

Coupled Simulation with Two Coupling Approaches on Parallel Systems

Neda Ebrahimi Pour, Verena Krupp, Harald Klimach, and Sabine Roller

Abstract The reduction of noise is one of the challenging tasks in the field of engineering. The interaction between flow, structure, and an acoustic field involves multiple scales. Simulating the whole domain with one solver is not feasible and out of range on today's supercomputer. Since the involving physics appear on different scales, the effects can be spatially separated into different domains. The interaction between the domains is realised with coupling approaches via boundaries. Different interpolation methods at the coupling interfaces are reviewed in this paper. The methods include the Nearest-Neighbor Interpolation (first order), the Radial-Basis Function (second order) as well as the direct evaluation of the state representation at the requested points (arbitrary order). We show which interpolation method provides less error, when compared to the monolithic solution of the result. We present how the two coupling approaches *preCICE* and *APESmate* can be used. The coupling tool *preCICE* is based on a black box coupling, where just the point values at the surface of the coupling domains are known. In contrast *APESmate* has knowledge about the numerical schemes within the domain. Thus, *preCICE* needs to interpolate values, while *APESmate* can evaluate the high order polynomials of the underlying Discontinuous Galerkin scheme. Hence, the *preCICE* approach is more generally applicable, while the *APESmate* approach is more efficient, especially in the context of high order schemes.

1 Introduction

With increasing computational resources also the idea of simulating more complex and larger simulations gets more and more important, since they allow a better understanding of physical phenomena and the optimisation in product design. In the recent years the energy turnaround in renewable resources gained more and more popularity, which lead to an increasing number of e.g. wind turbines. Wind turbines emit noise, which is caused by the rotor-wind interaction, where turbulent

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flow appears. With the increasing number and size of the turbines, the reduction of noise becomes important, due to the noise emission in the range of hundreds of meters or up to a few kilometres. The interaction of flow, structure and acoustic field (FSA) has to be studied in more detail, to improve the understanding of these factors, that can help to reduce the noise propagation. Solving the whole domain with a single equation (monolithic) up to the smallest scales is not feasible and still out of reach on today's supercomputers. Therefore we use partitioned coupling, where the physical space is divided into smaller domains and each of the subdomains covers a dedicated physical setup, as the different physical effects appear on different scales. Hence the separation of the domains allows different numerical treatments of the large and complex problem, which is than feasible as different equations as well as mesh resolutions can be used for each of them.

For the communication and the data exchange between the subdomains coupling approaches are used. They are based on a heterogeneous domain decomposition, where the different domains are connected to each other via boundary conditions. Considering compressible flows, we make use of explicit time stepping schemes that enable a straightforward data exchange at the coupling interfaces. Applying a proper data exchange at the coupling boundaries allows the deployment of various schemes and equations in each domain. Thus the numerical approximation can be adapted to the requirements of each domain. Especially for the acoustic far field, where no or few obstacles are present and only the wave propagation has to be considered, high order methods with low dissipation and dispersion are beneficial. Therefore the high order modal Discontinuous Galerkin Method (DGM) [5] is considered.

In this paper we investigate the two different coupling approaches. One coupling approach is a black-box tool, which allows the coupling of different solvers without any knowledge of each discretisation, while the other one is an integrated approach, which has knowledge about the underlying scheme and makes use of that. At first two interpolation methods: Nearest-Neighbor (NN) and Radial-Basis Functions (RBF) with and without providing equidistant points, provided by the coupling tool *preCICE* [1, 2] are presented. Afterwards the direct evaluation of the state representation at requested points, provided by the coupling approach *APESmate* [6] is introduced.

The final section is devoted to simulation results with a small academic testcase, in order to compare the different interpolation methods and the resulting error. Finally we come to an end, by concluding our results.

2 Data Mapping Methods

This section describes the different interpolation methods as well as the evaluation of the state variables, in order to exchange point values at the coupling interfaces. Therefore first the interpolation methods in the coupling approach *preCICE* are introduced, afterwards the integrated coupling approach *APESmate* is presented.

