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General Purpose Code Coupling for Particulate Methods Using the Multiscale Universal Interface

SPH-SIG/CCP-WSI Joint Meeting 1 - Bristol

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UK FLUIDS NETWORK

CCP-WSI
a Collaborative Computational Project in Wave Structure Interaction

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Why do we need to couple codes?

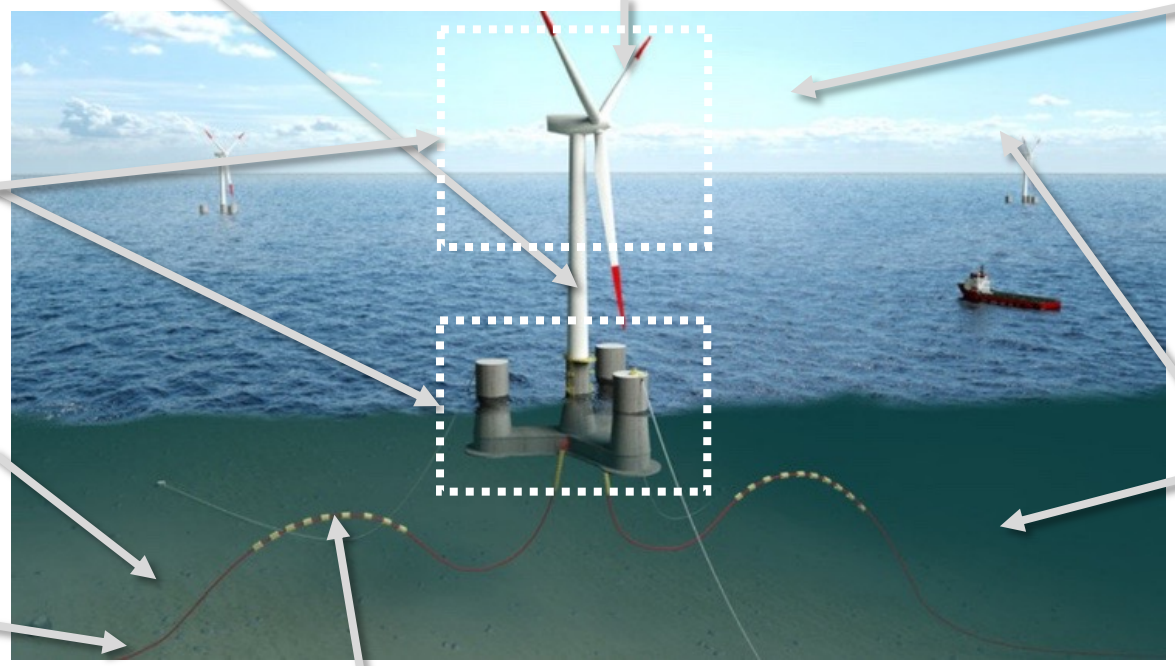
Complex multiphysics/multiscale problems

Rigid floating body dynamics

Flexible structural mechanics

Atmospheric modelling

Near-field: multi-phase fluid dynamics and single-phase aerodynamics



Far-field: Potential flow for fluid dynamics and aerodynamics

Seabed (soil mechanics)

Anchors (soil-structure dynamics)

Flexible tethering

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www.ccp-wsi.ac.uk/data_repository/test_cases/test_case_015

CCP-WSI a Collaborative Computational Project in Wave Structure Interaction

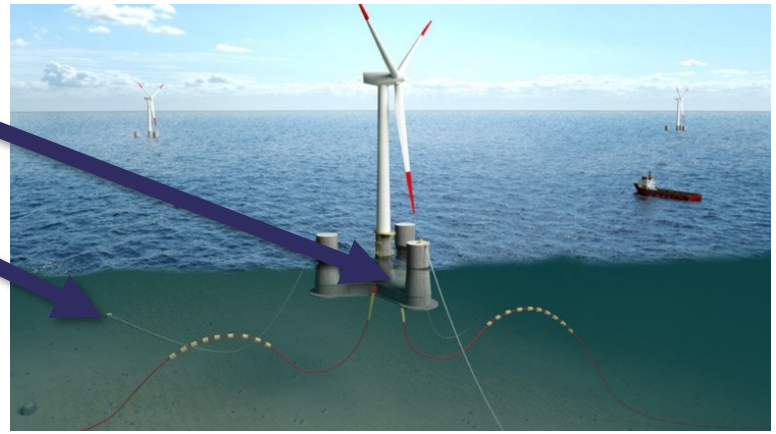
www.ccp-wsi.ac.uk

HEC-WSI a High End Computing Consortium for Wave Structure Interaction

www.hec-wsi.ac.uk

Why do we need to couple codes?

