Foundational AI Directions for CFD and Multi-Physics Modelling

CCP-WSI Working Group, 2nd April 2025

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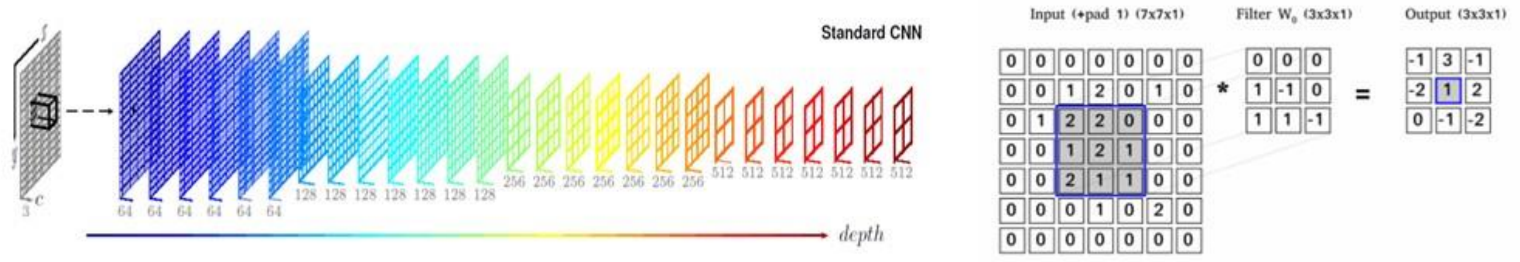
PREMIERE, RELIANT, COTRACE, TRACK, PROTECT, COVAIR, TAPAS, RECLAIM

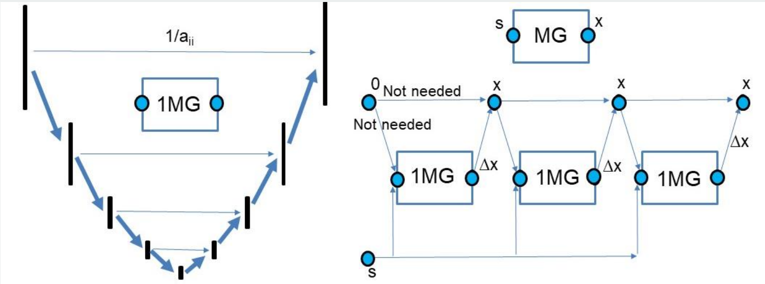
AI-RESPIRE

Convolutional Neural Networks



AI4PDEs applied to CFD

Multigrid-solution methods



- AI technology provide novel solution of complex problem
- Exascale CFD simulation – a wide range of turbulent scales
- Develop GPU-based solver to relax the limitation of computational cost
- Cerebras systems with 1M node chip
- Summary speed - total 10^6 - 10^9 faster; AI models 10^3 - 10^6 faster; AI computer 10^3 faster
- Applications: indoor ventilation and urban flows

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Methodology – AI4PDEs

- Design the values of kernels in ANNs without data training
- Represent the discretization of PDEs on structured mesh
- Produce identical solution to classical approaches

Advantage

✓ Easy implementation
✓ Less quantities of code
✓ More computational efficient than conventional CFD solver (~100 times)
✓ More accessible to optimize by GPU and AI computer
✓ Digital twins assimilating data and performing uncertainty quantification
✓ Long term model/code supported by community and AI software

Airflow modelling using AI4PDEs: South Kensington area

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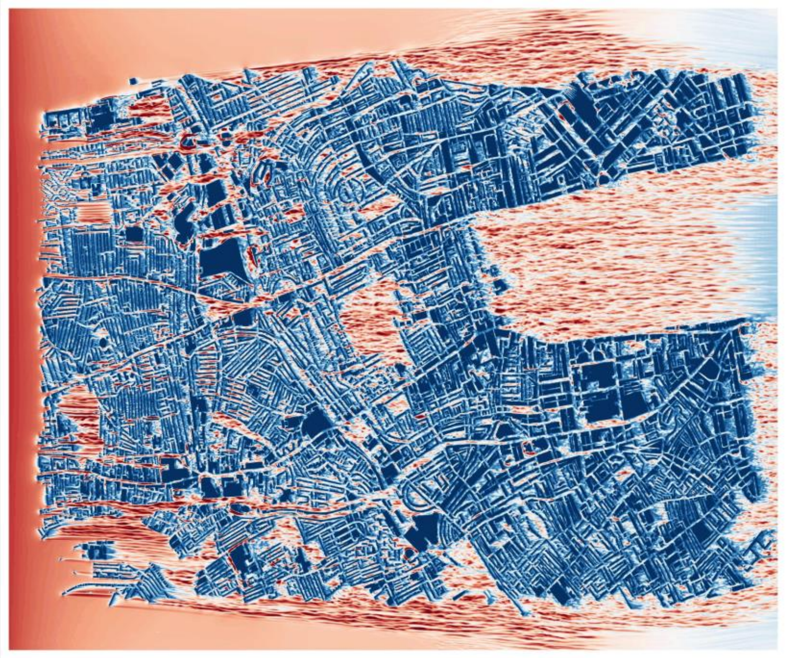
- 3D South Kensington area (5km x 4km)
- One-hour computational time → 5 hours
- Uniform inflow speed (from left to right) – 1 m/s
- 2 Billion nodes London – 4 A100 GPUs

Schematic diagram of the area



Airflow speed (m/s)

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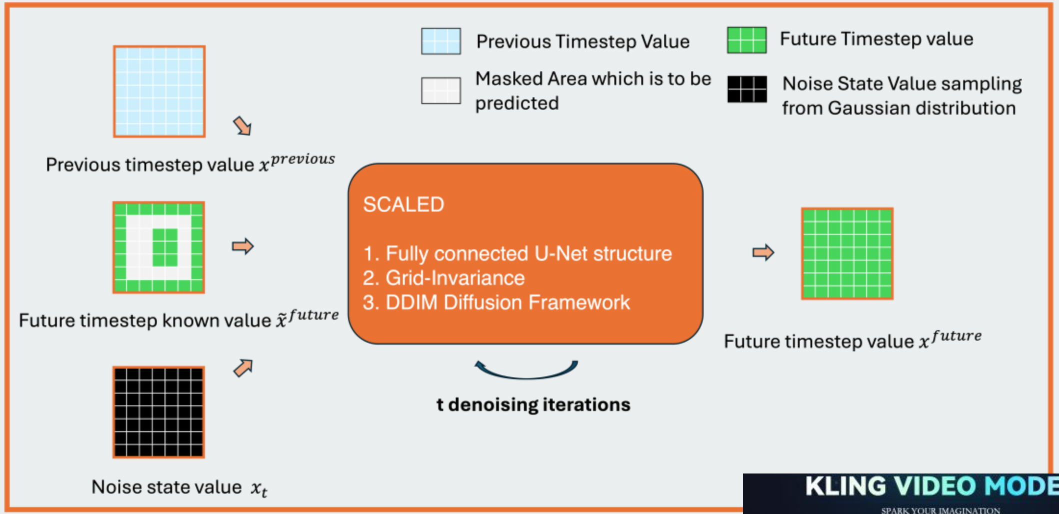
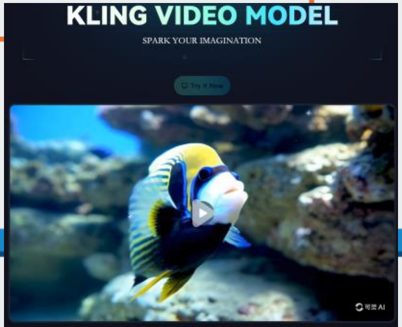
Foundational Methodology – diffusion model: Overview of SCALED – AI Surrogate model – grid and geometry invariant

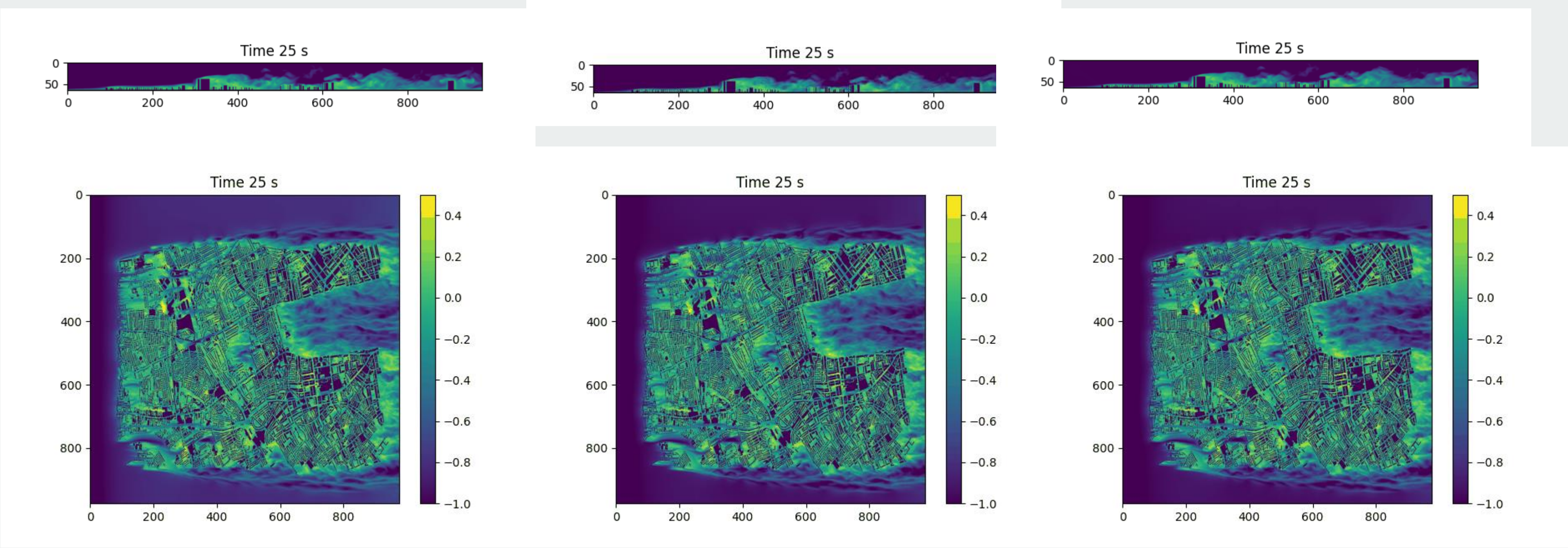


SCALED model structure for predicting the future timestep value, with 3 inputs: the previous timestep value, future timestep known value and the noise state value sampling from gaussian distribution. The future timestep known value could come form

