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Region Coupling Algorithms in OpenFoam

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Abstract

Region coupling is an interesting approach to combine different solvers in complex multi-physics problems. In OpenFoam® region coupling is usually employed to couple the temperature between solids and fluids but it is generally not limited to this type of problem. For example when simulating a porous medium in a fluid flow it is necessary to not only couple temperature but also pressure, species concentration and velocity of the porous medium and the surrounding fluid in order to be able to combine appropriate solvers for each of the two regions. Such a coupling for porous media was implemented in OpenFoam®-7 based on the loose coupling approach. The influence of grid size and number of solver iterations on the on the coupled solution and it's divergence from an uncoupled reference solution was investigated. The coupled approach is shown to perform better with increasing number of cells in the simulation domain, as opposed to treating the whole simulation domain with a pure two-fluid approach. However, its accuracy depends on additional iterations for the coupling.

Introduction

As the availability of numerical resources for researchers keeps increasing, increasingly complex problems can be investigated by simulations. These problems are often multi-physics problems combining different physical phenomena in a single simulation. Reactive flows, where fluid dynamics and chemistry are coupled, are a common example for these complex problems. It is important to combine effective solution strategies for each of the sub-problems to ensure efficiency [1].
One way to handle complex multi-physics problems in an efficient manner is to split the problem in distinct regions according to the prevalent physical phenomena. Those regions can then be solved separately using specialized solvers and the individual solutions are coupled through an interface. Such a procedure has been successfully employed for the coupling of solvers for compressible and incompressible fluids [2], as well as for the coupling of LES and RANS solvers to model turbulent flows [3]. The motivation for the coupling algorithm presented in this work is to couple single and two-phase Euler simulations to simulate porous particles surrounded by a stream of gas.
chtMultiRegionTwoPhaseEulerFoam implemented in the ESI OpenFOAM® version v1906 [4] and a similar in-house developed solver provide the basis for the current implementation of the multi-region solver. Both developments are capable to couple solid and fluid or solid and two-fluid phases. The new in-house solver is also capable to couple fluid regions with two-phase regions that contain a fluid as well as a solid part. The mixed coupling boundary conditions for temperature are the basis for implementing the coupling of species, pressure and velocity in the in-house solver which is based on OpenFOAM®-7 [5].

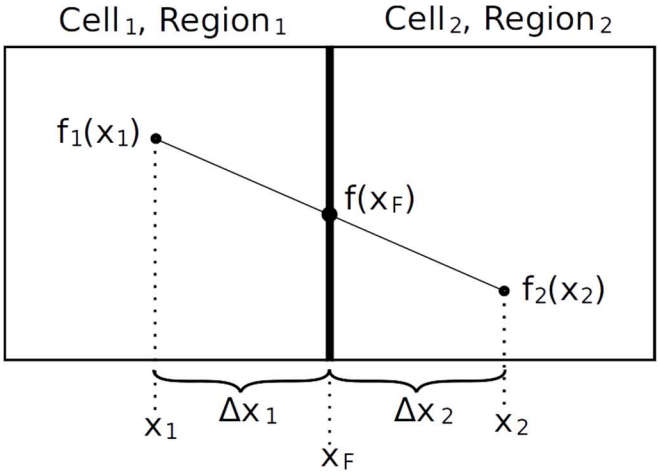

Figure 1: Schematic illustration of the discretization of the region coupling approach. Two neighboring cells belonging to two different regions, where the function $f_i(x)$ has a distinct value in each cell center. The distance from each cell center to the interface is Δx_i, while the interface is located at x_F and the value of f(x) at the interface has to be calculated by assuming a continuous function across both regions.

Region Coupling Boundary Conditions

In general, OpenFoam® employs a loose coupling approach for coupling different simulation regions. This approach is also known as explicit Robin-Neumann coupling, for details see [1]. Loose coupling means that the solution of the first region is obtained using the initial conditions specified at the interface between the coupled regions. This solution is then used to set the boundary condition value at the interface to the second region. The second region is now solved based on the already known solution of the first region at the interface as an initial condition. This introduces a hierarchy of solutions where the second region's solution depends on the previously obtained first region's solution. In order to break up this hierarchy an iterative solution procedure is employed, where, without advancing the time step, both regions are repeatedly solved based on each other's previous solutions as initial conditions. This approach is analogous to the one employed by the ESI OpenFoam® version v1906 and the procedure is repeated until convergence or a maximum number of iterations is reached. In order to couple two simulation domains through an interface any function *f(x)* (e.g. species concentration, pressure or velocity) needs to be continuous at that interface. This can be treated analogous to most boundary value problems with periodic boundary conditions in physics, where a continuous solution is needed, by requiring *f(x)* and its derivative *df(x)/dx* to have the same values at each side of the interface. This means the following two equations must hold true exactly at the interface:

