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TIME STEPPING ALGORITHMS FOR PARTITIONED MULTI-SCALE MULTI-PHYSICS IN PRECICE

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Abstract. Using the partitioned approach, specialized single-physics solvers with different numerical properties may be combined to solve a multi-physics setup. This allows us to use expert solvers for every considered phenomenon. To handle their respective problems in the most efficient way solvers use non-matching meshes – both in the spatial and temporal domain (multi-scale) – and different discretization techniques (inhomogeneous setup).
The coupling library preCICE provides methods for an appropriate treatment of non-matching spatial meshes, but it currently lacks advanced techniques for the treatment of non-matching temporal discretization. To maintain order and stability of time stepping, special care must be taken and simply exchanging nodal values at the coupling interface does not suffice.
This contribution presents different setups that arise in partitioned multi-physics problems. Different temporal scales and different discretization techniques are considered. Challenges and requirements that stem from the partitioned approach are derived and various candidate techniques for multi-rate time stepping are introduced and evaluated. Convergence studies for a simple benchmark scenario are performed and implementation aspects are presented – with the final goal of implementing multi-rate time stepping in preCICE.

1 INTRODUCTION

The coupling library preCICE [1] has been developed to provide a flexible, minimally invasive way to couple independent existing solvers in surface-coupled multi-physics simulations, such as aeroelasticity [2, 3] , cardio-vascular flow [4] or conjugate heat transport in fluids and structures [5, 6]. It provides various options for three important ingredients of coupling thus eliminating the need for re-implementation in every coupled simulation setup. The first ingredient is the technical communication between processes of several parallel solvers, which is realized in a scalable point-to-point manner via MPI or TCP/IP [7]. The second ingredient

is data mapping. Here, preCICE provides both consistent and conservative mapping methods to map physical coupling data, such as velocities or forces, from the surface of one solvers mesh to the (non-matching) discretization points of another solver at the same surface [8]. The third ingredient, iterative coupling, implements several methods to speed up the solution of the interface fixed-point equations based on pure input and output data [9].
However, a proper coupling for multi-rate timestepping is still neglected. Additionally, we would like to be able to couple solvers that are using different timestepping schemes. This would enable efficient surface-coupled and also multi-scale simulation. Naively coupling solvers with two different timestepping schemes or using two different timestep sizes leads to a degradation of the overall timestepping to first order convergence [10, 11, 12], and it affects the stability, even if we couple implicitly [12]. Whereas various approaches have been proposed to recover at least second-order consistency [2, 4, 12], we aim at providing more general solutions for timestepping with arbitrary order while still following the black-box philosophy of preCICE: Our approach should only require the exchange of input/output data and not the exchange of (time) discretization details of the involved solvers. This contribution is motivated by fluid-structure-acoustic (FSA) interaction, explained in more detail in Section 2. Further applications with clear multi-scale characteristics are, for example, powder bed based additive manufacturing processes [13] or multi-scale structural mechanics [14, 15].
The remainder of the paper is organized as follows: In Section 2, we present requirements for multi-rate coupling based on characteristics of the physics, on the one hand, and the black-box paradigm in preCICE, on the other hand. In particular, we focus on surface coupling, which is different from volume coupling as it resembles both time splitting schemes and domain partitioning. In Section 3, we provide an overview of existing coupling schemes for surface coupling. In Section 4, we run numerical experiments using these existing schemes; the experimental setup is a linear one dimensional heat transport model on a partitioned domain. In Section 5, we finally assess the numerical properties of the coupling schemes based on our previous experiments and give conclusions and further directions with regards to an implementation of multi-rate coupling schemes in preCICE.

