IFPRI Round Robin Progress Report 2023

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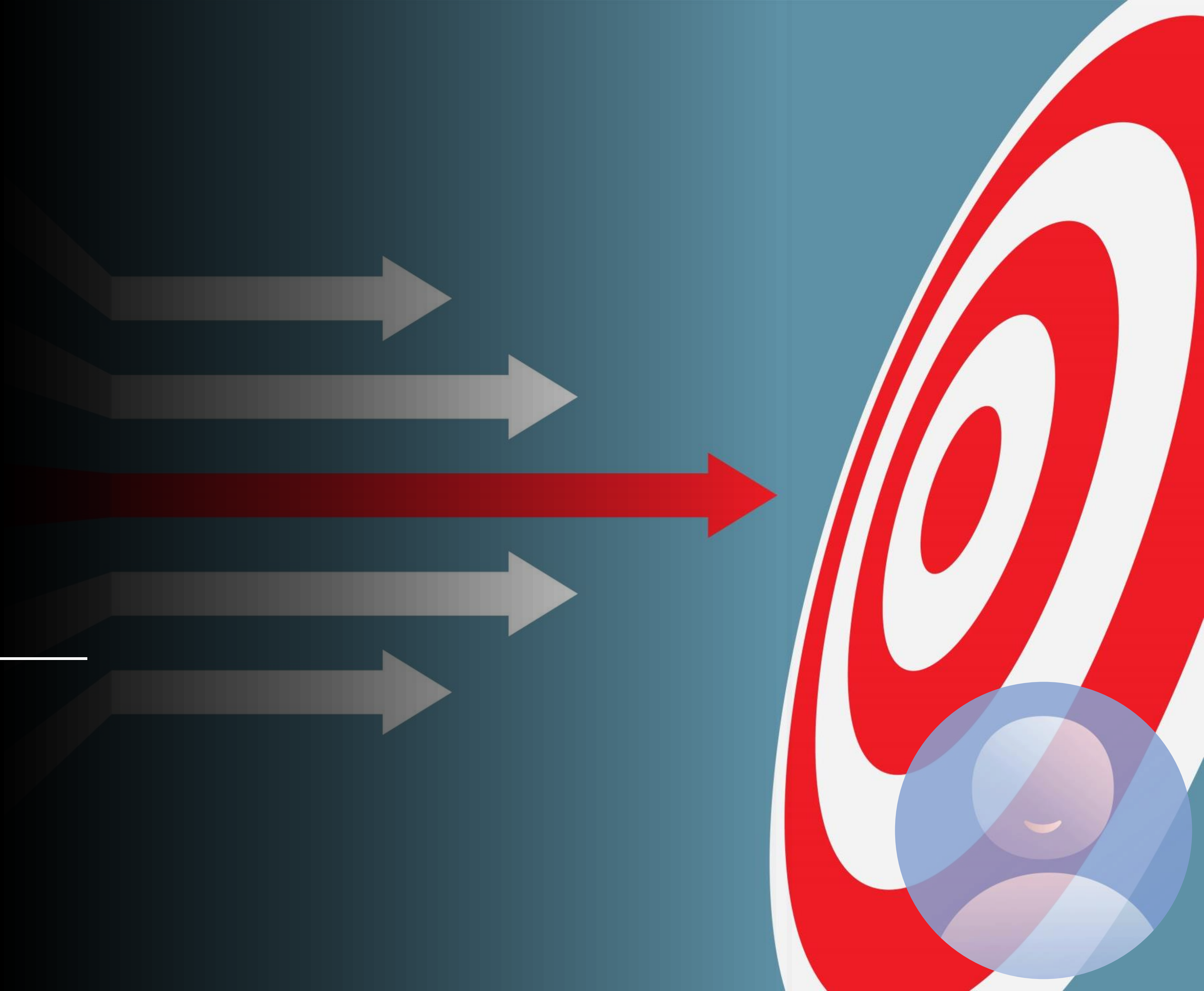
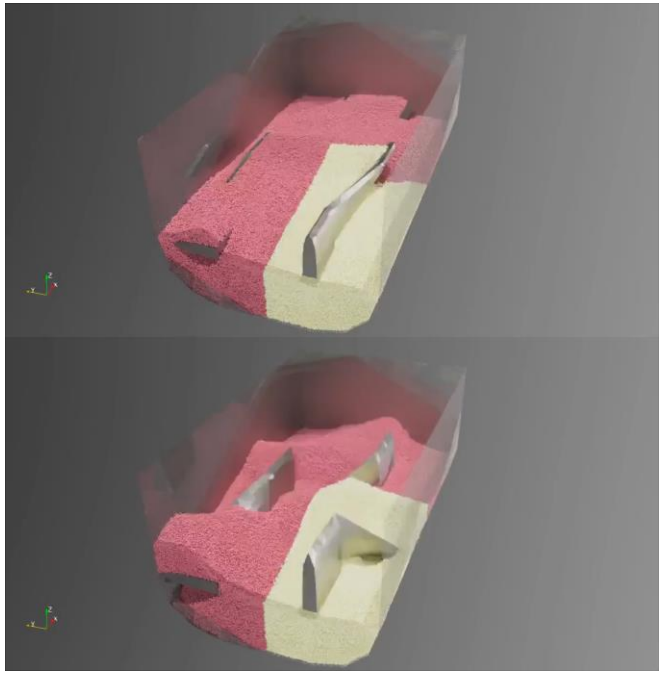
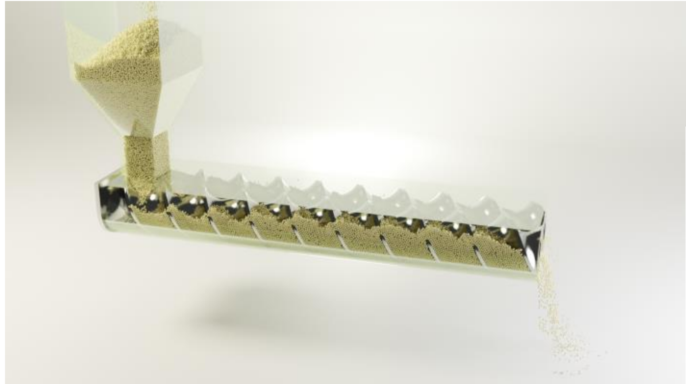
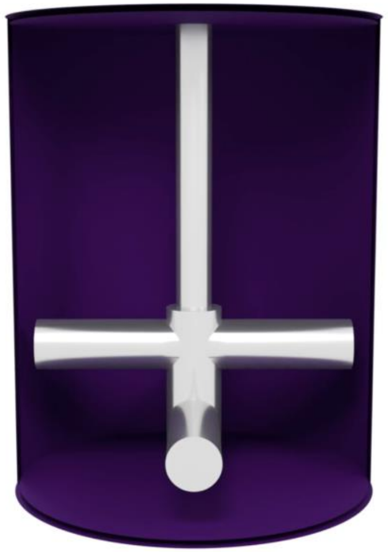
Recap: Motivation, Aims and Objectives



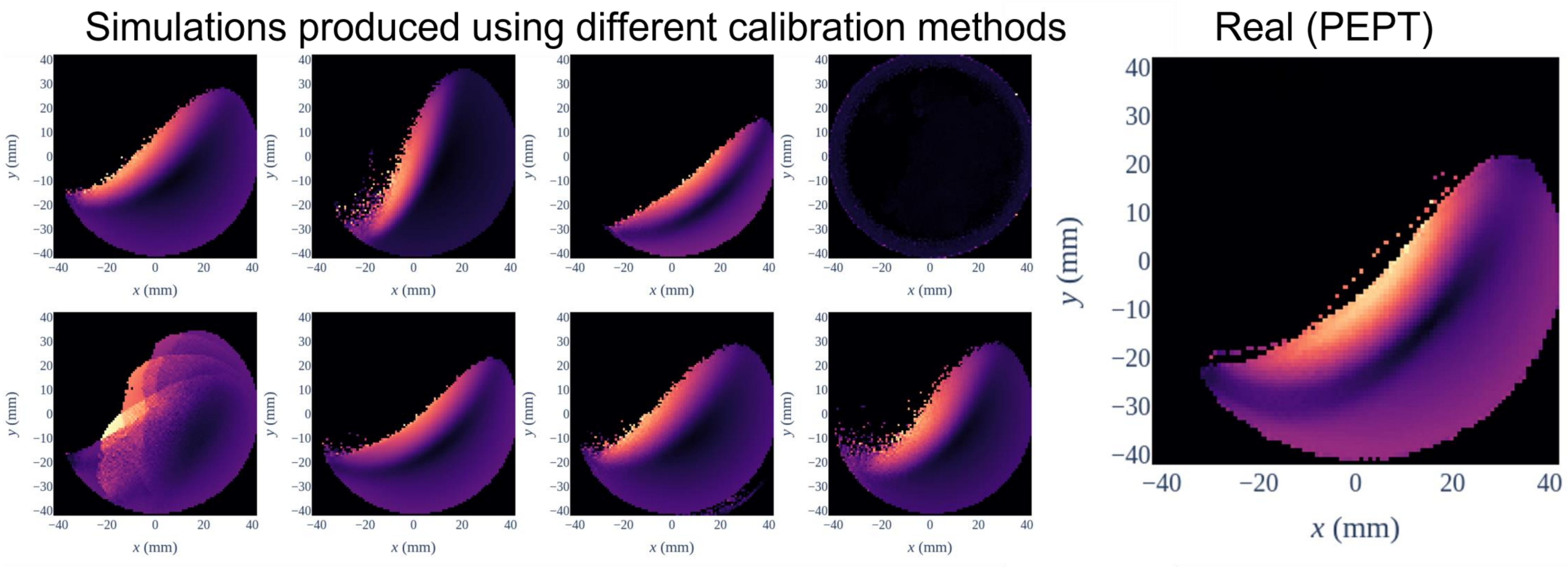






DEM – its value, and its weaknesses

- A powerful tool for the modelling, development & optimisation of industrial systems
- If properly calibrated can quantitatively reproduce the dynamics of complex industrial systems