- Can’t the FOWT problem be solved just using particle approaches?
- A **monolithic methodological** approach is possible, but is it sensible?
- A **monolithic software** approach is also feasible, but again, is it sensible?
- A **partitioned** approach using the best method and software solution for each aspect of the problem is often the most sustainable method:
  - Particle methods for some aspects
  - Mesh-based approaches for others



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The Multiscale Universal Interface

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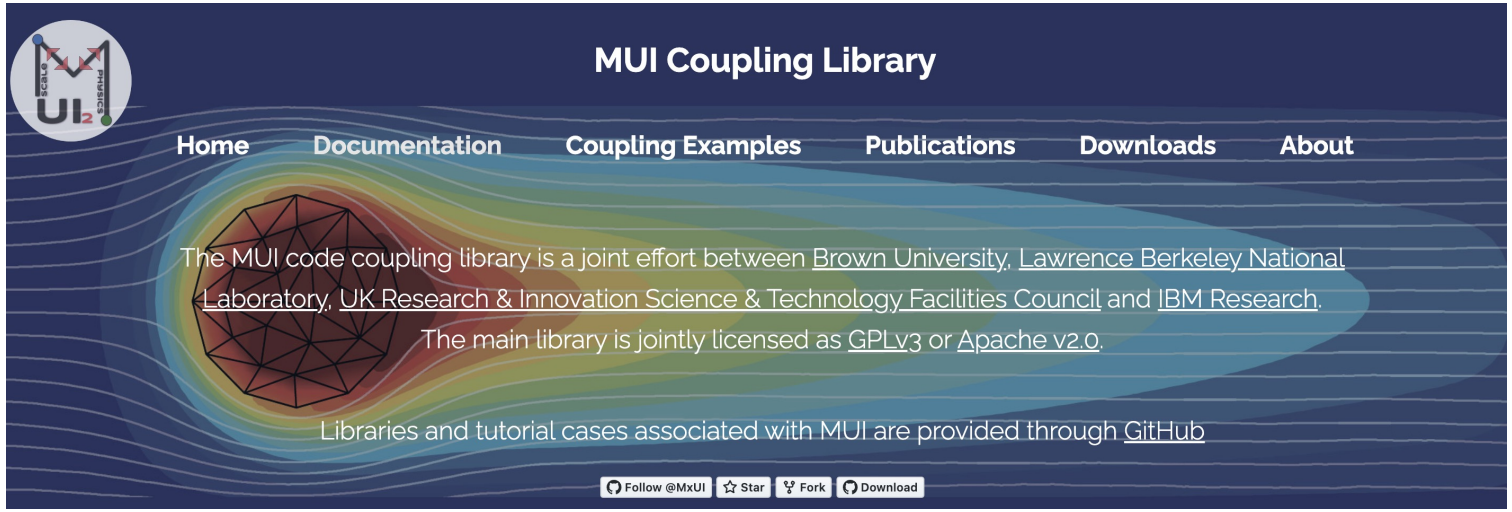
The Multiscale Universal Interface (MUI)

- Written in C++11 (with wrappers for C, Fortran and Python)
- Open-source, licensed at the user's choice as either **GPLv3** or **Apache 2.0**
- Header-only design with only external dependency being MPI
- Creates a peer-to-peer MPI based *interface* between two or more codes
- **Website:** https://mxui.github.io/
- **Library:** https://github.com/MxUI/MUI
- **Demos:** https://github.com/MxUI/MUI-demo
- **Benchmarking Framework:** https://github.com/MxUI/MUI-Testing



