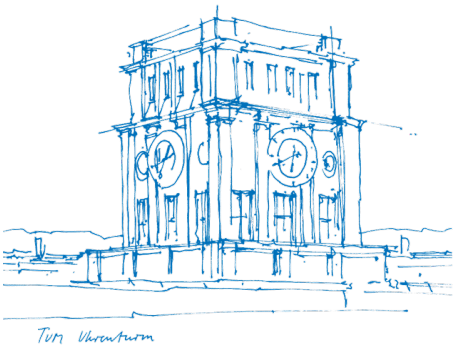
What is new in preCICE?

preCICE Workshop 2021

Frédéric Simonis
Technical University of Munich

Recorded on 19. February 2021



Flashback to preCICE Workshop 2020

- Productive hands-on sessions
- A lot of user discussions
- World Café
- User support session

Toooooooooo of Feedback!

Condensed feedback preCICE Workshop 2020

- Restructure documentation and website
- Extend tutorials on writing adapters
- Provide reference virtual machine with preCICE installed
- Allow solver-based data mapping
- Improve error messages
- Improve building experience
- Keep investing in Spack
- Create Youtube videos

Condensed feedback preCICE Workshop 2020

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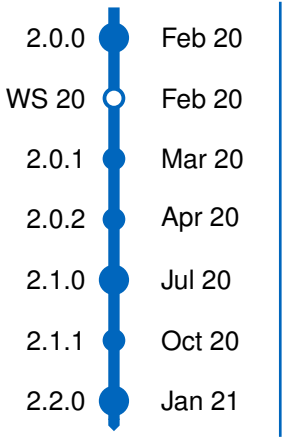
With this in mind. Let's see what happened!

Part I

The preCICE library

Highlights


2.0.0
Feb 20
WS 20
Feb 20
2.0.1
Mar 20
2.0.2
Apr 20
2.1.0
Jul 20
2.1.1
Oct 20
2.2.0
Jan 21

Highlights

2.0.0	**Feb 20**
WS 20	**Feb 20**
2.0.1	Mar 20
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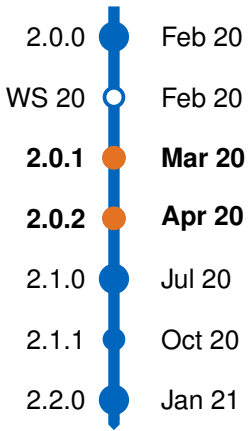
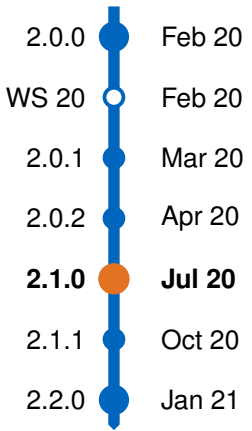
Covered in *Frédéric Simonis, preCICE 2.0 and beyond, preCICE Workshop 2020* `https://youtu.be/l1m1rdU36EI`

Highlights



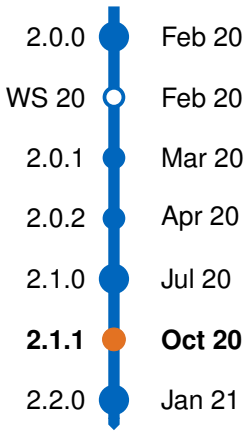
- Implemented feedback from user session.
- Mainly compatibility and bug fixed.

Highlights



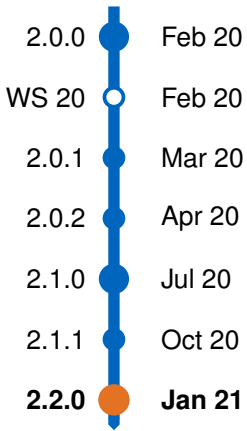
- Reworded and extended **all error messages** in preCICE
- Support of Quads
- Parallel RBF mapping without PETSc
- Clarified action timings
- Improved and extended convergence measure logging
- Reduce verbosity of profiling

