A Unified SPH Framework for Flexible Fluid-Structure Interaction with DualSPHysics

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Overview

- Background & Motivation
- Methods & Implementation
- Validation & Results
- Summary & Conclusions
- Current Work: Accelerating SPH

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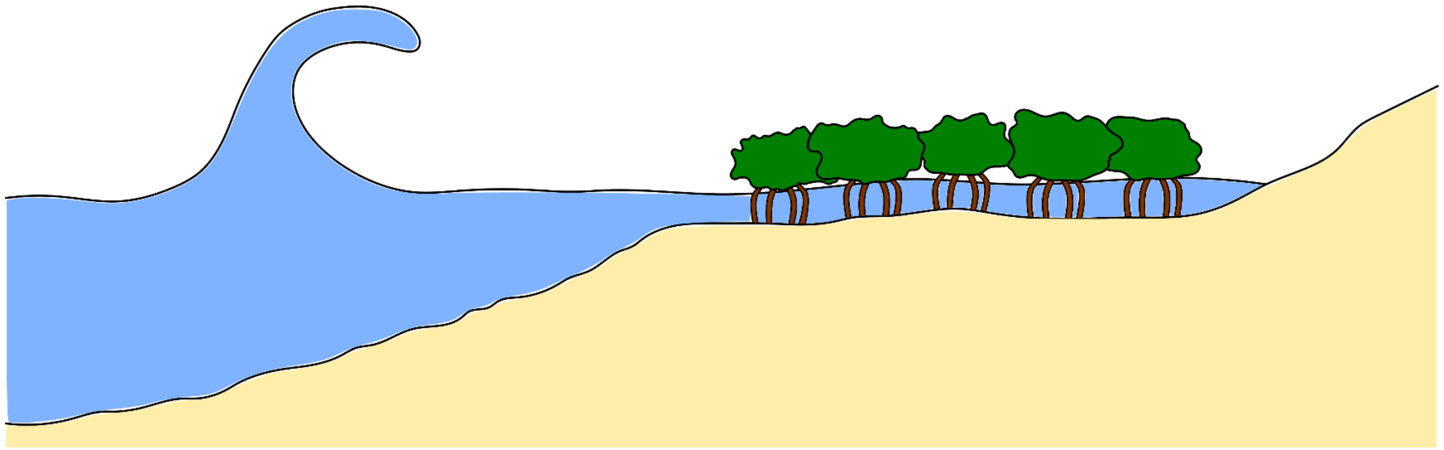
Flexible Fluid-Structure Interaction

- Many real-world engineering and natural phenomena are governed by flexible fluid-structure interactions (FSI)
  - This includes vegetation, biological flows, coastal/marine infrastructure, and many more…

- However, the resulting physics can be extremely difficult to model and analyse
  - Multiphysics models
  - Interfacial coupling
  - Monolithic vs partitioned
  - Deforming domains
  - Different sound speeds
  - Dynamical instabilities
  - Resonance/lock-in



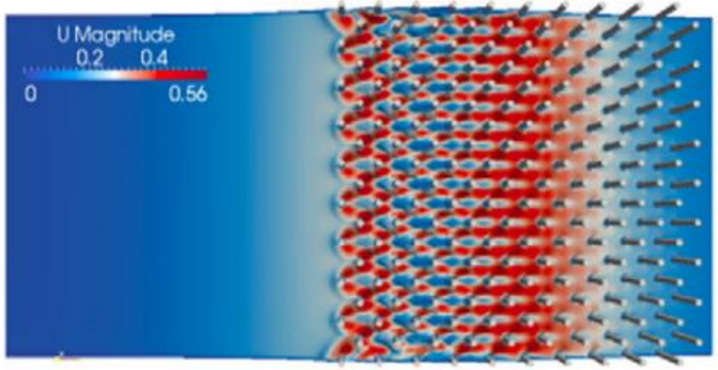
Wave-vegetation interactions can be exploited for coastal protection.

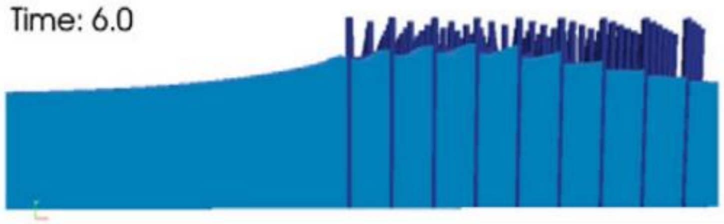
Modelling Fluid-Structure Interactions

- Often some form of reduced-order modelling with certain simplifying assumptions is adopted
  - For example, neglecting structural deformation or using a porous layer for dense arrays of structures

- However, in some cases this can lead to incorrect physics (e.g. under-predicting forces or over-predicting wave attenuation)

- Higher-fidelity models that capture the physics we need would be useful





Flow velocity and surface elevation of wave through array of rigid emergent cylinders (Maza et al. 2015).

Overview

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Fluid Modelling with SPH

- The governing equations for (Lagrangian) weakly-compressible SPH are:

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\nabla\cdot\mathbf{u}$$ **Conservation of mass**

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = \frac{1}{\rho}\nabla\cdot\boldsymbol{\sigma} + \mathbf{g}$$ **Conservation of momentum**

- The Cauchy stress is split into an isotropic and deviatoric part:

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{g}$$

- The mass and momentum equations are coupled via an equation of state

- Finally, the SPH discretisation provides operators for the derivatives

Structural Modelling with SPH

- We opted to use SPH to model the structure as well
  - Easier integration within DualSPHysics (e.g. GPU implementation)
  - Monolithic/unified schemes provide enhanced stability over partitioned approaches
  - Better suited to modelling certain additional physics (e.g. fracture)

- Recall the momentum equation for a continuum:

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = \frac{1}{\rho}\nabla \cdot \boldsymbol{\sigma} + \mathbf{g}$$

- One option is split stress tensor into an isotropic and deviatoric part and solve just like we do with fluids (with different state equation and constitutive model)
  - This approach exhibits three main problems: tensile instability, linear inconsistency, rank deficiency/hourglassing

Overcoming Tensile Instability

- Tensile instability arises due to shape of smoothing kernel and leads to unphysical particle clumping that can ruin the simulation