$$\frac{df_1(x)}{dx}|_{x=x_F} = \frac{df_2(x)}{dx}|_{x=x_F} = \frac{df(x_F)}{dx}, \quad (1)$$

$$f_1(x)|_{x=x_F} = f_2(x)|_{x=x_F} = f(x_F). \quad (2)$$

Here x_F is the spatial location of the interface, as illustrated in Figure 1. To convert these requirements into a boundary condition, the conservation equations have to be discretized at the boundary for each region. The first order approximation of the discretized first derivative is:

$$\frac{df(x)}{dx} \approx \frac{f(x_a) - f(x_b)}{\Delta x_{ab}}, \tag{3}$$

here x_a and x_b are two points at a small distance Δx_{ab}. At the interface this yields:

$$\lambda_1 \frac{f(x_F) - f_1(x_1)}{\Delta x_1} = \lambda_2 \frac{f_2(x_2) - f(x_F)}{\Delta x_2}, \tag{4}$$

Here λ_1 and λ_2 are transport coefficients, for e.g. thermal conductivities or diffusion coefficients, and Δx_1 and Δx_2 are the distances between the cell center and the interface. Solving the discretized equation for the boundary value gives the following expression for the interface value:

$$f(x_F) = \frac{\frac{\lambda_1 f_1(x_1)}{\Delta x_1} + \frac{\lambda_2 f_2(x_2)}{\Delta x_2}}{\frac{\lambda_1}{\Delta x_1} + \frac{\lambda_2}{\Delta x_2}}. \tag{5}$$

In OpenFoam® 7 [5] the coupling condition is implemented as mixed boundary condition (BC), which is a linear combination of a Van Neumann and a Dirichlet boundary condition and has the following form:

$$f(x_F) = \zeta \cdot \Phi + (1 - \zeta) \cdot \tag{6}$$

Here ζ is the weighting factor between the Van Neumann and Dirichlet conditions:

$$\zeta = \frac{\frac{\lambda_1}{\Delta x_1}}{\frac{\lambda_1}{\Delta x_1} + \frac{\lambda_2}{\Delta x_2}}. \tag{7}$$

The reference value Φ is the boundary value for the Dirichlet part of the BC and $\frac{\partial \Phi}{\partial x}$ is the surface gradient at the interface used together with the function value $f_i(x_i)$ of the adjacent cell center for the Van Neumann part of the BC:

$$\frac{\partial \Phi}{\partial x} = \left(|S_f| \frac{f(x_2) - f(x_1)}{|d|} \right) \left(\frac{S_f \cdot d}{|S_f| \cdot |d|} \right), \tag{8}$$

with $\boldsymbol{S_f}$ being the surface vector of the interface and d being the vector connecting the two adjacent cell centers [2]. This gradient expression is only used in the pressure and velocity coupling at the interface.

Region Coupling Single-Phase and Two-Phase Regions

The coupling of a single-phase and a two-fluid region requires special attention since the heat flux from the boundary face to the adjacent cell center proceeds via two phases. Discretizing equation 4 for two-phase fluid gives the following equation at the region interface:

$$\lambda_1 \frac{f(x_F) - f_1(x_1)}{\Delta x_1} = \lambda_2{}' \alpha_2{}' \frac{f_2{}'(x_2) - f(x_F)}{\Delta x_2} + \lambda_2{}'' \alpha_2{}'' \frac{f_2{}''(x_2) - f(x_F)}{\Delta x_2}. \tag{9}$$

On the right-hand side of equation 9 contributions of both phases in the two-phase region is needed, where λ_2' and λ_2" are the transport coefficients and α_2' and α_2" are the phase fractions of each phase.
The temperature boundary condition uses an effective thermal conductivity κ_{eff} at the interface, which is the sum of the thermal conductivity in each phase, weighted with the phase fraction α of each phase, similar to OpenFOAM®-v1906 [4]:

$$\kappa_{eff} = \alpha_1 \kappa_1 + \alpha_2 \kappa_2. \tag{10}$$

For species diffusion the contribution of the solid phase is negligible and only the fluid phases of both regions are coupled. A weighted or effective diffusion coefficient D_{eff} is needed to account for the reduced fluid volume in the two-phase region:

$$D_{eff} = \alpha_{fluid} D_{fluid}. \tag{11}$$

OpenFoam® 7 [5] uses Schmidt analogy to determine the mass diffusion coefficient D from the viscosity μ:

$$SC = \frac{\nu}{D} = \frac{\mu}{\rho D} \tag{12}$$

where ν is the kinematic viscosity and ρ the fluid's density.

