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# AI for Scientific Discovery and Multiscale Modelling: - Demonstrating AI4PDEs and AI4Particles

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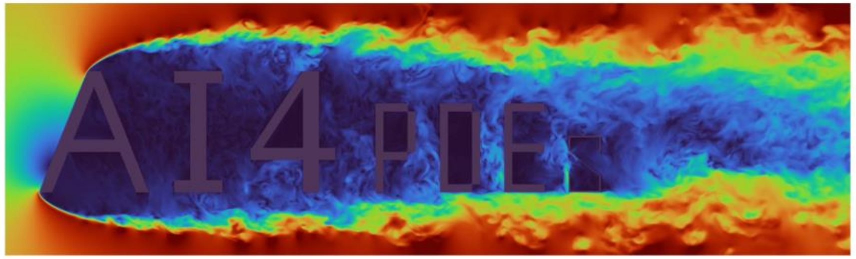
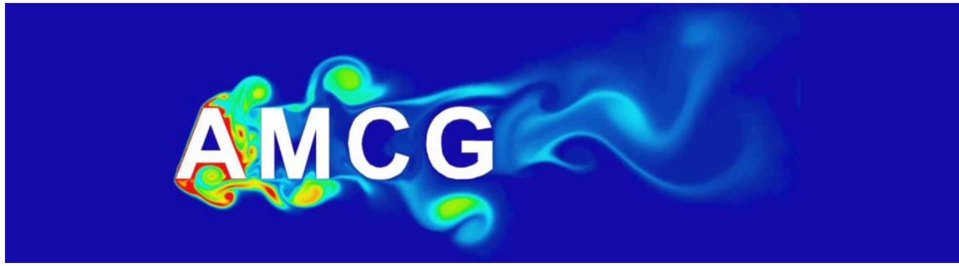



25 Mar 2025
ECO-AI Workshop
Edinburgh, UK



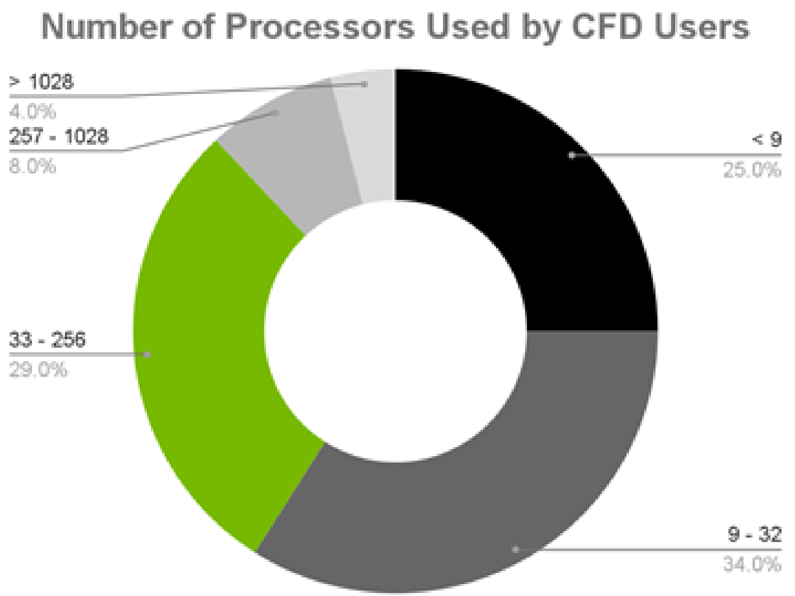
# Background and Motivation

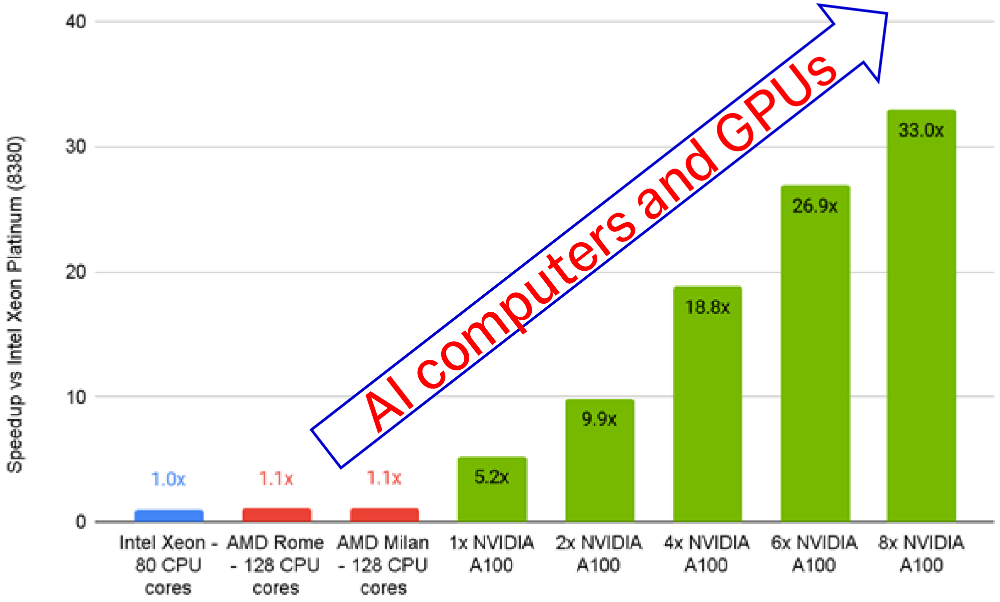
- AI & ML technology provide novel solution of complex problem
- Large-scale CFD simulation (exascale computing)
- Numerical modelers intend to develop GPU-based solver

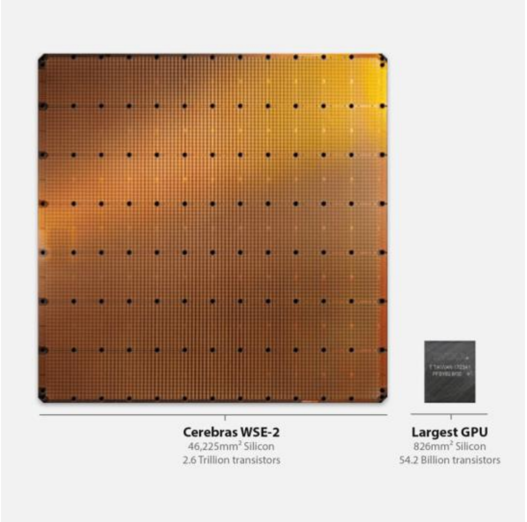
Relax the limitation of computational cost

- New AI computers
- Summary speed - total $10^6$~$10^9$ faster

AI models $10^3$~$10^6$ faster; AI computer $10^3$ faster




Cerebras 1M node chip


GRAPHCORE IPU

# Methodology – AI4PDEs

Artificial Intelligence for Partial Differential Equations (AI4PDEs)

Neural Networks for Partial Differential Equations (NN4PDEs)

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

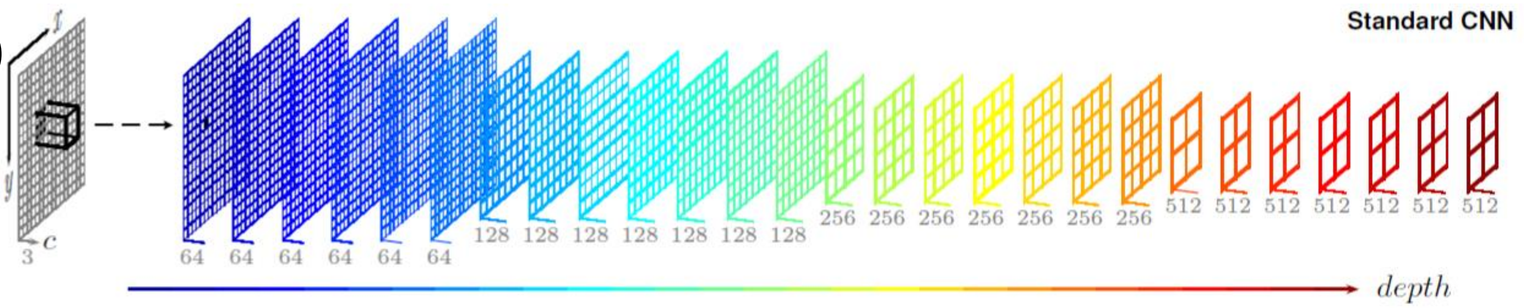

**Advantage**

✓ 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

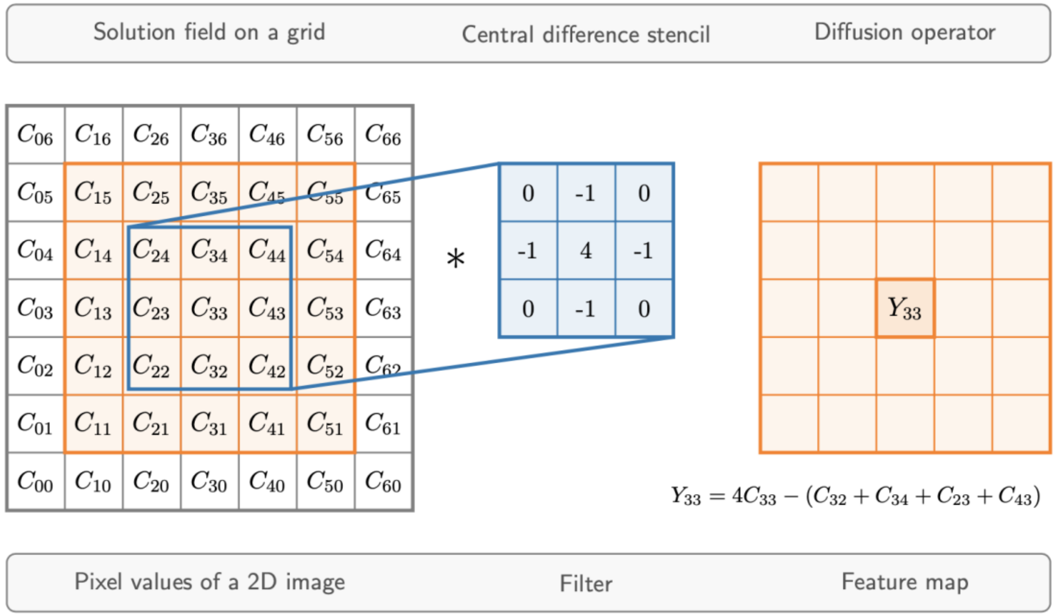
# Methodology - Convolutional neural networks

