UNIVERSITY OF BIRMINGHAM | COLLEGE OF ENGINEERING AND PHYSICAL SCIENCES

DEM Round Robin: Toward a Best Practice for Powder Flow Simulation

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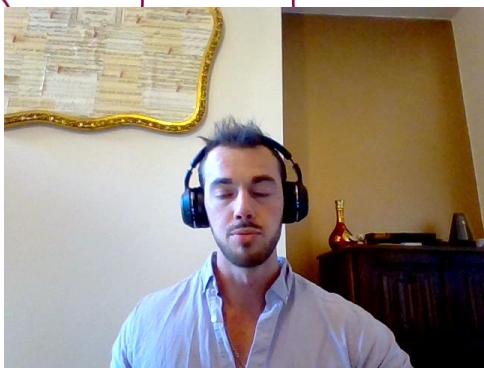
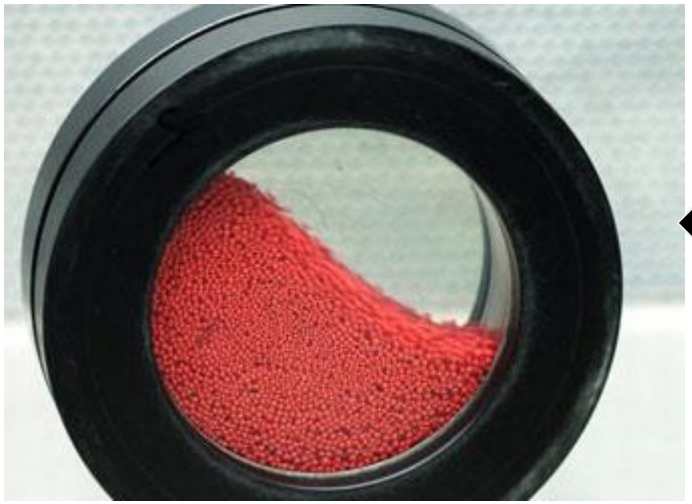
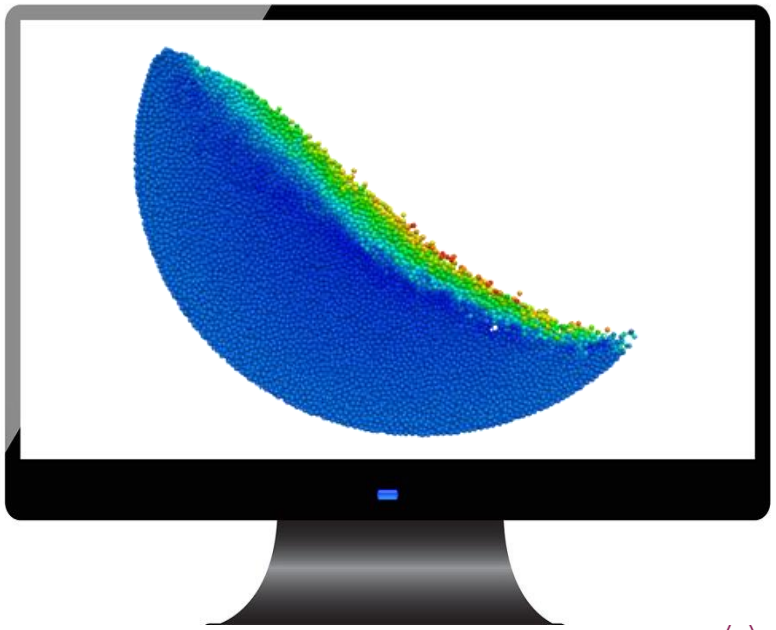
School of Chemical Engineering

The University of Birmingham



Background: What is DEM, and why do we care?





DEM is a tool for numerically modelling powders and particulates

Provides **more information**, **more cheaply** than any experimental

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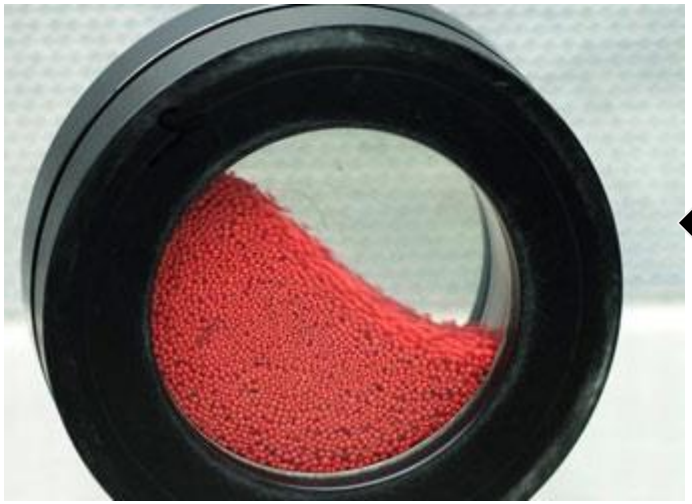