Highlights



- Improved compatibility with Intel compilers

Highlights



- Multiple mappings from and to a mesh
- Watch integral of a mesh
- Improved support for macOS
- Upgrade to C++14
- Robust PETSc discovery

Highlights

Improvements

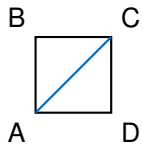
Support of quads

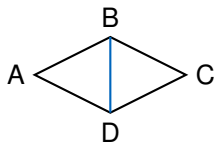
API `setMeshQuad(AB,BC,CD,DA)` `setMeshQuadWithEdges(A,B,C,D)`

Requirement Planar Quad

Implementation Triangulation, split longest diagonal

Consequence `<export:vtk />` contains triangulated mesh





Parallel RBF mappings without PETSc

Context	Builds interpolant using Mesh + RBF Solve one or more linear systems
PETSc	Use GMRES to solve the systems Works for parallel and serial participants
Without PETSc	Eigen QR decomposition with triangular solve Works for serial participants
New	Gather scatter approach for parallel participants Slower, but it works

When PETSc is enabled one can still request the Eigen implemenation:

```
<mapping:rbf-compact-tps-c2 support-radius="0.05" constraint="consistent"
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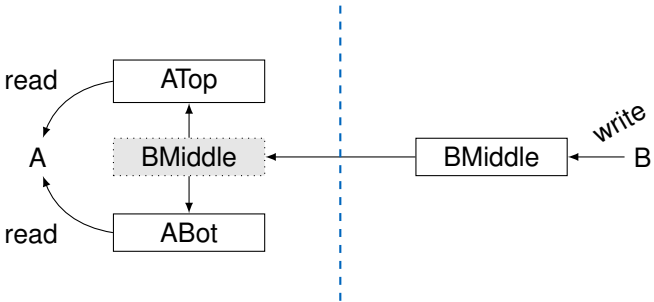
Kyle Davis, Data mapping in preCICE, **preCICE Workshop 2021**

Multiple mappings from and to a mesh

Use-cases Sum up multiple meshes on another mesh.
Map a received mesh to various internal meshes.



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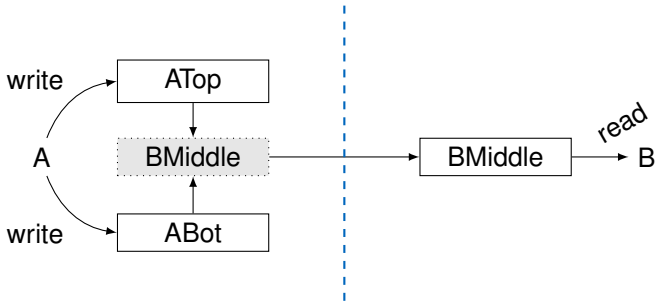

Watch integral of a mesh

Use-cases Determining the total force on a geometry in an FSI simulation.
Determining the flow rate for a fluid-fluid coupling.

New Watch the integral value of a whole Mesh.
`<watch-integral mesh="..." name="..." />`
Either scale with area or sum up data on vertices.

```
<participant name="MySolver1">
  <use-mesh name="MyMesh1" provide="yes"/>
  ...
  <watch-integral mesh="MyMesh1" name="MyWatchIntegral"
                  scale-with-connectivity="yes"/>
  ...
</participant>
```

Highlights

Reworded and extended all error messages in preCICE

git: “What went wrong. How to proceed from here.”

Our Guideline

- Use names for meshes, data and participants.
- State what went wrong.
- Provide a next step *if possible*
  configuration example, documentation, instructions

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  configuration example, documentation, instructions

Old