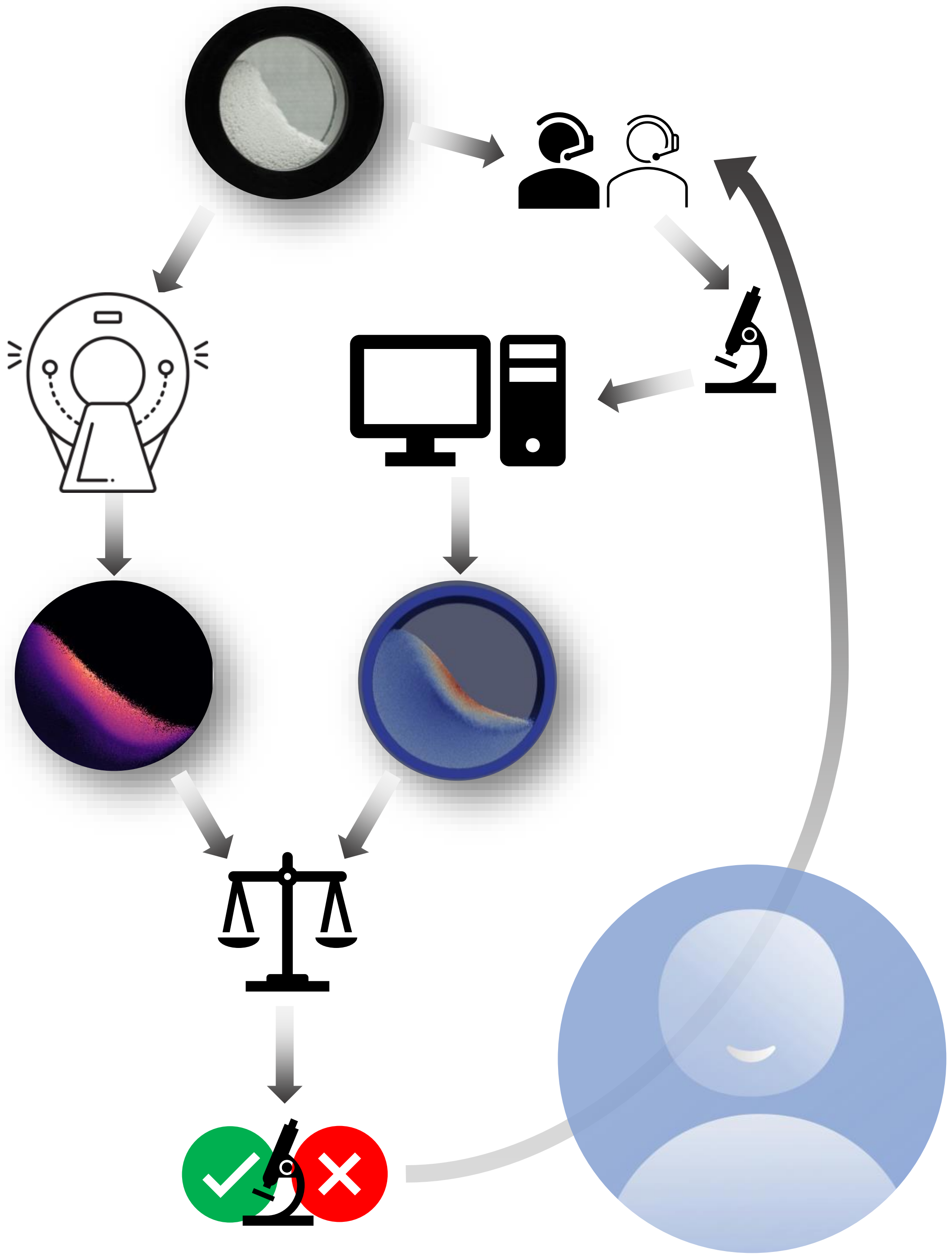
DEM – its value, and its weaknesses

Round robin goals:

1. Establish current industry practices
2. Assess their efficiency
3. Highlight ineffectual methodologies, **distil best practice**

Round Robin Format

1. Choose an industry-relevant system to model
2. Interview industry participant regarding their proposed calibration procedures
3. Reproduce their calibration procedures
4. Simulate system using the calibration parameters obtained
5. Obtain detailed PEPT data from real system
6. Compare simulations with PEPT "ground-truth" data
7. **Learn!**
8. Repeat

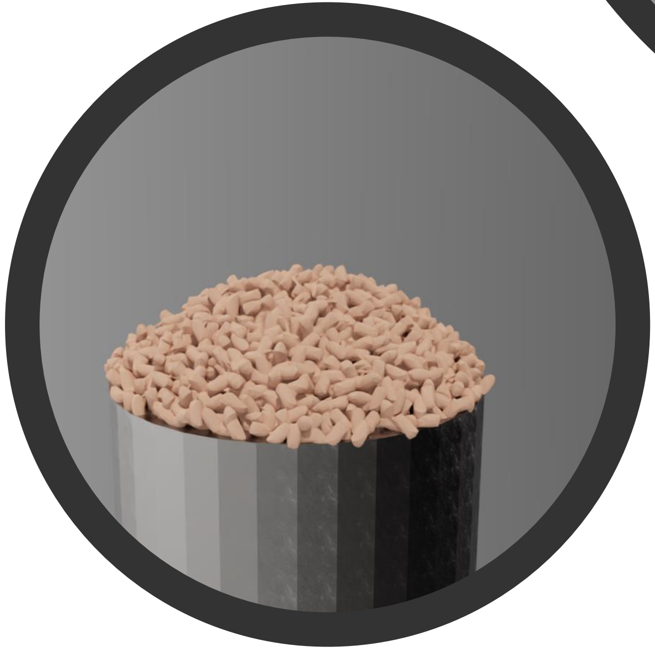


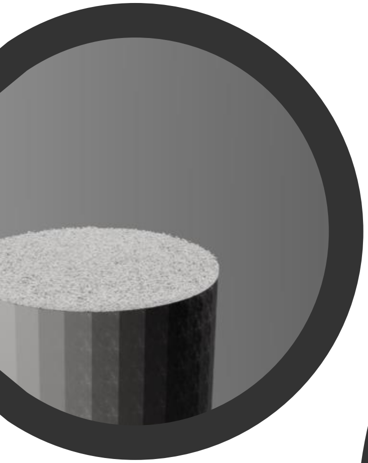
“The 7 Phases”

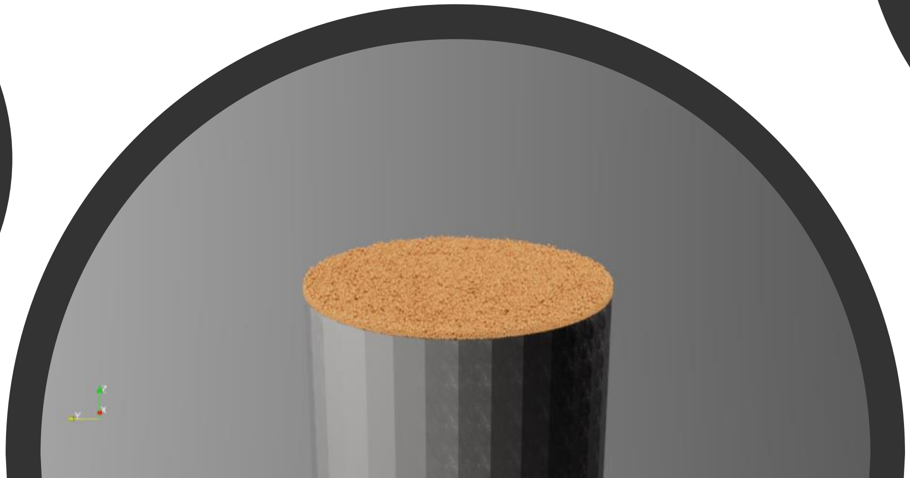
Providing a comprehensive challenge for DEM practitioners!