1. sensor data and buildings information,
2. entire domain boundary conditions and
3. information exchange between neighbours

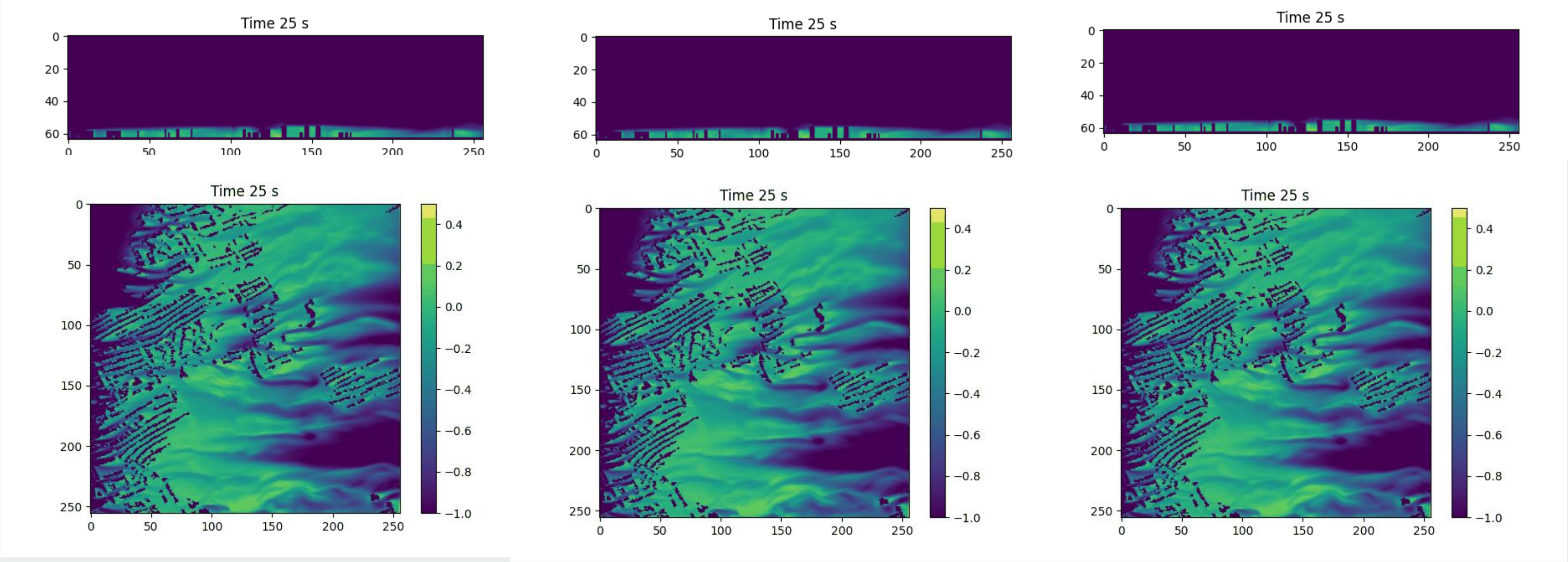


Model Result demonstration - Flow Past South Kensington



Gound Truth　　SCALED Result　　UNET Result

Model Result demonstration - Flow Past Generated Area



Gound Truth

SCALED Result

UNET Result

Multiphase flow using AI4PDEs : Collapsing water column

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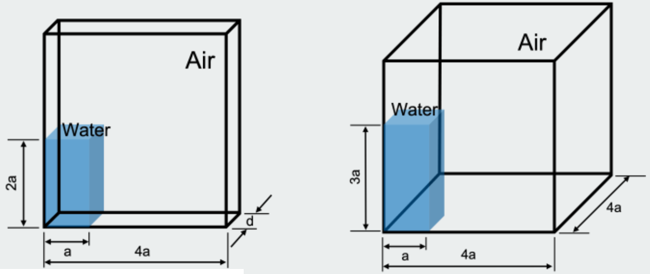
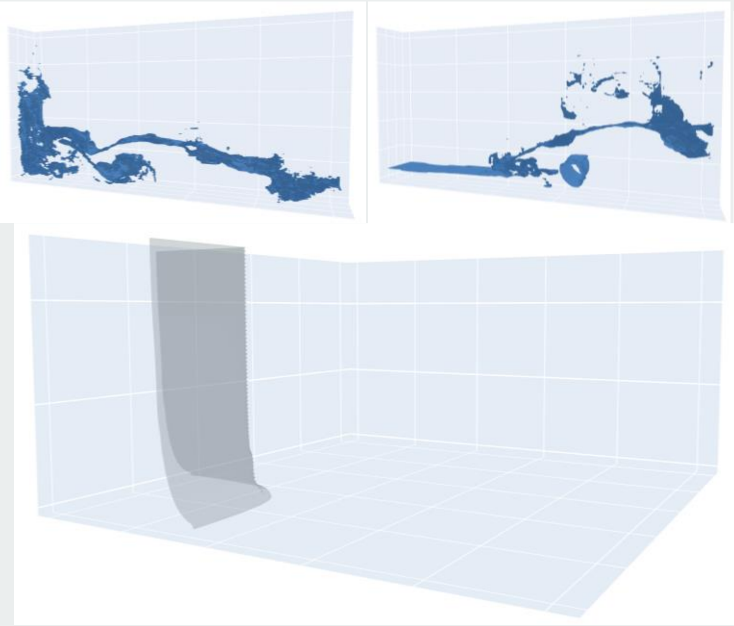
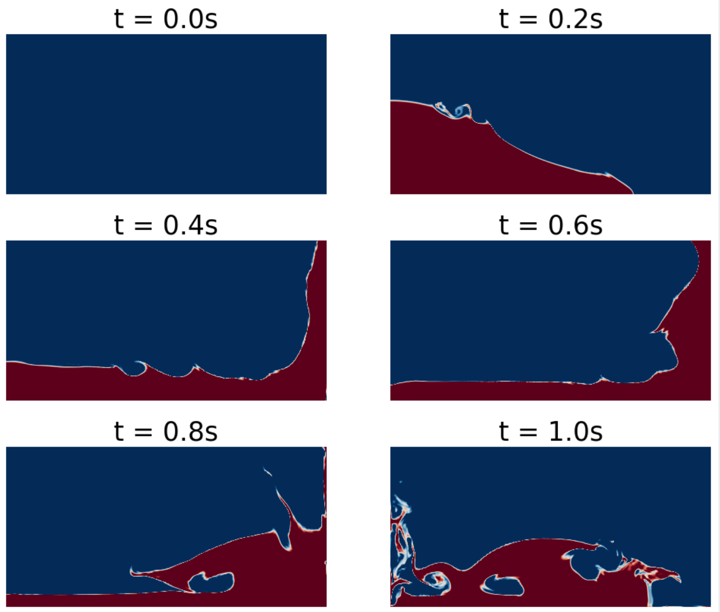
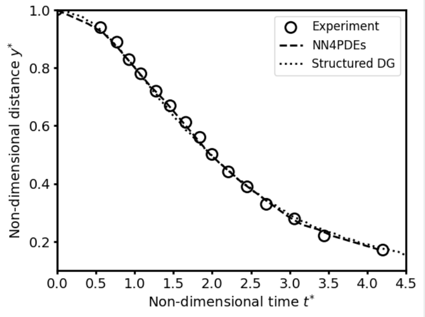
- Cubic domain size: 0.5 (m) x 0.5 (m) x 0.5 (m)
- Grid point: 512 x 512 x 512 (0.256 billion nodes)
- One single GPU









Multiphase flow using AI4PDEs: 3D flooding modelling

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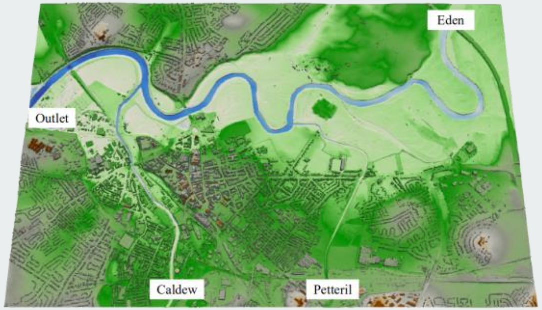
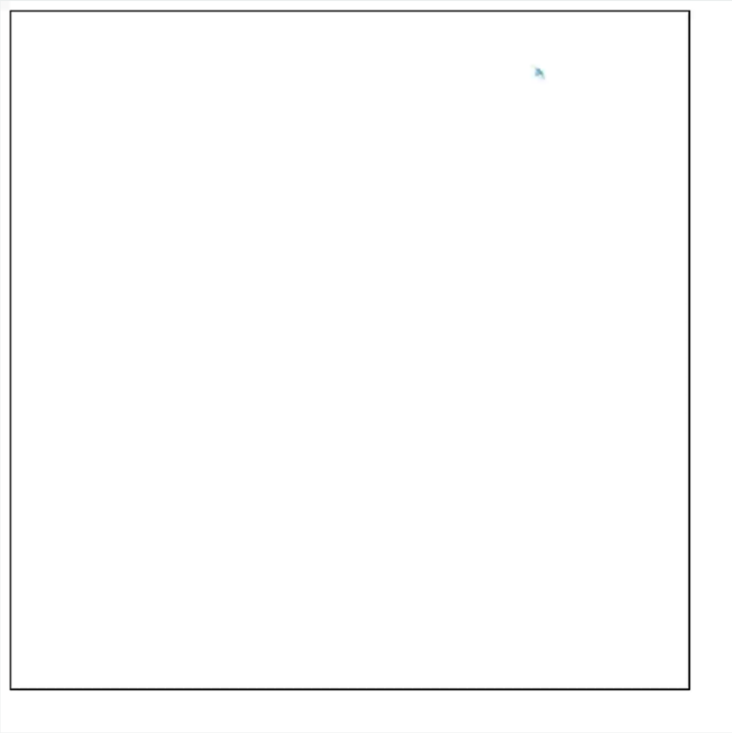


