Frameworks for DCE

with gradient based optimisation

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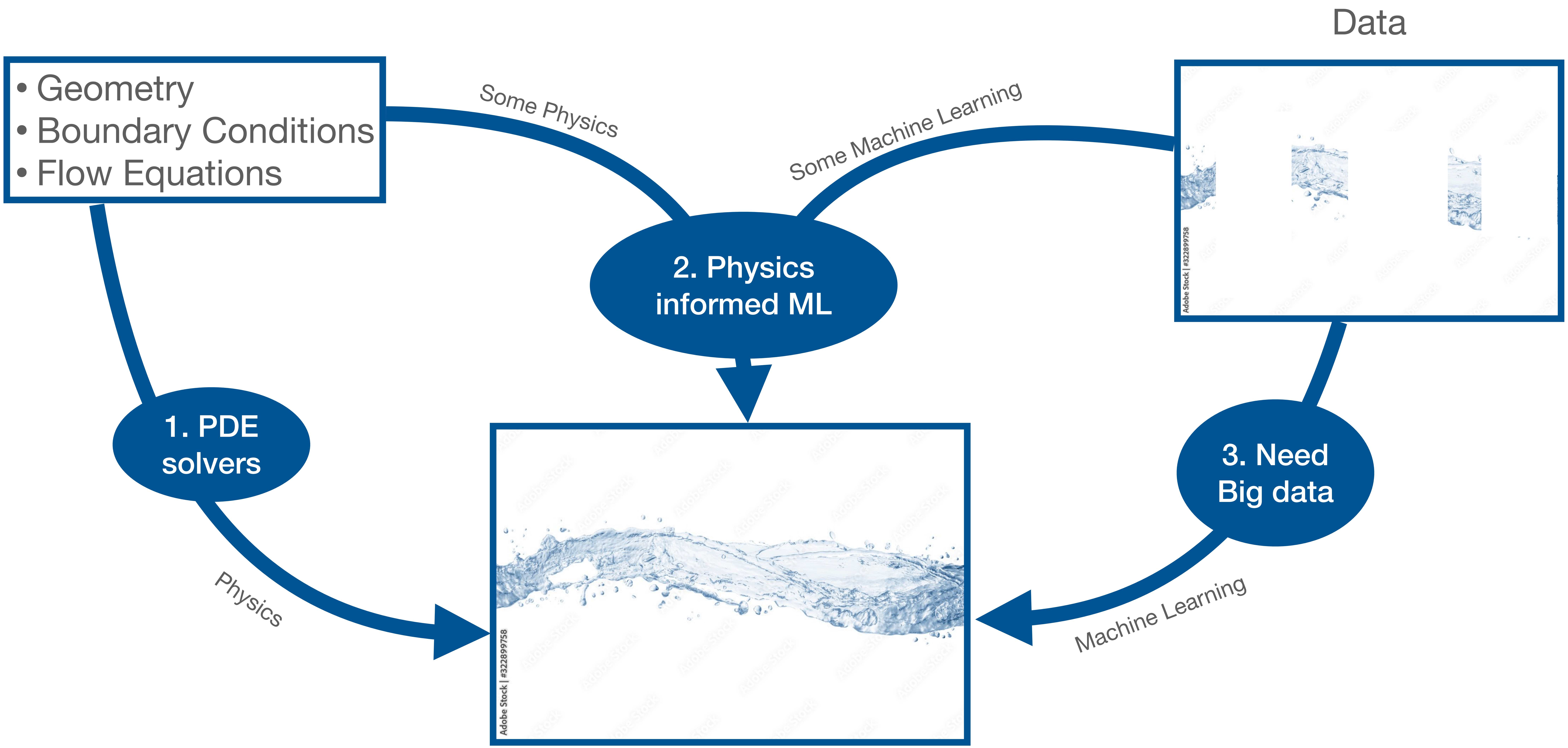
Physics Informed Machine Learning