- Convolution neural networks (CNN)
- ✓ Matrix-free discretization of PDEs
- ✓ No training of the network
- ✓ Known weights in the filters
- Convolutional FEM (ConvFEM)
- ✓ Linear, quadratic and cubic finite element
- Rapid multigrid algorithms
- ✓ U-net structure of F-cycle and V-cycle

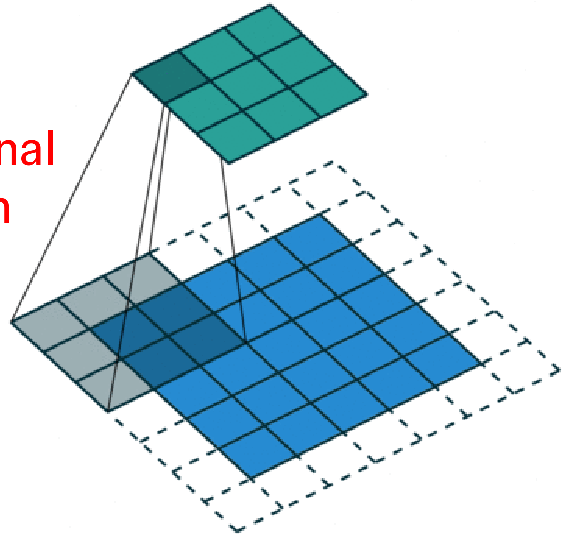
Restriction in multigrid



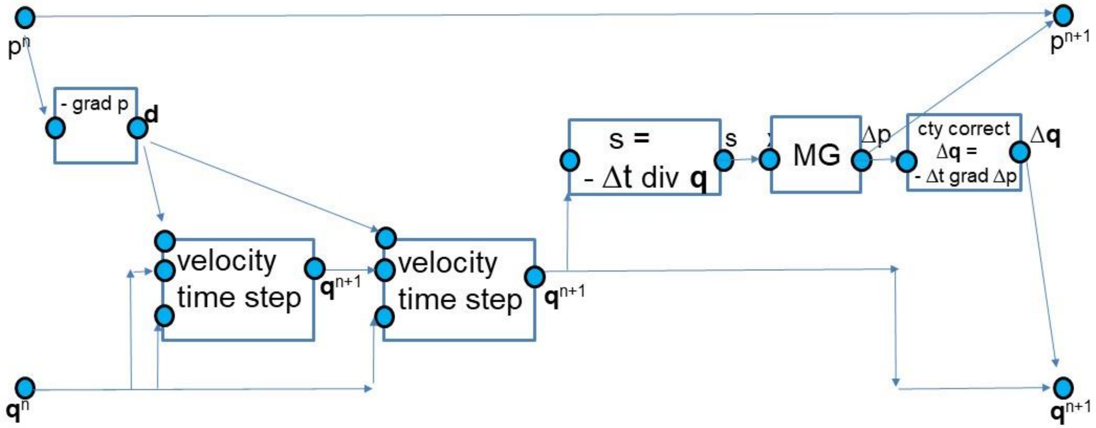

Weights in CNN filters




Convolutional operation



# Methodology - Solving CFD with AI Libraries



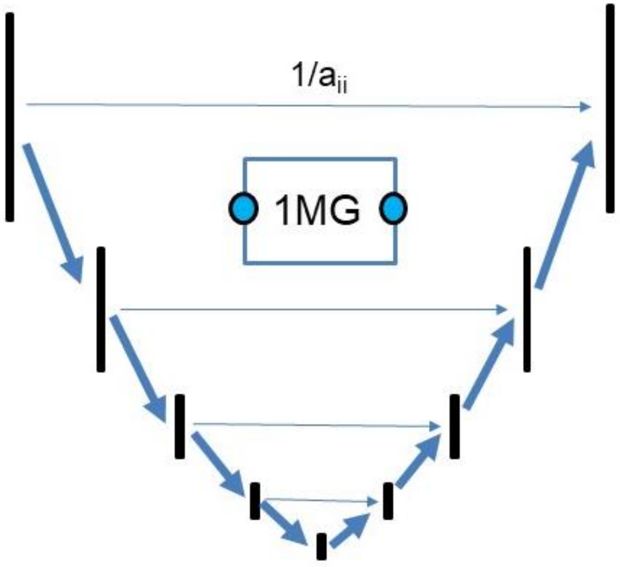

Pressure-velocity coupling

- Two-step time scheme
- Finite differencing method (FDM)
- Finite element method (FEM)
- F-cycle multi-grid for solving pressure
- Projection method
- Petrov-Galerkin stabilisation

$\nabla^2 \phi \longrightarrow$ Central differencing

FDM $\begin{pmatrix} 0.0 & 1.0 & 0.0 \\ 1.0 & -4.0 & 1.0 \\ 0.0 & 1.0 & 0.0 \end{pmatrix}$

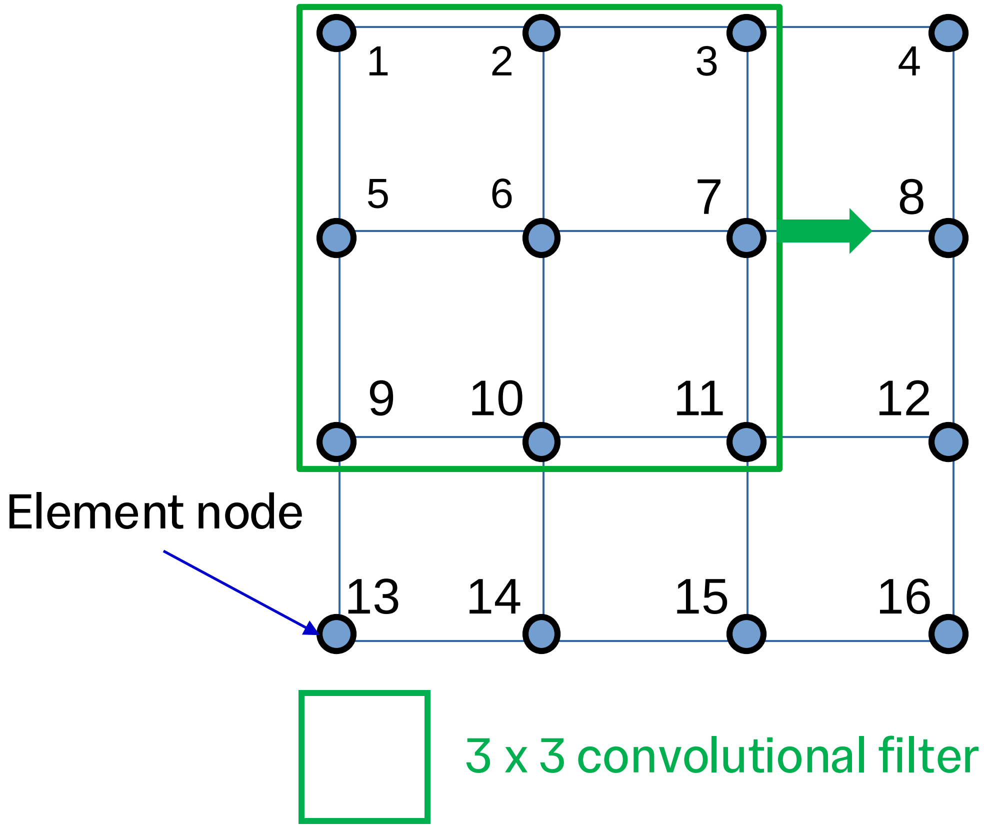
FEM $\begin{pmatrix} 0.25 & 0.5 & 0.25 \\ 0.5 & -3.0 & 0.5 \\ 0.25 & 0.5 & 0.25 \end{pmatrix}$