2.1 Interpolation

preCICE is an multi-solver, which allows the coupling of different solvers, considering them as a *black-box*. Thus it has no information about the discretisation of each solver, while exchanging input and output values via the coupling interfaces using coupling points. For the exchange of values at requested points, the coupling tool provides different interpolation methods, in this paper, we are going to review three of them. More information about *preCICE* can be found in [1] and [9]. Since the domains, which are involved in the coupling, request point values located at arbitrary positions at the coupling interface, hence providing values has to be done on those requested point positions. Therefore interpolation methods are necessary to compute values from one domain to the other.

The easiest applicable interpolation method is the *Nearest-Neighbor* (NN) interpolation (see Fig. 1a) [3]. In order to use this method, the solver does not have to provide any information beside the variable values at its exchange points. Coupling from domain B to A, this method searches for the closest point on B and copies the value to the requested point on A. If more than one point of domain A is in the near of one point in domain B, than all those points get the same value. Therefore this interpolation method is just first order accurate and useful, when having a matching coupling.

The *Nearest-Projection* (NP) method (see Fig. 1b) looks for the closest neighboring point of domain A among domain B, while computing the projection point of the point in B on the point in domain A. Thus a linear equation has to be solved, which leads to a second order accuracy. In order to make use of this method, the solver has to provide neighborhood information, in form of triangles or edges [3].

A second order accurate method, where no neighborhood information is necessary, is the *Radial-Basis-Function* method (RBF).

$$g(x) = \sum_{i=1}^{N_B} \gamma_i \cdot \phi(\|x - x_i\|) + q(x) \quad (1)$$

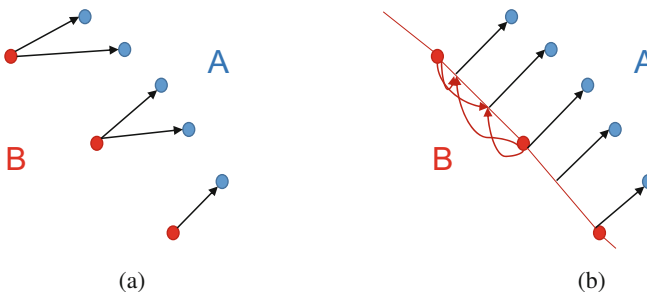


Fig. 1 (a) Nearest-Neighbor, (b) Nearest-Projection interpolation [3]

For the mapping from domain B to A, the radial-basis-function creates a global interpolant on B, which is evaluated on A. The basis are radially symmetric basis functions, which are centred at the coupling points of domain B. Equation (1) presents the equation, which has to be solved internally by *preCICE* for the RBF. To make sure, that constant and linear functions are interpolated exactly, the basis has an additional first order global polynomial $q(x)$. The variable ϕ is the basis function, chosen by the user. In this paper we use the Gaussian function as basis function for the interpolation [3]. Using this basis function requires to predefine a shape-parameter s (see Eq. (2)), which defines the width of the Gaussian function.

$$s = \frac{\sqrt{-\ln(10^{-9})}}{m \cdot h} \quad (2)$$

Where m is the number of points which has to be covered by the Gaussian function and h the average distance between the points. It has to be mentioned, that the distribution of the coupling points has a major influence on the quality of the simulation results as well as on the convergence of the linear equation system, which has to be solved. Different situations can be thought of, where the sampling points on a domain interface are non-equidistant. One is the use of high order Discontinuous Galerkin (DG) schemes, where the sampling points are the Gaussian integration points which are not equally distributed. While at the corners of the cells the points are more concentrated, in the middle of the cell the distance is much larger. The size of the shape-parameter has an great impact on the convergence of the system, while selecting a high m leads to an increase in the quality of the simulation, it also influences the condition number, which also increases [7]. In the DG context, the variable h is set to the maximum distance between the points, to also cover the points in the middle of the cell, which have a larger distance to each other. The distance is calculated by considering the distance between the Chebyshev nodes.

