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Positron Emission Particle Tracking: A technique for the high-speed, high-resolution imaging of multiphase flows

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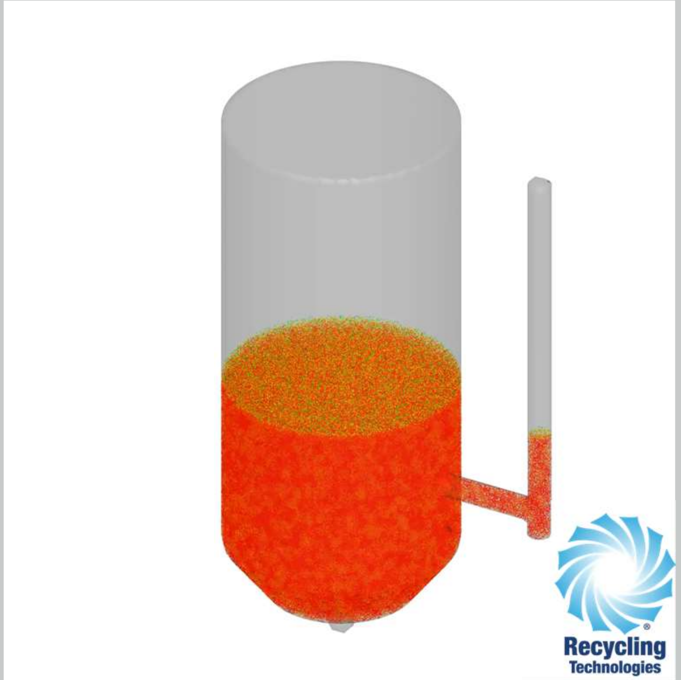
Overview & Motivation

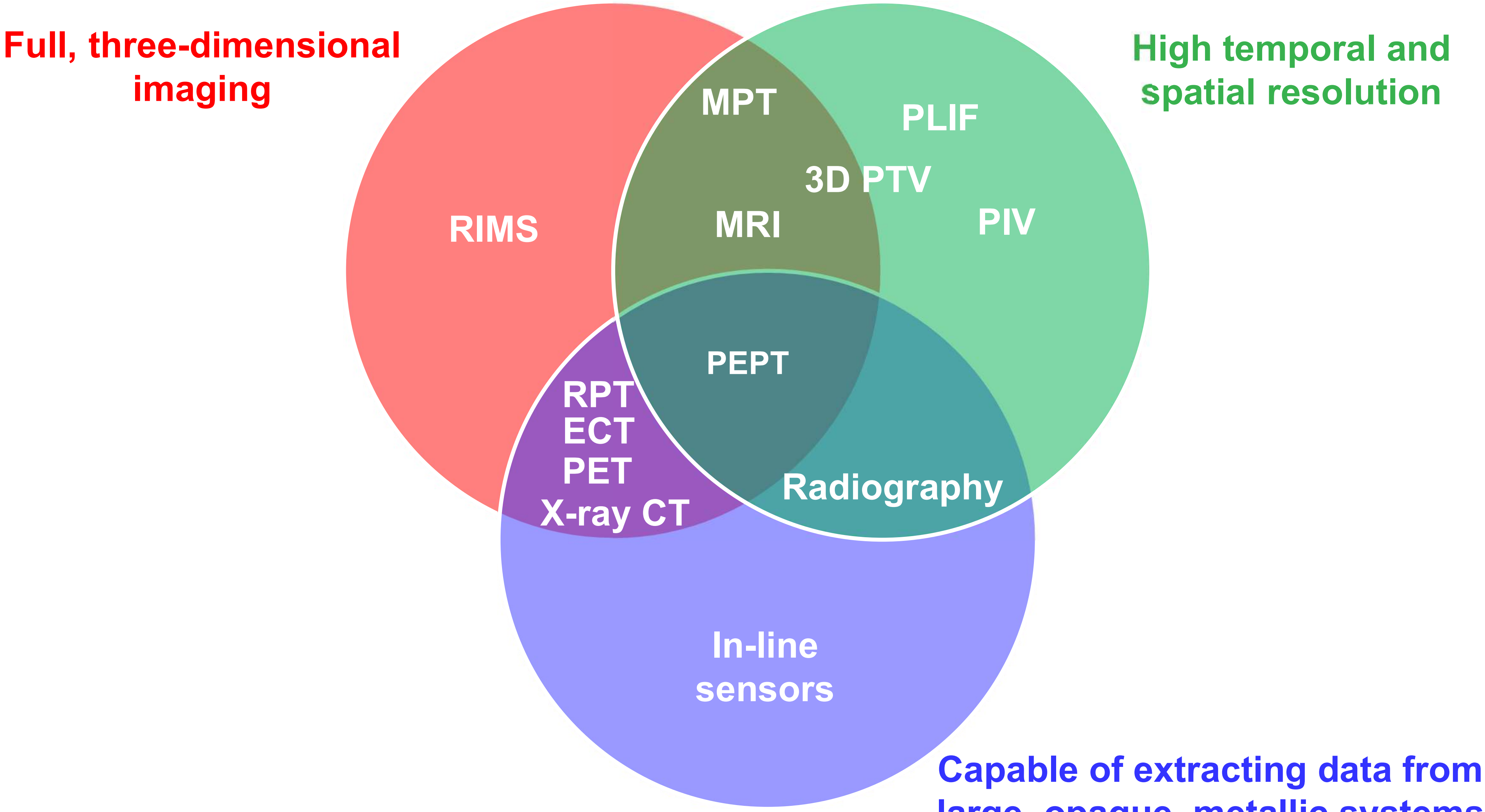
How do we better understand industrial systems?

- Understanding the dynamics of multiphase flows is crucial to the optimisation of diverse process equipment
- …but these large, metal systems are near-impossible to accurately image using conventional methods



How do we better understand industrial systems?

- Numerical methods (DEM, CFD, MP-PIC…) can provide insight
- **But** without experimental validation, simulations may be **misleading**
- → We still need to find a way to experimentally investigate these large, opaque systems!


Full, three-dimensional imaging
High temporal and spatial resolution
Capable of extracting data from large, opaque, metallic systems
RIMS
MPT
MRI
3D PTV
PLIF
PIV
PEPT
RPT
ECT
PET
X-ray CT
Radiography
In-line sensors

Talk Overview

I) An Introduction to PEPT

II) Case Study

III) The Synergy of PEPT and Numerical Simulation

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I. An Introduction to PEPT

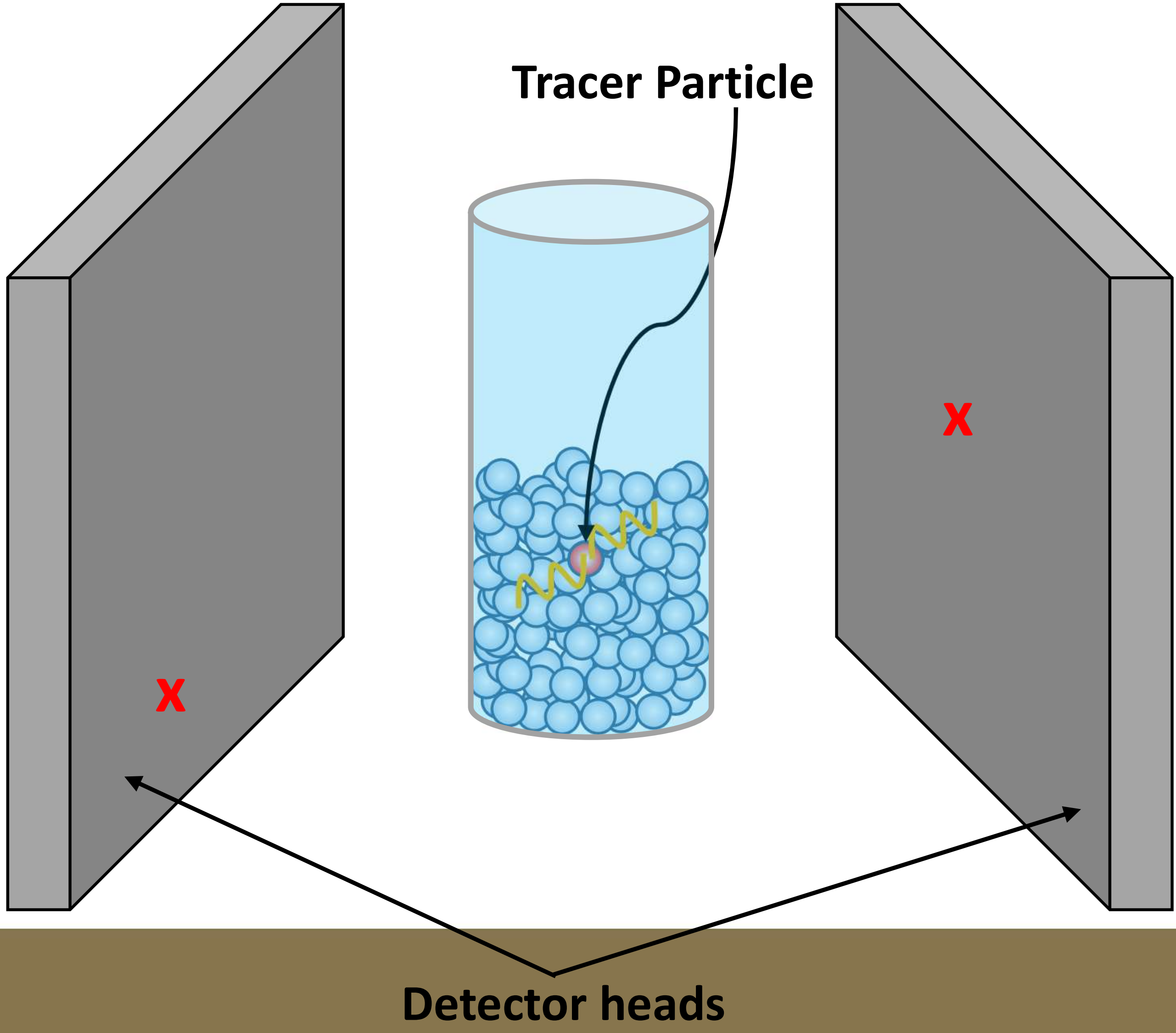
Positron Emission Particle Tracking (PEPT)

Uses highly-penetrating gamma radiation to **directly track** the three-dimensional motion of particulate, fluid and multiphase systems, with **high temporal and spatial resolution**.