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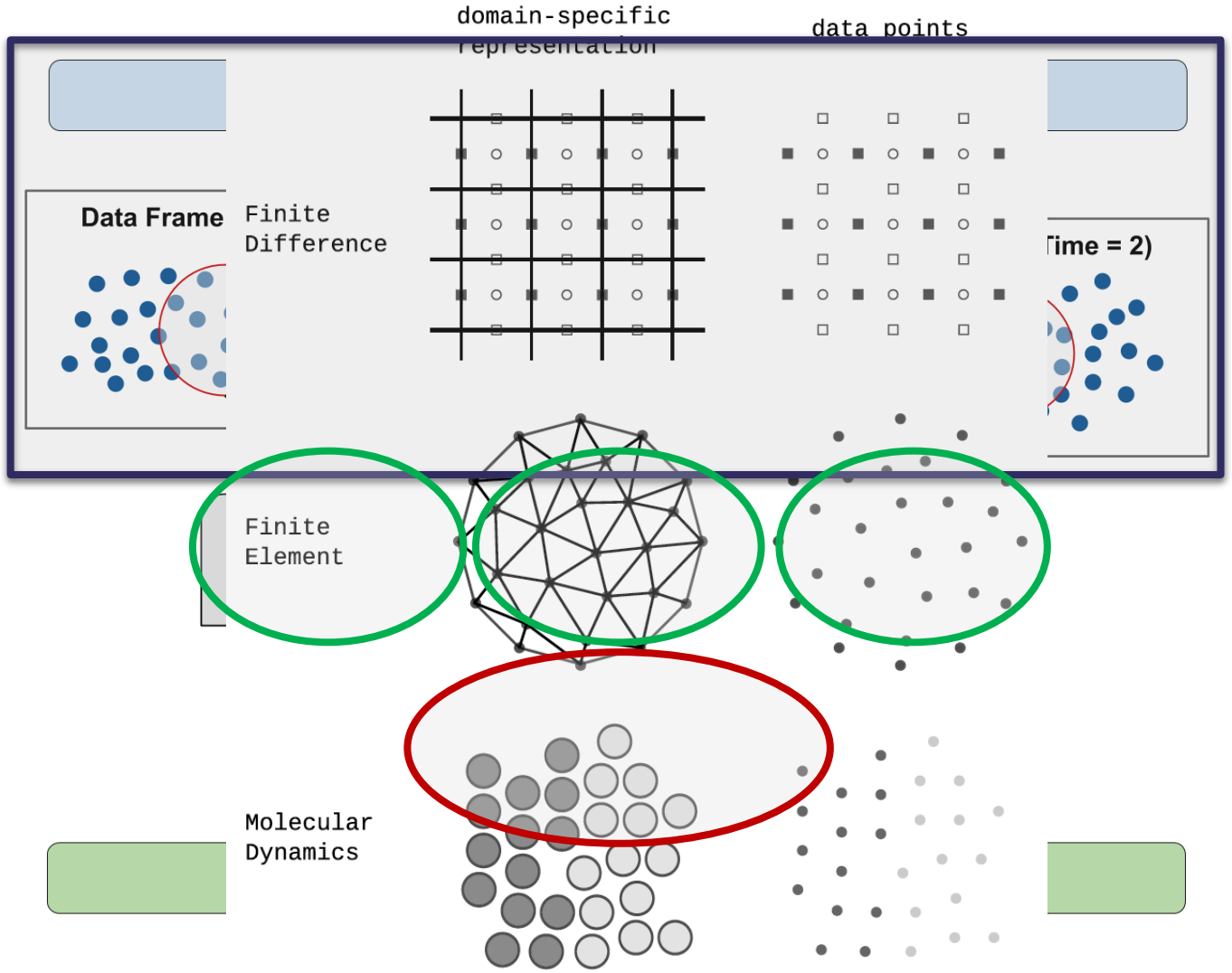
Multi-physics/scale coupling using MUI?

