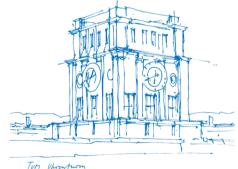


What is new in preCICE?

preCICE Workshop 2022

Gerasimos Chourdakis Frédéric Simonis Technical University of Munich Recorded February 2022





What is new in preCICE? The preCICE library

Speaker: Frédéric Simonis



- Resulting state of the solver
- Why did it finish
- What was the last residual norm



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- Resulting state of the solver
- Why did it finish
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- Resulting state of the solver
- Why did it finish
- What was the last residual norm



PETSc RBF - solver behaviour

Solver	Log level	preCICE
converges	INFO	continues
diverges	ERROR	stops



PETSc RBF - solver behaviour

Solver	Log level	preCICE
converges	INFO	continues
stops	WARNING	continues
diverges	ERROR	stops

Reaching max iter is actionable.

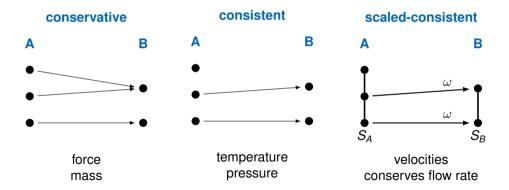


Readable convergence output

User feedback
 Readable names ResRel(Forces)
 Convergence in fixed scientific format
 Iterations and timesteps in fixed width
 tail -f precice-A-convergence.log
 2.13325385e-01
 3.84809185e-02
 3.72078735e-04
 3.34837628e-06

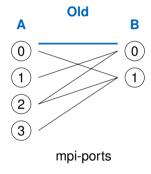


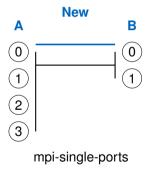
Scaled-consistent mappings





M2N communication - changed m2n:mpi







Socket communication

run preCICE without network connection fails #45





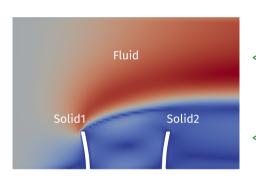
Memory usage of meshes

- Deep refactoring
- · Reduced heap allocations
- Improved data locality

primitive	rel. red.
vertices	50%
edges	62%
triangles	55%



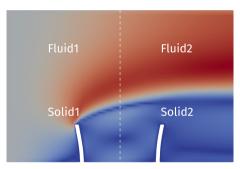
Multi-coupling extension



```
<coupling-scheme:multi>
  <participant name="Fluid" control="yes" />
  <participant name="Solid1" />
  <participant name="Solid2" />
  ...
</coupling-scheme:multi>
```



Multi-coupling extension



Limitation: Non-centric controller needs to run in serial.

```
<coupling-scheme:multi>
  <participant name="Fluid1" control="yes" />
  <participant name="Fluid2" />
  <participant name="Solid1" />
  <participant name="Solid2" />
  ...
</coupling-scheme:multi>
```



Adjusted build experience

- \$ cmake ..
 - Shared library
 - Debug and trace logging
 - Assertions

- \$ cmake -DCMAKE_BUILD_TYPE=Release ..
 - Shared library
 - Optimized
 - No debug or trace logging
 - No assertions



Experimental features

Explicitly activate in the config



Experimental features - direct access

```
<participant name="MyParticipant">
    <use-mesh name="Mesh" from="Other" direct-access="true" />
    <write-data name="Data" mesh="Mesh" />
</participant>
```



Experimental features - direct access

```
// Specify region of interrest
mid = precice.getMeshID("Mesh");
precice.setMeshAccessRegion(mid, aabb);
// Initialize preCICE
precice.initialize();
// Inspect received mesh
n = precice.getMeshVertexSize(mid);
precice.getMeshVerticesAndIDs(mid, n, ids, coords);
// Write data directly
did = precice.getDataID("Data", mid);
precice.writeBlockScalarData(did, n, ids, data);
```



Upcoming changes

Mostly release 2.4.0



Bigger features

High-order and multi-rate time stepping with preCICE

preCICE Workshop 2020, Munich, Germany

https://youtu.be/7NhBmcx_MmI

From low-order to high-order coupling schemes

preCICE Workshop 2022, Munich, Germany

Wed. 23 10:00-12:00 CET, 3rd talk



Configuration checker

\$ precice-tools check precice-config.xml ERROR: Data with name "forces" used by mesh "Solid" is not defined. Please define a data tag with name="forces".