$$h_{max} = \left[\cos\left(\frac{2 \cdot (n_h + 1) - 1}{2 \cdot nO} \cdot \pi\right) - \cos\left(\frac{2 \cdot n_h - 1}{2 \cdot nO} \cdot \pi\right) \right] \cdot \frac{dx}{2} \quad (3)$$

The value nO represents the scheme order, n_h the half value of the scheme order and dx the cell size. Providing non-equidistant sampling points for the RBF reconstruction leads to instability of the convergence of the matrix, while equidistant points lead to its stabilisation. Keeping that in mind, the need of a method, which overcomes these challenges becomes more important. Thus evaluating polynomials for each domain directly, instead of using an additional interpolation method for the reconstruction, allows to overcome the convergence challenge as well as increasing the quality of the simulation results.

2.2 Data Mapping by Evaluation

The integrated coupling approach *APESmate* [6] is implemented in our *APES* framework [8, 10], thus it has access to solver specific data. Therefore exchanging data at arbitrary number of exchange points with our DGM solver *Ateles* at the coupling interface can be realised by the direct evaluation of the polynomial representations at the requested points. Hence no additional interpolation is necessary. One of the main beneficial of our coupling approach is, that with a higher order a higher accuracy in the context of simulation errors can be obtained [6].

3 Results

This section deals with the simulation results, when using the two different coupling methods, interpolation and evaluation. Therefore we use a Gaussian density pulse, which travels from the left domain to the right domain, to compare the different methods. We created three different testcases, (a) matching, (b) non-matching with same number of coupling points and (c) non-matching with different number of coupling points. For the simulation we change the cell size and the scheme order. The matching testcase (a) has on both domains the same number of cells as well as the same scheme order, thus the number of coupling points are also the same. For non-matching testcase (b) the left domain is kept same as for (a), while on the right domain a two times greater cell size and scheme order has been chosen, which still results in the same number of coupling points as for the left domain. Testcase (c) is also a non-matching testcase, here the left domain is again the same as in (a) and (b), while the right domain has a four times bigger cell size and the scheme order is equal to the right domain in testcase (b).

3.1 Configuration of the Simulation

For our testcases we provide a 4×4 plane, which is divided into two domains. We solve both domains with the nonlinear Euler equation and choose a Gaussian density pulse, which travels from the left domain to the right, due to the advection of the flow in x-direction. The amplitude of the pulse is set to 1.0 and a halfwidth of 0.316. The pressure p is set to 8.0 and the density ρ to 1.0. The velocity has a constant value of $\mathbf{v} = [12.5, 0.0, 0.0]$. Figure 2 presents the point distribution in the cells for all investigated testcases, when using DG. Table 1 provides a short overview of the investigated testcases with the different configurations.

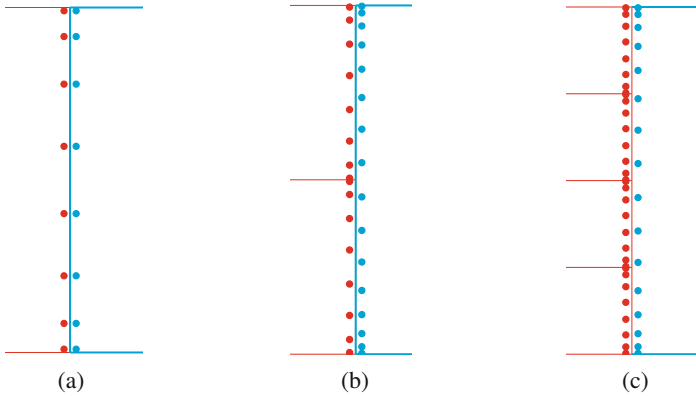


Fig. 2 Point distribution in cells, when using DGM: (a) matching testcase a, (b) non-matching testcase b and (c) non-matching testcase c

Table 1 Three testcases for the investigation of the interpolation methods

	Testcase a matching		Testcase b non-matching		Testcase c non-matching	
	Left	Right	Left	Right	Left	Right
Number of cells	512	512	512	256	512	128
Number of coupling points	128	128	128	128	128	64
Scheme order	8	8	8	16	8	16