2 REQUIREMENTS FOR MULTI-RATE COUPLING IN PRECICE

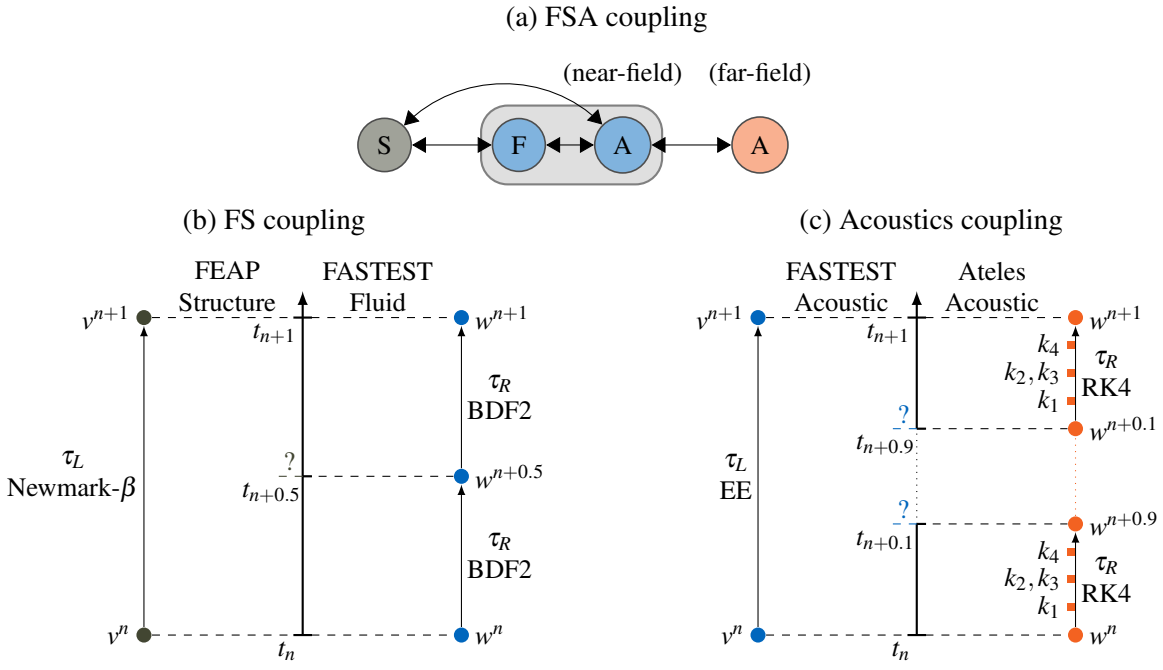
The requirements for multi-rate coupling can be split into two classes: (i) requirements stemming from the type of surface-coupled multi-physics and multi-scale applications introduced above and (ii) requirements stemming from the preCICE paradigm of coupling black-box solvers not giving access to any discretization details.

(i) *Application specific requirements.* From an application point of view, being able to couple different timestepping schemes using different timestep sizes as shown exemplary in Figure 1 is the ultimate goal. The need for combining different timestepping methods stems from different requirements in terms of stability (stiffness of the underlying different models), whereas different timestep sizes are imposed by the need to efficiently tackle multi-scale problems. The showcase we ultimately target is FSA interaction, where, in particular, the coupling between a full fluid simulation around an elastic structure, in the near-field, and the noise propagation, in the far-field, features multi-scale behavior: For the flow part the natural scale is much larger

than for the acoustic wave propagation. For a partitioned coupling approach, the resulting challenge is to provide suitable surface data for both sides of the coupling interface not only at the common global timestep, but also for substeps in case of different timestep sizes and for stages of Runge-Kutta methods. We seek for a way that preserves the minimum of the convergence orders of both coupled timestepping method.

(ii) *Software specific requirements.* preCICE [1] is implemented as a library with a clearly defined application user interface (API) providing high-level functions that are called by solver-specific adapter codes. The API is designed such that it can be used also for commercial closed-source (black-box) solvers. To guarantee the necessary flexibility, the whole coupling functionality has to be based on input and output data of the solvers without access to further solver discretization details. Thus, the multi-rate coupling proposed in this work also has to follow this rule. This means, for example, that we do not want to use tailored approaches to communicate the intermediate stages of Runge-Kutta schemes.

Figure 1: (a) Our exemplary fluid-structure-acoustics (FSA) setup with temporal multi-scale characteristics: (b) fluid-structure (FS) coupling between structure dynamics in FEAP [16] using Newmark-β timestepping and fluid dynamics in FASTEST [17] using BDF2 and subcycling; (c) acoustics coupling between acoustic near-field in FASTEST using explicit Euler (EE) timestepping and acoustic far-field in Ateles [18] using fourth-order Runge-Kutta (RK4) and subcycling.



