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The *Multiscale Universal Interface* Code Coupling Library

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Scene Setting (or, why something like MUI?)

- Coupling the **physics** of a problem can be achieved in **software** terms:
  - Monolithically – everything in the same executable
  - Partitioned – discrete executables exchanging data

- A partitioned approach is often desirable (sometimes unavoidable):
  - Provides a separation of concerns (individual codes remain separate)
  - Offers increased flexibility in HPC terms (load balancing per domain, mixed-architecture solutions for heterogenous systems etc.)

- Partitioned approach requires data exchange:
  - Preferable solution is a generalised approach using a code coupling middleware/library
  - Using high-performance and portable data exchange methods

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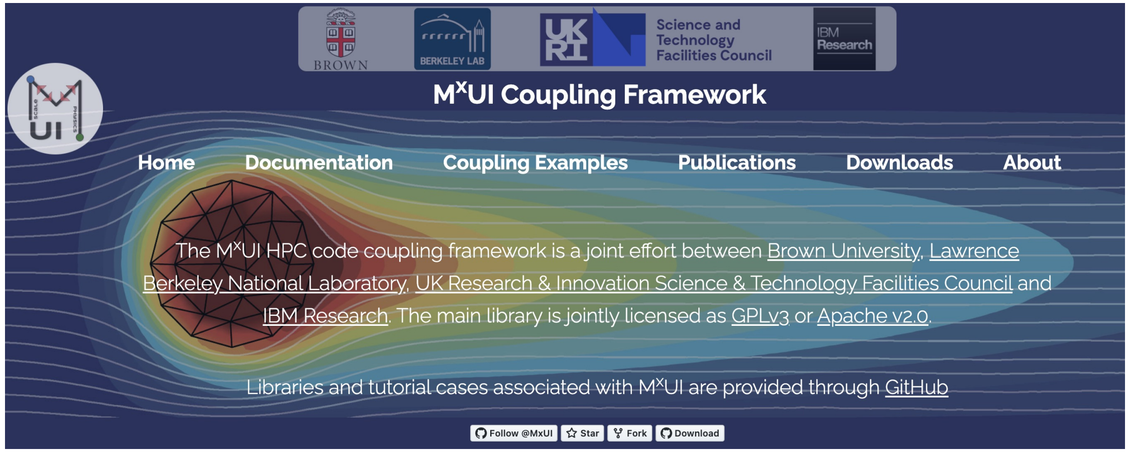
General Code Coupling with MUI

What is MUI?

Tang Y.-H., Kudo, S., Bian, X., Li, Z., & Karniadakis, G. E. **Multiscale Universal Interface: A Concurrent Framework for Coupling Heterogeneous Solvers**, *Journal of Computational Physics*, 2015, 297.15, 13-31. https://doi.org/10.1016/j.jcp.2015.05.004

- The **M**ultiscale **U**niversal **I**nterface code coupling library
- Collaboration between Brown University; Lawrence-Berkeley National Lab, UKRI-STFC at Daresbury Lab and IBM Research
- Written in C++11 (with wrappers for C, Fortran* and Python)
- Open-source, licensed as either **GPLv3** or **Apache 2.0**
- Header-only design (with caveats)
- 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



** Currently being fully implemented*

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Multi-physics/scale Coupling With MUI?

- Provides *tool-kit* to create new couplings between methods:
  - Mesh to particle
  - Mesh to mesh (fixed or moving)
  - Particle to particle
- Also provides ability to couple across both length- and time-scales:
  - **Reasonable** length scales can be tackled due to the point-based nature (interpolation is our friend)
  - **Reasonable** time scales can be tackled using the libraries *frame* based concept (described in more detail later)
- At a point, **direct** multi-scale coupling becomes unfeasible, at which point MUI can still be used purely for tagged data transport to enable complex abstractions

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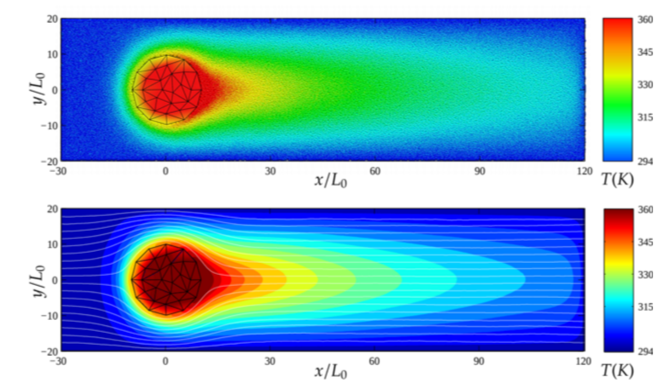
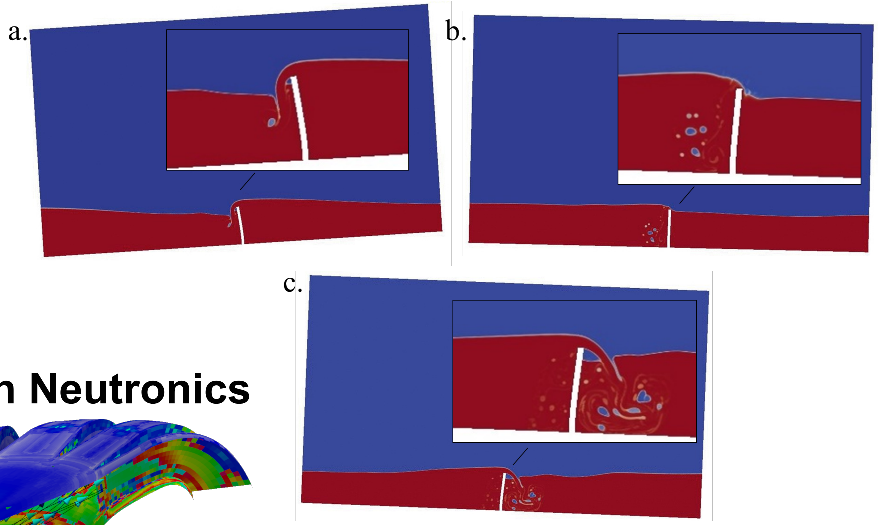
MUI Coupling Examples