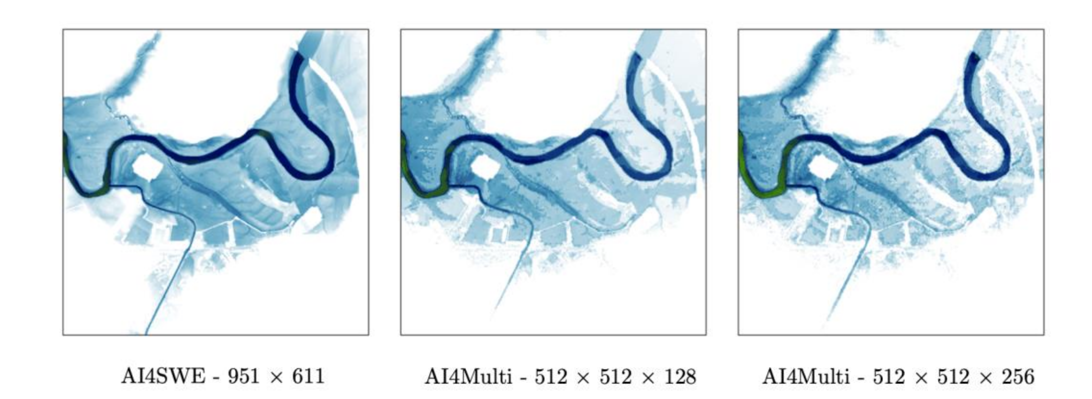
Carlisle area

- Carlisle 2005 flooding event
- 10-hour real time simulation
- Three water sources
- Comparison with 2D AI4PDEs model

water depth from 0 to 10 hours



2D 3D 3D



Spatial variation of water depth in the flooded area

Vehicle airflow modelling using AI4PDEs – AI surrogate is similar

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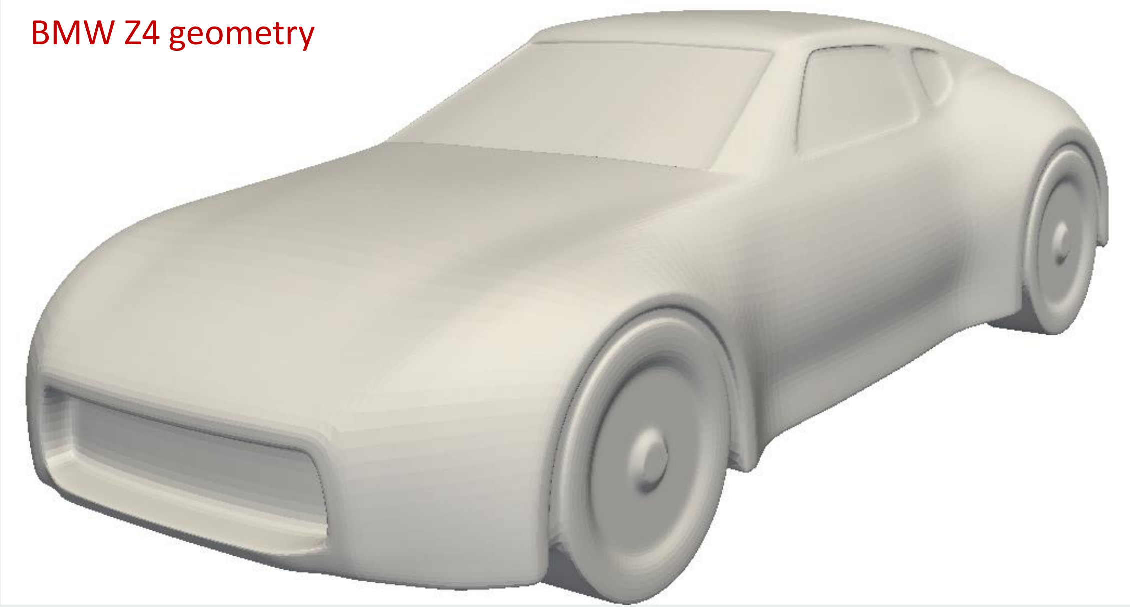
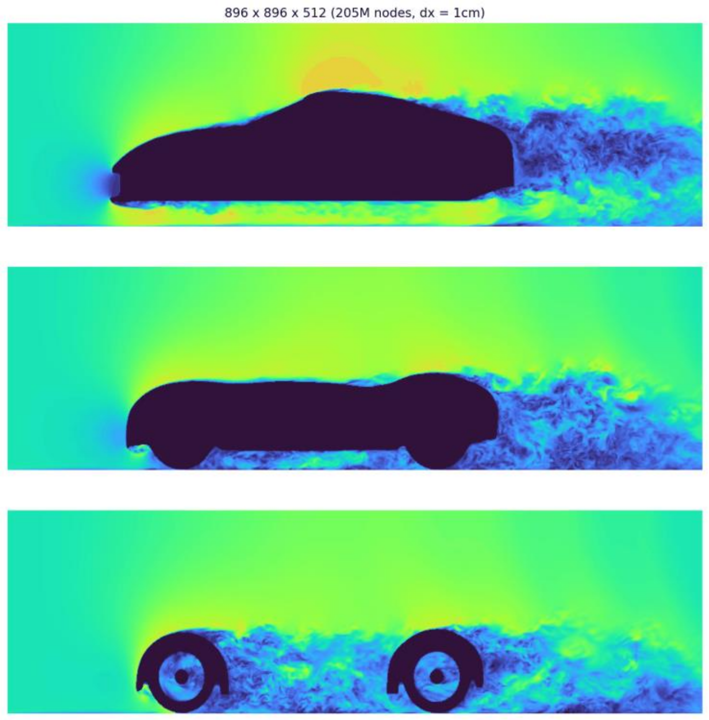
- BMW Z4
- 400M quadratic finite elements
- dx = dy = dz = 1cm

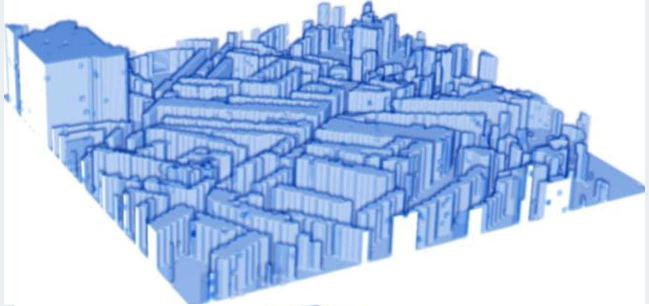
BMW Z4 geometry

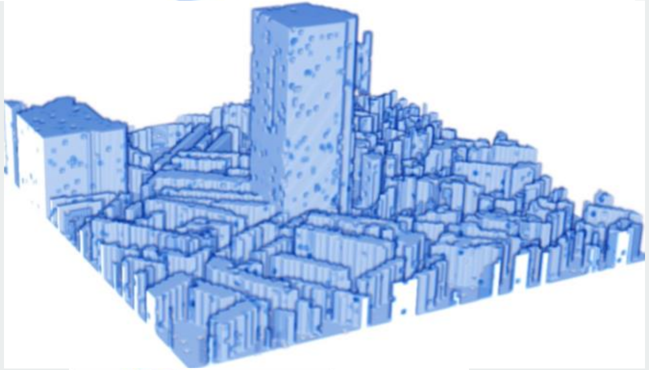


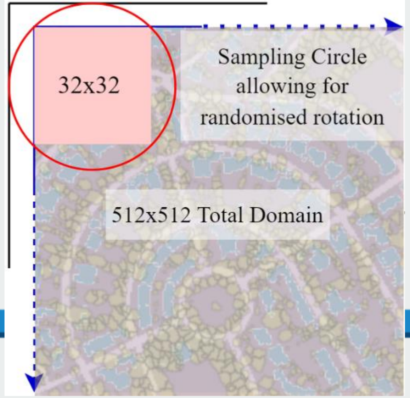
Air flow speed in middle plane

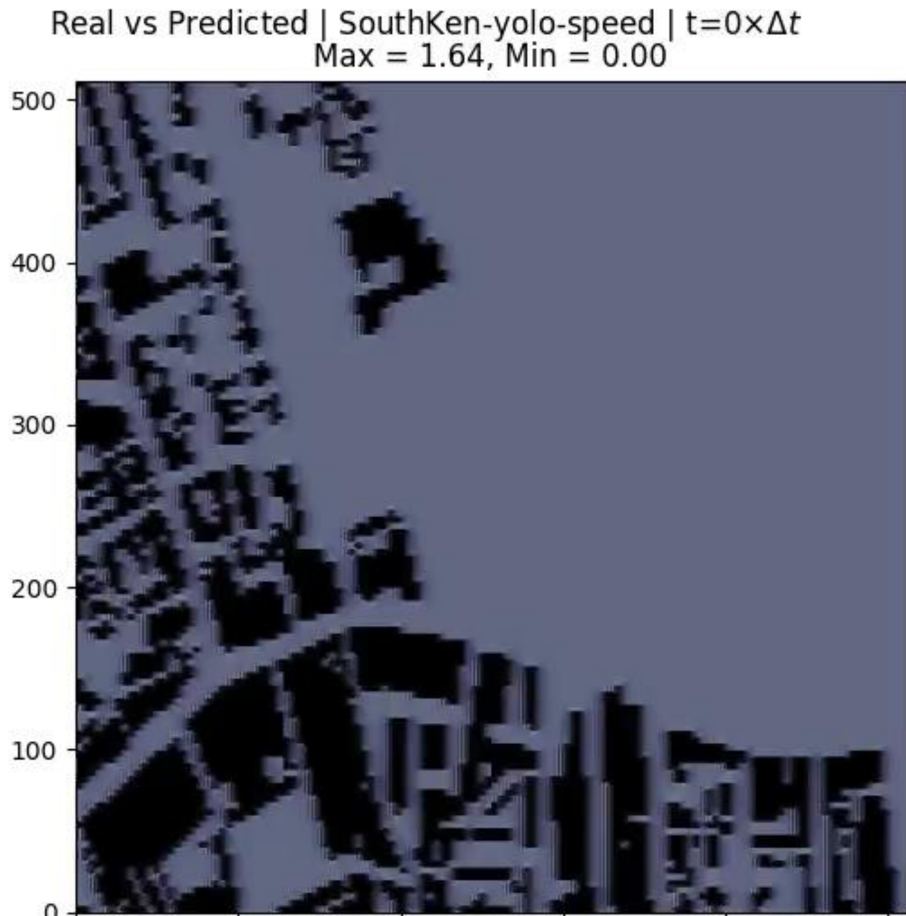


Generators (Buildings+Greening – left) and AI surrogate (10K x faster CFD & trained for car flow - right)