Uses highly-energetic gamma rays, capable of penetrating opaque media, including aluminium and steel

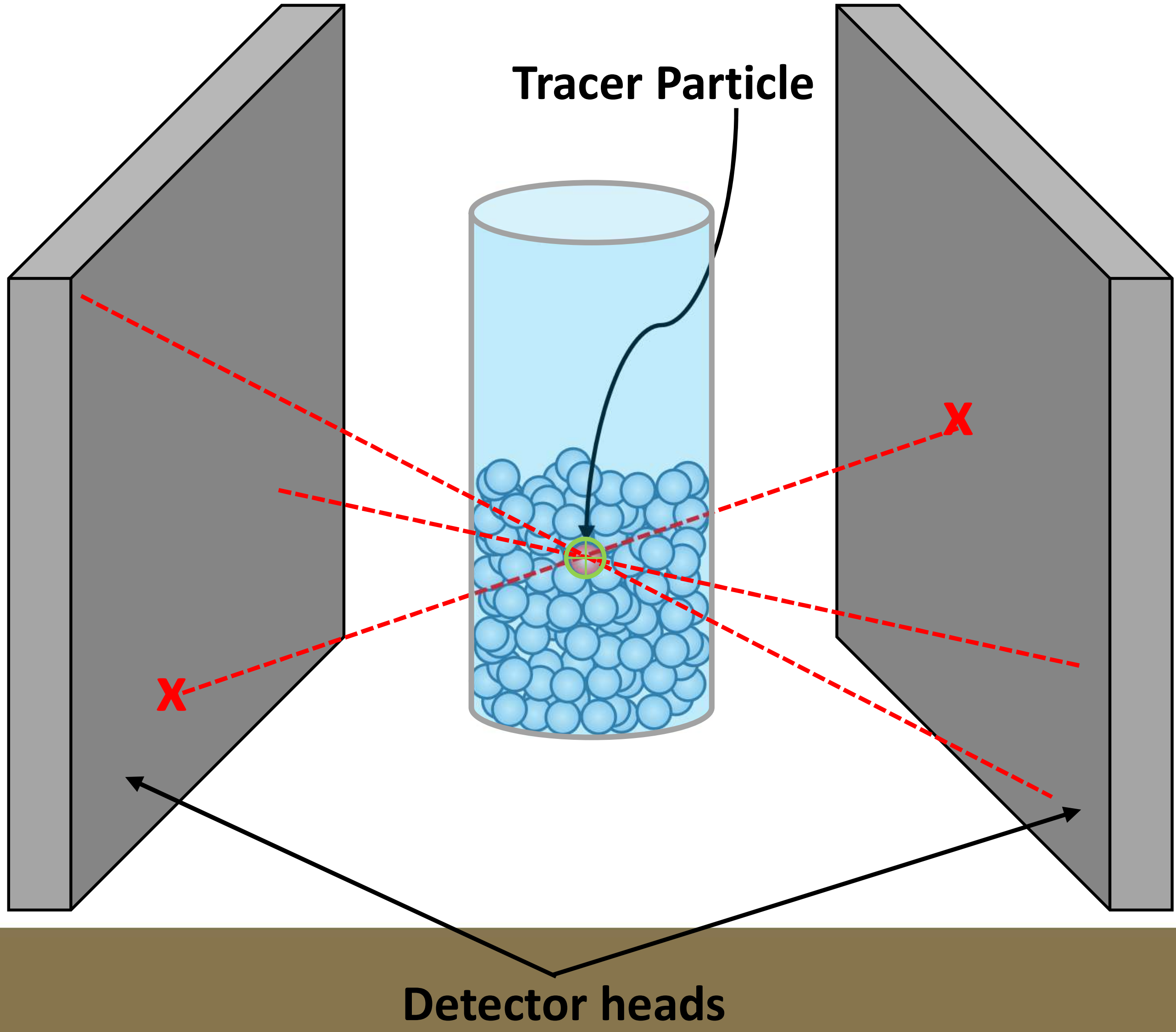
In essence, PEPT allows us to **'see inside' opaque systems**.

How does it work?



Windows-Yule, C. R. K., Seville, J. P. K., Ingram, A., & Parker, D. J. (2020). Positron Emission Particle Tracking of Granular Flows. *Annual Review of Chemical and Biomolecular Engineering*, *11*.

How does it work?



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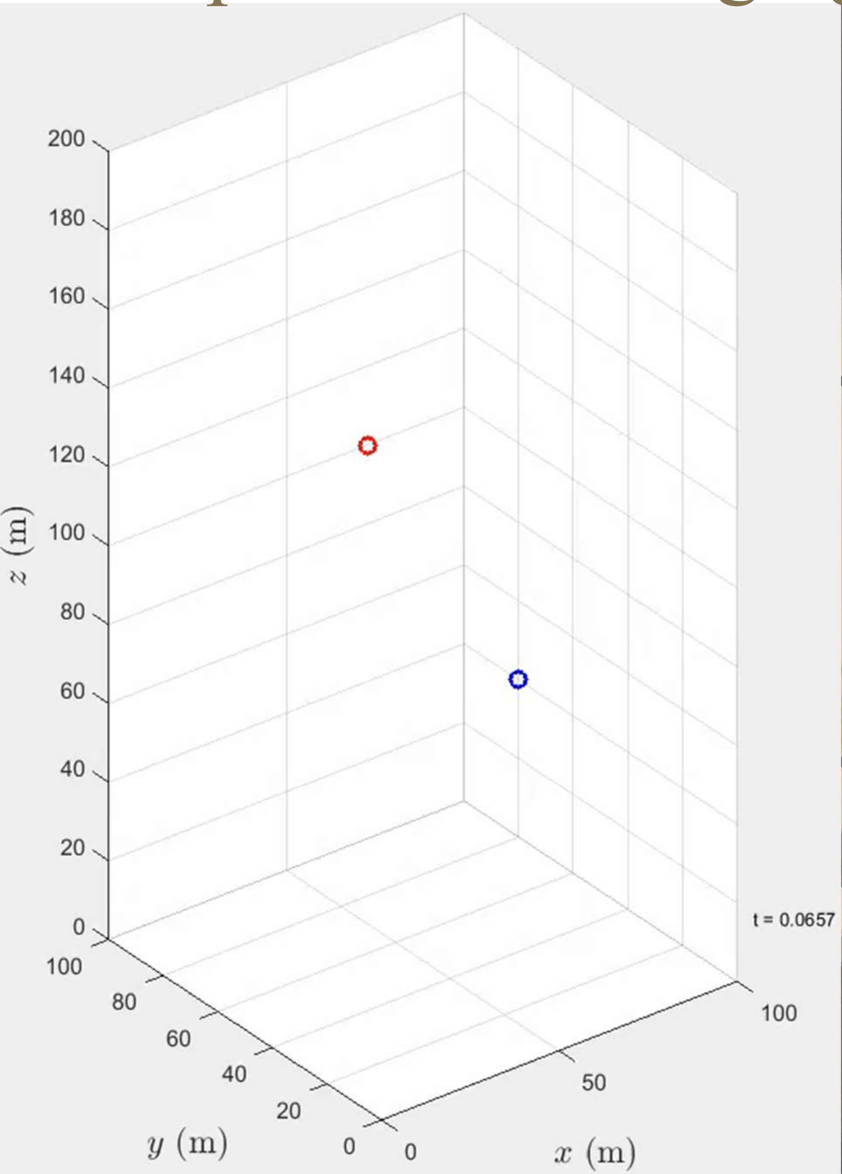
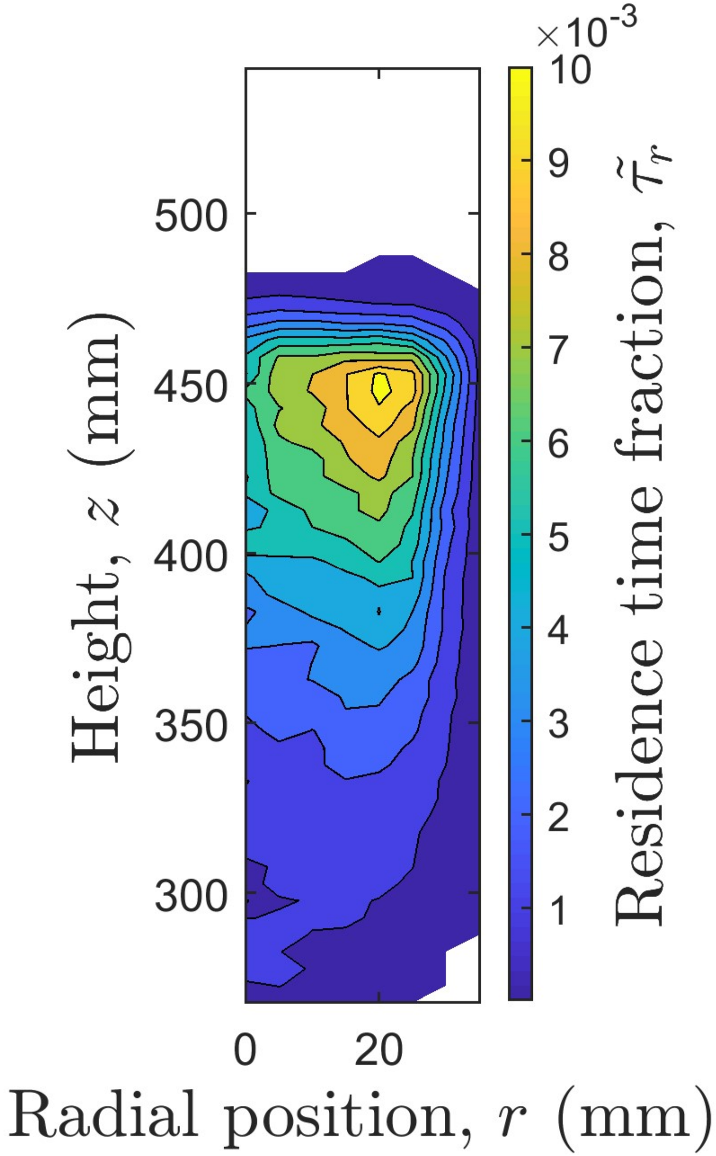
Example: PEPT imaging of a fluidised bed





