Coupling of TAU and TRACE for parallel accurate flow simulations

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Abstract

To simulate flow phenomena that include exterior aircraft as well as turbomachinery aerodynamics like a stalling aircraft engine nacelle, a method of coupling two specialized flow solvers is developed. The flow data exchange is based on an overset grid approach and allows for flexible and independent grid generation. Two test cases are used to validate the method with respect to accuracy and robustness and to demonstrate the ability to run simulations on a massively parallel high performance computing cluster.

Nomenclature

f	weighting factor
$\vec{x}_P$	coordinates of an interpolation point
$\vec{x}_{P^*}$	coordinates of a virtual interpolation point
$\vec{x}_S$	coordinates of point on surface
$\vec{\varepsilon}$	projection vector

1 Introduction

One of the major goals of the FOR 1066 project is to simulate the effects of disturbed flow conditions on the compressor of an aircraft engine caused for example by a stalling engine nacelle. To achieve this, the exterior flow including separation processes as well as the internal compressor flow has to be simulated accurately. As there is no monolithic RANS solver available to the FOR 1066 consortium suited for both fluid domains, the flow solvers TAU and TRACE will be used in a coupled simulation, where the TAU code is applied to the external flow and TRACE is used to simulate the internal flow. The coupling is performed using the Chimera technique which allows for exchanging data between the grids of the two flow domains by means of interpolation in an overlapping region, introduced by Benek et al [1].

The TAU code [3] is developed at the Institute of Aerodynamics and Flow Technology to simulate exterior aircraft aerodynamics by solving the Reynolds-averaged Navier-Stokes (RANS)

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equations. It uses an unstructured finite volume discretization and is capable of simulating both steady and unsteady flows. By default a cell-vertex metric is used for the flux balance. The TAU code is capable of using both explicit and implicit time integration schemes and features a multigrid algorithm to accelerate numerical convergence. The flow solver TRACE [4] of the Institute of Propulsion Technology is developed to simulate turbomachinery flows and uses a block-structured finite volume discretization with a cell-centered metric to solve the RANS equations. For time integration different implicit methods are implemented. The TRACE code does not feature a Chimera method with an overset grid approach. The coupling method is implemented in an external coupling module that provides the necessary functionalities to exchange the flow data between the simultaneously running solvers.

In this paper an overview of the implemented coupling method and technical aspects of its implementation are presented. In chapter 2 an introduction to the code coupling method concerning data interpolation including a wall projection technique to improve accuracy and robustness is given. Furthermore some technical aspects of the parallel implementation of the code coupling method are presented. In chapter 3 the application of the code coupling method to different test cases is presented. The simulation of a two-dimensional channel flow is used to validate the method and to demonstrate the wall projection method. Additionally, a configuration of a compressor test rig is used to evaluate the parallel performance of the implemented method. The paper closes with a conclusion and an outlook towards further usage of the coupling method.

2 Coupling method

To perform a coupled flow simulation, the flow data has to be exchanged at the coupling boundary during the iterative time stepping process of the flow solvers. To update the data accurately on each coupling boundary point of one grid, the data is interpolated from the overlapping region of the grid of the opposing flow solver. This approach requires a search of an appropriate donor cell as data source for each coupling target point on both grids. This donor cell search and the calculation of the interpolation coefficients has to be performed only once in simulations with no relative movements of both grids. In case of relative grid movement in a time-accurate simulation the mapping and the interpolation coefficients have to be recomputed. The calculated point mapping and the interpolation coefficients can then be used for the data exchange in the solution process.

2.1 Coupling point mapping

To compute the coupling point mapping and the associated interpolation coefficients, both flow solvers have to send the grids of their flow domains to the coupling module. Then an appropriate donor cell for data interpolation is searched for each coupling boundary point of both grids. Finally the located donor cell, respectively the associated donor points have to be transmitted back to the flow solvers. This mapping procedure is shown in figure 1.

