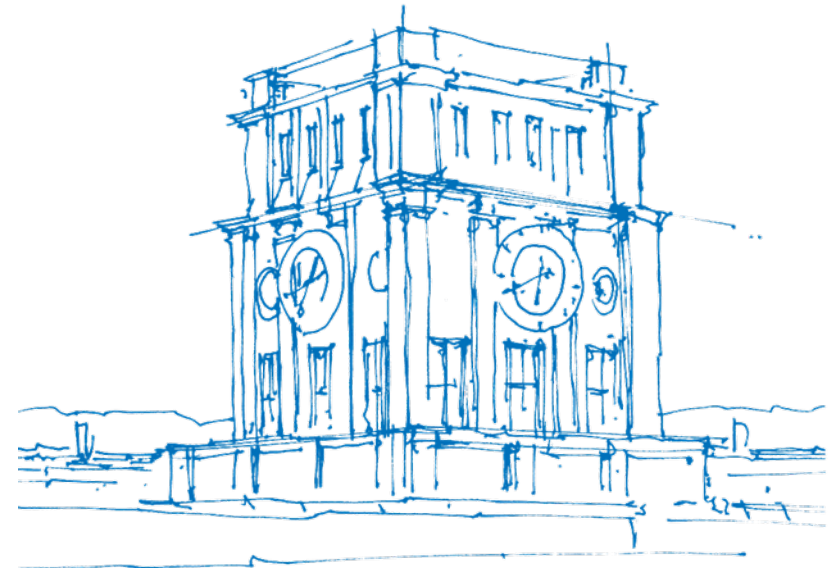


Time stepping algorithms for partitioned multi-scale multi-physics in preCICE

Benjamin R uth, Benjamin Uekermann, Miriam Mehl, Hans-Joachim Bungartz

Technical University of Munich
Department of Informatics
Chair of Scientific Computing

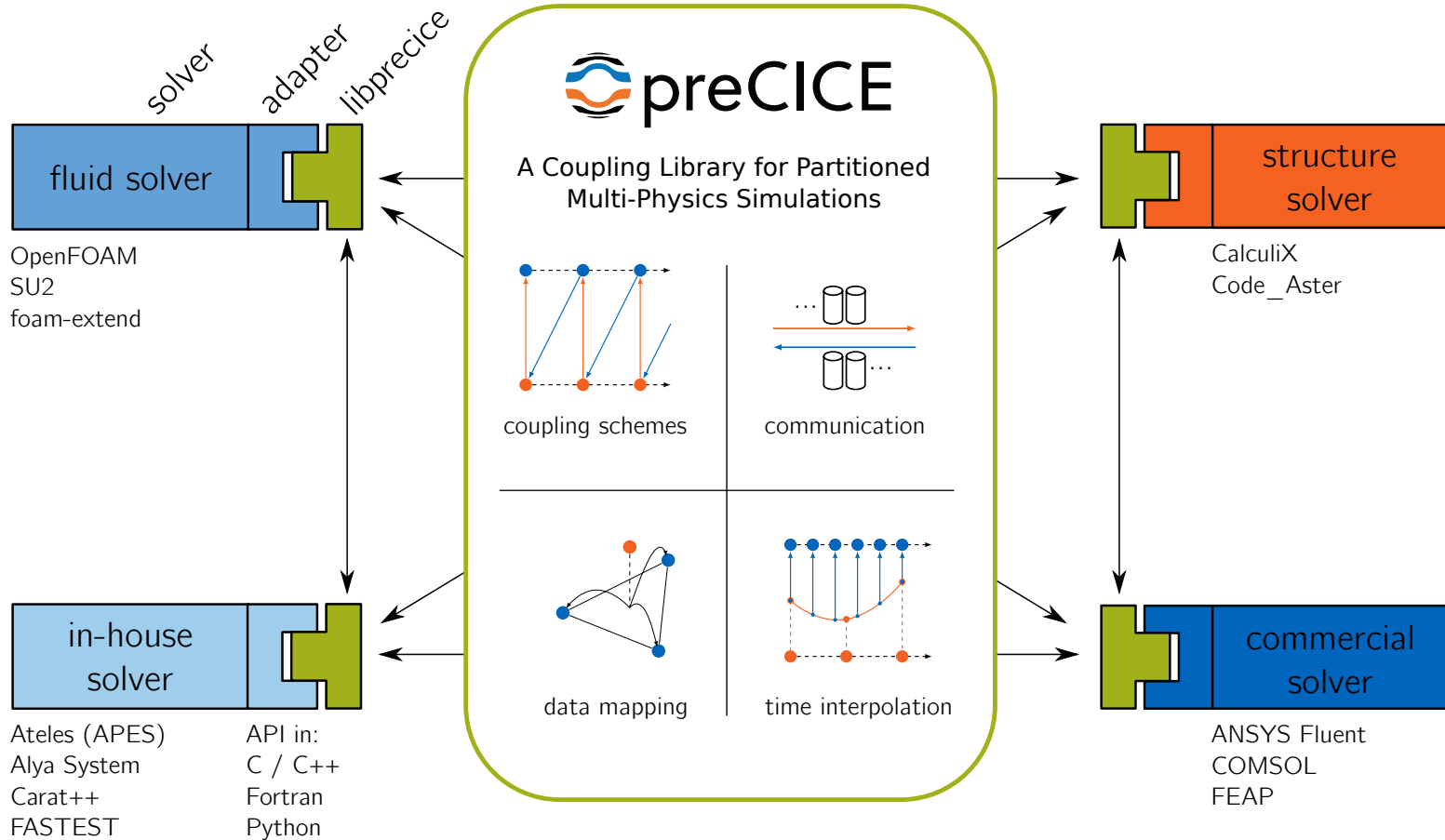
ECCM 6 / ECFD 7
Glasgow, UK
14. June 2018



TUM Uhrenturm

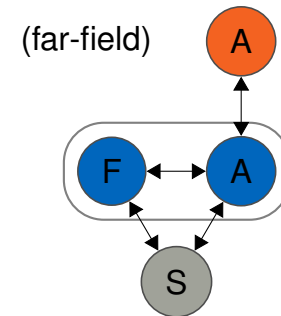
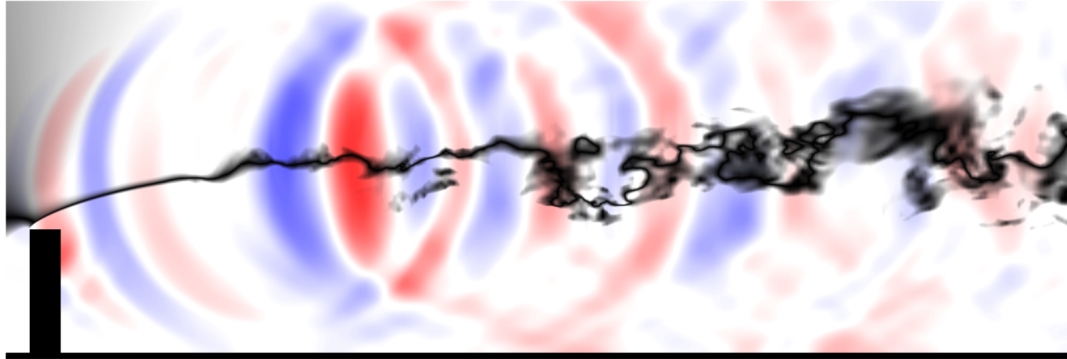
Partitioned multi-physics

preCICE



Partitioned multi-physics

Example application: fluid-structure-acoustics



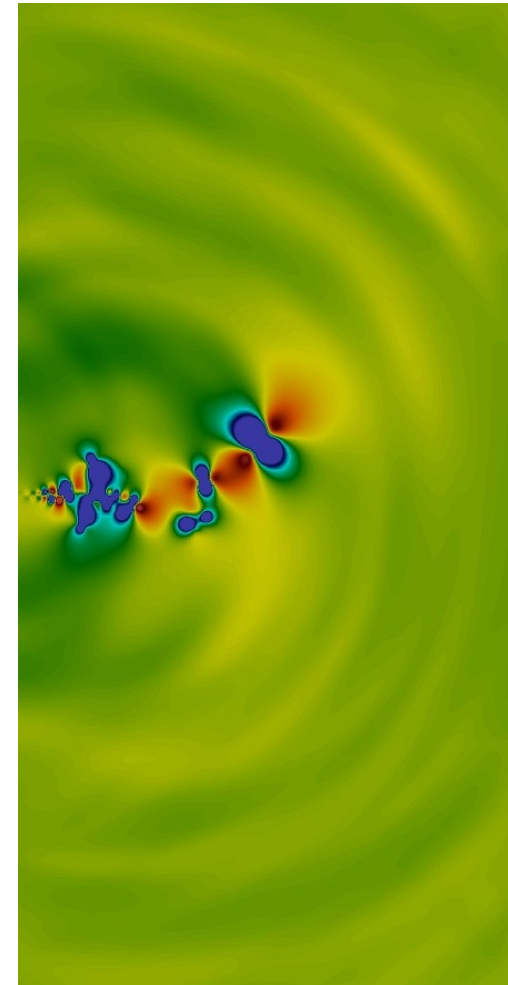
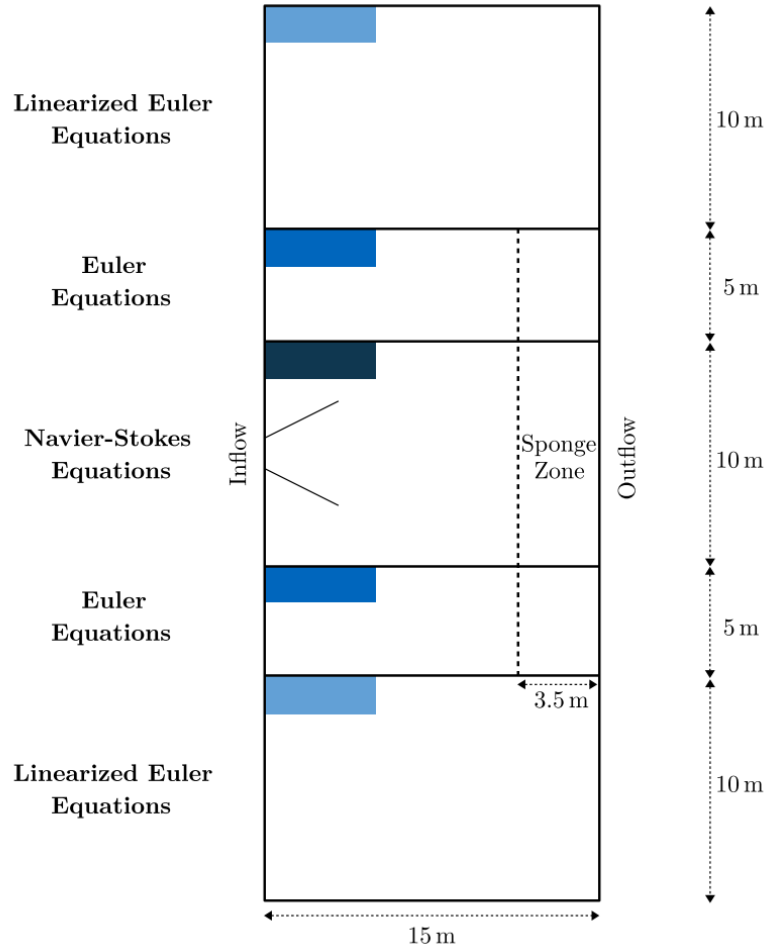
Fluid-structure-acoustics simulation and partitioned setup¹.

physics	timescale	solver	scheme	order
(A)	small	Ateles	RK	2 or 4
(A)	small	FASTEST	EE	1
(F)	medium	FASTEST	CN	2
(S)	large	FEAP	N- β	1 or 2

¹Reimann, T., et al. (2017). Aspects of FSI with aeroacoustics in turbulent flow. In 7th GACM Colloquium on Computational Mechanics.