- Provides *tool-kit* to create new couplings between methods:
  - Mesh to particle
  - Mesh to mesh (fixed or moving)
  - Particle to particle
- Offers ability to couple across both length- and time-scales:
  - **Reasonable** length scales can be tackled (interpolation is our friend)
  - **Reasonable** time scales can be considered using a *data frame* concept
- At the point where **direct** multi-scale coupling no longer feasible, MUI can still be used purely for tagged data transport to enable complex abstractions
- MPI multi-program multi-data (MPMD) design allows large numbers of apps to be coupled together simultaneously

MUI overview

- 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-stamped data frame** using **non-blocking** operations
  3. Other solver requests data at specific location and time from MUI interface using **spatial** and **temporal** samplers and **blocking** fetch operations



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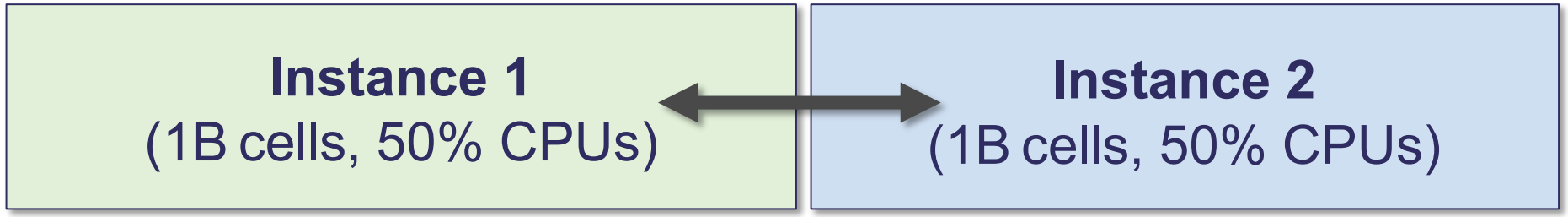
What is in the MUI toolkit?

- API to create an MPI based interface between 2 or more apps
- Extensible frameworks of spatial and temporal samplers as well as *coupling helpers*:
  - 10 spatial samplers: simple Gaussian, quintic SPH approach, Radial Basis Function (RBF) approach with both conservative and consistent modes and many others.
  - Temporal samplers allowing simple concepts like summation or averaging in time but with scope for more complex operations.
  - *Coupling helpers* to provide the functions to enable common approaches like the Aitken's iterative method used in FSI
- A custom linear algebra solution for both dense and sparse problems, currently used within the RBF spatial filter but able to be called from any filter or coupling helper

MUI Performance

- AMD EPYC HPE Cray EX (~750K cores)
- Representative of a typical 3D CFD problem coupled to itself:
  - Simulated local computation load
  - Simulated local MPI transfer using standard MPI 3D Cartesian decomposition
  - **Assumes linear scaling of CFD solver**
- 1 billion points transferred per instance (2B total) – full volumetric coupling
- Total of 48GB of data transferred via MUI
- Both with and without Gaussian spatial interpolation



