eff} \mathbf{D}(\mathbf{u})) - \nabla \left( \frac{2}{3} \mu_{eff} (\nabla \cdot \mathbf{u}) \right), \quad (2)$$

where,  $p, \mathbf{g}, \mu_{eff}, \mathbf{D}(\mathbf{u})$  are static pressure, gravitational acceleration, effective viscosity, rate of strain tensor, respectively.  $\mu_{eff}$  is a sum of molecular viscosity and turbulent viscosity and  $\mathbf{D}(\mathbf{u})$  is defined as  $\mathbf{D}(\mathbf{u}) = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ .

##### Energy equation

Energy equation can be solved by using internal energy  $e$  or enthalpy  $h$  as follows.

$$\nabla \cdot (\rho \mathbf{u} e) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \mathbf{u} K) + \nabla \cdot (p \mathbf{u}) = \nabla \cdot (\alpha_{eff} \nabla e) + \rho \mathbf{u} \cdot \mathbf{g}, \quad (3)$$

$$\nabla \cdot (\rho \mathbf{u} h) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho \mathbf{u} K) - \frac{\partial p}{\partial t} = \nabla \cdot (\alpha_{eff} \nabla h) + \rho \mathbf{u} \cdot \mathbf{g}, \quad (4)$$

where,  $K \equiv |\mathbf{u}|^2/2$  is a kinetic energy per unit mass and  $h$  can be written as  $h \equiv e + p/\rho$ . Effective thermal diffusivity  $\alpha_{eff}$  is calculated as  $\alpha_{eff} = \rho v_t / Pr_t + \mu / Pr = \rho v_t / Pr_t + k / c_p$  and  $k, c_p, \mu, v_t, Pr, Pr_t$  are thermal conductivity, specific heat, viscosity, turbulent kinematic viscosity, Prandtl number and turbulent Prandtl number, respectively.

#### 2.2 *laplacianFoam* solver

Conductive heat transfer through solid can be solved by *laplacianFoam* for which governing equation is written as follows.

$$\frac{\partial T}{\partial t} = \nabla \cdot (\alpha \nabla T), \quad (5)$$

where,  $\alpha = k / (\rho c_p)$  is a thermal diffusion coefficient and  $k, \rho, c_p$  are thermal conductivity, density, and specific heat of solid, respectively. For steady state simulation, the time term is removed.

#### 2.3 *chtMultiRegionSimpleFoam* solver

Solution procedure using the *chtMultiRegionSimpleFoam* which tightly coupled *buoyantSimpleFoam* and *laplacianFoam* is illustrated in Fig. 1. Mesh is generated for full domain and split into fluid and solid regions. For each regions, boundary conditions and properties are separately defined by a utility program.

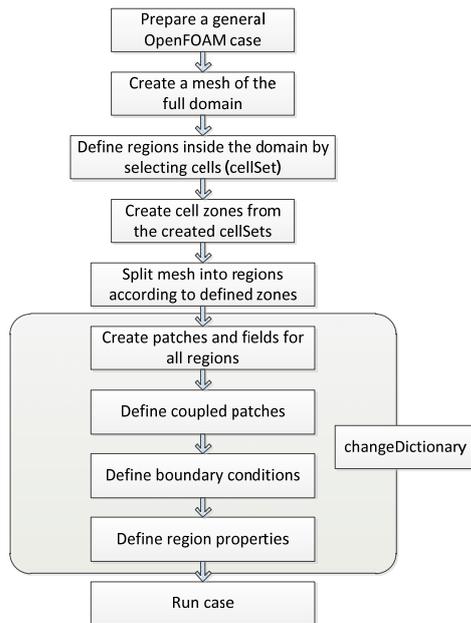


Fig. 1. Work flow of *chtMultiRegionSimpleFoam* [3]

#### 2.4 preCICE coupling library

preCICE (Precise Code Interaction Coupling Environment) is a coupling library for partitioned multi-physics simulations, including, but not restricted to fluid-structure interaction and CHT [4]. As shown in Fig. 2, preCICE can couple commercial codes, open source codes and in-house codes by using adapters.