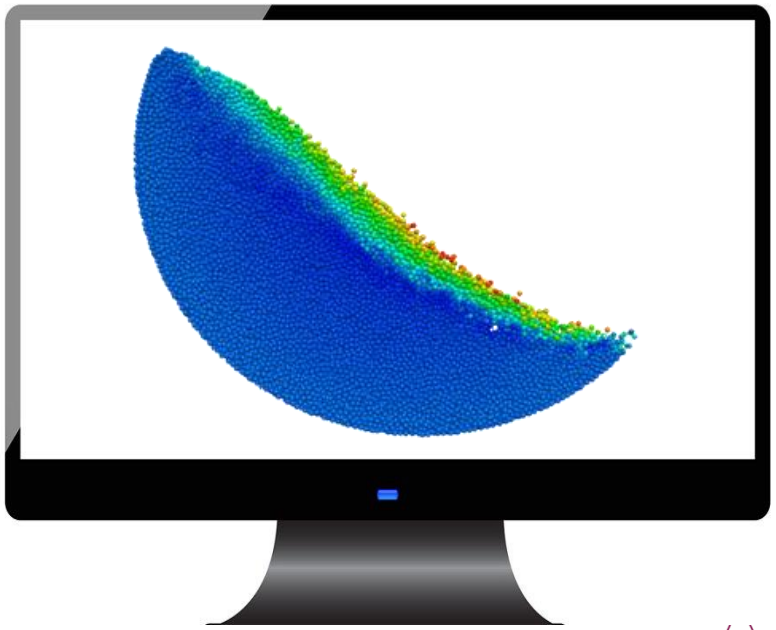

If well calibrated, DEM is capable of quantitatively reproducing dynamics of ‘real’ systems, making it a powerful tool for
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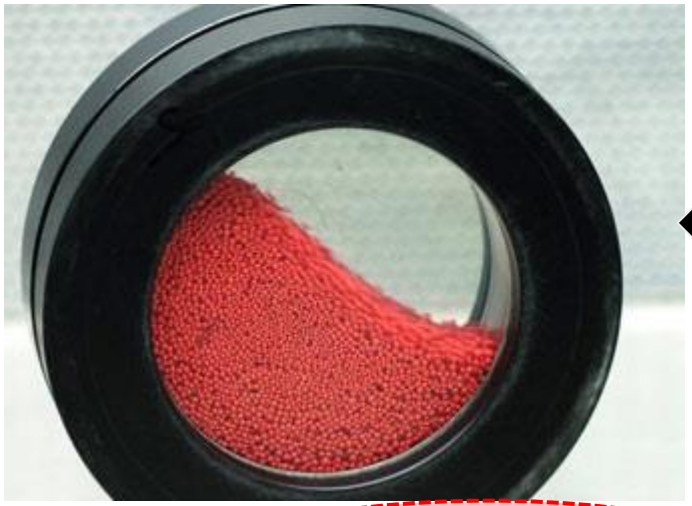
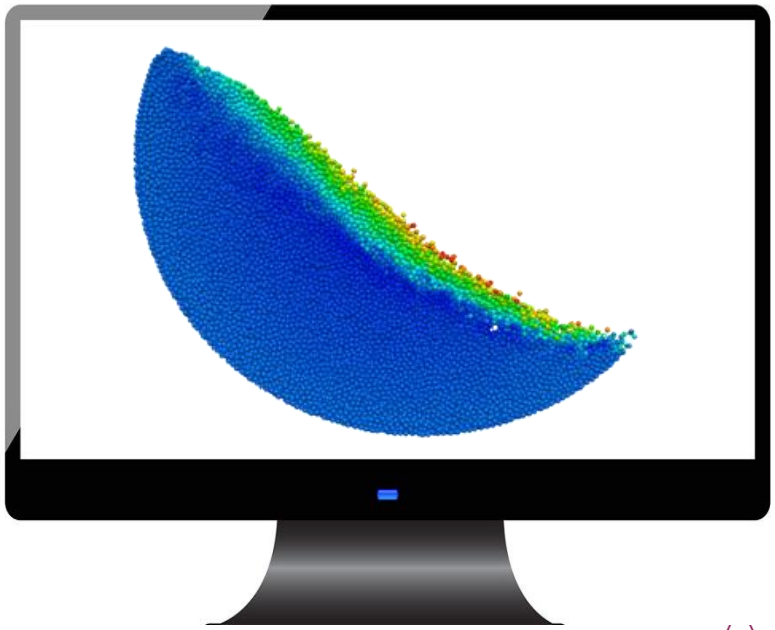
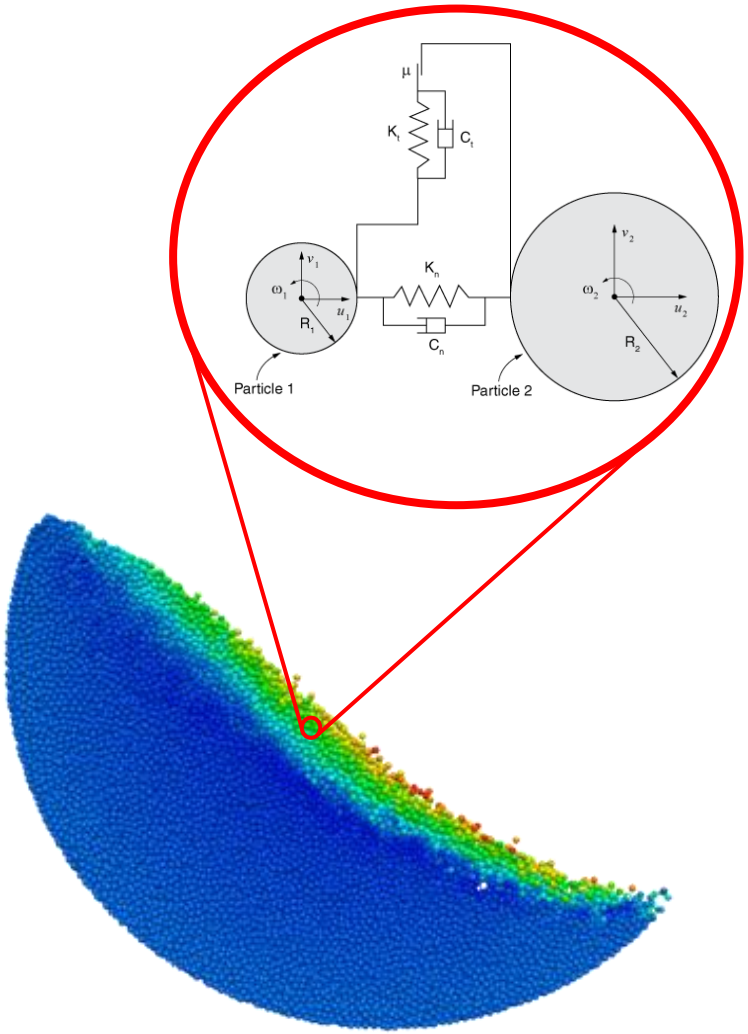




If well calibrated, DEM is capable of quantitatively reproducing dynamics of 'real' systems, making it a powerful tool for design and optimisation of industrial equipment

This is a **big if!**

Background: DEM's Limitations

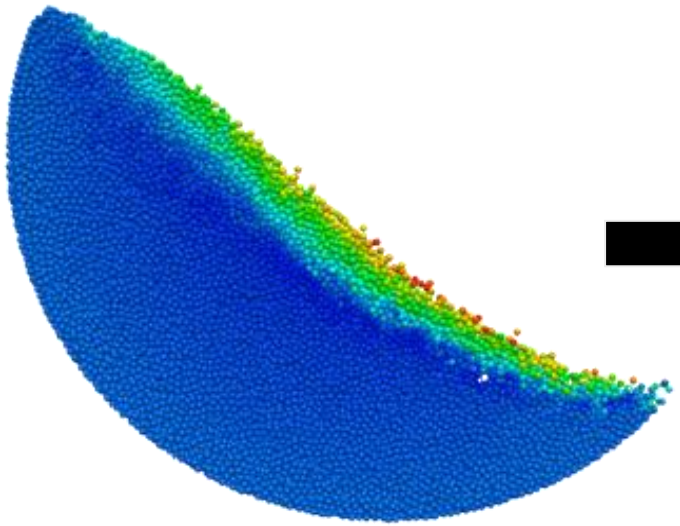


DEM's main limitation is that it is *just a model*

Like any model, it requires certain **assumptions** and **simplifications**

To make an **accurate model**, we require **detailed calib**

Background: DEM's Limitations



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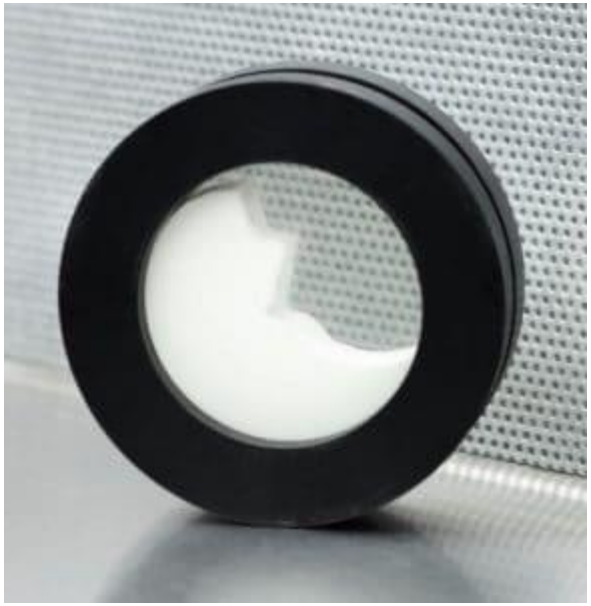
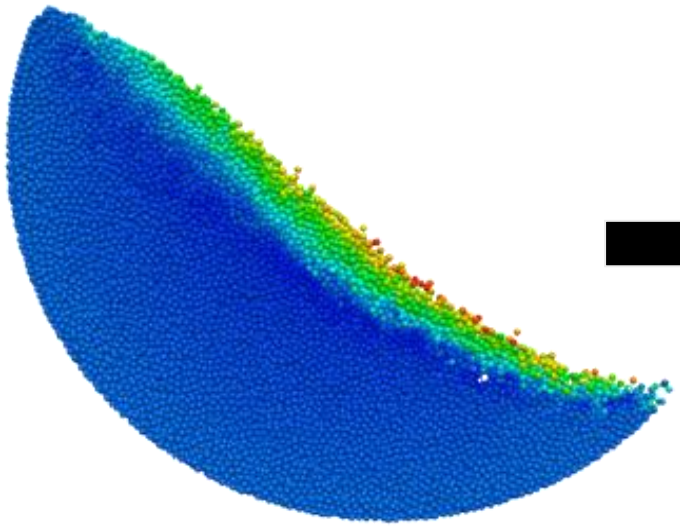


The problem:

1) Calibration is **not simple** – certain properties (e.g. cohesion, particle shape) are both **characterise** and hard to **model**