3 REVIEW OVER EQUATION COUPLING SCHEMES

In this section, we provide a review over different techniques for the coupling of partitioned problems. We consider a partitioned setup with two participants L and R and their respective spatially discretized partial solutions v and w, in $\Omega^L_{h_L}$ and $\Omega^R_{h_R}$, respectively. The partitioned setup solves the overall coupled problem $u = (v, w)$, in $\Omega_h = \Omega^L_{h_L} \cup \Omega^R_{h_R}$.
The spatially discretized partitioned system can then be written as

$$\begin{pmatrix} \dot{v}(t) \\ \dot{w}(t) \end{pmatrix} = \begin{pmatrix} f_L(v(t), w(t), t) \\ f_R(v(t), w(t), t) \end{pmatrix}. \tag{1}$$

We define the temporal discretization $t_n = n \cdot \tau, n \in \mathbb{N}, t_n \in [0, T]$, where T denotes the maximum simulation time and τ denotes the macro timestep size τ. We denote $u^n = u(t_n)$ and call the interval $T_n = [t_n, t_{n+1}]$ a window. To realize subcycling we introduce micro timesteps τ_L and τ_R for the respective participants on a window. The relationship between the macro timestep size τ and the micro timestep sizes τ_L and τ_R is defined as $N_L \tau_L = N_R \tau_R = \tau$ with $N_L, N_R \in \mathbb{N}$.

3.1 Classical coupling techniques

Classical coupling schemes use a very simple and easy to implement approach of exchanging data associated to different timesteps between solvers, which basically corresponds to constant interpolation in time. Classical coupling schemes can be based on a sequential, Gauss-Seidel-like execution of both solvers or a simultaneous, Jacobi-like execution[9]. For simplification, we only consider sequential coupling in this contribution. Furthermore, classical coupling schemes come in two flavors: explicit and implicit coupling.
Explicit coupling – often also referred to as weak or loose coupling [20] – relies on the explicit exchange of coupling conditions. This means that the result of one participant is directly used as a boundary condition for the next timestep of the other participant. No iterations are used, which leads to low computational cost, but also to characteristic instabilities [21, 22]. One of the involved solvers always uses interface data of the old time step t_n for its calculations during a global time step (Figure 2a)[1] Implicit coupling schemes – also referred to as strong coupling [20] – are used to avoid the aforementioned instabilities at the cost of an iterative approach, where a fixed point equation for interface degrees of freedom is solved at every timestep to guarantee consistent and stable solutions. The participants iteratively update their respective boundary conditions until they match at the interface. To avoid high cost and to speed up computations, acceleration schemes are widely used [9, 23]. These implicit schemes result in a converged solution where all solvers use coupling data from their partners corresponding to t_{n+1} (constant interpolation backwards in time, Figure 2b).
Due to the constant interpolation in time, the order of the coupled timestepping scheme degrades to one for both approaches [10, 11, 12]. Additionally, even implicit time stepping schemes show instabilities for large timesteps [12].

[1] The second solver uses data associated to the next step t_{n+1}.

3.2 Semi explicit-implicit coupling

For simple one-step methods without intermediate stages, using a mixture of implicit and explicit coupling can help to avoid order degradation to first order and tackle stability issues [12, 20]. The resulting scheme still relies on (expensive) iterations to implicitly determine consistent values for the coupling variable at the interface. We illustrate this for the example of the second order consistent trapezoidal rule, which reads

$$\begin{pmatrix} v^{n+1} \\ w^{n+1} \end{pmatrix} = \begin{pmatrix} v^n \\ w^n \end{pmatrix} + \frac{dt}{2} \begin{pmatrix} f_L(v^n, w^n, t_n) + f_L(v^{n+1}, w^{n+1}, t_{n+1}) \\ f_R(v^n, w^n, t_n) + f_R(v^{n+1}, w^{n+1}, t_{n+1}) \end{pmatrix} \tag{2}$$

if applied monolithically to Equation 1. On the other side, classical implicit coupling using the trapezoidal rule in both solvers would give