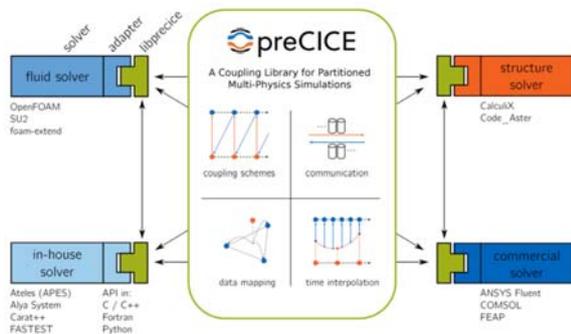


Fig. 2. Concept of preCICE library [4]

Coupling configuration is set by `precice-config.xml` file. The xml file has 5 parts for configuration which are composed of coupling data, mesh information for mapping, coupling participants, communication channel and coupling schemes as in Fig. 3.

```
<precice-configuration>
  <solver-interface dimensions="3">
    <data .../>
    <mesh .../>
    <participant .../>
    <m2n .../>
    <coupling-scheme .../>
  </solver-interface>
</precice-configuration>
```

Fig. 3. Configuration file for preCICE

There are two types of mapping constraints for preCICE, i.e., consistent and conservative. Consistent constraint is applied for normalized quantities such as temperature and pressure and the value at coarse nodes is the same as the value at the corresponding fine node. Conservative constraint is applied for absolute quantities such as force and mass and the value at a coarse node is calculated as an aggregation of the corresponding fine nodes, such that the total coupling value on the coarse and fine mesh is the same [5].

To find a corresponding node, there are two key methods. “nearest-neighbor” is a first-order method and “nearest-projection” is a second-order method which first projects onto mesh elements and then uses linear interpolation within each element as shown in Fig. 4. The latter method is relatively fast and numerically superior to the former.

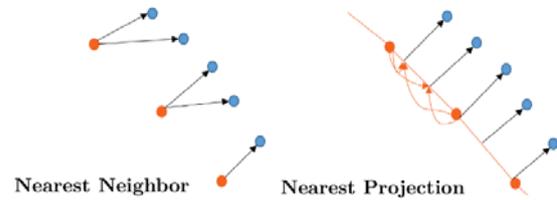


Fig. 4. Mapping methods [5]

A coupling scheme can be one of four sets, i.e., serial-explicit, serial-implicit, parallel-explicit and parallel-implicit. For serial coupling, all the programs are run in a sequential manner, i.e., one participant after the other. For parallel coupling, all the programs are run simultaneously. Explicit and implicit denote time marching schemes. Implicit scheme is more stable than explicit scheme but for implicit scheme acceleration techniques need to be applied. There are three different types of acceleration techniques in preCICE which are constant (constant under-relaxation), aiten (adaptive under-relaxation), and various quasi-Newton variants (IQN-ILS, IQN-IMVJ). Quasi-Newton methods are usually recommended for a stable acceleration.

#### 2.4 Results using chtMultiRegionSimpleFoam solver

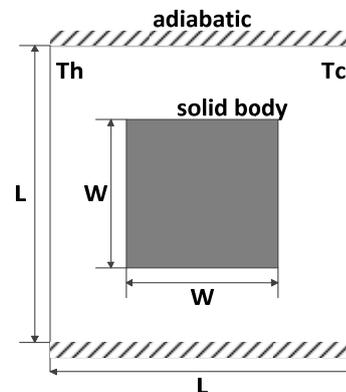


Fig. 5. Layout of a conjugate heat transfer case

For a CHT analysis, a cavity having a solid inside was chosen [6]. Boundary conditions are set as shown in Fig. 5. For this case, natural circulation characteristics is influenced by the conductivity value of the solid block. Temperature difference between two facing vertical walls induces natural circulation.

Ratio between length of one side of the solid block and height of the vertical wall was set to  $W/L=0.5$ . Non-dimensional numbers were set to  $Pr=0.71$ ,  $Ra=10^5$ . Rayleigh number is defined as  $Ra = \rho g \beta \Delta T L^3 / (\alpha \nu) = Gr * Pr$ , where  $\rho, g, \beta, \Delta T, L, \alpha, \nu$  are fluid density, gravitational acceleration, thermal expansion coefficient, temperature difference between the vertical walls, thermal diffusivity, kinematic viscosity, respectively. By using Prandtl number and Rayleigh number, Grashof number is calculated as  $Gr = 140,845$ . Then, the height of the vertical wall can be calculated as  $L = [Gr \mu^2 / (\rho^2 g \beta \Delta T)]^{1/3} = 0.0444 \text{ m}$ . Thermal properties of fluid and solid were given at 300 K.