Background: DEM's Limitations

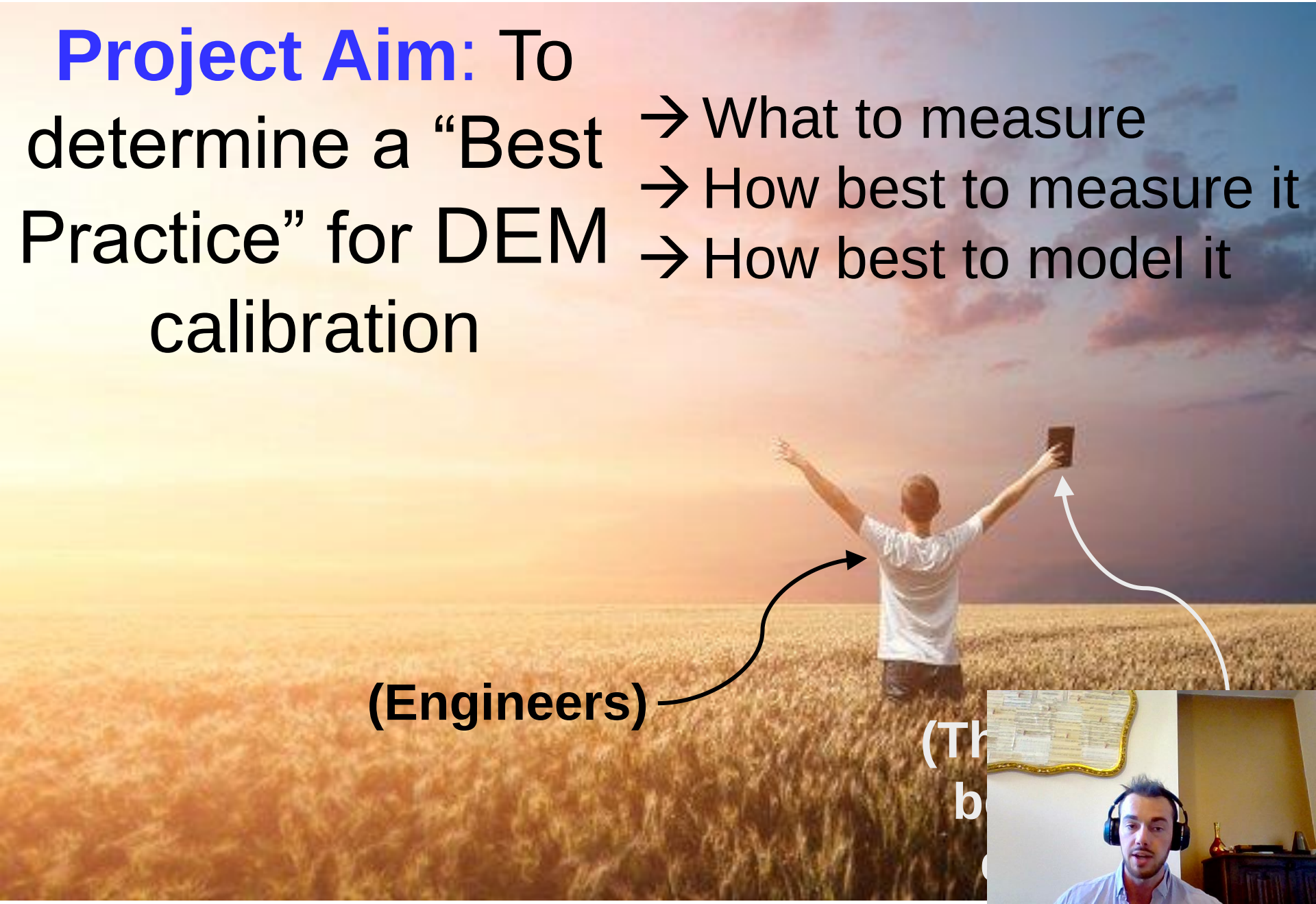


?

2) There is **no reliable, standard procedure** for DEM calibration – different companies & i
take very different approaches

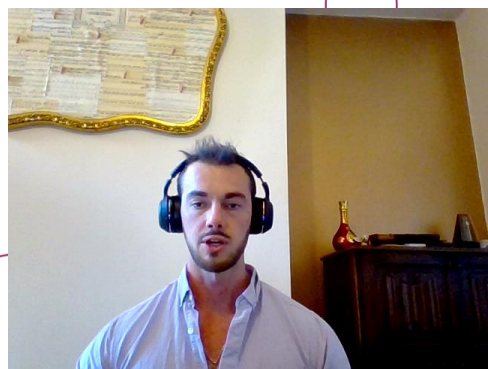
Project Aim: To determine a "Best Practice" for DEM calibration

→ What to measure
→ How best to measure it
→ How best to model it



How to Determine Best Practice?

- Need to be able to **objectively** and **quantitatively** assess how well a given methodology reproduces the dynamics of a given system.
- We require the **direct, detailed comparison** of simulation data to experimental data
- This requires both
  - a suitable system
  - a suitable experimental technique



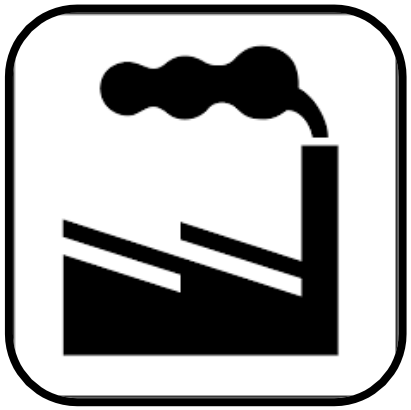
How to Determine Best Practice?

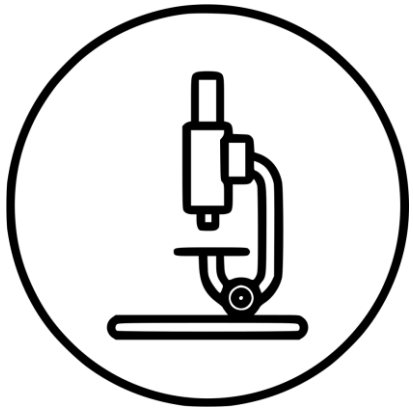
Choose experimental system(s) to model

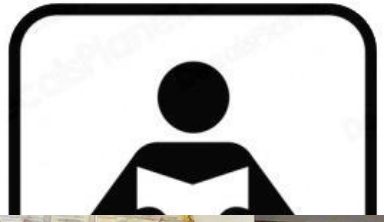
Acquire experimental data using suitable technique

Produce simulations following current industry practices

Compare simulations to experiment → **best practice**





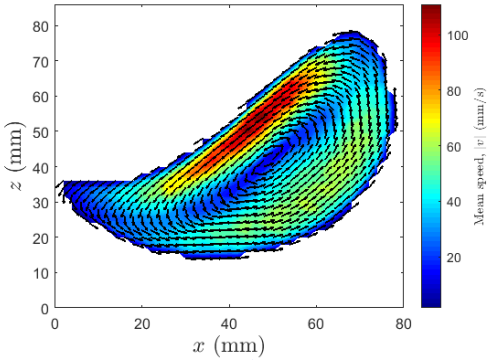


System Selection

- Criteria:
  1. Industrially-relevant systems
     - (→ meaningful outcome)
  2. Suitable for imaging
     - (→ steady state, interesting dynamics)
  3. Explore all regimes (frictional, collisional, intermediate)
     - (→ ensure models suitable for **all** li states)

System Selection 1 – Granutools GranuDrum

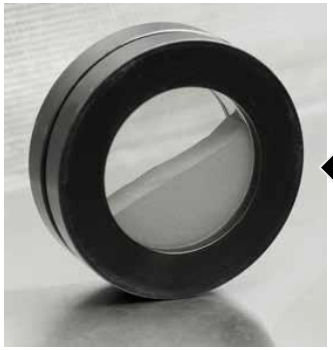
PEPT Data
(45rpm – "cataracting" state)

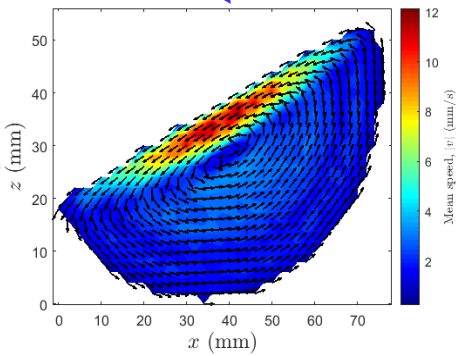


Criterion 3: Can explore both frictional *and* collisional regimes by altering rotation rate ✓

Criterion 1: Rotating drum geometry – common in industry ✓

Same material, varying RPM





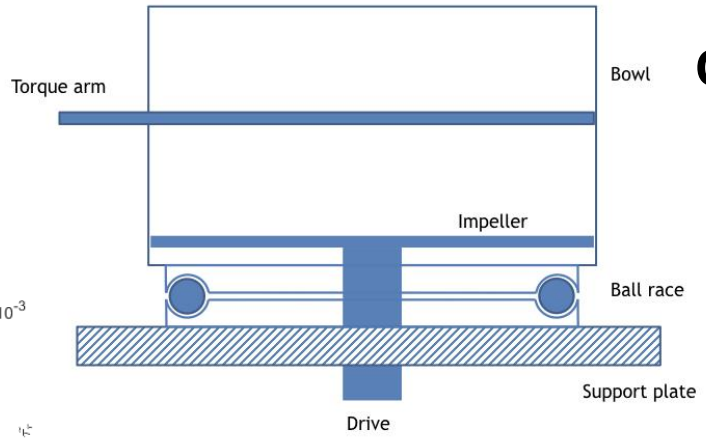
PEPT Data
(5rpm – "rolling" state)