ML Framework for Engineering

Classical physics

ML Framework for Engineering

Classical physics + machine learning

ML Framework for Engineering

Optimise controls

$$\frac{\partial C}{\partial x'} = \frac{\partial z}{\partial x'} \longleftrightarrow \frac{\partial \mathscr{L}}{\partial z}$$

Optimisation Framework

AutoDiff with PyTorch

- Analytical derivatives: chain rule as code runs
- Complex models
- Gradient-based optimisation
- Probabilistic models by re-parameterisation trick

$$\frac{\partial C}{\partial x'} = \frac{\partial z}{\partial x'} \qquad \longleftrightarrow \qquad \frac{\partial \mathscr{L}}{\partial z}$$

Opportunities for DCE

Physics informed neural net: Solve PDEs with NN

- Solve for all possible parameters
- Include data

$$\mathscr{L} = w_{\text{data}}\mathscr{L}_{\text{data}} + w_{\text{PDE}}\mathscr{L}_{\text{PDE}}$$

- Design NN architecture to satisfy physical laws
- Can NNs always find good solutions?
- Uncertainty propagation through PDE

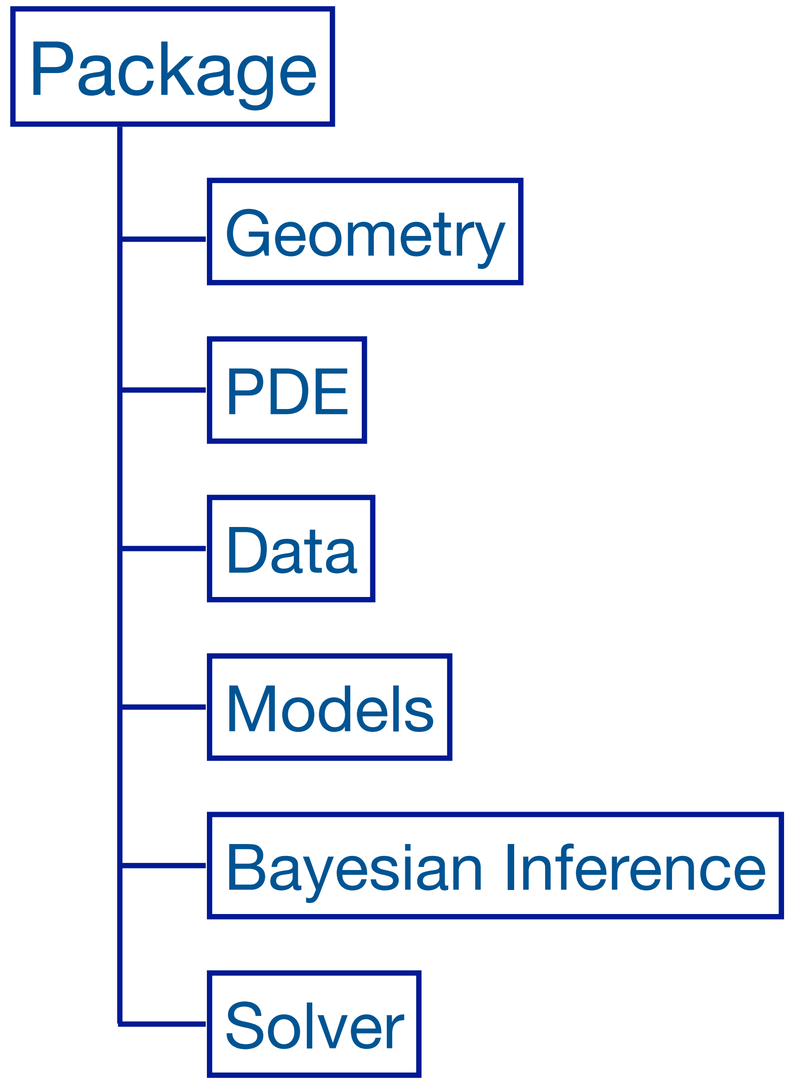
$$\frac{\partial C}{\partial x'} = \frac{\partial z}{\partial x'} \longleftrightarrow \frac{\partial \mathscr{L}}{\partial z}$$