Since the data exchange is based on a linear interpolation, the mapping and the corresponding interpolation coefficients have to be computed with respect to the flow data localization of the grids. In the unstructured grids used in TAU, the cell vertices on the coupling boundary and their first neighbors are marked as the interpolation target points, as shown on the left in figure 2. These points are excluded from the flow computations performed by the solver, since they are updated by the coupling procedure. In block-structured grids with a cell-centered met-

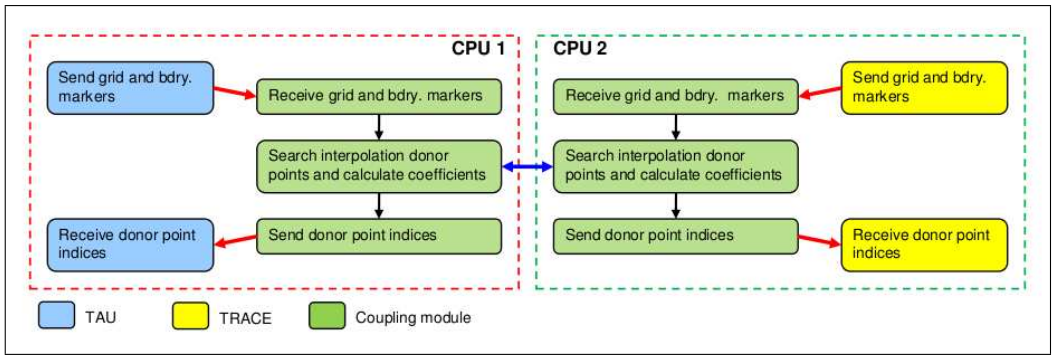

Figure 1: Coupling point mapping and calculation of interpolation coefficients.

ric used in TRACE, two layers of ghost cells are constructed around each block to implement the boundary conditions. Therefore the cell centers of the ghost cells at the coupling boundary are marked as interpolation target points. To compute interpolation coefficients with respect to the TRACE grid, a dual grid based on the cell centers has to be constructed. The cells of this grid serve as donor cells for the linear interpolation (see figure 2 on the right). The dual grid extends into the first layer of ghost cells of each block to cover the hole physical flow field. Otherwise interpolation close to an adjacent grid boundary would be impossible.

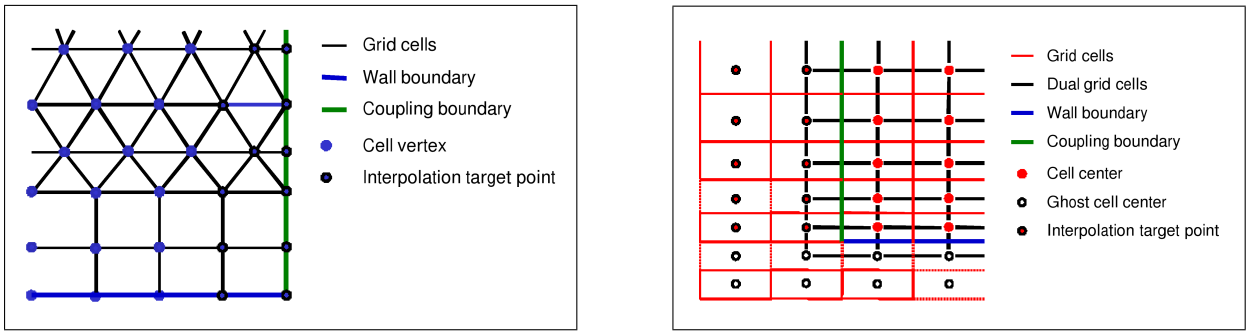

Figure 2: Localization of flow data and coupling boundary in TAU grid (left) and TRACE grid (right).

In case the TRACE grid contains several blocks, the hexahedra of the dual grid blocks can be gathered to one set of cells, since the mapping process does not take any block-structure of a grid into account.

2.2 Coupled flow computation

Within the iterative time stepping procedure a close coupling between the flow solvers is applied. In simulations of steady flows with a local time stepping method the data can be exchanged during each time step to result in a converged flow solution with both solvers. In time-accurate simulations with dual time stepping the data can be exchanged in each pseudo time step to converge to a quasi-steady state in each physical time step. To exchange the flow data, both flow solvers send the data from the mapped donor points to the coupling module. Then the calculated interpolation coefficients are applied to compute the flow data updates for the coupling boundary points of the opposing grid. After that, both solvers perform the next iteration of the flow computation as shown in figure 3.