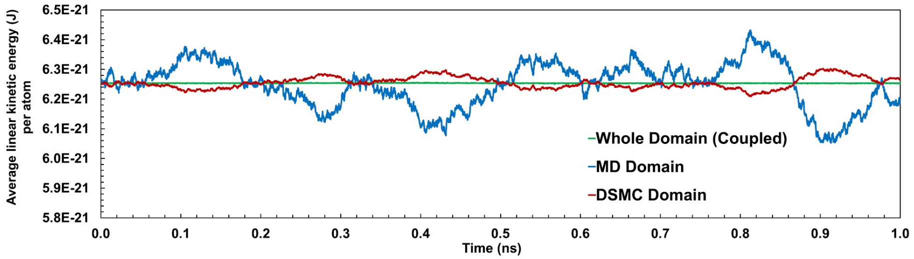
eDPD & Finite Element

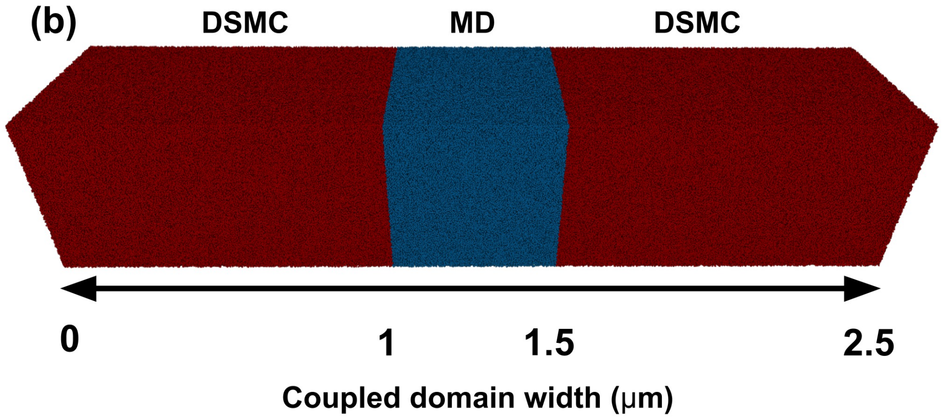


CFD & Structural Mechanics (FSI)

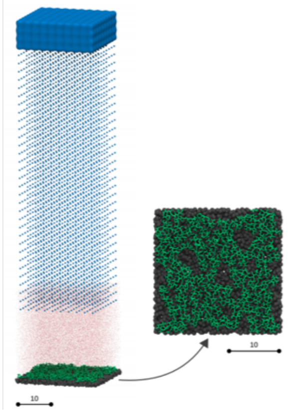


Molecular Dynamics (MD) & Direct Simulation Monte Carlo (DSMC)

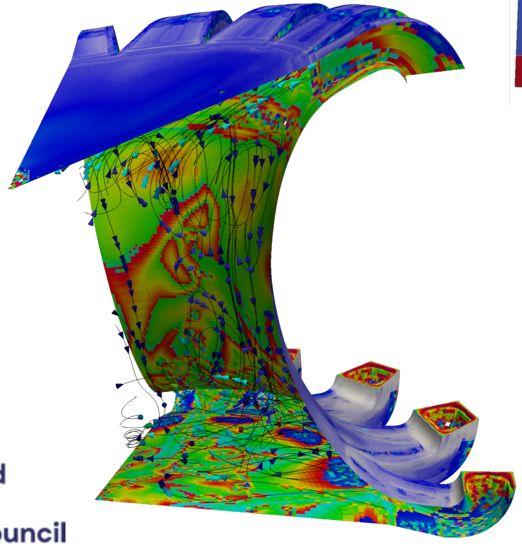




Particle CFD (SPH) & DPD



CFD with Neutronics



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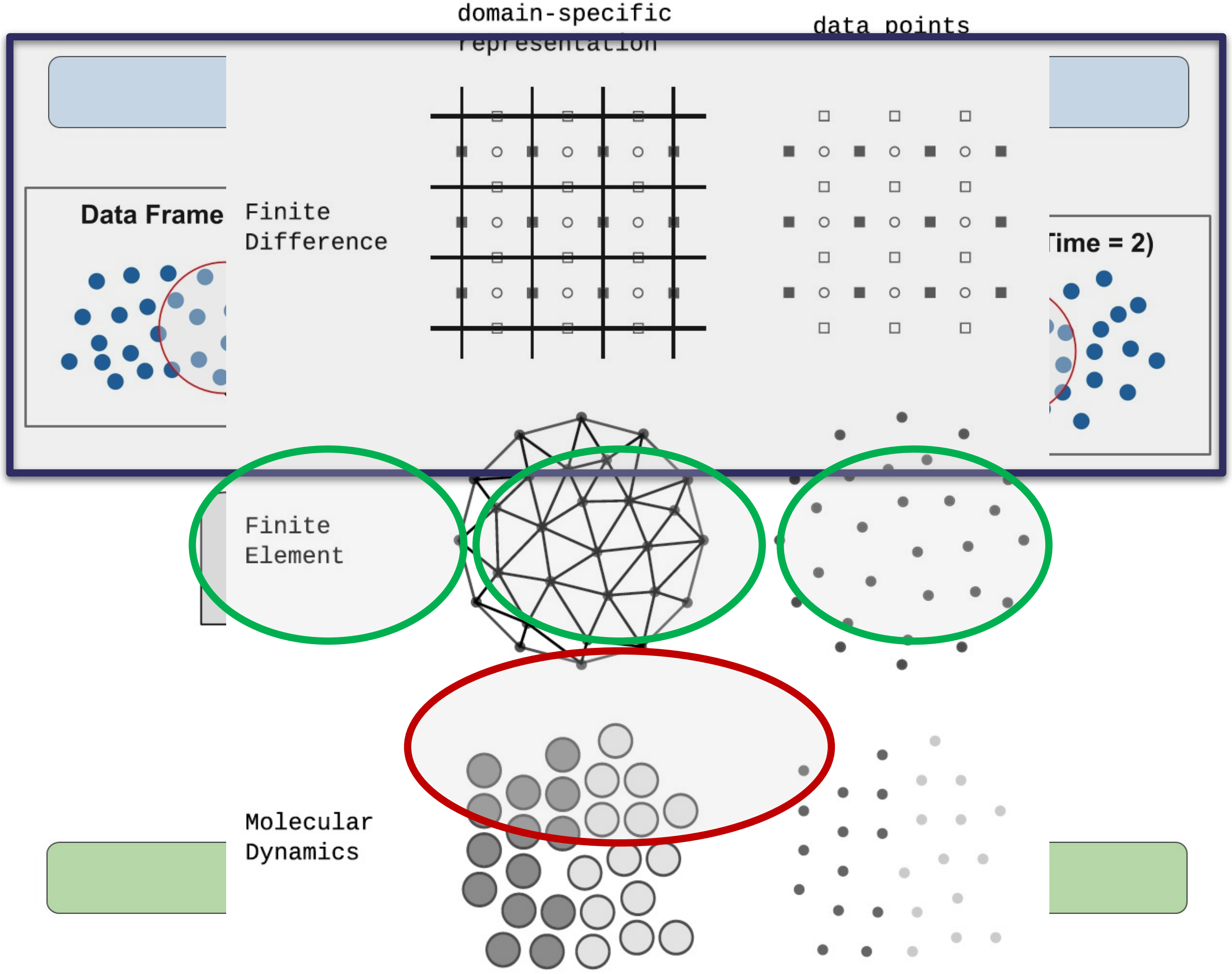
Overview of MUI