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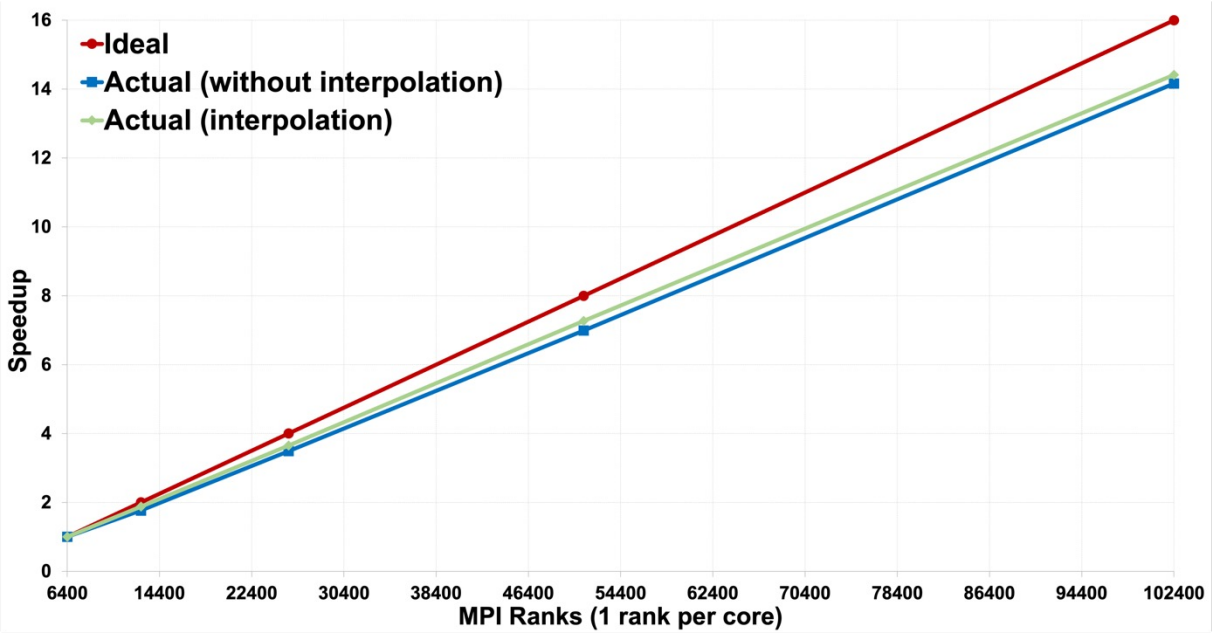
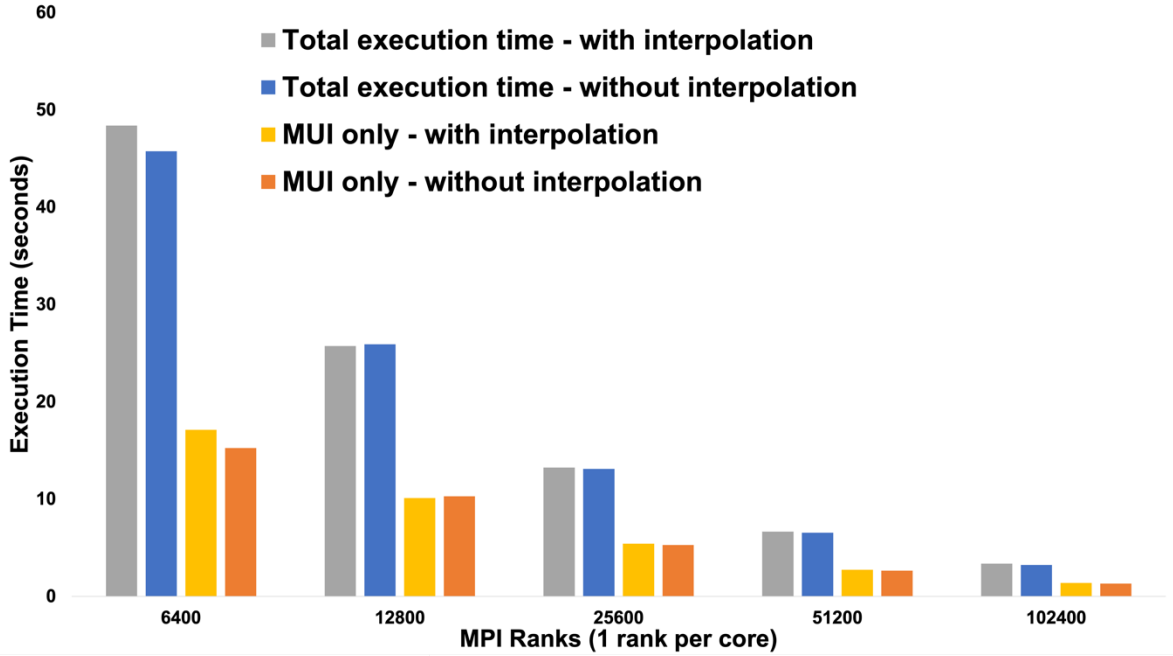
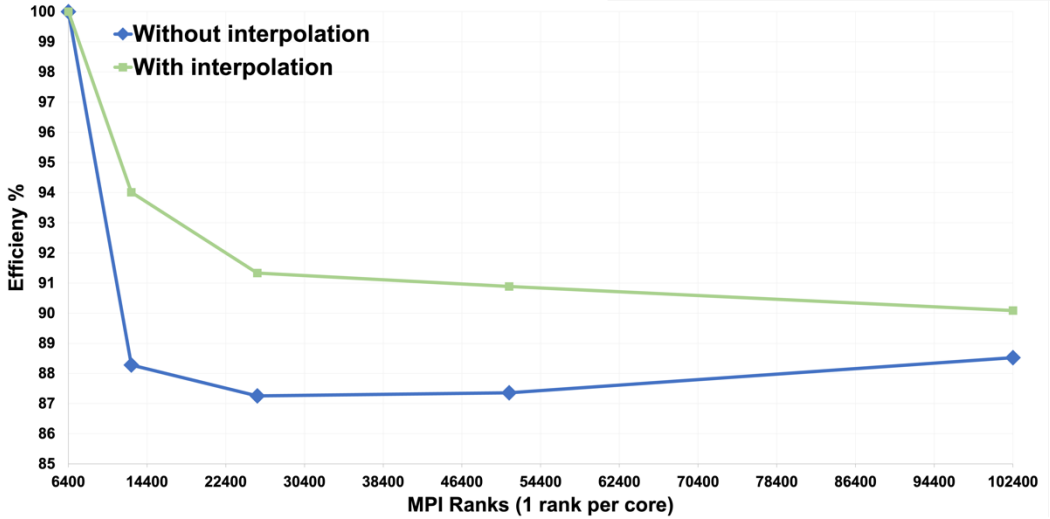
https://github.com/MxUI/MUI-Testing