The 7 phases

- 6 materials + 1 binary combination
- Aiming to hit the main challenges raised by participants:
  - Aspherical particles
  - Elongated particles
  - Cohesive particles
  - Mixtures



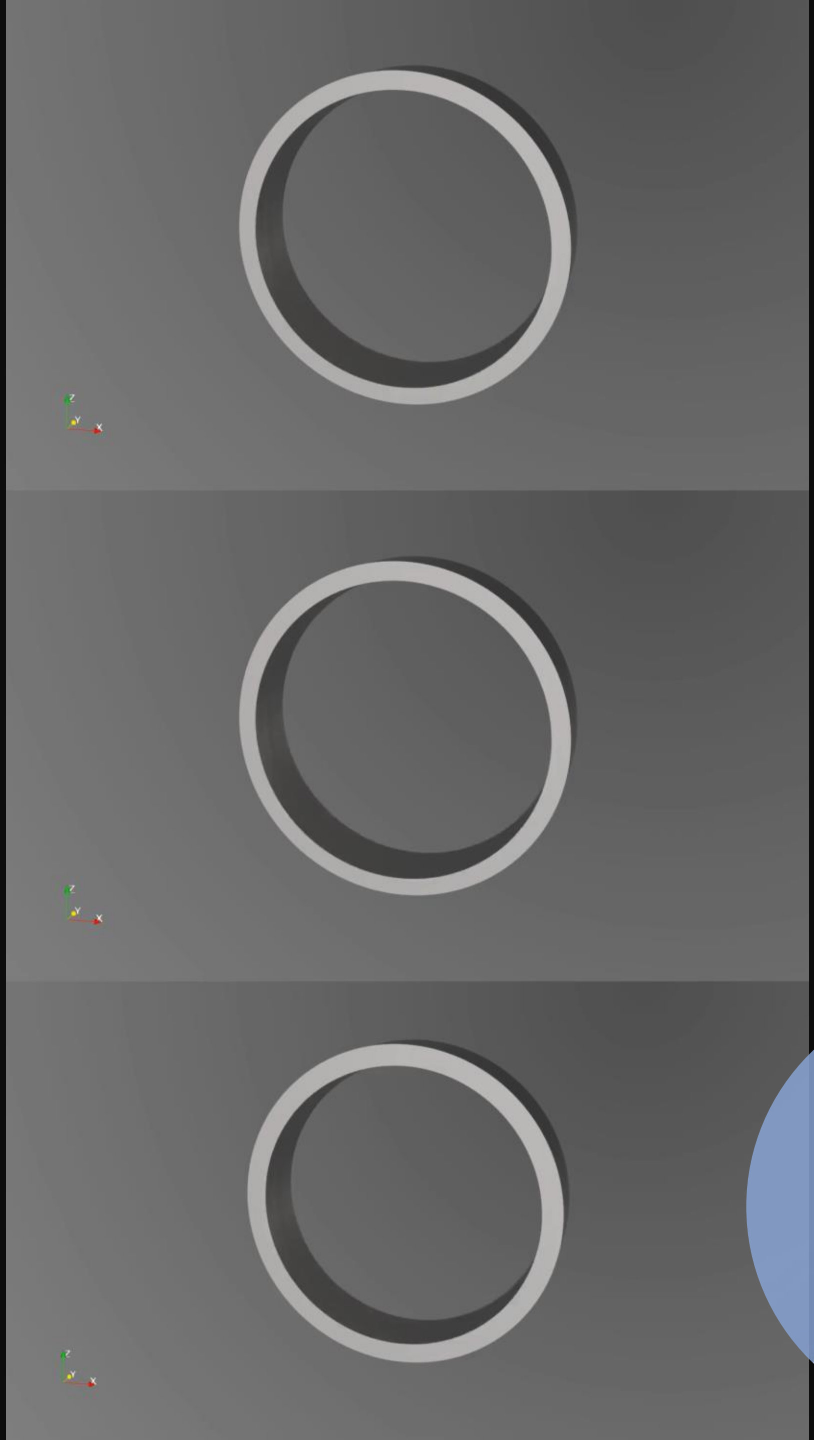




Test Systems

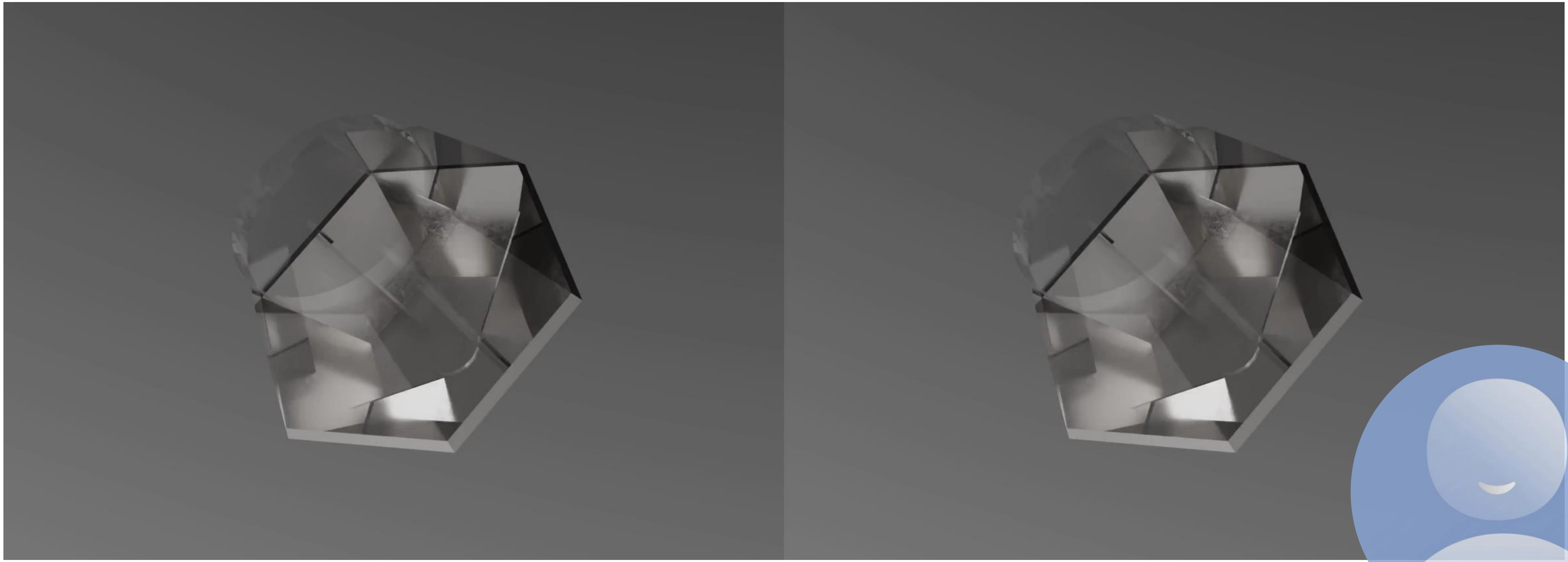
Granutools GranuDrum

- Small, simple, but capable of producing varied dynamics
- → A good differentiator for ability to calibrate **material properties**, without need to simulate large numbers of particles



Pascall Mixer

- Industry relevant
- Similar dynamics to GranuDrum but **significantly larger scale**
- → Rigorously test methods' abilities to handle large numbers of particles

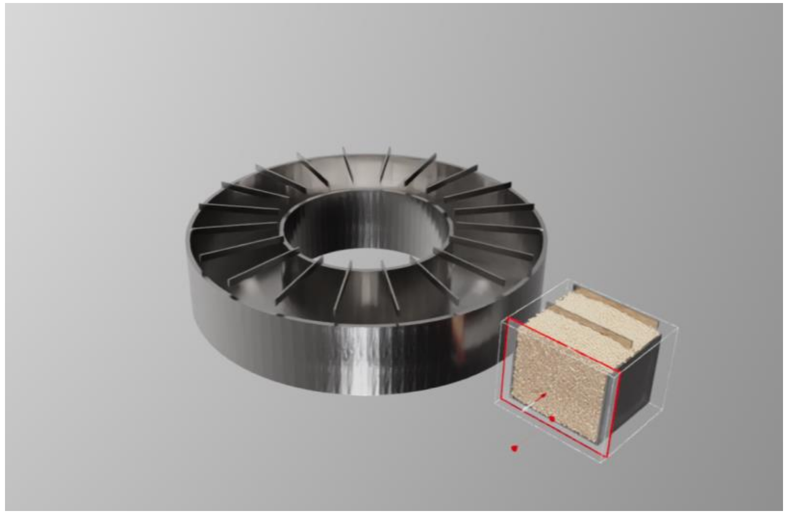


Resodyn Acoustic Mixer

- Industry relevant
- Strongly differing dynamics to previously-explored systems
- Addressing question highlighted I prior AGM – what about restitution?

DEM Digital Twins of Powder Characterisation Tools

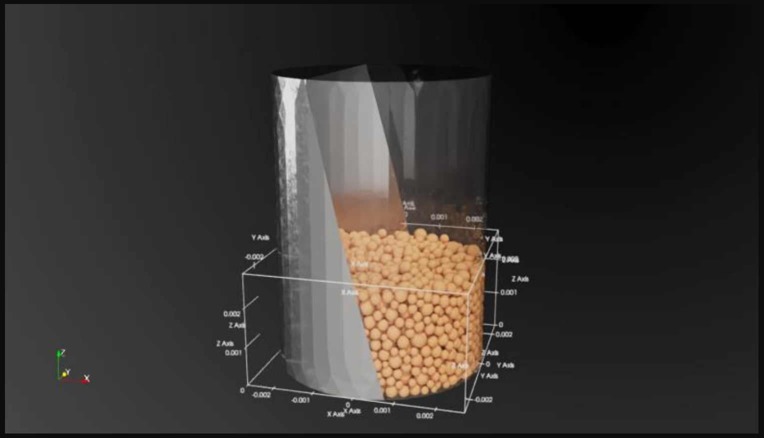
Freely available to all IFPRI members!