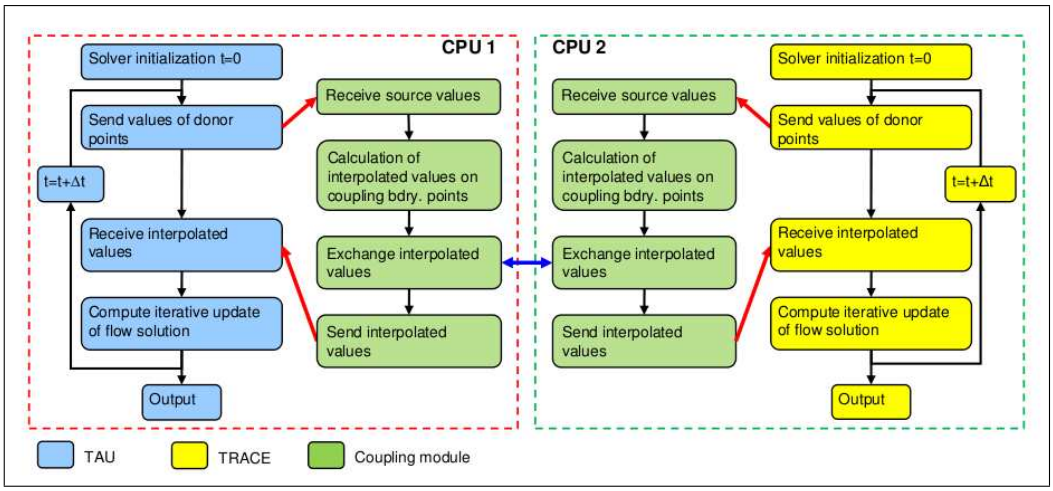

Figure 3: Data exchange during iterative time stepping.

The data exchange synchronizes the time stepping procedure of both flow solvers, so that a proper load balancing in coupled simulations is crucial with respect to computational time. Apart from choosing an appropriate ratio of computing resources for the solvers, the load balancing can be improved by a coupling time step stride that can be applied for each flow solver individually, specifying a defined number of pseudo time step to be calculated before the flow data is exchanged. Between the data exchanges the flow data at the coupling boundary is kept constant.

2.3 Robustness

In case of curved wall boundaries in the overlapping grid region, the different discretizations in both grids may lead to large interpolation errors. Although both grids represent the same geometry, a node of one grid may be located at a wrong distance to the wall with respect to the other grid. This effect would lead to inaccurate data interpolation, especially in boundary layers, and therefore distort the flow solution. Furthermore a grid node may also be located completely outside of the other grid so that no appropriate donor cell can be found. These effects are addressed by a wall projection method to calculate virtual interpolation target points with a correct wall distance with respect to the opposing grid. The implemented method is based on the wall projection technique developed by Schwarz [2]. However, the projection vector is weighted slightly different to compute the virtual target point coordinates.

At first the nearest wall boundary point S for each interpolation target point P is searched within the own grid. After that, the marked wall point is projected to the corresponding wall boundary of the opposing grid. Finally the target point is displaced according to the projection vector $\vec{\varepsilon}$ and a weighting factor f as follows:

$$\vec{x}_{P^*} = f \cdot \vec{\varepsilon} + \vec{x}_P \tag{1}$$

with

$$f = \begin{cases} 1 - \frac{|\vec{x}_S - \vec{x}_P|}{|\vec{\varepsilon}| \cdot c} & \text{if} \quad |\vec{x}_S - \vec{x}_P| < |\vec{\varepsilon}| \cdot c \\ 0 & \text{if} \quad |\vec{x}_S - \vec{x}_P| \geq |\vec{\varepsilon}| \cdot c \end{cases} \tag{2}$$

This implementation restricts the target point displacement to a region close to the wall boundary and creates a smooth decrease of the target point displacement in the flow field,

depending on the prescribed value c. To the author's experience a value of $c = 100$ shows good results.

To apply the wall projection in a coupled simulation including the TRACE code, the surface grids of each block have to be provided to the coupling module, since the interpolation coefficients are calculated with respect to a dual grid, which does not represent the actual grid boundaries. The cell-vertex grid metric used for TAU include the actual boundaries, so that the primary surface grid is used in the wall projection method.

The robustness of the mapping process is further improved by a nearest neighbor search approach. If no appropriate donor cell is found, the nearest point in the opposing grid is used to update the flow data. The resulting data transfer is less accurate than a linear interpolation of the flow data, but might still be acceptable for flow conditions with small gradients. However, this feature ensures a complete target point mapping to run a coupled simulation.