- Model calibration

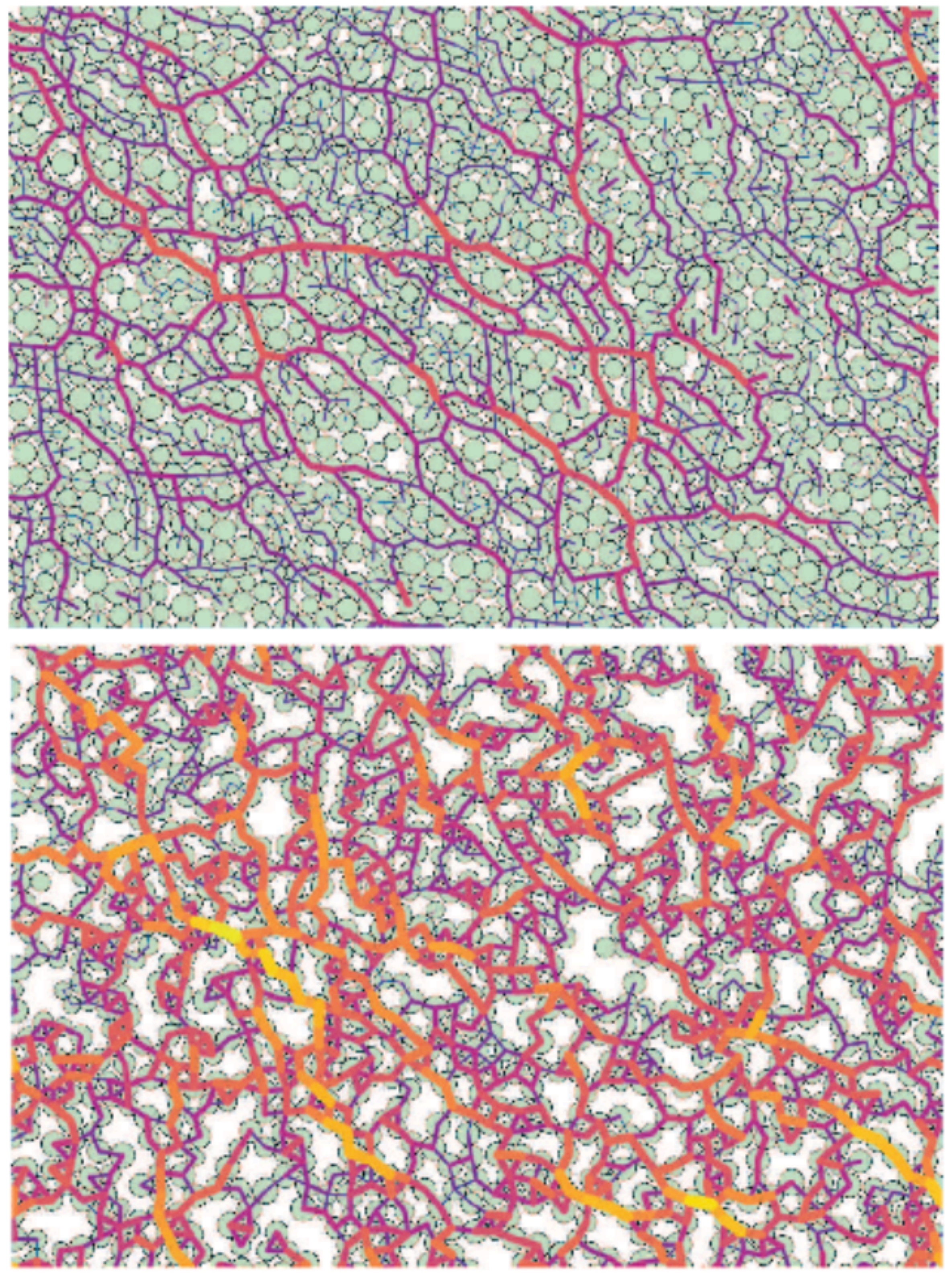
Opportunities for DCE

Application to Digital twins

- Develop or extend a python package
  - Specifically for digital twins
  - Real-time data
  - Probabilistic or deterministic models and NN