- Available out of the box
- Checks XML structure
 Typos in tags and attribute names
- Checks names of Participants, Meshes, Data
- Cannot check coupling logic
 Is data actually exchanged in a coupling scheme?



Exporter overhaul

- \$./fluid
- \$ ls *vtk

fluid-Mesh-dt1.vtk

- \$ mpirun -n 2 ./fluid
- \$ ls *vtu

fluid-Mesh-dt1.pvtu fluid-MeshA-dt1_r0.vtu fluid-MeshA-dt1_r1.vtu



Exporter overhaul - VTK exporters

VTK UnstructredGrid

```
<participant name="fluid">
    <export:vtu />
</participant>
$ ./fluid
$ ls *vtu
fluid-Mesh-dt1.vtu
$ mpirun -n 2 ./fluid
$ ls *vtu
fluid-Mesh-dt1.pvtu
fluid-MeshA-dt1 r0.vtu
fluid-MeshA-dt1_r1.vtu
```

VTK PolyData

```
<participant name="fluid">
    <export:vtp />
</participant>
$ ./fluid
$ ls *vtp
fluid-Mesh-dt1.vtp
$ mpirun -n 2 ./fluid
$ ls *vtp
fluid-Mesh-dt1.pvtp
fluid-MeshA-dt1_r0.vtp
fluid-MeshA-dt1_r1.vtp
```



Exporter overhaul - CSV exporter

- Point data only
- Separate rank files
- Easy to postprocess
 R, Pandas, Matlab, LibreCalc, Excel
- pseudo coordinates

PosX; PosY; Rank; Temperature; ForcesX; ForcesY



Exporter overhaul - CSV processing

```
def loadParallelCSVSeries(name)
  import re, glob, pandas
  l = [(re.search("dt(\d+)_", s).group(1), s)
            for s in glob.glob(f"{name}.dt*_*.csv")]
  return pandas.concat(
            [pandas.read_csv(file, sep=";").assign(dt=dt)
            for dt, file in l], ignore_index=True)
```



Extended release builds

Debugging adapter using mesh connectivity?

```
$ cmake -DCMAKE_BUILD_TYPE=Release \
    -DPRECICE_RELEASE_WITH_DEBUG_LOG=YES ...
```

Slower, but usable.