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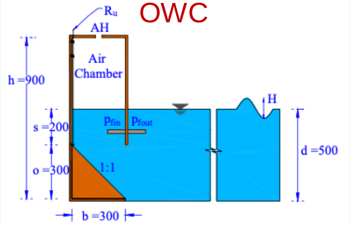
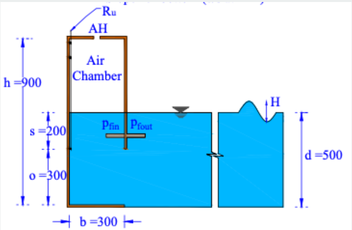
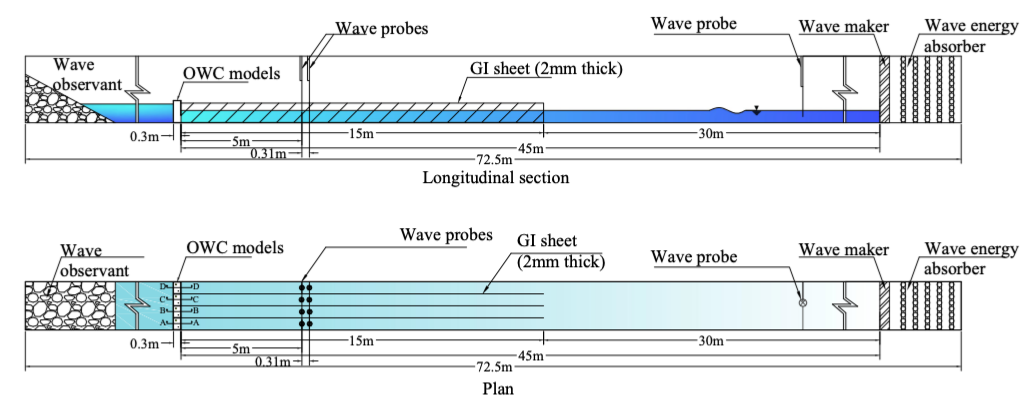
AI4Wave - Oscillating water column (OWC) energy device

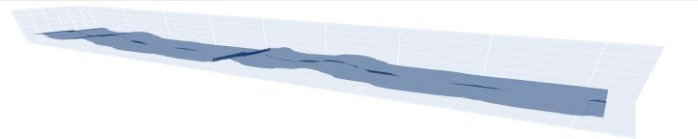
Schematic diagram of experimental set-up

Two types of OWC

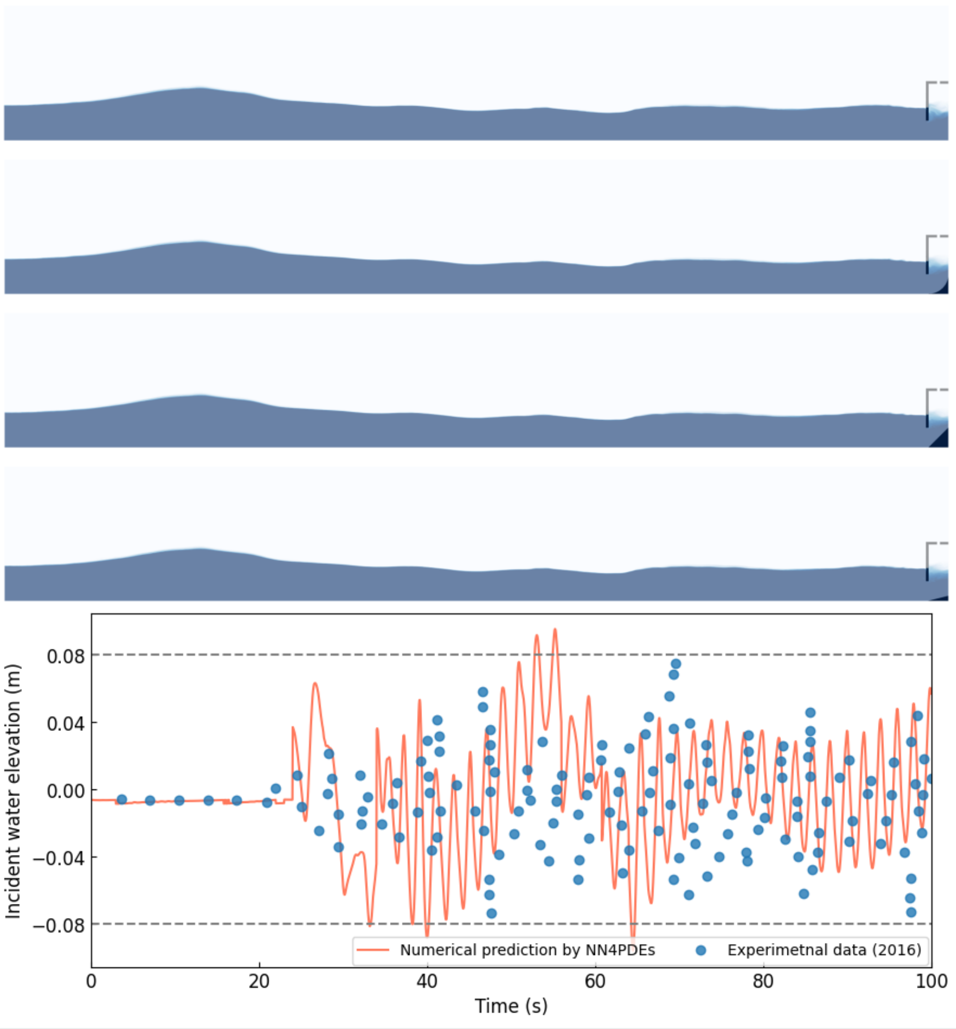
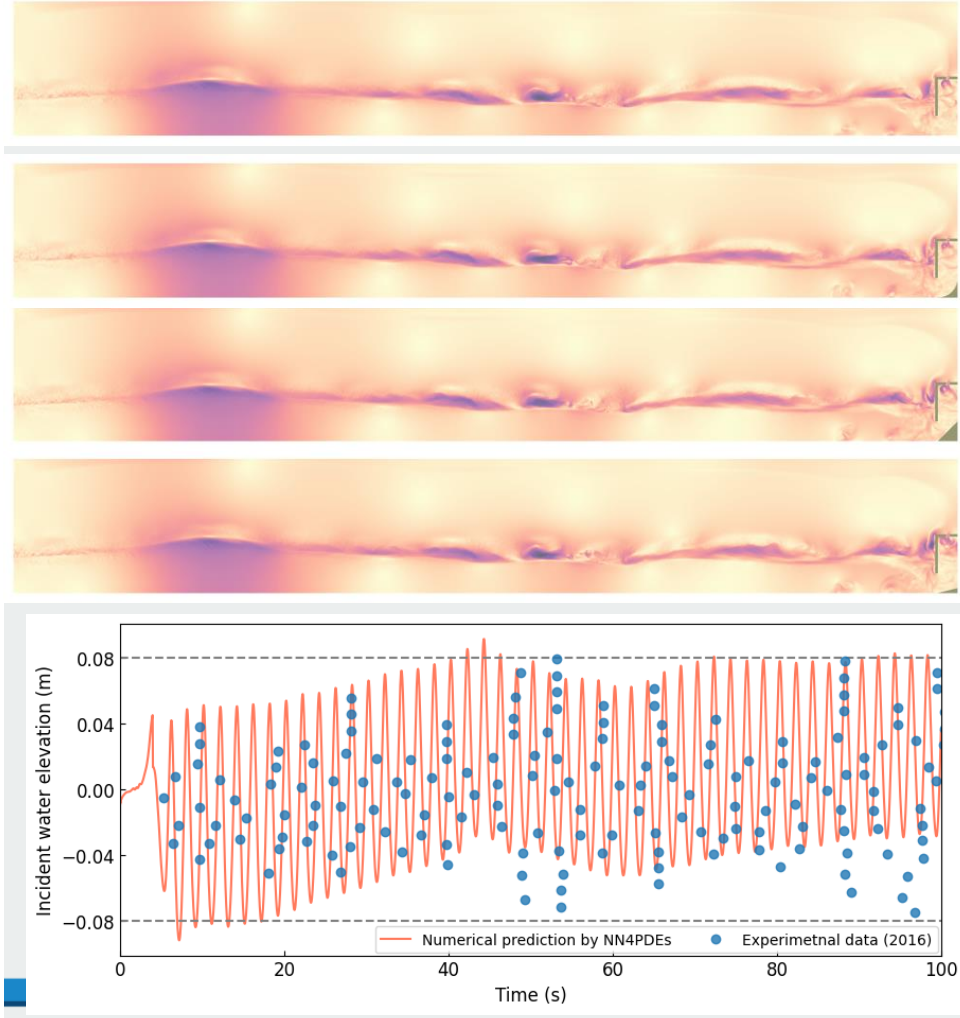