Partitioned multi-physics

Example application: acoustics-acoustics



Three-field flow coupling around a 2D subsonic free jet¹

¹Uekermann, B. (2016). Partitioned Fluid-Structure Interaction on Massively Parallel Systems.

Partitioned multi-physics

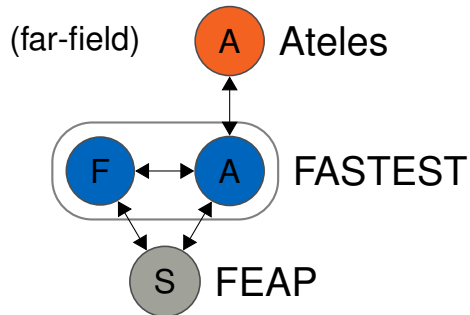
Time stepping requirements

Engineering:

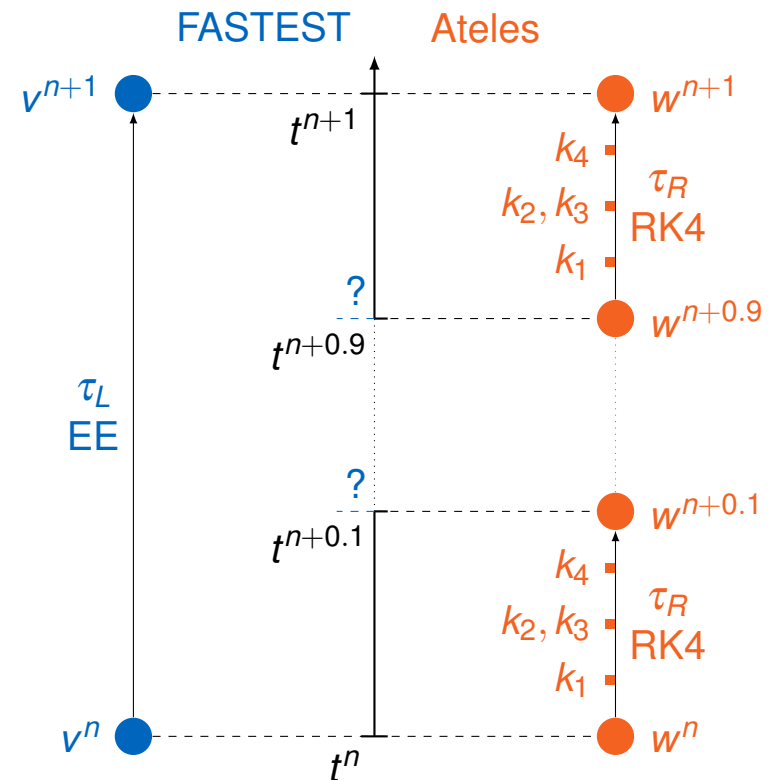
- use different solvers (EE + RK4)
- use different time discretization
- no degradation of solver performance

Informatics:

- black-box approach (nodal data)
- parallel (Exa-Scale)



Multi-Scale Multi-Physics

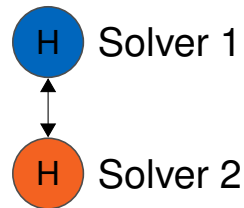


Partitioned heat transport equation

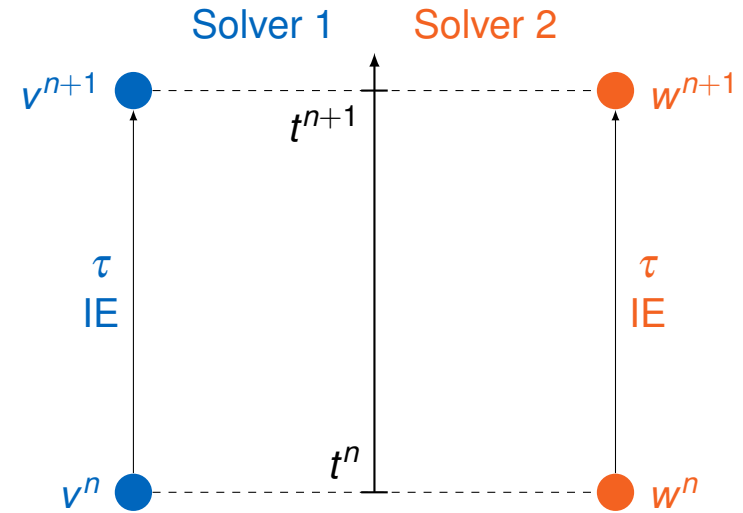
A simple model problem

Partitioned heat transport equation

- introduce a model problem
- review different coupling schemes
- evaluate performance of schemes



Simple setup



Partitioned heat transport equation

Monolithic setup

Heat Transport equation

$$\frac{\partial u(x, t)}{\partial t} = \alpha \frac{\partial^2 u(x, t)}{\partial x^2}, x \in \Omega, t \in \mathbb{R}^+$$

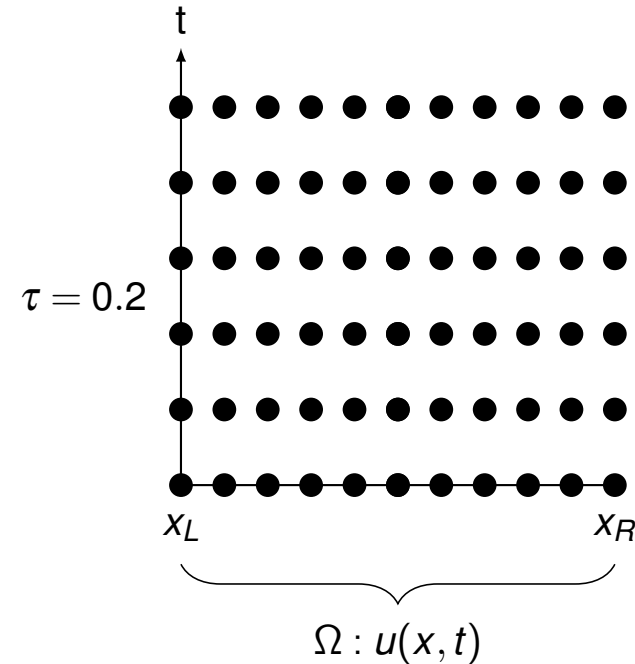
Dirichlet boundary conditions

$$u(x = x_L, t) = u_L^D, u(x = x_R, t) = u_R^D$$

Initial condition

$$u(x, t = 0) = u_0(x)$$

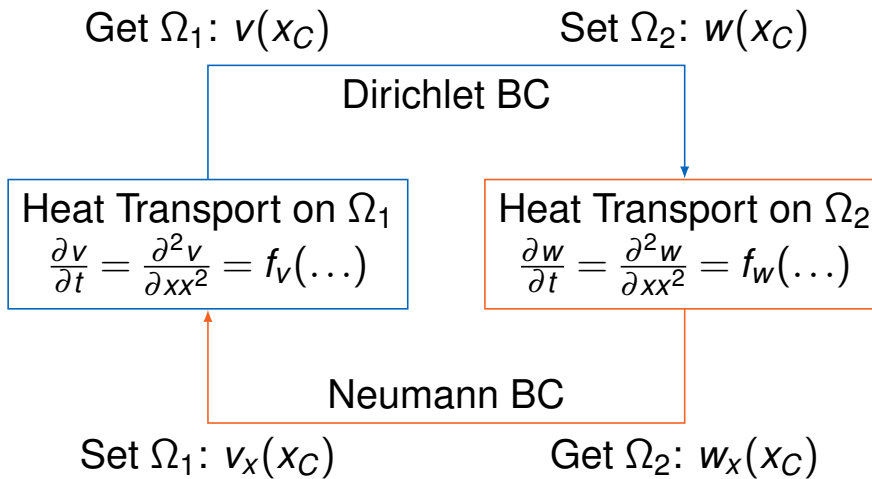
Discretization



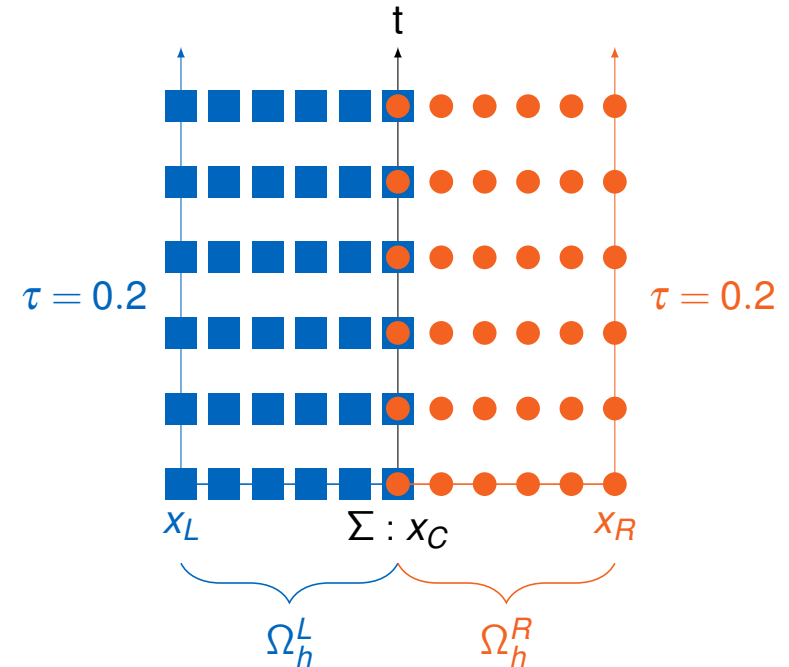
Partitioned heat transport equation

Partitioned setup

Dirichlet-Neumann coupling



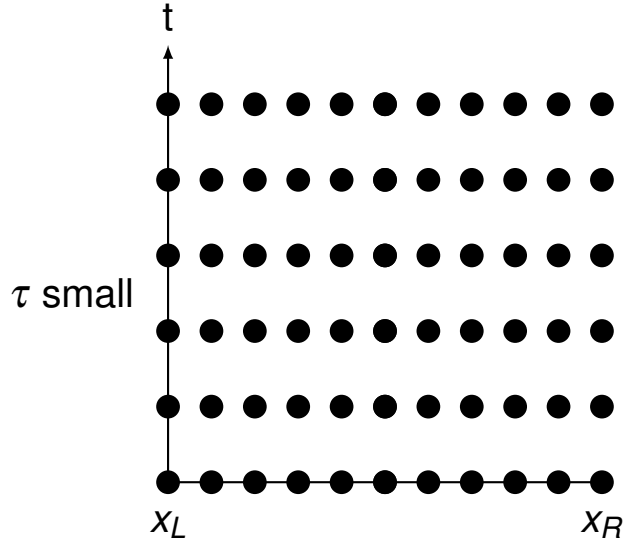
Partitioning



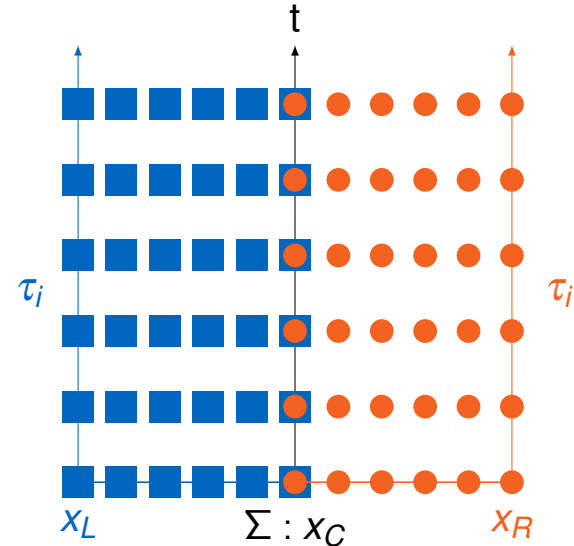
We are interested in higher order coupling