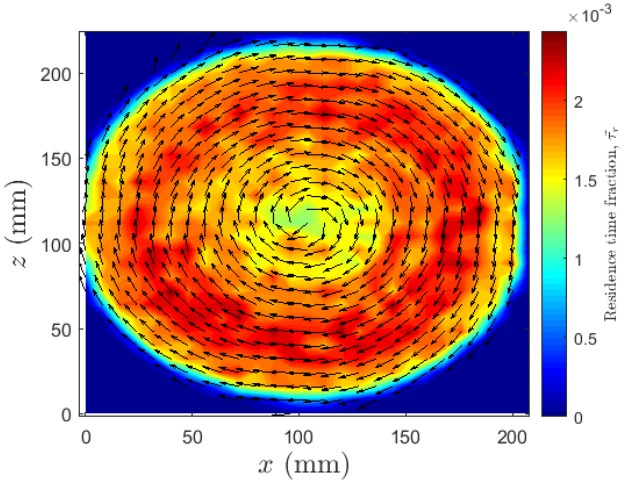
Criterion 2: Interesting and well-researched ste dynamics ✓

System Selection 2 – High Shear Mixer-Granulator

Criterion 3: “High shear” nature and large size complements relatively small, “low shear” rotating drum systems ✓

Criterion 1: Common industrial process equipment ✓





Criterion 2: Interesting and well-researched steady-state dynamics ✓

System Selection: Progress

- Systems agreed and chosen
- Tests conducted to ensure:
  - Compatibility with chosen materials
  - Compatibility with PEPT
- Experiments conducted for Phase 1 materials
- Experiments conducted for Phase 2 materials
- Phase 3 experiments scheduled for April cancelled due to Covid-19 closure
  - Will perform as soon as lab re-opens.

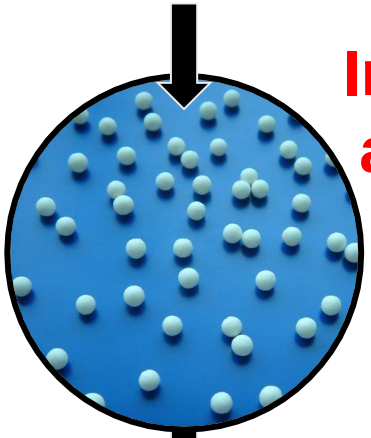
Material Selection

Why these choices?

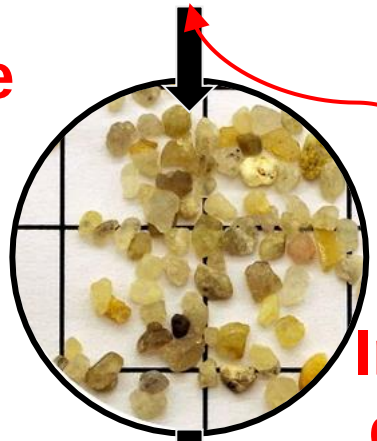
1. Test fundamental abilities

2. Test ability to model particle shape

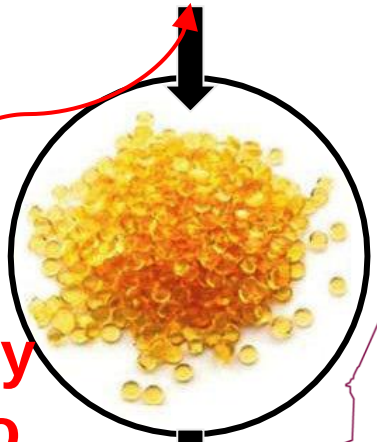
3. Test ability to model cohesion



In case we are doing it *really badly*



Infamously difficult to model



MCC
Simple, spherical geometry
Non-cohesive

Angular Sand
Complex, angular geometry
Non-cohesive

Si
Va

Material Selection

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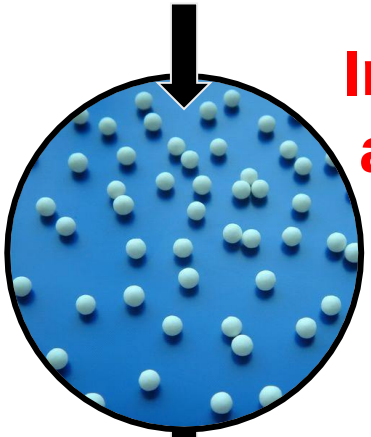

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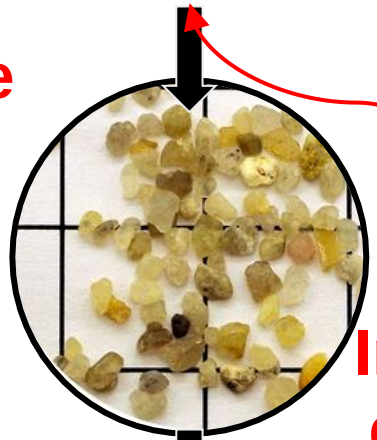

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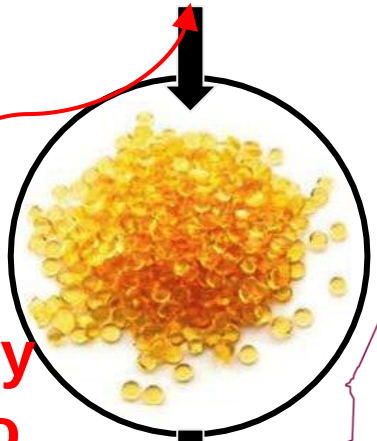
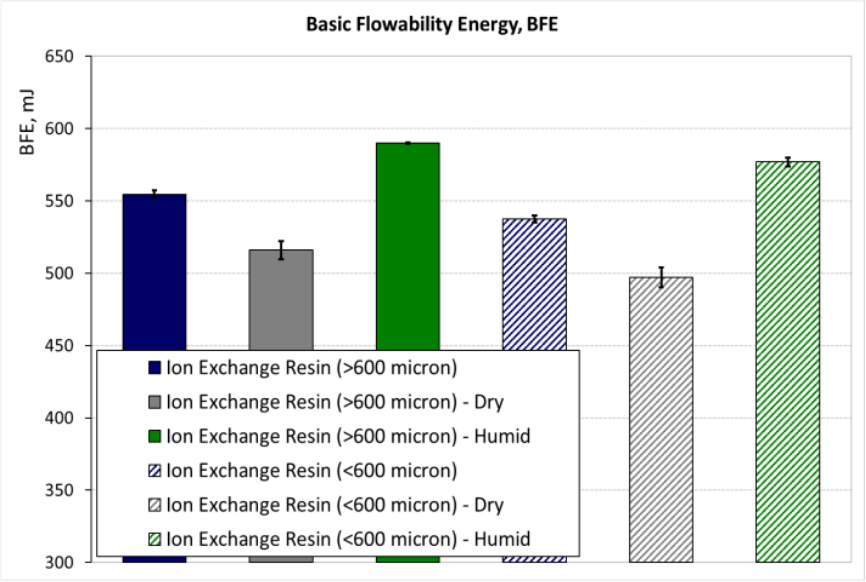


$d \in [1000,1400]\mu m$
$\rho = 1.58\ g/cm^3$

$d \in [1200,2400]\mu m$
$\rho = 2.65\ g/cm^3$

d

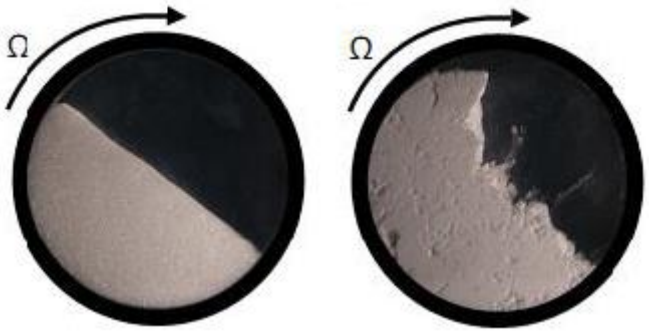
Material Selection: More on Material 3

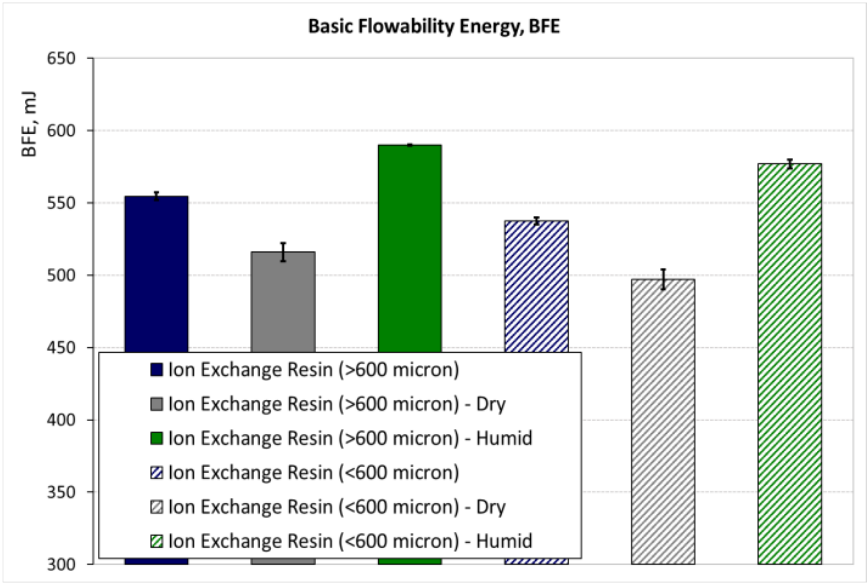


- Tests performed by Freeman Technology show cohesion varies with humidity.