Example: PEPT imaging of a **serious** fluidised bed

Modular cameras provide additional, flexible imaging area

Main ADAC camera heads

Large, opaque vessel
$(D = 300\text{mm}, H > 1\text{m})$
Solid steel walls

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Example: PEPT imaging of a **real, industrial** fluidised bed

ACCES

Featured in *Ingenia* magazine:

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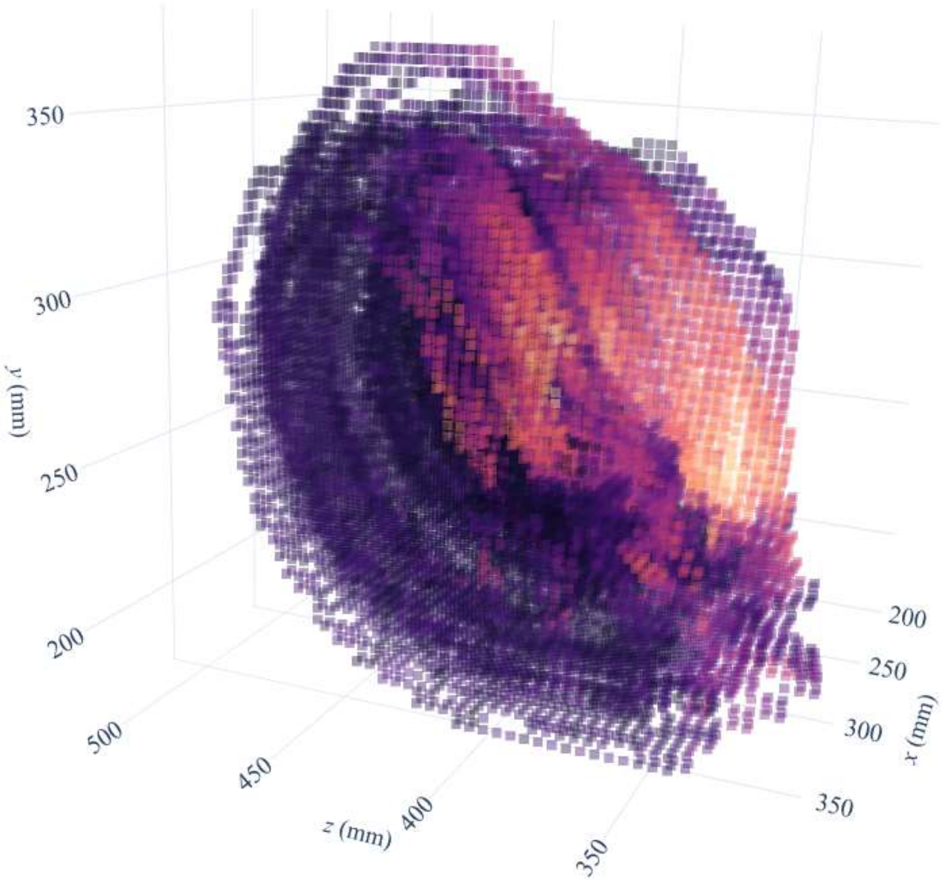
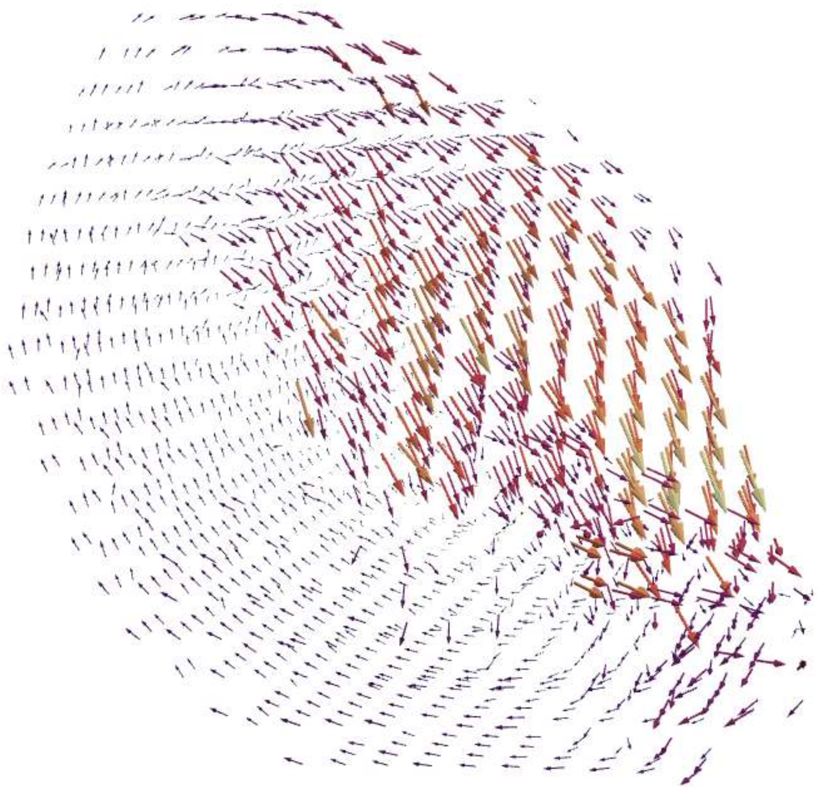
High-resolution, three-dimensional data





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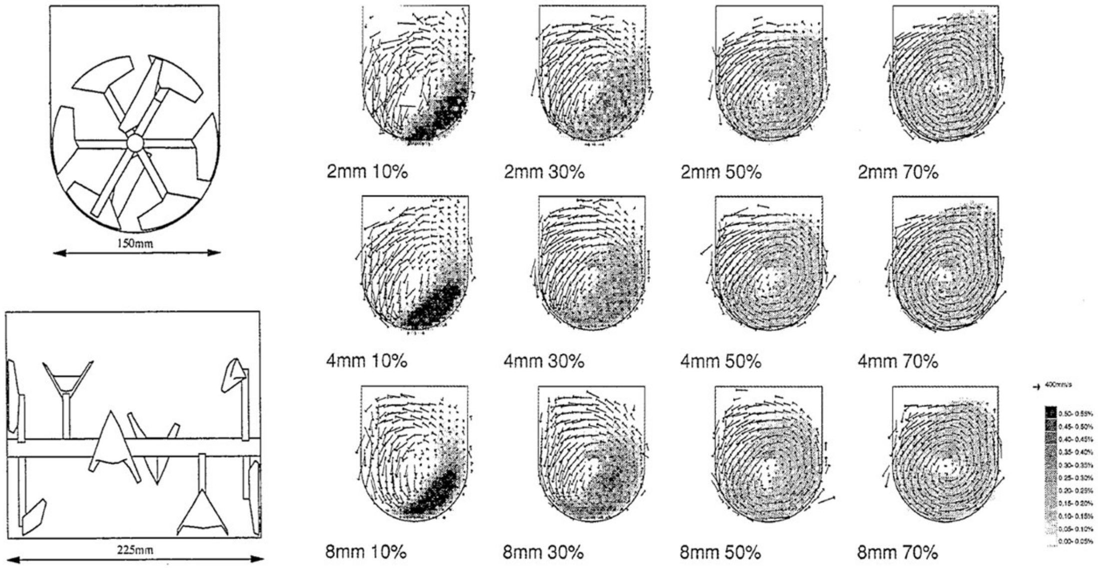
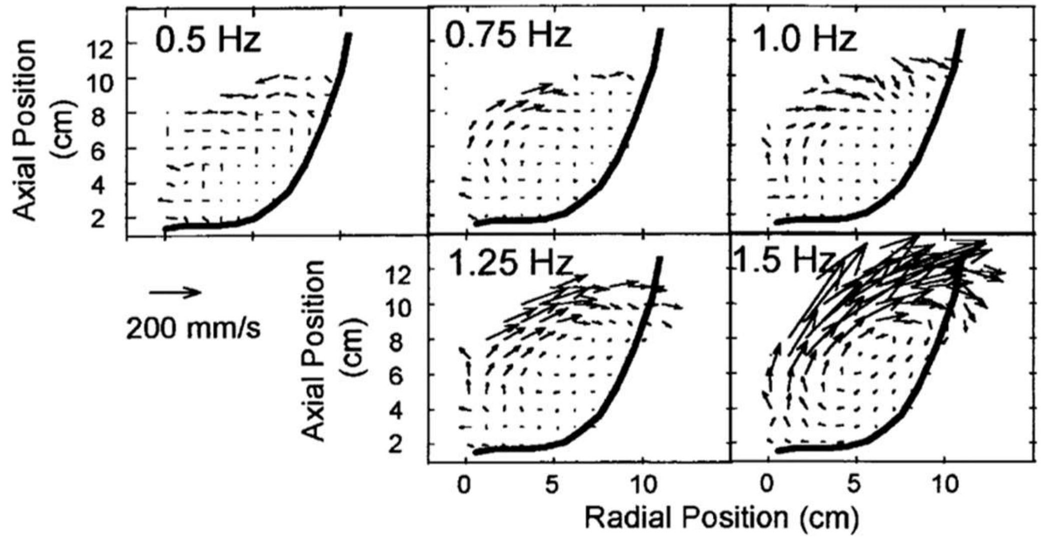
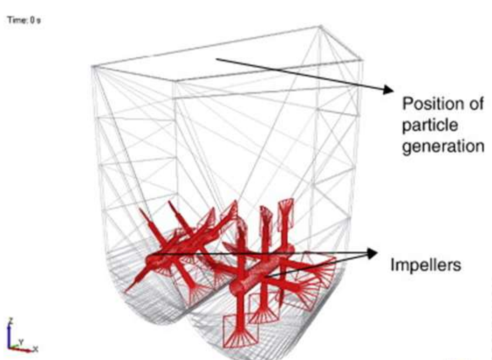
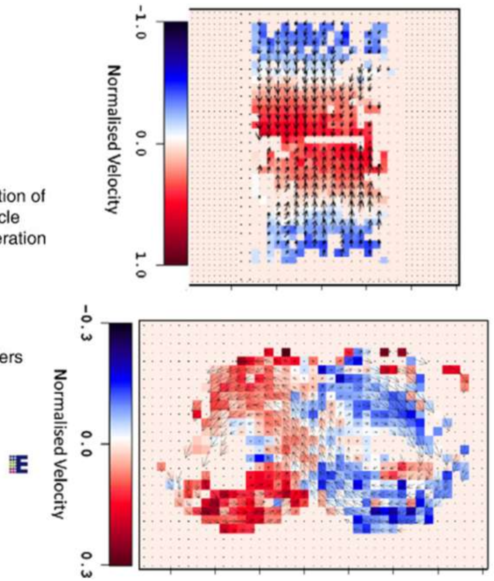
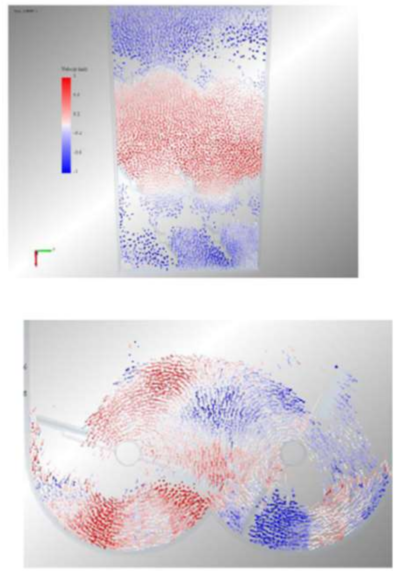