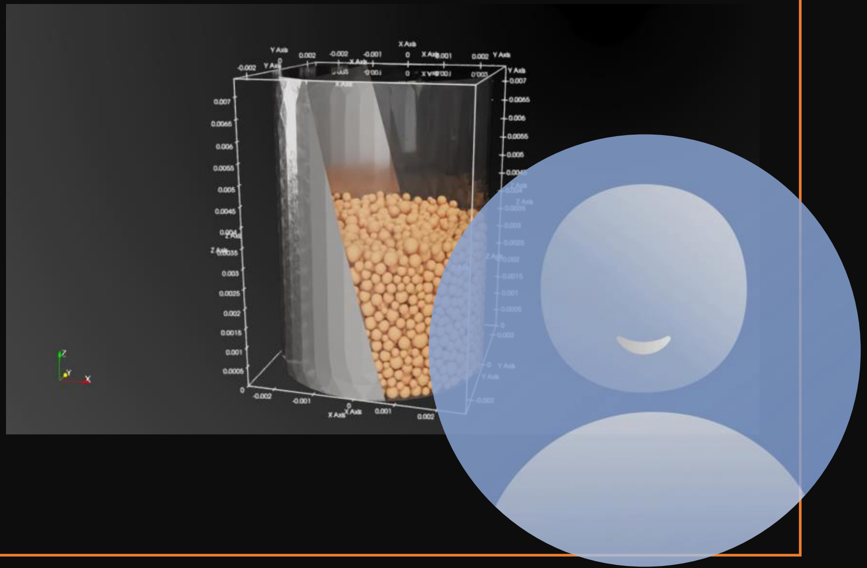


Digital Twins

The AutoBeaker – the calibration tool you didn't know you needed!

- Packing density of particles varies **dramatically** with friction & cohesion
- → Simulating (for example) GranuDrum at fixed particle **number** can give **very problematic** results
- AutoBeaker can be automatically run before "real" calibration to ensure a fixed **volume** as opposed to a fixed **number** of particles





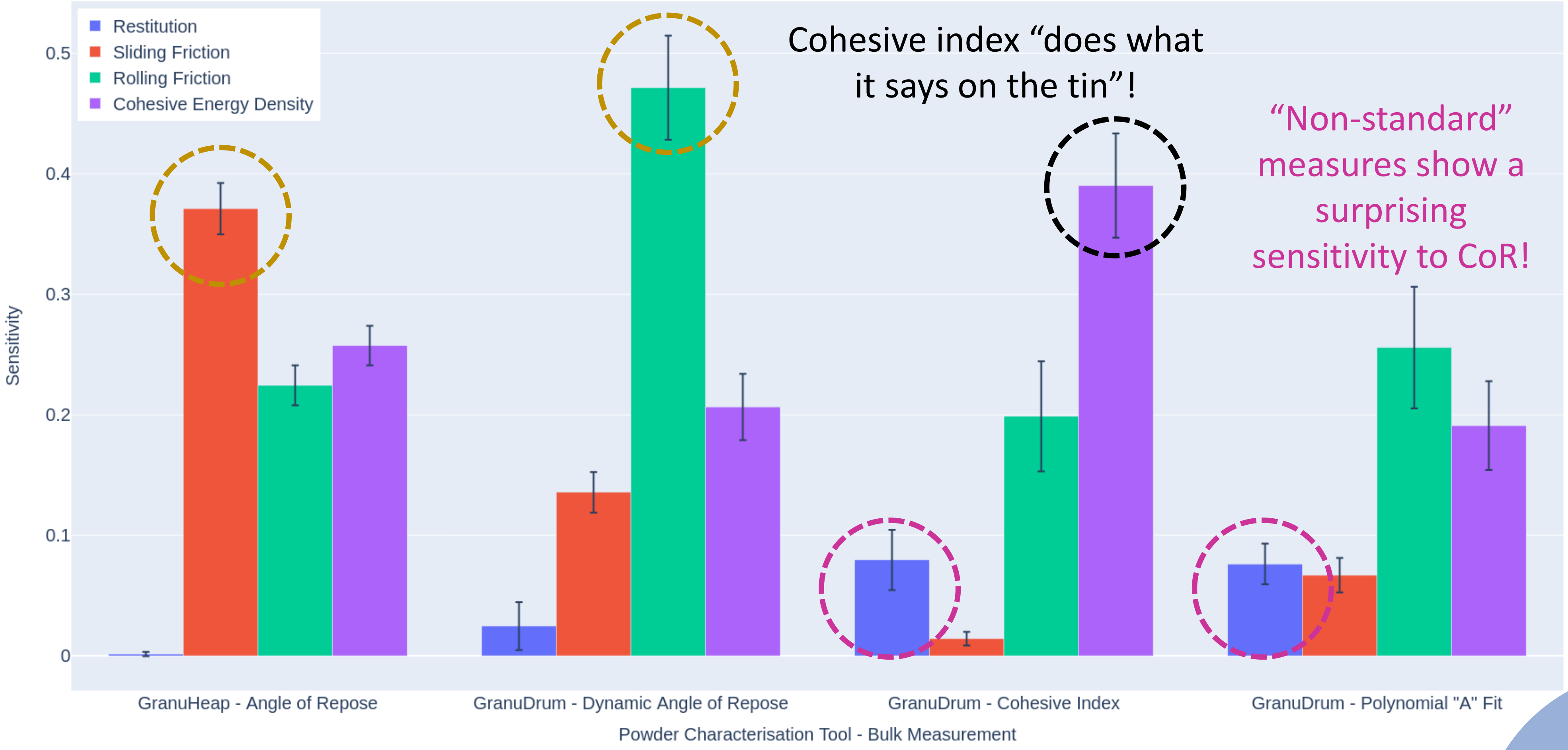
Sensitivity analysis – establishing the best tool for the job

- There are many characterisation tools available
- However, as illustrated in Part 1 of the project, not all tools work for all situations
- We have used our digital twins to perform a sensitivity analysis to determine which tools are best suited to calibrating which parameters

Question:

Would you expect a static angle of repose tester and a dynamic angle of repose tester to be sensitive to different parameters?

Static AoR more sensitive to sliding friction, dynamic AoR more sensitive to rolling friction



Cohesive index “does what it says on the tin”!

“Non-standard” measures show a surprising sensitivity to CoR!

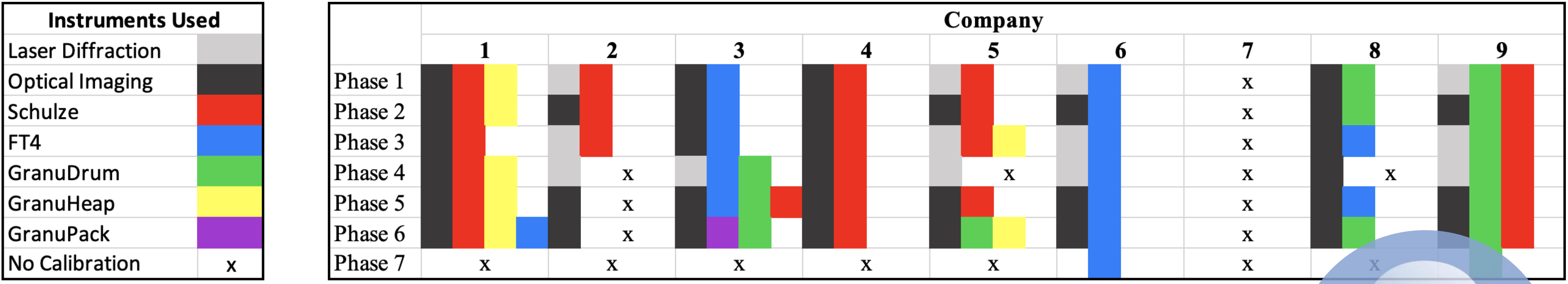
Sensitivity Analysis

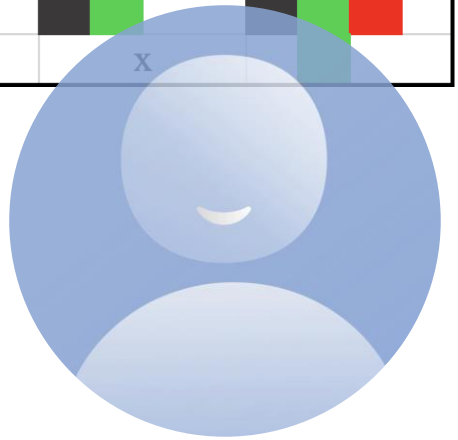
Data acquired using high dimensional model representation (HDMR)