Water volume frac. on the middle plane


Incident water elevation (m)
0.08
0.04
0.00
−0.04
−0.08
0
20
40
60
80
100
Time (s)
Numerical prediction by NN4PDEs
Experimetnal data (2016)

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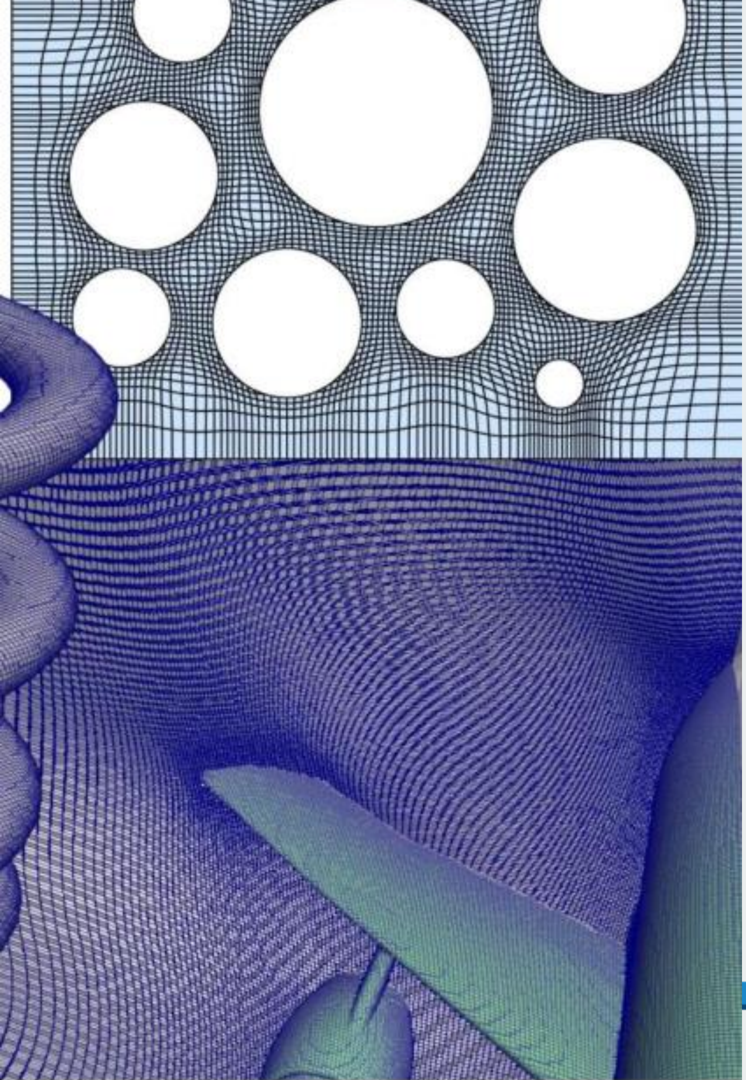
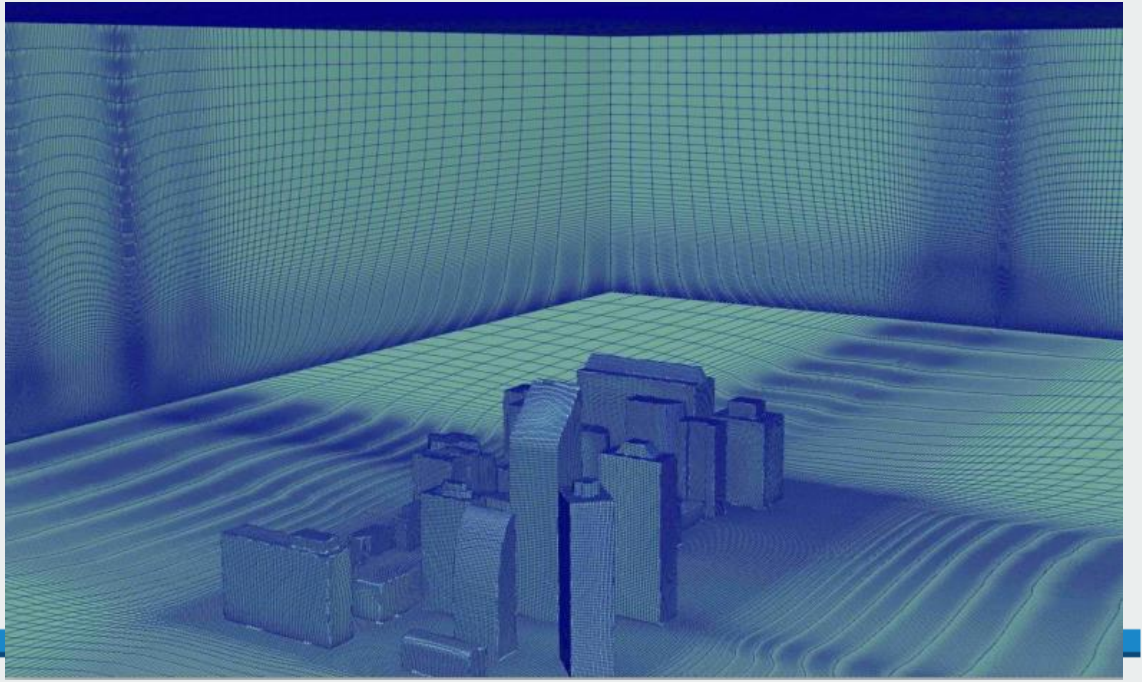


Distorted structured convolutional grids – future direction



Unstructured meshes – future direction - Graph neural network AI4PDE unstructured grid model - Turek FSI3 benchmark animation

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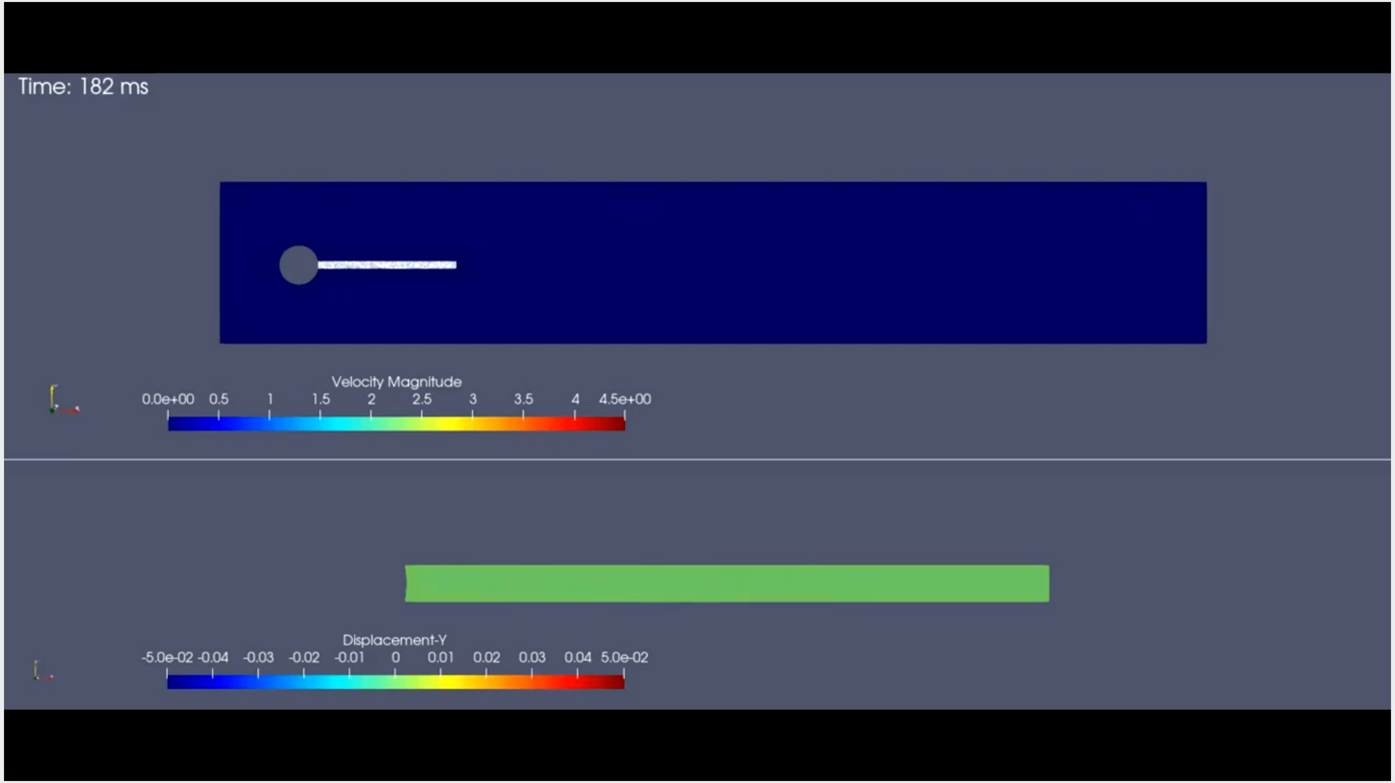