The Library

- Couples using a set of discrete data samples through an **interface**:
  1. Convert domain-specific representations (mesh) to a general form (cloud of points with associated data).
  2. Solver **imparts** data (at a point in space) to MUI interface with an **associated time-stamp or frame.**
  3. Other solver requests data at specific location and time from MUI interface using **spatial** and **temporal** sampler.
- Uses MPI Multi-program, Multi-data (MPMD)
- Wrappers for Fortran (partial), C (complete) & Python (ongoing)



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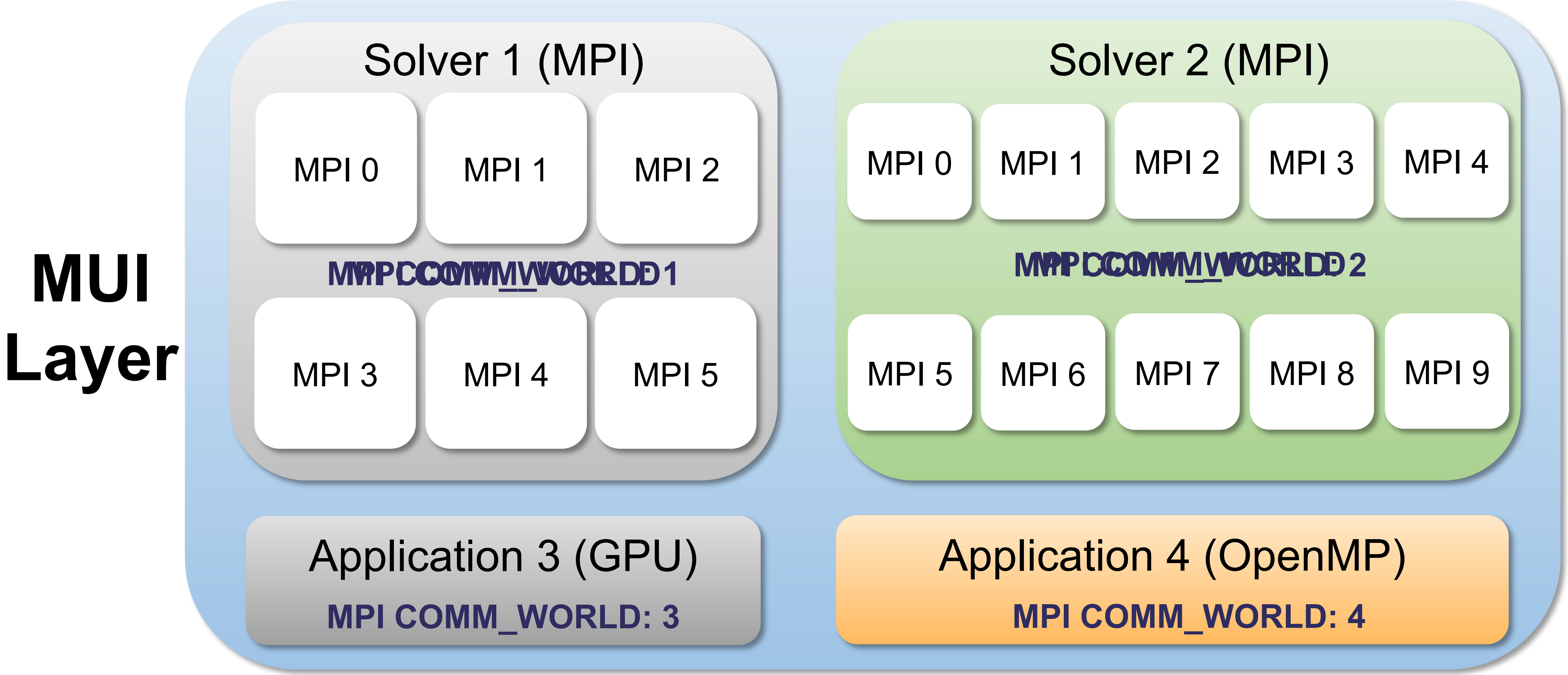
Why MUI?

- *lightweight* coupling library design.
- No other library requirements other than MPI (*one spatial interpolation method requires Eigen).*
- Works with almost any compiler/runtime environment combination as long as a C++11 compliant and MPMD compatible MPI implementation available.
- Introduces minimal extra computational overhead (*this is problem specific, MUI isn't magical and can't hide MPI communications!*)
- Designed from the ground-up for use on HPC systems

- **In ideal situations you can integrate MUI into a code in around 10 lines of code.**