- Solution (for structures) is to adopt a Total Lagrangian approach where the momentum equation is reformulated with respect to the initial configuration

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = \frac{1}{\rho}\nabla \cdot \boldsymbol{\sigma} + \mathbf{g} \quad \Rightarrow \quad \frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = \frac{1}{\rho_0}\nabla_0 \cdot \mathbf{P} + \mathbf{g}$$

- Cauchy stress tensor is replaced with nominal (first Piola-Kirchoff) stress tensor and standard SPH discretisation is applied

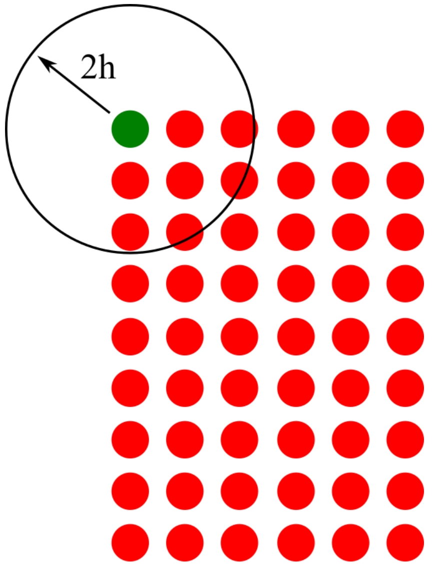
- Everything is measured with respect to initial configuration
  - No need to recompute kernel derivatives, neighbouring particles, or continuity equation

Overcoming Linear Inconsistency

- Boundaries pose a challenge for SPH due to incomplete support
- For fluids, typically extra layers of particles are added to the boundaries to fill in the support
- Can't do this for structures without changing the geometry
- Solution is to introduce a kernel correction that ensures the gradient of a linear field can be recovered:

$$\tilde{\nabla}_a W_{ab} = \mathbf{L}_a^{-1} \nabla_a W_{ab}$$

$$\mathbf{L}_a = \sum_b \frac{m_b}{\rho_b} \mathbf{x}_{ba} \otimes \nabla_a W_{ab}$$



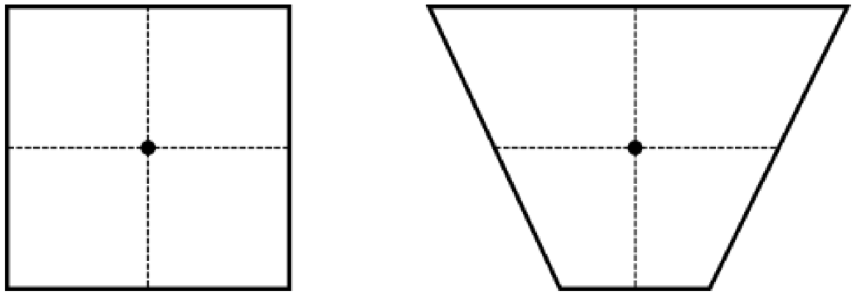
Particles near edge do not have full support within kernel radius.

Overcoming Rank Deficiency/Hourglassing

- Collocated nature of SPH means that different particle arrangements within the kernel support can give rise to same deformation gradient tensor

- This rank deficiency leads to zero-energy modes which are not suppressed and eventually become unstable (similar to reduced-order elements in FEM)

- Various solutions:
  - Stress integration points, mixed-base reformulation, corrective force



Reduced order elements cannot capture certain deformation modes.

- Corrective force penalises any deformation which is not exactly described by the deformation gradient tensor
  - Efficient and easy to implement but modifies stiffness and introduces a tuning parameter

Discretisation & Material Model

- Finally, the discrete form of the momentum equation of the structure is:

$$\frac{\mathrm{D}\mathbf{u}_a}{\mathrm{D}t} = \sum_b m_{0b} \left(\frac{\mathbf{P}_a \mathbf{L}_{0a}^{-1}}{\rho_{0a}^2} + \frac{\mathbf{P}_b \mathbf{L}_{0b}^{-1}}{\rho_{0b}^2} \right) \cdot \nabla_{0a} W_{0ab} + \frac{\mathbf{f}_a^{HG}}{m_{0a}} + \mathbf{g}$$

- The first Piola-Kirchhoff stress is related to the second Piola-Kirchhoff stress:

$$\mathbf{P} = \mathbf{F}\mathbf{S}$$

- The second Piola-Kirchhoff stress is related to the Green-Lagrange strain via the Saint Venant-Kirchhoff constitutive model:

$$\mathbf{S} = \lambda \mathrm{tr}(\mathbf{E})\mathbf{I} + 2\mu\mathbf{E}$$

- Where the Green-Lagrange strain and deformation gradient are given by:

$$\mathbf{E} = \frac{1}{2}\left(\mathbf{F}^T\mathbf{F} - \mathbf{I}\right) \qquad \text{and} \qquad \mathbf{F} = \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}\mathbf{x}_0}$$

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Fluid-Structure Coupling

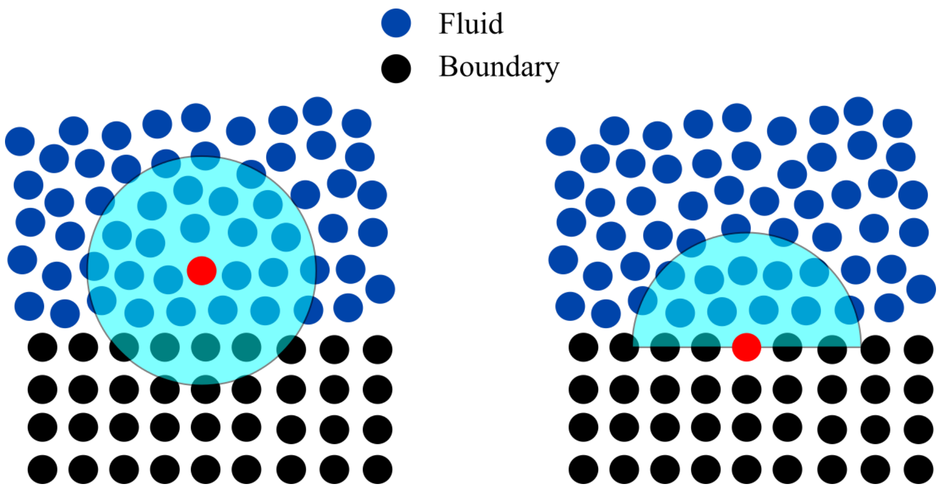
- The dynamic boundary condition is the basic pre-existing boundary condition within DualSPHysics