Velocity magnitude

y displacement

Indoor airflow modelling using AI4PDEs and AI4Particle

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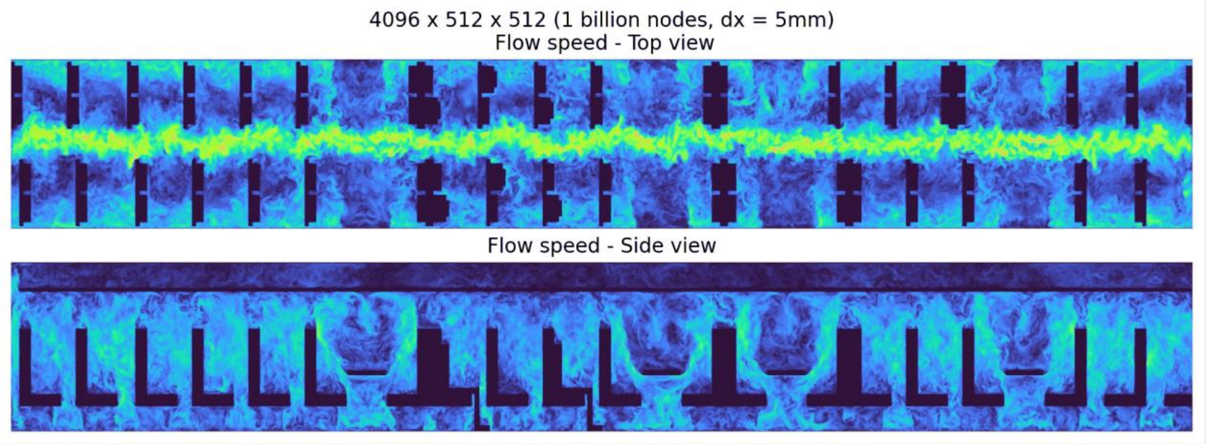
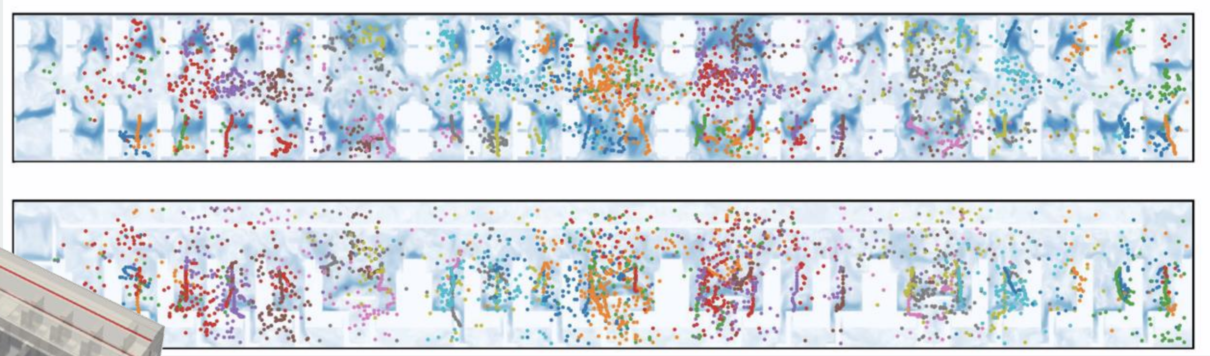
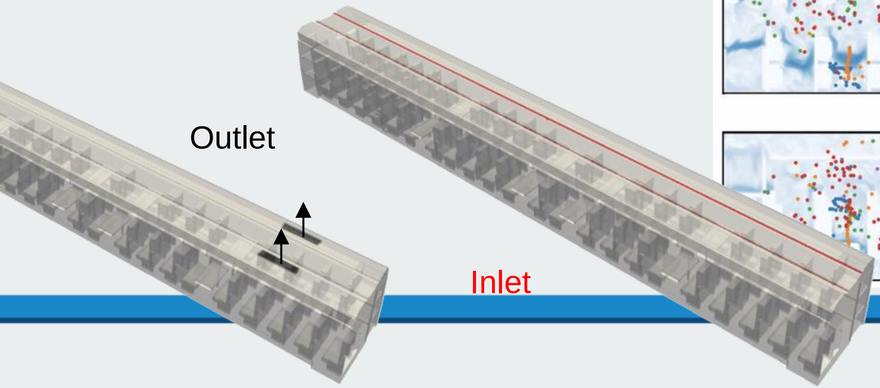
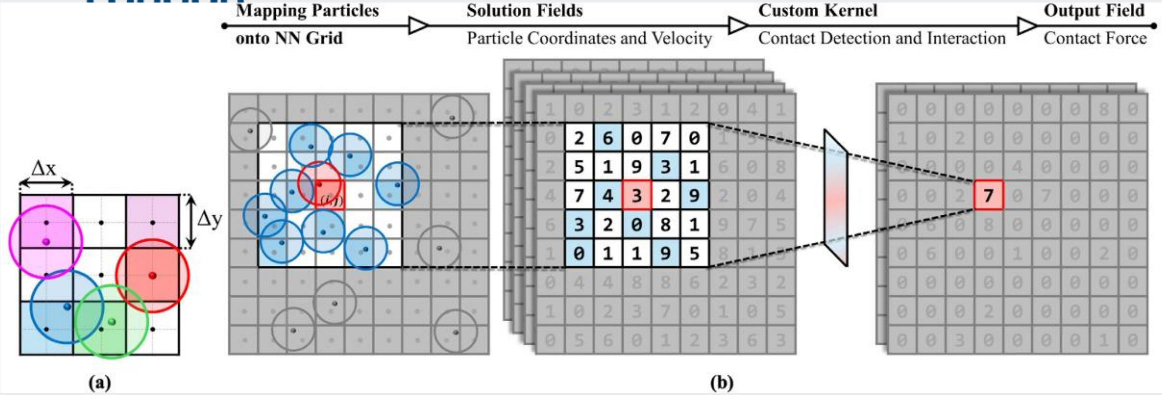
- Ventilated train carriage
- Message Passing Interface (Parallisation)
- 1 billion FEM nodes – 4 A100 GPUs
- AI4Particle/AI4System
- Tackle individual transmission



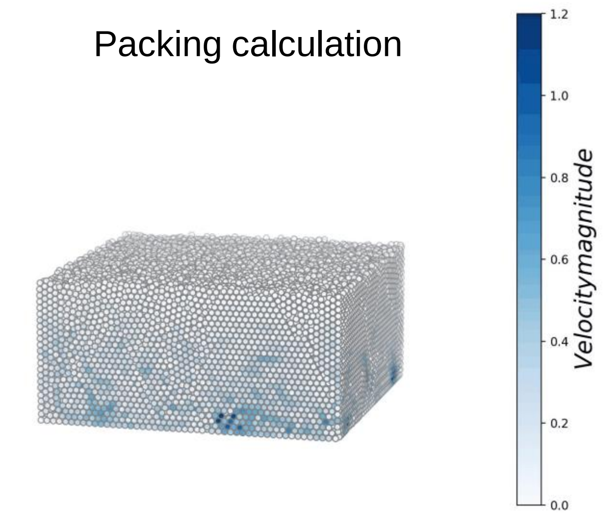




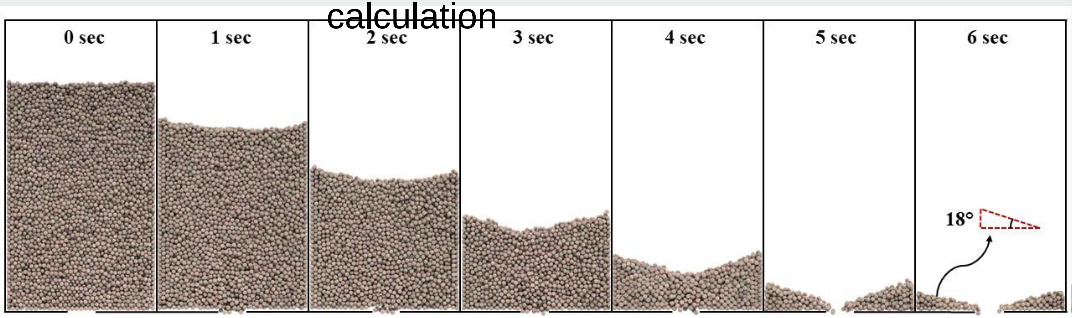
Design and optimizing Neural Network for Discrete Element Method



