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CCP-WSI
a Collaborative Computational Project
in Wave Structure Interaction

OpenFOAM® Based Code Coupling

Dr Stephen Longshaw

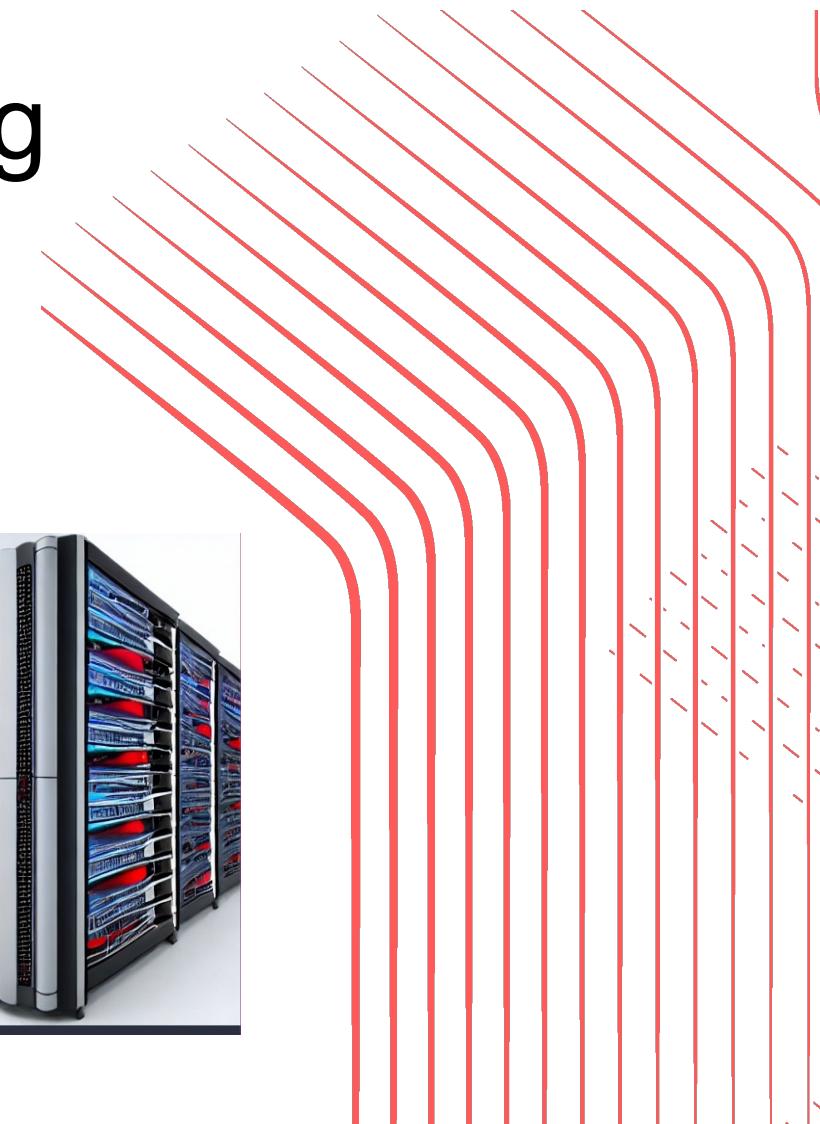
OpenFOAM Parallel Performance Engineering Workshop

[Register](#) [Agenda](#)

5 - 6 June 2023
Time TBC
Daresbury Laboratory, Keckwick Lane, WA4 4AD



OpenFOAM



Introduction

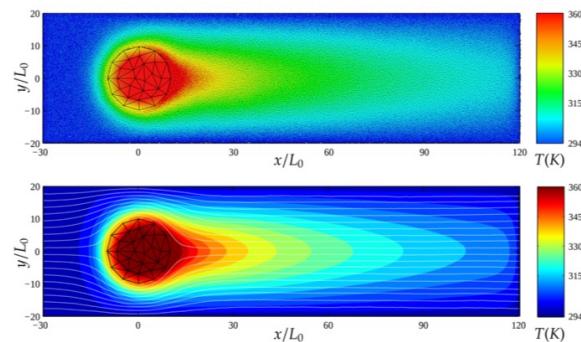
- Coupling allows **multi-physics** or **multi-scale** problems to be solved
- May involve a single or multiple solvers
- Some solutions are solved simultaneously
- Some couplings are 1-way, some 2-way, some tight, some loose
- ... some definitions needed

Nomenclature

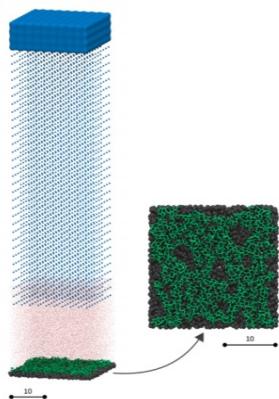
- **Multi-physics:** Coupling different methods or solvers to simulate a single problem involving multiple physical aspects (e.g. structural mechanics and fluid dynamics)
- **Multi-scale:** Coupling different methods or solvers to simulate a physical process while considering significantly different length or time scales
- Code coupling can be: **monolithic** or **partitioned**:
 - **Software:** single executable *or* multiple executables with inter-process communication
 - **Algorithmic:** single system of equations *or* multiple discrete systems joined through a connective term such as a boundary condition
- Partitioned solutions need complex inter-process communication and generalised capabilities like spatial interpolation