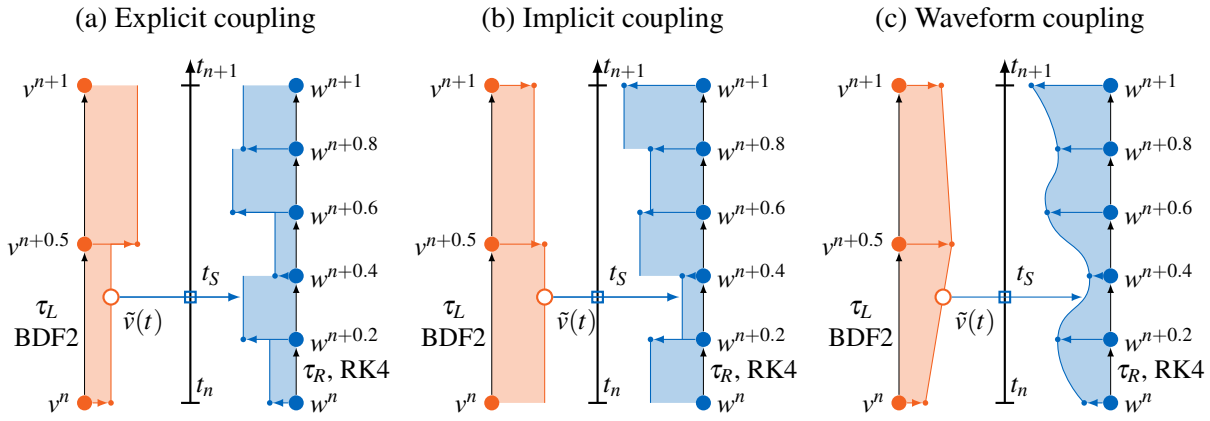
$$\begin{pmatrix} v^{n+1} \\ w^{n+1} \end{pmatrix} = \begin{pmatrix} v^n \\ w^n \end{pmatrix} + \frac{dt}{2} \begin{pmatrix} f_L(v^n, w^{n+1}, t_n) + f_L(v^{n+1}, w^{n+1}, t_{n+1}) \\ f_R(v^{n+1}, w^n, t_n) + f_R(v^{n+1}, w^{n+1}, t_{n+1}) \end{pmatrix}.$$

It can be shown easily that this results in only first order convergence. To recover the original scheme (see Equation 2) and, thus, second order, we have to change the t_{n+1} values in the right-hand side terms associated to t_n back to v^n and w^n respectively, i.e., use a scheme that couples implicitly in the second part of the right-hand side and explicitly in the first.

3.3 Predictor-based coupling

Where semi explicit-implicit coupling helps to recover the order for implicit timestepping schemes, for explicit coupling, predictor schemes are helpful to speed up convergence [24]

Figure 2: Coupling schemes. Colored areas resemble approximations of the solution v and w on the respective subdomains. approximation $\tilde{v}$ is sampled at t_S: (a) explicit coupling with subcycling, constant extrapolation $\tilde{v}(t) = v^n$ is used for $t_n < t < t_{n+0.5}$; (b) implicit coupling with subcycling, constant extrapolation $\tilde{v}(t) = v^{n+0.5}$ is used for $t_n < t < t_{n+0.5}$; (c) waveform relaxation coupling with subcycling, the waveform $\tilde{v}(t)$ is a time continuous function on the window $T_n = [t_n, t_{n+1}]$.