- different coupling schemes
- use constant spatial meshwidth h
- refine temporal meshwidth τ
- compare partitioned result to monolithic solution \mathbf{u}^n with fine τ

Monolithic setup



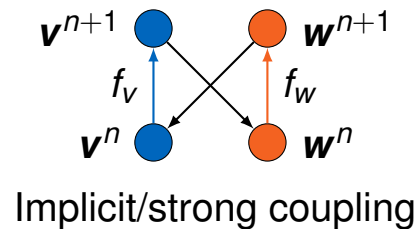
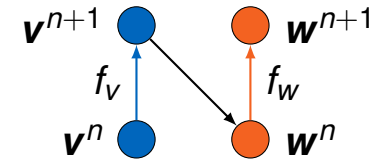
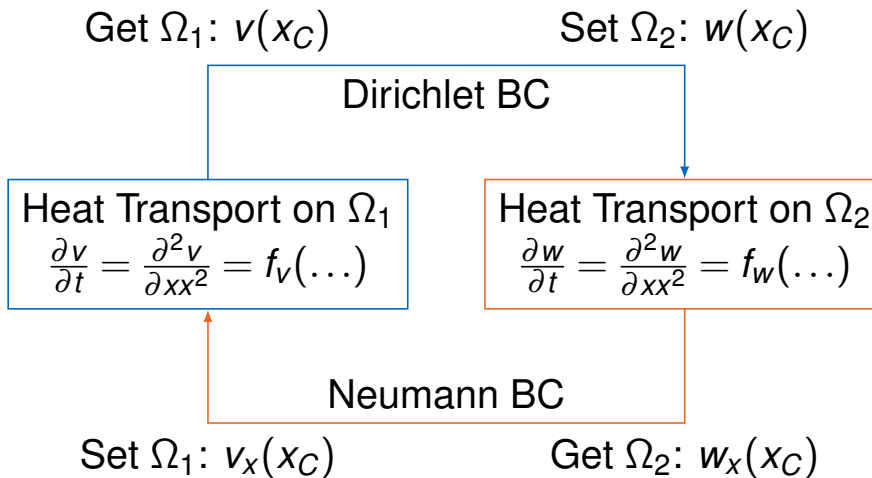
Partitioned setup



Review and experiments on coupling schemes

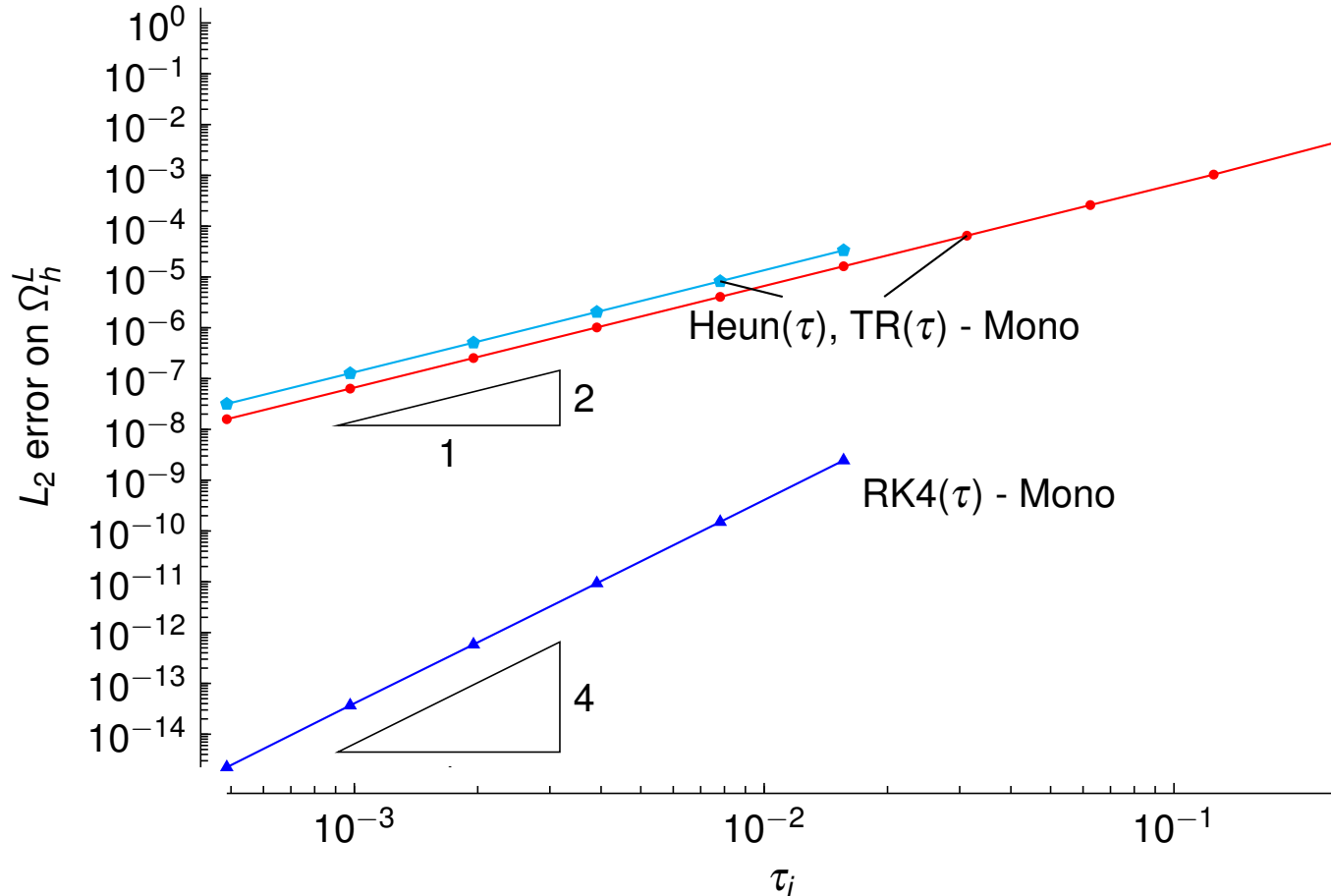
Classical coupling schemes

Dirichlet-Neumann coupling



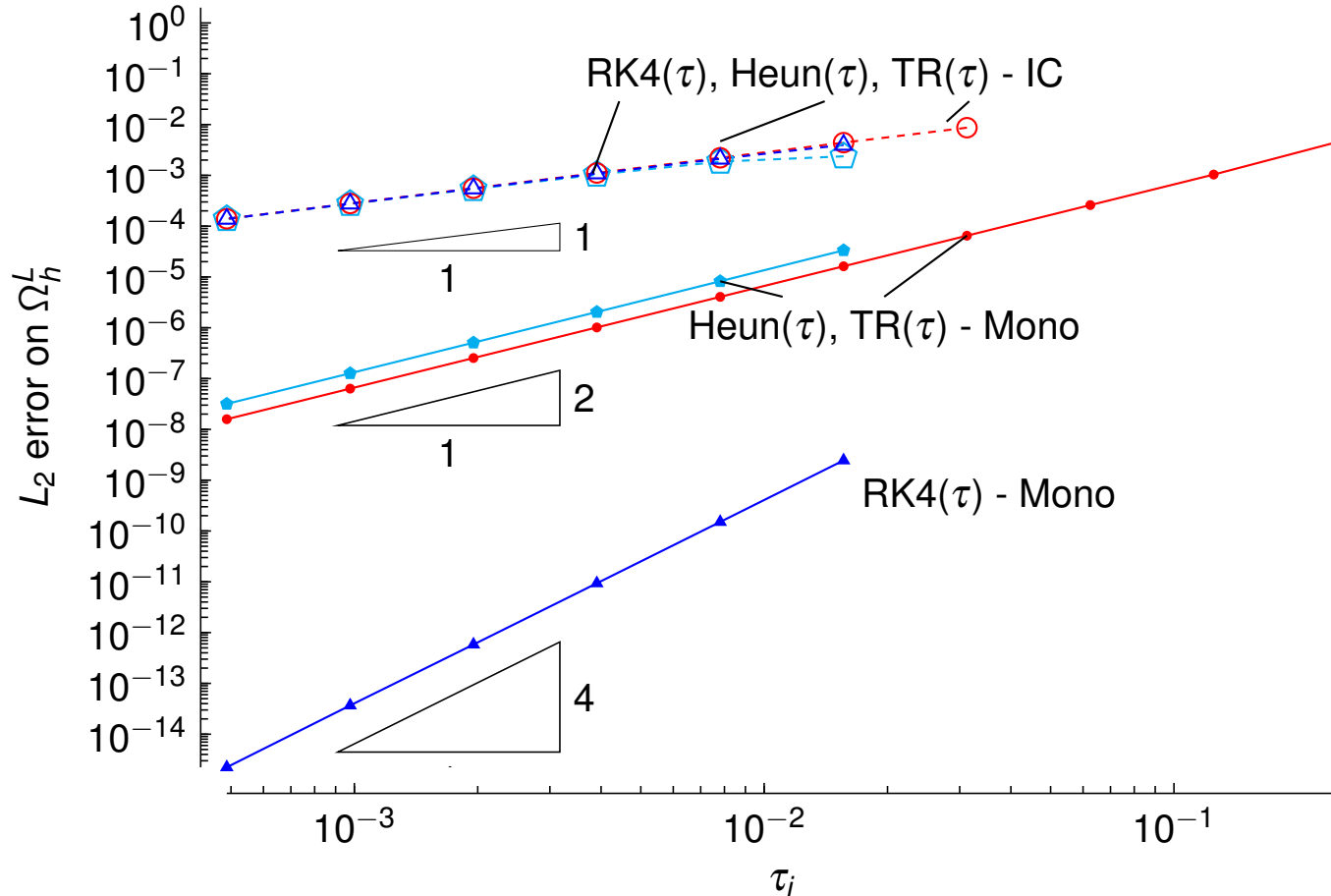
Review and experiments on coupling schemes