MUI in a Heterogeneous HPC Environment



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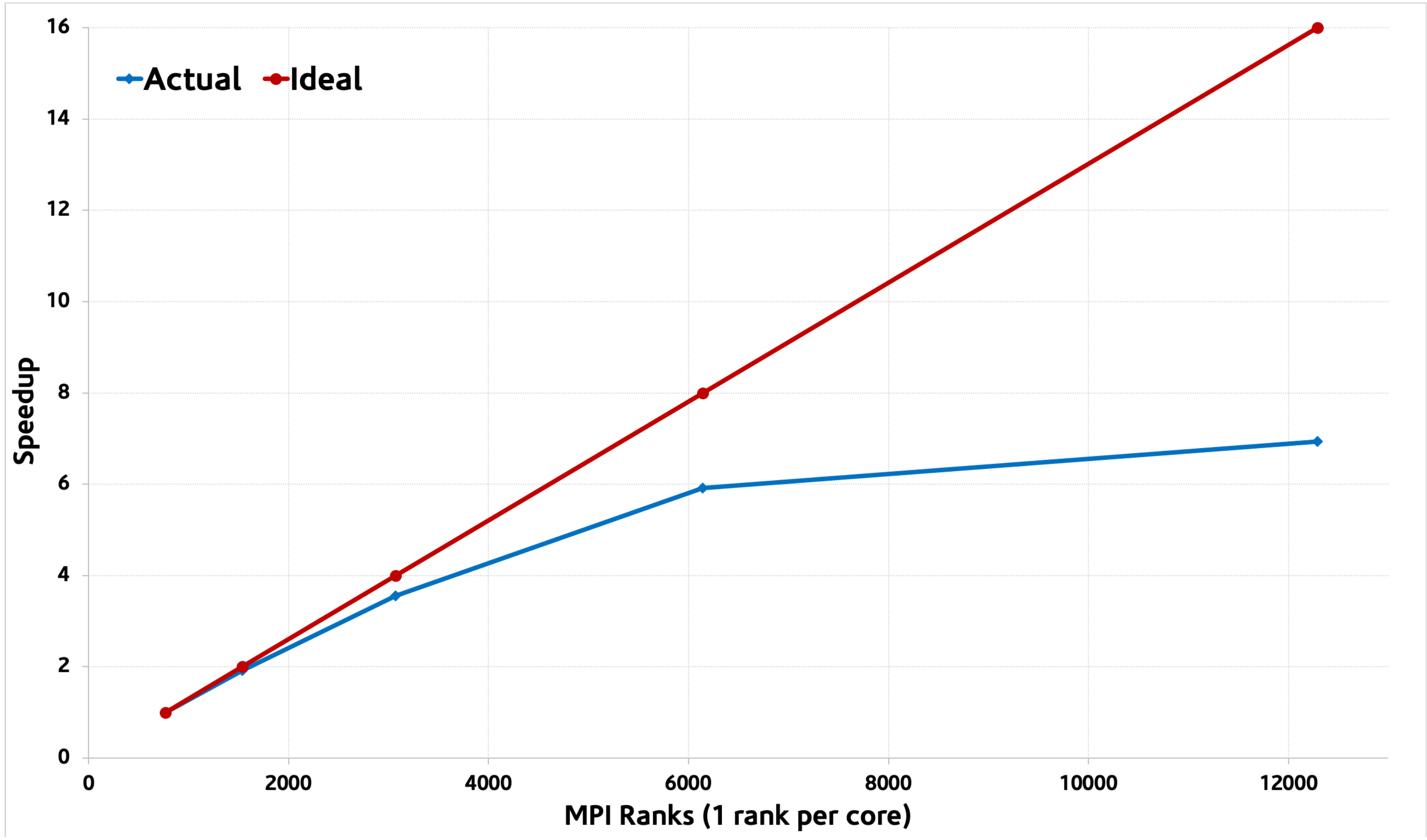
Benchmarks

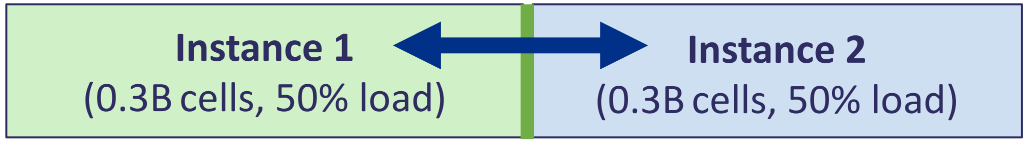
Artificial Benchmarking

- MUI Testing Framework (https://github.com/MxUI/MUI-Testing)
- General purpose testing and benchmarking tool for MUI
- Couples to itself
- Allows for a wide-range of complex coupling scenarios to be simulated
- Produces a 3D Cartesian grid structure which is then sent and received by one (or more) MUI interfaces with various controllable options.
- Includes simulation of computational overhead:
    - Local MPI data transfer based on 3D Cartesian decomposition
    - Artificial barrier to allow for inclusion of delay to simulate processing time of host application

Benchmark Performance



- Emulates a typical CFD workflow
- 0.3B points transferred per instance (volumetric)
- 32 - 512 nodes
- Equal load-balancing
- **Reading values directly from MUI interface**
- **Using Gaussian spatial interpolation**



S. M. Longshaw, R Pillai, L Gibelli, D. R. Emerson, D. A. Lockerby (2019) ***Multiscale Simulation of Evaporation Using the Multiscale Universal Interface.*** *The 31st International Conference on Parallel Computational Fluid Dynamics: ParCFD'2019, 2019 (Antalya, Turkey)*