Demonstrator Ideas In Mineral Processing



Theory

Adapt physics informed neural nets to grains

- NN for grain kinematics (as opposed to PDEs)
    - Grain specific loss function
- Inverse problem: what is the physical law or material?
    - E.g. geotechnical: porosity, permeability, strength
    - E.g. transient response

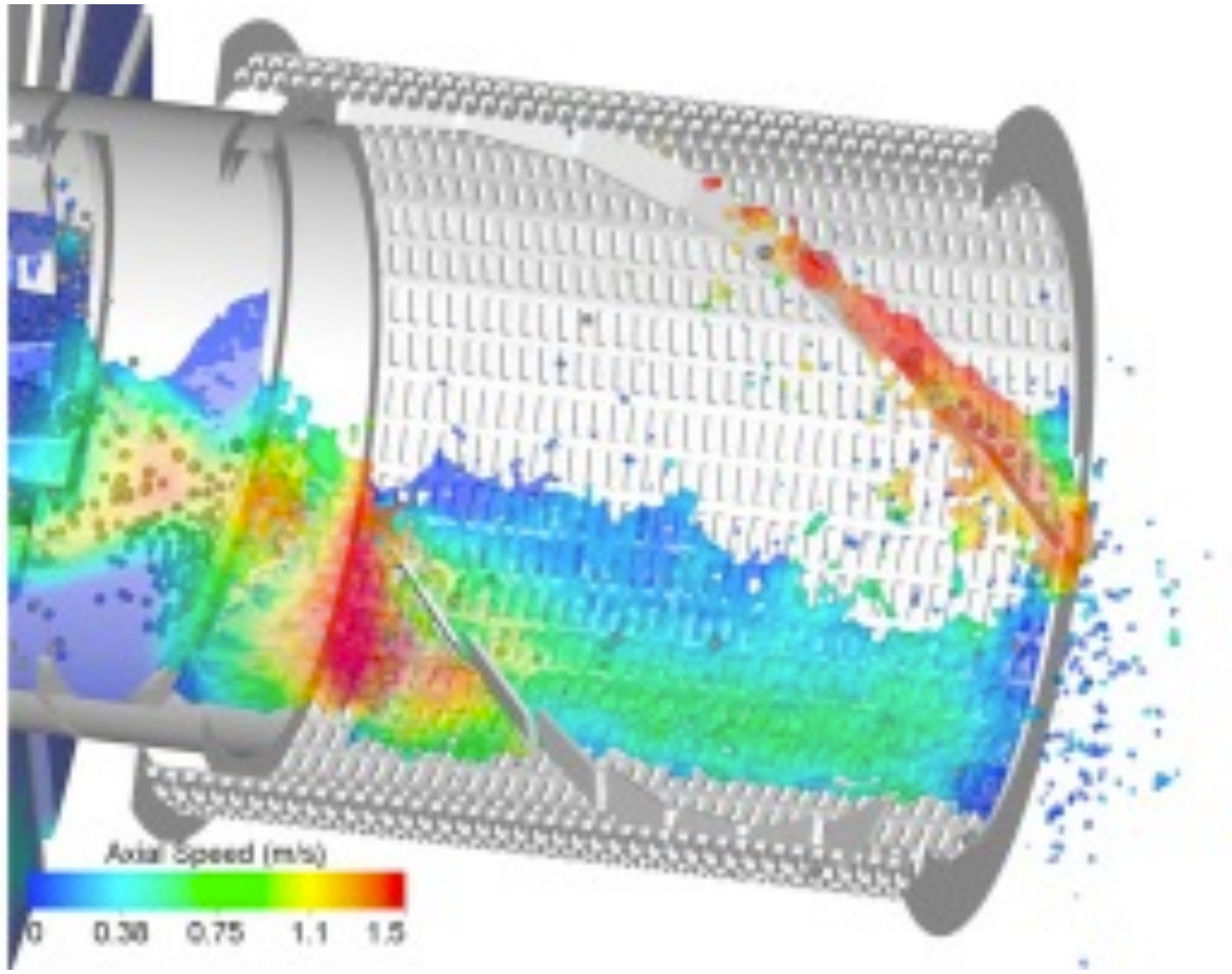
$$\mathscr{L} = w_{\text{data}}\mathscr{L}_{\text{data}} + w_{\text{PDE}}\mathscr{L}_{\text{PDE}}$$