Classical coupling schemes



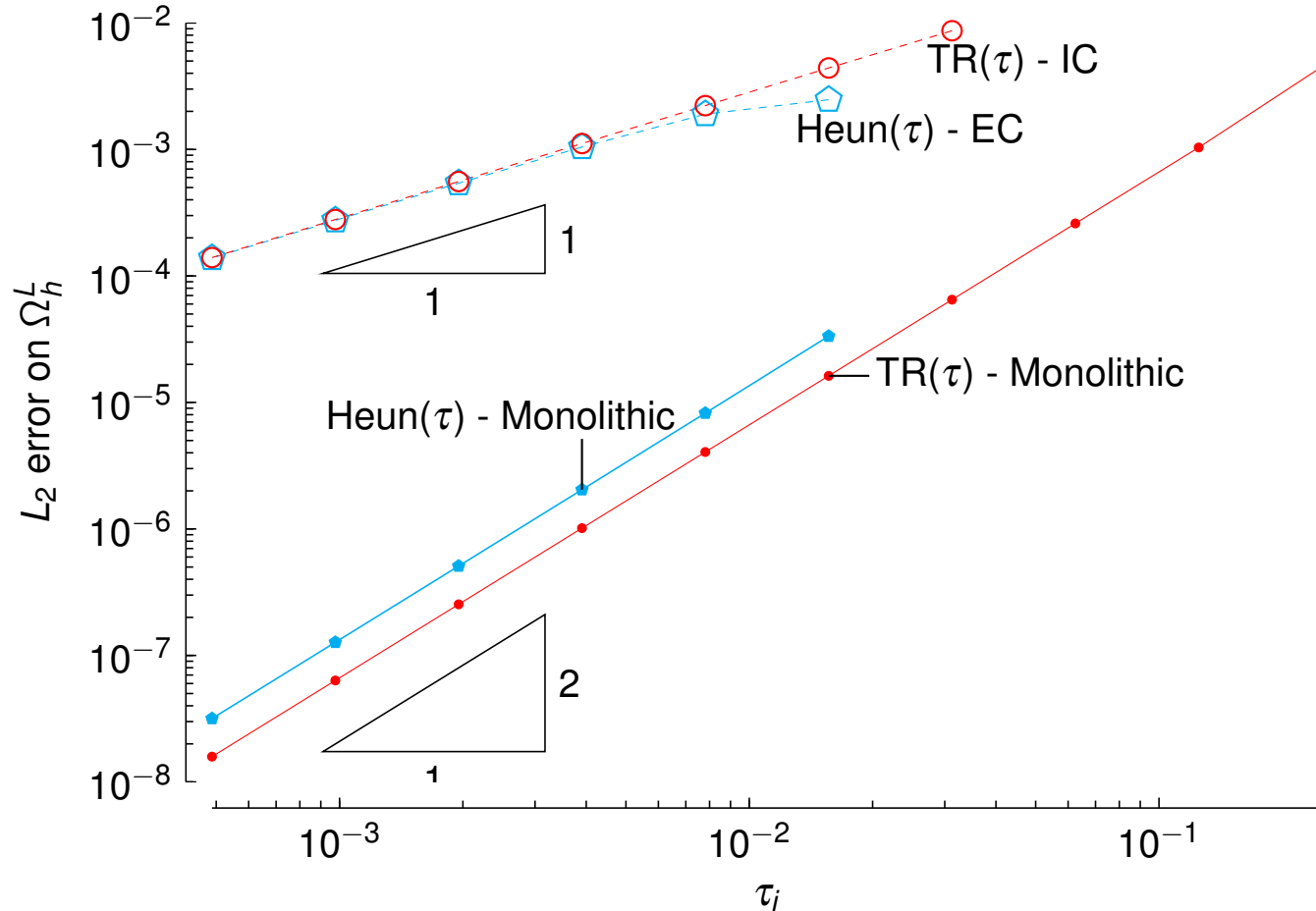
Review and experiments on coupling schemes

Classical coupling schemes



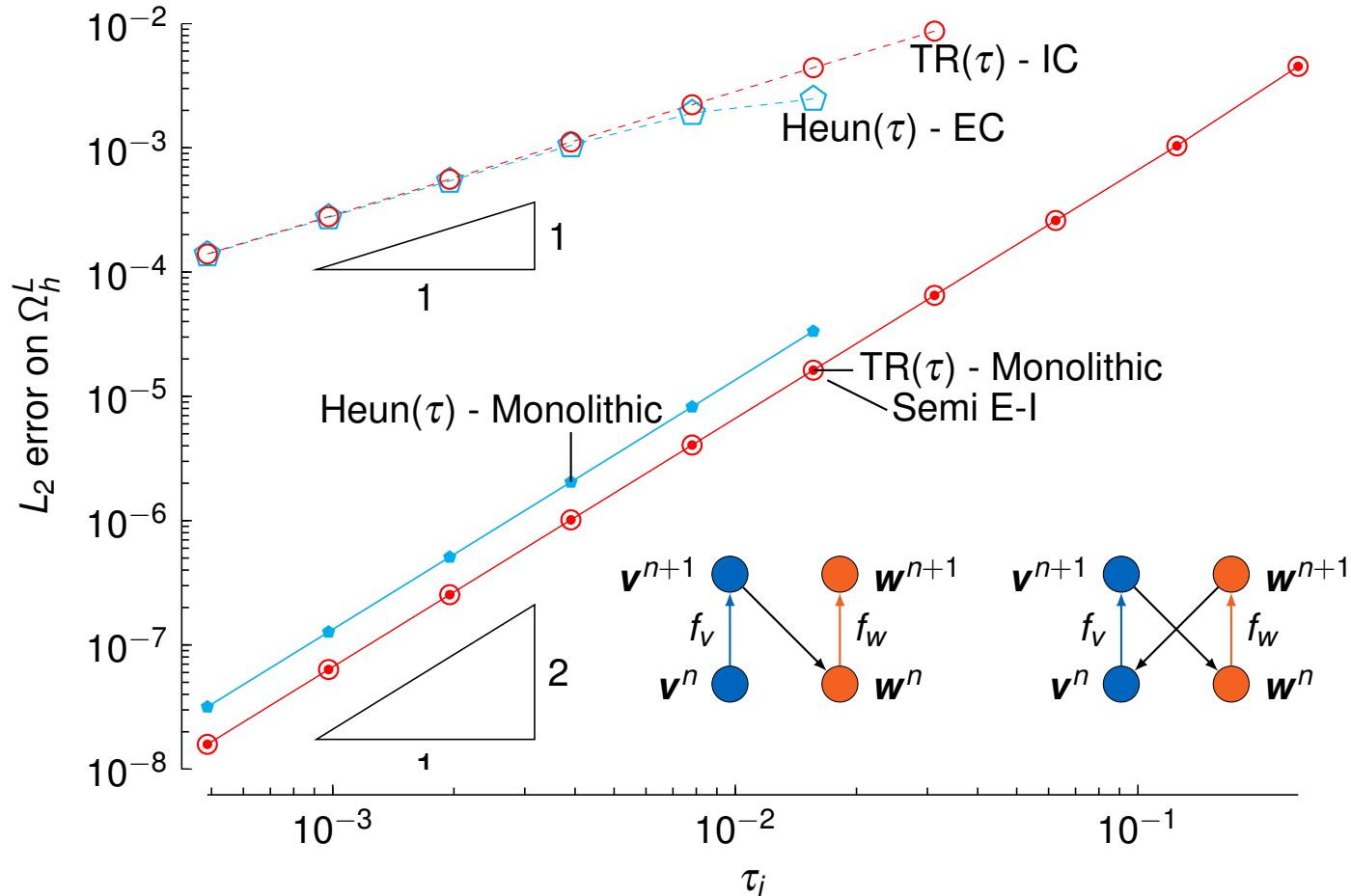
Review and experiments on coupling schemes

Customized 2nd order schemes



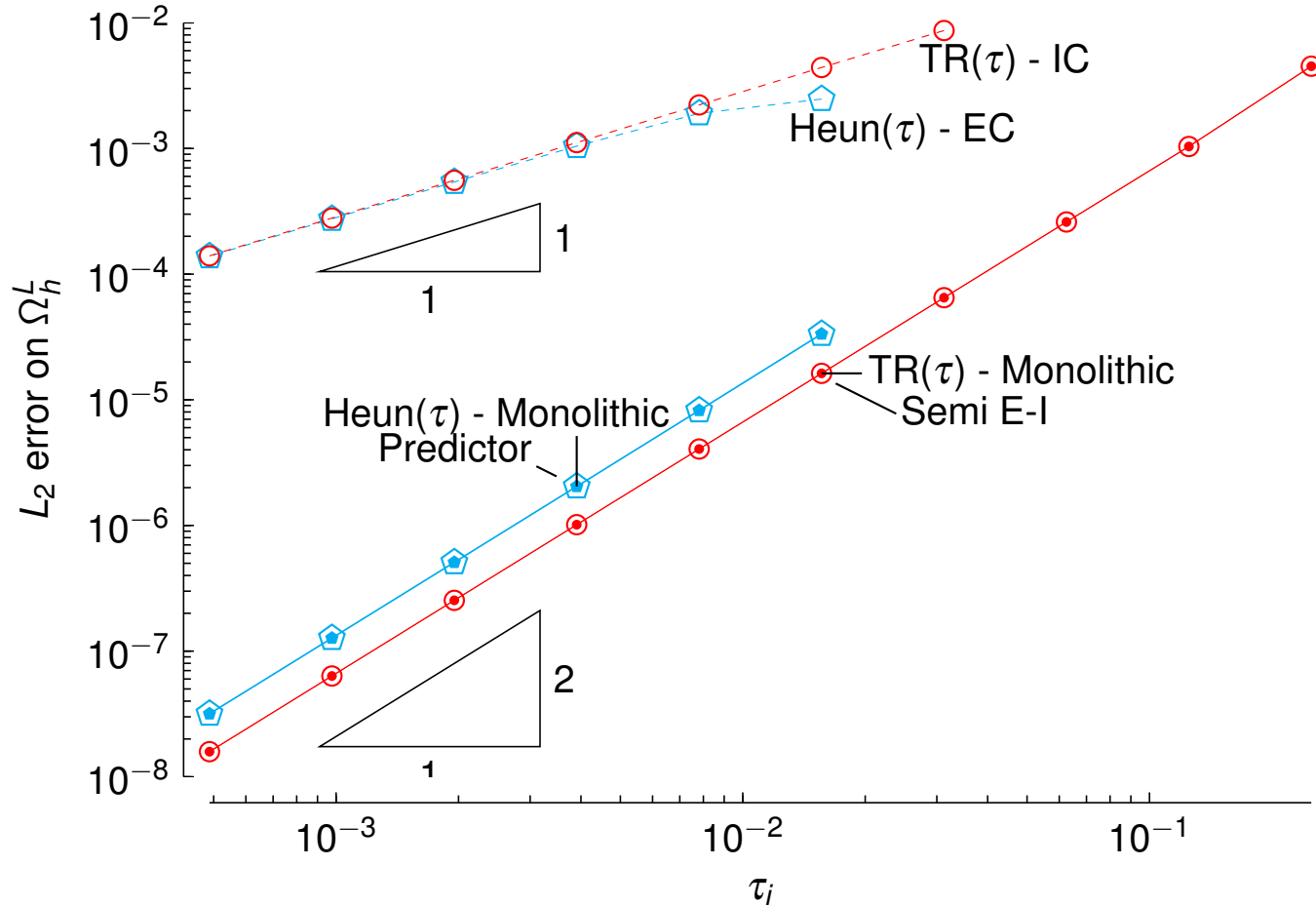
Review and experiments on coupling schemes