Thermal conductivity of the solid block was changed by controlling the ratio of solid conductivity and fluid conductivity,  $k^* (=k_s/k)$ , as keeping the fluid conductivity constant.

Mesh sensitivity was tested with several grid systems (refer to Fig. 6). blockMesh utility was used for mesh generation. Mesh was clustered near the walls. CHT inside the cavity was calculated by using *chtMultiRegionSimpleFoam* solver. Fig. 7 and Fig. 8 show temperature distributions and velocity distributions, respectively. In Fig. 8, top figures display velocity vectors as well. Air rises at the hot wall and goes down along the cold wall. Difference is not significant depending on number of meshes. Averaged Nusselt number was calculated at the left wall and compared with each other. Table I shows that Nusselt number converges after 40x40 grid system.

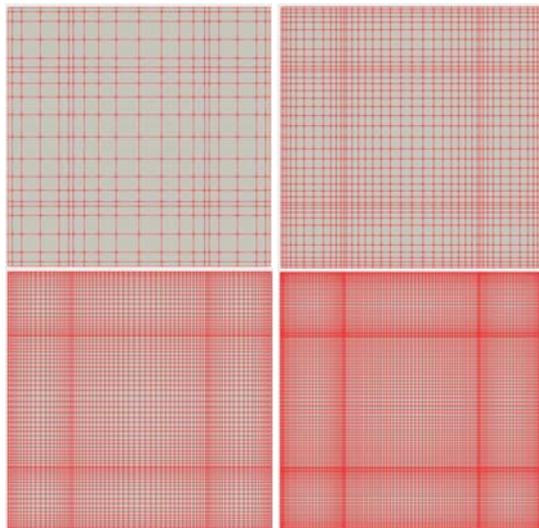


Fig. 6. Grid systems, 20x20, 40x40, 80x80, 120x120 (clockwise from top left corner)

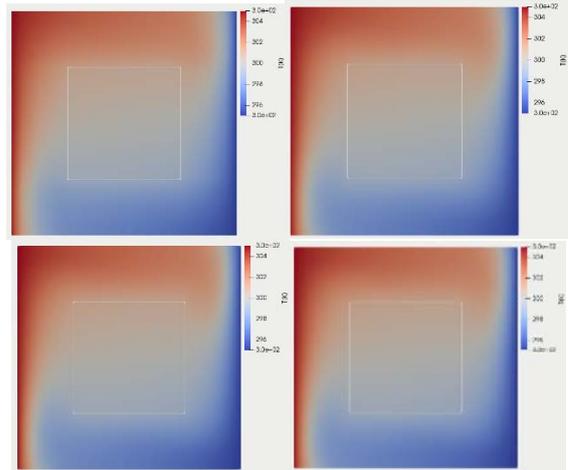


Fig. 7. Temperature distribution, 20x20, 40x40, 80x80, 120x120 (clockwise from top left corner)

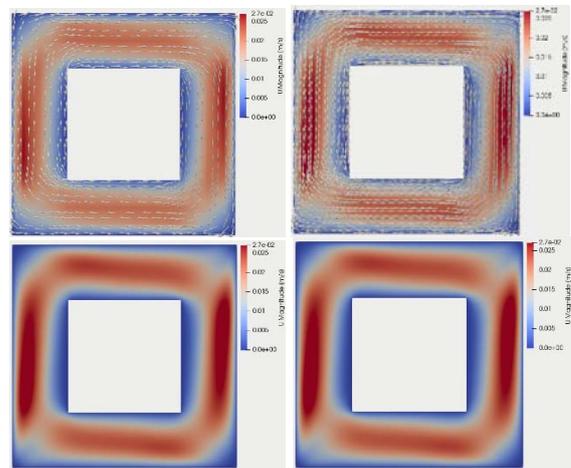


Fig. 8. Velocity distribution, 20x20, 40x40, 80x80, 120x120 (clockwise from top left corner)

Table I. Average Nusselt number on the left wall

	House [6]	chtMultiRegionSimpleFoam			
		20x20	40x40	80x80	120x120
Nusselt No.	4.322	4.308	4.317	4.317	4.317

Fig. 9 shows influence of the thermal conductivity of the solid block. As the thermal conductivity of the solid block becomes smaller, flow temperature around the block gets higher. This means that heat transfer via fluid increases because heat conduction through the solid decreases. This fact was confirmed by the averaged Nusselt number calculated at the left wall (refer to Table II).