- Density of boundary particles is evolved via continuity equation as normal

- Momentum equation is not computed for boundary particles

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{g}$$

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\nabla\cdot\mathbf{u}$$

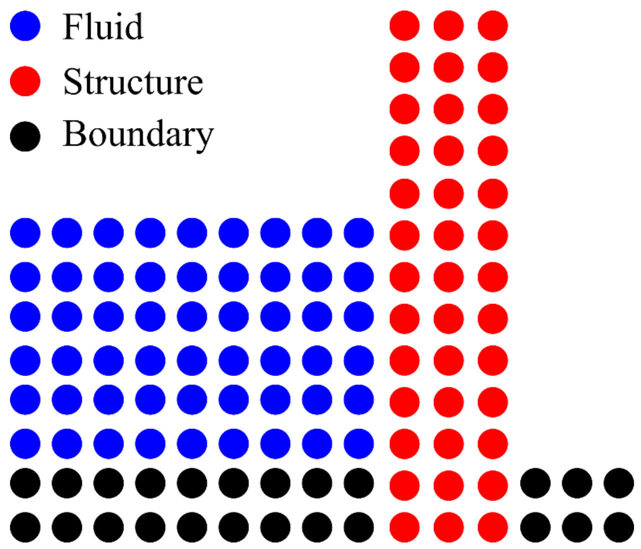


$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\nabla\cdot\mathbf{u}$$

Kernel stencil for fluid (left) and boundary (right) particle.

Fluid-Structure Coupling

- The fluid-structure coupling is handled via the dynamic boundary condition
- Fluid sees structural particles as normal boundary particles (with a velocity)
- Structure sees fluid particles in the same way a boundary particle does
- Momentum equation is integrated for structure particles but not for boundary particles
- No need to know any geometric information about interface (e.g. surface normals)

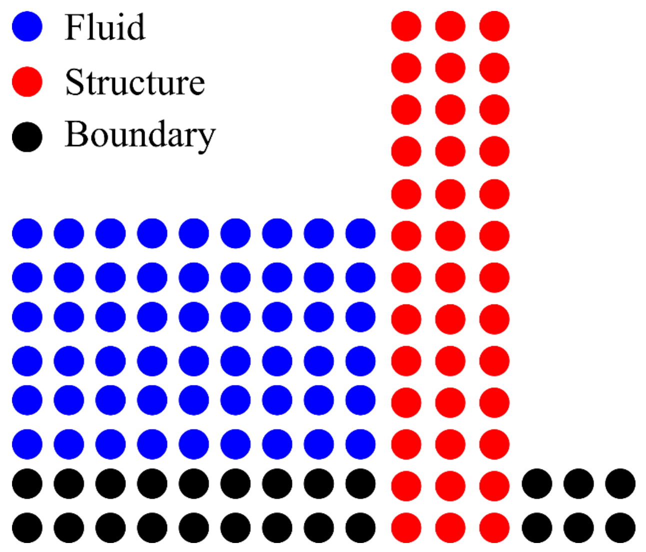


Particle types used for fluid-structure coupling.

Fluid-Structure Coupling

- Total force on a particle is sum of contributions from neighbouring fluid, structure and boundary particles

- Note that the last two terms in the structure equation use the Total Lagrangian form



Particle types used for fluid-structure coupling.

Fluid Particle

$$\frac{D\mathbf{u}_a}{Dt} = -\sum_b m_b\left(\frac{p_a}{\rho_a^2}+\frac{p_b}{\rho_b^2}\right)\nabla_a W_{ab} - \sum_b m_b\left(\frac{p_a}{\rho_a^2}+\frac{p_b}{\rho_b^2}\right)\nabla_a W_{ab} - \sum_b m_b\left(\frac{p_a}{\rho_a^2}+\frac{p_b}{\rho_b^2}\right)\nabla_a W_{ab}$$

Structure Particle

$$\frac{D\mathbf{u}_a}{Dt} = -\sum_b m_b\left(\frac{p_a}{\rho_a^2}+\frac{p_b}{\rho_b^2}\right)\nabla_a W_{ab} + \sum_{b0} m_{0b}\left(\frac{\mathbf{P}_a}{\rho_{0a}^2}+\frac{\mathbf{P}_b}{\rho_{0b}^2}\right)\cdot\tilde{\nabla}_{0a} W_{0ab} + \sum_{b0} m_{0b}\left(\frac{\mathbf{P}_a}{\rho_{0a}^2}+\frac{\mathbf{P}_b}{\rho_{0b}^2}\right)\cdot\tilde{\nabla}_{0a} W_{0ab}$$