```
Data with name "Forces" is not defined on mesh with ID 1.
```

New

```
Data with name "Forces" is not defined on mesh "FluidMesh".
Please add <use-data name="Forces"/> under <mesh name="FluidMesh">.
```

Reset write data to zero in `advance()`

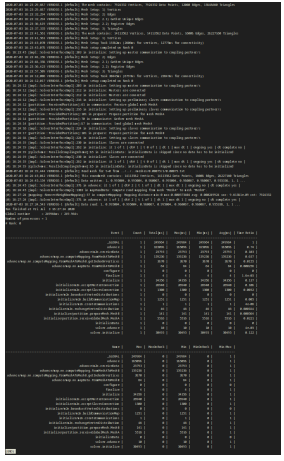
Common mistake Forgetting to write data for implicit coupling

Problem Very difficult to debug (data looks realistic)

Solution Reset `<write-data ... />` in each `advance()`

Minuscule impact, major gain!

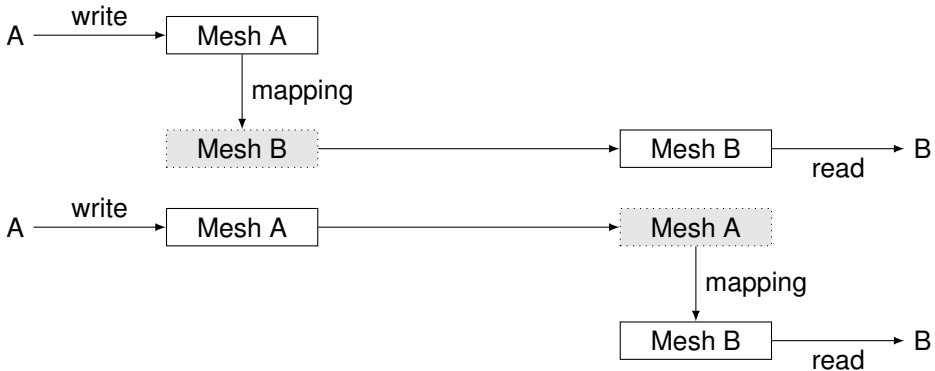
Reduce verbosity of profiling



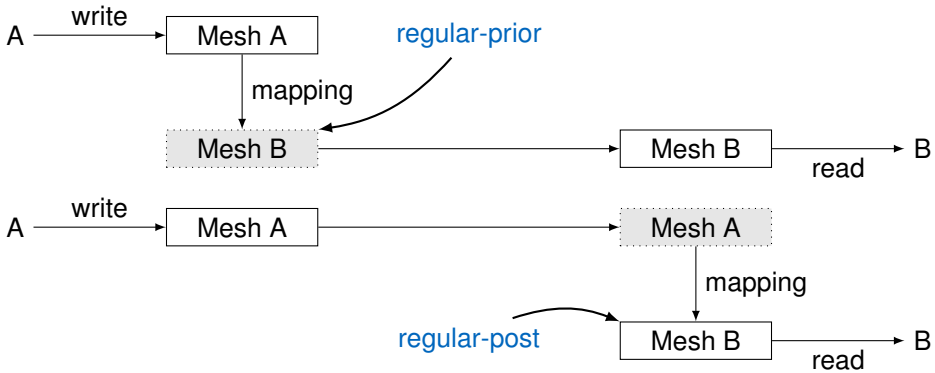
Output of participant A

precice-A-events-summary.log

Clarified action timings



Clarified action timings - Old



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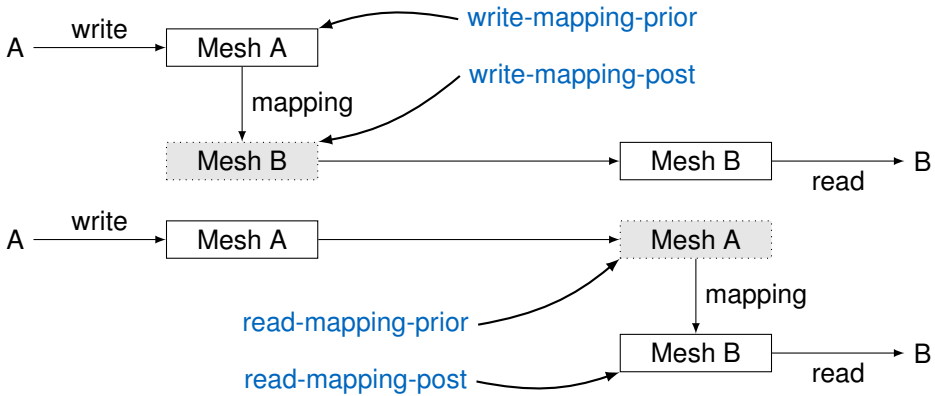


Strict convergence measures

New Strict convergence measures
Ends simulation if not fulfilled

Use-case Saves resources if things go very wrong

Example