Coupling Examples

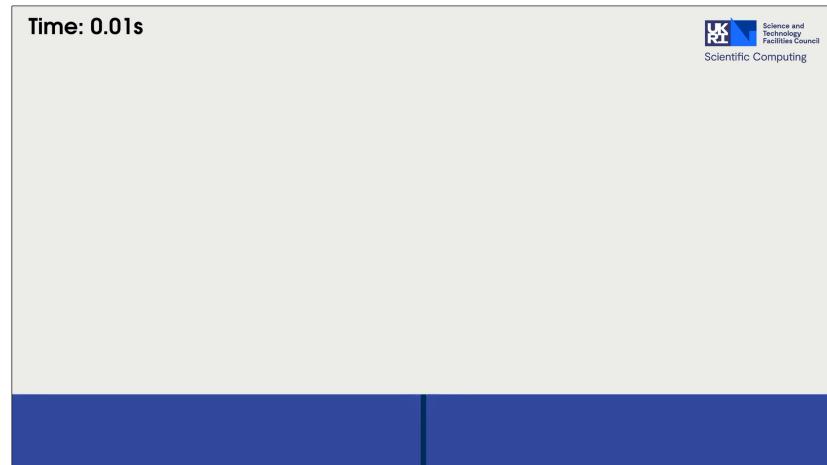
eDPD & Finite Element



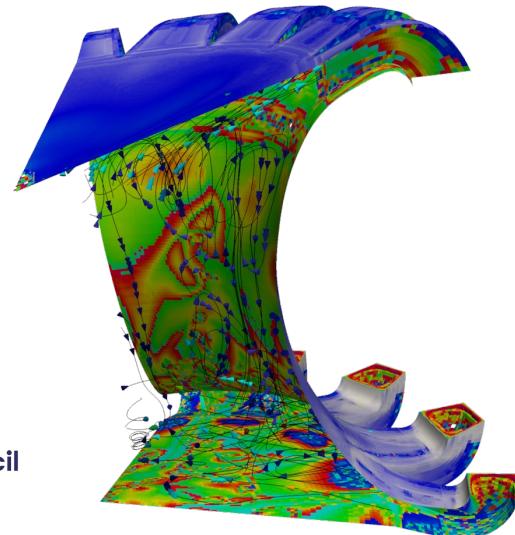
SPH & DPD



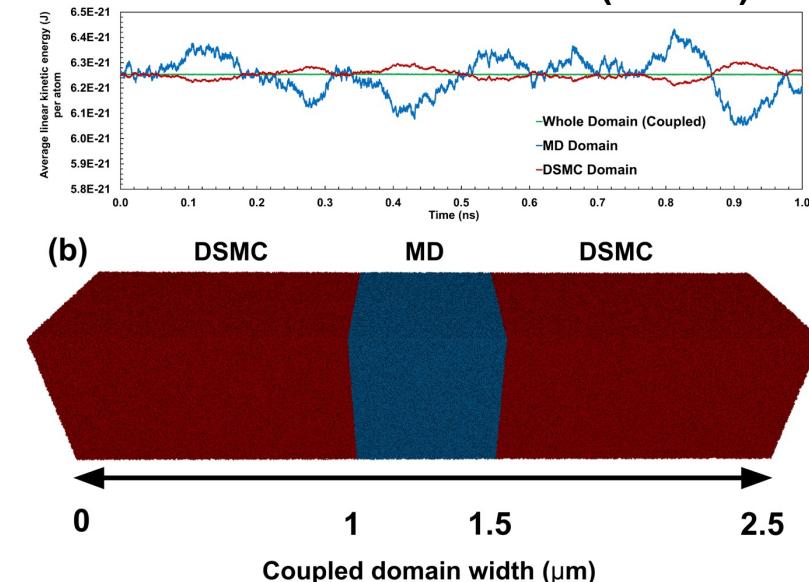
Fluid & Structural (FSI)



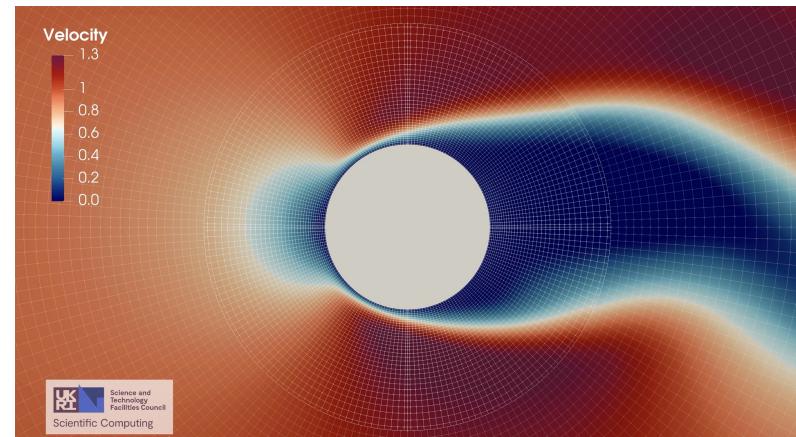
Fluid & Neutronics



Molecular Dynamics (MD) & Direct Simulation Monte Carlo (DSMC)



Fluid to Fluid





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Creating Coupled Solutions with OpenFOAM®



OpenFOAM's Coupling Capabilities

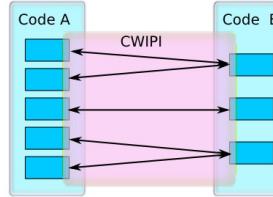
- Coupling is primarily achieved using inbuilt boundary patch types:
 - AMI (Arbitrary Mesh Interface):
 - Coupling between disconnected adjacent mesh domains
 - Well tested (available in OpenFOAM for a while), robust, generally applicable
 - Does not... guarantee conservation!
 - NCC (Non Conformal Coupled):
 - Coupling between non-conformal patches
 - Introduced into ESI OpenFOAM in 2022
 - Guarantees conservation (within the limits of the Finite Volume method)
- Both provide a way to create a *monolithic* coupled software solution
- **Neither** are suitable should you wish to introduce a solution that cannot be solved directly by OpenFOAM (e.g. Finite Element)

Extending its Capabilities

- A number of general purpose *code coupling* libraries exist
- These can be integrated into OpenFOAM and used to either couple its own solvers together or to other external codes