$$\mathscr{L} = w_{\text{data}}\mathscr{L}_{\text{data}} + w_{\text{Grain}}\mathscr{L}_{\text{Grain}}$$

Applications

Predict flow features

- Energy efficiency of mineral processing equipment
- Particle Mixers
- Powder “flowability”
- Granular wear and tear

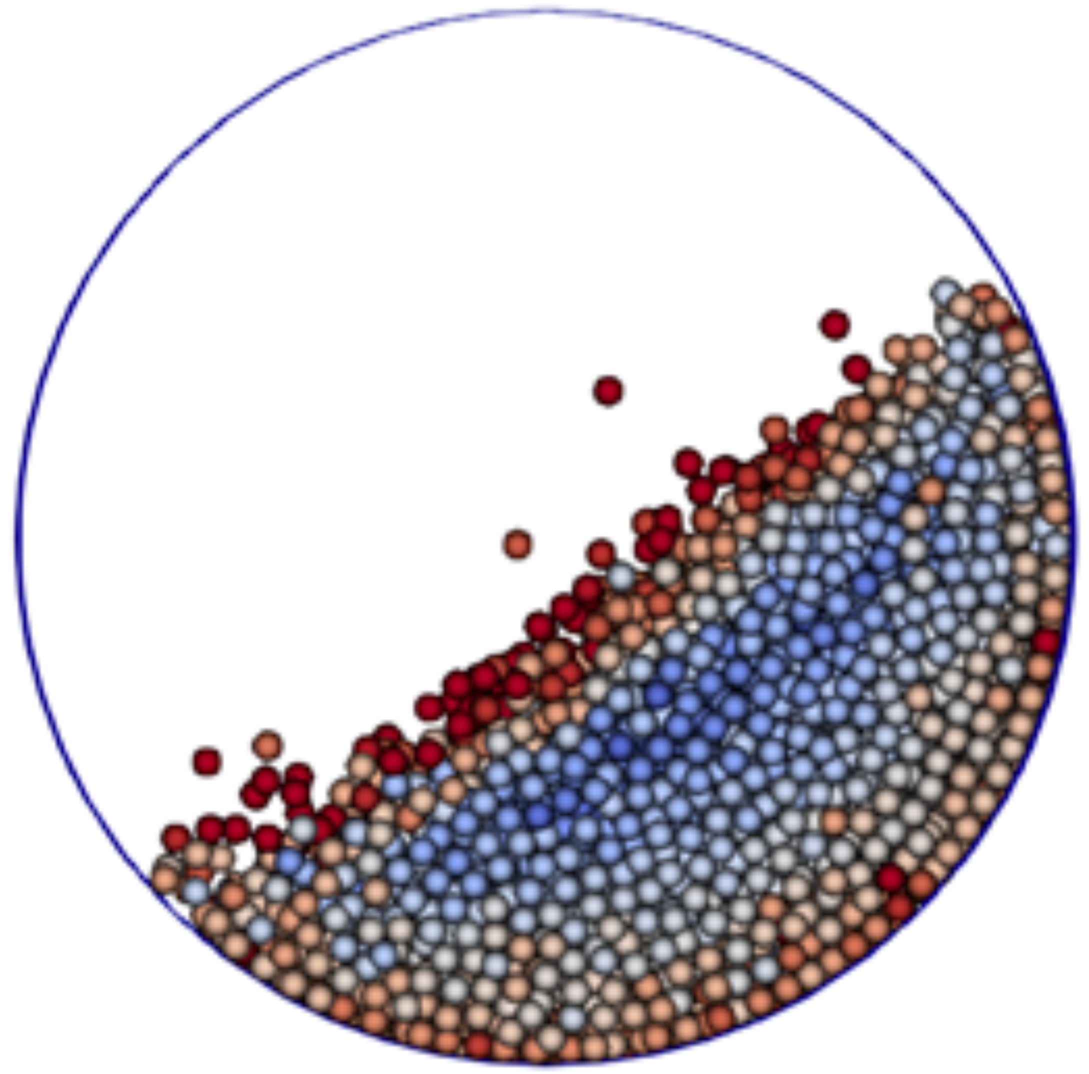