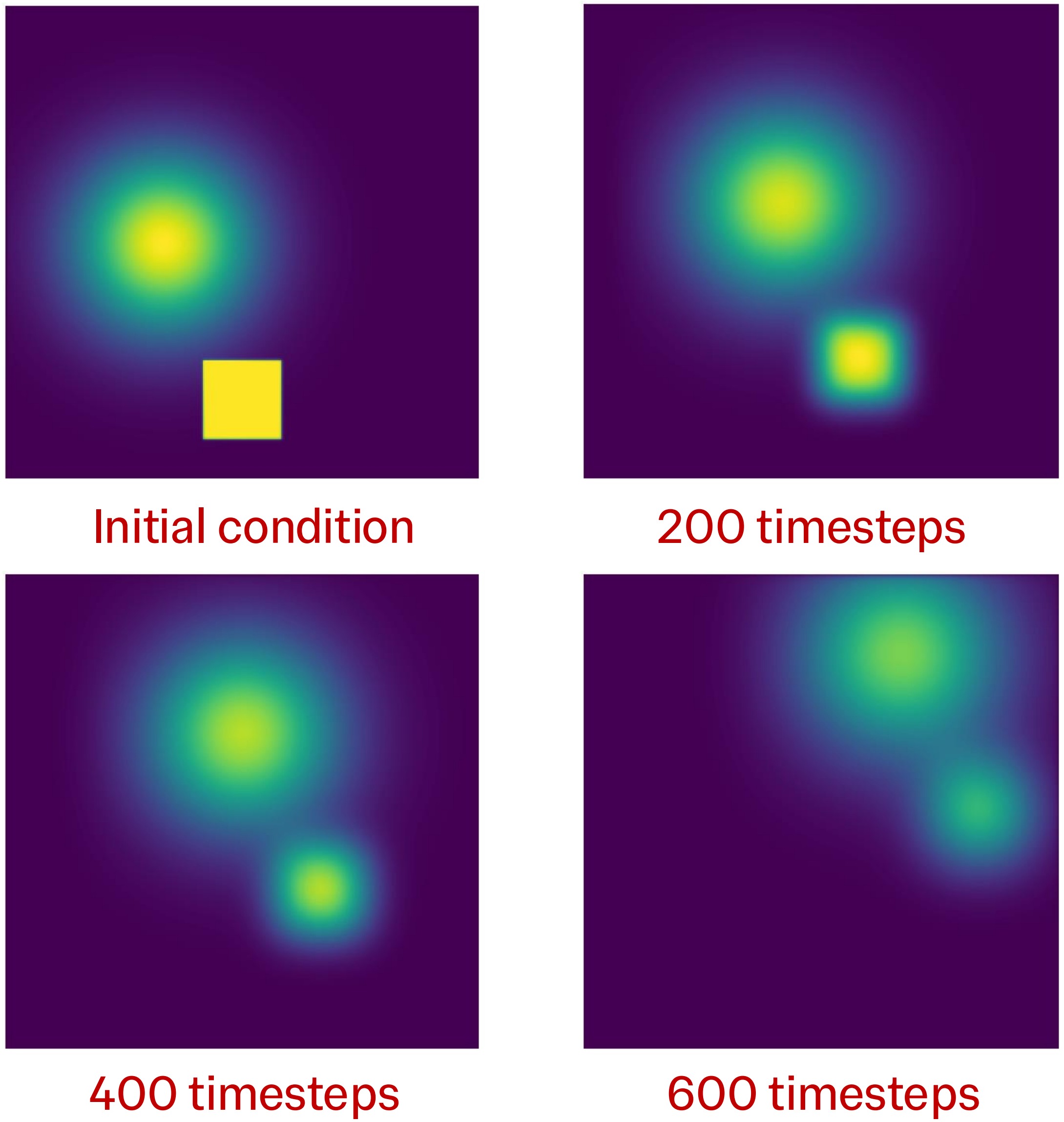



Multigrid with U-net structure

# Methodology - example of solving PDEs using AI libraries

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} - \nu\nabla^2 T = s$$

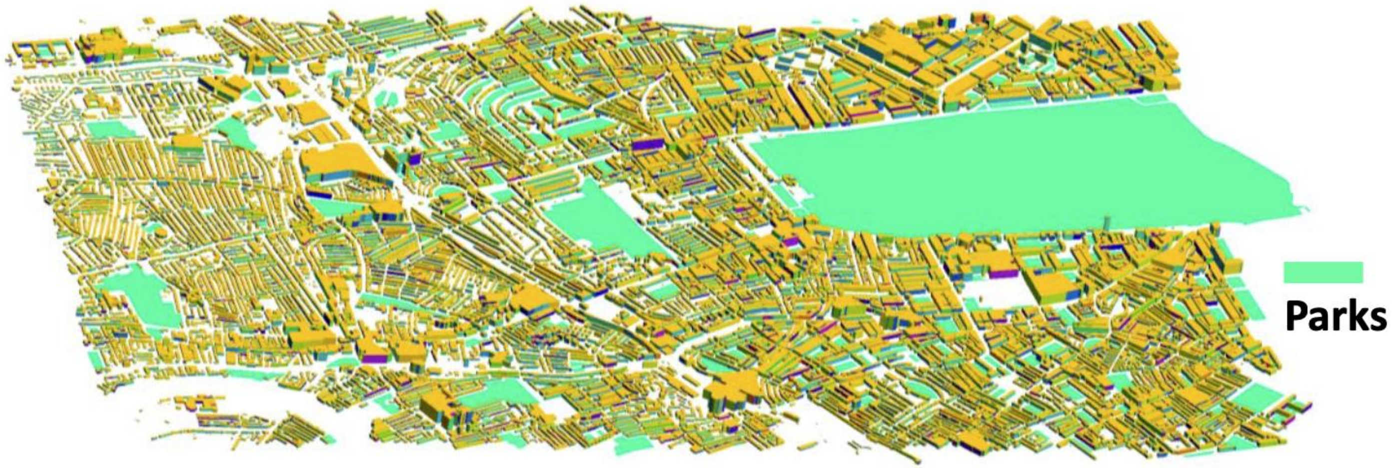


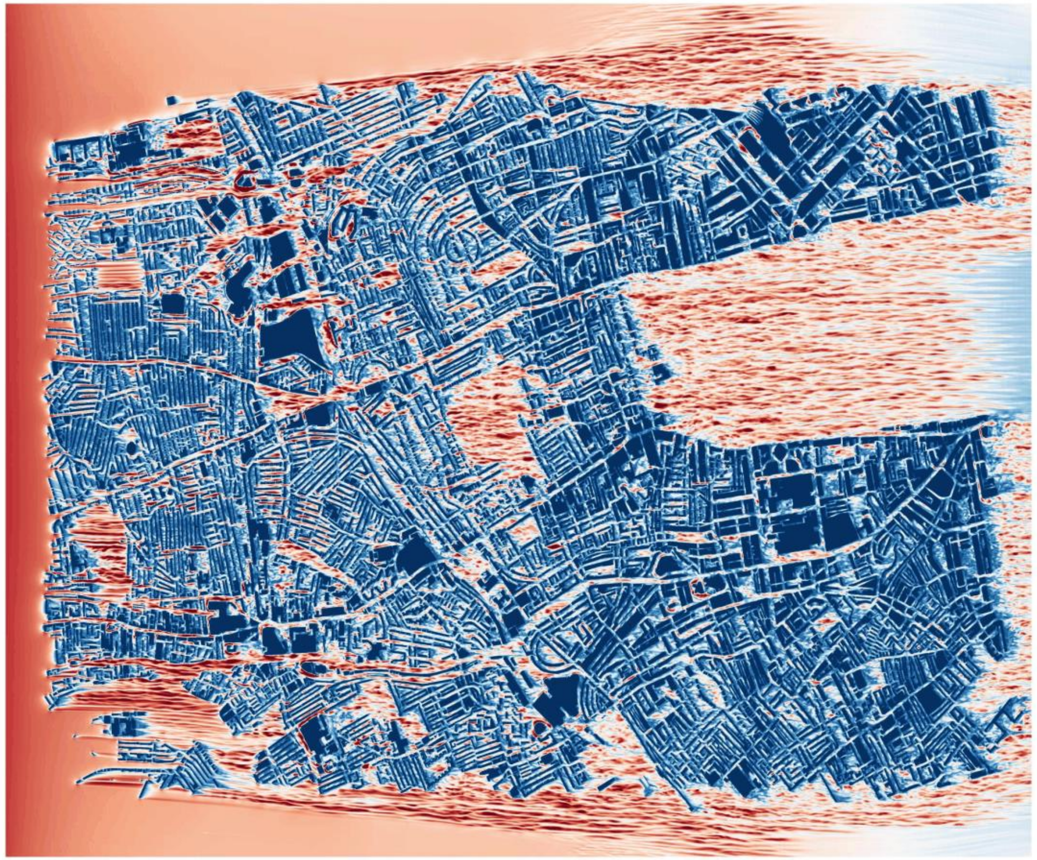
# Airflow modelling using AI4PDEs: South Kensington area

$$\frac{\partial q}{\partial t} + u\frac{\partial q}{\partial x} + v\frac{\partial q}{\partial y} + \sigma q - \nu\nabla\cdot\nabla q = -\nabla p \qquad \nabla\cdot q = 0$$

- 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 – 4 A100 GPUs




Schematic diagram of the area



Airflow speed (m/s)

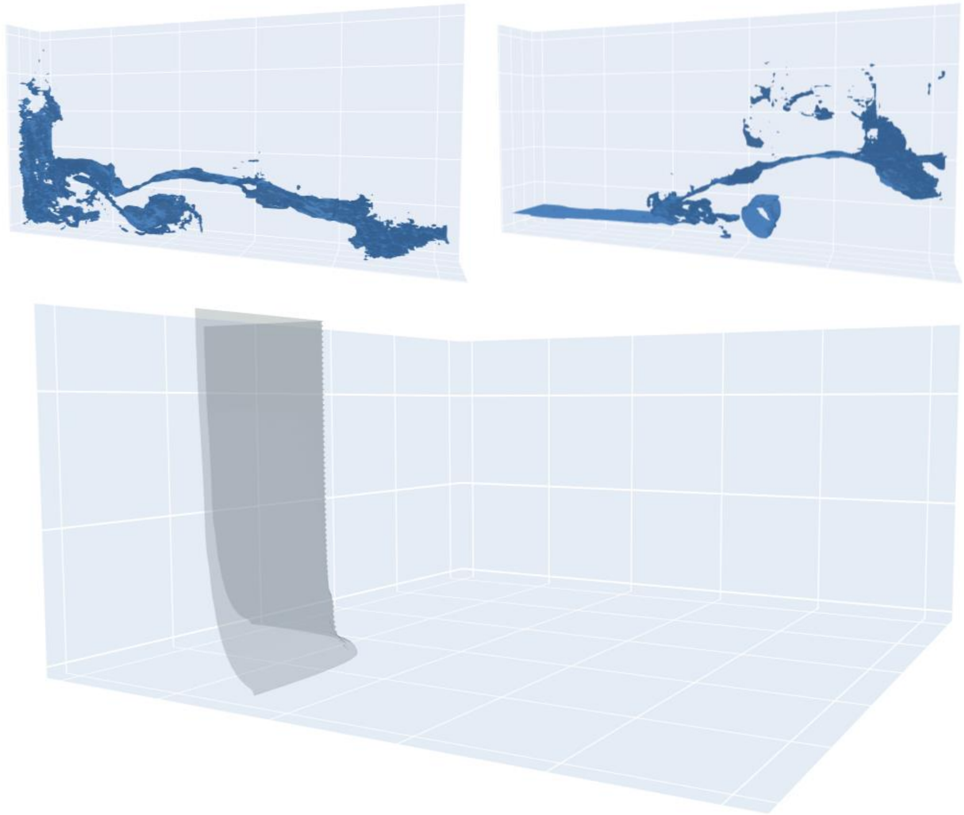
# Multiphase flow using AI4PDEs : Collapsing water column