Multiscale Universal Interface (MUI)
<https://mxui.github.io>



Coupling With Interpolation
Parallel Interface (CWIPI)
<https://w3.onera.fr/cwipi/bibliotheque-couplage-cwipi>

PLE

Parallel Location and
Exchange
[www.code-
saturne.org/documentation/
ple-2.0/html/index.html](http://www.code-saturne.org/documentation/ple-2.0/html/index.html)



Precise Code Interaction
Coupling Environment
<https://precice.org>

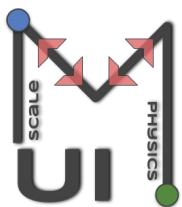
MUSCLE 3

Multiscale Coupling Library and
Environment (MUSCLE)
<https://github.com/multiscale/muscle3>

Coupling Library Overview

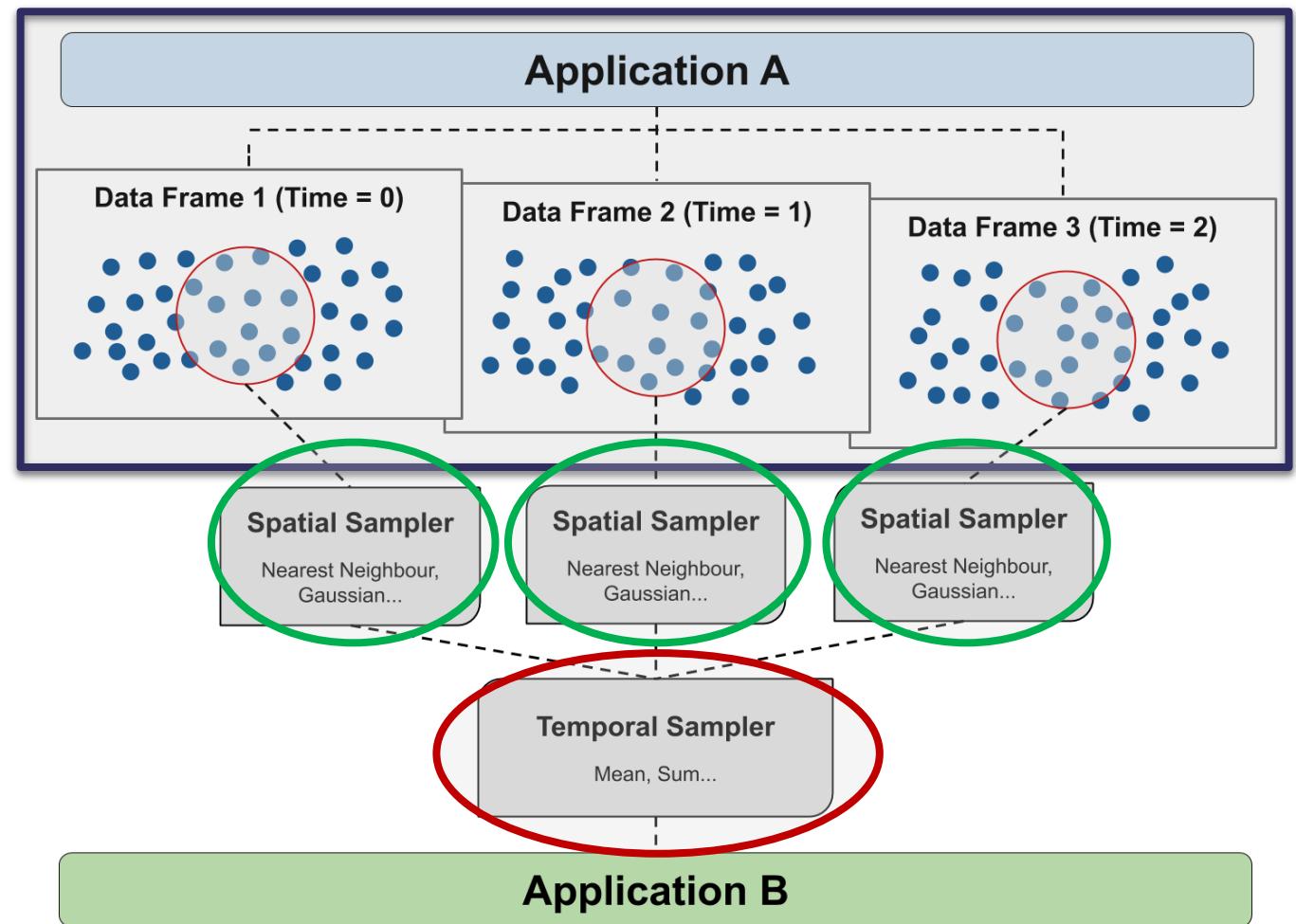
- Create an **interface** for data transfer between codes:
 - *Mesh-based* (preCICE / CWIPI / PLE)
 - Potential for re-use of mesh data from coupled domains for collocated problems
 - Harder to use for particle-based couplings
 - *Particle-based* (MUI)
 - Coupling dissimilar methods (e.g. Lagrangian to Eulerian) conceptually simple
 - Relies on spatial interpolation to convert this data back to a useful form for each domain
 - Potential introduction of loss of accuracy when used with higher-order methods.
- Data transfer typically performed using MPI (rarely TCP/IP) for performance
- Provide interpolation methods to map data back to coupled domains*:
 - Some also provide temporal interpolation (e.g. MUI/preCICE)
 - Some also define specific coupling methodologies (e.g. Aitken's for FSI)