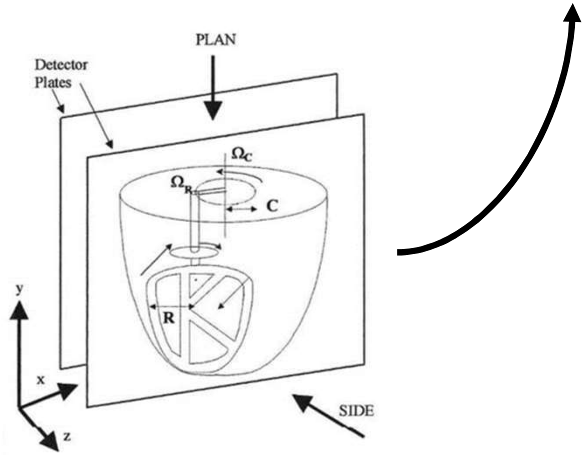


Industrial Mixers

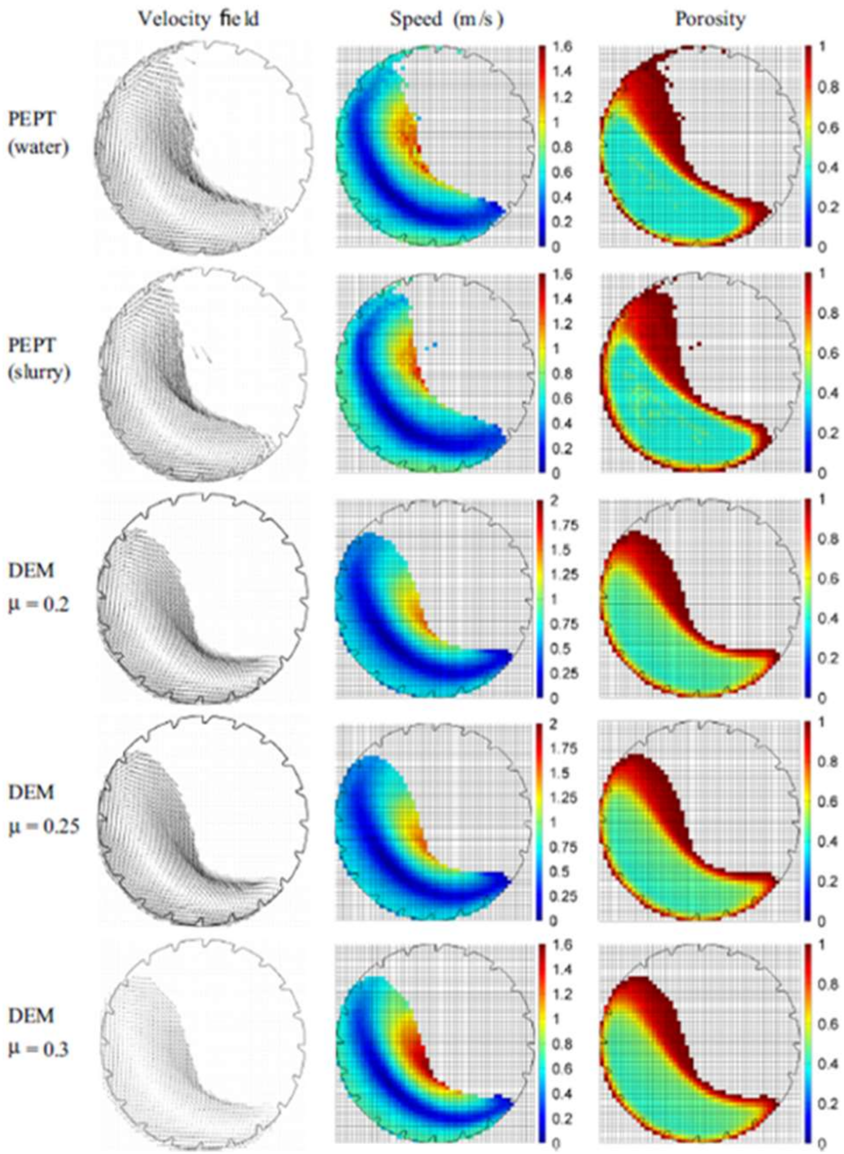


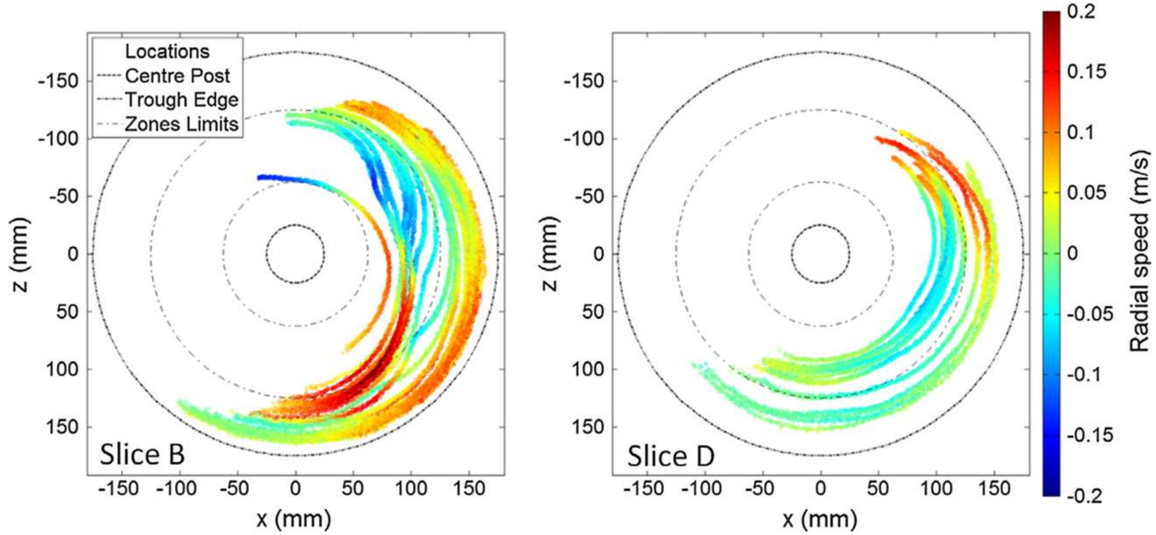




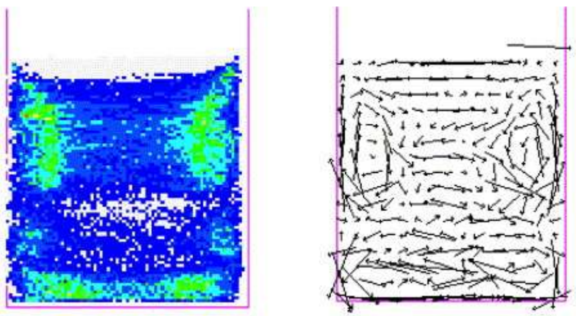


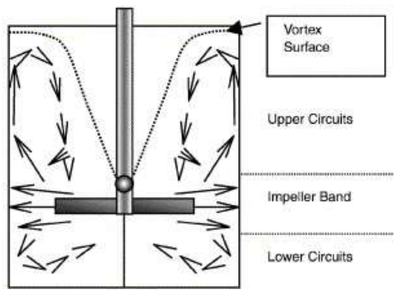
Windows-Yule, C. R. K., Nicuşan, A.L., Herald, M. T., Manger, S. & Parker, D.J., *PEPT, a Comprehensive Guide*, IoP Publishing, 2022