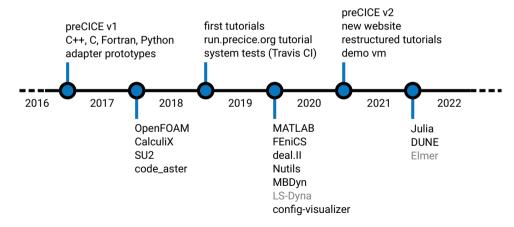


What is new in preCICE? The preCICE ecosystem

Speaker: Gerasimos Chourdakis

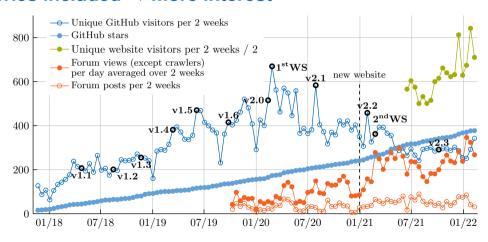


From a library to an ecosystem



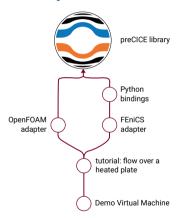


Batteries included → more interest



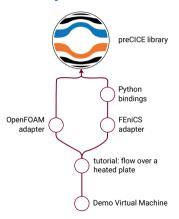


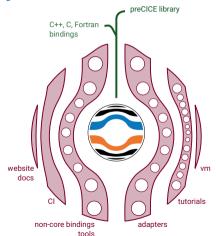
Multiple components, in multiple layers





Multiple components, in multiple layers







Tutorials news

New structure, new cases and more



Tutorials: starting points for your simulations



48 solver cases in 15 tutorials



Tutorials: a new, modular structure

Structure of a tutorial

Our tutorials generally follow a file structure similar to this:

```
- <tutorial>/
             # e.g. perpendicular-flap/
 - README.md
                        # description of the case

    precice.config.xml

                        # a works-with-all preCICE configuration file
 - clean-tutorial.sh
                         # a symbolic link (see ../tools/)
 - <visualization scripts> # gnuplot or simple Python scripts
                        # anv images used by the documentation
 - images/
 - <participant1-solver1>/ # e.g. fluid-openfoam/
   - run.sh # a short script to run the solver1 case
   - clean.sh
                        # a short script to clean the solver1 case
   - <the solver1 files>
 - - cparticipant2-solver2>/ # e.g. solid-dealii/
   - run sh
   - clean sh
   - <the solver2 files>
```

Contribute your own case setup!



Tutorials: v202202.0

New tutorials and several changes (workshop is coming!) (Lalest)





New year, new tutorial cases!

In this scheduled release (part of the preCICE Distribution 2202.0 and in the context of the preCICE Workshop 2022), you can find:

A new volume coupled diffusion tutorial with EFniCS.

MakisH released this 6 days ago 🕒 v202202.0 -o- 5cab2c5 🕢

- Our first tutorial case with DUNE: a solid solver for the perpendicular flap tutorial.
- · An OpenFOAM version of the partitioned heat confuction tutorial.
- A FEniCS version of the elastic tube 3D tutorial.

Additionally, this release brings several changes changes, Most importantly, we changed the type of elements that CalculiX uses in the perpendicular flap tutorial (from Cabe to Cabe 1), which now performs very similarly to the rest of the cases. We also cleaned up several configuration files from confusing unnecessary details. See the changelog or all file changes for more details.

Once more, this release was a collective effort by the complete preCICE team. It includes code contributions by @IshaanDesai. @BenjaminRodenberg. @DavidSCN. @MakisH. further contributions by @fsimonis, @KyleDavisSA, and @uekerman, as well as first-time community contributions by @AndresPedemonteFIUBA, @maxfirmbach, and @mohamad-altaweel.

Contributors











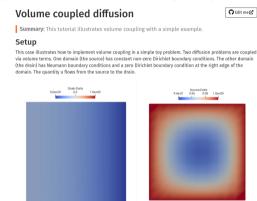


IshaanDesai, BenjaminRodenberg, and 8 other contributors



Tutorials: new example for volume coupling





Available solvers and dependencies

FEniCS. Install FEniCS of and the FEniCS-adapter . Additionally, you will need to have preCICE and the python
bindings installed on your system.

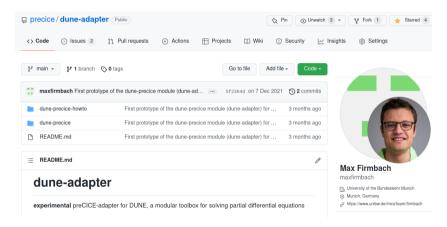


Adapter news

New DUNE adapter, CalculiX adapter release, FEniCS adapter paper and more



New DUNE adapter





CalculiX adapter release v2.19.0





FEniCS adapter paper

SoftwareX 16 (2021) 100807



Contents lists available at ScienceDirect

SoftwareX

iournal homepage: www.elsevier.com/locate/softx



Original software publication

FEniCS-preCICE: Coupling FEniCS to other simulation software



(http://creativecommons.org/licenses/by/4.0/).

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ARSTRACT

The new software FERICS-preCICE is a middle software layer, sitting in between the existing finiteelement library FERICS and the coupling library preCICE. The middle layer simplifies coupling explices (FERICS-preCICE) and the coupling library preCICE. The middle layer simplifies coupling complication codes to other simulation software via preCICE. To this end. FERICS-preCICE meth and data structures, provides easy-to-use coupling conditions, and manages data checkpointing for implicit coupling. The new software is a library itself and follows a FERICS-thate stych obly a few lines of additional code are necessary to prepare a FERICS application code for coupling. We illustrate the functionality of FERICS-preCICE by two examples: at PERICS hast conduction code coupled to OpenPOMA and a FERICS inter exclusive code coupled to openPOMA and a FERICS inter exclusive code coupled to the PERICS hast conduction are compared with other simulation software showing good agreement.