3.2 Coupled Simulation Results

As the investigated testcase is small enough, we can obtain a monolithic simulation, running the entire testcase in one single non-split domain, and use this as the reference solution without coupling error (Fig. 3). Then we split the domain into halves, while keeping the same cell size and order. I.e. all differences between splitted and monolithic simulation results are due to the coupling error. In the following, we then change the settings in the right domain, such as to adopt the scheme order and cell size to the needs of the domain. Thus, additional errors are introduced now, due to the non-matching conditions. For the monolithic simulation, where we consider the settings as for testcase a, the error is computed from the difference between the result of the simulation and the analytical solution [6]. The error in the middle area of the domain is due to the shape of the pulse and its location at the beginning of the simulation. Since the pulse was located in the striking distance of the left boundary, oscillations appear, which traveled with the pulse through the entire domain. Which does not have any influence for the comparison of the different methods. Figure 4 shows the pulse after passing the interface for all three testcases using the RBF interpolation. As can be recognise no significant

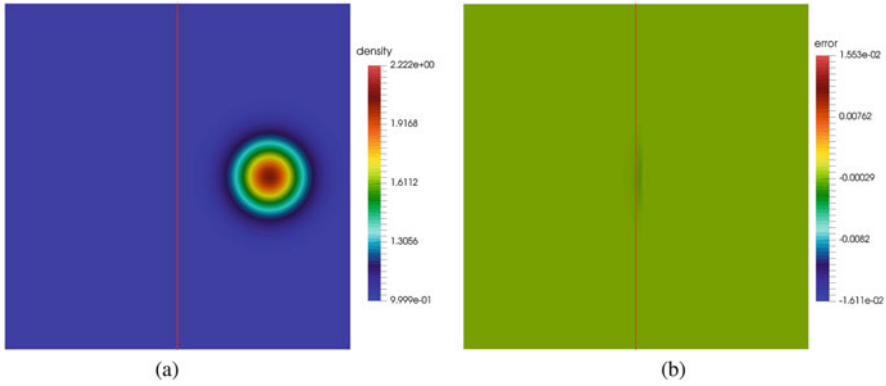


Fig. 3 (a) Monolithic solution of the simulation and (b) Error of the simulation

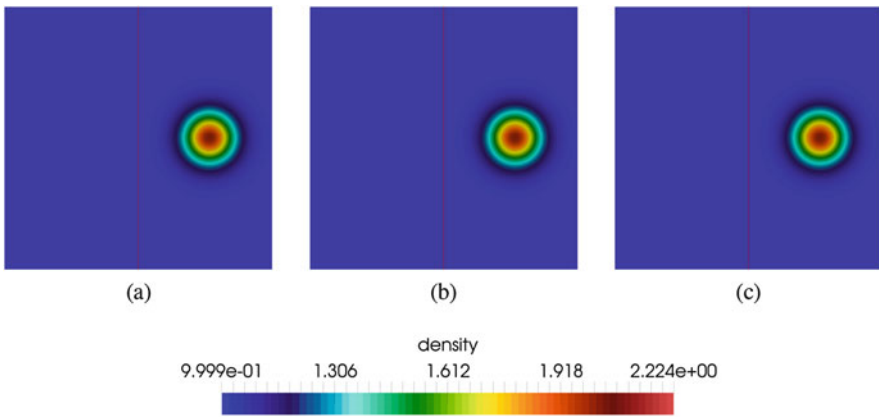


Fig. 4 Solution of the Gaussian density pulse, which has traveled from the left domain to the right: (a) Testcase a, (b) Testcase b and (c) Testcase c

change of the pulse can be observed. To clarify which method shows the lowest error, we investigate the simulations in more detail. The error for the following coupled simulations are calculated from the difference between the coupled solution and the monolithic solution Fig. 3a. Thus this should just provide the error, which is due to the coupling of the domains, using interpolation or the evaluation of the polynomials respectively. In Fig. 5, a stronger impact of the matching and non-matching setup is visible. For the NN interpolation, it becomes apparent, that the error has an increasing behaviour, when having an increasing non-matching coupling interface (see Fig. 5b, c). For the matching coupling interface Fig. 5a, the error is similar to the monolithic solution, which is due to the fact, that the points on both sides coincide. Thus, the NN interpolation is a pure injection, no interpolation error is introduced. For the RBF interpolation we have to compute the shape-parameter (Sect. 2) for each domain before running the simulation. Thus