or to reduce error [2]. We use a customized explicit predictor for one participant to provide the missing data at the stages of the other participant (i.e., stages of a Runge-Kutta scheme). As an example, we apply Heun's method monolithically to Equation 1:

$$\begin{pmatrix} v^{n+1} \\ w^{n+1} \end{pmatrix} = \begin{pmatrix} v^n \\ w^n \end{pmatrix} + \frac{dt}{2} \begin{pmatrix} f_L(v^n, w^n, t_n) + f_L(\tilde{v}^{n+1}, \tilde{w}^{n+1}, t_{n+1}) \\ f_R(v^n, w^n, t_n) + f_R(\tilde{v}^{n+1}, \tilde{w}^{n+1}, t_{n+1}) \end{pmatrix},$$

where $\tilde{v}^{n+1}$ and $\tilde{w}^{n+1}$ are computed from an explicit Euler step for Equation 1. In a partitioned explicit coupling approach, $\tilde{v}^{n+1}$ in f_R and $\tilde{w}^{n+1}$ in f_L are not available. We have to rely on v^n in f_R or w^n in f_L instead, which contradicts Heun's method.
A predictor improves this situation: Each participant performs an explicit Euler and provides the predicted values $\tilde{\tilde{v}}^{n+1}$ and $\tilde{\tilde{w}}^{n+1}$ to the other participant. This results in the following scheme:

$$\begin{pmatrix} v^{n+1} \\ w^{n+1} \end{pmatrix} = \begin{pmatrix} v^n \\ w^n \end{pmatrix} + \frac{dt}{2} \begin{pmatrix} f_L(v^n, w^n, t_n) + f_L(\tilde{v}^{n+1}, \tilde{\tilde{w}}^{n+1}, t_{n+1}) \\ f_R(v^n, w^n, t_n) + f_R(\tilde{\tilde{v}}^{n+1}, \tilde{w}^{n+1}, t_{n+1}) \end{pmatrix}$$

3.4 Splitting methods

Another alternative to couple inhomogeneous timestepping schemes are Splitting methods [26]. In the following, we concentrate on Strang splitting [25], which allows second order accuracy in time if the substeps are also solved with at least second order accuracy. For (1), one timestep of Strang splitting reads

1. participant L solves $\dot{v}(t) = f_L(v(t), w^n, t)$ in $[t_n, t_{n+1/2}]$, yielding $v^{n+1/2}$,
2. participant R solves $\dot{w}(t) = f_R(v^{n+1/2}, w(t), t)$ in $[t_n, t_{n+1}]$, yielding w^{n+1},
3. participant L solves $\dot{v}(t) = f_L(v(t), w^{n+1}, t)$ in $[t_{n+1/2}, t_{n+1}]$, yielding v^{n+1},

where $t_{n+1/2} := t_n + \tau/2$.

3.5 Waveform relaxation

Waveform relaxation (WR) or dynamic iteration is a method where so-called waveforms at the coupling interface are exchanged between participants. The original idea comes from electrical circuits that are split into subsystems exchanging their waveforms at the system interface [27]. A waveform is a continuous functional approximation $\hat{v}(t)$ of the coupling variable $v(t)$ on a window T_n. The continuous approximation $\hat{v}(t)$ allows to transfer significantly more information than the snapshots in time v^n, v^{n+1} as used in the classical coupling techniques (cf. Section 3.1). Similar to implicit coupling, the approximation is iteratively improved until convergence. T_n can be subdivided using arbitrary time step sizes τ_L, τ_R for both participants, since the temporal discretization at the interface is hidden by the waveform (Figure 2c). For more details on WR, we refer to [27, 28]. WR has already been successfully used in partitioned multi-physics simulations with subcycling [29]. One timestep of the iterative version of WR for (1) reads

1. participant L solves $\dot{v}(t) = f_L(v(t), \hat{w}_k(t), t)$ in T_n and provides $\hat{v}_k(t), t \in T_n$,

2. participant R solves $\dot{w}(t) = f_R(\hat{v}_k(t), w(t), t)$ in T_n and provides $\hat{w}_{k+1}(t), t \in T_n$,
3. if $\hat{v}_k, \hat{w}_k$ not converged continue iterating ($k \to k+1$).

Note that the waveforms $\hat{v}_k$ and $\hat{w}_k$ are provided by the participants L and R using, for example, appropriate interpolation techniques.

4 NUMERICAL EVALUATION: PARTITIONED HEAT TRANSPORT EQUATION

A thorough convergence study of the partitioned heat transport equation is performed to evaluate the performance of the previously introduced coupling schemes.