Spiral mineral concentrators

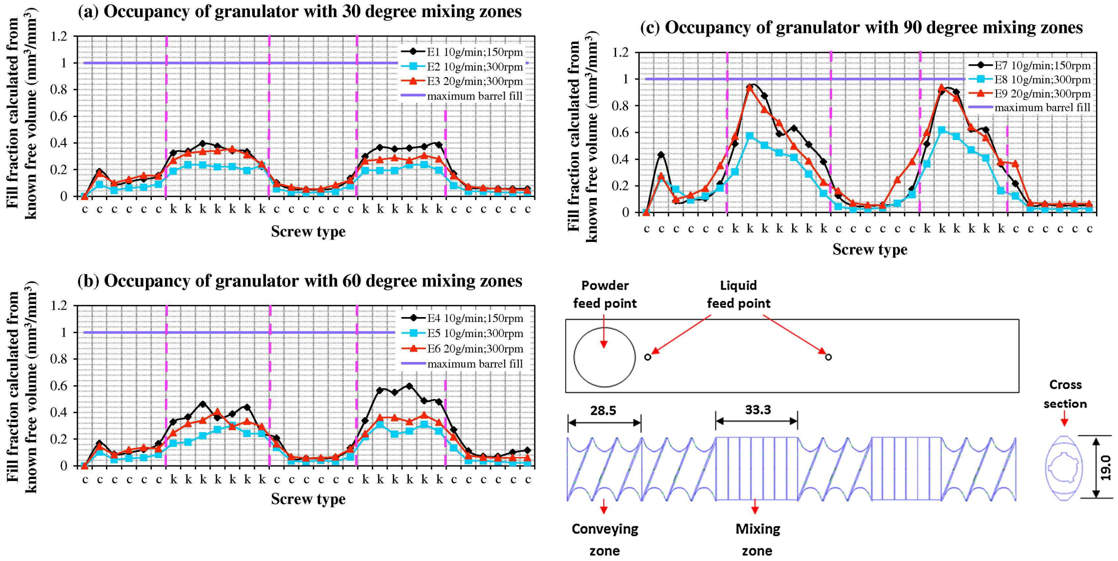


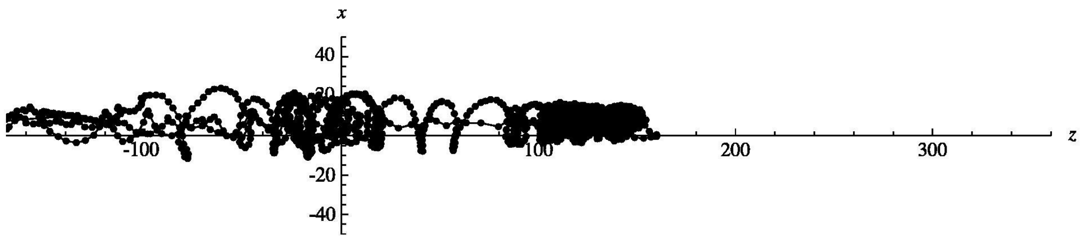


Mills

Windows-Yule, C. R. K., Nicuşan, A.L., Herald, M. T., Manger, S. & Parker, D.J., *PEPT, a Comprehensive Guide*, IoP Publishing, 2022

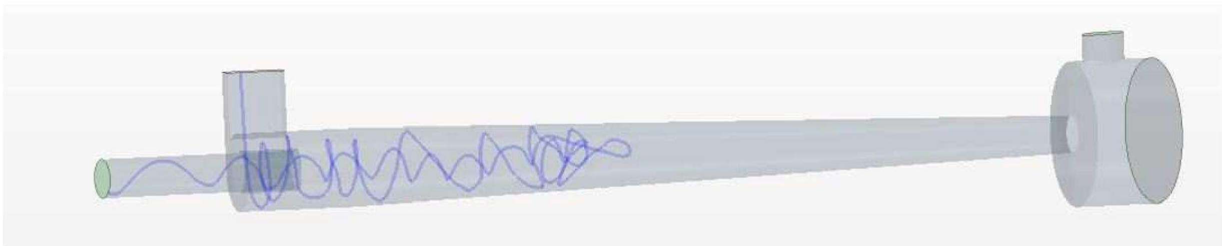
Twin screw granulators



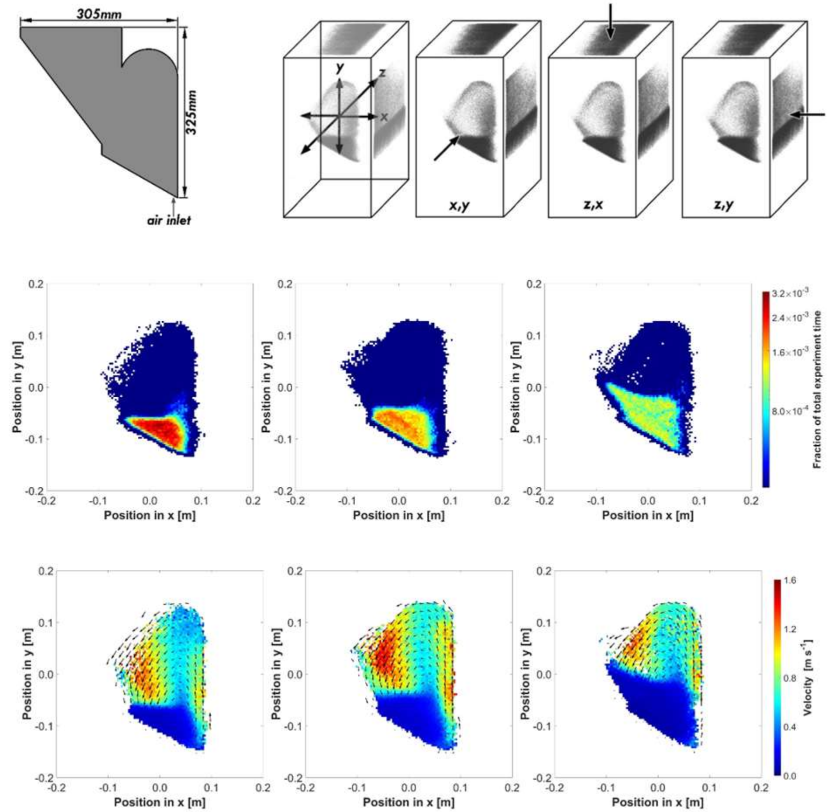


(a)

Gas-/hydro-cyclones

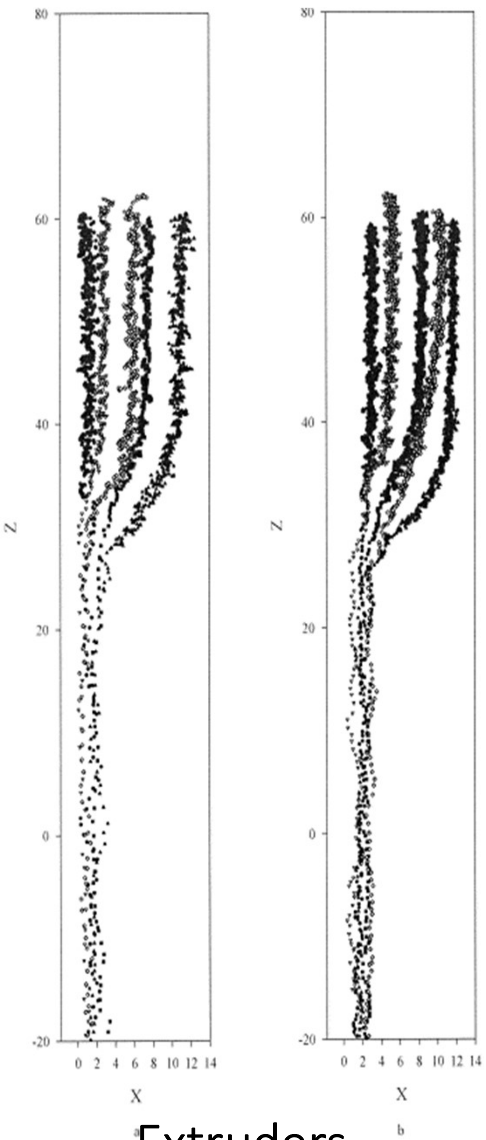


(b)

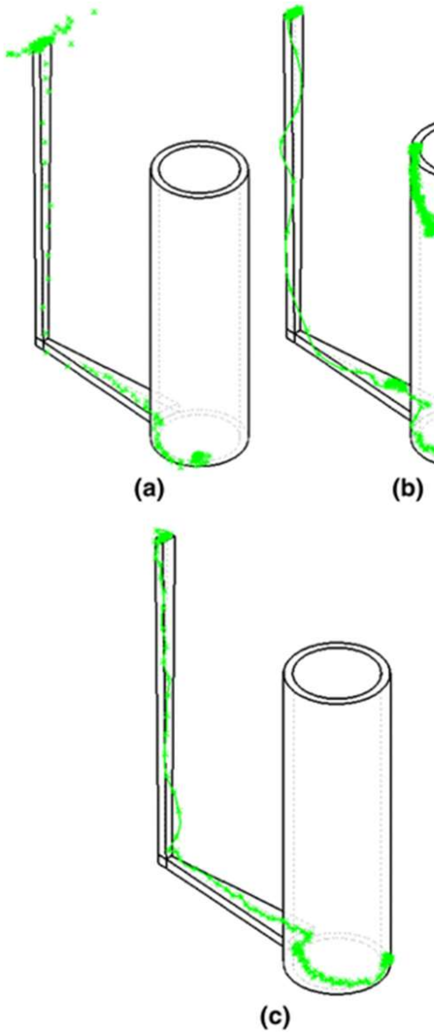


Coffee roasters

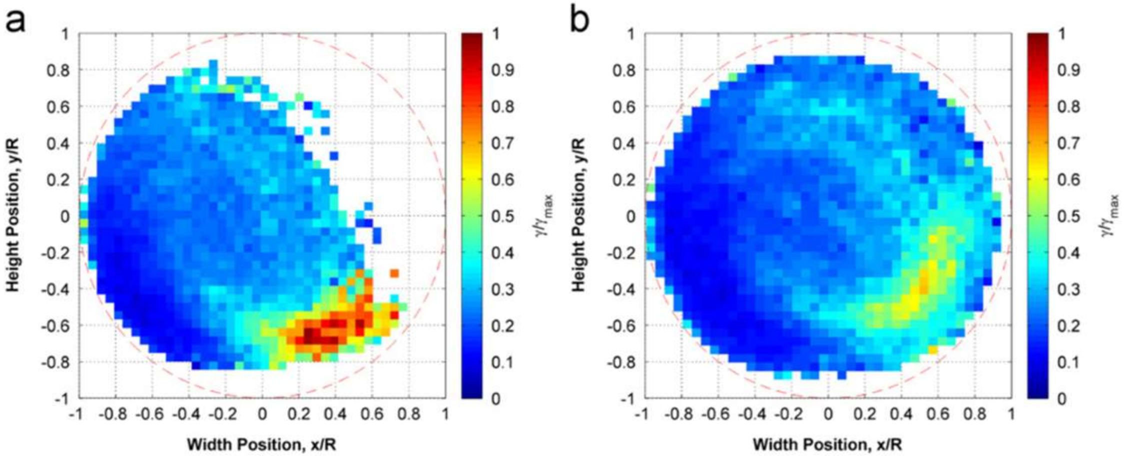
Windows-Yule, C. R. K., Nicuşan, A.L., Herald, M. T., Manger, S. & Parker, D.J., *PEPT, a Comprehensive Guide*, IoP Publishing, 2022