Customized 2nd order schemes



Review and experiments on coupling schemes

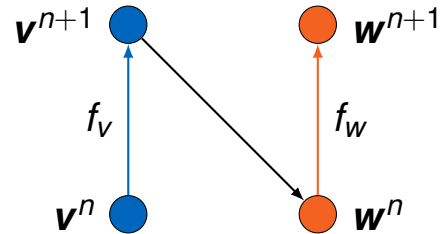
Customized 2nd order schemes



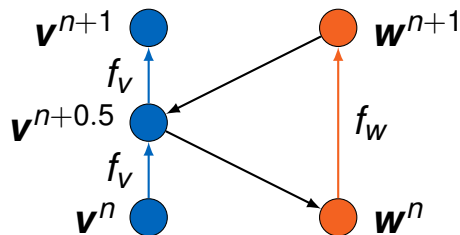
Review and experiments on coupling schemes

Splitting methods

Godunov splitting (= explicit coupling)

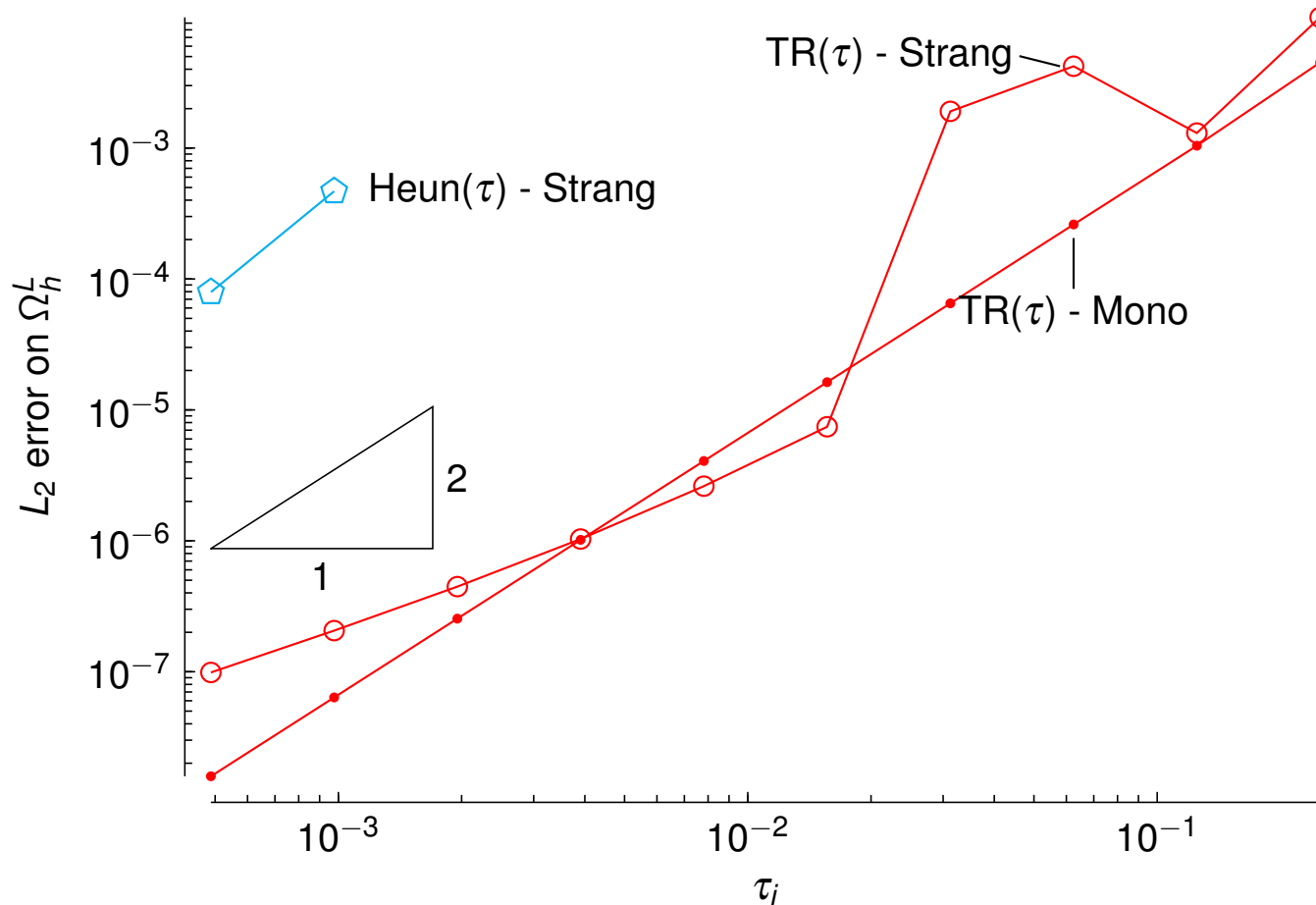


Strang splitting



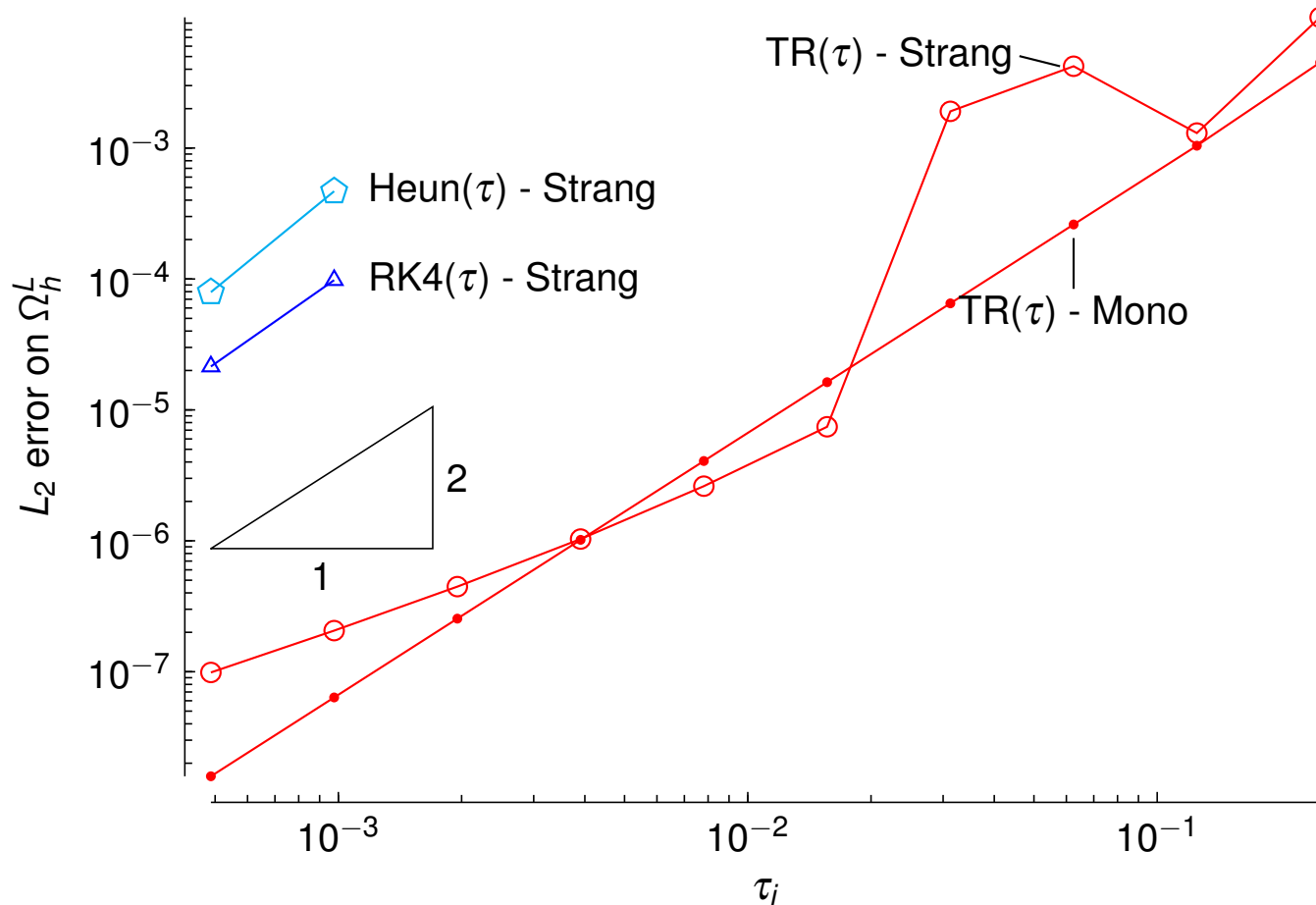
Review and experiments on coupling schemes