Rock + slurry. Sinnott, 2017, Minerals Engineering (data 61)

Rotating drum

Optimise milling efficiency

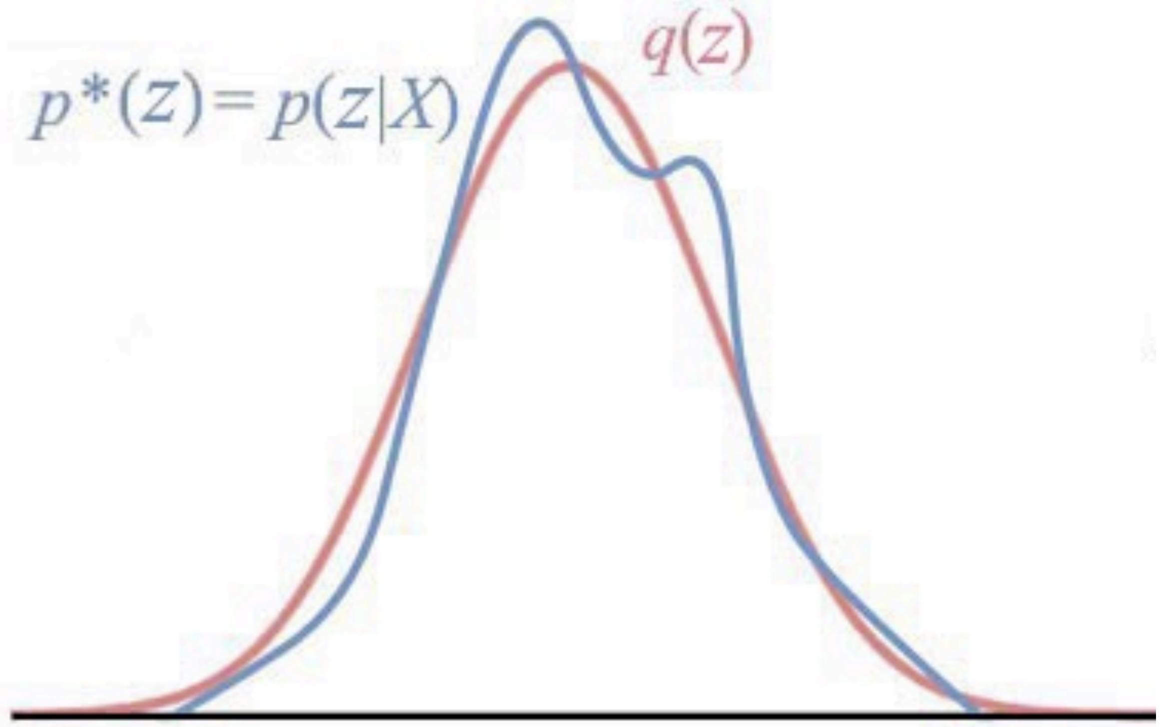
1. Input: grain size, geometry, …



2. Train NN to results of DEM.
   Predict: kinematics and/or energy

[Option: Bayesian Variational Inference]