Example of Granutools GranuHeap and GranuDrum

Key Findings

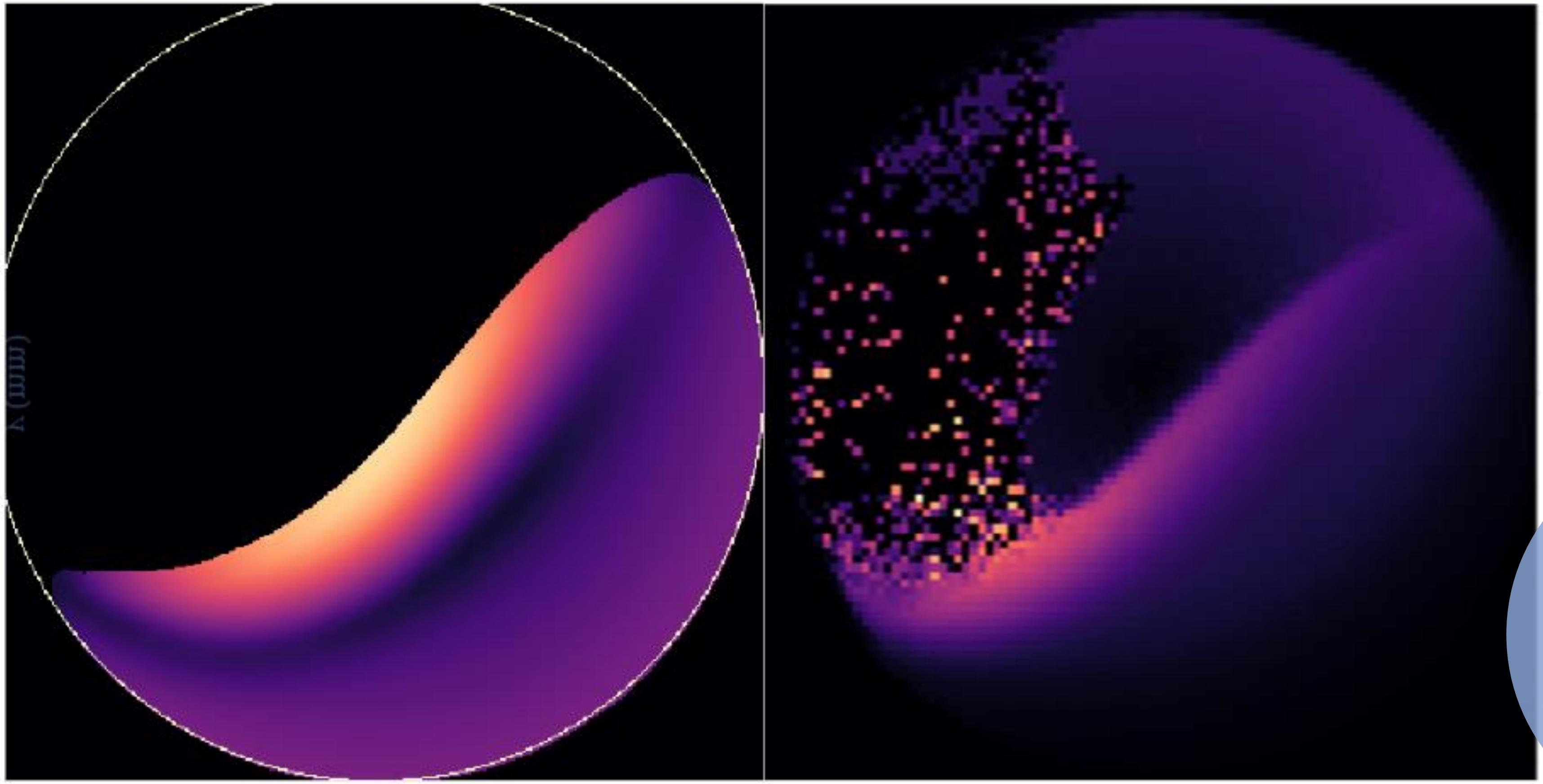
1) We **really** need standardisation





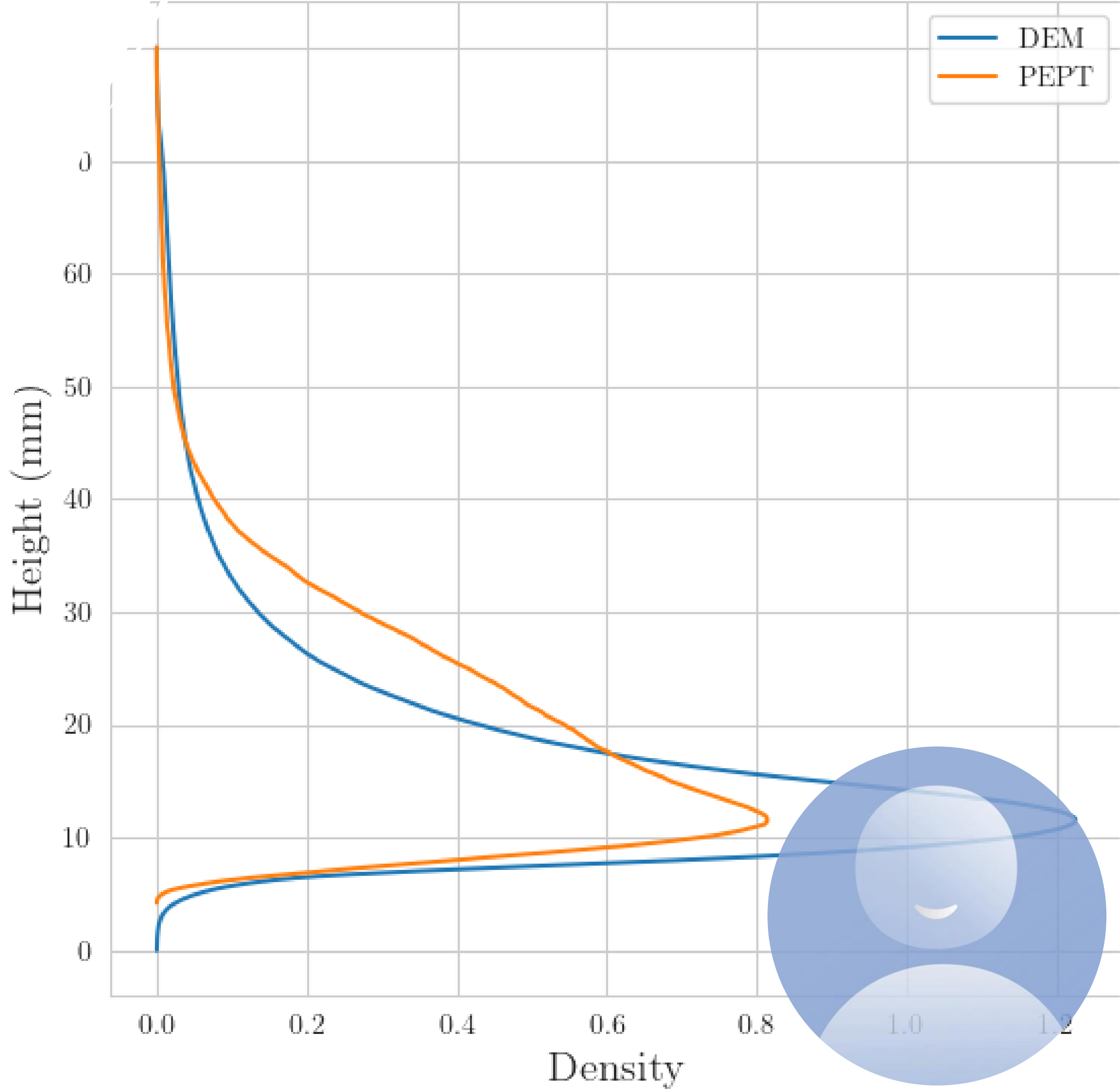
2) We **really** need to calibrate - Default values don't cut it

PEPT "Values from Literature"

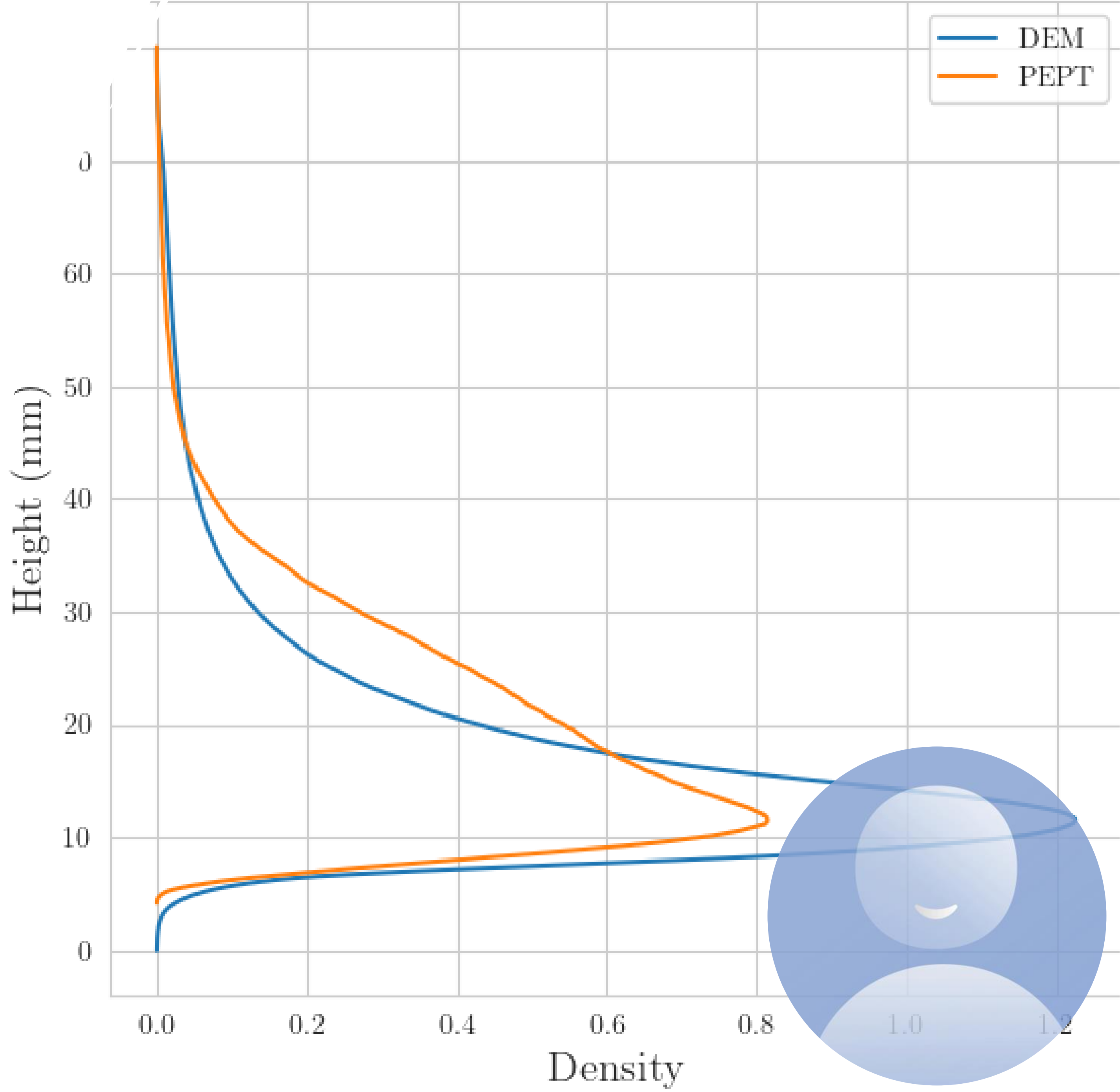


3) What works for one system...