* *PLE provides data transport and mapping but **not** interpolation methods*

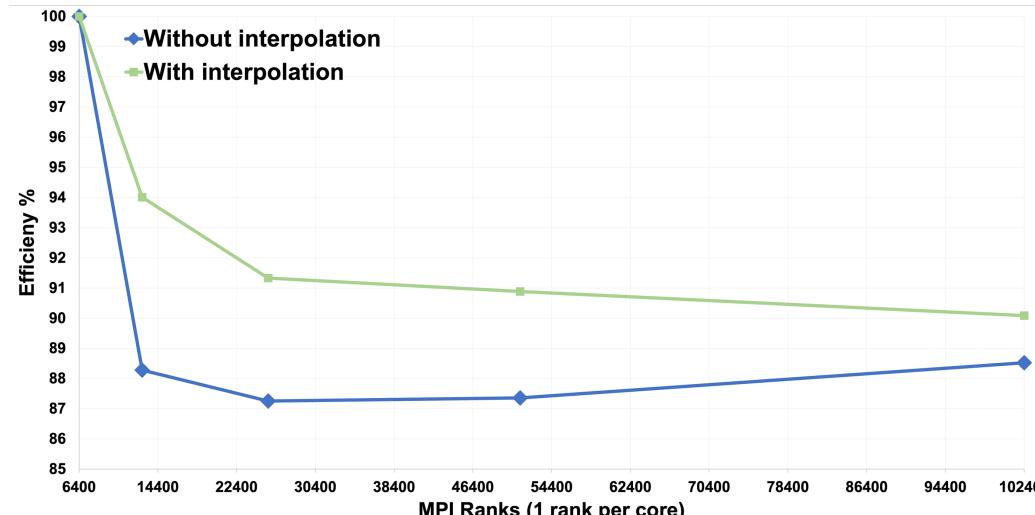
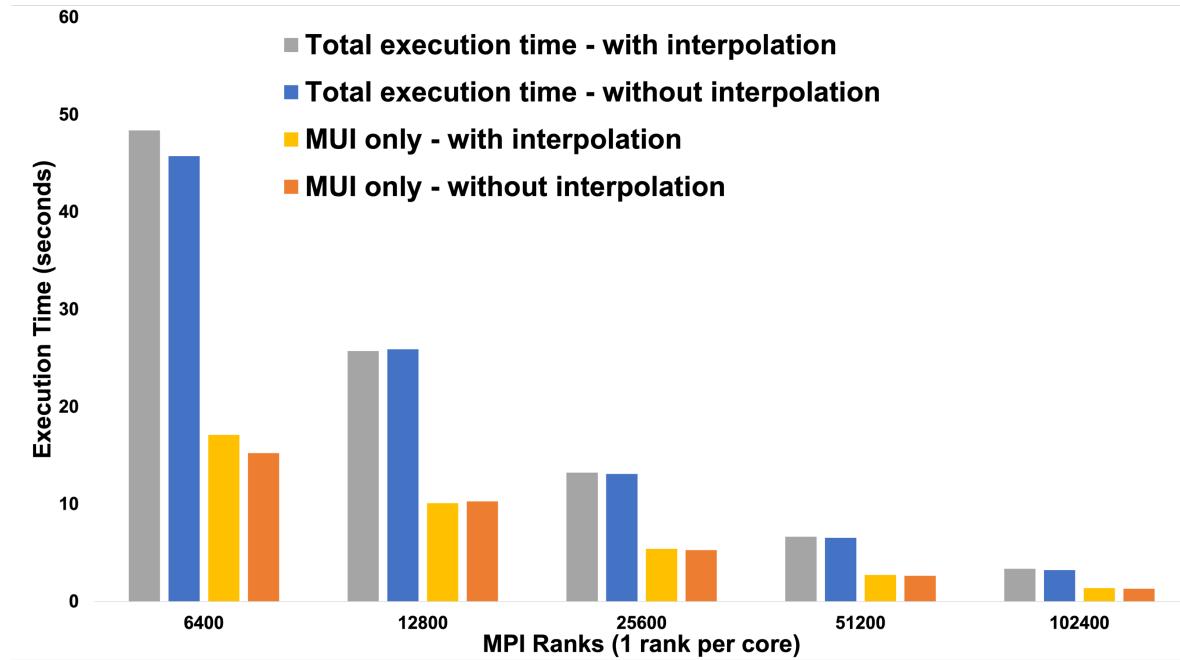
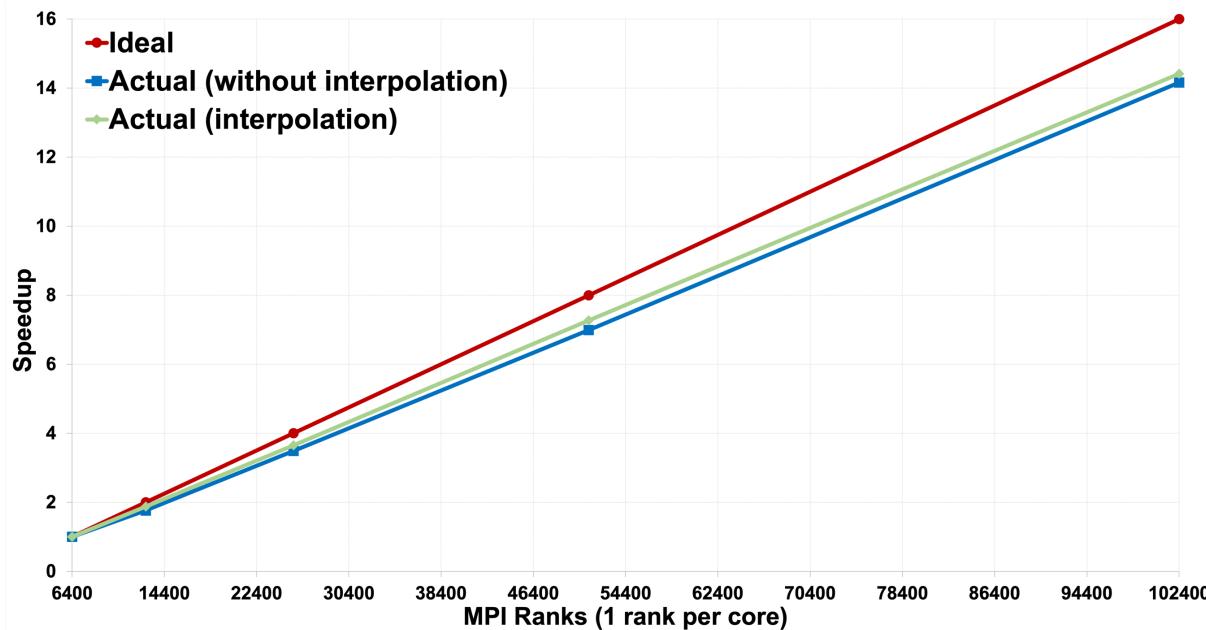


