GRaiNNs: Graph Neural Network Simulation for particulate processes

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CCC-ParaSolS Project

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Science and Technology Facilities Council
CoSeC Computational Science Centre for Research Communities
NPRAISE National Platform for Research Technical Professional on AI for Science and Engineering
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What's that?

- The National Platform for Research Technical Professionals on **AI** for Science and Engineering (NPRAISE) is one of the UKRI's Strategic Technical Platforms (STPs)
  - Funded by UKRI through EPSRC and its central DRI programme
  - Is designed to improve the skills of Research Technical Professionals (RTPs) on AI for Science and Engineering (AI4SE) in the UK
  - NPRAISE is run by STFC Scientific Computing
- A call for proposals went out in January to identify RTPs that will benefit from some training:
  - Up to 12 months at 80% FeC
  - https://www.cosec.ac.uk/what-is-cosec/npraise-projects/
  - https://www.cosec.ac.uk/what-is-cosec/npraise-projects/john-morrissey/

So what are you doing?

- Aimed at three different levels: Learn, **Explore**, Excel
- Exploring the use of Graph Neural Networks for the simulation of particulate solids
- Graph networks with their nodes and edges are quite a similar topology to a DEM simulation with particles and contacts
  - Initially works from Google DeepMind
  - NE3 Krishna Kumar presented some work on the topic

[1] Sanchez-Gonzalez et al. (2020): https://doi.org/10.48550/arXiv.2002.09405.
[2] Choi & Kumar (2024). https://doi.org/10.1016/j.compgeo.2024.106374.
[3] Kumar & Vantassel (2022): https://doi.org/10.48550/arXiv.2211.10228.
[4] Mayr et al. (2023): http://arxiv.org/abs/2106.11299.

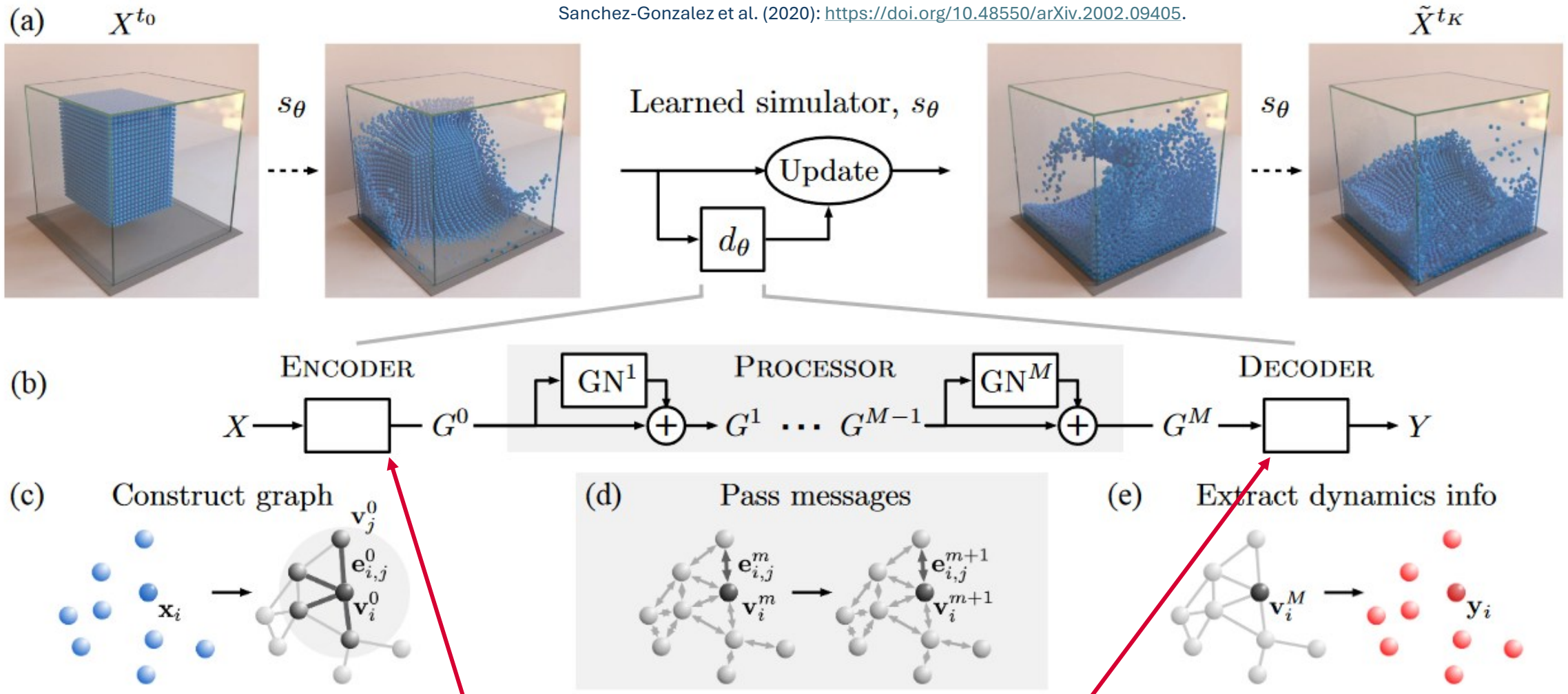
Why GNNs?