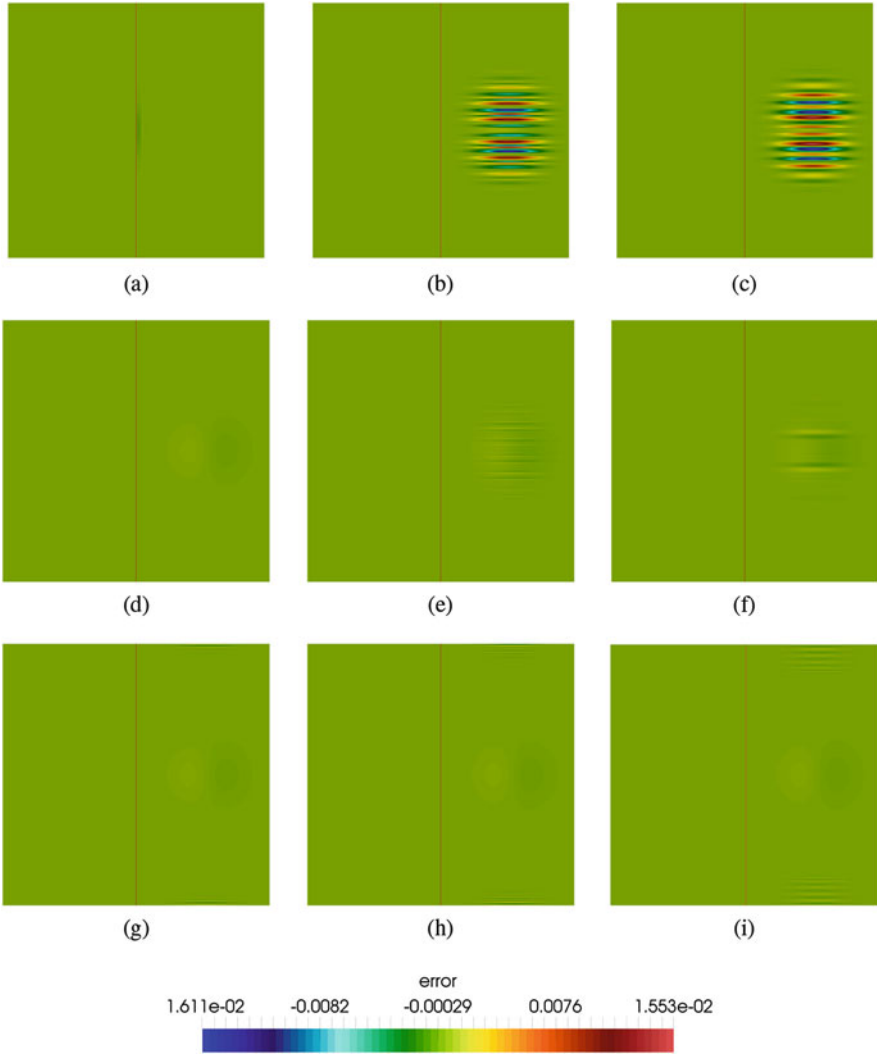


Fig. 5 Error of the traveled Gaussian density pulse when using RBF interpolation with non-equidistant point distribution: (a) Testcase a with NN, (b) Testcase b with NN, (c) Testcase c with NN, (d) Testcase a with RBF non-equidistant Points, (e) Testcase b with RBF non-equidistant Points, (f) Testcase c with RBF non-equidistant Points, (g) Testcase a with RBF equidistant Points, (h) Testcase b with RBF equidistant Points and (i) Testcase c with RBF equidistant Points

for each testcase the maximal distance between the non-equidistant points has to be determined. Considering the results in Fig. 5d–f, the error, when using the RBF interpolation also increases with stronger non-matching coupling interfaces (Fig. 5e, f), while for the matching testcase Fig. 5d the error is similar to the monolithic solution. Taking Table 2 into account, we can recognise, that stronger non-matching