9.2021 The AUMON SPRINGS AND Also: 3D extensions in v1.3.0



Coming up

Julia bindings, Elmer adapter, ASTE updates



Coming up: Julia bindings

PreCICE.jl

license LGPL-3.0

This package provides Julia language bindings for the C++ library preCICE. It is a Julia package that wraps the API of preCICE.

Adding the package to a Julia environment or script

You can use the Julia bindings for preCICE by adding them as a package in a Julia environment or also directly including the package in a Julia script. For both usages you need to have preCICE installed on the system. For preCICE installation you can look at the installation documentation. You can directly add the Julia bindings to your Julia environment in the following way:

```
julia> ]
pkg> add https://github.com/precice/julia-bindings.git
Then exit the package mode with $\frac{1}{40}$ or Ctrl + c
julia> using PreCICE
```





Coming up: Elmer adapter

elmer-adapter

experimental preCICE-adapter for the open source multiphysical simulation software Elmer FEM

Getting started

Dependencies & Installation Instructions

- preCICE
 - Recommended: Install debian package, please refer to https://precice.org/installation-overview.html for installation
- Elmer
 - o Recommended: Install debian package, please refer to http://www.elmerfem.org/blog/binaries/

Packages

No packages published Publish your first package

Contributors 2



BenjaminRodenberg Benjamin Rode...



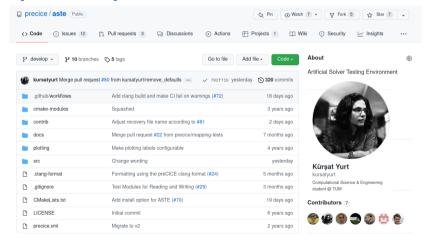
HishamSaeed Hisham

Languages

- Fortran 93.5% GLSL 6.2%
- Shell 0.3%



Coming up: ASTE updates





Outer layers

Demo Virtual Machine, preCICE Distribution and more



Demo Virtual Machine



Demo Virtual Machine

○ Edit me 🗹

Summary: A sandbox to try preCICE and all the adapters without having to install them on your system.

Do I need this?

You probably only want to use this if you are very new to preCICE and want to learn, for example during our preCICE Workshops or other conferences where we may be present with a training session.

After trying this out for a few days, you probably want to just delete it and install only the components you need

directly on your target system. What is this?

This is a Vagrant obus, essentially a VirtualBox of virtual machine image, with additional automation to make it easier for you to use and for us to maintain.

This contains all the solvers and adapters used in our tutorials, already built and configured for you to enjoy.





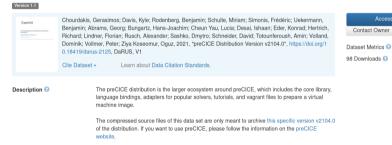
Shara

Contact Owner

A citable preCICE Distribution



preCICE Distribution Version v2104.0



v2202.0 released last week, to appear on DaRUS soon



New reference paper

PRECICE V2: A SUSTAINABLE AND USER-FRIENDLY COUPLING LIBRARY

A PREPRINT

Gerasimos Chourdakis^{1,*}, Kyle Davis^{2,*}, Benjamin Rodenberg^{1,*}, Miriam Schulte^{2,*}, Frédéric Simonis^{1,*}, Benjamin Uekermann^{3,*,†} Georg Abrams², Hans-Joachim Bungartz¹, Lucia Cheung Yau¹, Ishaan Desai², Konrad Eder¹, Richard Hertrich¹, Florian Lindner², Alexander Rusch¹, Dmytro Sashko¹, David Schneider³, Amin Totounferoush², Dominik Volland¹, Peter Vollmer², and Oguz Ziya Koscomur¹

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What to cite?

preCICE v1 paper: Now, or whenever specifically writing about preCICE v1

preCICE v2 paper: Soon, whenever writing about preCICE

Adapter papers: Whenever using an adapter

Distribution: For reproducibility (specific versions)



Wrapping up



Don't miss

Support program: Talk by Bejnamin Uekermann

Developer talks: Updates on:

Macro-micro coupling

Testing the ecosystem

High-order coupling schemes

Data mapping

Summer meeting: preCICE Minisymposium at ECCOMAS Congress 2022, June 5-9, Oslo



2022 resolution

be part of the "What's new in preCICE" list in the preCICE Workshop 2023.

(or simply manage to catch up on all these updates)