Splitting methods



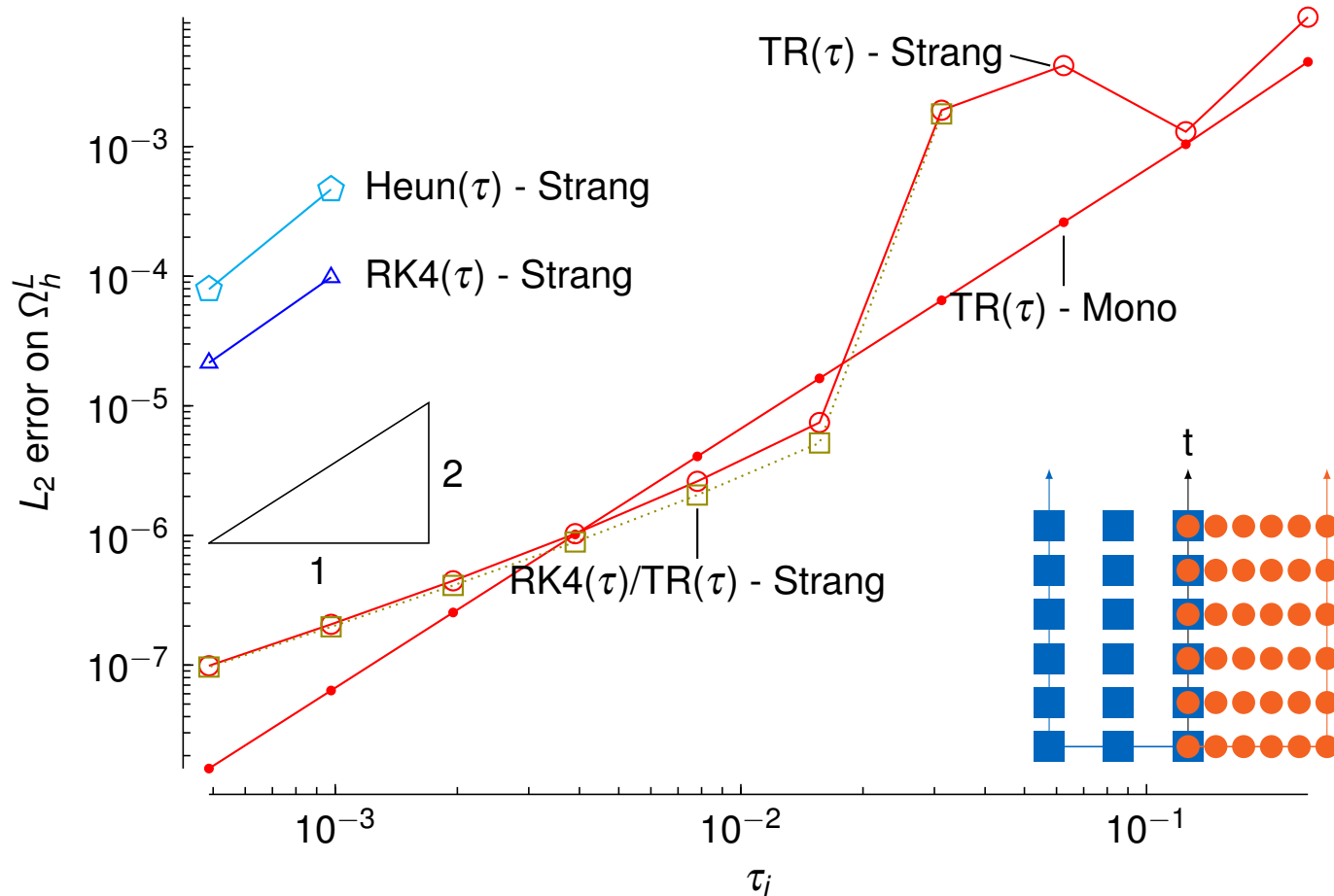
Review and experiments on coupling schemes

Splitting methods



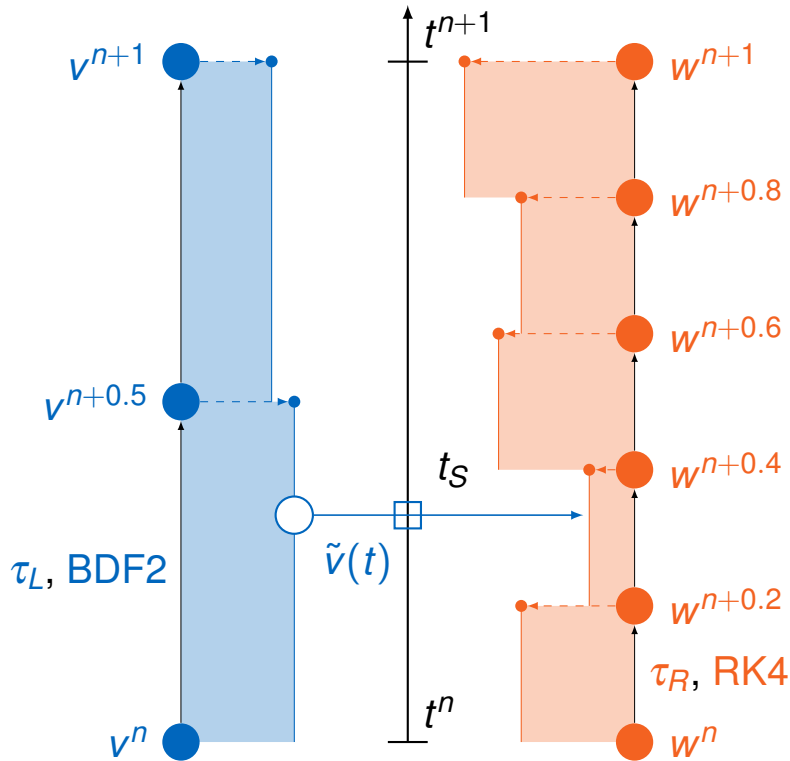
Review and experiments on coupling schemes