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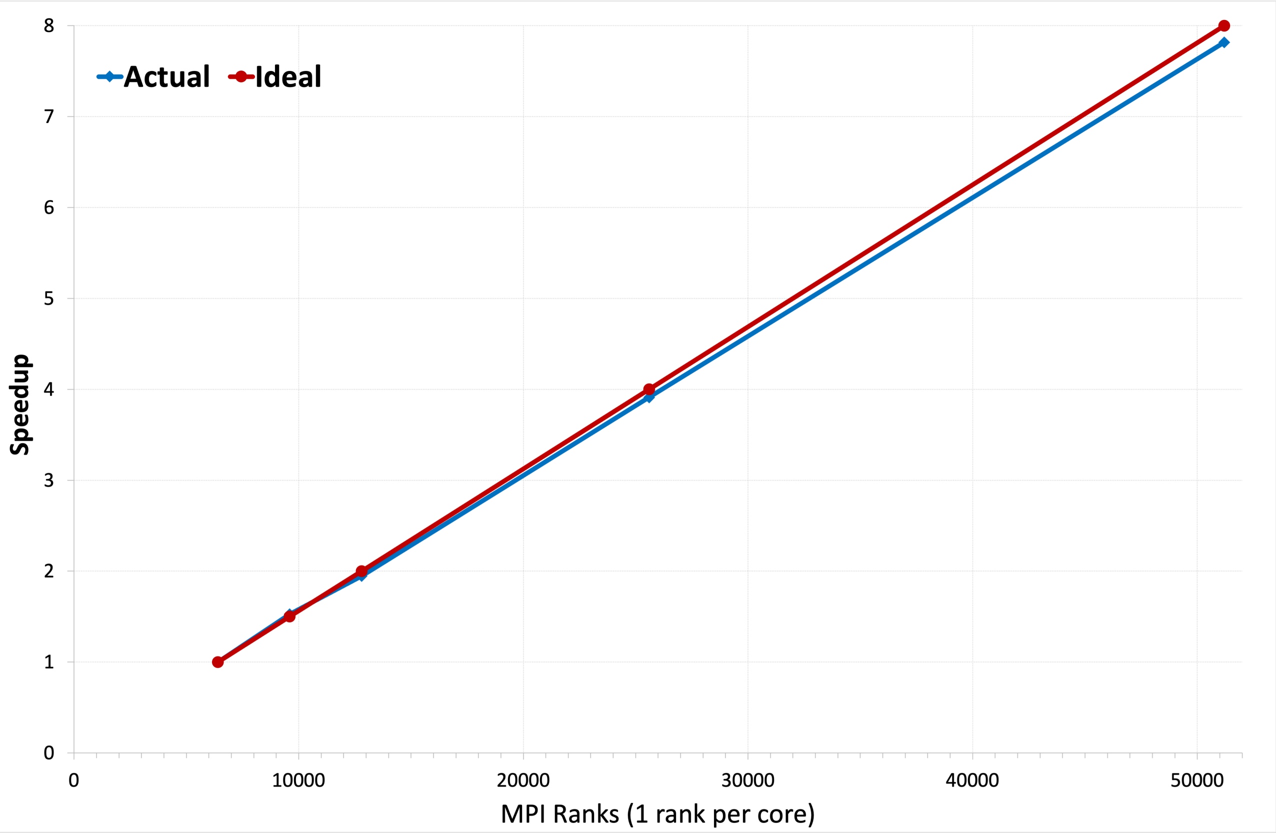
ARCHER2 Preliminary Results

- HPE Cray EX (peak ~28 Pflop/s)
- 5860 nodes, giving total of 750,080 AMD EPYC 7742 cores



- Same artificial testing tool and assumed CFD workflow
- ~0.5B points transferred per instance (volumetric)
- 50 - 400 nodes
- Equal load-balancing
- **Reading values directly**

- ARCHER2 displaying odd behaviour around MPI fabric – results currently unpredictable

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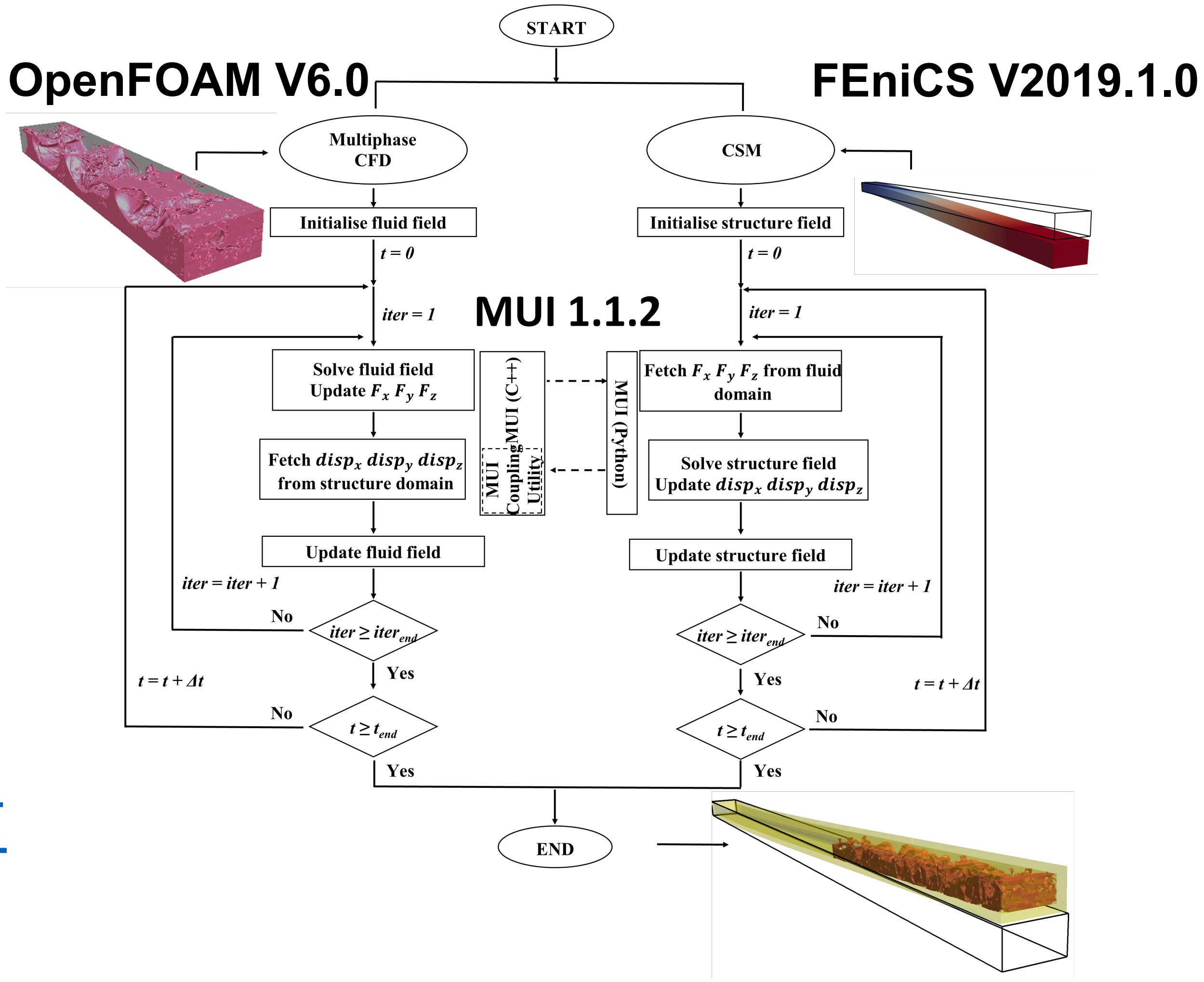
Real-world Example: Fluid-Structure Interaction (FSI)