Posterior Distribution of Energy Efficiency



z = controls e.g. rotating speed

3. Optimise energy required by auto-diff through NN - with gradients

Rotating drum

Optimise milling efficiency

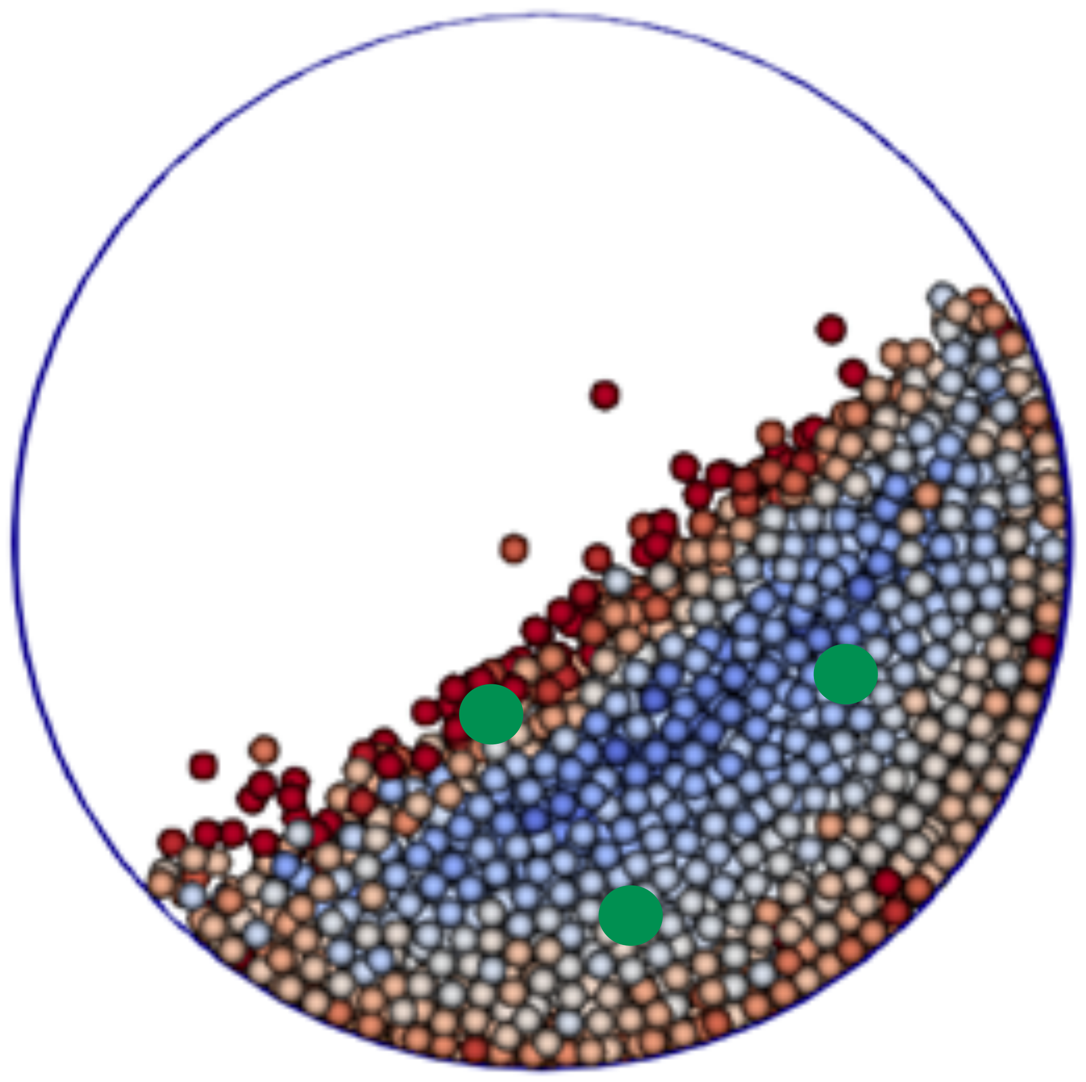
1. Input: grain size, geometry, …

2. Train NN to results of DEM.