Table 2 Computed shape-parameter for non-equidistant point distribution

Testcase	h_{max}		m		s	
	Left	Right	Left	Right	Left	Right
a	0.0244	0.0244	4	4	46.642	46.642
b	0.0244	0.0245	4	3	46.642	61.936
c	0.0244	0.0245	4	2	46.642	46.452

Table 3 Computed shape-parameter for equidistant point distribution

Testcase	h_{max}		m		s	
	Left	Right	Left	Right	Left	Right
a	0.0156	0.0156	7	7	41.621	41.621
b	0.0156	0.0156	7	7	41.621	41.621
c	0.0156	0.0313	7	7	41.621	20.810

interfaces lead to a decreasing number of points m , which can be covered by the Gaussian function. Additional in [7] a more detailed study pointed out, that non-equidistant point distribution leads to instability of the system, thus to the not convergence of the matrix. Therefore it was suggested to consider equidistant points, to stabilise the system, hence aiming for a faster convergence. Thus in our next simulations, we provide equidistant points to *preCICE*, while asking for point values, which are non-equidistant distributed. Since we make use of the modal DG, providing and asking *preCICE* for equidistant point values would lead to higher computational effort, due to additional transformation from points to polynomials. Again we calculated according to Eq. (2) the shape-parameter for the new setup. As in Table 3 pointed, the variable m , can be chosen much higher. Furthermore the system converged much faster, which leads to the decreasing of computational effort. The simulation results for the equidistant point distribution illustrate for all testcases oscillations near the upper and lower boundaries, which increase with stronger non-matching coupling interfaces (see Fig. 5h, i). The oscillations did not appear, using the NN and the RBF method with non-equidistant points. This behaviour is due to the *Runge's* phenomenon [4], which appears, when using high order polynomials over equidistant interpolation points. Thus providing equidistant points for the interpolation leads to the stabilisation of the system, but decreases the quality of the simulation results. In Fig. 6 as well as in Fig. 7 the solution for all testcases show the same behaviour, thus even for the strongest non-matching testcase Fig. 7c, the error is comparable to the matching testcase Fig. 7a. Besides the visualisation of the simulation results, we also consider the L2error for the simulations to have a better comparison between the different methods. The presented Table 4 gives an overview, which method allows the lowest error, when running coupled simulations. Therefore we just consider the right domain, where the pulse reaches its final position, after passing the coupling interface. From Table 4 it can be pointed out, that for the RBF with non-equidistant points as well as for the NN interpolation with stronger non-matching coupling interfaces (c) also the error increases, while for NN this increase is distinguished. The RBF with equidistant points show already a high error for testcase (a), while a significant trend as for RBF

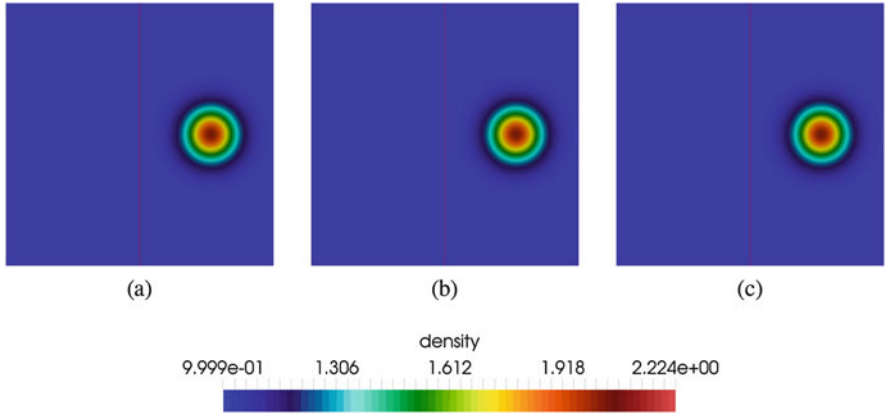


Fig. 6 Solution of the Gaussian density pulse, which has traveled from the left domain to the right using *APESmate*: (a) Testcase a, (b) Testcase b and (c) Testcase c