```
<relative-convergence-measure
    mesh="Fluid_Nodes" data="Pressure"
    limit="1e-5" strict="1" />
```

Improved and extended convergence measure logging

Example

```
<relative-convergence-measure
    mesh="Fluid_Nodes" data="Pressure"
    limit="1e-5" />
```

Output

```
relative convergence measure:
```

Old

```
two-norm diff = 2.6036e-08, relative limit = 1.0005e-08, conv = true
```

New

```
relative two-norm diff = 2.6023e-05, limit = 1e-05,
normalization = 0.00100051, conv = false
```

Improved and extended convergence measure files

`precice-MySolver-iterations.log`

Additional information on QN columns.

```
TimeWindow  TotalIterations  Iterations  Convergence \
    QNColumns  DeletedQNColumns  DroppedQNColumns
1   6  6  1   5  0  0
2   9  3  1   7  0  0
3  12  3  1   9  0  0
```

`precice-MySolver-convergence.log`

Measures now display the data name.

```
TimeWindow  Iteration  ResRel(Temperature)  ResRel(Heat-Flux)
1           1          1.0000000000000000   1.0000000000000000
1           2          0.0009551938284061   0.4856546284783871
1           3          0.0008506916349598   0.0211064920997584
```

Improved support for macOS

Big Shoutout Oguz Ziya Koseomur **@oguzziya**

Done Port to macOS Catalina 10.15

Future CI on macOS

In a nutshell:

1. ```
   $ brew install cmake eigen  libxml2 boost petsc openmpi python3 numpy
   $ port install cmake eigen3 libxml2 boost petsc openmpi python3 numpy
   ```
2. Get the sources
3. Build as usual
   ```

Upgrade to C++14

- Long planned
- Required by Boost.geometry 1.75
- Cleaner internals
- Allows many improvements

Toolchain	New	Old	Comment
GCC	5	5	
Intel	**17**	**15**	requires GCC 5
Cray	8.**6**	8.**4**	requires GCC 5
Clang	3.**4**	3.**3**	

Example: Deprecated API methods:

```
/.../Solver.cpp:42:16: warning: 'hasToEvaluateSurrogateModel' is deprecated: The manifold mapping feature is no longer supported. [-Wdeprecated-declarations]
  if (interface.hasToEvaluateSurrogateModel()) {
                ^
/.../precice/SolverInterface.hpp:260:5: note: 'hasToEvaluateSurrogateModel' has been explicitly marked deprecated here
[[deprecated("The manifold mapping feature is no longer supported.")]] bool hasToEvaluateSurrogateModel() const;
```

Robust PETSc discovery

Official	use pkg-config
Old	use community FindPETSc
New	custom pkg-config wrapper
Features	• Drop-in replacement • Lists considered prefixes • Invalid prefixes
Distros	All but CentOS

Part II

Outlook

Outlook

v3 and beyond

Two-level parallel initialization

- No mesh gather on master
  Allows for larger meshes
- Close to complete
- Does not yet cover all corner-cases
- Enable using
  `<m2n use-two-level-init="on">`

Amin Totounferoush, Two step parallel communication initialization for preCICE,
preCICE Workshop 2021, `https://youtu.be/ioU8DcOACyE`

Usability of parallel RBF

pre 2.1

```
Interpolation matrix C is not invertible.
RBF [Polynomial] linear system has not converged.
```

2.1