- Graph-based Neural Networks (GNNs) offer a logical starting point for modelling dynamics granular systems
  - This enables GNNs to learn underlying interaction laws that govern the particle dynamics.
  - GNN-based tools are often able to make reasonable predictions of particle dynamics but currently do not predict forces or stresses in a system
  - limited usefulness for making engineering decisions about complex industrial systems, e.g., predicting the pressures within a silo

- Current state-of-the-art GNN-based simulators can handle simple geometry primitives but not complex boundaries and dynamic systems.
- A further limitation is that GNNs have high memory demands.
  - A typical desktop GPU with 16GB of memory may be limited to just 20,000 particles: far fewer than needed to model most industrial systems
  - However, next-gen systems such as Isambard-AI create the opportunity to apply such tools on a much larger scale, offering faster training and ability to solve larger problems

What is a GNN?

Sanchez-Gonzalez et al. (2020): https://doi.org/10.48550/arXiv.2002.09405.



Distance Calculation

Predicted position & velocity

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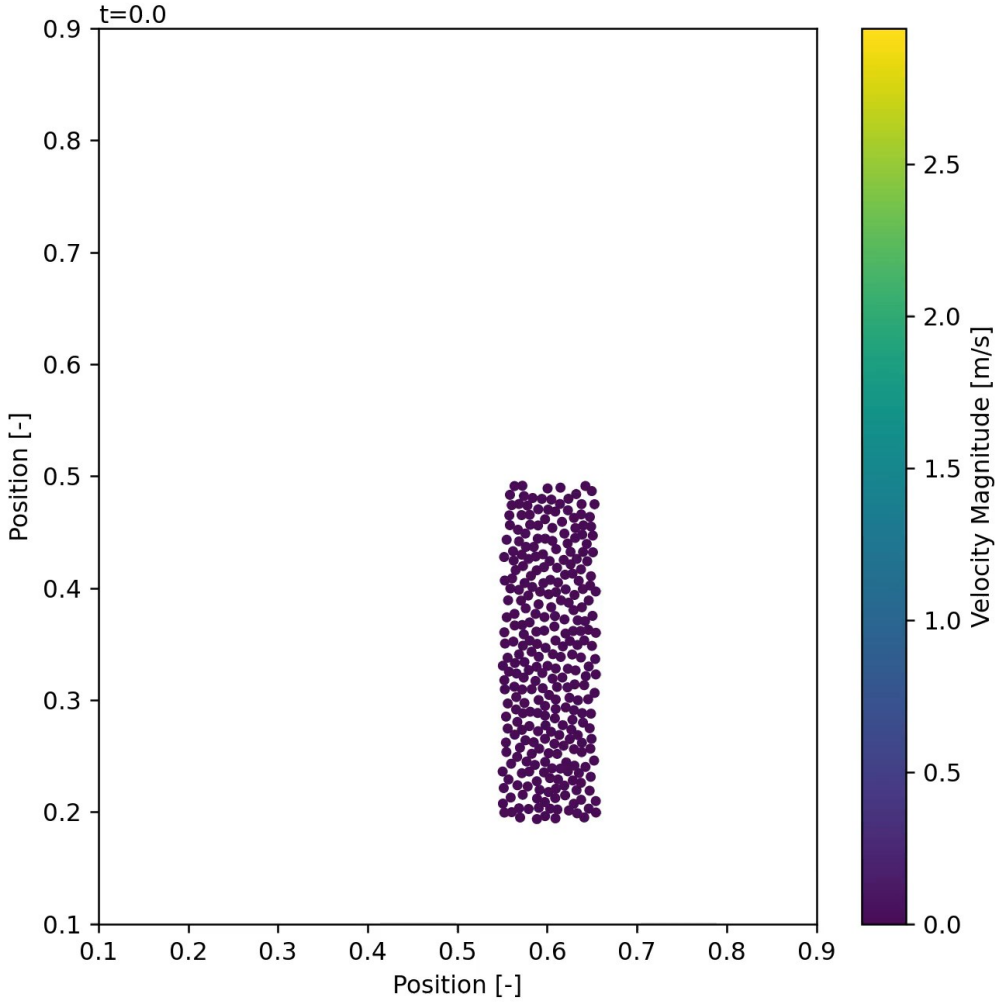
Work to be “Explored”