4.1 Experimental setup

Monolithic and partitioned model We perform numerical experiments with the transient 1D heat transport equation on the domain $\Omega = [x_L, x_R]$:

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2}, x \in \Omega, t \in [0,T] .$$

We apply Dirichlet boundary conditions at the left $x_L = 0$ and right $x_R = 2$ boundary of the domain, such that $u(x_L,t) = u_L^D$ and $u(x_R,t) = u_R^D$. We use initial conditions $u(x,t_0) = u_0(x) = x - x^2$, and consistently set $u_L^D = u_0(x_L), u_R^D = u_0(x_R)$. We consider a monolithic setup, where the equation is solved on the whole domain Ω, as well as a partitioned setup (already described in Section 3), where we split the domain Ω at $x_C = 1$ and solve one heat transport equation on each of the subdomains Ω_L and Ω_R. At the coupling point x_C, we require C^1-continuity,

$$v(x_C,t) = w(x_C,t) \text{ and } \frac{\partial}{\partial x} v(x_C,t) = \frac{\partial}{\partial x} w(x_C,t) .$$

We split these coupling conditions in a Dirichlet-Neumann manner: On Ω_L, a heat transport equation subject to a Dirichlet boundary condition at the left part of the domain $v(x_L,t) = u_L^D$ and Neumann boundary condition at the right part of the domain $\frac{\partial}{\partial x} v(x_C,t) = u_C^N$ is solved. On Ω_R, the heat transport equation is subject to Dirichlet boundary conditions on both sides of the domain $w(x_C,t) = u_C^D$, $w(x_R,t) = u_R^D$. u_C^D and u_C^N are continually exchanged between both heat equations.

Discretization To discretize Ω, we introduce the mesh $x_{i,L} = x_L + ih_L, h_L = \frac{x_C - x_L}{M_L}$ and $x_{i,R} = x_C + ih_R, h_R = \frac{x_R - x_C}{M_R}$, with M_L and M_R denoting the number of cells in the regions left and right, of x_C, respectively. For the monolithic setup this results in a single, possibly non-regular (if $h_L \neq h_R$), mesh of $M_L + M_R + 1$ points, Ω_{h_L/h_R}. For the partitioned setups, we obtain two regular meshes with $M_L + 1$ and $M_R + 1$ points, $\Omega_{h_L}^L$ and $\Omega_{h_R}^R$, respectively. In our experiments, we consider a regular mesh $\Omega_{h/h}$ and a non-regular mesh $\Omega_{h/0.25h}$ with $h = 0.2$. All occurring spatial derivatives are discretized using second order finite difference schemes. For the temporal discretization explicit or implicit timestepping schemes of second and fourth order are used.

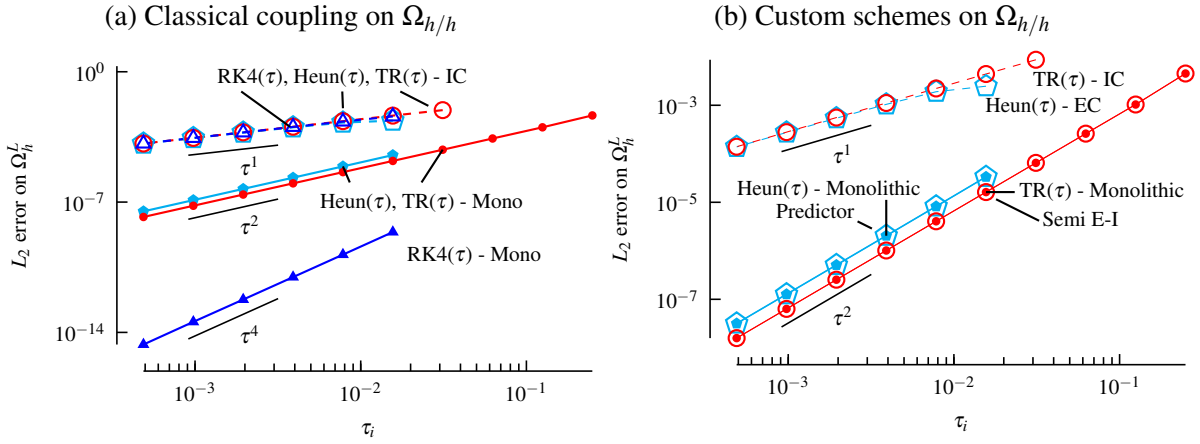
Convergence study setup The aim of our experiments is to determine the convergence order and accuracy in time of the partitioned setup introduced above. Different coupling schemes (see Section 3) are compared and evaluated. For this purpose, we compare the solution obtained through a partitioned or monolithic experiment to a monolithic reference solution u_{ref}. We consider the error e in the $L_1(\Omega_L)$-norm at the final time T: $e = \sum_{j=0}^{N} ||v_j(T) - u_{\text{ref},j}(T)||/N$. Here, j denotes the vector index of the discretized solution. The convergence study is performed by varying the timestep size $\tau_i = \tau_0/2^i, i = 0 \dots 9$ with $\tau_0 = T/4$. u_{ref} results from a temporal resolution $\tau_{\text{ref}} = 0.5 \min \tau_i$.