Splitting methods

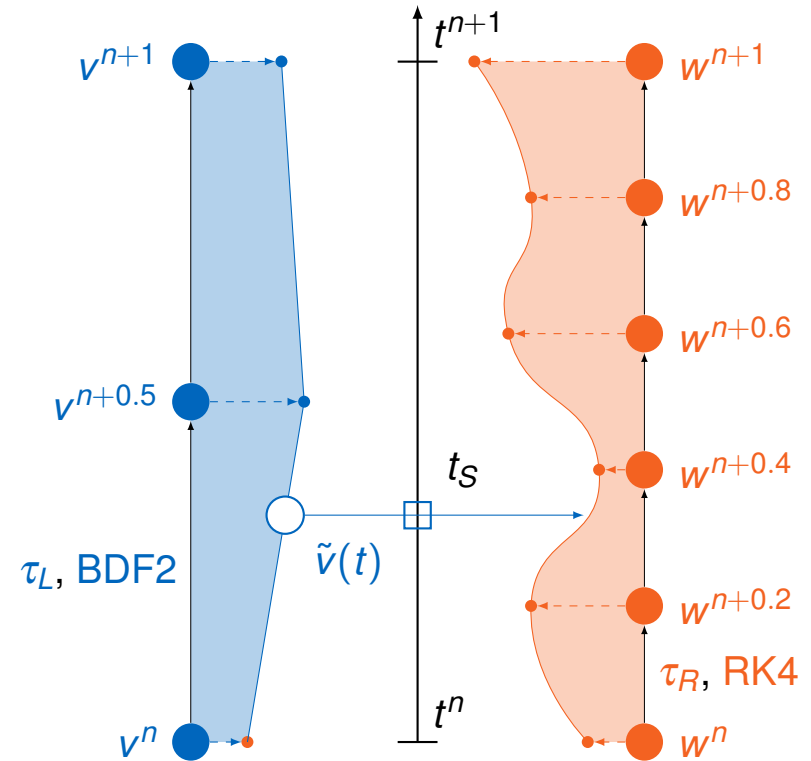


Review and experiments on coupling schemes

Waveform relaxation



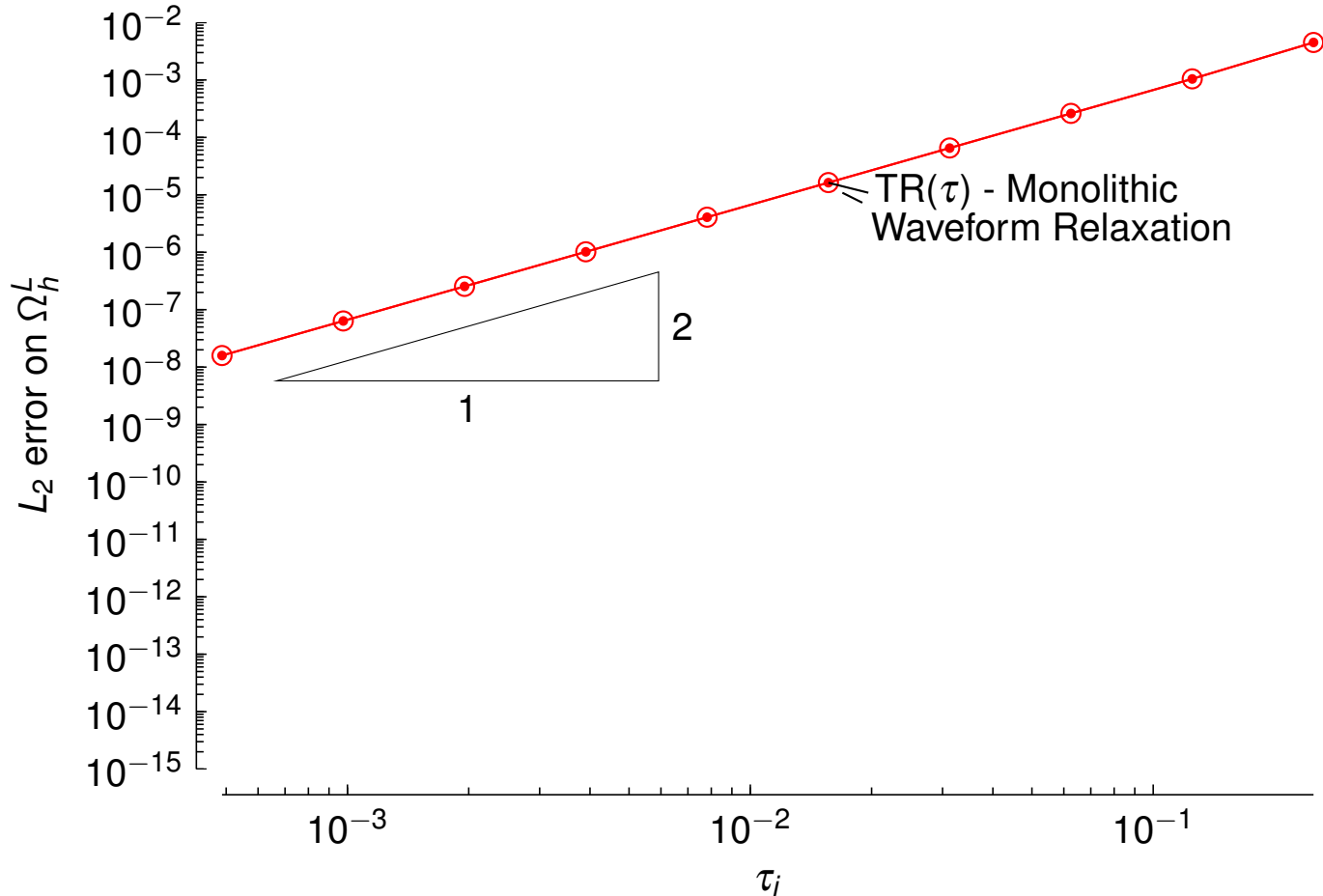
Implicit/strong coupling



Waveform relaxation

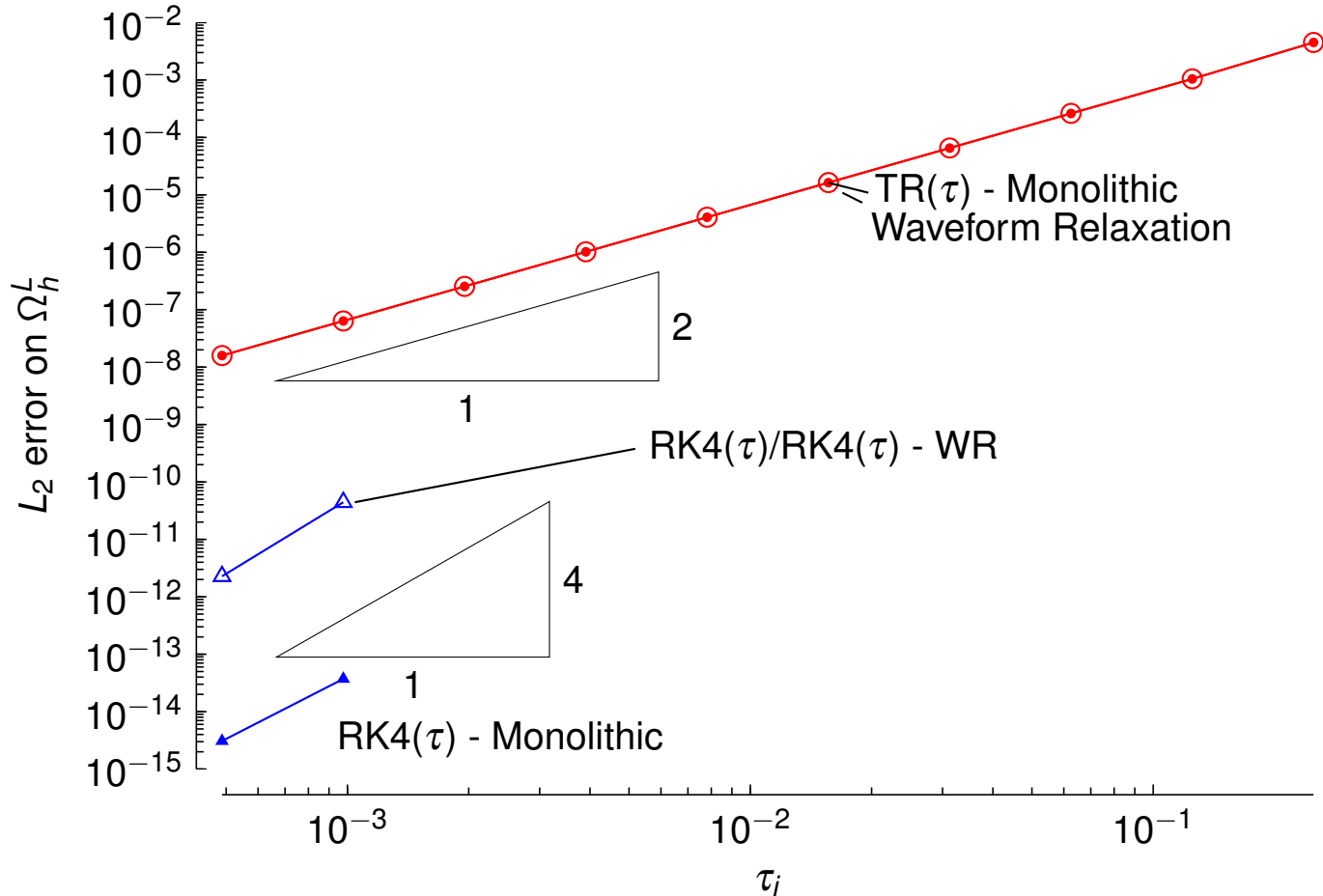
Review and experiments on coupling schemes

Waveform relaxation



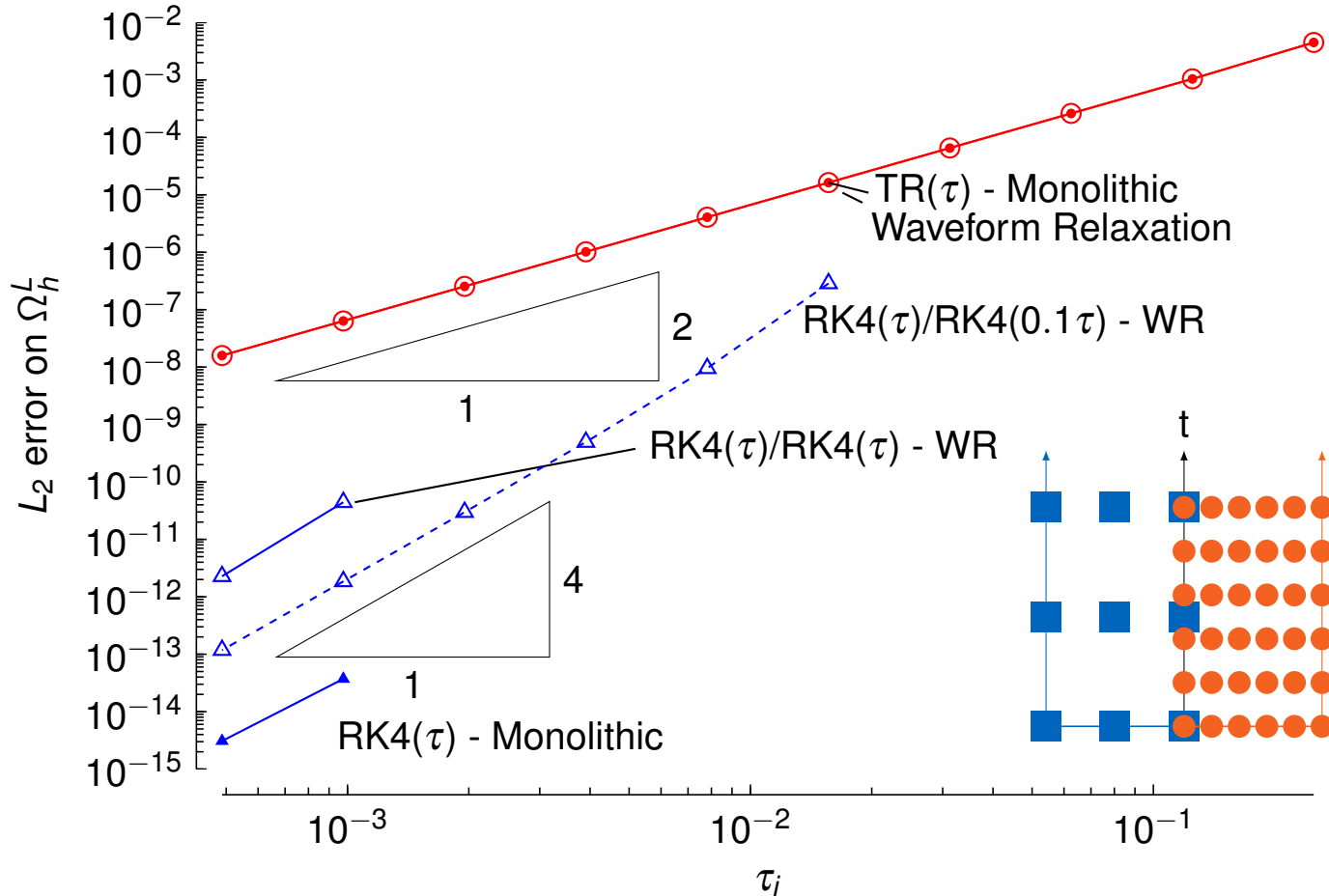
Review and experiments on coupling schemes

Waveform relaxation



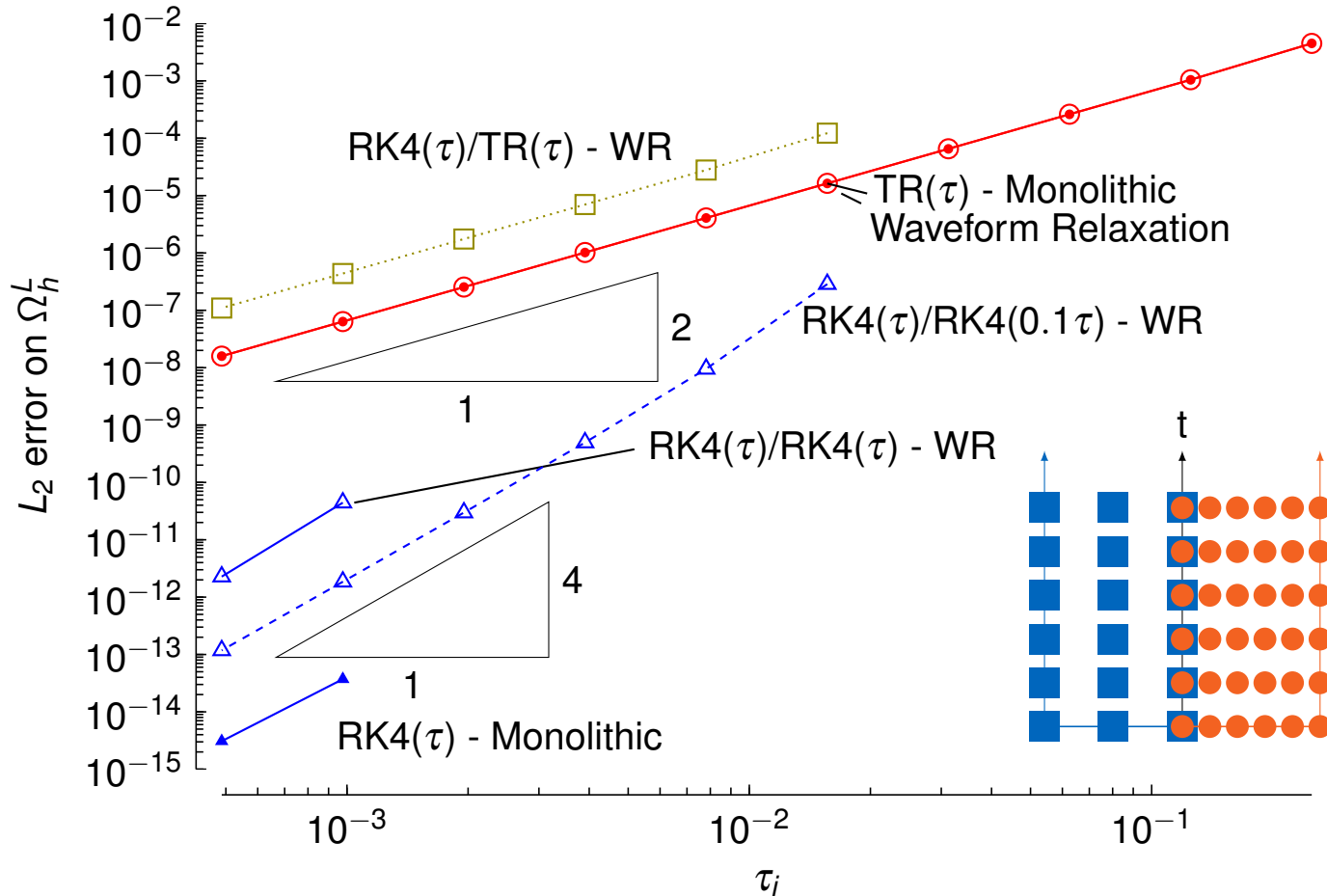
Review and experiments on coupling schemes