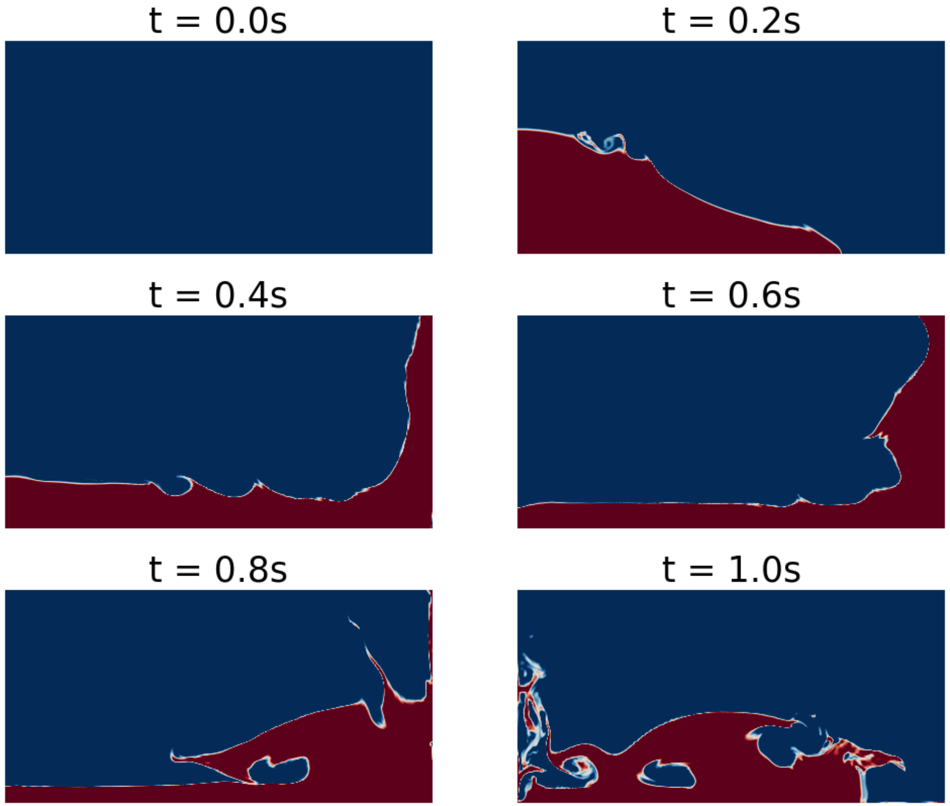
- Cubic domain size: 0.5 (m) x 0.5 (m) x 0.5 (m)
- Grid point: 512 x 512 x 512 (0.256 billion nodes)
- One single GPU

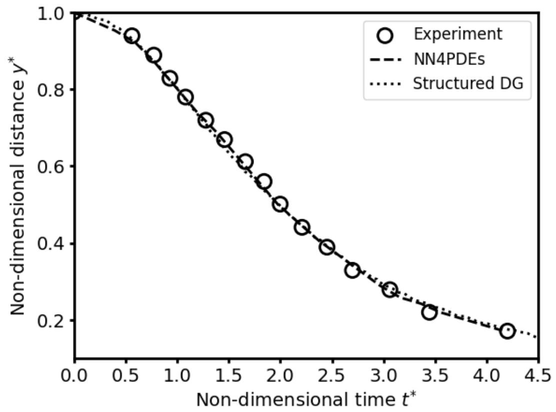
$$\rho\left(\frac{\partial q}{\partial t} + q \cdot \nabla q\right) + \sigma q - \nabla \cdot (\mu \nabla q) = -\nabla p + s_q + s_t$$

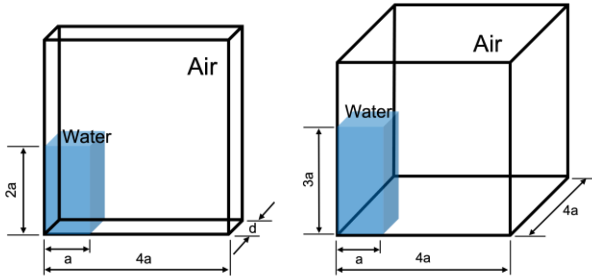
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho q) = 0$$

$$\frac{\partial C}{\partial t} + q \cdot \nabla C = 0$$



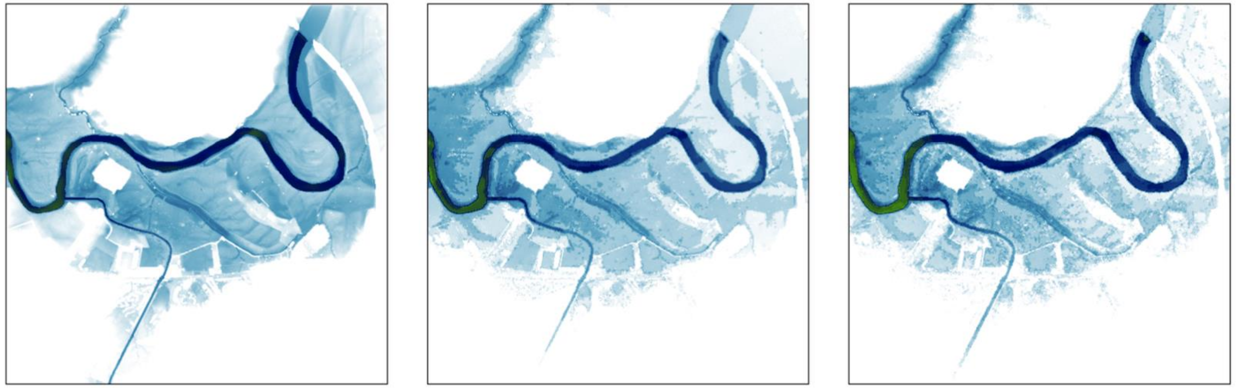


# Multiphase flow using AI4PDEs : Carlisle 2005 flooding

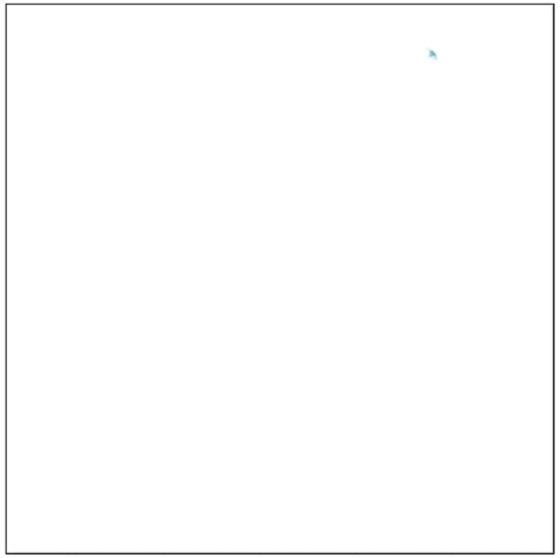
3D flooding using AI4Multiphase and comparison with 2D flooding model