- Tests will be performed with identical particles under both dry and humid conditions
- → Provide clear and rigorous test of ability of DEM m to simulate cohesion.

Material Selection: More on Material 3



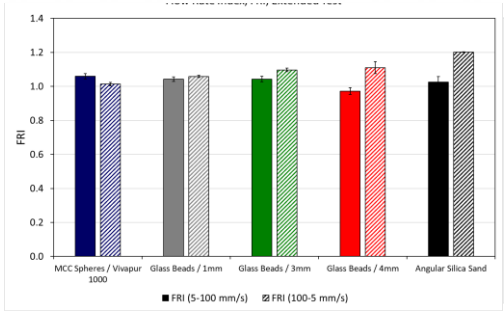


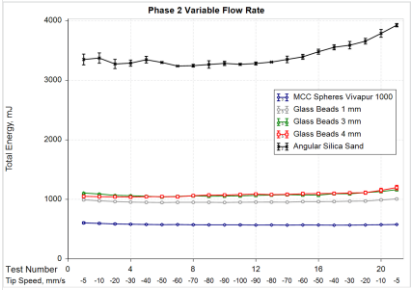
- Use of (air-tight) GranuDrum
- Samples prepared in glove box at desired humidtity
- → allows experiments to be performed under caref controlled conditions

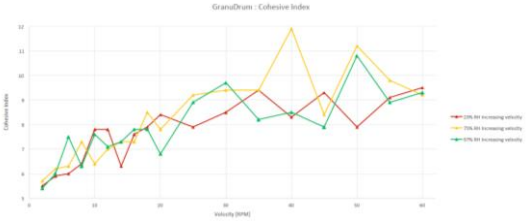
Material Selection: Progress

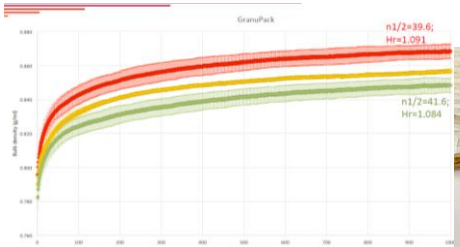
- All 3 materials agreed, chosen and acquired
- Samples sent to “Characterisation Partners” Freeman Technology and Granutools
- Full, detailed characterization received
- Participants at various stages of characterization

freeman*technology*
a micromeritics® company









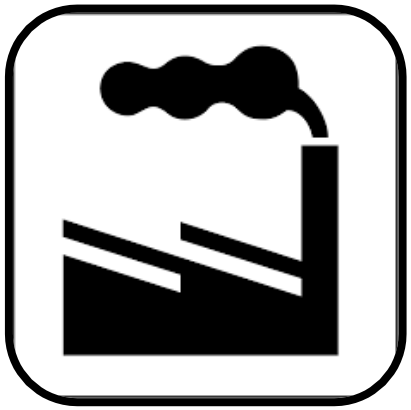
How to Determine Best Practice?

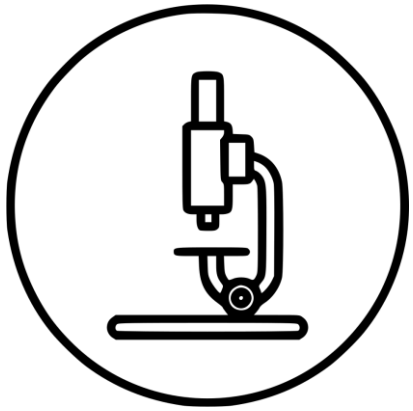
Choose experimental system(s) to model

Acquire experimental data using suitable technique

Produce simulations following current industry practices

Compare simulations to experiment → **best practice**





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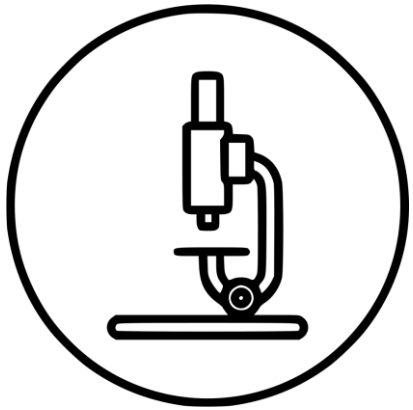
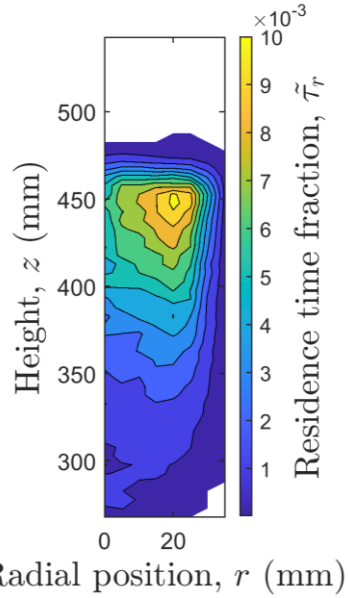


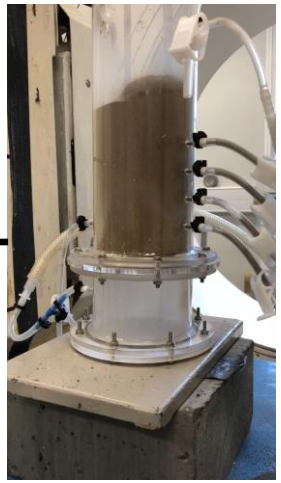
Experimental Method Selection

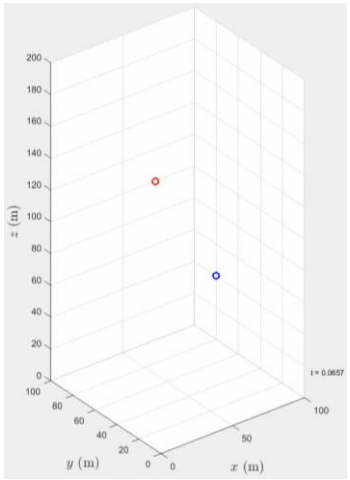
- Requirements:
  1. Can acquire full, three-dimensional data from opaque systems
  2. Both particle-level (microscopic) and bulk (macroscopic) information
  3. Dynamical data and force data
  4. Detailed, multi-point validation

Experimental Method Selection

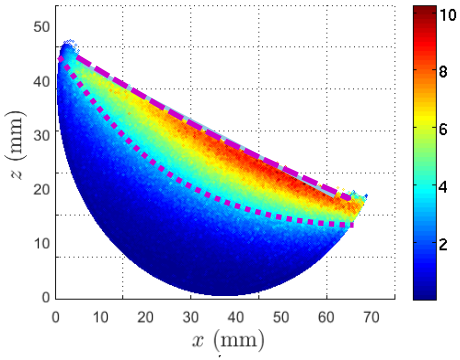


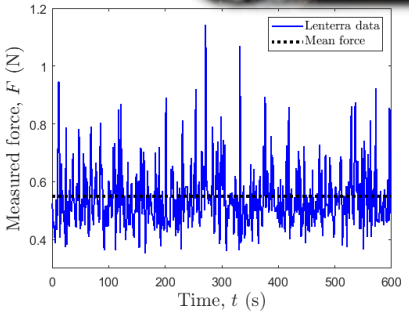
Criterion 2: Both micro- and macro-scale information ✓