Test Case Setup

For the analysis of the region coupling method presented in this work, the five 1D test cases with different grid spacings, shown in Figure 2, were employed.

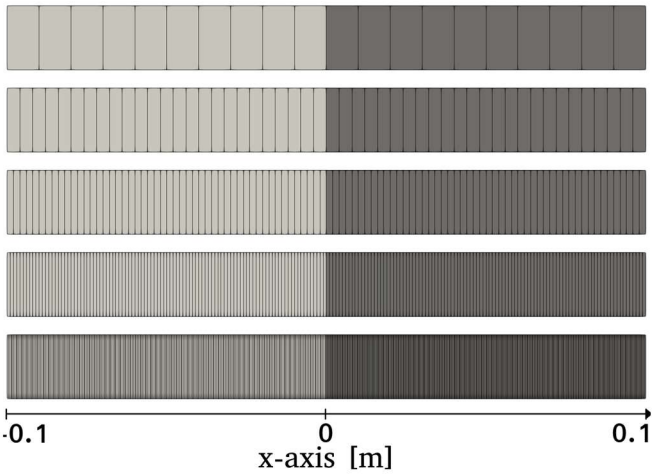

Figure 2: Illustrations of the 5 grids that were used to investigate dependency of solution accuracy on grid spacing. The total number of cells in each grid from top to bottom are: 20, 50, 100, 200 and 500.

Each case is setup identically with a single-phase region extending to the negative x direction and a two-phase region extending to the positive x direction. The interface between the regions is located at x=0 m.
Subsequently, the single-phase region will be referred to as region 1 and the two-phase region will be referred to as region 2. The initial and boundary conditions are identical for each case and are summarized in Table 1.
The solid phase fraction was set to zero in region 2 to allow for a smooth solution in this initial simple test case. The solid phase's temperature at the region interface is set to the same value as the fluid phase temperature to satisfy the initial condition of uniform temperature. Furthermore, the concentrations of N_2 and O_2 are only coupled for the fluid phases in both regions and their concentration is assumed to be constant zero in the solid phase of region 2. The pressure coupling is independent of the two phases in region 2 since the two-fluid model uses the shared pressure [6].
Each case is simulated with the multi-region setup described in Table 1 and an identical single-region setup to evaluate the influences of the coupled boundary conditions by determining the deviation between both solutions.

Table 1: Boundary conditions (BC) and initial values for the single-phase region 1 (R1) and the two-phase region 2 (R2). Here a inletOutlet boundary condition is either a zero gradient condition, when there is an outward flow or a fixed value condition (inletValue) when there is an inward flow. The value-keyword sets the initial value at the patch. The fixedFluxPressure boundary condition calculates the pressure value at the boundary according to the flux set in the velocity boundary condition.

Field	BC R1	Initial Value R1	Initial Value R2	BC R2
T_{fluid} [K]	zero-gradient	2000	1000	zero-Gradient
T_{solid} [K]	-	-	1000	zero-Gradient
$N_{2,fluid}$ [mass fraction]	fixedValue = 0	0.8	1	inletOutlet= inletValue(0), value(1)
$O_{2,fluid)}$ [mass fraction]	fixedValue = 1	0.2	0	inletOutlet= inletValue(1), value(0)
C_{solid} [mass fraction]	-	-	1	zero- Gradient
P_{rgh} [Pa]	fixedFlux-Pressure	100000	100000	fixedValue= internal-Field
U_{fluid} [m/s]	(0 0 0) to (0.08 0 0) in 3s	(0 0 0)	(0 0 0)	inletOutlet= inletValue(0 0 0), value(internalField)

Figure 3 shows the temporal evolution of the single-region solution to give an impression of how the system is supposed to evolve over a time of 10s.