2.4 Parallel implementation

The presented coupling method is implemented as an external module that performs the data interpolation and manages the data transfer. This approach allows for coupling flow solver, that do not provide a Chimera-like interpolation technique on their own. Furthermore, only a simple communication interface has to be implemented within the flow solvers to reduce the effort of both development and maintenance of the coupling method.

To perform coupled simulations of large configurations on a high performance computing (HPC) cluster, the flow solvers do not only have to run simultaneously, but also run in parallel mode themselves. Therefore each grid and also its coupling boundary may be distributed to an arbitrary number of subdomains. This issue is addressed by a parallel implementation of the coupling module that has to run with a parallel process associated to each parallel process of both flow solvers. As the data exchange has to be performed between different running applications and without file access, the communication between coupling module and flow solver is realized via socket communication. To minimize communication load on the HPC cluster network, the socket communication is designed to transfer data only on each HPC cluster node, so that no connection using the actual network is needed. The coupling module itself uses the message passing interface (MPI) to compute the interpolation coefficients and exchange the interpolated flow data internally.

Due to the parallelization concept, an appropriate donor cell will always be located in a grid subdomain that is associated to a different parallel process as the coupling boundary point. Therefore the donor cell search is based on a two-stage parallel mapping procedure. In this approach all subdomains are searched for, where a donor cell may be contained. Then the target point is transmitted to the associated processes of these subdomains, where the actual donor cell is searched. As the Chimera interpolation is performed with respect to a single donor cell, the flow data needed to compute the values for a specific coupling boundary point is not distributed to several grid subdomains. Therefore the flow data interpolation can be performed in parallel and independent on each process associated to a grid subdomain containing donor cells. After that the interpolated flow data is exchanged internally and then transmitted to the flow solver to update the coupling boundary points.

3 Applications of the code coupling method

The presented coupling method is demonstrated by coupled simulations of two test cases with the flow solvers TAU and TRACE. The simulation of a simple two-dimensional channel flow is used to examine effects of different time stepping settings for the flow solver TAU on convergence rates and to demonstrate the improved robustness and accuracy by using the wall projection. Additionally, the parallel performance is shown with a large test case of a compressor test rig configuration.

3.1 2D channel flow

The test case of a two-dimensional channel flow with one viscous wall is used to simulate the development of a turbulent boundary layer. The boundary conditions at the side boundaries of the flow domain is set to symmetry conditions in the TAU grid and to inviscid wall condition in the TRACE grid, as shown in figure 4 on left. To obtain an accurate flow solution a correct data transfer in the coupling region is crucial, especially in the boundary layer, where interpolation errors due to gradients of the flow data may disturb the solution. The reference conditions of the inflow are set to a Mach number of $Ma = 0.2$ and a Reynolds number of $Re = 500000$. As a result of a coupled simulation isolines of the Mach number in the boundary layer at the overlapping region are visualized in figure 4 on the right.

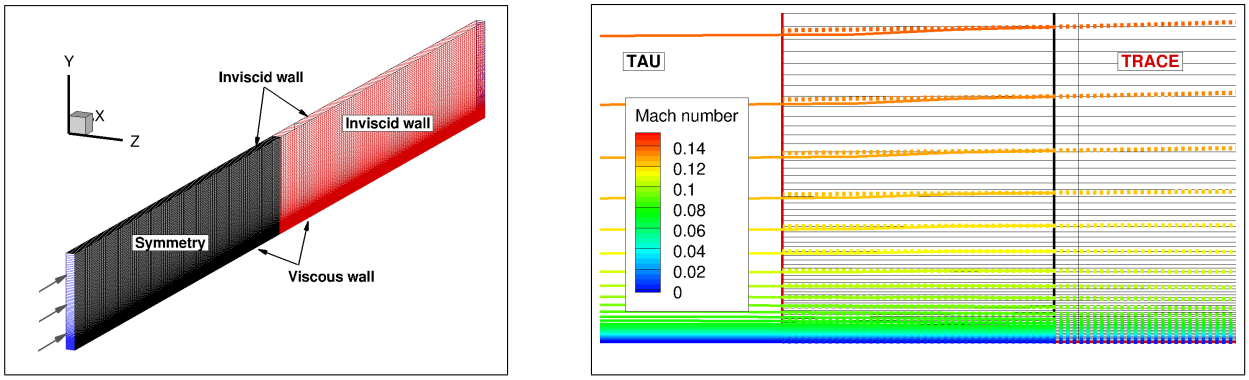

Figure 4: Test case of two-dimensional channel flow (left) and isolines of Mach number in the overlapping region of the boundary layer.