AI4SWE - 951 × 611 AI4Multi - 512 × 512 × 128 AI4Multi - 512 × 512 × 256

Spatial variation of water depth in the flooded area after 10 hours as predict

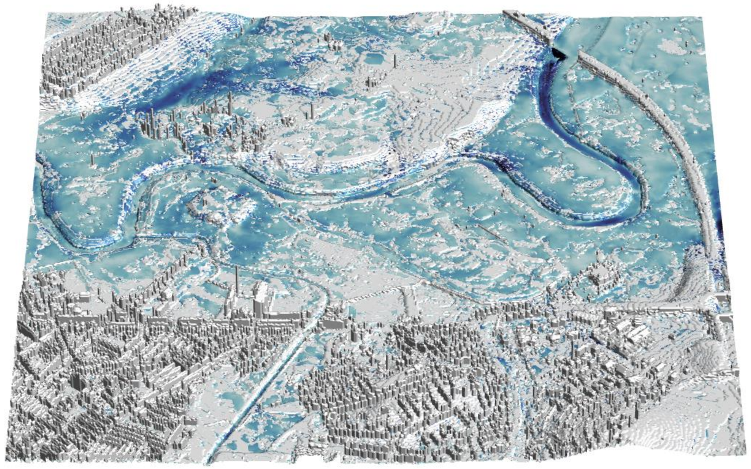
Water depth from 0 to 10 hours



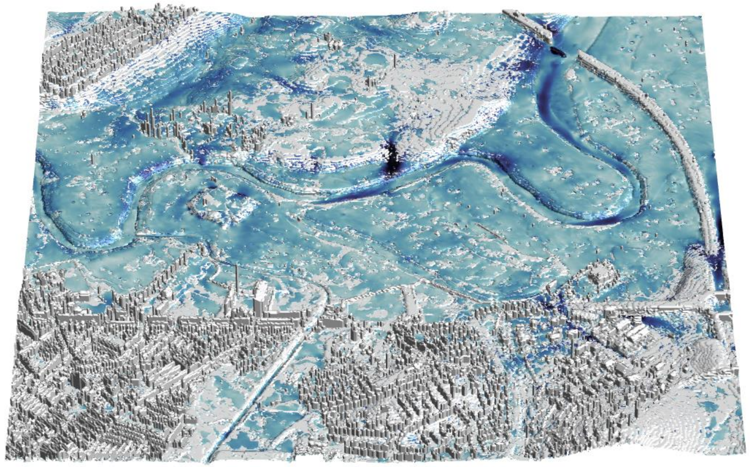
Google Map

Iso-surface colored by water speed (m/s) at two different time levels

T1



T2



# Multiphase flow using AI4PDEs : porous media flow

- Domain size: 0.05 (m) x 0.05 (m) x 0.05 (m)
- Grid spacing: 0.1mm x 0.1mm x 0.1mm
- Number of pellets: ~2000
- Application: $CO_2$ storage
- Surface tension model
- Pressure drop comparing with Ergun equations

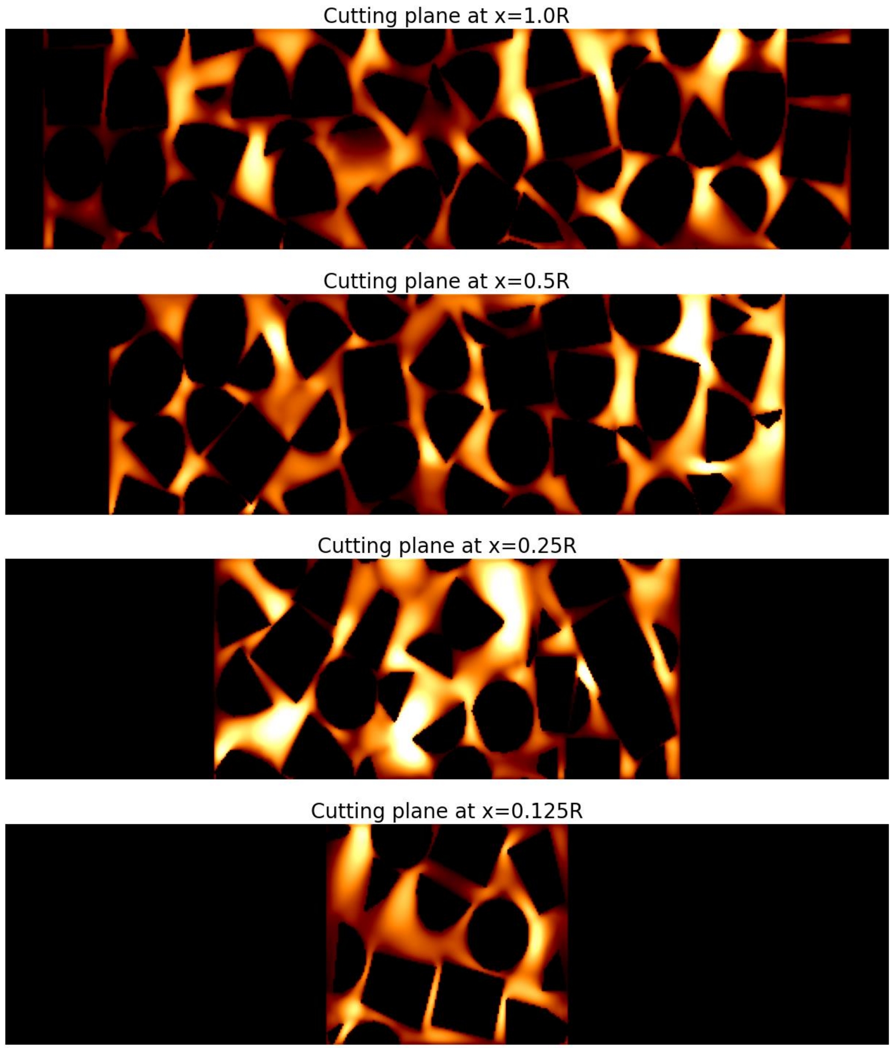
Two scenarios:

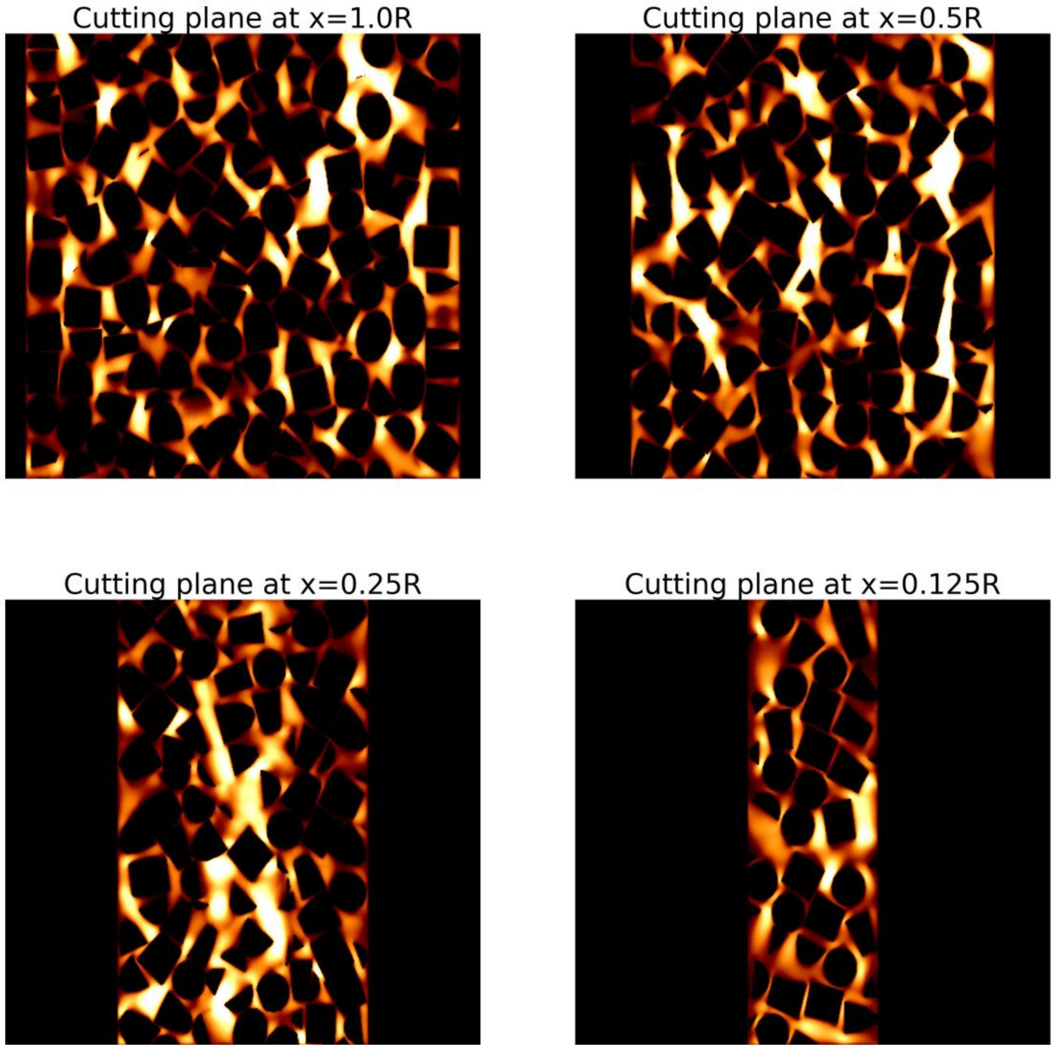
❖ Air is injected from bottom to top (single-phase)

❖ Air is injected into water from bottom to top (multi-phase)