Example: Multiscale Universal Interface

- Couples using a set of discrete data samples and an **interface**:
 1. Convert domain-specific representations to a general form (a cloud of points with associated data)
 2. Solver **imparts** data (at a point) to interface with an **associated time-stamp** using **non-blocking** operations
 3. Other solver requests data at specific location and time from MUI interface using **spatial** and **temporal** sampler using **blocking** operations
 4. Data is transferred between solvers using the MPI multi-program multi-data (MPMD) method



MUI Performance



- MUI & artificial benchmark
- AMD EPYC HPE Cray EX
- 2 billion data items transferred
- Total of 48GB of data transferred
- With and without spatial interpolation



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Using Coupling Libraries with OpenFOAM

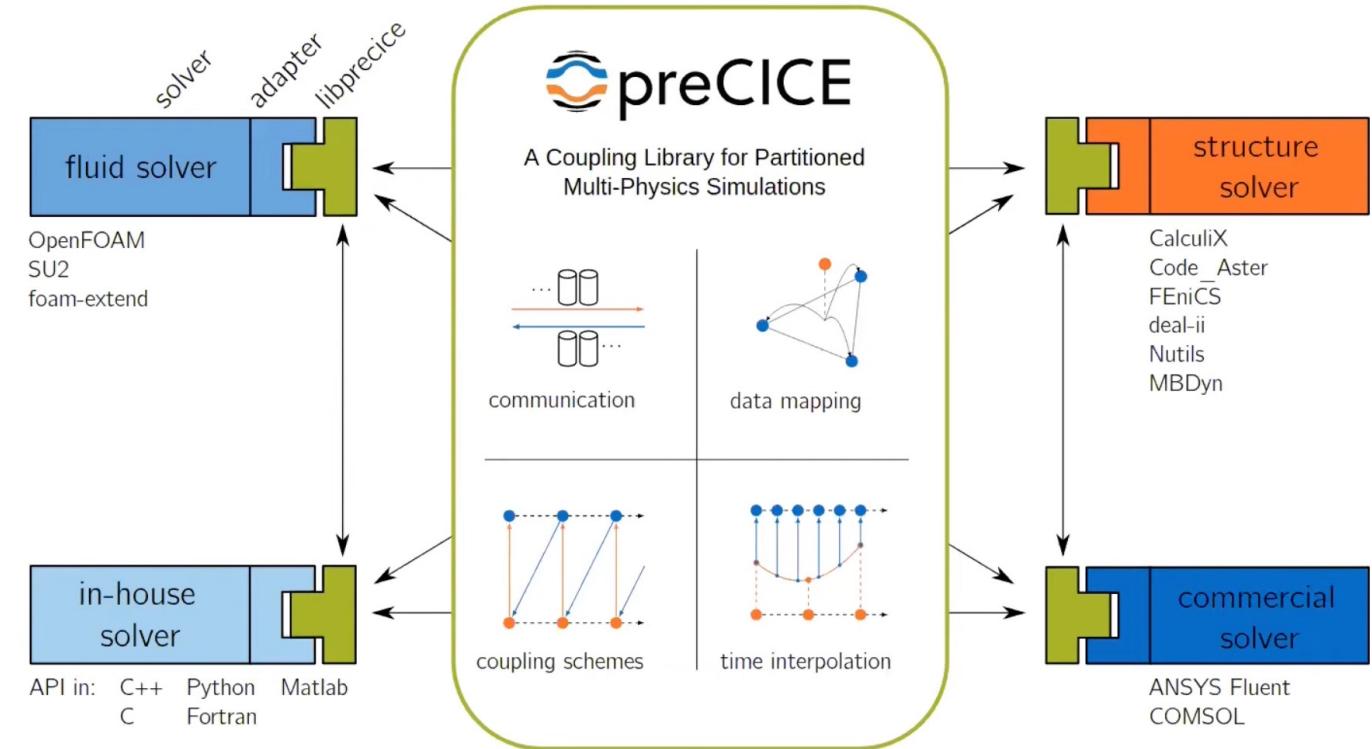


Existing Implementations

- Recent versions of ESI OpenFOAM provide support for using the ADIOS2 I/O library, this can enable high performance **inter-process** communication
- Recent ESI OpenFOAM also directly supports creating custom split MPI communicators – you can communicate data between solvers using MPI
- The **preCICE** coupling library offers a specific capability for coupling OpenFOAM with itself or other solvers
- CoSeC have directly integrated the **MUI** coupling library into OpenFOAM and use it as part of our general-purpose multi-physics simulation package, the **Parallel Partitioned Multiphysics Simulation Framework (ParaSiF)**

preCICE

- Provides support for recent OpenFOAM versions to couple to external solvers (or itself) to enable:
 - Fluid Structure Interaction (FSI)
 - Conjugate Heat Transfer (CHT)
 - Fluid-fluid coupling (FFC)
- Can be extended to enable other coupling types
- <https://precice.org/adapter-openfoam-overview.html>



Chourdakis, G., Schneider, D., & Uekermann, B. (2023). OpenFOAM-preCICE: Coupling OpenFOAM with External Solvers for Multi-Physics Simulations. OpenFOAM® Journal, 3, 1–25. [DOI: 10.51560/ofj.v3.88](https://doi.org/10.51560/ofj.v3.88)