archer2

MUI Performance







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What are we working on right now?

- Porting the linear algebra portion of MUI to the heterogenous programming model SYCL:
  - Work ongoing through an EPSRC ExCALIBUR project and through an Intel Centre of Excellence hosted at Daresbury Lab.
  - Enables cross-vendor GPU acceleration of dense/sparse matrix operations, initially in the RBF spatial filter.
- Integrating the matrix data types defined within the linear algebra solution so they can be used generally through the interface (i.e. you can pass them between codes directly).
- Considering how to integrate data science (AI/ML) workflows directly into the library to allow for use within coupling algorithms.

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Coupling Examples

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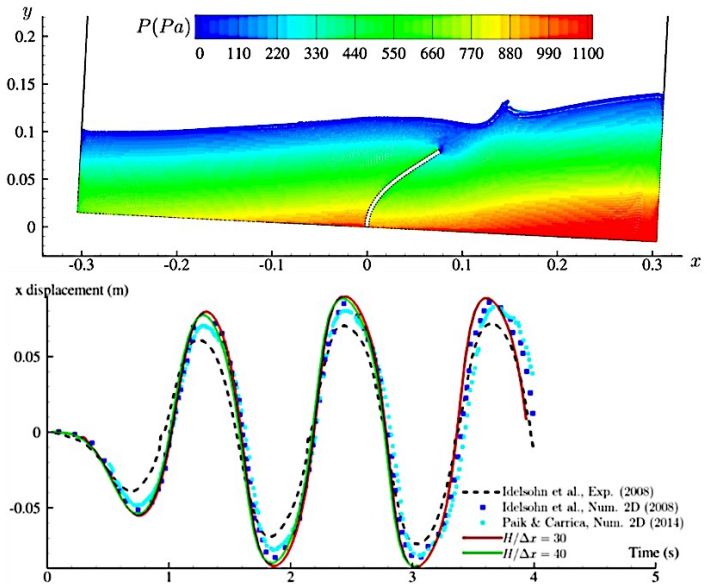
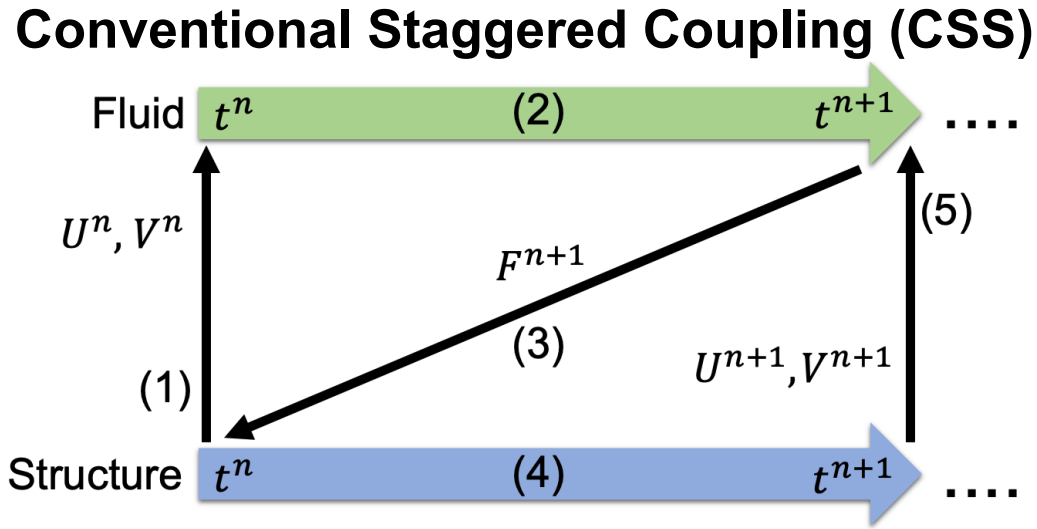
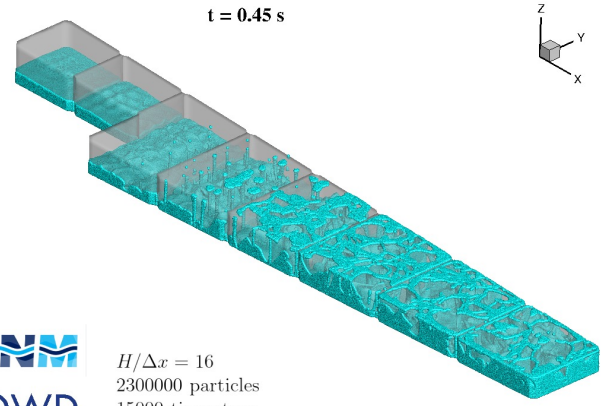
Fluid Structure Interaction (FSI)