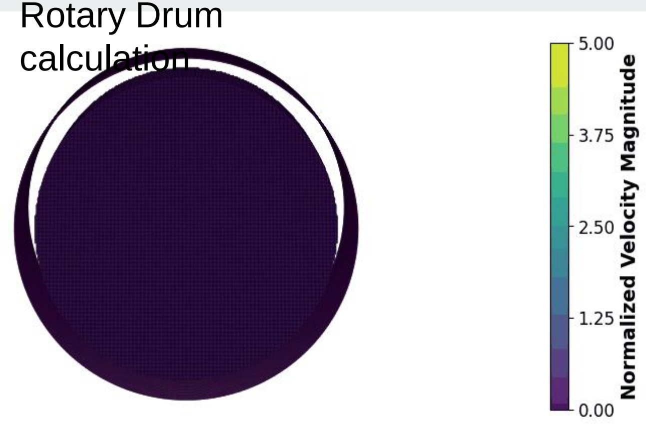
Packing calculation



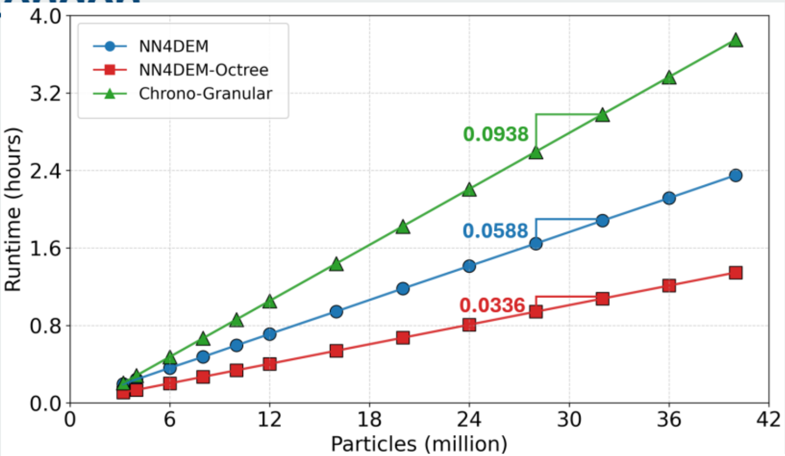
Hopping case calculation

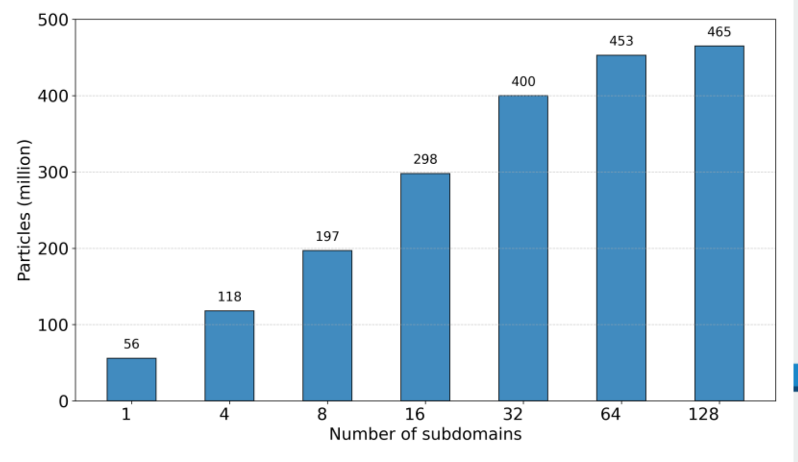


Rotary Drum calculation

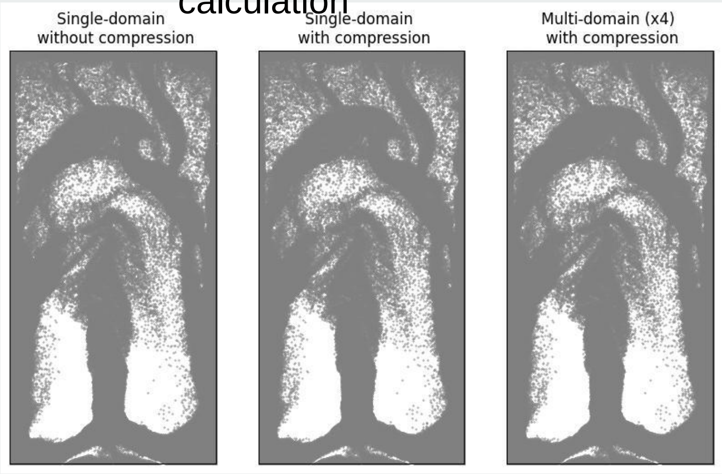


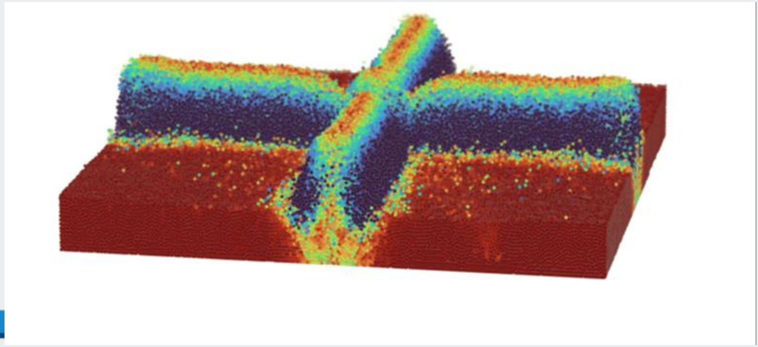
GPU profiling results of NN4DEM with domain decomposition methods and Octree based methods





Fluidized bed calculation





SCALED-X: extend scaled to multi-physics problems

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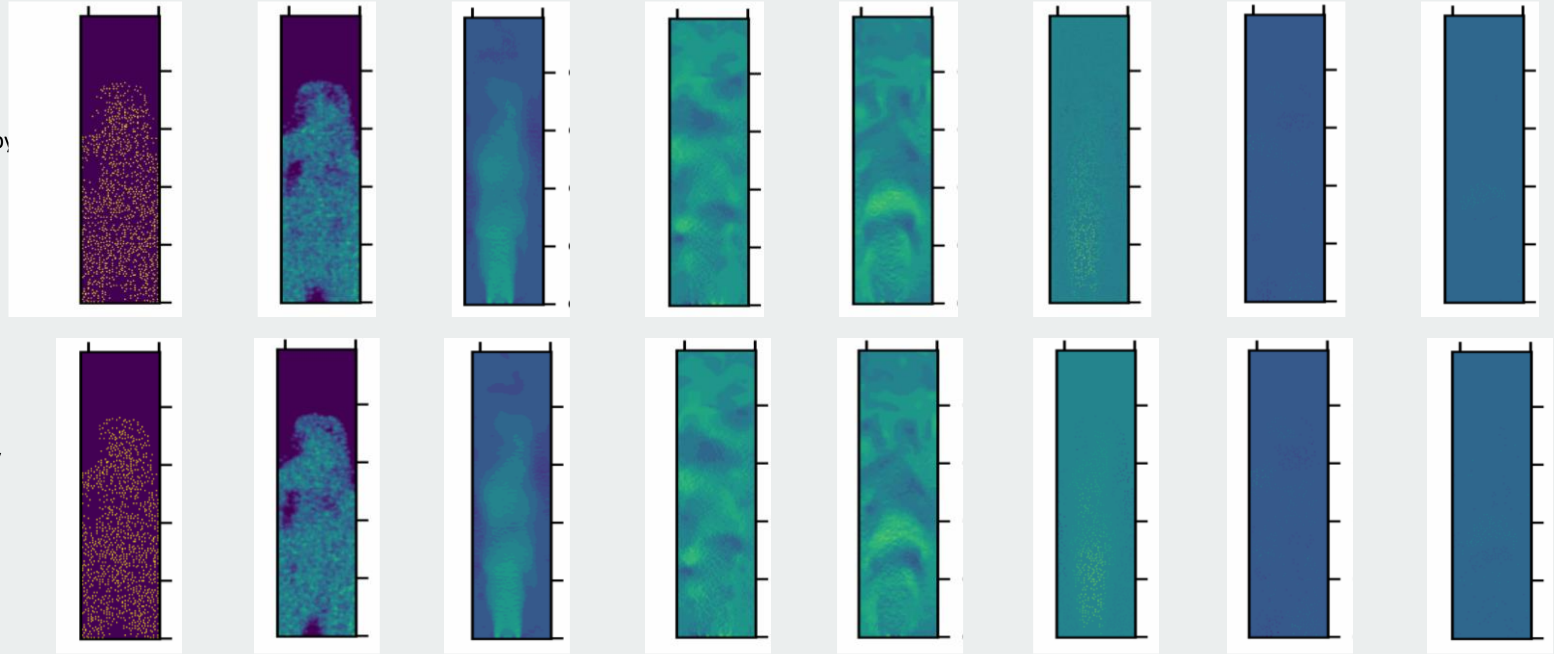
Result Generated by SCALED

Result Generated by numerical solver



Particle Position

Particle Volume

flow velocity on z direction

flow velocity on y direction

flow velocity on x direction

Particle velocity on z direction

Particle velocity on y direction

Particle velocity on x direction

Particle on fluidized bed problems

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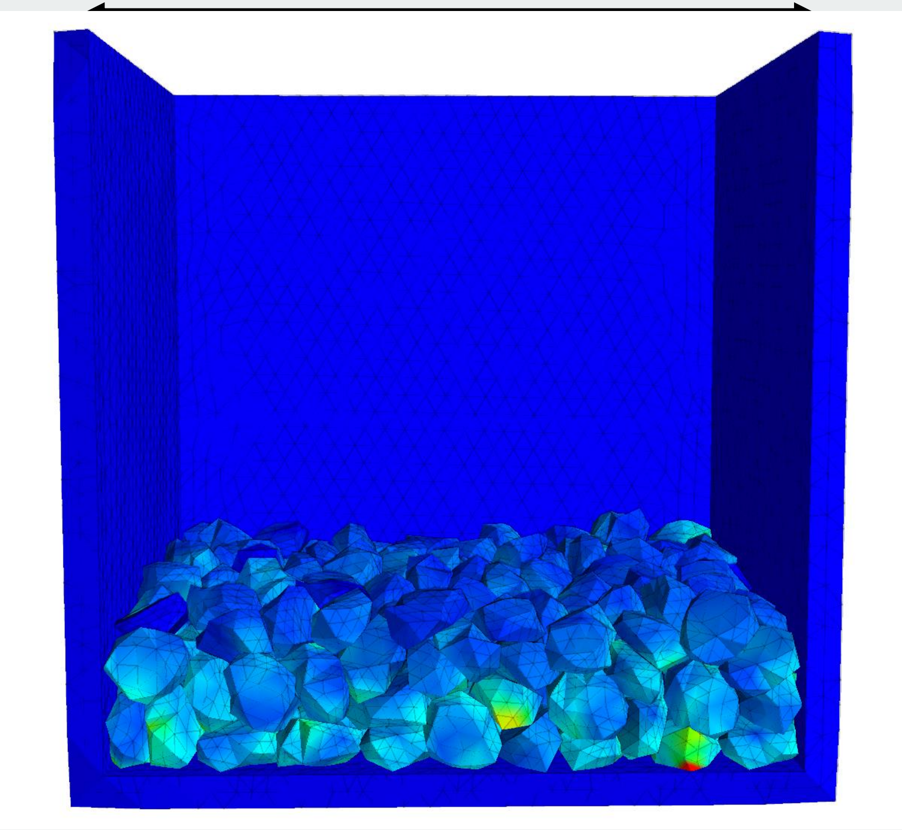
FEMDEM: Dynamic Multi-Body Packing