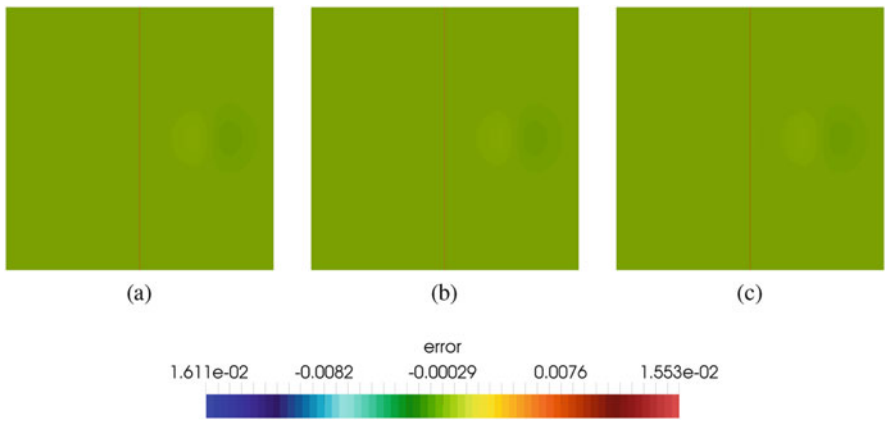


Fig. 7 Error of the traveled Gaussian density pulse when using *APESmate*: (a) Testcase a, (b) Testcase b and (c) Testcase c

Table 4 Comparison of the L2error for the different methods

$\times 10^{-3}$	a	b	c
Nearest-Neighbor	1.606	27.774	52.344
Radial-Basis-Function: non-equidistant points	1.606	1.986	2.326
Radial-Basis-Function: equidistant points	1.606	5.101	3.485
APESmate	1.606	1.593	1.599
Monolithic	1.05870		

with non-equidistant points and for the NN can not be observed. The increase of error values in testcase (b) and the decrease for testcase (c) are due to the changes of order and cell size in testcase (b), where the number of non-equidistant points in the corners of a cell is more dominant for a 16th order than for a 8th order simulation. The error decreases for the testcase (c), since the cell size on the right domain is two times larger than in testcase b), thus less cells are involved in the coupling, which also decreases the error. The results of *APESmate* are noticeable, even for testcase (c), where all interpolation methods provided by *preCICE* show a high error, the simulation results of our coupling approach shows the smallest and the most stable error over all simulations.

Beside the error of the simulation results, the performance of each method is an important factor, which allows the fast computation of the simulation. Therefore also investigate the performance of the used methods.

3.3 Performance of the Mapping Methods

For the performance runs we consider the same settings as in Sect. 3.1, while using testcase c as a three dimensional setup. The left domain has 16,384 cells and the right domain 256. The number of coupling points at the coupling interface is 65,536 and 16,384 respectively. Since the left domain has just 256 cells, the number of cores is chosen according to this limitation. Figure 8 presents the time for the simulation