# Multiphase flow using AI4PDEs : porous media flow

## Flow speed (m/s) in the tank – single phase flows



# Multiphase flow using AI4PDEs : porous media flow

## Flow speed (m/s) in the tank – multi phase flows

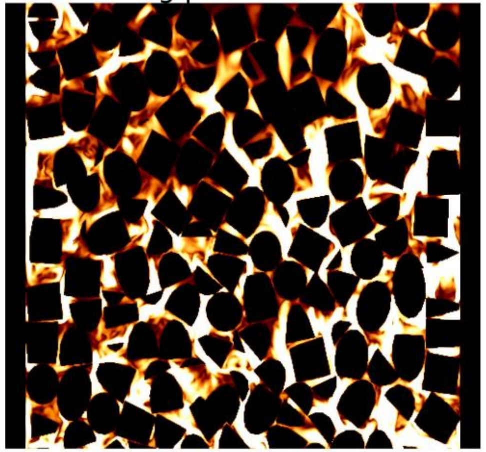
Cutting plane at x=1.0R

Cutting plane at x=0.5R

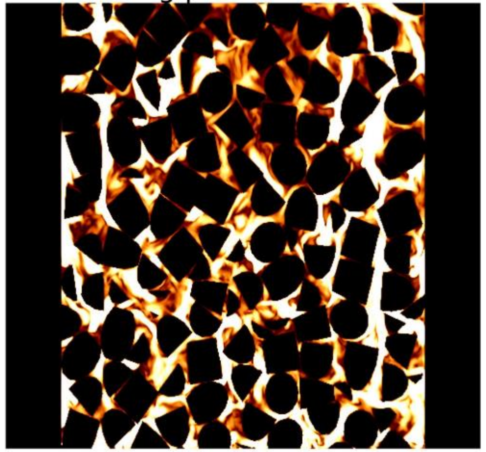
Cutting plane at x=0.25R

Cutting plane at x=0.125R

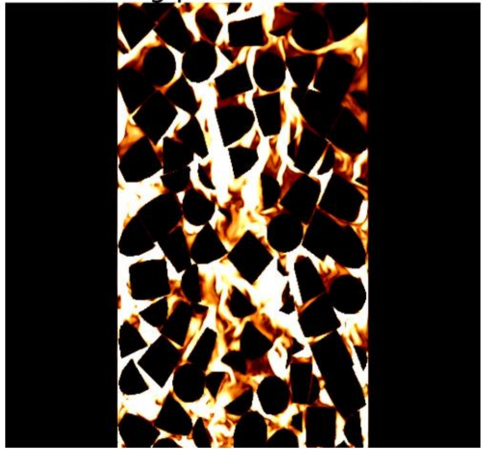
Cutting plane at x=1.0R



Cutting plane at x=0.5R



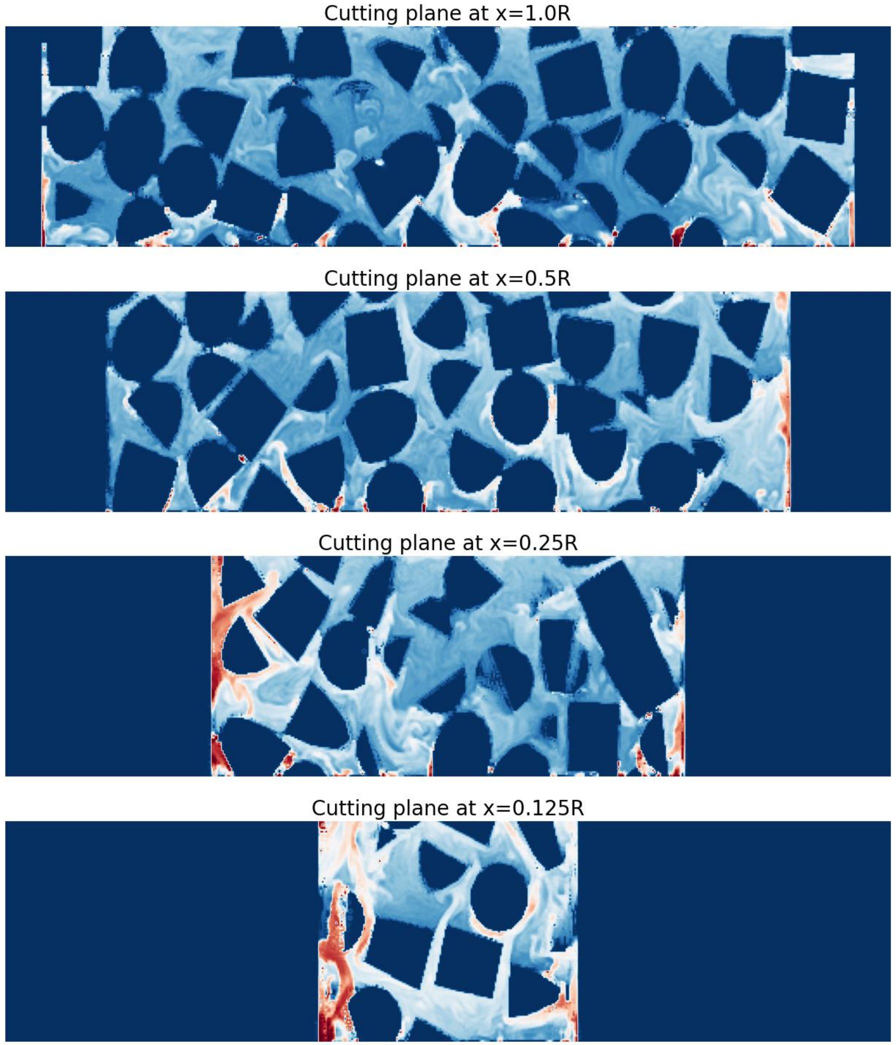
Cutting plane at x=0.25R

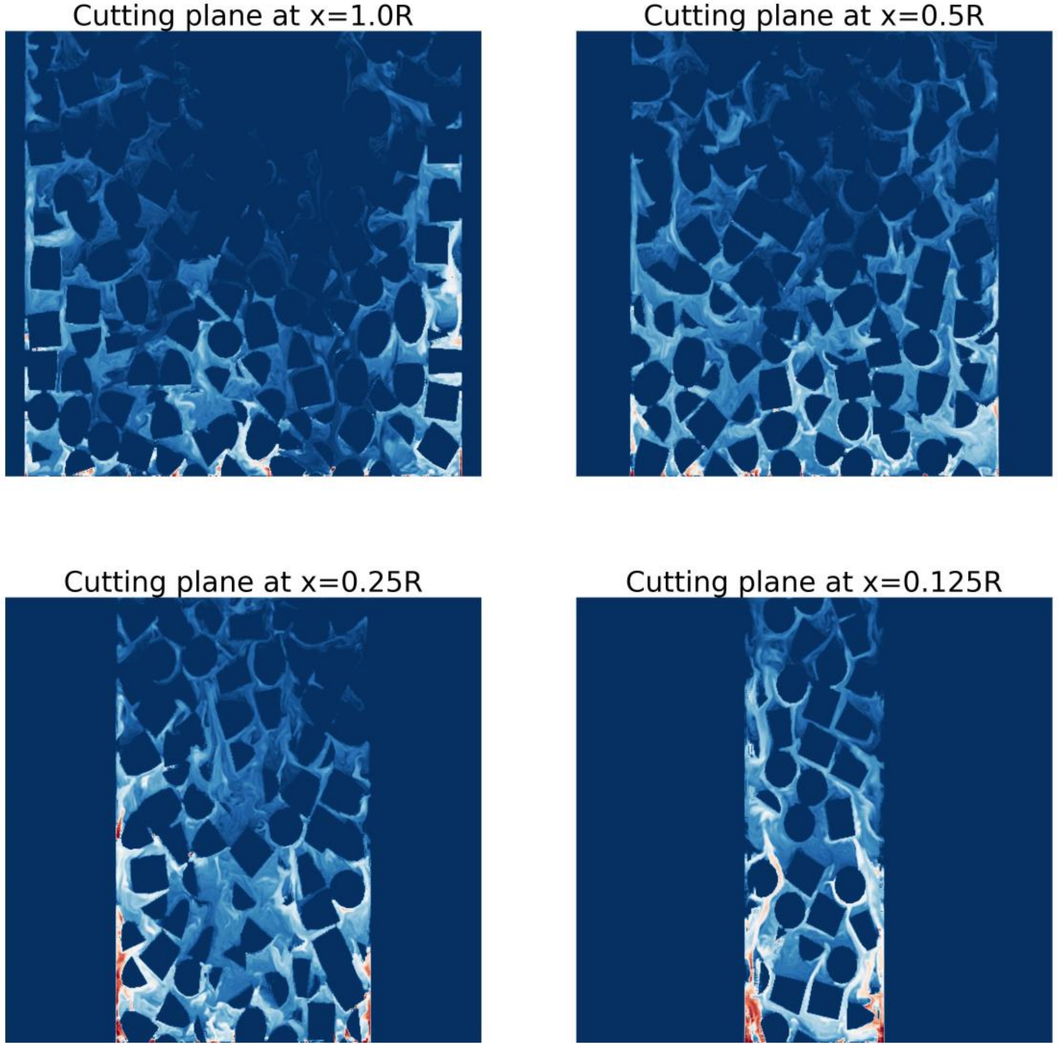


Cutting plane at x=0.125R

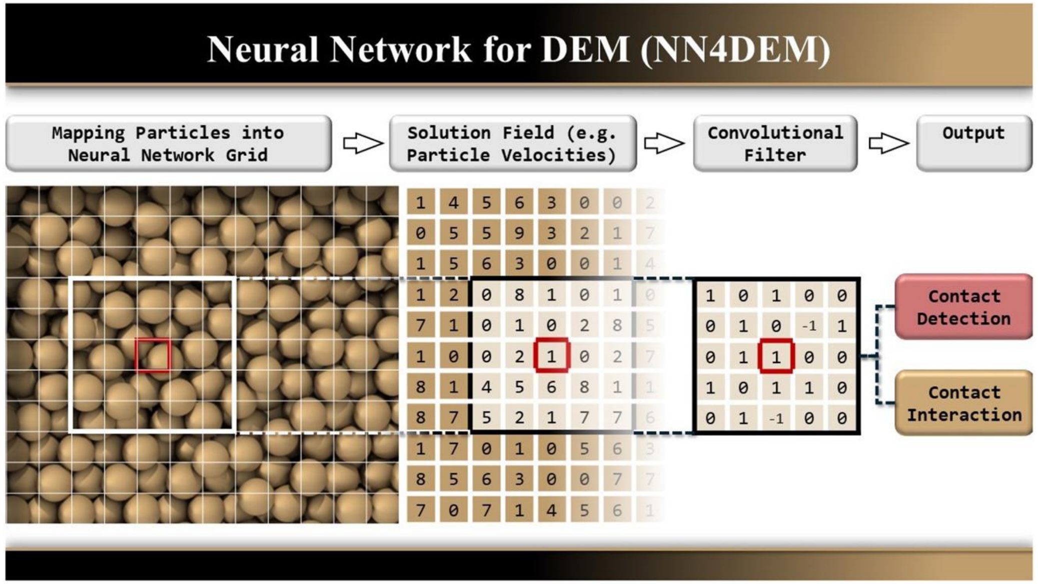
# Multiphase flow using AI4PDEs : porous media flow