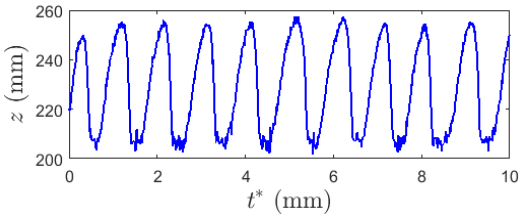


Criterion 1: Full, high-resolution imaging of opaque, 3D systems ✓

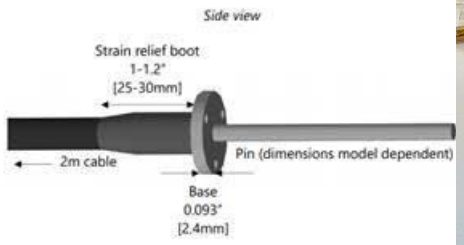




Criterion 3: Additional force data from Freeman Technology's Lenterra force sensor ✓



Criterion 4: Detailed multi-point data



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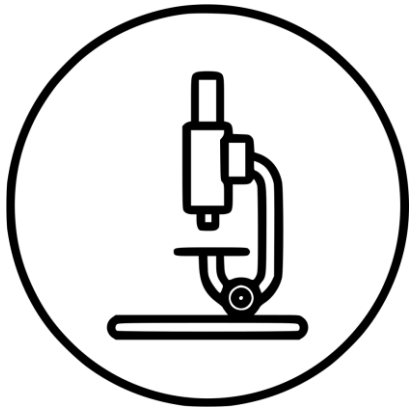
Compare simulations to experiment → **best practice**



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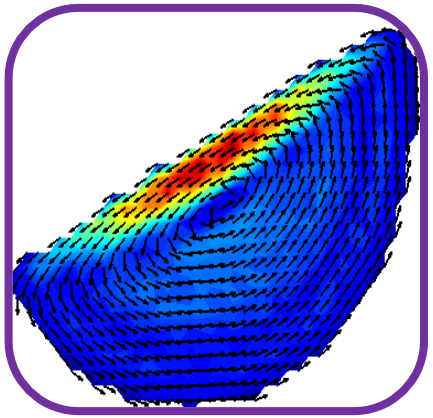
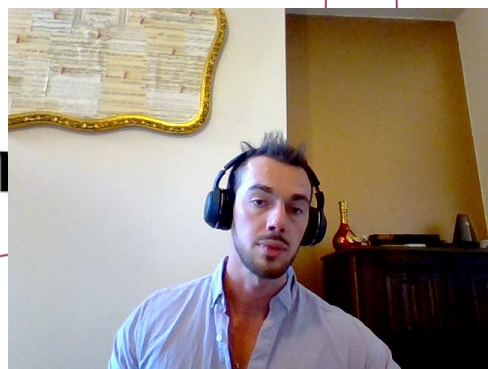


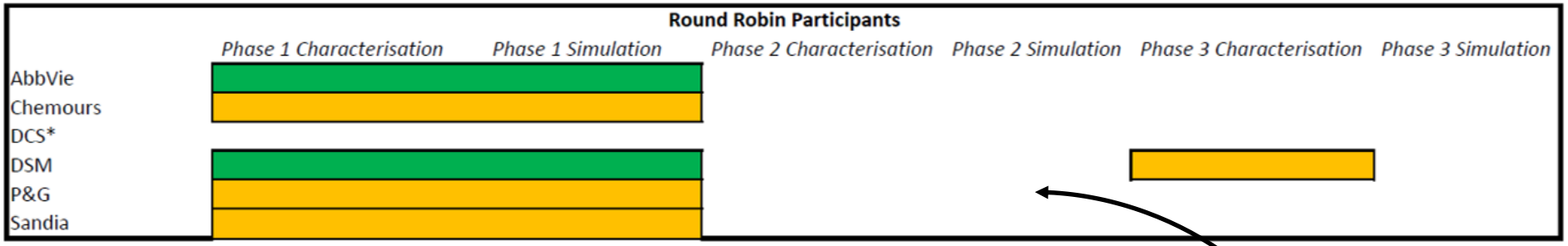
Replicating current industry practice

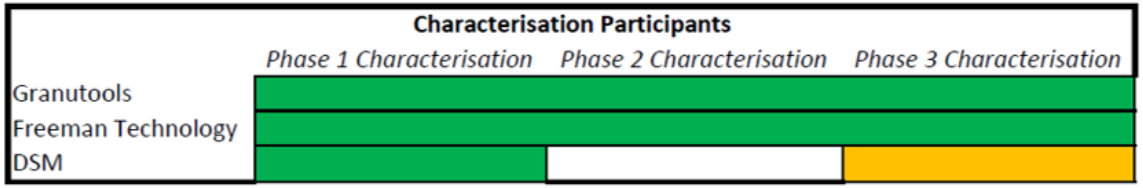
- The best way to replicate industry practice?
  - Let industry practice!
- Industry participants will:
  - Simulate the 2 systems & 3 materials chosen
  - Provide precise details of their calibration methods
  - Provide their simulation data for comparison with experiment



Simulation: Progress

- Participants at various stages of progress (see below)
  - Covid-19 and other issues have delayed participant progress
- EngD student recruited to aid participants and add additional simulation data
  - → More comprehensive & detailed analysis





*Due to time and manpower constraints, DCS have had to step down from the Round Robin

M
Pharı

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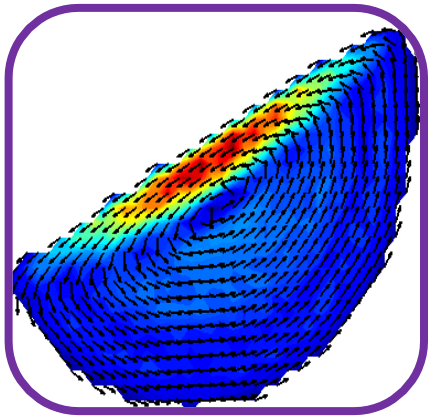
Produce simulations following current industry practices

Compare simulations to experiment → **best practice**



How to Determine Best Practice?

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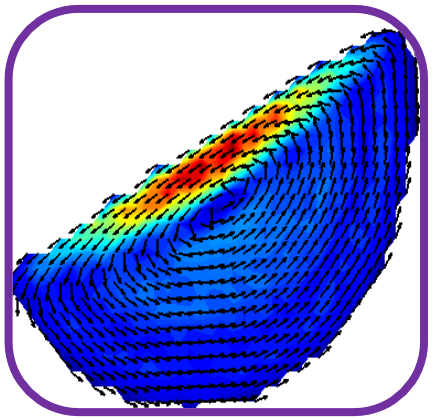
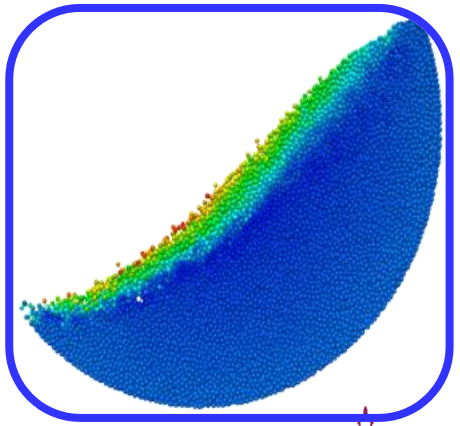
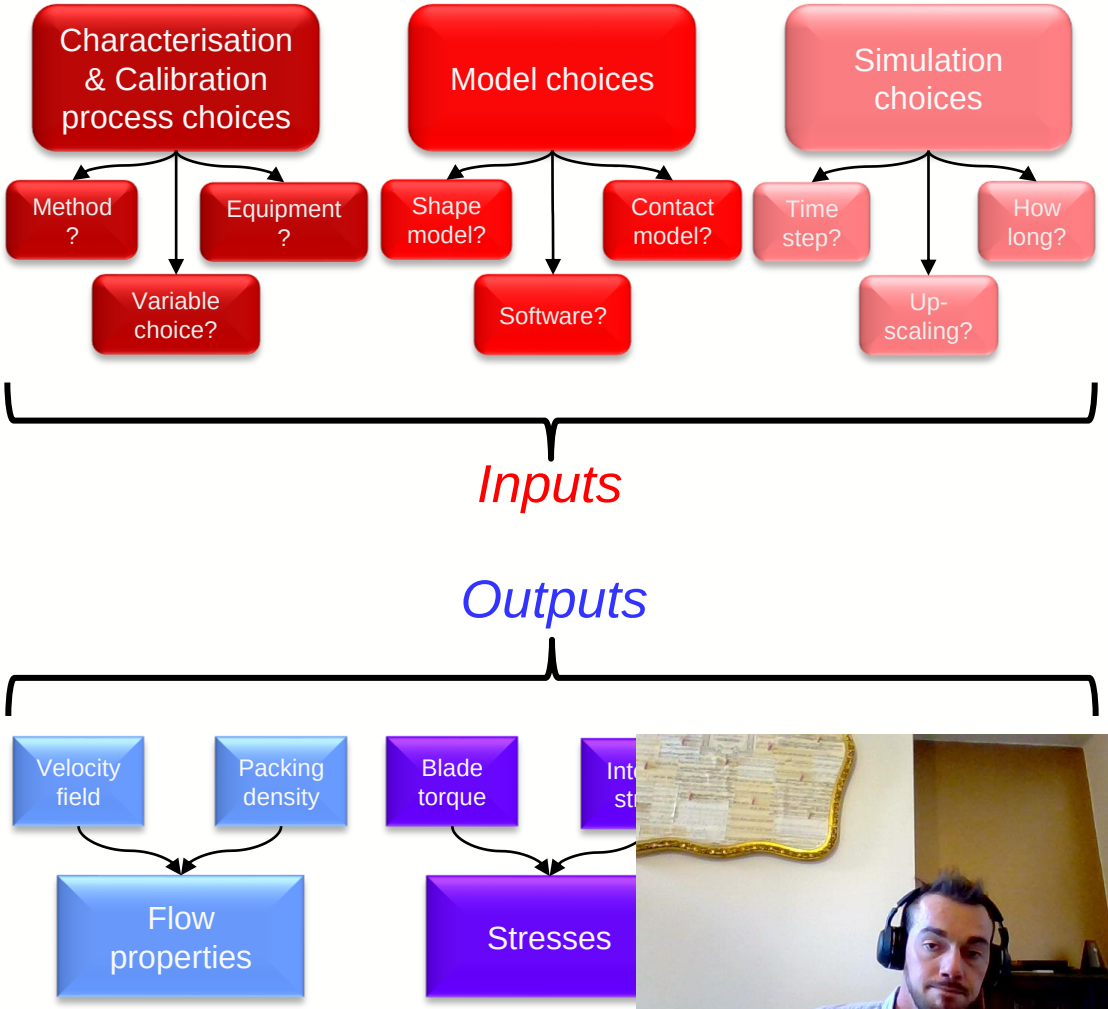