4.2 Covergence study

Figure 3 and Figure 4 show the results for the regular mesh $\Omega_{h/h}$ and the non-regular mesh $\Omega_{h/0.25h}$, respectively[2]. For $\Omega_{h/h}$, we observe an order degradation to first order for implicit coupling as well as for explicit coupling. This means that the implicit trapezoidal rule, Heun's method and Runge-Kutta 4 produce all similar error. On the other hand, if we apply customized coupling schemes such as the semi explicit-implicit coupling for the implicit trapezoidal rule, or a predictor scheme for Heun's method, we are able to recover second order.
Strang splitting recovers second order on the non-regular grid $\Omega_{h/0.25h}$ for arbitrary explicit schemes. Fourth order schemes, such as Runge-Kutta 4, are reduced to second order. Strang splitting allows us to use an explicit solver on the coarse domain Ω_h^L and an implicit solver

[2] `github.com/BenjaminRueth/TimeSteppingAlgorithms`

Figure 3: Convergence studies for different timestepping and coupling schemes for the 1D partitioned heat transport equation on a regular grid $\Omega_{h/h}$ with monolithic reference solution (Mono) and constant spatial resolution h for both subdomains Ω_h^L and Ω_h^R: (a) order degradation for the implicit trapezoidal rule (TR), Heun's method (Heun) and Runge-Kutta 4 (RK4) timestepping schemes with explicit (EC) and implicit coupling (IC); (b) semi-explicit-implicit (Semi E-I) and predictor coupling schemes recovering second order for trapezoidal rule (TR) and Heun's method (Heun).