Extruders

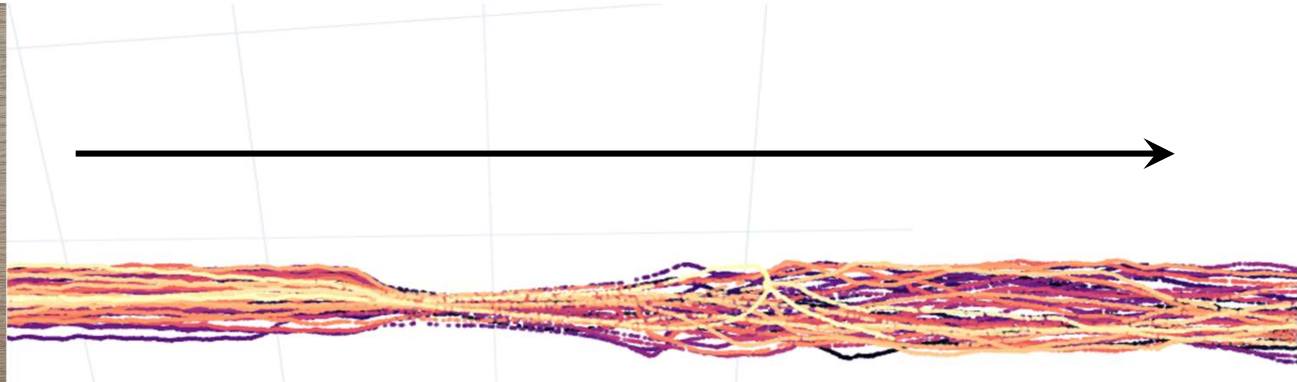


Metal casting



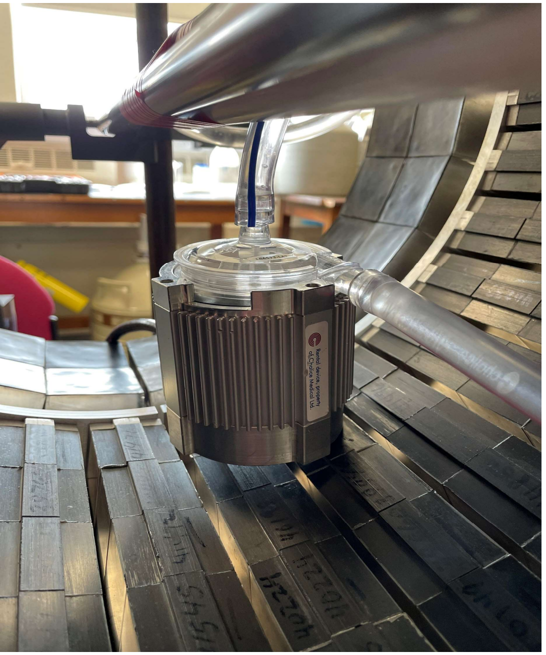
Domestic systems

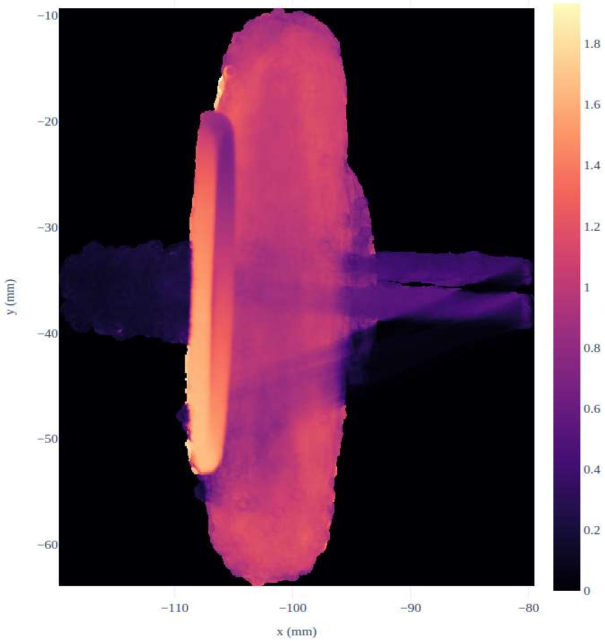
Windows-Yule, C. R. K., Nicuşan, A.L., Herald, M. T., Manger, S. & Parker, D.J., *PEPT, a Comprehensive Guide*, IoP Publishing, 2022

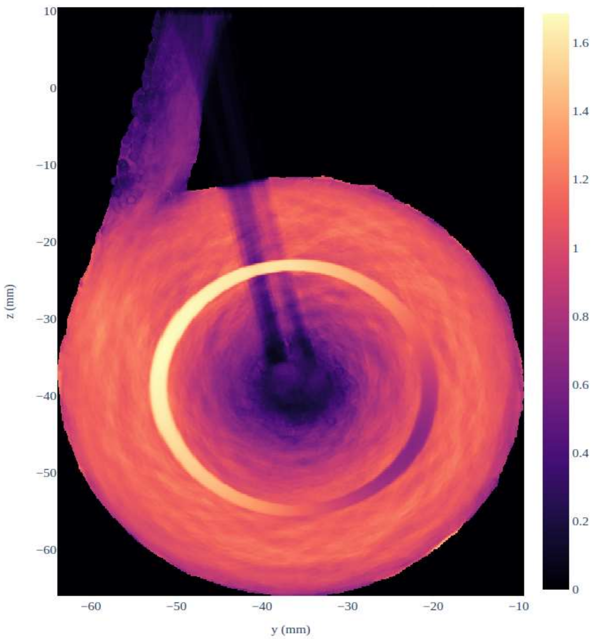


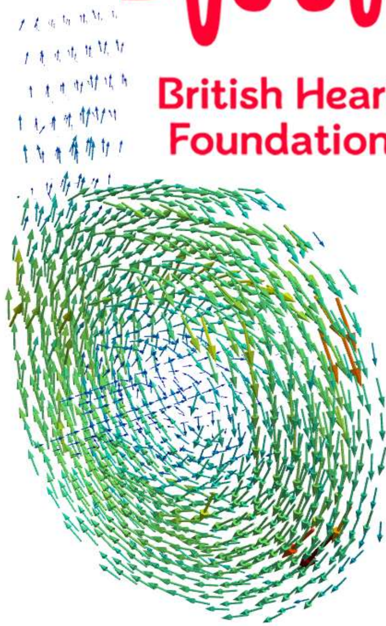
The human body?

British Heart Foundation









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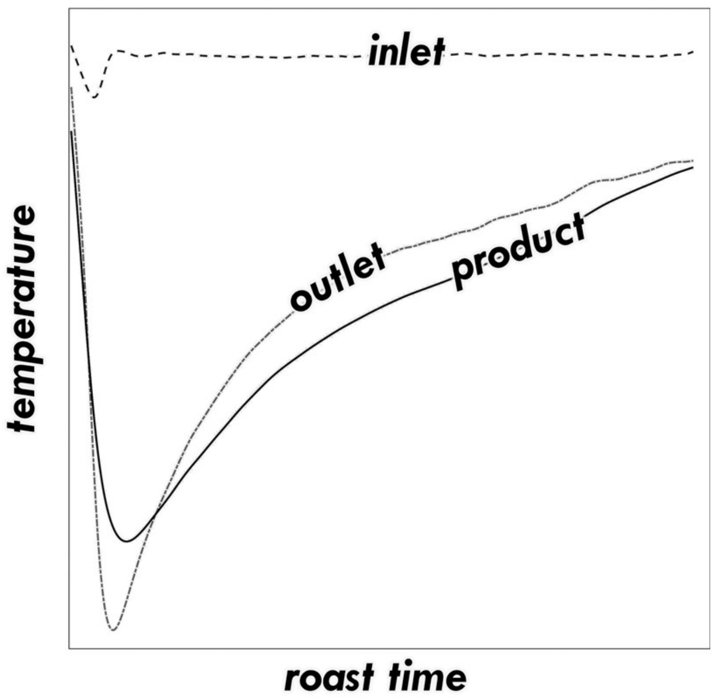
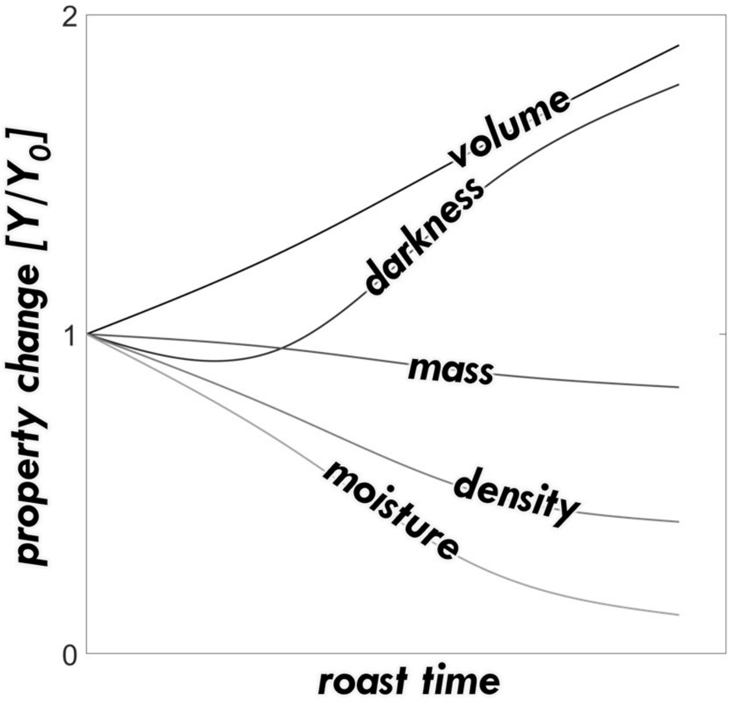
JDE
JACOBS DOUWE EGBERTS