```
The [polynomial] linear system of the RBF mapping from mesh MeshA to mesh MeshB has not converged.
This means most probably that the mapping problem is not well-posed.
Please check if your coupling meshes are correct.
Maybe you need to fix axis-aligned mapping setups by marking perpendicular axes as dead?
```

Problem

- What went wrong?
- Divergence or stop?
- What are the residual limits?
- How many iterations?
- More configuration options?
- RBF convergence log files?

Parallel RBF without PETSc

Currently	Gather-Solve-Scatter
Problem	Compute and memory imbalance *“It works”*
Desirable	Parallel sparse decomposition

Windows support

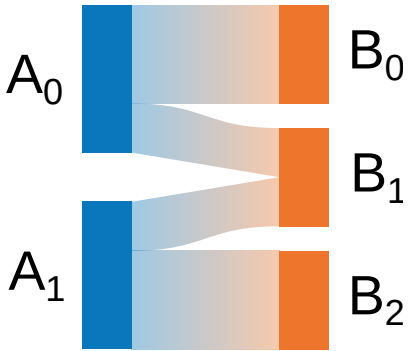
- Visual Studio Community 2019
- Already quite some progress made
- Some required fixes already released
- Ongoing task

Nearest projection for volume coupling

- Mapping on interface or volume
- Changes in mapping scheme
- 3D-Elements tetrahedra, octahedra

Contiguous mapping

- Matching meshes: Currently NN Mapping
  We can do better!
- Matching meshes with identical vertex order?
- Order as in time of registration
- Mapping of sub-ranges



Bulk Functions for Setting Meshes

- Edges and triangles
- API input sanitization
- API calls guarantee consistent state
- Bulk functions vastly more efficient

```
void SolverInterface::setMeshEdges(
     int meshID,
     int size,
     const int* vertexIDs,
     int* edgeIDs);

void SolverInterface::setMeshTriangles(
     int meshID,
     int size,
     const int* edgeIDs);
```

Outlook

Guide to major features

Geometric Mutli-Scale Mapping

Gerasimos Chourdakis, Geometric multi-scale coupling prototypes with preCICE, **SIAM CSE 21**

Consistent Time Interpolation

Benjamin Rüth, High-order and multi-rate time stepping with preCICE, preCICE Workshop 2020, `https://youtu.be/7NhBmcx_MmI`

Dynamic Adaptive Meshes

Frédéric Simonis, Adaptive Dynamic Meshes for Fully-Parallel Partitioned Multi-Physics in preCICE, ECCOMAS WCCM 2020, `https://slideslive.com/38944678`

Macro-Micro Coupling

Benjamin Uekermann, Macro-Micro Coupling in preCICE, **preCICE Workshop 2021**, `https://youtu.be/i12Fgz8yvhg`

Part III

The preCICE ecosystem

Restructured tutorials

Current format `./Physics/Case/SolverA-SolverB/...`
`./CHT/flow-over-plate/buoyantPimpleFoam-fenics/...`

Future format `./Case/...`

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Future format `./Case/...`

perpendicular-flap

- Select solvers
- Run them
- Same results

Fluid options

- nutils
- OpenFOAM
- SU2

Solid options

- CalculiX
- deal.ii
- FEniCS

News about Spack

Python bindings on Spack

```
spack install py-pyprecice@2.2.1.1
```

xSDK 0.6.0

Includes preCICE version 2.1.1
May be preinstalled on your local cluster

The preCICE virtual machine

All-in one sandbox to test and experiment.

```
$ mkdir somewhere && cd somewhere
$ vagrant init precice/precice-vm
get a cup of tea, or coffee, or both
$ vagrant up
```

Login and password `vagrant` via GUI or ssh.

Contains:

- preCICE
- Solvers
- Tutorials
- Shared folder with the host system
- Common tools (paraview)

The new website!

Our problem

- Distributed documentation
- Out-of-date info/links
- Confused users/developers
- Website barely useful

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Our strategy

- Unify access to documentation
- Integrate everything into website
- Restructure the information
- Searchable

preCICE is growing!

Benjamin Uekermann
Group for Usability and Sustainability of Scientific Software

Ishaan Desai
Adaptive and Flexible Macro-micro Coupling of Software

David Schneider
Flexible and Efficient Data Mapping for Simulation of Coupled Problems

Thank you for listening!

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simonis@in.tum.de