Coupling CFD (SPH Flow) with FEA (MSC Nastran) for sloshing problems:

- Commercial SPH solver – explicit time-stepping; mesh-based boundary condition
- Commercial Finite Element (FE) solver – implicit time-stepping
- MUI used to transfer data and synchronise







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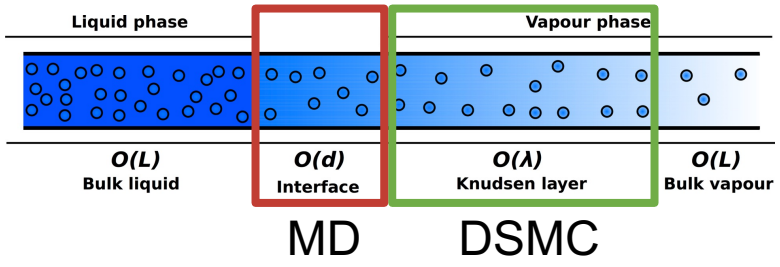
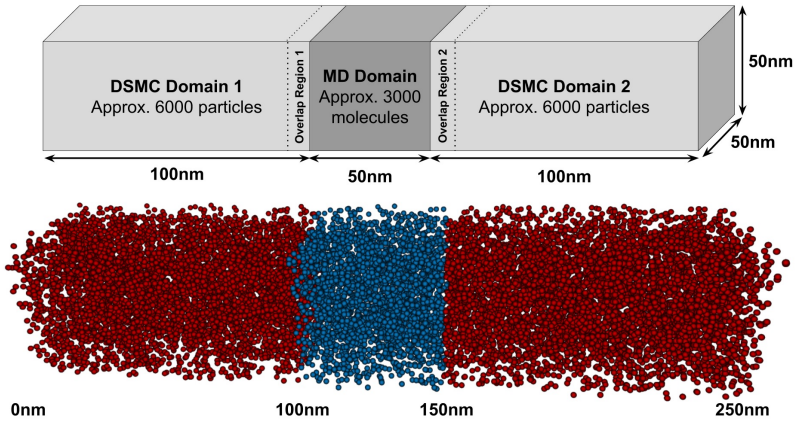
S. M. Longshaw et al. *A Coupled FSI Framework Using the Multiscale Universal Interface.* International Forum on Aeroelasticity and Structural Dynamics, Madrid, Spain. 2022.