The depicted isolines in the TAU and the TRACE domain show a very good agreement in the coupling region and indicates an undisturbed boundary layer flow. The small deviation of less than the local cell height may result from an interpolation error in the postprocessing within the TRACE code, since the cell-centered flow data is interpolated to the cell nodes.

To investigate the effects of different time stepping parameters of the TAU code on convergence behavior of both flow solvers, a series of coupled simulations have been performed. The time stepping method of the TRACE code was set to a Backward-Euler scheme with a CFL-number of 50 and was maintained throughout all simulations of this test case. The parameters of the TAU code in the coupled simulation are varied with respect to chosen relaxation solver, CFL-number and usage of the multigrid algorithm. For the simulations with explicit Runge-Kutta method (RK), the CFL-number is set to 1.0 and 1.8. Beyond these values the simulation became unstable. In the simulations performed with the implicit Backward-Euler scheme using the LUSGS-method the CFL-number was set to 5.0 and 50.0.

In figure 5 the convergence histories of the different simulations of both flow solvers are shown. It is clearly visible that the convergence rate of the TAU code is very poor with the explicit Runge-Kutta scheme, but it benefits from the acceleration of the multigrid algorithm. On the contrary, the implicit LUSGS-method does not show a benefit from the multigrid algorithm but the convergence rate is greatly increased by using a large CFL-number. The convergence history of the TRACE code is hardly influenced by the settings used for TAU. The residual of the simulation with TAU using the Backward-Euler scheme, 4w-multigrid cycle and a CFL-number of 50.0 shows heavy oscillations in both codes, but seems to decrease near the end of the fixed number of 40000 time steps, but this behavior is left to further investigations. However, the best convergence rate is achieved with settings similar to the parameters used for the TRACE code, so that these settings are used for further simulations regarding this test case.

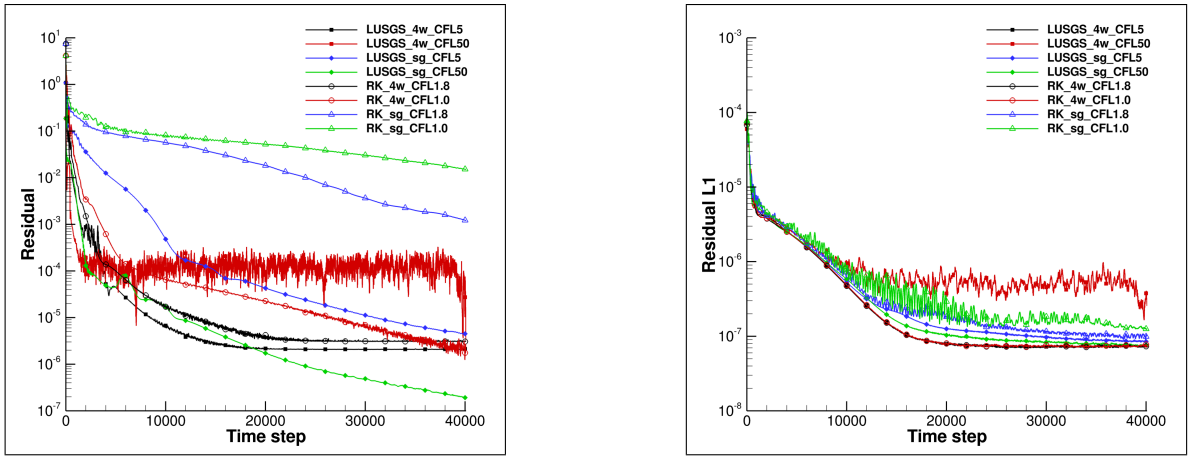

Figure 5: Convergence history of density residual in coupled simulations of TAU (left) and TRACE (right).

It should be mentioned, that these results concerning convergence rates give only a hint of preferable parameter settings.

The effect of the wall projection method is demonstrated with a simulation of the two-dimensional channel flow with an offset between the grid domains in wall normal direction. On the left side of figure 6 the result of the simulation without the use of the wall projection technique is shown.