MUI

- Integrated into OpenFOAM (currently v6.0, next release ESI v2212)
- **Currently working to integrate into future ESI OpenFOAM releases directly**
- Adding MUI capability to a new or existing FOAM solver involves:
 - Adding a couple of new lines to the code and creating a new dictionary to define coupling interfaces
 - Implementing your coupling algorithm by employing data transfer, spatial and temporal interpolation methods and using its *coupling helper* classes to calculate the values needed for common coupled approaches such as the Aitken's method for FSI problems.
- Allows you to couple OpenFOAM solvers with themselves or with other external solvers also instrumented with MUI
- Available in our ParaSiF repository: <https://github.com/ParaSiF>



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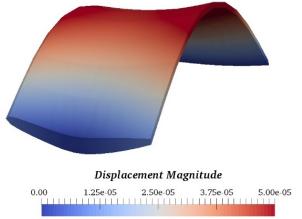
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Coupling Examples Involving OpenFOAM



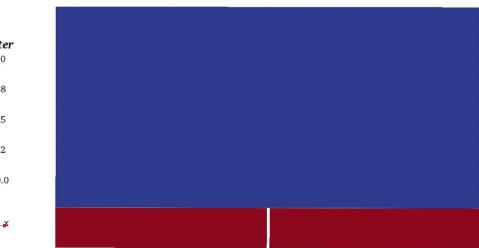
Fluid Structure Interaction (FSI)

Coupling CFD (OpenFOAM) with FEA (FEniCS) for FSI problems

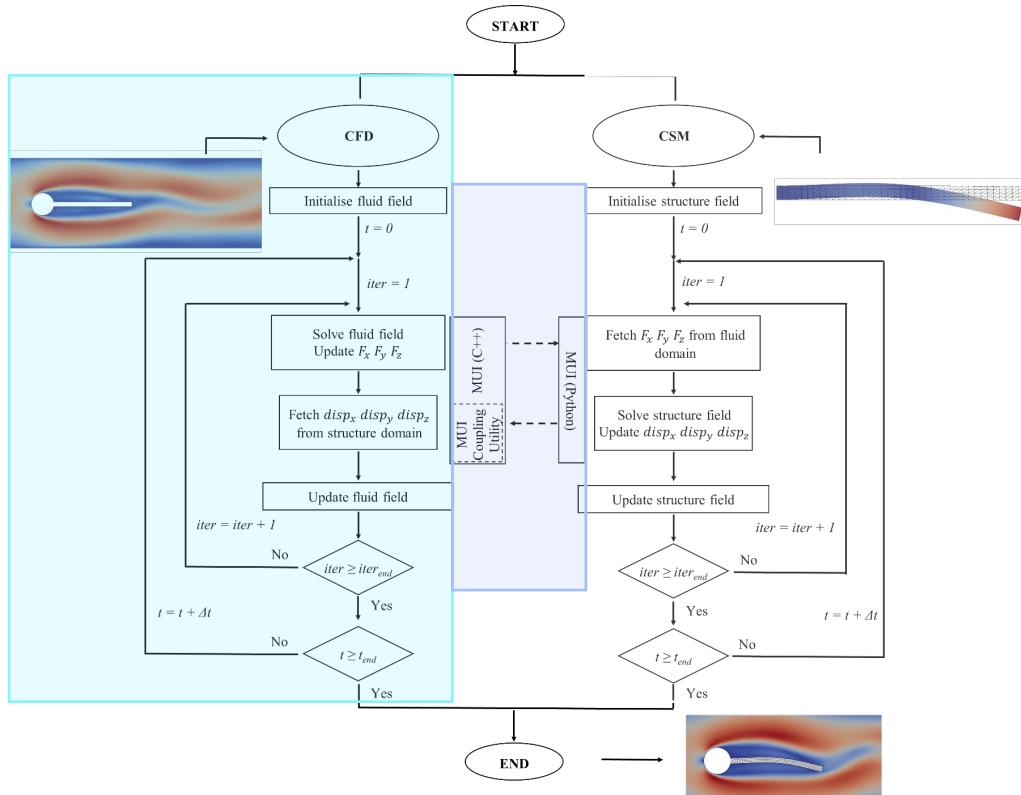


Vortex-induced vibration of the trailing edge of a hydrofoil

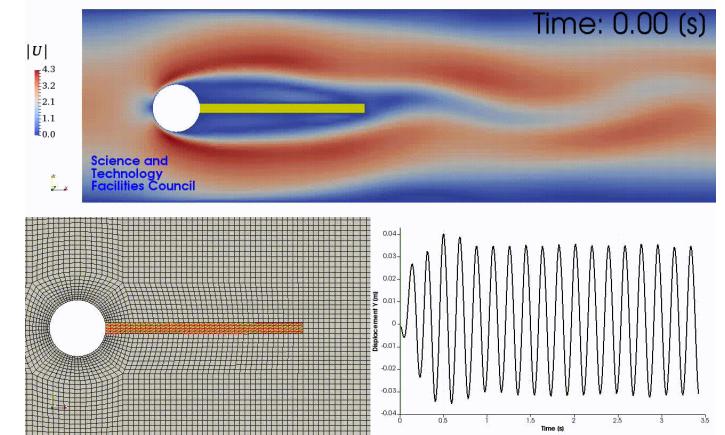
Time: 0.007 [s]