...does not necessarily work for another



4) Almost nobody calibrates restitution – and sometimes it matters!

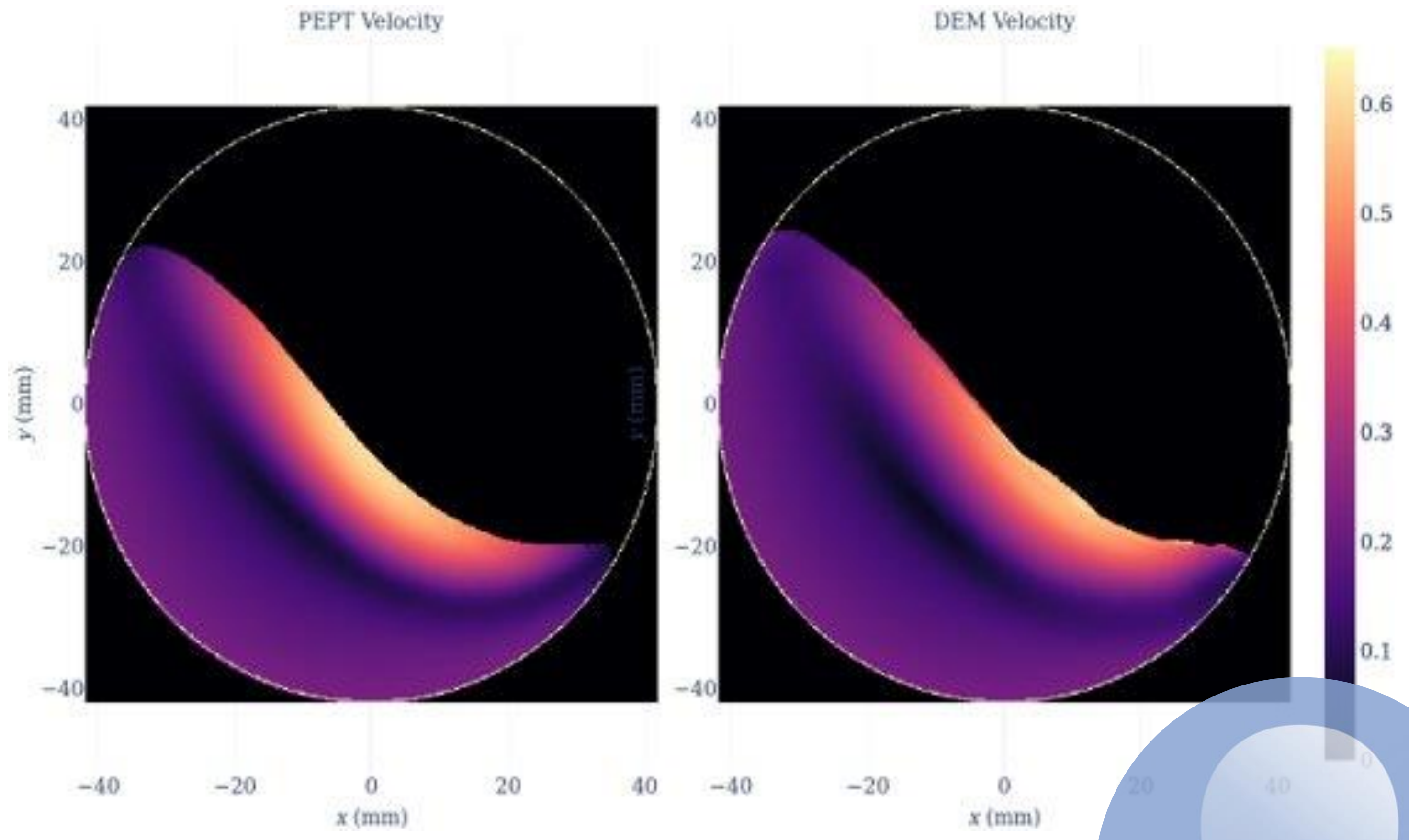


Added Value

New tools & techniques developed during the project

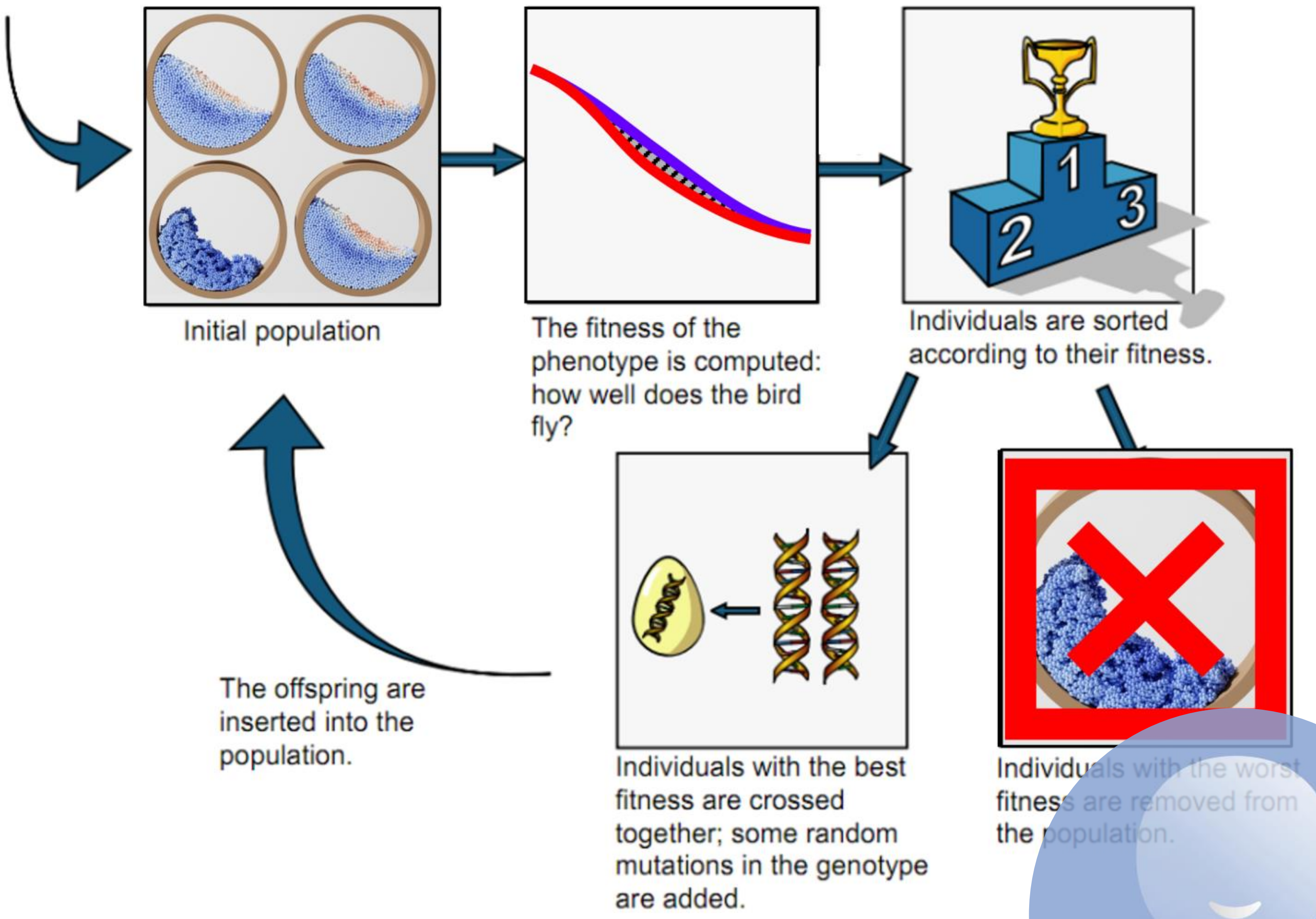
Universal Post-Processor for Particulate Processes (UP^4)

- A tool allowing DEM, PEPT (PTV, RPT, MP-PIC…) data to be analysed in a **truly identical manner**
- Facilitates the **most rigorous** validation possible