Motivation

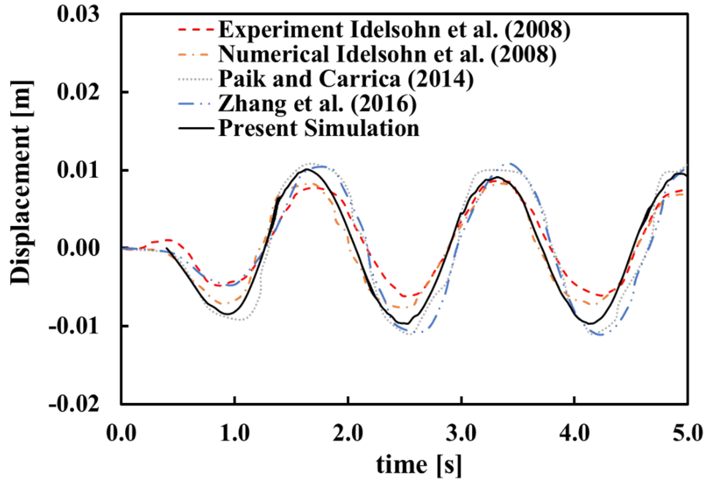
- Important physical interaction for many engineering problems:
  - Fundamental to many Wave Structure Interaction problems
  - Particularly important (and challenging) when the fluid has a **free surface**
- Approaches (and associated problems) for FSI well documented
- Open-source solutions for HPC FSI not as clear!

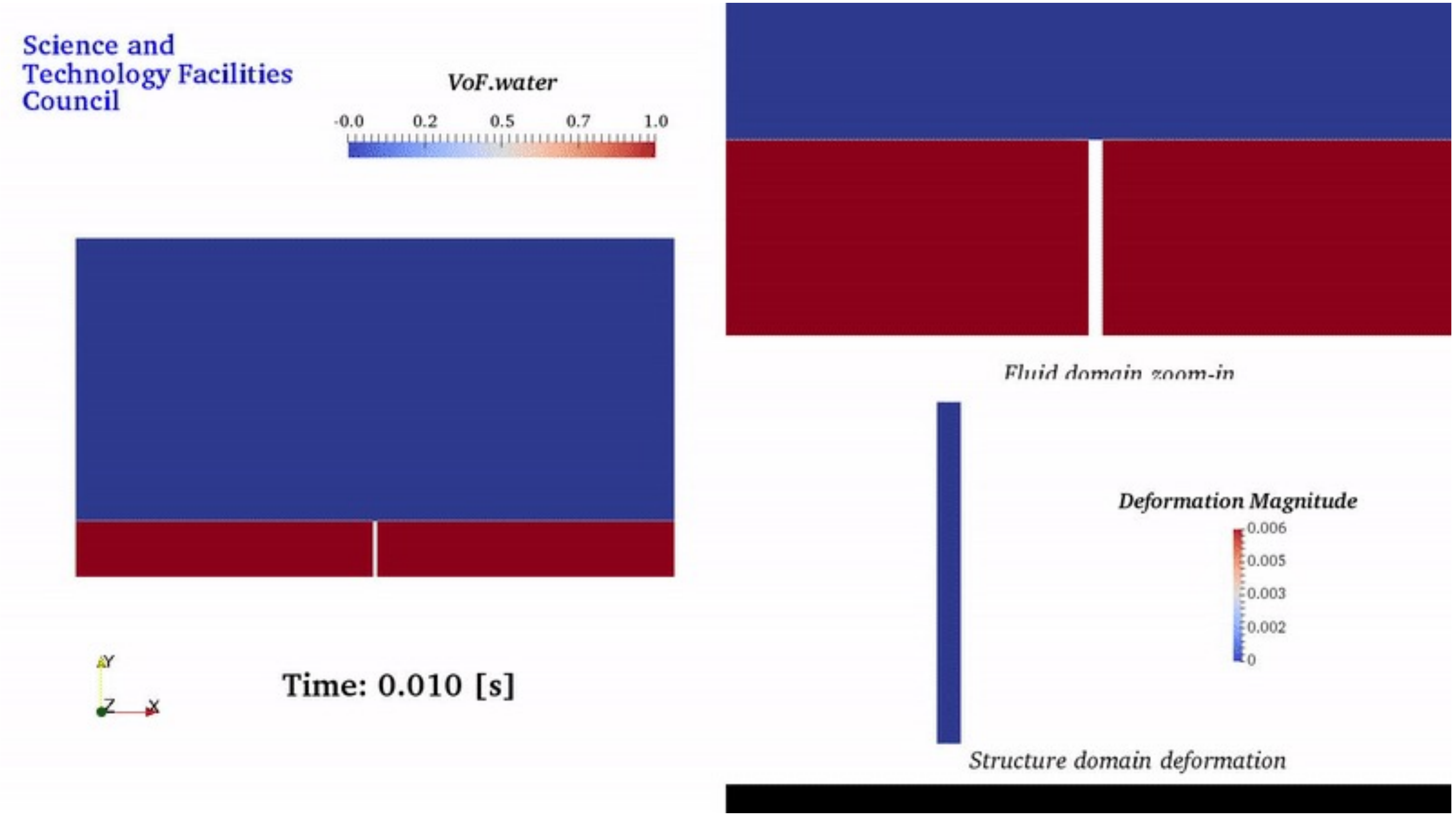
Coupled Design

- Couples:
  - Multiphase Volume of Fluid CFD
  - Elastic structural Finite Element solver
- Partitioned approach
- Quasi-Newton coupling strategy
- Radial Basis Function **spatial** sampling provided by MUI
- https://github.com/parMupSiF/parMupSiF



Results (Roll Tank)





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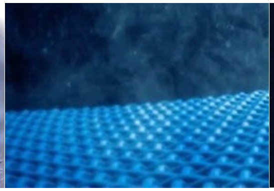
Real-world Example: Modelling Evaporation