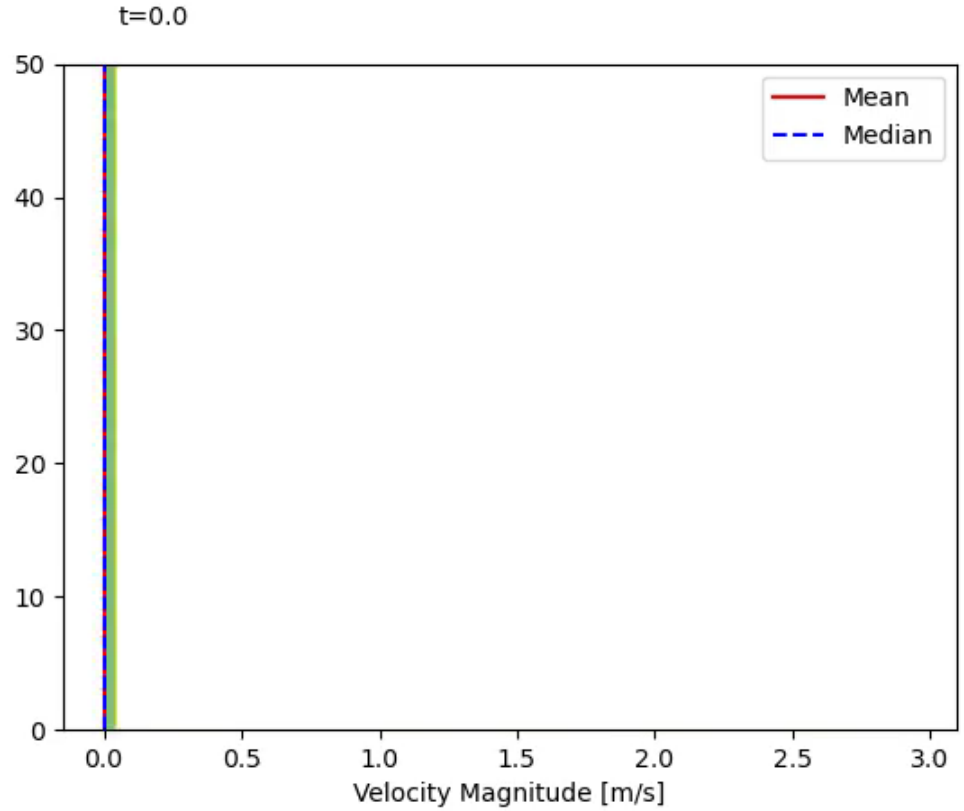
- New encoder and decoder architectures to attempt;
  - Inclusion of complex geometries and dynamics
  - Force predictions

- Generating some high quality DEM datasets for industrial problems
  - Silo discharge (see previous talk)
  - Rotating drum or mixer?

- Exploring hybrid use:
  - GNN to predict particle positions (very large timestep / cheap contact search)
  - Full DEM force calculation and update

Example – Trained from public dataset





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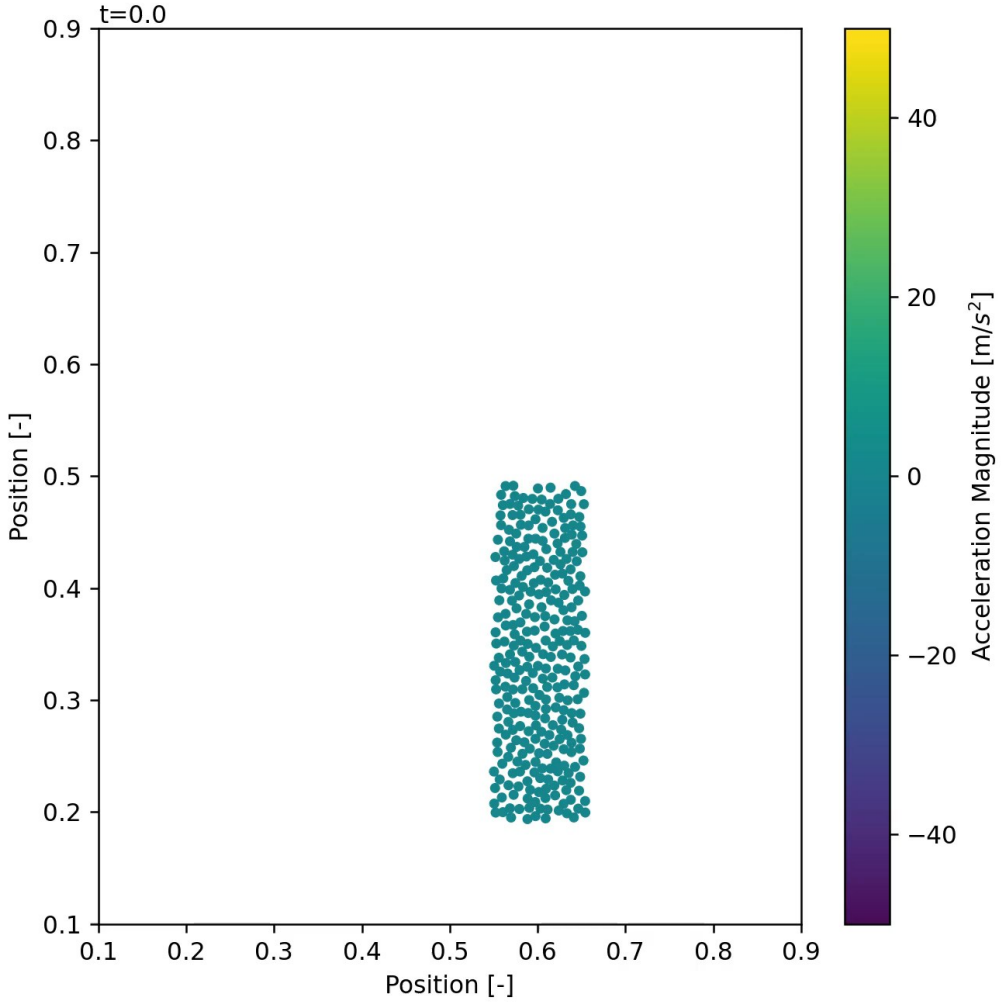