Table II: Average Nusselt number on the left vertical wall

conductivity	Nusselt Number	
	House[6]	chtMultiRegionSimpleFoam
$k^*=5$	4.322	4.317
$k^*=1$	4.506	4.502
$k^*=0.2$	4.626	4.622

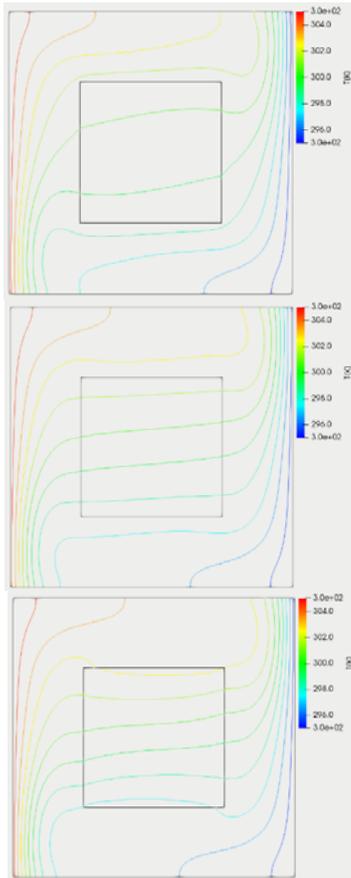


Fig. 9. Temperature contours,  $k^*=5, 1, 0.2$  (from top to bottom)

### 2.5 Results using preCICE coupling

For coupling between two solvers, implicit scheme with acceleration technique of quasi-Newton method was applied. At the interface between fluid region and solid region, heat flux data calculated by *laplacianFoam* solver were mapped into the fluid mesh and temperature data obtained from *buoyantSimpleFoam* solver were mapped into the solid mesh.

Fig. 10 displays meshes for the fluid solver and the solid solver. Fig. 11 shows calculation result of temperature field. For three cases with different thermal conductivity of the solid block, calculations with the preCICE coupling library were carried out. Averaged Nusselt number at the left wall was calculated and compared with other data in Table III. The integrated solver and the coupled solver with the preCICE library gave same results.

### 3. Conclusions

Coupling technique of solvers for different physics is very useful in that pre-existing codes can be utilized and new integrated multi-physics solver is not required to be developed. The preCICE coupling library to simulate a conjugate heat transfer was adopted and calculation results were compared with reference data and results using an integrated solver. Coupling using the preCICE

library was found to be robust and efficient. This coupling library is going to be utilized extensively for multi-scale and multi-physics problems, especially, in severe accident simulations.

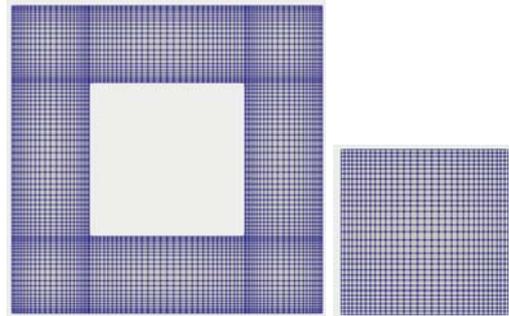


Fig. 10. Meshes for fluid solver (left) and solid solver (right)

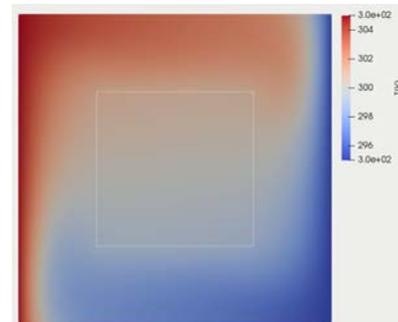


Fig. 11. Temperature distributions for whole domain

Table III Average Nusselt number on the left vertical wall

conductivity	Nusselt Number		
	House[6]	chtMultiRegion-SimpleFoam	preCICE coupling
$k^*=5$	4.322	4.317	4.318
$k^*=1$	4.506	4.502	4.502
$k^*=0.2$	4.626	4.622	4.621

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