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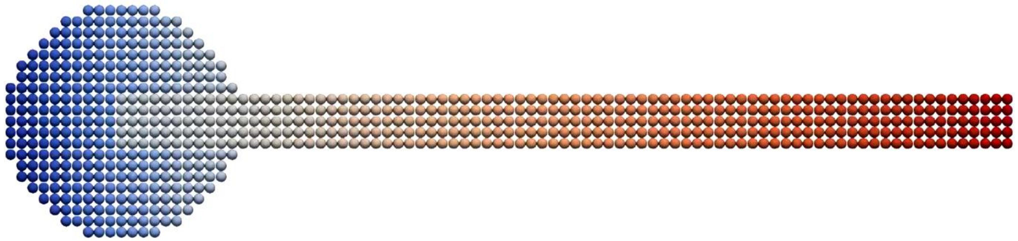
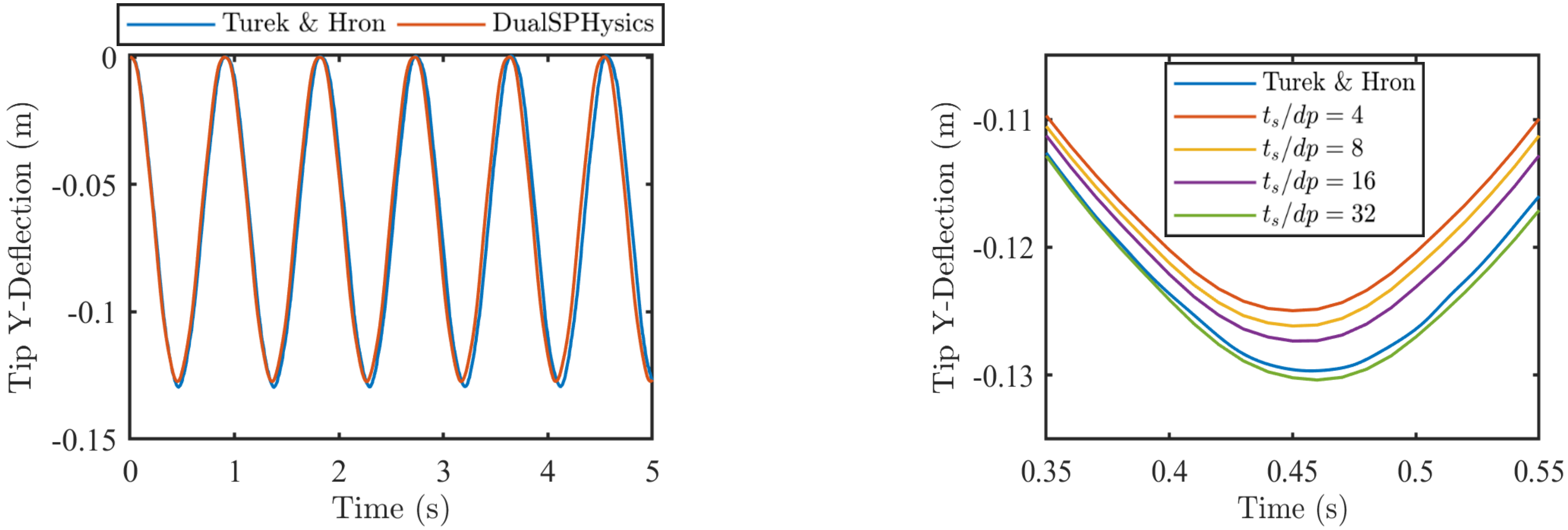
Structural Model Validation

- Tip deflections agree very well with benchmark data (FEM)
- Converges towards benchmark solution with increasing resolution



Animation of structural model validation. Particles coloured by particle ID.

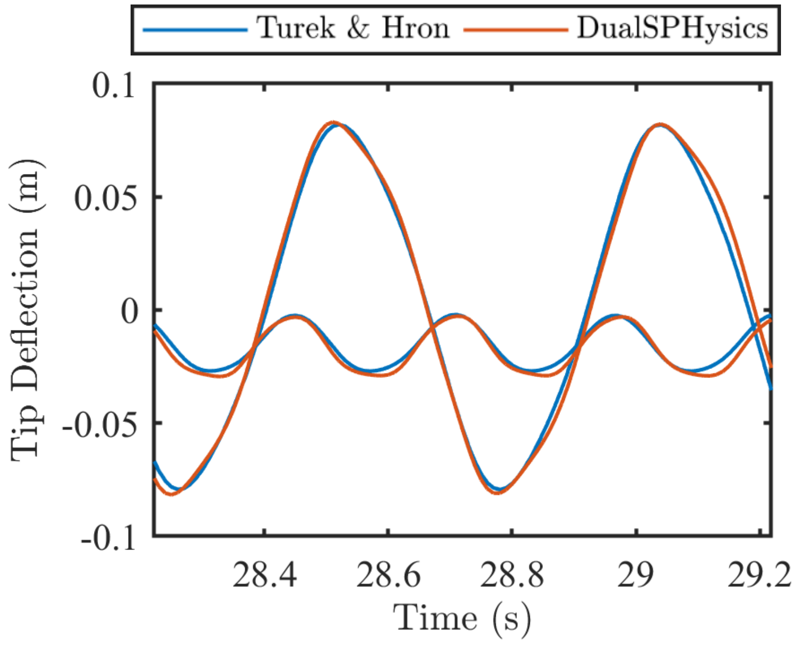


Tip deflection history compared against benchmark for t/dp = 16 (left) and different particle resolutions (right).

FSI Validation – Flapping Beam

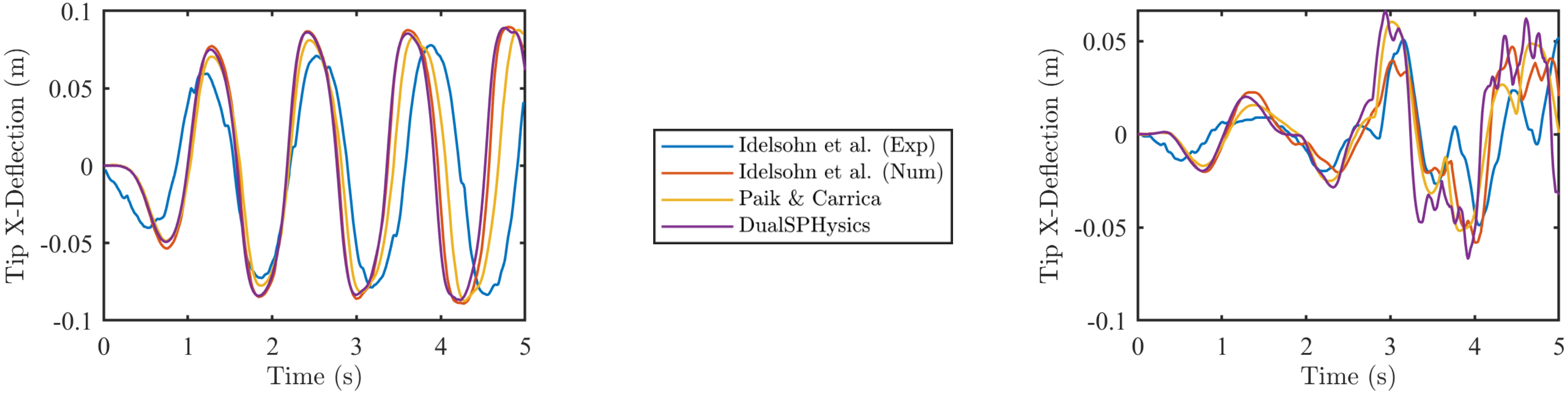
- Rigid cylinder with attached flexible beam at Re = 100