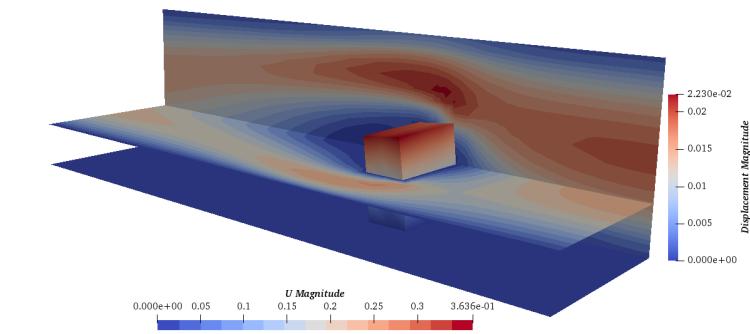
2-D roll tank with flexible beam



<https://github.com/ParaSiF>



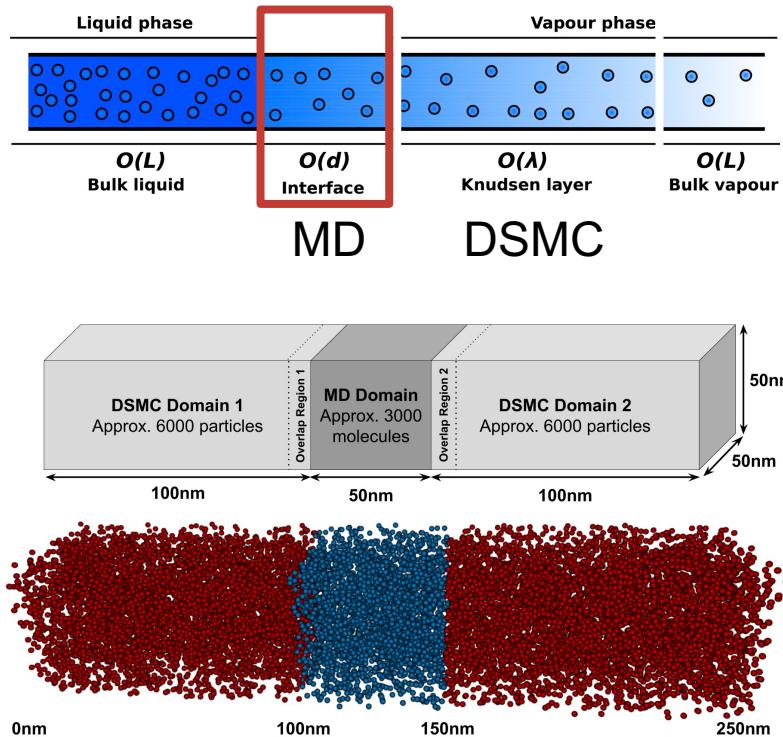
2-D Flow Pass Elastic Plate Behind a Rigid Cylinder



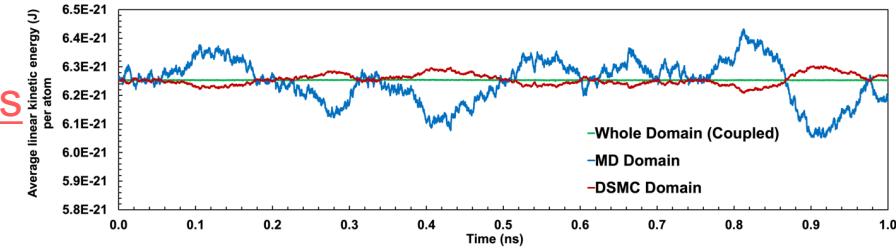
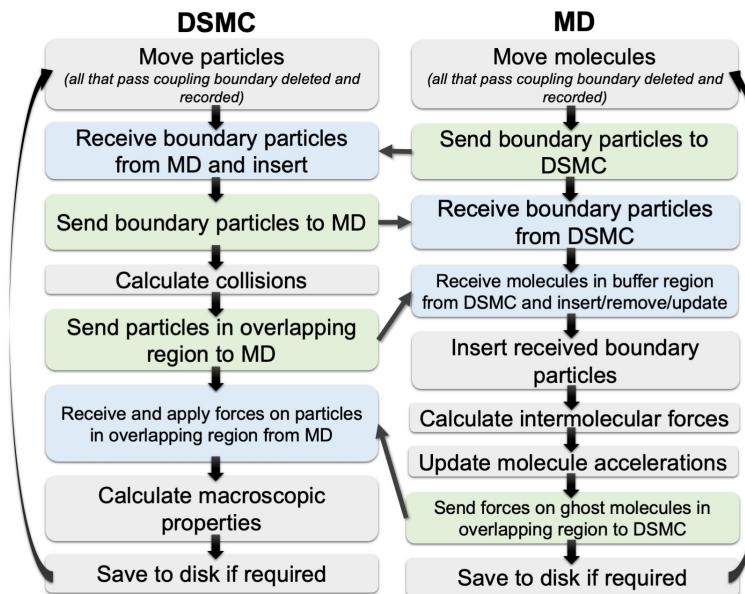
3-D Channel Flow Over an Elastic Beam with different levels of elasticity

Molecular Modelling of Gas Dynamics

Coupling OpenFOAM based Molecular Dynamics (MD) with Direct Simulation Monte Carlo (DSMC) to simulate the process of evaporation



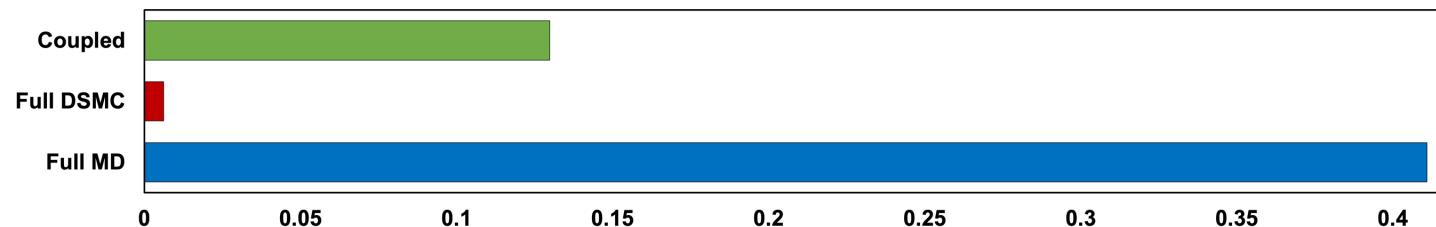
<https://github.com/MicroNanoFlows>



Coupled Linear Kinetic Energy (J)