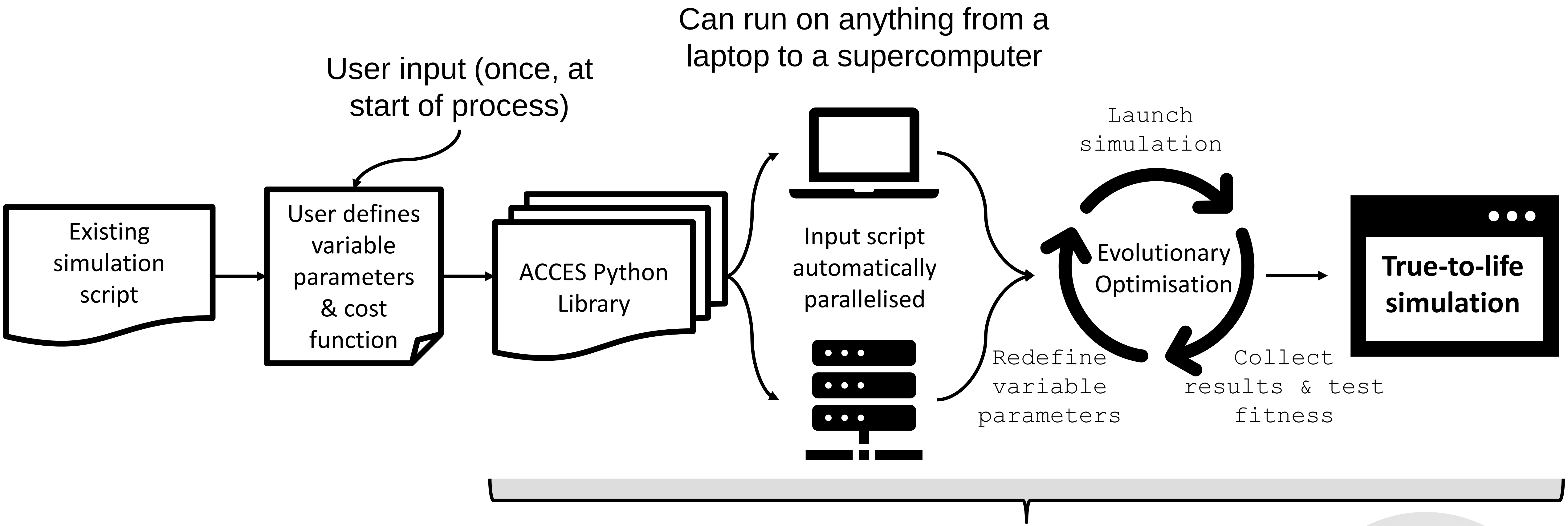


Autonomous Characterisation & Calibration using Evolutionary Simulation (ACCES)

- Fully automates the calibration procedure
- Evolutionary optimisation addresses the non-smooth, non-convex nature of the parameter space explored



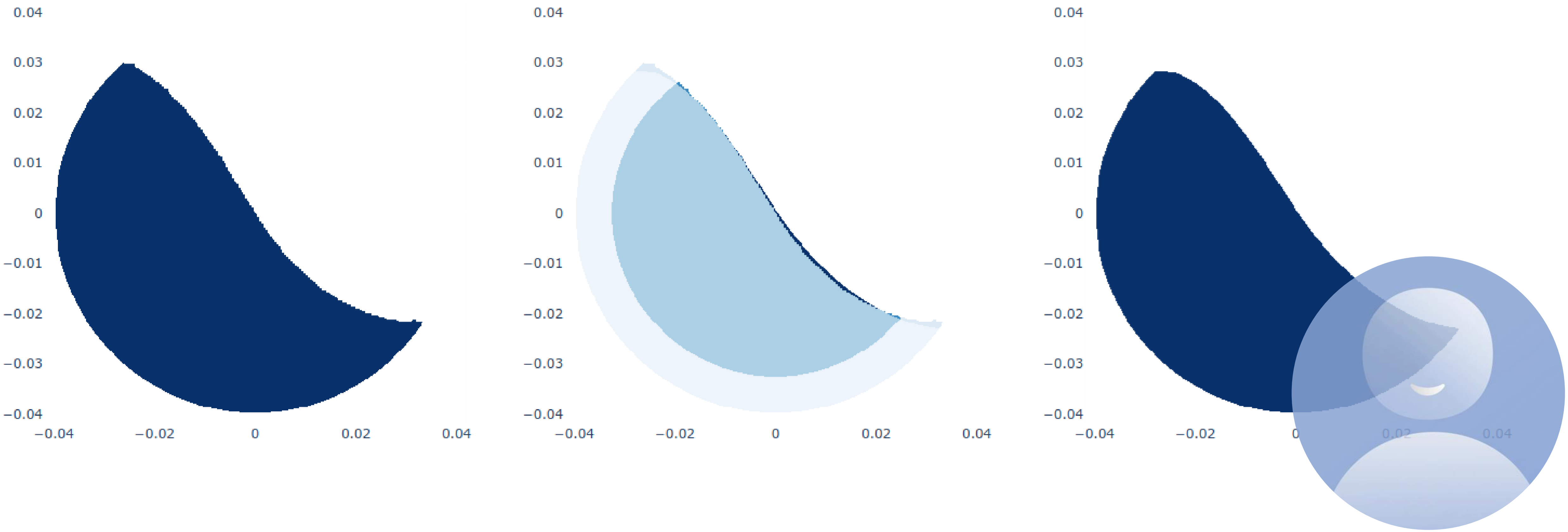
ACCES

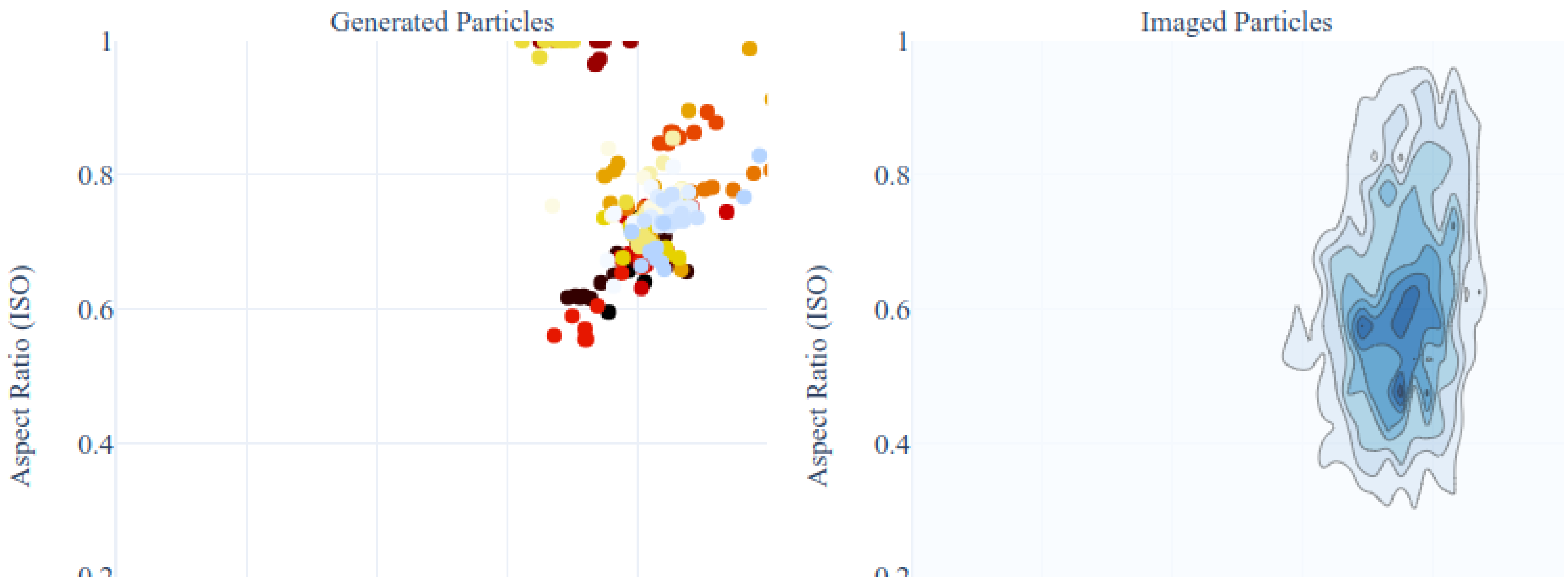


Absolutely no user input required!

Metaprogramming (code that writes code): ACCES takes input scripts, understands them, hacks them, and modifies them to run in fault-tolerant massively parallel environments