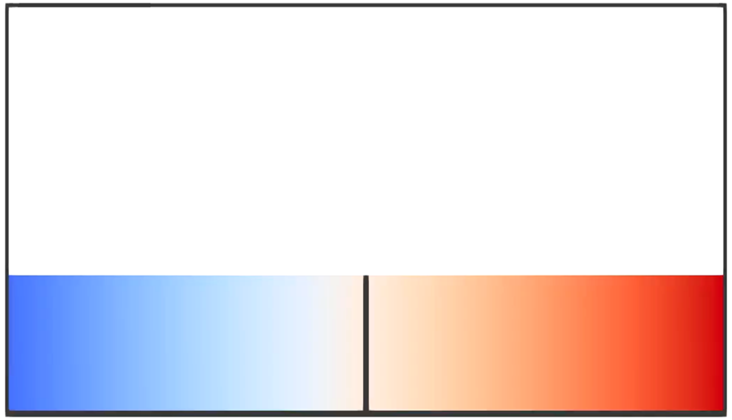
- Benchmark solution is calculated via a fully implicit monolithic FEM-ALE solver

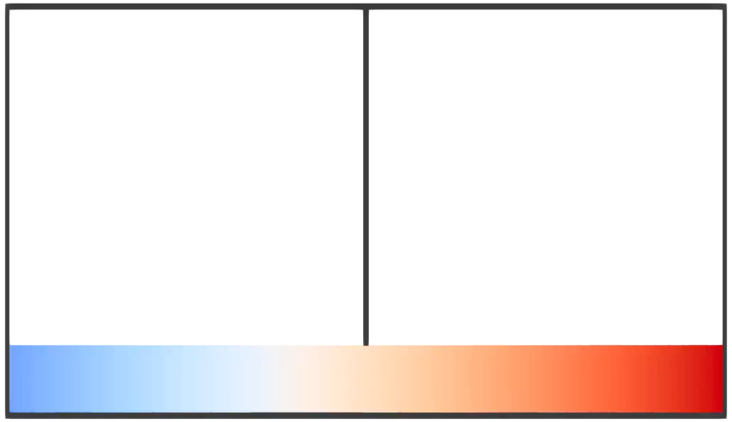


Animation and tip deflection for flapping beam case. Particles coloured by velocity magnitude.

FSI Validation – Rolling Tank





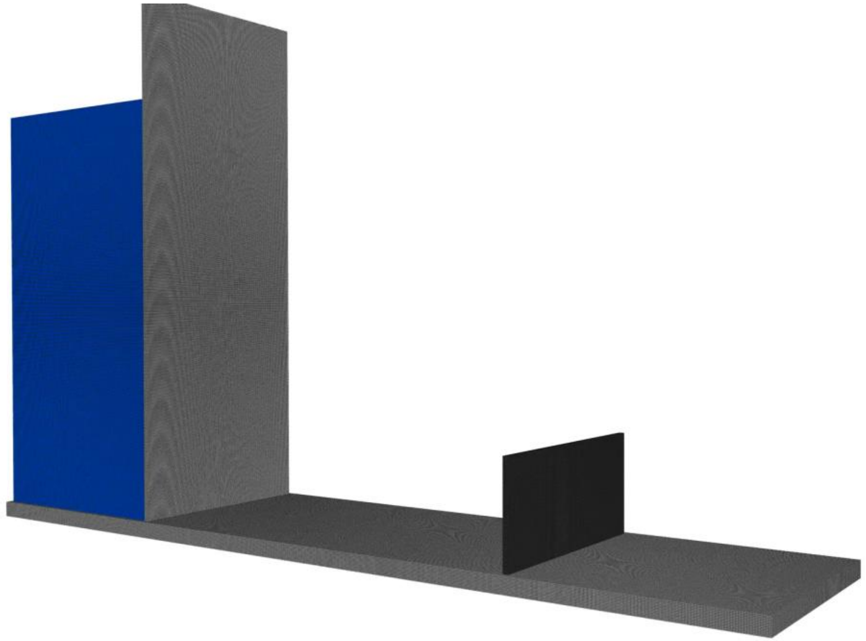


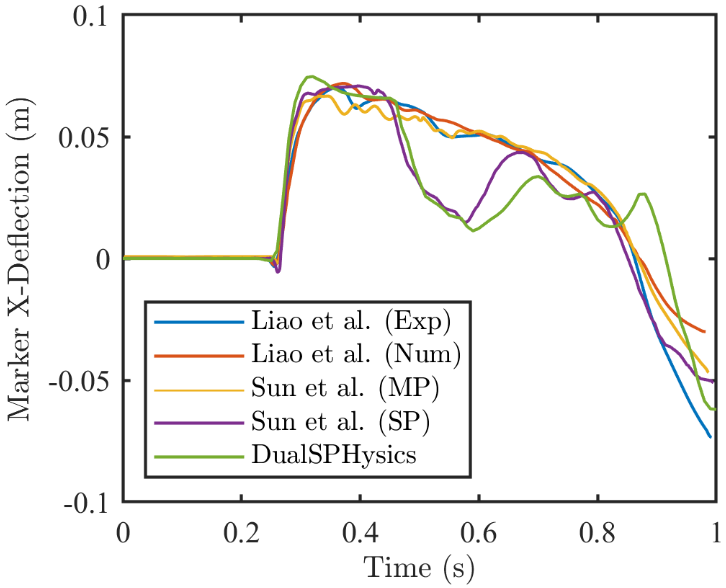
Animation and tip deflection for rolling tank case. Particles coloured by particle ID.

FSI Validation – 3D Dam Break

- Comparison with 2D results in literature shows reasonable agreement

- However, the single-phase (SP) vs multiphase (MP) comparison shows that it is important to correctly model the air entrainment





Animation and tip deflection for the dam break case. Particles coloured by velocity magnitude.