## Indicator field (0 to 1) in the tank - multi phase flow



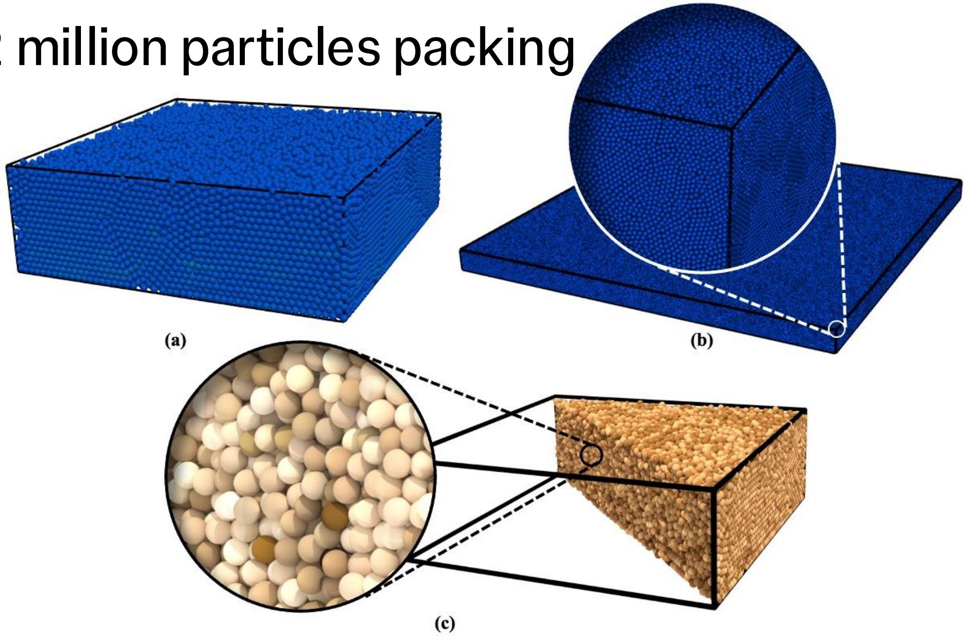



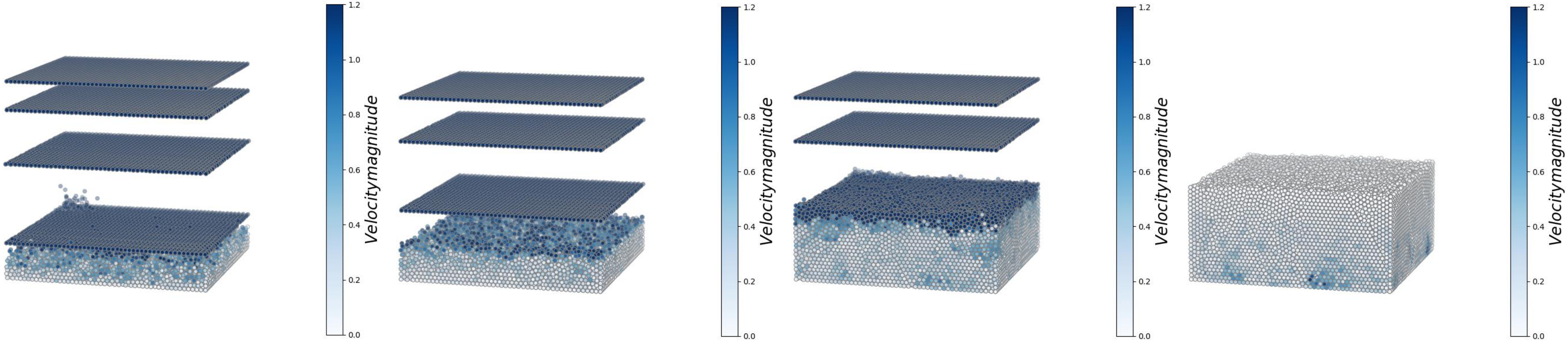
# Example of particle packing using AI4particle/systems




$$\dot{\vec{v}} = \frac{\vec{F}}{m} + \vec{g}\,,$$
$$\dot{\vec{\omega}} = \frac{\vec{T}}{I}\,.$$

32 million particles packing

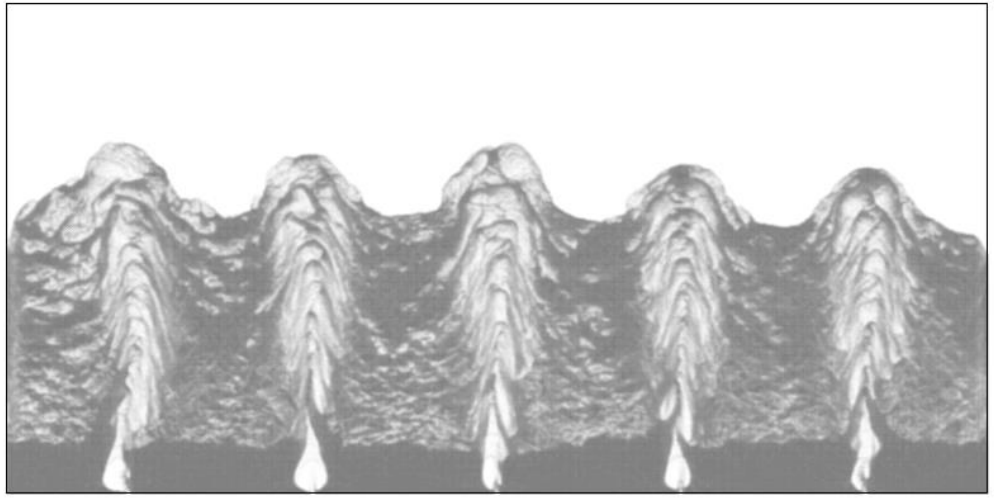


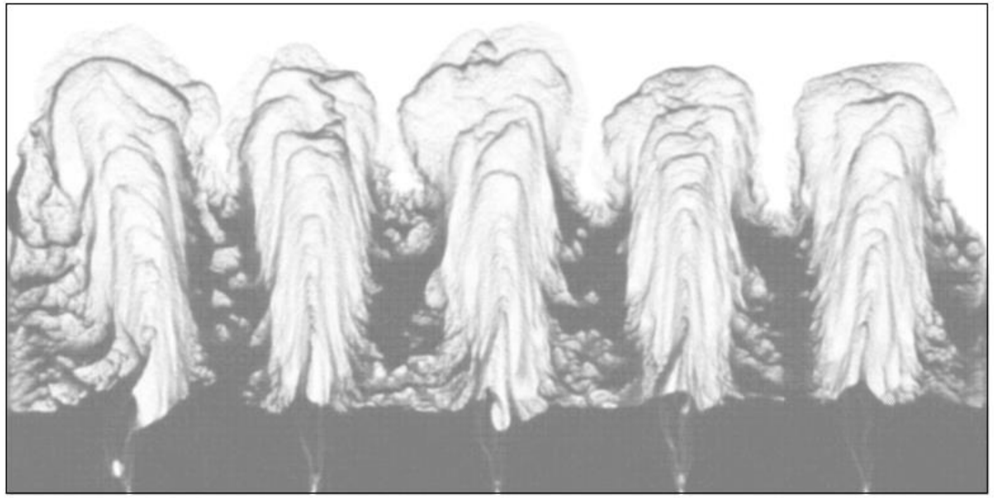
# Fluidised bed flow modelling – AI4Sytems (AI4PDEs + DEM)