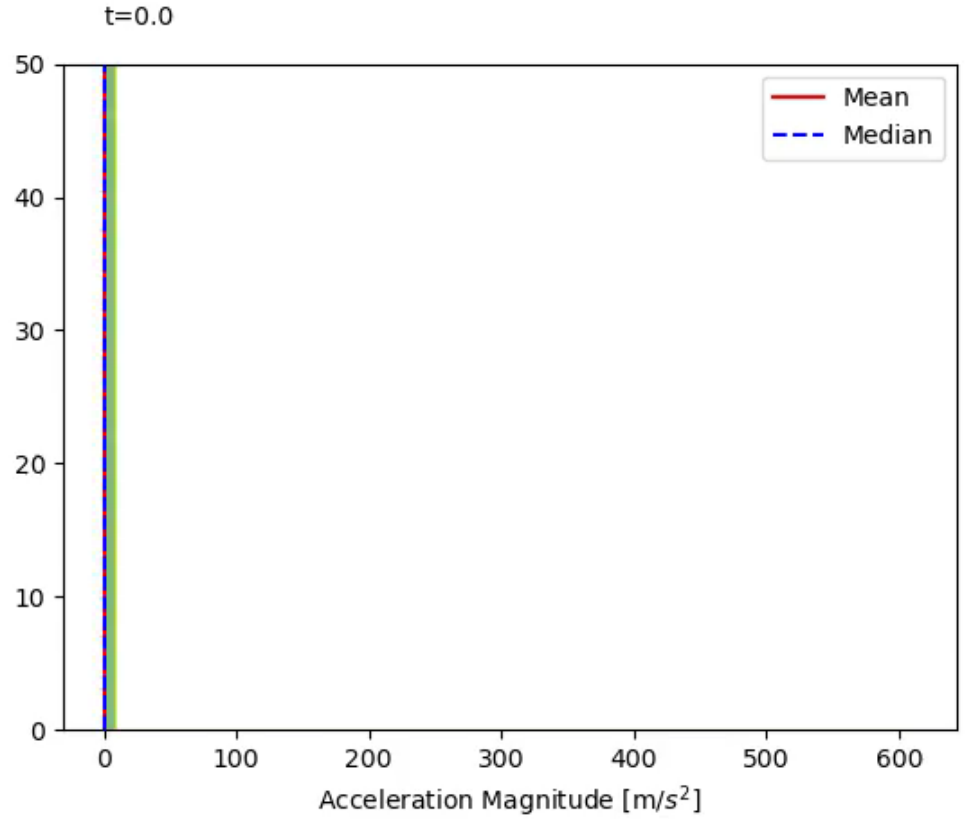

What's in it for the Community?

- A GNN based solver that can run on UK architecture and support complex geometries and dynamics
  - Boundary interactions
  - Improved temporal performance by using LSTM or Transformers
  - Investigating suitable loss functions
  - Investigating kd-Tree vs FRNN (with USP) for search
- Some high-quality DEM training datasets
- Documentation and tutorials on how to train/use to promote software sustainability
- A webinar (*or series of*) to further build upon training provided at previous events

When is this happening?

- Starting from 1st of September 2026
  - 50% time for twelve months

- Possible webinars in 2027 from February to October
  - To be decided based on progress

Questions?

ParaSolS

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Discourse https://parasols.discourse.group/

https://www.linkedin.com/company/ccc-parasols/