Overview

Summary & Conclusions

- The aim of this work was to develop a fluid-structure interaction model for violent free-surface flows and flexible structures

- Model is based on a unified SPH framework (fluid and structure solved via SPH)
  - Deficiencies addressed via Total Lagrangian approach with kernel correction and hourglass suppression
  - Coupling is handled via existing boundary condition (dynamic boundary condition)

- Validation against popular benchmark cases shows very good agreement for both the structure on its own and the fully-coupled FSI model

- Model is included in latest release of DualSPHysics (v5.2)
  - Please get in touch if you have any questions/issues using it – I'm always happy to help!

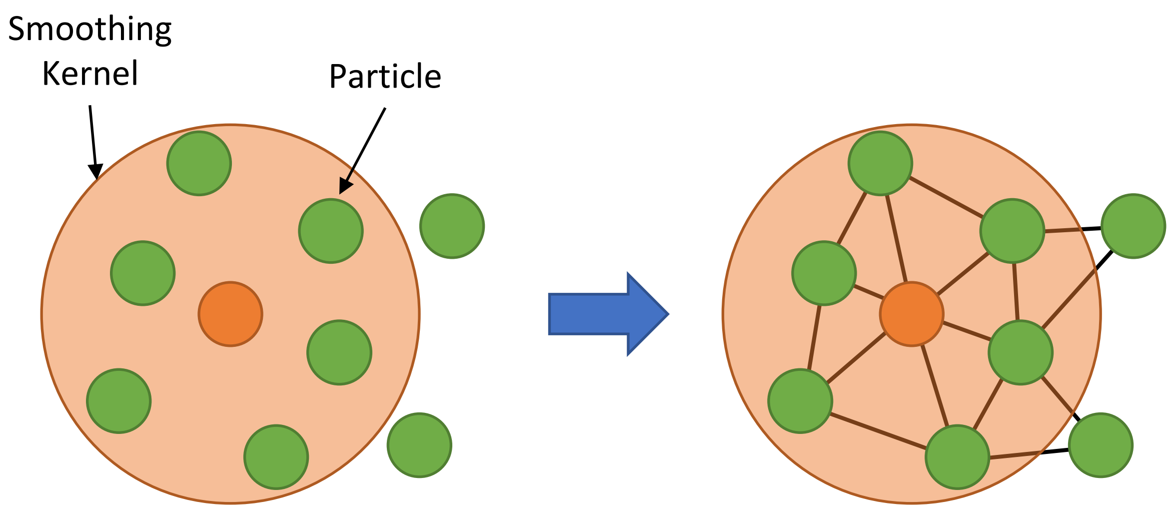
Overview

Motivation for Accelerating SPH

- Large-scale simulations and campaigns are essential for real-world applications
  - Real-world problems exhibit physical behaviours spanning a range of disparate spatial and temporal scales
  - Workflows involving optimisation/uncertainty quantification (UQ) require hundreds/thousands of simulations
- However, the cost/node/timestep is much higher in SPH than traditional CFD
  - A lot more neighbours and a lot more work per neighbour
- Advances in compute hardware (e.g. GPUs) have helped a lot, but there is a limit to how far traditional parallel decomposition strategies can go
- How else can we accelerate SPH and make real-world problems more tractable?

Surrogate Modelling with Graph Neural Networks (GNNs)

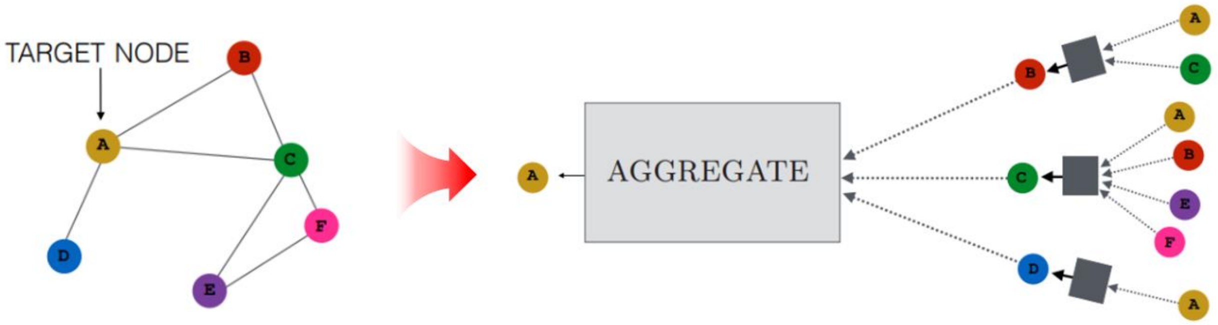
- Machine learning has had some success accelerating traditional CFD methods (e.g. using convolutional neural networks to solve PDEs)
  - However, so far, its application to SPH is still relatively limited
- GNNs show particular promise for low-fidelity modelling of high-fidelity SPH
  - Can be applied directly to unstructured data (unlike CNNs, which require interpolation to grid)
  - Particle-based simulations can be readily described as message passing on a graph
- So far, some proof-of-concept studies but very limited rigorous analysis



SPH convolution can be viewed as message passing on a graph.

GNN Architecture

- Encoder transforms node and edge features into latent space
  - Node features: particle type and velocity
  - Edge features: relative positions and distance



Aggregation function is a permutation-invariant function (e.g. sum, mean, max) that collects message from each edge.

- Followed by multiple message passing layers
  - Edge update, edge aggregation, node update

$$\mathbf{e}_{ij}^{k} = f^{e}\left(\mathbf{e}_{ij}^{k-1}, \mathbf{v}_{i}^{k-1}, \mathbf{v}_{j}^{k-1}\right)$$ **Edge Update**