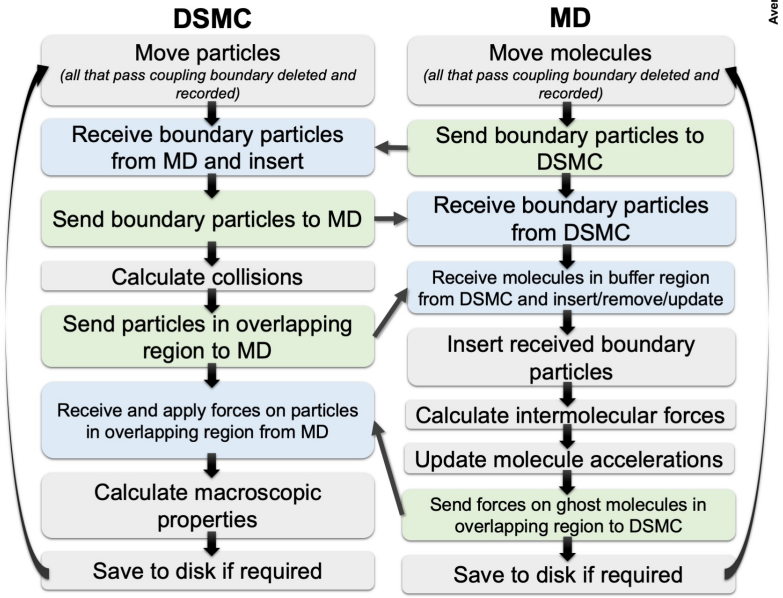
Molecular modelling of gas dynamics

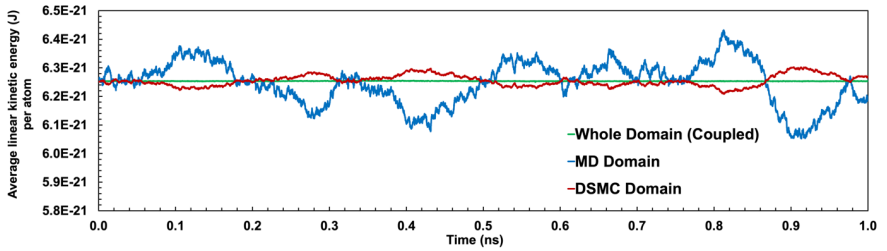
Coupling OpenFOAM based Molecular Dynamics (MD) with Direct Simulation Monte Carlo (DSMC) to simulate the process of evaporation





https://github.com/MicroNanoFlows

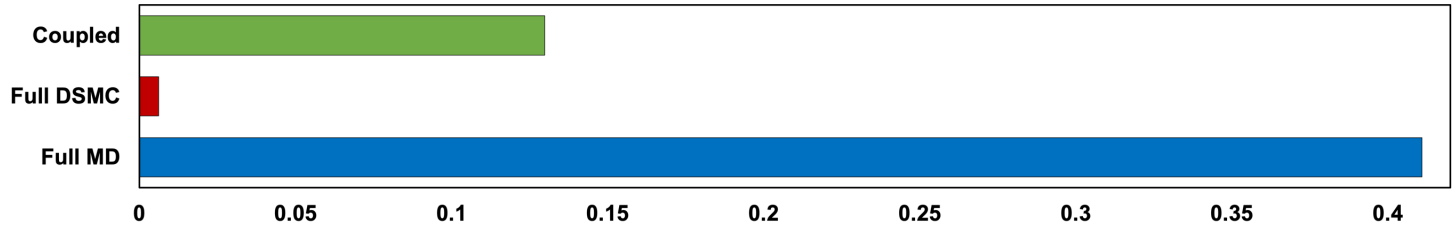




Coupled Linear Kinetic Energy (J)

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)



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Conclusions

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- The Multiscale Universal Interface is a general-purpose coupling library with a particle-based approach at its core.
- It can be used for both multiphysics and multiscale problems.
- It is suited for creating coupled approaches between methods with different discretisation methods and time-stepping methods.
- It is under active development within STFC and a core part of our coupling activities with communities like CCP-WSI.

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Questions?