20M particles in 2D – running on one single GPU

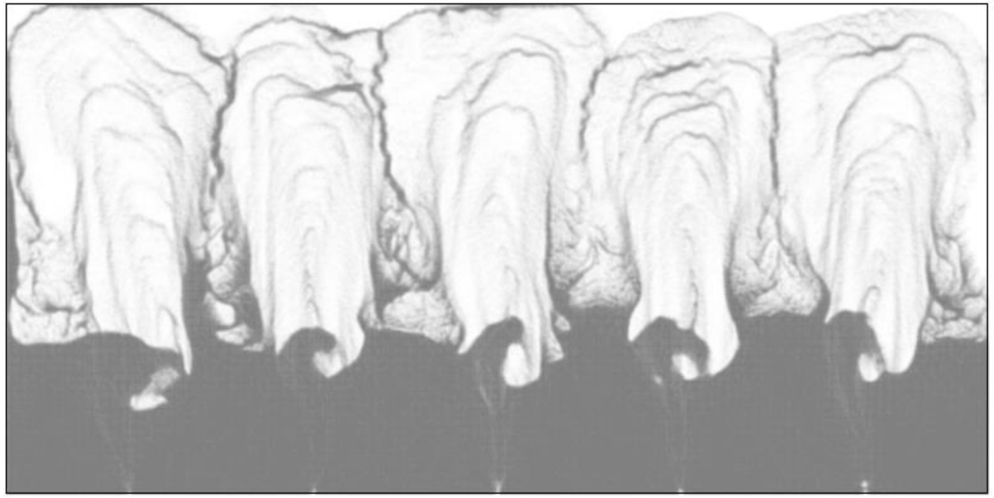
T1



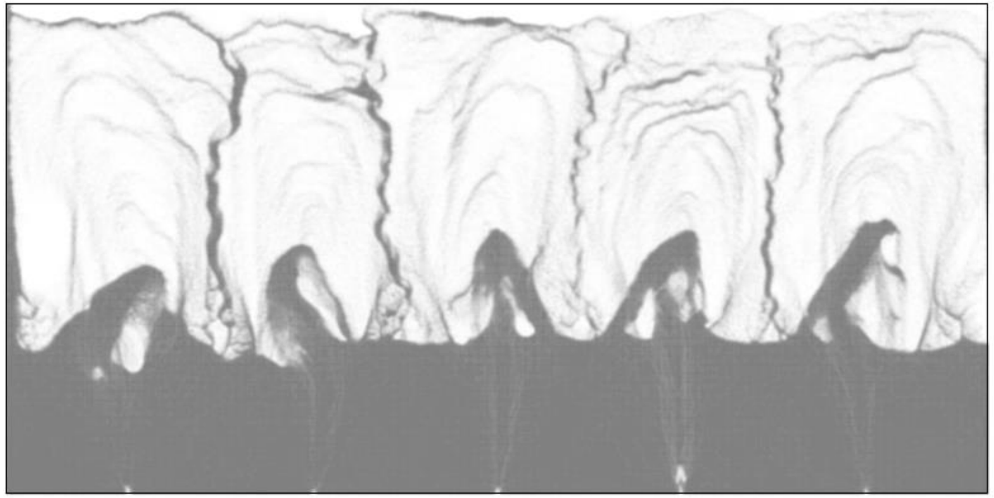
T2



T3



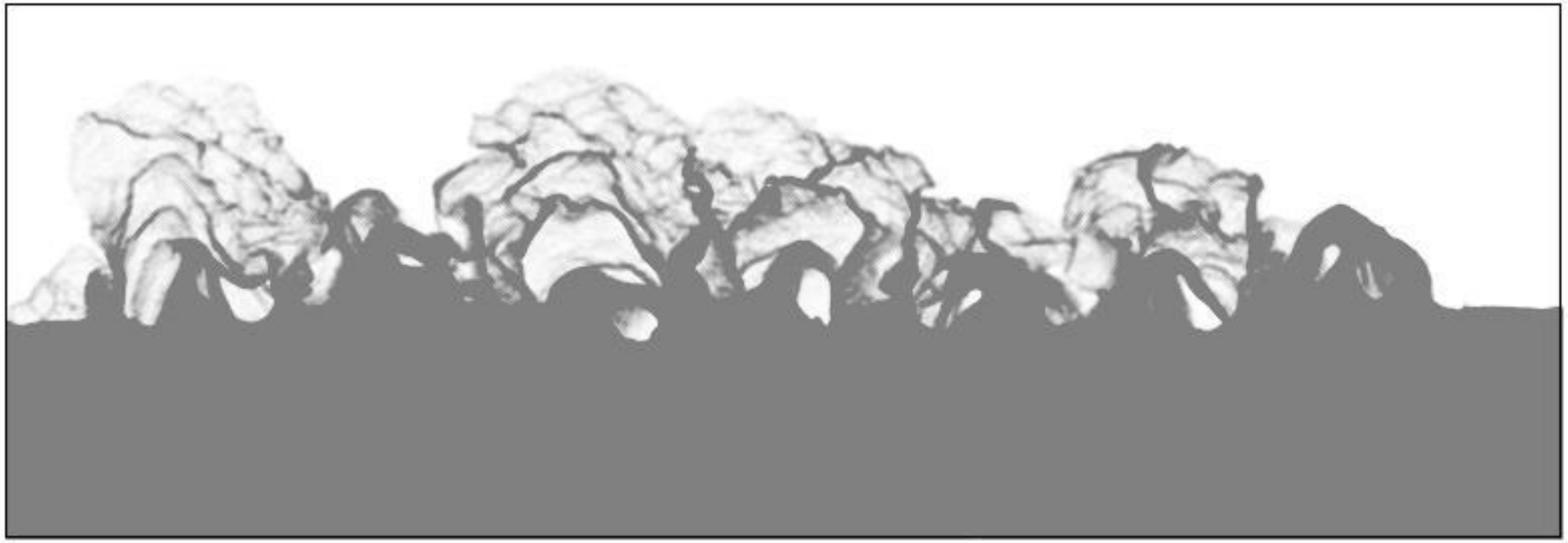
T4



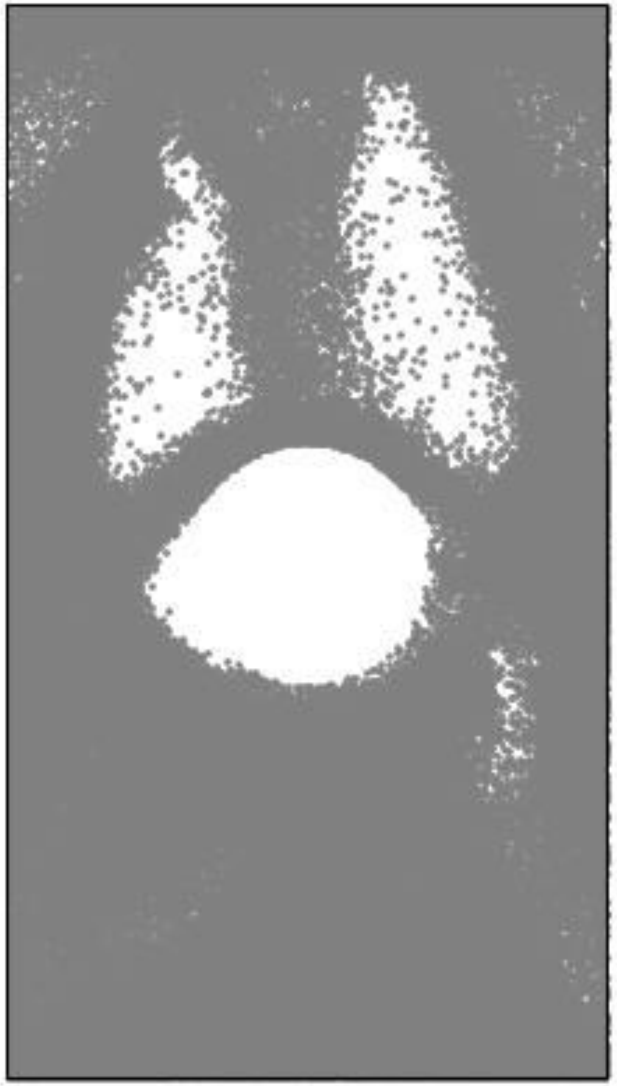
# Example of 2D fluidised bed coupling NN4Particle/System with fluid solver

- CFD-DEM simulation (NN4PDEs + NN4Particles)
- Molecular modelling application

Fluidised bed with an obstacle



40M particles in 2D – running on one single GPU



# Summary and conclusion (NN4PDEs)

- A new numerical solver using AI libraries is proposed, namely NN4PDEs or AI4PDEs. (NVIDIA Modulus)
- The new approach has been validated to predict physical mechanics.
- This approach has been demonstrated on a number of benchmark and realistic problems.

Single-phase flows, multi-phase flows, solid mechanics

- We found the advantage of this approach.

Flexible → CPUs, GPUs and new AI computers

Rapid Computing → digital twins, sensitivity and optimization

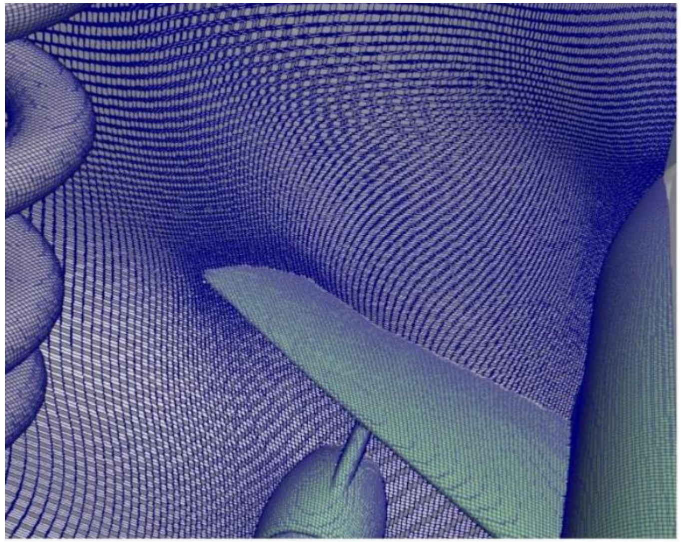
Portable → easy to maintain and develop further

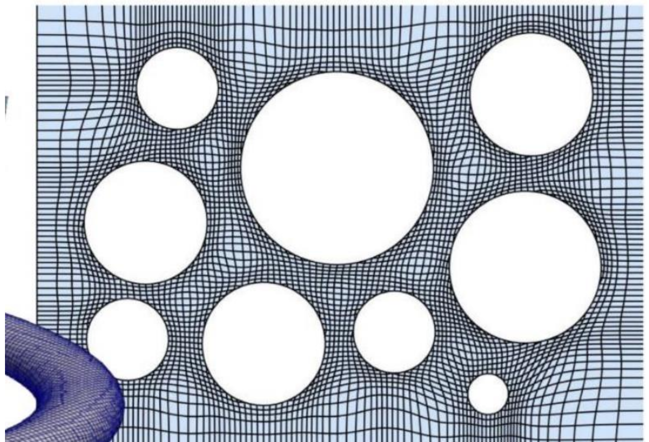
- Further work

Multi-physics solver (molecular dynamics, reservoir system)

Exascale computing (NVIDIA)

Complicated mesh system (distorted and unstructured mesh)





# References (NN4PDEs)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# Thank you