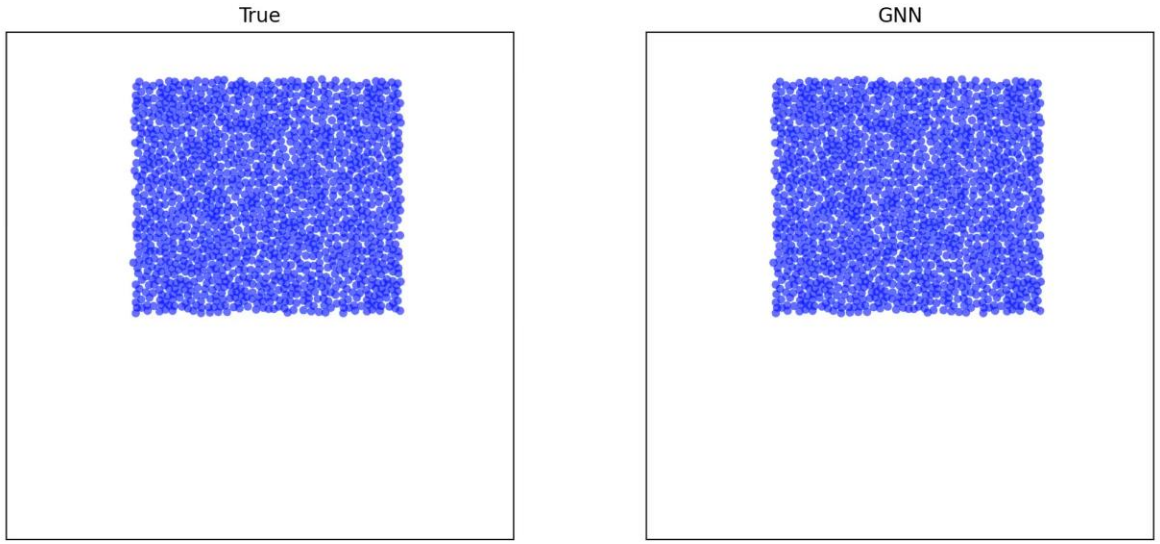
$$\overline{\mathbf{v}}_{i}^{k} = \sum_{j \in \mathcal{N}_i} \mathbf{e}_{ij}^{k}$$ **Aggregation (Sum)**

$$\mathbf{v}_{i}^{k} = f^{v}\left(\mathbf{v}_{i}^{k-1}, \overline{\mathbf{v}}_{i}^{k}\right)$$ **Node Update**

- Decoder transforms output of MP layers into something useful
  - Output: nodal (particle) accelerations

Training & Data

- Loss is computed based on particle accelerations for single time step
- Dynamics are then computed using standard time integration (e.g. Euler)
- Noise added to improve robustness over long time trajectories
- Dataset generated from MPM solver
  - 1000 train trajectories (100 test)
  - Each with 600 time steps and ~1000 particles
  - Sanchez-Gonzalez et al. (2020) from Deepmind
  - Approximately 12 hours for 3 epochs on a V100



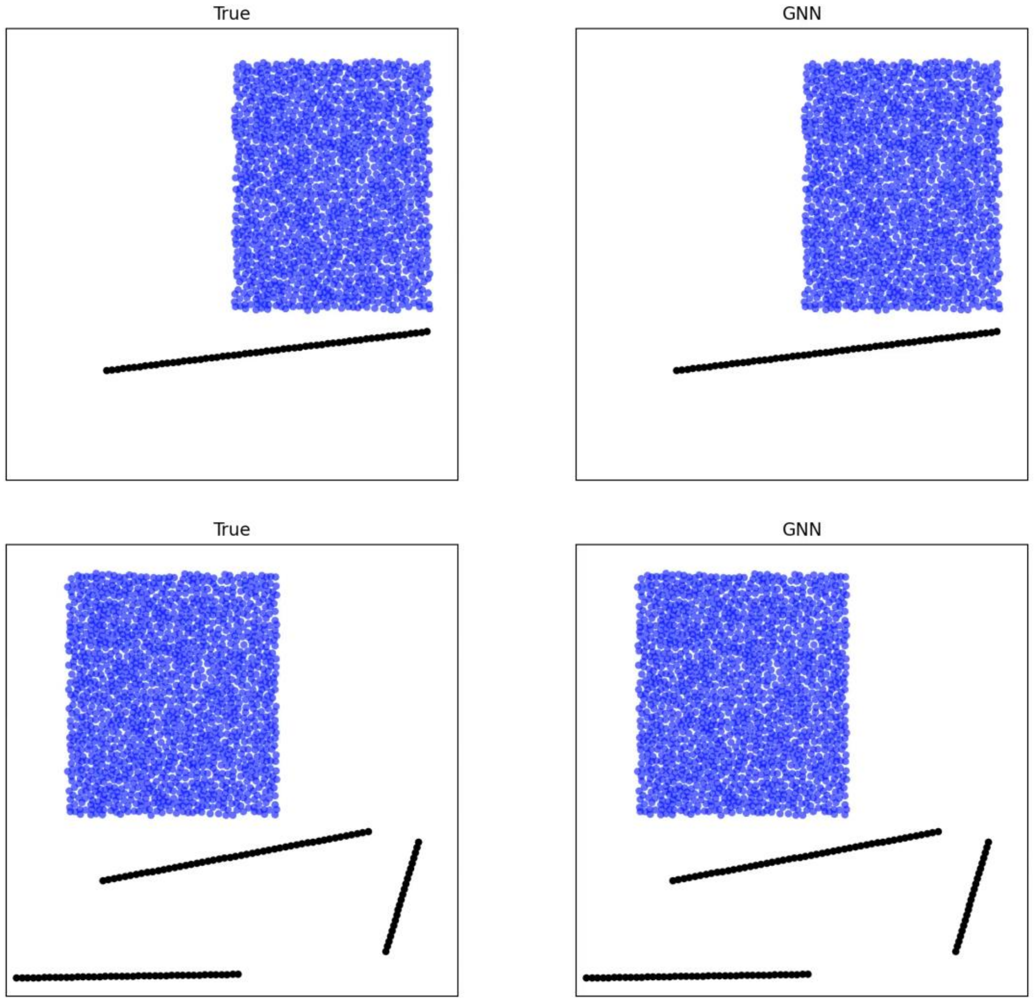
Comparison of true solver vs GNN simulator for example rollout.

Example Rollout Trajectories

- Encoding particle type allows modelling of boundaries

- Generalises well to unseen geometries

- Next steps:
  - Generate own dataset with SPH solver
  - Quantitative validation
  - Integrate with DualSPHysics
  - Detailed performance benchmarking
  - Architecture improvements (e.g. anti-symmetric networks for momentum conservation)



Comparison of true solver vs GNN simulator for example rollouts.