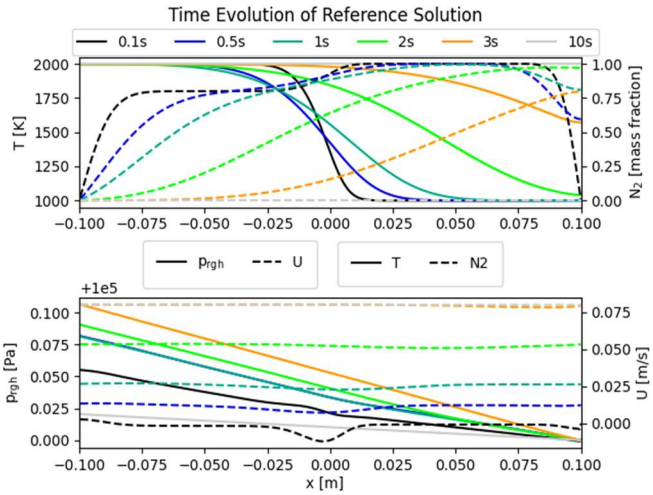

Figure 3: The temporal evolution of the single-region's solution for 500 grid points. The simulation approaches a steady state towards the maximum simulation time of 10s.

Grid Space Influence on Region Coupling

Mesh resolution is a key parameter in any CFD simulation. Especially, when using multi-region coupling. As can be seen in equations 1 and 2 the gradient and values of any function in both regions need to be identical at the interface. Equation 1 also shows that the numerical derivative is calculated in a first order approximation using the patch value and the adjacent cell center properties. However, to satisfy the boundary condition the derivatives need to match exactly at the face center of the boundary. Due to the first order approximation of the derivative its error is inversely correlated to the distance between the face and adjacent cell center. As this effect is only relevant for cells at the interface between two regions, local mesh refinement at the boundary is sufficient to capture the coupling correctly. This greatly reduces the computational cost of coupled multi-region simulations.

A uniform grid resolution was chosen for studying the grid dependence of the region coupling approach, due to its easier evaluation. Figure 4 compares snapshots of solutions for identical multi- and single-region simulations. It is clearly visible that the two solutions for lower grid resolution diverge

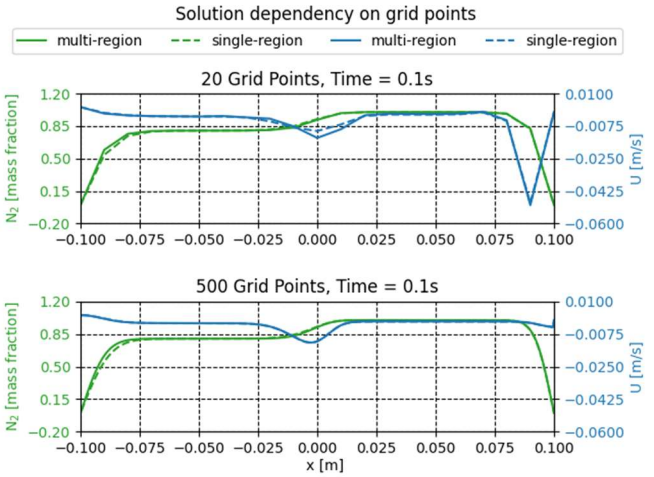

Figure 4: The solutions for identical multi-region and single-region simulations of N_2 concentration and velocity at two different grid resolutions (20 and 500 cells). All simulations were performed using 10 coupling loops of each of the three types (PIMPLE, PISO and Coupling iterations).

more for the velocity since the coupling also depends on the surface normal gradient (equation 8). Figure 5 shows a quantitative analysis of the deviation of single- and multi-region simulations by comparing the root mean square error (RMSE) as a function of the iteration settings and grid resolution. The figure also reveals the dependence of the multi-region coupling on the iterative solution procedure, which will be discussed in the next section.

Coupling iterations

Due to the loose region coupling in OpenFoam® an iterative solution is needed to ensure proper coupling of the boundary conditions at the region interfaces. Three types of iterations were investigated in the current work: PIMPLE, PISO and Coupling iterations. PIMPLE iterations recalculate the whole set of conservation equations including the matrix coefficients (outer iterations). PISO iterations only recalculate the pressure equation (inner iterations). Coupling iterations recalculate the conservation equations of the coupled quantities.

To identify the solution dependence on the different iteration loops, a case study has been conducted for the five grid spacings used in the previous section. The case study considered all possible combinations of 2, 5 and 10 iterations for PIMPLE, PISO and Coupling iterations. The RMSE was calculated using the multi-region and single-region simulations of identical grid size and varying the number of iteration loops of the multi-region simulation to assess the solution accuracy. Figure 5 reveals that the RMSE depends on both grid size and number of coupling iterations.