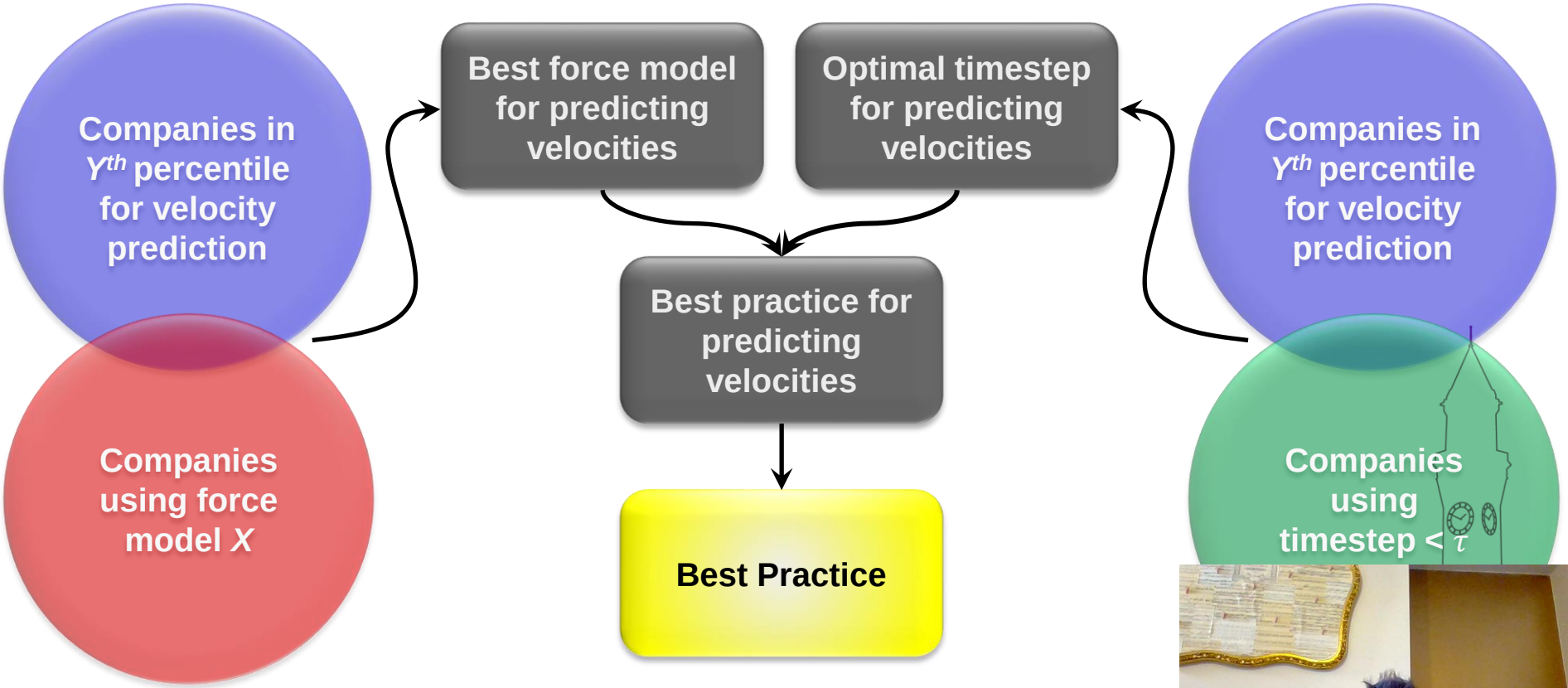


Toward a Best Practice

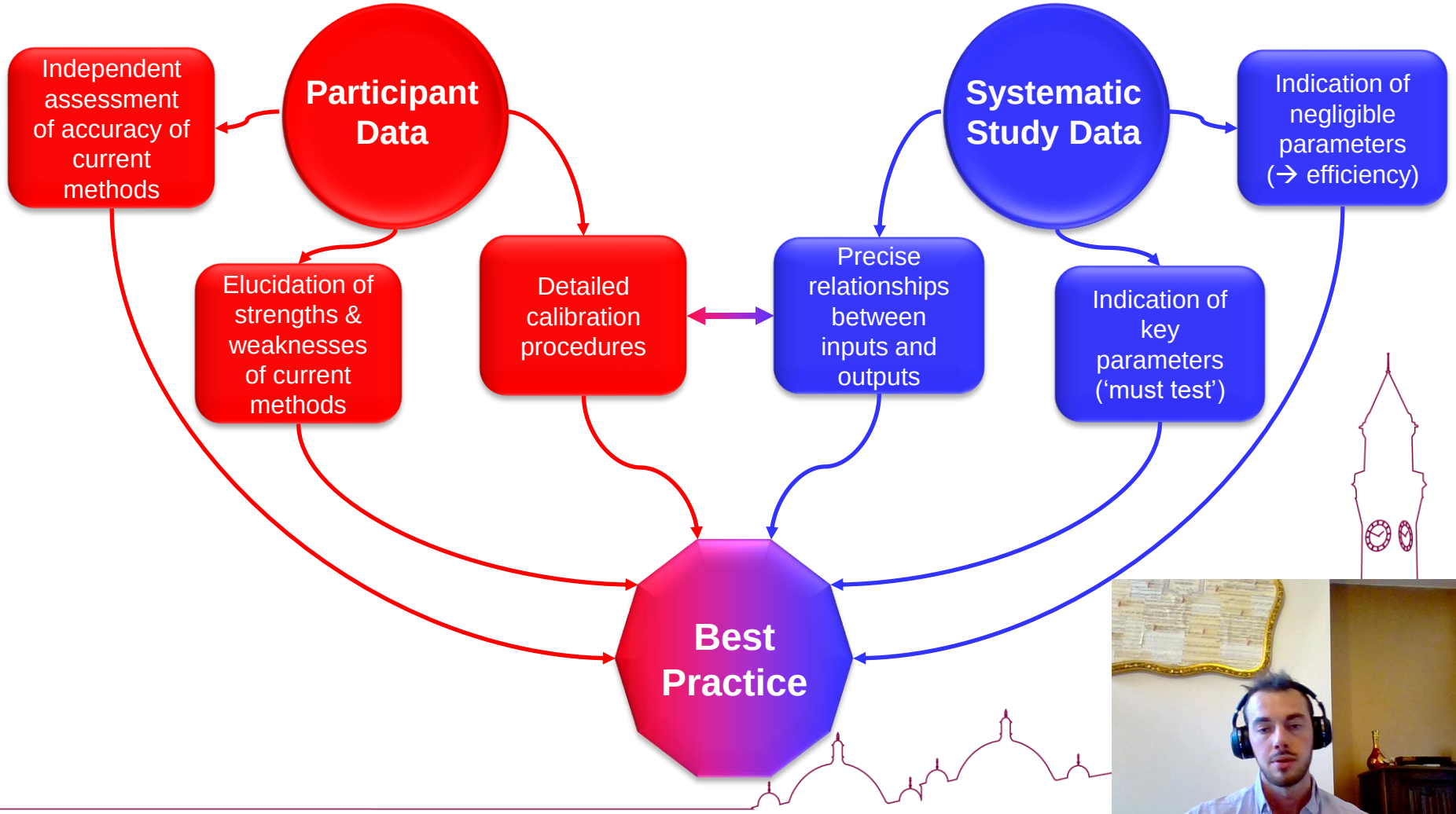
- Clearly, the chosen **inputs** to a model will influence the accuracy of the **outputs**.
- Our goal is to determine how the choice of each given input affects each given output…
- …and thus identify the **best choices**