Accelerating Single Simulations

- Fast low-fidelity models for SPH open the door for novel multi-fidelity and parallel-in-time strategies

- Parareal is the most popular parallel-in-time method
  - Low-fidelity model performs initial (serial) prediction
  - Multiple high-fidelity simulations are then started from different points in time to correct solution
  - Each high-fidelity simulation uses low-fidelity prediction as initial condition

- Some additional unique challenges posed by particle-based techniques

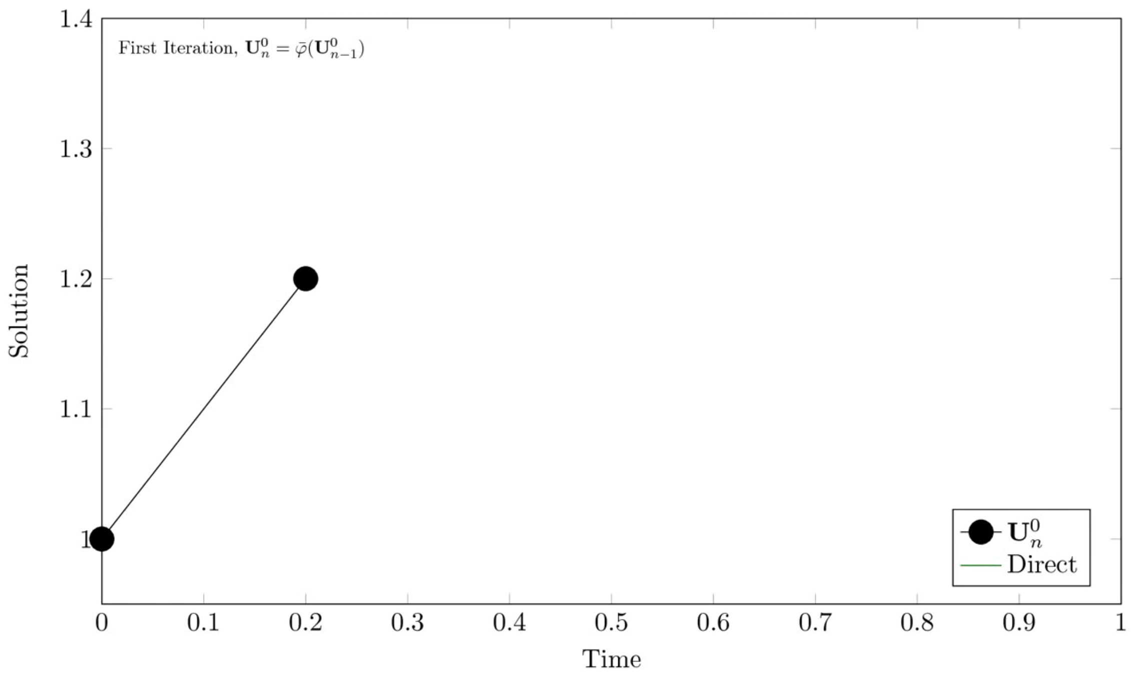


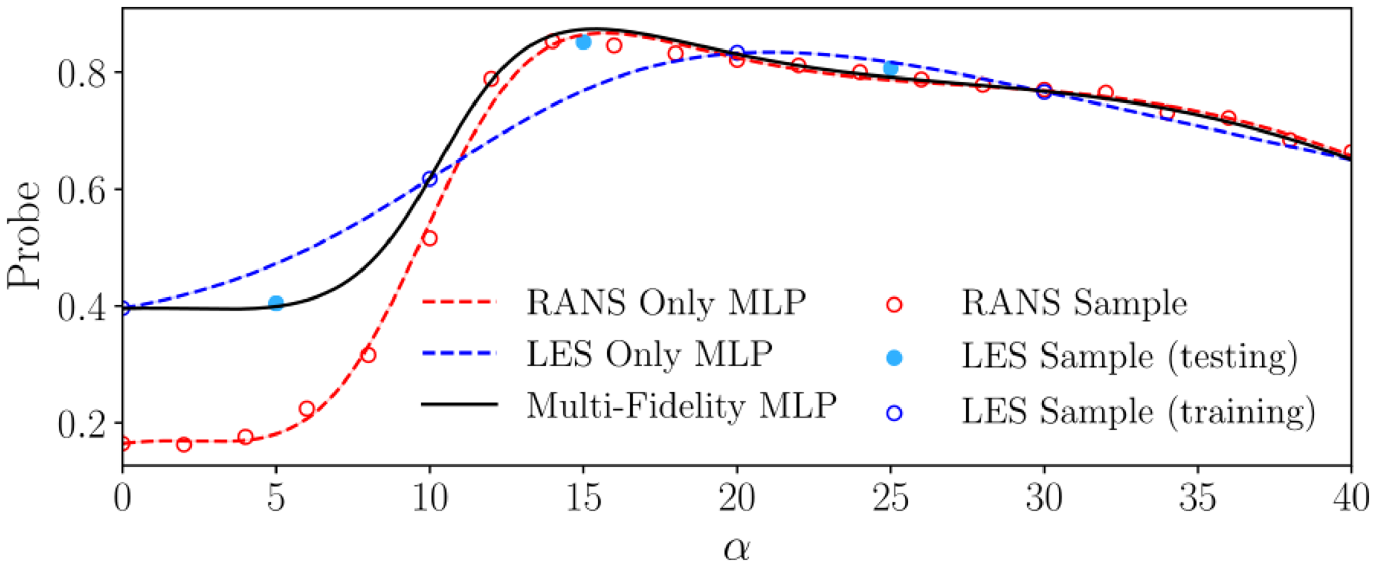
Illustration of Parareal algorithm for an example toy problem.

Accelerating Large Campaigns of Simulations

- Fast low-fidelity models for SPH will also enable targeted-fidelity strategies for large campaigns (e.g. optimisation, UQ)

- Build surrogate models from multiple sources of data
  - Small number of high-fidelity simulations
  - Large number of low-fidelity simulations

- Improved surrogate model for same overall budget
  - Can then be directly integrated with existing optimisation/UQ techniques



Combined multi-fidelity model shows better agreement with the test data than LES-only (high-fidelity) or RANS-only (low-fidelity) models (Mole et al. 2023).

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