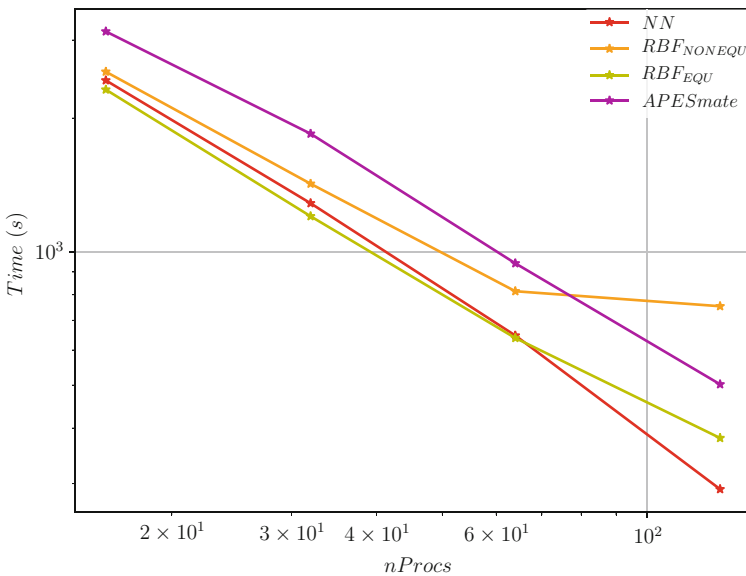


Fig. 8 Strong scaling of the different methods

with the different methods, while changing the number of cores from 16 to 128. It is clearly visible, that the interpolation method NN, is the fastest in the computation, which is as expected, since this method just copies data from one domain to the other. But we also have to keep in mind, that apart from the fast computation, this method provides the highest error, when having non-matching coupling interfaces (see Fig. 5c). A closer look at the RBF method with different point distribution illustrates also here, that the simulation with equidistant point distribution (RBF_{EQU}) behaves as expected faster than the non-equidistant point distribution, since the equidistant points reduce the condition number and thus the computational time. In contrast the performance of the non-equidistant point distribution (RBF_{NONEQU}) gets flat, with increasing number of cores. Since our integrated approach *APESmate* evaluates polynomials for the coupling, the computation is higher, when compared to the interpolation methods provided by *preCICE*. But as was shown before the simulation results (see Fig. 7) is outstanding and in the same magnitude range as for the monolithic run.

4 Conclusion

The simulation of multi-scale problems is still a challenging task in the engineering field. Solving these problems with one approach is still expensive, thus a more feasible strategy is required. The partitioned coupling is one of the most promising methods, which allows the decomposition of the whole problem into smaller ones, by subdividing the whole domain. Hence each domain can be solved according to its physics by using numerical methods, which are perfectly designed for each domain.

We presented how the two coupling approaches use different methods to exchange point values at the coupling interface. Therefore we considered for the external library *preCICE* the first order accurate *Nearest-Neighbor* (NN) method and the second order accurate *Radial-Basis-Function* (RBF) method. Beside the interpolation method, we are also able to do the direct evaluation of the polynomials at requested coupling points, using our integrated coupling approach *APESmate*. Thus no additional interpolation is here necessary. For our investigation we solved our domains using the Discontinues-Galerkin Method (DGM), where the coupling points (Gaussian integration points) are not equidistant distributed on the cell surface.

Our investigation clarified, that the interpolation method NN is not qualified for the usage of non-matching coupling interfaces, which is necessary, when coupling different solvers with different numerical resolution, thus the simulation results showed a high error, when compared to the monolithic solution. The second order accurate interpolation method RBF illustrated a lower error, when using non-equidistant point distribution. But the condition number of the linear equation system, which has to be solved, as well as the selected number of points, which have to be covered by the basis function is unsatisfactory. Thus the condition number increases with higher scheme order and at the same time the computational

effort. In order to decrease the condition number and stabilise the system, we provided *preCICE* equidistant points at the coupling interface, while asking for non-equidistant distributed points. By applying the equidistant points for the interpolation, we were able to increase the number of points, which has to be covered by the Gaussian function (basis function). Furthermore the condition number decreases and thus the stabilisation of the system could be archived. But taking also the quality of the simulation results into account, we could recognise, that oscillation occur at the lower and upper boundary, which we could not observe before, when using the NN or the RBF method with non-equidistant point distribution. These oscillations appear, due to the *Runge's* phenomenon, when using equidistant points for the interpolation of non-equidistant point distribution. The results of the simulations, when using our integrated approach *APESmate*, depict the lowest error, when compared to the monolithic solution. Even for the non-matching coupling interface, where the interpolation methods in *preCICE* show the highest error, our approach illustrated an outstanding behaviour, by having an almost constant L2error for all simulations, which is in the same magnitude range as the monolithic one.

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