II. Case Study: Spouted Bed Coffee Roaster (Jacobs Douwe Egberts)

Context – Coffee Roasting

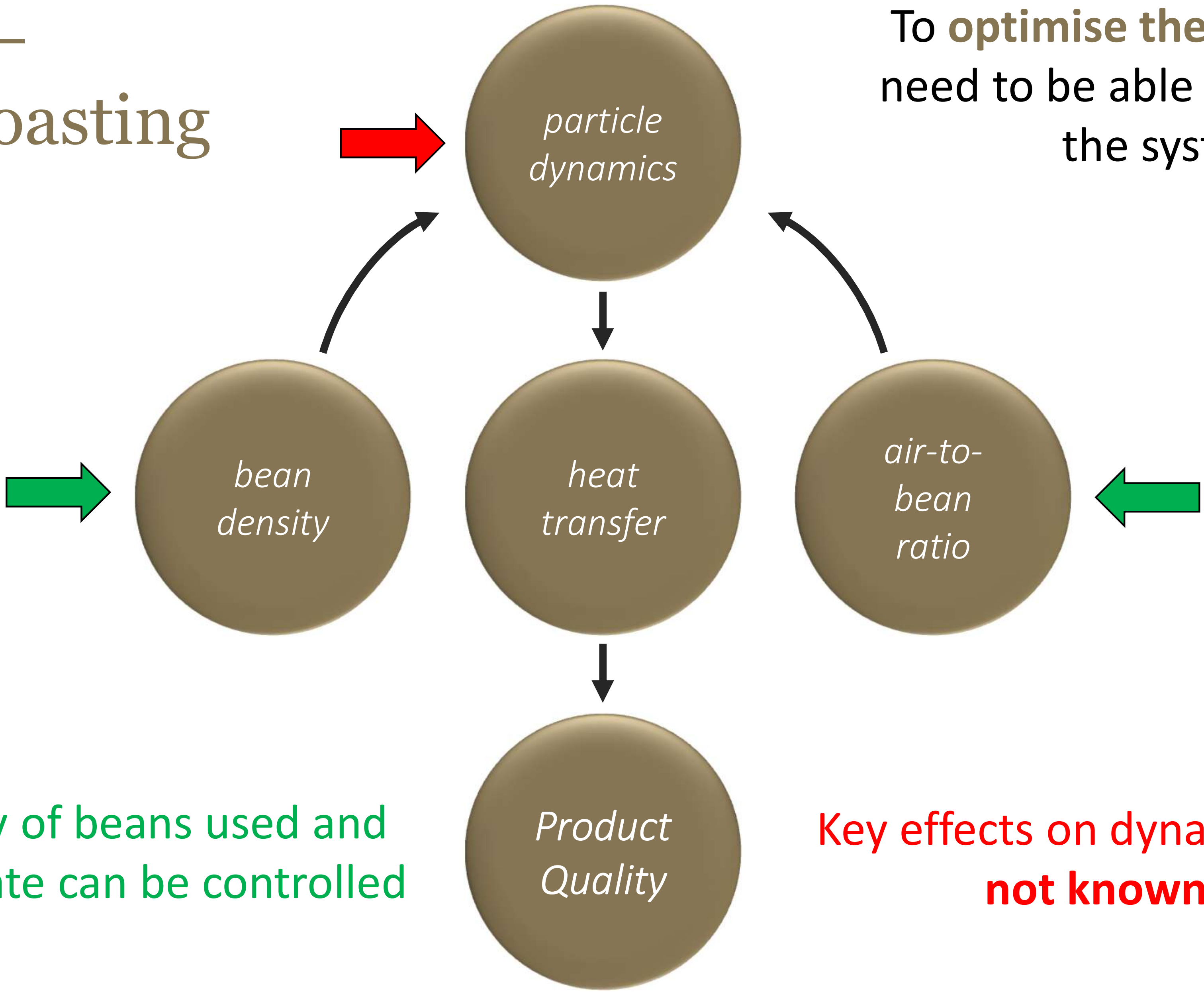
Transformations during roasting





Context – Coffee Roasting

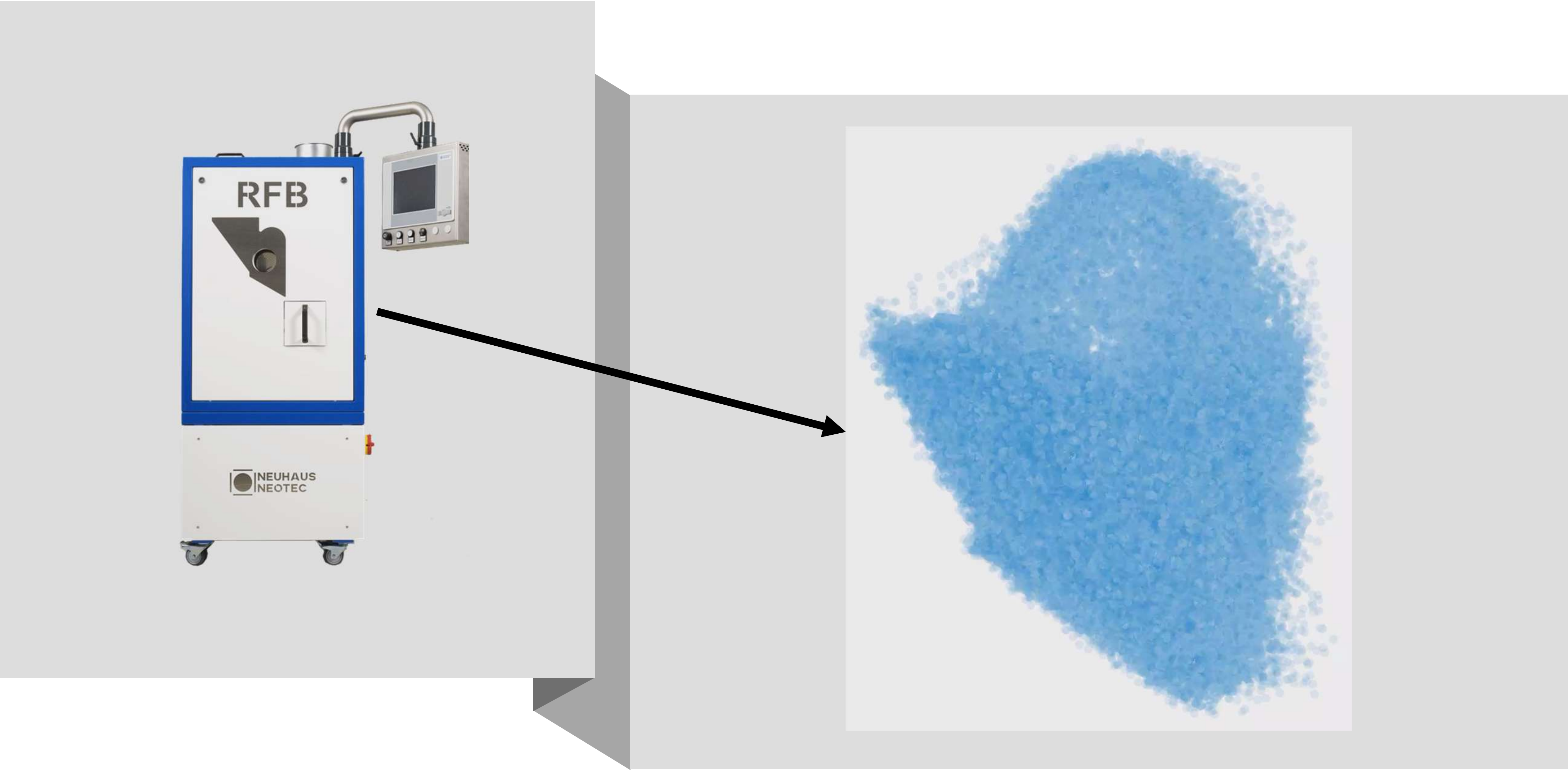
To **optimise the product** we need to be able to **see inside** the system



Quantity of beans used and airflow rate can be controlled

Key effects on dynamics are **not known**

Experimental set-up


RFB
NEUHAUS
NEOTEC

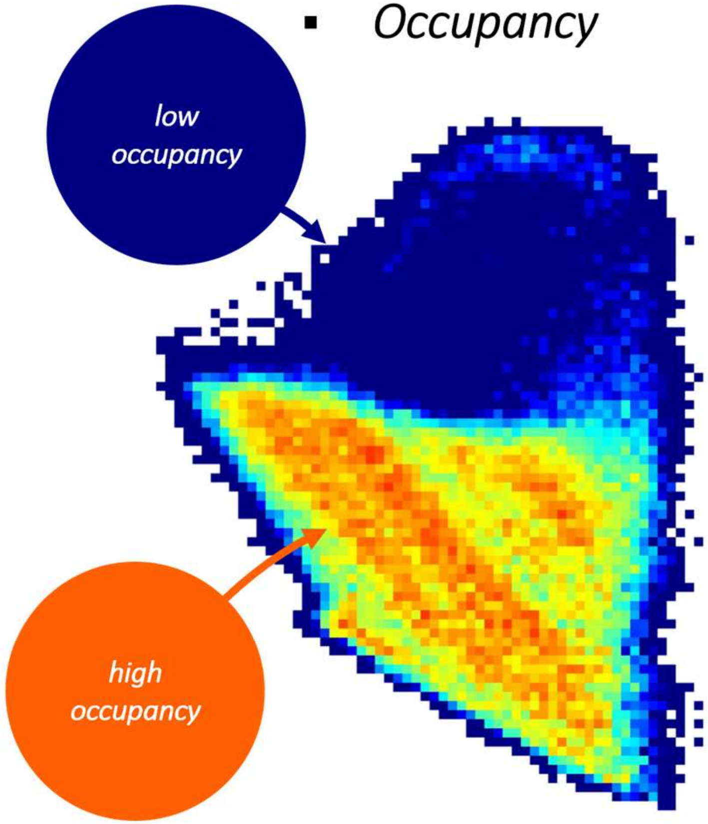
Extracting Data from PEPT

Al-Shemmeri, **Windows-Yule**, *et al.* (2021). Coffee bean particle motion in a spouted bed measured using Positron Emission Particle Tracking (PEPT). *Journal of Food Engineering*, 110709.