At least two PIMPLE iterations were needed in the investigated cases for a stable simulation. This is reasonable due to the loose coupling and that the first region to be solved is otherwise solely responsible for setting the solution at the interface while the second region has no influence on the interface. That can lead to unphysical simulation results. The RMSE can be seen to converge at a reasonably low total number of iterations and a good coupling across all fields and grid sizes could be achieved using 5 PIMPLE-, 2 PISO- and 5

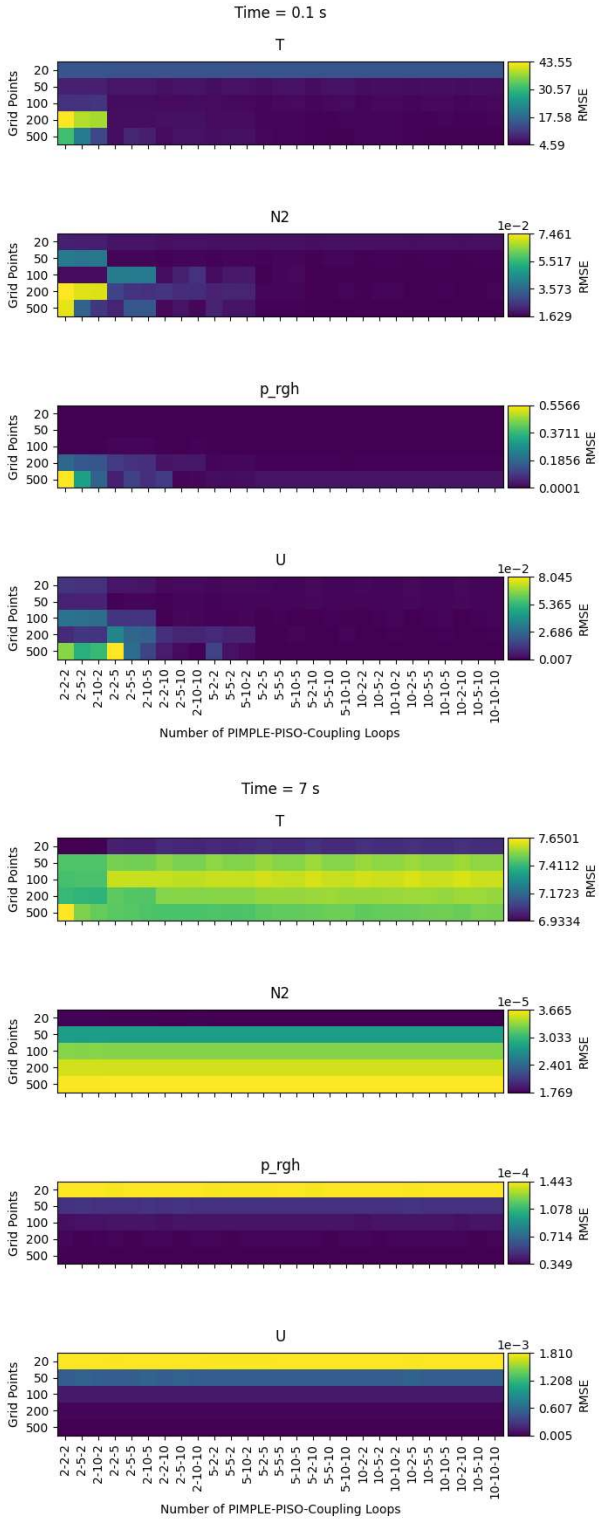

Figure 5: Root mean square error (RMSE) of the solution between the single and multi-region case for various grid sizes and combinations of PIMPLE, PISO and Coupling iterations at 0.1 s and 7 s.

Coupling loops. PIMPLE and Coupling loops show a higher influence on the solutions than PISO loops which is confirmed by Figure 5, since the RMSE is lower when more PIMPLE and Coupling loops were used. Between those two the PIMPLE iterations are more important than the Coupling iterations, as can be seen in Figure 5 for the velocity at 0.1 s with 500 grid points.

When increasing the number of grid cells the RMSE can increase for smaller numbers of solver iterations. This indicates that the minimum number of solver iterations needed for a reasonable loose coupling can increase with the number of grid points. However, the minimum of the RMSE can also converge at a lower value when using more grid points. The velocity solution is the most dependent on the number of grid points as is visible in Figure 4, as well as Figure 5. Overall an increase in the number of grid cells is favorable for accurate region coupling.