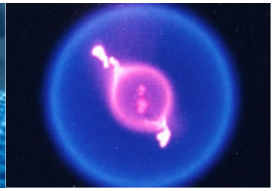
Motivation

Cometary Atmospheres

Laser induced vaporisation

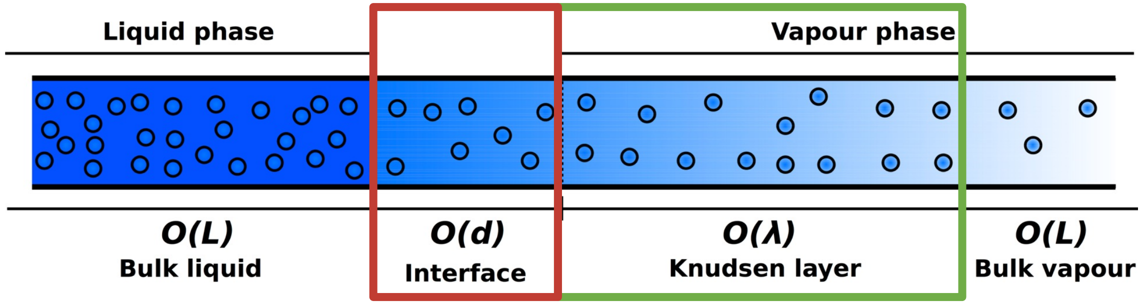


Capillary cooling



Fuel droplet dynamics

- Physical processes like evaporation often simulated using CFD:
  - Micro and mesoscopic effects are introduced using parameters in the macroscopic model
  - The reality is this sort of process is truly multi-scale…
  - There is a non-equilibrium gaseous layer on the vapour side
  - And a liquid-vapour interface between the phases



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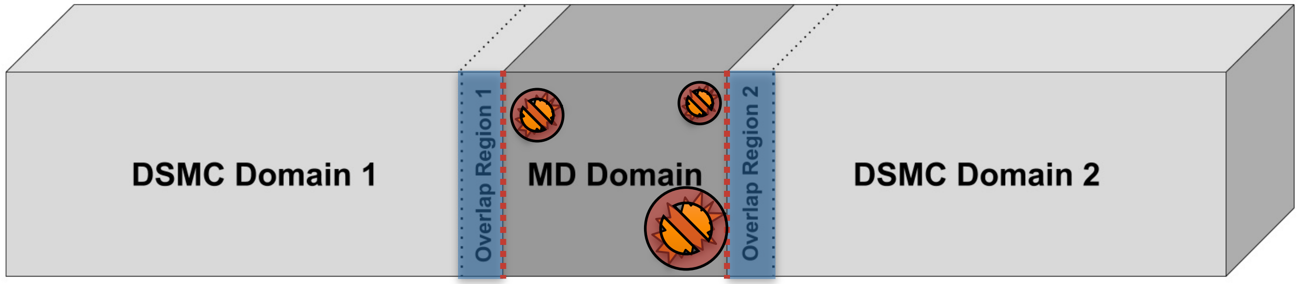
Coupled Design

- Provides a 1:1 atom/molecule to DSMC particle mapping:
  - For cases where system accuracy is paramount and relative domain scales are similar (i.e. fundamental studies of evaporation)
  - Not applicable when coarse graining needed in DSMC (more than 1 atom/molecule per particle)
  - Direct transference of mass and momentum between domains via MUI (**no interpolation**)

- Coupling region at the edge of the DSMC domains:
  - DSMC particles are mirrored as a special type of atom/molecule in the MD domain
  - Deletion/insertion boundaries between the domains
  - MD insertion takes special care to preserve physical location while avoiding potentially explosive effects from inserting too close based on the forcefield



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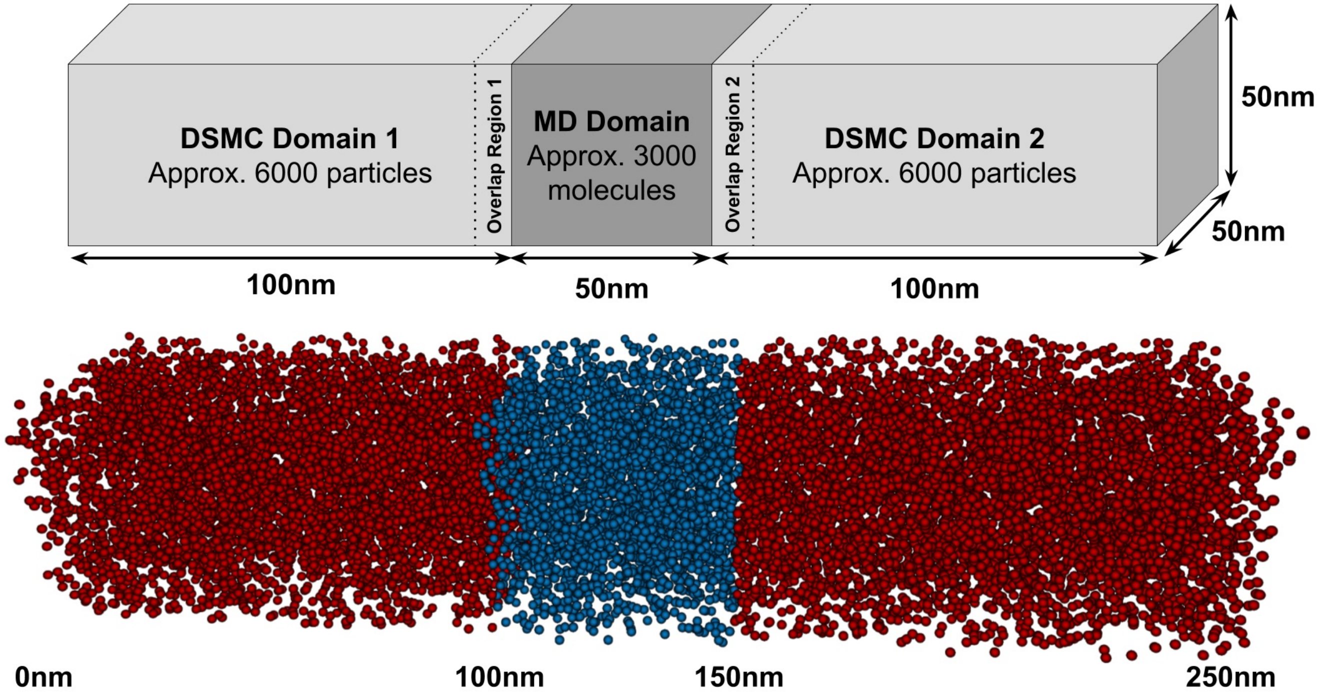
Results: Case Setup