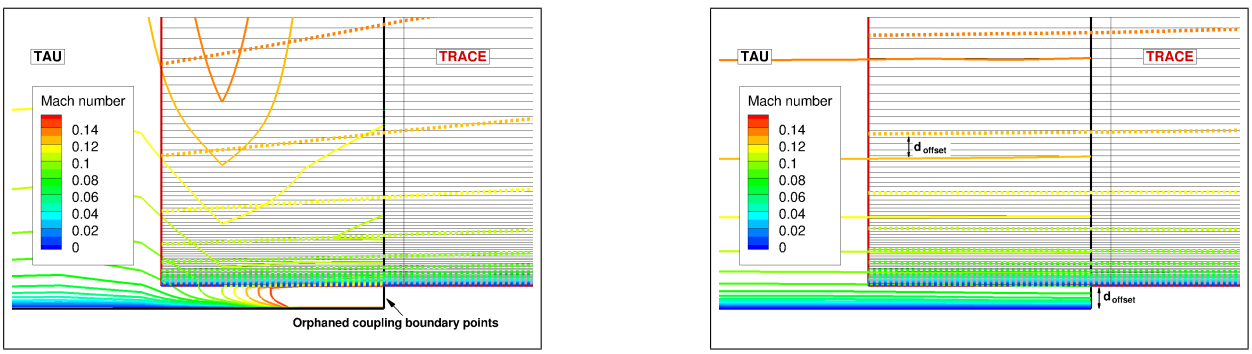

Figure 6: Isolines of Mach number in coupled simulations with an offset of the wall boundary using only nearest neighbor search (left) and using wall projection (right) to complete target point mapping.

The orphaned coupling boundary points of the TAU grid received a flow data update from cells of the TRACE grid found by nearest neighbor search. Due to the dual grid approach to determine donor points in a TRACE grid, the values originate from the first ghost cell layer which introduces an unphysical flow condition in the TAU grid. Applying the wall projection before calculating the interpolation coefficients, the offset of the Mach number isolines between both grids shows a very good agreement with the offset of the grids, which results from the correct wall distance of the computed virtual target point coordinates, as shown in figure 6 on the right.

3.2 Compressor test rig

To demonstrate a coupled simulation in a massively parallel HPC environment, a large three-dimensional configuration representing the Rotor1 compressor test rig of the Technical University of Darmstadt is used. This configuration is to be examined both experimentally and numerically in FOR 1066 and shows a rotor stage of an axial compressor and a device to disturb the onflow of the rotor stage to represent significant flow phenomena of a stalling aircraft engine including a disturbed onflow of the engine compressor. To realize the rotation of the compressor stage in this time-accurate simulation, the TRACE grid was set up with a non-rotating inlet block at the code coupling interface and an internal sliding mesh interface between inlet block and rotor stage. The TAU grid covers the compressor inlet including the flow disturbing device and the cone end of the spinner and consists of about 15.8 million grid points. The initial TRACE grid represents the compressor rotor stage with its 16 blades, divided into 145 grid blocks and consisting of about 19.8 million cells in total.

The inflow conditions are prescribed by the experimental setup with reference values of velocity of $v = 160m/s$, pressure of $p = 85kPa$ and temperature of $T = 300K$. The static pressure behind the rotor stage is set to $p_{out} = 118kPa$. The physical time step size is set to $\Delta t = 9.87 \cdot 10^{-7}$ to perform 190 time steps for each blade passage. In figure 7 a snapshot of the velocity in axial direction at the symmetry plane of the configuration is shown. The isolines of the velocity show a good agreement across the code coupling interface, so that shedded vortices can be introduced accurately into the TRACE grid.