The temporal evolution of the test problem shown in Figure 3 compared to the RMSE of the solutions at 7 s indicates that the number of iterations becomes less important if the gradients at the interface are small. It can be concluded that the number of iterations required for an accurate multi-region solution increases with increasing solution complexity at the interface. A possible reason for having to use a higher number of solver iterations at a higher number of grid cells could be a similar increase in complexity at the interface due to being able to resolve finer details of the solution, which can lead to larger gradients at the interface. For steady state problems the results indicate that no decidedly coupling loops are required.

The RMSE of the solutions at 7 s for temperature and N_2 concentration increases with number of grid cells, independently of solver iterations. However, for those two figures the actual variation of within the RMSE are very small. For the temperature, the difference between maximum and minimum RMSE is in the order of 1 and for the N_2 concentration it is in the order of 10^{-5}. Both variations are lower than what can be seen at 0.1 s. The minimum RMSE for the temperature is comparable for both times and the minimum RMSE is three orders of magnitude lower for the pressure solution at 7 s than at 0.1 s. Thus, the argument that an increase in number of grid points generally increases solution accuracy is not invalidated.

Scaling with number of cells in each region

In order to justify region coupling for large simulations, the computational cost needs to be smaller than for a pure two-fluid case. Employing the multi-region approach reduces the number of two-phase fluid cells compared to the single-region approach. For the comparison of simulation times a large three-dimensional simulation domain was set up with a spherical particle in a cubic box.

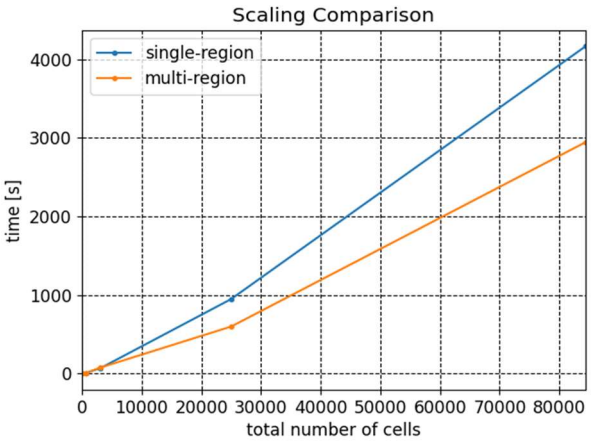

Figure 6: Comparison of the calculation time for the single- and multi-region versus the cell count.

This geometry leads to an unequal number of cells in the two regions. The cubic box includes more cells than the spherical particle. The number of cells in the sphere as well as the box are shown in Table 2 for each simulation. Figure 6 indicates that, for the given test case, the multi-region approach's performance scales better with the cell count of the simulation domain than the single-region approach.

Table 2: Number or cells in the two-phase region and surrounding single-phase region, as well as total number of cells in the simulation domain of the test case.

Total cells	675	3125	25000	84375
Two-phase cells	189	875	7000	23625
Single-phase cells	486	2250	18000	60750

The superiority of the multi-region approach depends on the required coupling iterations. However, it was shown in the previous section that a small number of coupling iterations should be sufficient for a reasonably accurate solution.

Summary & Conclusion

The region coupling algorithm for OpenFOAM® presented in this work has been tested for the coupling of temperature, species concentration, pressure and velocity between a fluid and a two-fluid region. The region coupling algorithm has been implemented in OpenFOAM®-7 [5] in the form of special boundary conditions for the coupling of temperature, species concentration, pressure and velocity for the case of coupling a fluid with a two-fluid region. The investigation of the existing coupling parameters showed that the multi-region approach gives similar results as the uncoupled approach.
The grid size and solver iterations were found to be crucial for accurate multi-region solutions. The solution accuracy increases with the number of PIMPLE and Coupling iterations and to a lesser extend with the number of PISO iterations. When the number of grid cells is increased, slightly more solver iterations are needed to reach the same RMSE. However, the minimum of the RMSE also decreases, which means the solution accuracy increases.
The region-coupling boundary conditions have a wide variety of possible applications and can be included in any existing OpenFOAM®-7 [5] solver that has the capability to simulate multiple regions. The idea is to couple single-phase fluid and two-phase porous regions for the simulation of heterogeneous processes, e.g. adsorption and solid fuel conversion.

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