Toward a Best Practice



How to determine best practice



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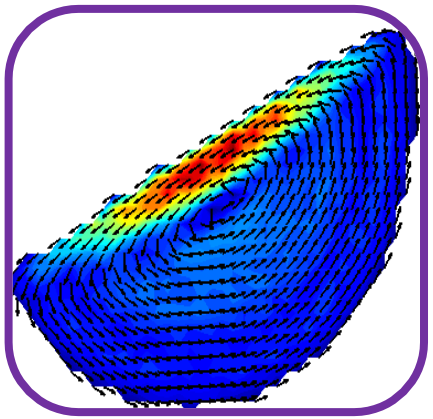

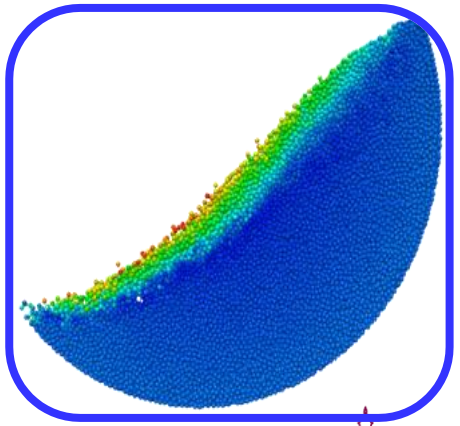

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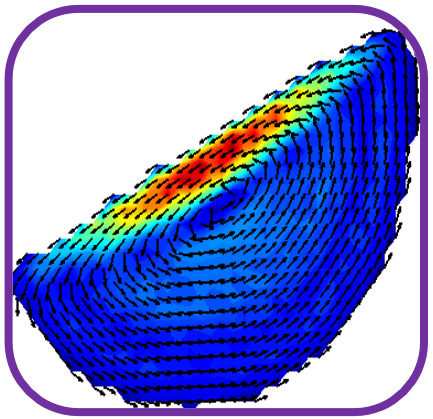
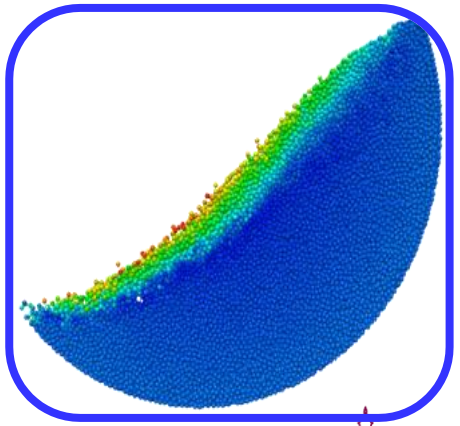
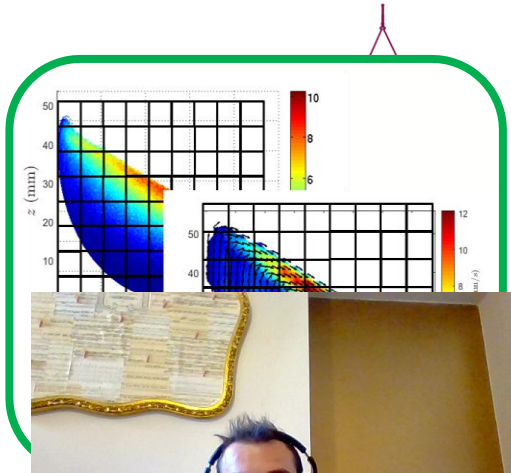
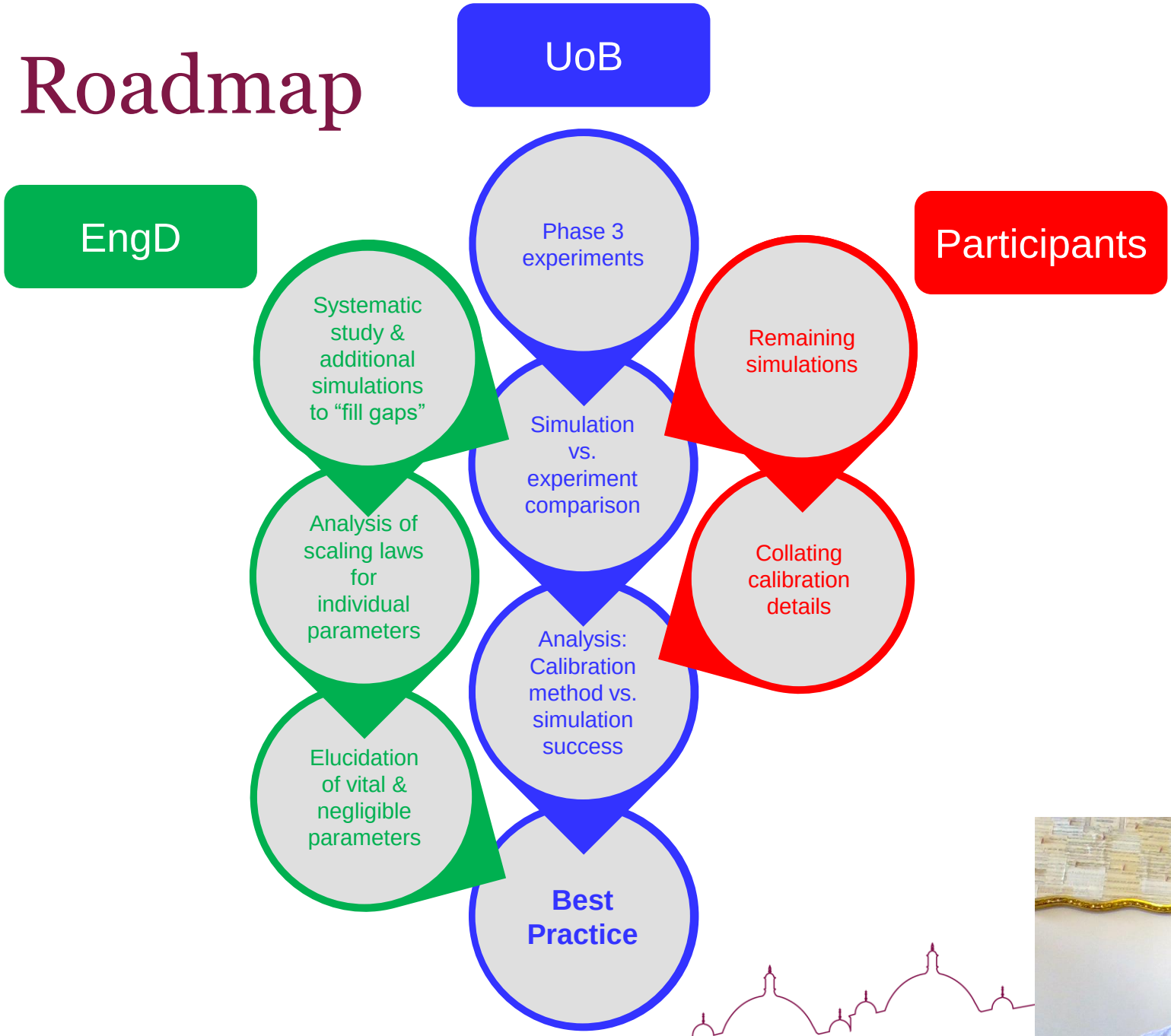






Roadmap


UoB
EngD
Participants
Phase 3 experiments
Systematic study & additional simulations to “fill gaps”
Remaining simulations
Simulation vs. experiment comparison
Analysis of scaling laws for individual parameters
Collating calibration details
Analysis: Calibration method vs. simulation success
Elucidation of vital & negligible parameters
Best Practice