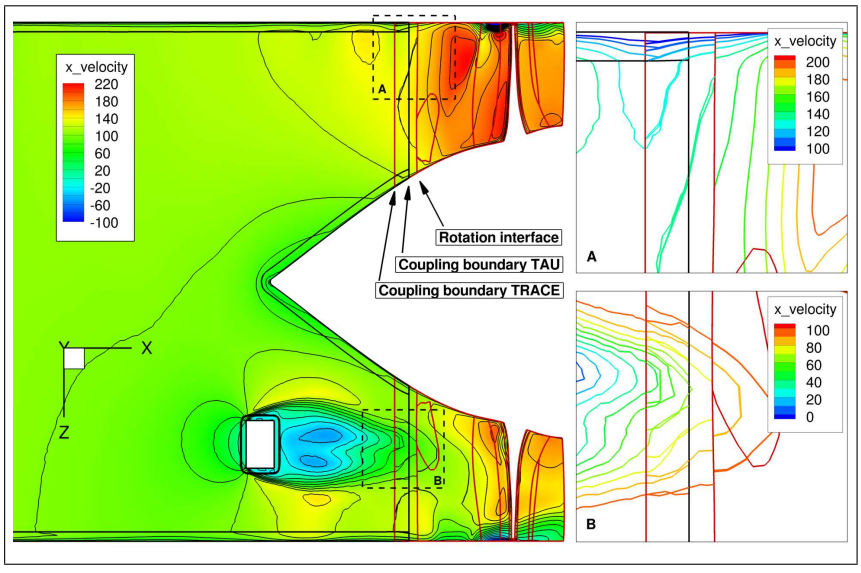

Figure 7: Snapshot of x-velocity of a time-accurate coupled simulation of the Rotor1 test rig.

Due to its size, this test case is well-suited to test parallel performance, since the grids are large enough to use high numbers of CPUs without losing parallel efficiency of each flow solver. The coupling module offers some time measurements statistics of coupled simulation, which helps to adapt the dedicated computing resources of each solver to the demands of the test case with respect to load balance and overall computational time. For this, the time needed for the mapping process, the flow data exchange and the time needed by the flow solver to compute the time step iteration are measured.

In table 1 information about four different parallel test runs of the time-accurate simulation and the measured wall times for mapping, data exchange and solver computations is given. In case of using a coupling time step stride the measured time for solver computations spans the number of computed time steps until the next data exchange.

The non-rotating grid block with the coupling boundary of the initial TRACE grid nevertheless affected the parallel efficiency of the TRACE code for it was the largest grid block and therefore became the bottleneck in simulations with high numbers of CPUs. This issue was addressed by splitting this block in circumferential direction into 16 blocks. This splitting also distributed the coupling boundary to 16 blocks which had a large impact on the parallel performance during the mapping process. For the last mentioned parallel setup further block splitting was used resulting in a total of 224 grid blocks.

Setup TAU-TRACE	t-mapping [s]	t-exchange [s]		t-computation [s]	
		TAU	TRACE	TAU	TRACE
CPU $48-48$ Stride $3-1$ 1 TRACE coupling block	1820.2	0.72	0.17	17.69	8.51
CPU $144-48$ Stride $2-1$ 1 TRACE coupling block	905.1	0.08	0.06	2.69	4.47
CPU $120-72$ Stride $2-1$ 16 TRACE coupling blocks	587.3	0.09	0.08	3.43	2.98
CPU $216-168$ Stride $4-2$ 16 TRACE coupling blocks	250.7	0.17	0.17	3.09	2.38

Table 1: Various settings of parallel runs on an HPC cluster and measured times for mapping process, data exchange and CFD computation time between data exchange.

Of course, the parallelization does not provide a linear scaling of performance, since communication increases drastically in massively parallel simulations. Furthermore, if computational time for a time step decreases, load imbalances become more significant. Therefore it is advisable to test different load balances for large simulations and use the coupling iteration stride if beneficial.

4 Conclusion and Outlook

To simulate flows with different physical properties like a stalling nacelle including the entry of the separated flow into the fan of the engine a method to couple two specialized flow solvers for external and turbomachinery flows has been developed with focus on accurate and robust data

transfer as well as parallel performance and modularity of the communication interface. The coupling environment is based on Chimera interpolation algorithms allowing a data exchange for any kind of mesh type and spatial discretization. Since the data interpolation will be applied not only inside the flow field but also near body surfaces, a projection method has been implemented to preserve the wall distances to prevent interpolation errors that would otherwise degenerate the quality of the flow solution, or result in unphysical flow conditions. A study of numerical parameters of the time stepping schemes has been performed and the accuracy of the data transfer has been demonstrated with a two-dimensional channel flow simulation and the parallel performance has been evaluated with a large three-dimensional compressor configuration.

Future work within FOR 1066 will be highly accurate simulations of gust encounters. To propagate the velocity disturbances of the gust through the flow field without unphysical dissipation, a Cartesian solver with a higher-order accurate spatial discretization method will be used in the far field. The near field will be simulated with the TAU code to allow for flexible grid generation to discretize the boundary layer. Both CFD codes will be coupled with the coupling method presented in this paper. A first demonstration of a coupled simulation using TAU and the Cartesian solver was already shown, but the interpolation technique has to be adapted to the higher-order discretization of the Cartesian solver to utilize the full potential of this application.

Acknowledgments

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