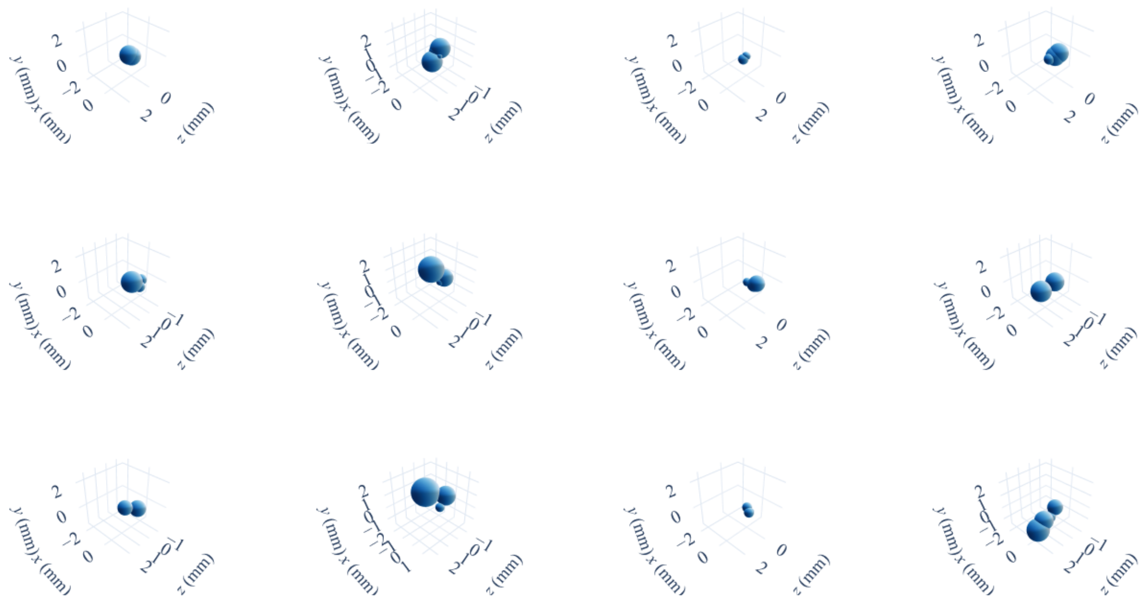
Example of an ACCES-calibrated system





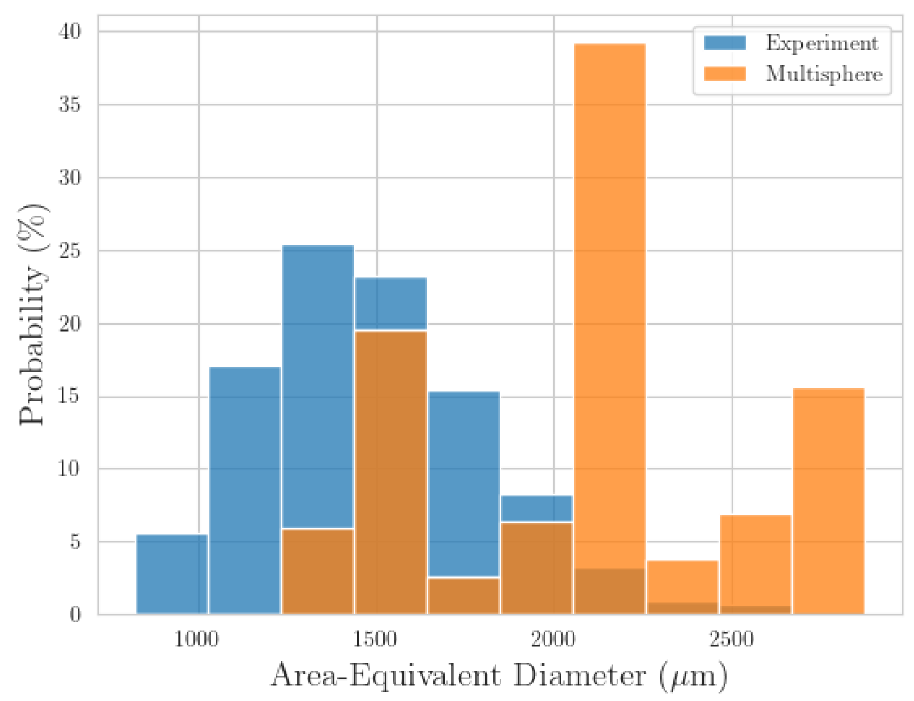
Using ACCES to Model the Particle *Shape* Distribution

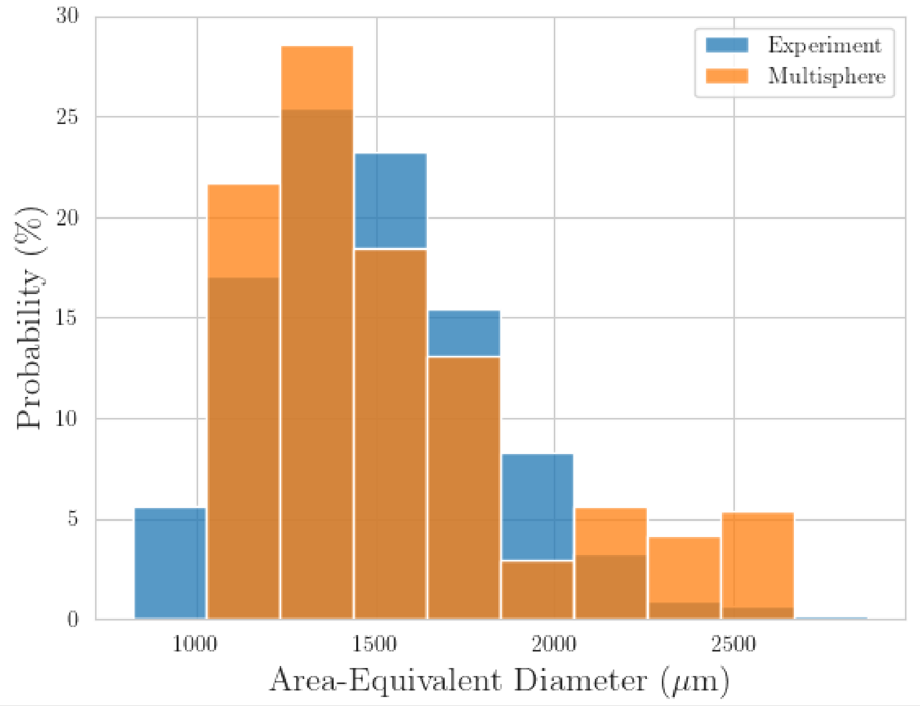
1. Use optical imaging to get a 2D distribution in EFF-AR space
2. Use MC to generate candidate particles falling within the bounds of this distribution



Using ACCES to Model the Particle *Shape* Distribution

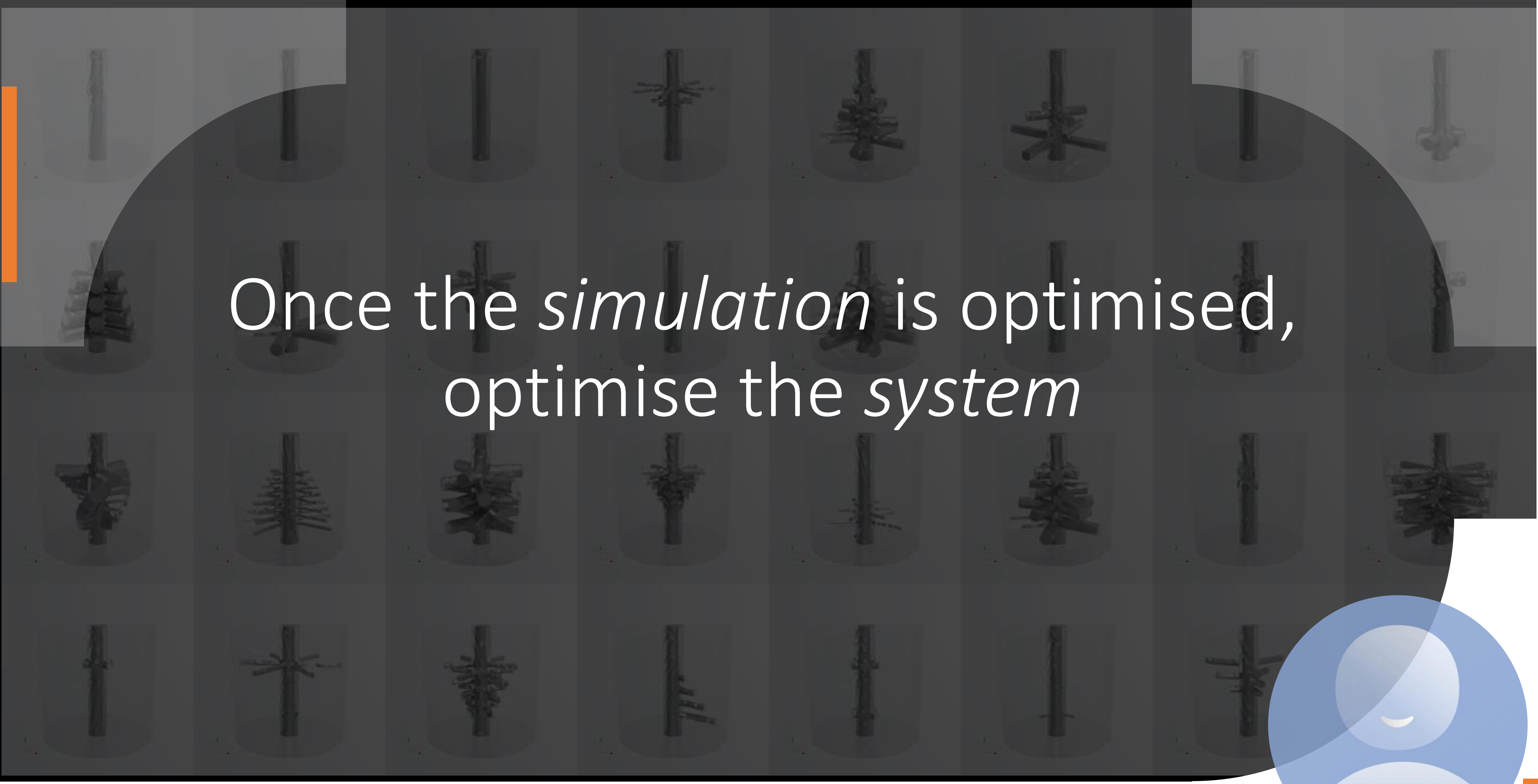
3. Choose *N* candidate shapes
4. From *N* candidates, produce *M*N* “candidate particles” by scaling initial candidates
5. Simultaneously with 4, determining the necessary fractions of each scaled candidate to correctly represent the distributions, creating a *2*M*N*-dimensional optimisation problem!





Before and after ACCES fitting

6. Solve the problem with ACCES → Correct fractions and scalings



Once the *simulation* is optimised, optimise the *system*