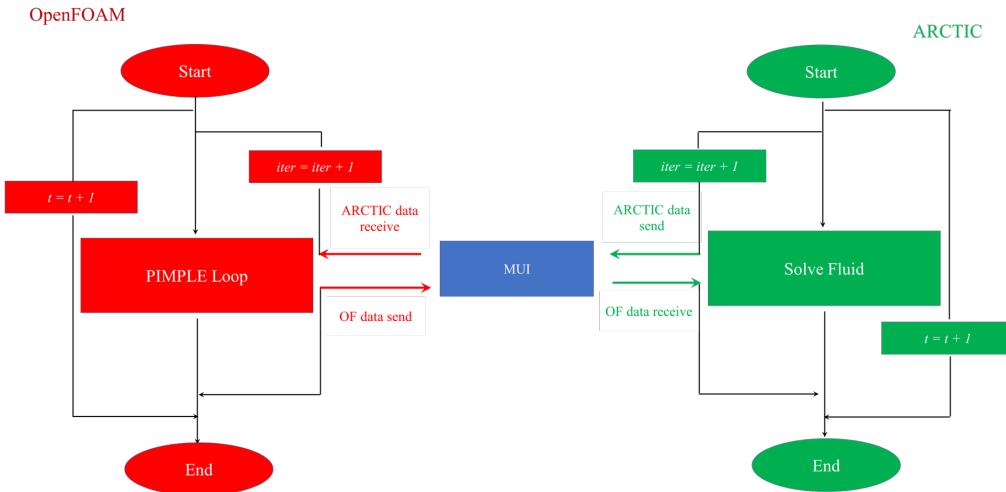
S. M. Longshaw et al., Coupling Molecular Dynamics and Direct Simulation Monte Carlo using a general and high-performance code coupling library, Computers & Fluids, 213, 104726, 2020.

Computational time per step (s)

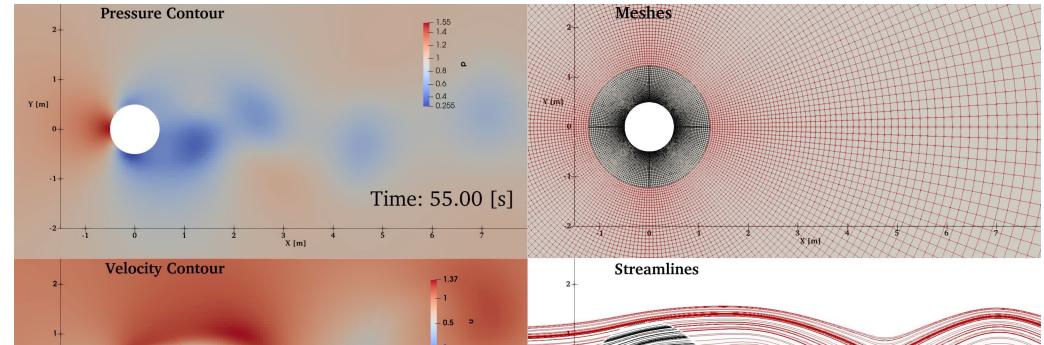


Fluid Fluid Interaction

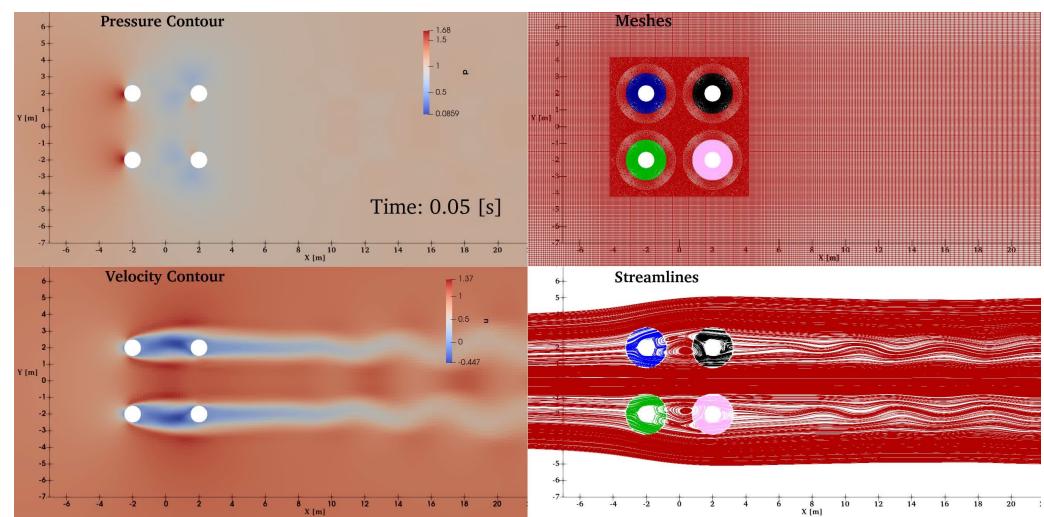
Coupling highly specialised (ARCTIC) and general purpose (OpenFOAM) CFD codes to handle complex rotor geometries in a large multi-physics domain



Single cylinder
Re=150



Four cylinders
Re=150



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Conclusions and the Future



- OpenFOAM is inherently capable of solving multi-physics and multi-scale problems where the solutions can fit into its existing framework (typically a Finite Volume approach)
- Where other methods are needed (such as Finite Element) then coupling libraries like MUI or preCICE can be used to extend its capabilities
- Some of OpenFOAM's solvers are *already* multi-physical in nature – interFoam provides 6 Degree-of-Freedom rigid body dynamics coupled with the FV VoF method

OpenFOAM is already a very capable set of solvers - It should now be used as part of wider coupled solutions that can stretch the capabilities in cutting edge supercomputing where using a single solver cannot



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Questions?