- Results for a canonical NVT (constant number of atoms *N*, volume V and temperature T):
  - Argon gas
  - 3 domains: DSMC – MD – DSMC
  - 250nm x 50nm x 50nm total size
  - T = 300K
  - No thermostat or control applied



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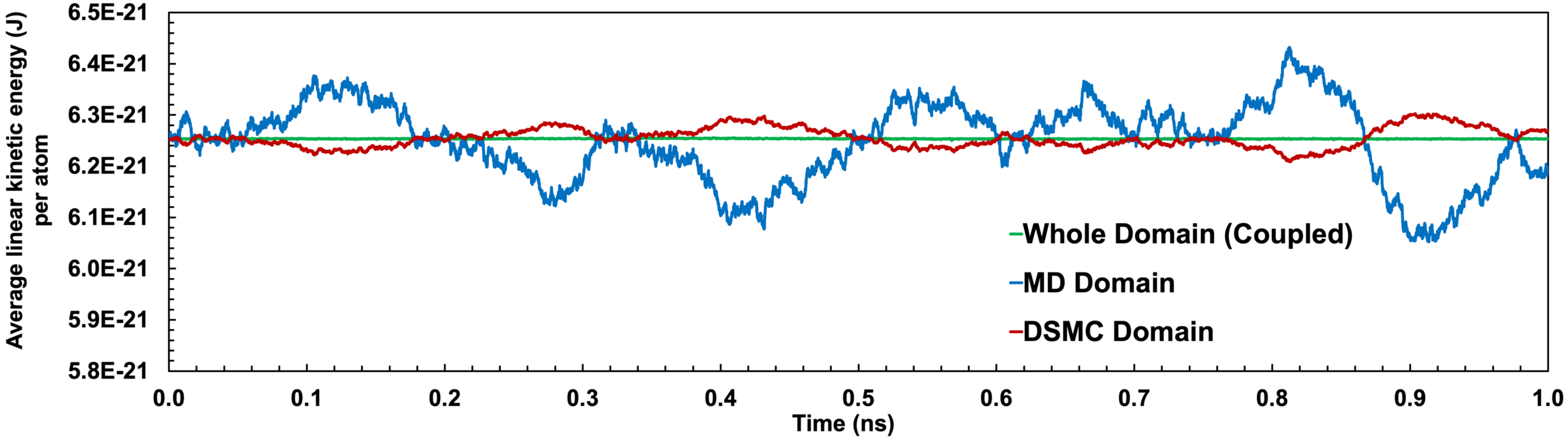
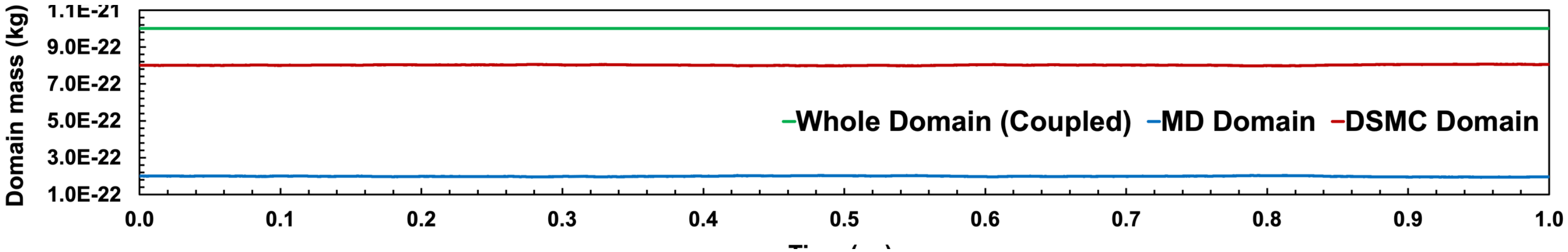
Results: Physics and Performance

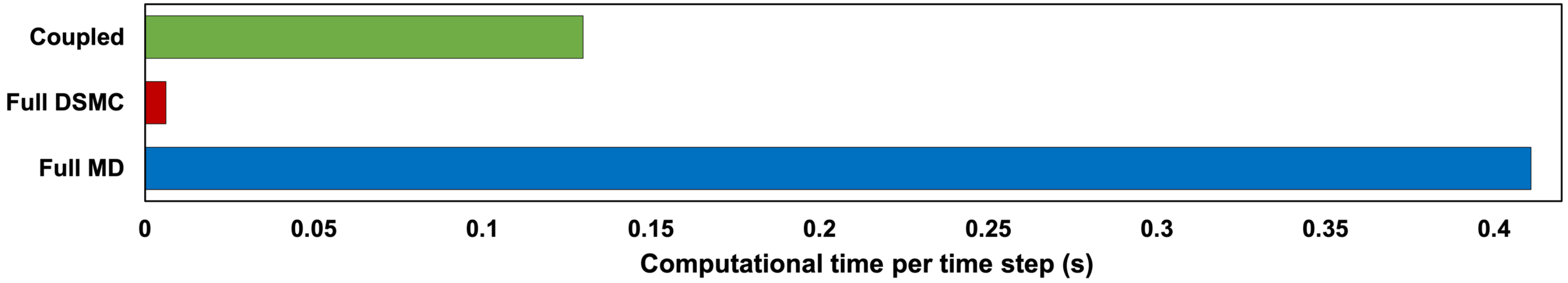
Linear KE (J)



Mass (kg)



Computational time per time step (s) – 8 MPI ranks (4/4)



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Conclusions

Conclusions

- MUI is lightweight and open-source.
- It is a header-only C++ library with wrappers for C, Fortran and Python.
- It can be used to couple two or more solvers together in a peer-to-peer way:
  - Either purely as a data transport layer
  - Or including spatial/temporal interpolation of the data
- Designed for use in HPC environments
- This ExCALIBUR project now looks to optimise this:
  - Analyse and improve MPI communication patterns – need to better understand scalability
  - Reduce memory overhead of frame storage (each currently needs its own bin structure)
  - Explore offload of spatial interpolation to accelerators within heterogeneous environments
  - Explore use of Spack to package and improve DevOps (CI on GitHub!)

https://github.com/MxUI

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