   Predict: kinematics and/or energy

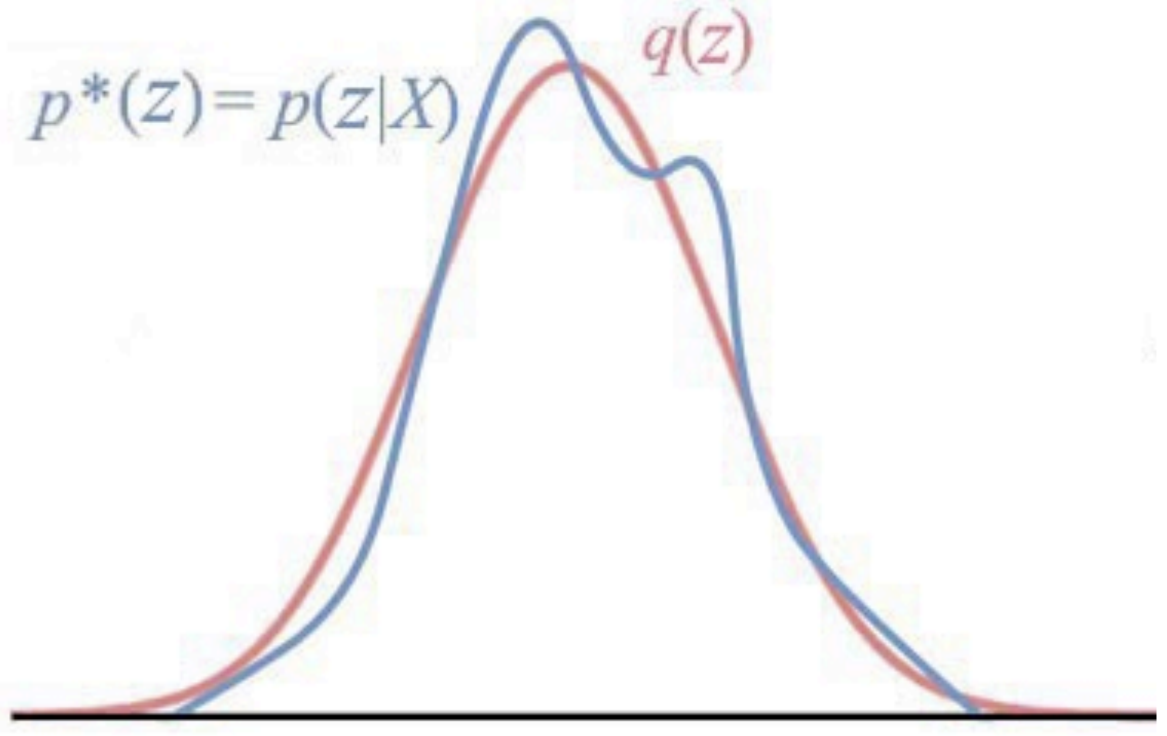
   [Option: Bayesian Variational Inference]

   - Add sensors as inputs

3. Optimise energy required by auto-diff through NN - with gradients



Posterior Distribution of Energy Efficiency



z = controls e.g. rotating speed