288 rocks

40 kg

D=0.31 m



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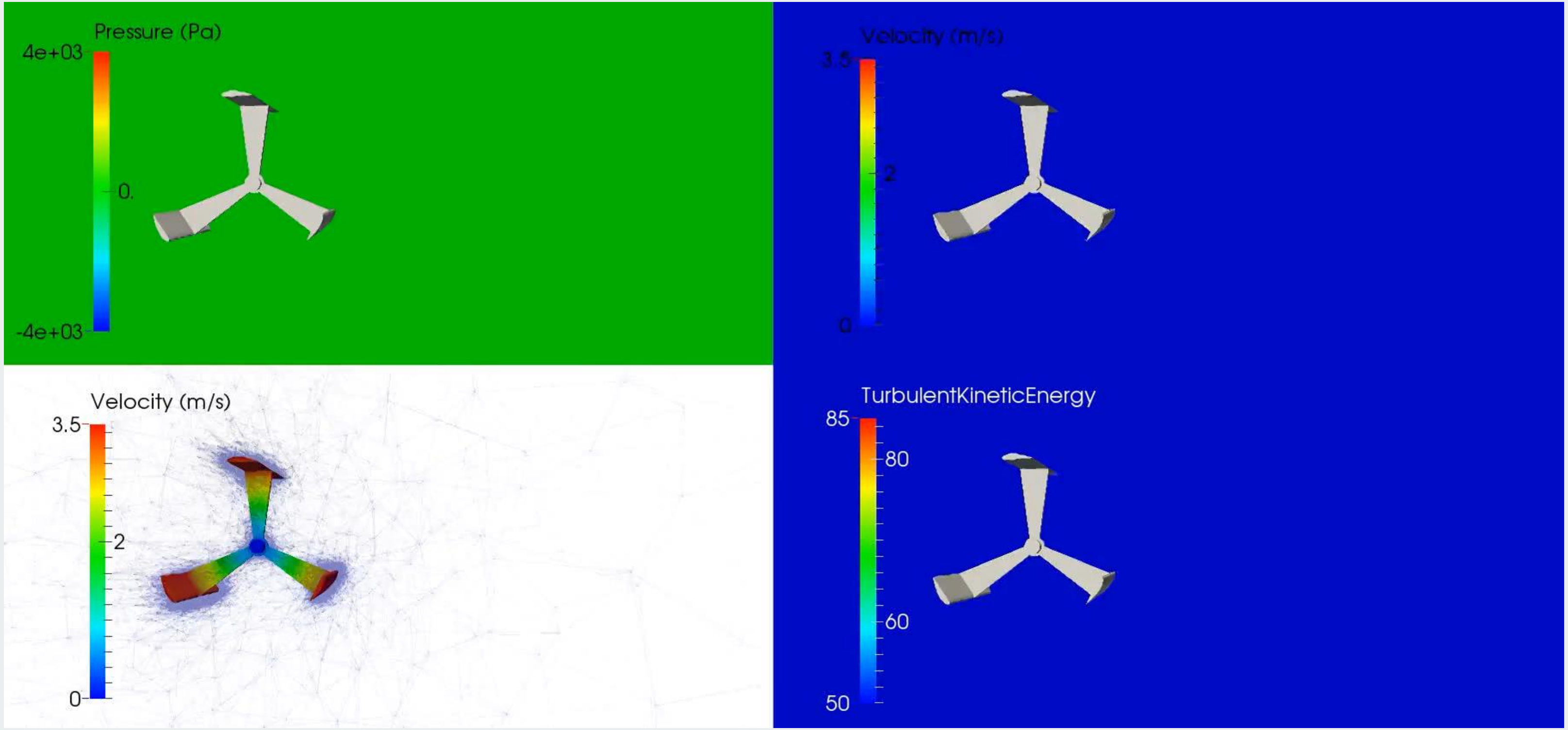
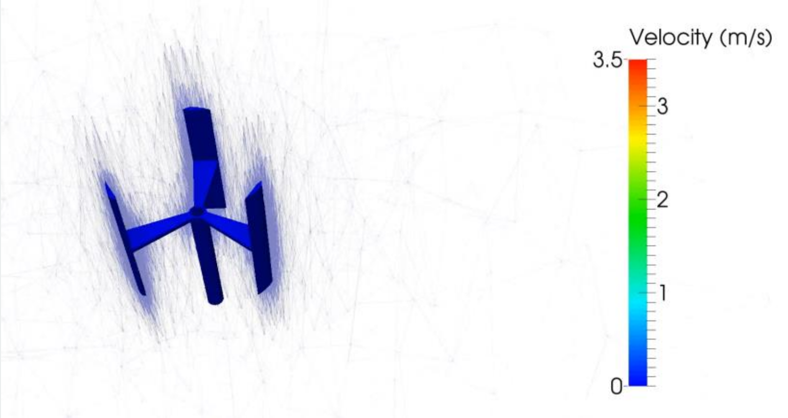
Flow past a 3D rotating VATT



Inlet velocity: 2.3 m/s, fluid mesh size: 0.002m, CFL<1.0, Re=147200

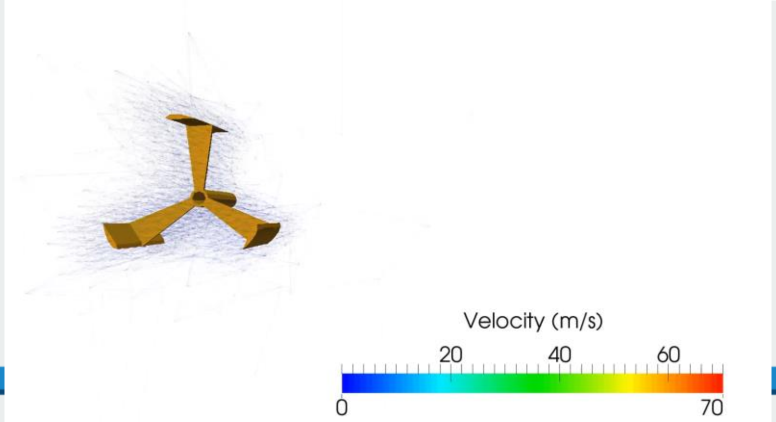
Flow-induced vibration and fractures



Inlet velocity: 2.3 m/s,

fluid mesh size: 0.002m,

CFL<1.0, Re=147200



Inlet velocity accelerating at

a=100m/s,

fluid mesh size: 0.002m,

CFL<1.0.

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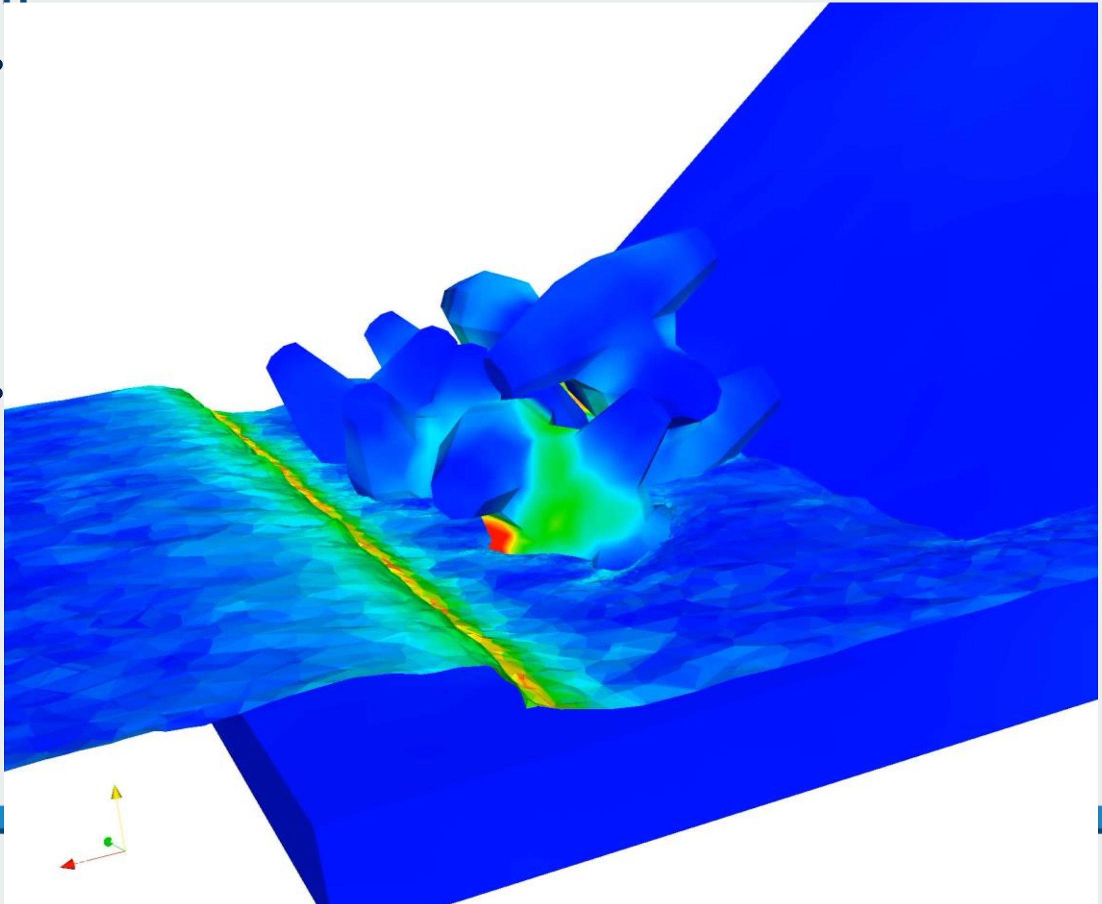
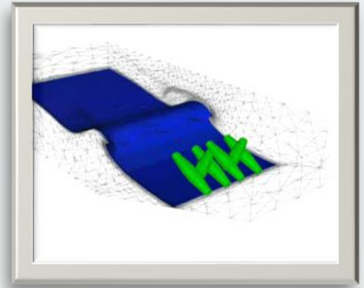
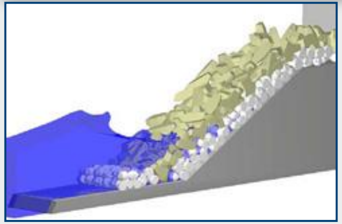
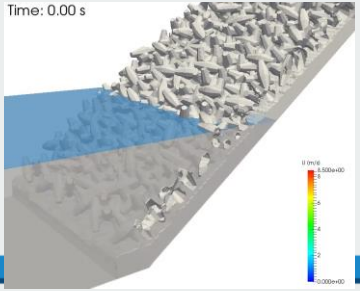
Wave-Structure Interaction (WSI)









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Thank you!

References and available code

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