Waveform relaxation



Review and experiments on coupling schemes

Waveform relaxation



Algorithmic requirements

- inhomogeneous setup
- subcycling
- black-box
- parallel

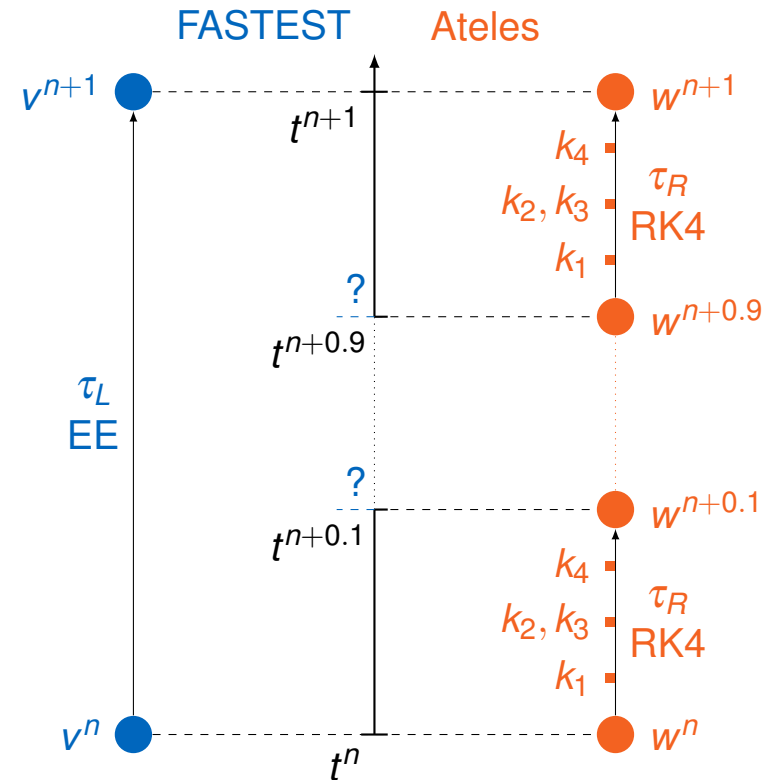
Partitioned Heat Transport

- model problem
- experimental study

Short discussion

- ✗ implicit/explicit
- ✗ semi explicit-implicit
- ✗ predictor
- ✓ Strang
- ✓ Waveform Relaxation

Multi-Scale

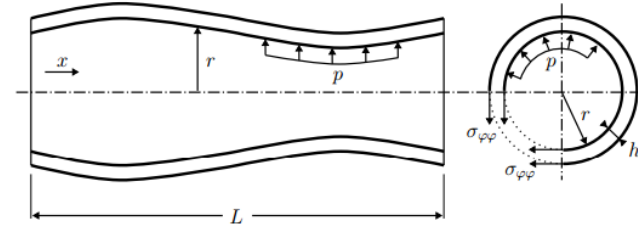


Implementation

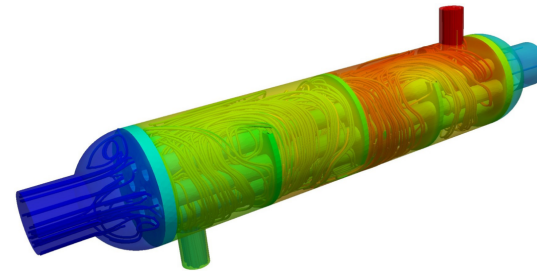
- Interpolation methods?
- Convergence of acceleration schemes
- Parallel performance

Tests

1D Tube¹:



preCICE examples²:



¹figure from Degroote, J., et al. (2008). Stability of a coupling technique for partitioned solvers in FSI applications. <https://doi.org/10.1016/j.compstruc.2008.05.005>

²figure from Cheung Yau, L. (2016). Conjugate Heat Transfer with the Multiphysics Coupling Library preCICE. TUM.

Thank you!¹

Website: precice.org

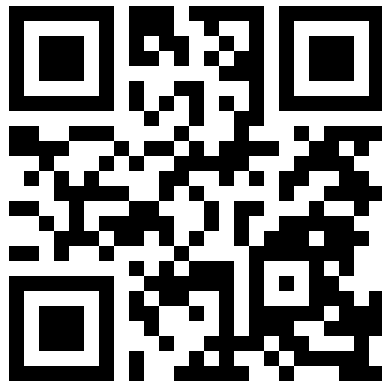
Source/Wiki: github.com/precice

Mailing list: precice.org/resources

My e-mail: rueth@in.tum.de

Homework:

- Follow a tutorial
- Join our mailing list
- Star on GitHub
- Send us feedback
- Ask me for stickers

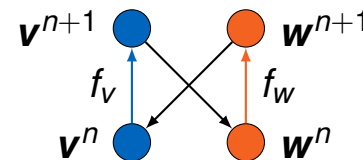
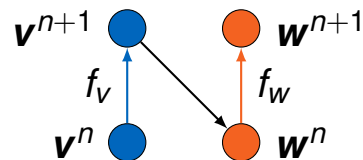


¹The financial support of the managing board of ECCOMAS and of SPPEXA, the German Science Foundation Priority Programme 1648 – Software for Exascale Computing is thankfully acknowledged.

Appendix

Semi Implicit-Explicit Coupling

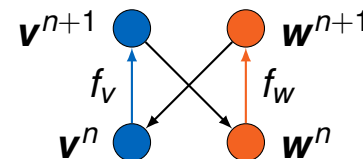
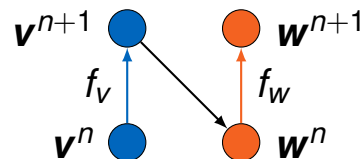
	update scheme	stability	order
fully explicit	$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\tau}{2} [f_v(\mathbf{v}^n, t_n) + f_v(\mathbf{v}^{n+1}, t_{n+1})]$ $\mathbf{w}^{n+1} = \mathbf{w}^n + \frac{\tau}{2} [f_w(\mathbf{w}^n, t_n) + f_w(\mathbf{w}^{n+1}, t_{n+1})]$	depends on τ	$\mathcal{O}(\tau)$
fully implicit	$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\tau}{2} [f_v(\mathbf{v}^n, t_n) + f_v(\mathbf{v}^{n+1}, t_{n+1})]$ $\mathbf{w}^{n+1} = \mathbf{w}^n + \frac{\tau}{2} [f_w(\mathbf{w}^n, t_n) + f_w(\mathbf{w}^{n+1}, t_{n+1})]$	depends on τ	$\mathcal{O}(\tau)$



Appendix

Semi Implicit-Explicit Coupling

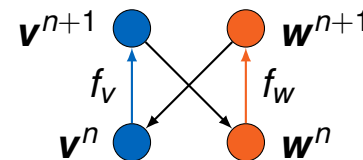
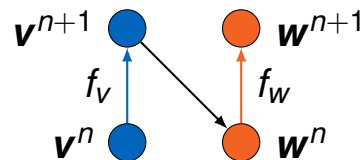
	update scheme	stability	order
fully explicit	$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\tau}{2} [f_v(\mathbf{v}^n, \mathbf{w}^n, t_n) + f_v(\mathbf{v}^{n+1}, \mathbf{w}^n, t_{n+1})]$ $\mathbf{w}^{n+1} = \mathbf{w}^n + \frac{\tau}{2} [f_w(\mathbf{v}^{n+1}, \mathbf{w}^n, t_n) + f_w(\mathbf{v}^{n+1}, \mathbf{w}^{n+1}, t_{n+1})]$	depends on τ	$\mathcal{O}(\tau)$
fully implicit	$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\tau}{2} [f_v(\mathbf{v}^n, \mathbf{w}^{n+1}, t_n) + f_v(\mathbf{v}^{n+1}, \mathbf{w}^{n+1}, t_{n+1})]$ $\mathbf{w}^{n+1} = \mathbf{w}^n + \frac{\tau}{2} [f_w(\mathbf{v}^{n+1}, \mathbf{w}^n, t_n) + f_w(\mathbf{v}^{n+1}, \mathbf{w}^{n+1}, t_{n+1})]$	depends on τ	$\mathcal{O}(\tau)$



Appendix

Semi Implicit-Explicit Coupling

	update scheme	stability	order
fully explicit	$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\tau}{2} [f_v(\mathbf{v}^n, \mathbf{w}^n, t_n) + f_v(\mathbf{v}^{n+1}, \mathbf{w}^n, t_{n+1})]$ $\mathbf{w}^{n+1} = \mathbf{w}^n + \frac{\tau}{2} [f_w(\mathbf{v}^{n+1}, \mathbf{w}^n, t_n) + f_w(\mathbf{v}^{n+1}, \mathbf{w}^{n+1}, t_{n+1})]$	depends on τ	$\mathcal{O}(\tau)$
fully implicit	$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\tau}{2} [f_v(\mathbf{v}^n, \mathbf{w}^{n+1}, t_n) + f_v(\mathbf{v}^{n+1}, \mathbf{w}^{n+1}, t_{n+1})]$ $\mathbf{w}^{n+1} = \mathbf{w}^n + \frac{\tau}{2} [f_w(\mathbf{v}^{n+1}, \mathbf{w}^n, t_n) + f_w(\mathbf{v}^{n+1}, \mathbf{w}^{n+1}, t_{n+1})]$	depends on τ	$\mathcal{O}(\tau)$
semi explicit-implicit	$\mathbf{v}^{n+1} = \mathbf{v}^n + \frac{\tau}{2} [f_v(\mathbf{v}^n, \mathbf{w}^n, t_n) + f_v(\mathbf{v}^{n+1}, \mathbf{w}^{n+1}, t_{n+1})]$ $\mathbf{w}^{n+1} = \mathbf{w}^n + \frac{\tau}{2} [f_w(\mathbf{v}^n, \mathbf{w}^n, t_n) + f_w(\mathbf{v}^{n+1}, \mathbf{w}^{n+1}, t_{n+1})]$	unconditionally	$\mathcal{O}(\tau^2)$



Appendix

Predictor Coupling

Heun's method

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

- $\tilde{v}^{n+1}, \tilde{w}^{n+1}$ from explicit Euler
- only coupling at the beginning of timestep happening

With predictor

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

- $\tilde{v}^{n+1}, \hat{v}^{n+1}, \tilde{w}^{n+1}$ and \hat{w}^{n+1} from explicit Euler
- coupling also for stages of scheme

Appendix

What is Waveform Relaxation?



Algorithm¹

We want to solve the coupled problem

$$F_v(v, c) = 0, F_w(w, c) = 0.$$

with v, w, c known for $t < t_n$ on the window $T_n = [t_n, t_{n+1}]$.

1. set $k = 0$ and extrapolate $c^0(t) = c_n$ for $t \in T$
2. solve decoupled F_v, F_w using c^k to obtain v^{k+1}, w^{k+1} for $t \in T$
3. use v^{k+1}, w^{k+1} to obtain c^{k+1}
4. if not converged:
 - a. set $k = k + 1$ and go to step 2,
 - b. otherwise proceed to next window T_{n+1}

¹Adapted from Schöps, S., et al. (2017). *Application of the Waveform Relaxation Technique to the Co-Simulation of Power Converter Controller and Electrical Circuit Models*. <https://doi.org/10.1109/MMAR.2017.8046937>