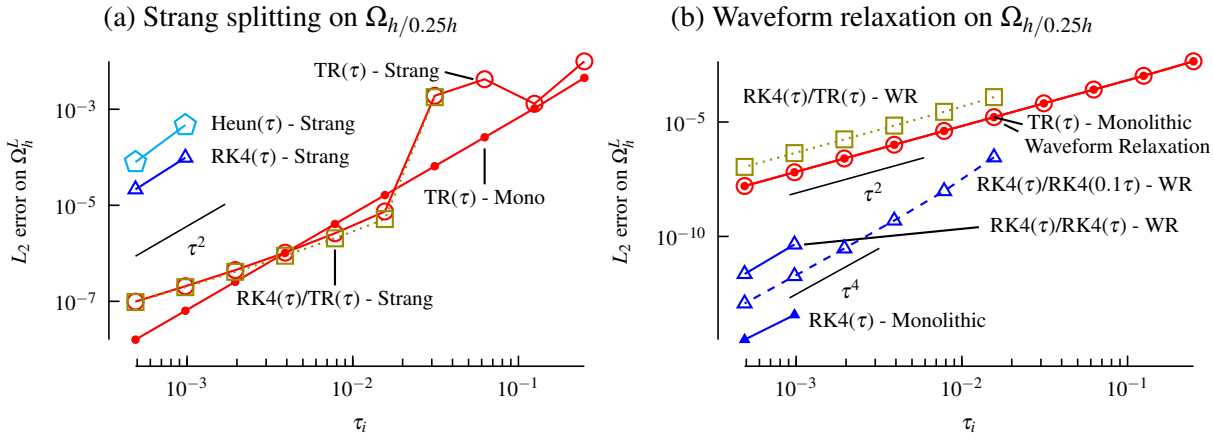


on the fine domain $\Omega^R_{0.25h}$. This avoids stability problems due to the finer mesh resolution on $\Omega^R_{0.25h}$. However, the order is reduced to one.
Waveform relaxation coupling completely avoids order degradation for all considered timestepping schemes. We use matching interpolation order for the different timestepping schemes: that is, linear interpolation for second order schemes and cubic spline interpolation or dense output interpolation [31] for Runge-Kutta 4. To take the irregular mesh into account, we use a combination of different timestepping schemes, here the locally lowest order scheme defines the global order. Alternatively we apply subcycling, where we use a finer timestep $\tau_R = 0.1\tau_L$ on $\Omega^R_{0.25h}$.

5 CONCLUSION

Based on numerical experiments with a partitioned 1D heat transport equation scenario, we assessed the numerical properties of different coupling schemes. We observed that classical explicit coupling and implicit coupling only require the exchange of snapshots (in time) and are, thus, easy to implement also for black-box coupling [1]. However, a degradation of accuracy in time to first order occurs, leading to a waste of computation time, since smaller timesteps are needed to obtain a given error threshold and the higher order of the involved participants' time stepping schemes is not exploited.
To avoid order degradation, we analyzed customized schemes, such as the explicit-implicit

Figure 4: Convergence studies for different timestepping and coupling schemes for the 1D partitioned heat transport equation on an irregular grid with monolithic reference solution (Mono). The right half $\Omega^R_{0.25h}$ of the domain $\Omega_{h/0.25h}$ is discretized through a refined mesh with resolution $0.25h$, while the left half Ω^L_h has a coarser resolution h: (a) Strang splitting (Strang) coupling scheme recovering second order for arbitrary explicit timestepping schemes, such as Heun's method (Heun) and Runge-Kutta 4 (RK4), while for combinations with trapezoidal rule (TR) no clear order is visible; (b) waveform relaxation (WR) coupling scheme recovering optimal convergence order for arbitrary timestepping schemes, such as Heun's method (Heun), implicit trapezoidal rule (TR) and Runge-Kutta 4 (RK4).



coupling or predictor schemes, and showed their ability to recover high order and stability for second order time stepping schemes, such as the trapezoidal rule or Heun's method. However, customized schemes depend on the solver setup and, thus, contradict the black-box paradigm.
Strang splitting, as an example for an operator splitting method, allows the combination of arbitrary time stepping schemes without the need of customization, since the method acts as an abstract interface hiding the timestepping methods from each other. However, operator splitting schemes are strictly sequential and with Strang splitting only second order can be reached at maximum and a splitting error is introduced. Though there are higher order splitting methods, this approach is still not sufficiently generic for our purpose and it would require a completely different coupling workflow depending on the requested order of the overall time stepping.
Finally, waveform relaxation allows to combine arbitrary time-stepping schemes with independent timestep size (subcycling) while maintaining the minimum order of the time stepping schemes in use. The resulting method is flexible and only requires an interpolation in time analogue to the interpolation in space already used in black-box spatial coupling.
In this sense, for the black-box library approach of preCICE, waveform relaxation coupling fits the requirements defined above. Strang splitting should be kept in mind as a simple and fast method, if only second order is required for a weakly coupled sequential setup. Only if solver details are known, semi explicit-implicit coupling or predictor schemes may also be considered.
So far, we applied waveform relaxation coupling only for the coupling between two heat transport equations. We will consider further test scenarios in the future, including fluid-structure interaction with its characteristic instabilities for incompressible fluids due to the added-mass-effect [21, 23]. Additionally, we will further investigate the software specific features of waveform relaxation coupling in preCICE, i.e. how to best communicate the interpolant in time at the coupling interface from a software engineering perspective. Also, new numerical questions, such as which data should be used in the iterative fixed-point equation solver at the coupling interface, arise. We want to study whether the applied quasi-Newton solves should be based on data at the end and beginning of time windows or, for example, also on support points of the time interpolant.

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