- *Trajectories*

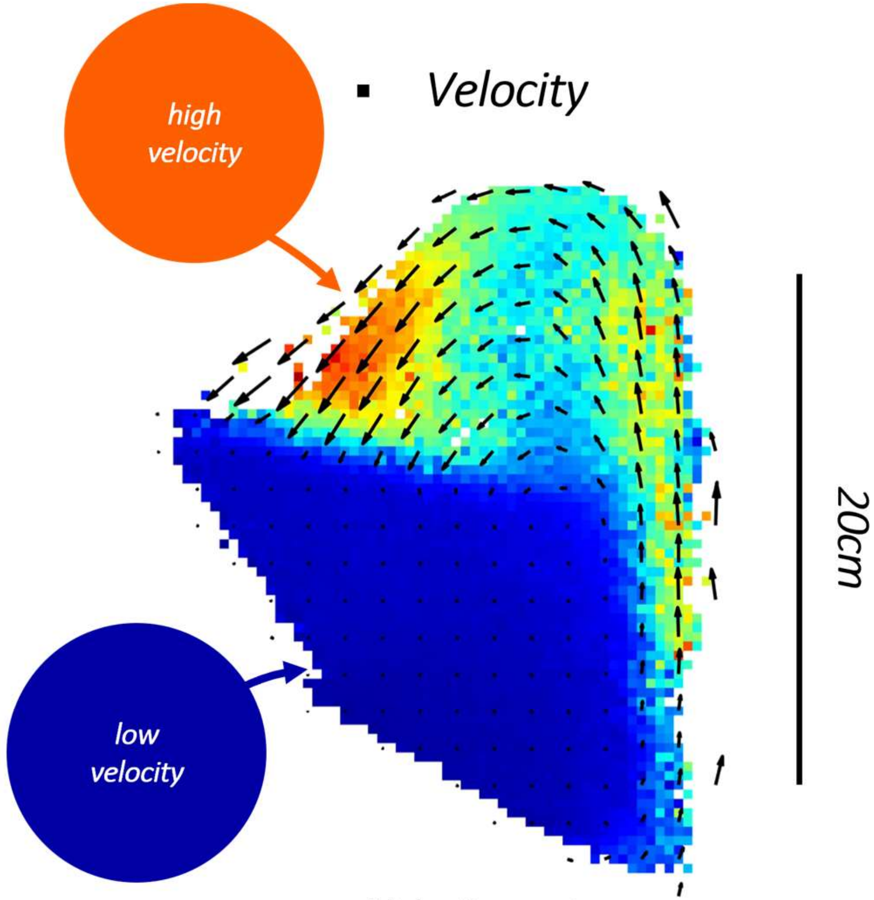
Trajectories identified via analysis of Cartesian co-ordinates (t,x,y,z)

- *Occupancy*



Fractional residence times determined using time-averaged Eulerian data

- *Velocity*

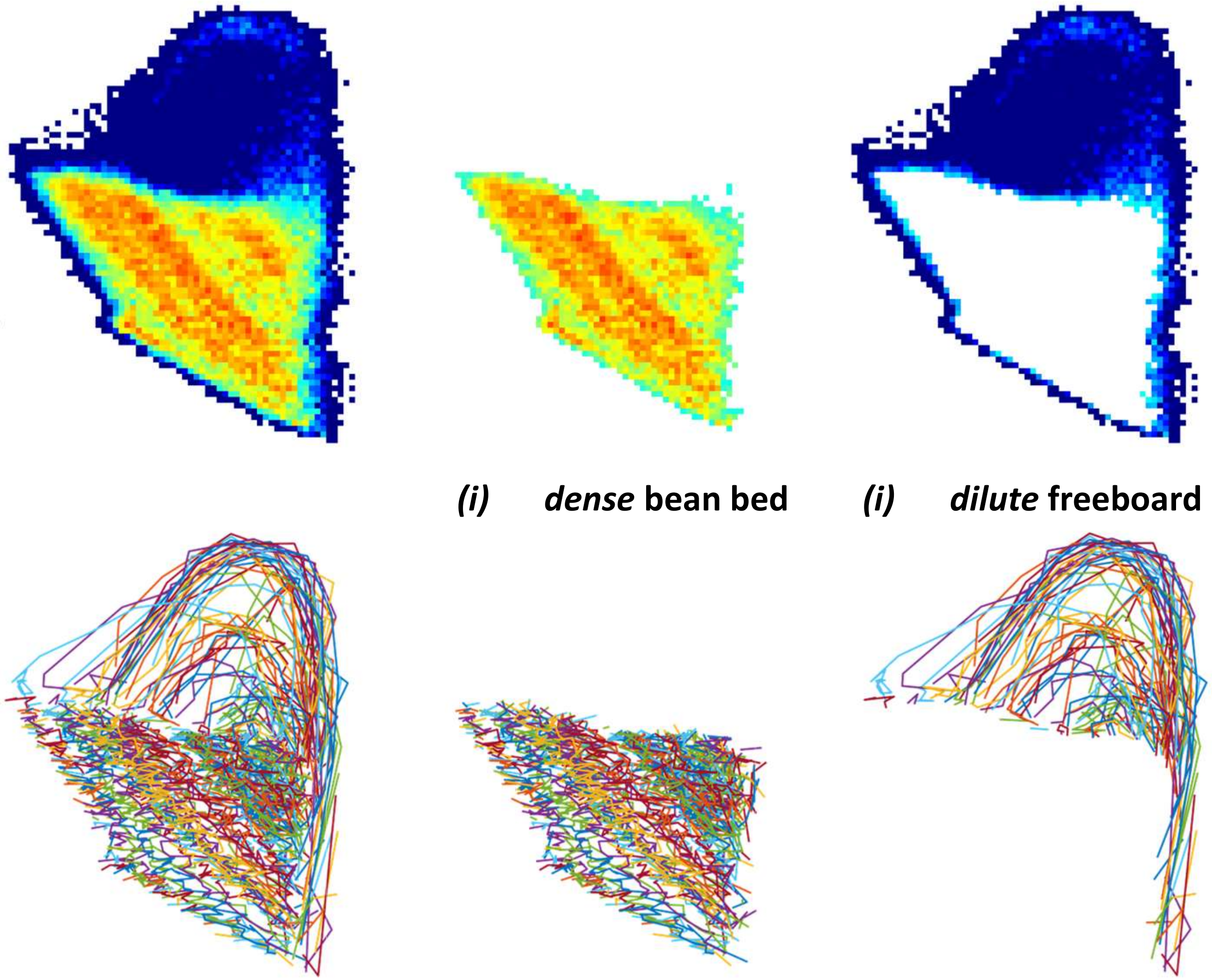


Velocity vectors determined using time-averaged Eulerian data

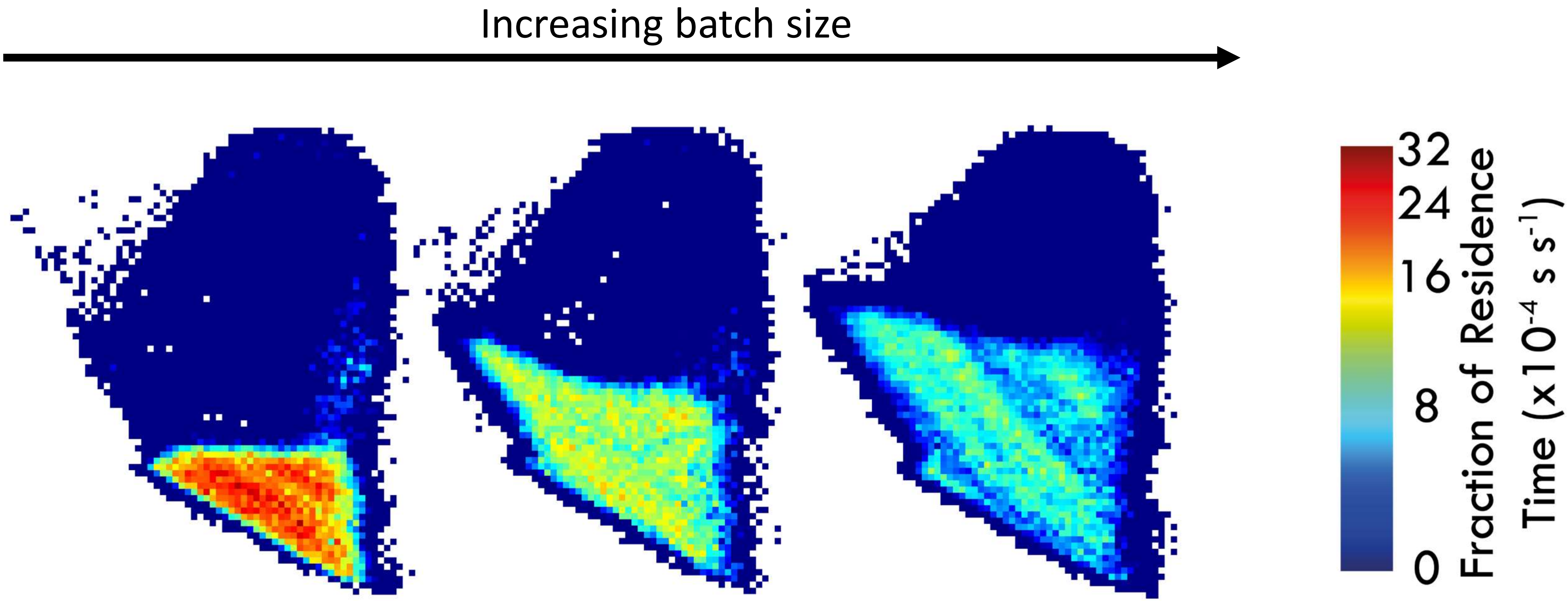
Extracting Data from PEPT

Al-Shemmeri, **Windows-Yule**, *et al.* (2021). Coffee bean particle motion in a spouted bed measured using Positron Emission Particle Tracking (PEPT). *Journal of Food Engineering*, 110709.

- Bean bed delineation
- Defined via Otsu method threshold
- Revealed Two distinct regions
  - (i) dense bean bed
    - Low velocity, high occupancy
    - Convective heat transfer limited
    - Lower temp. & heat transfer
  - (ii) dilute freeboard
    - high velocity, low occupancy
    - Convective heat transfer dominant
    - Higher temp. & heat transfer



Results – Effect of batch size

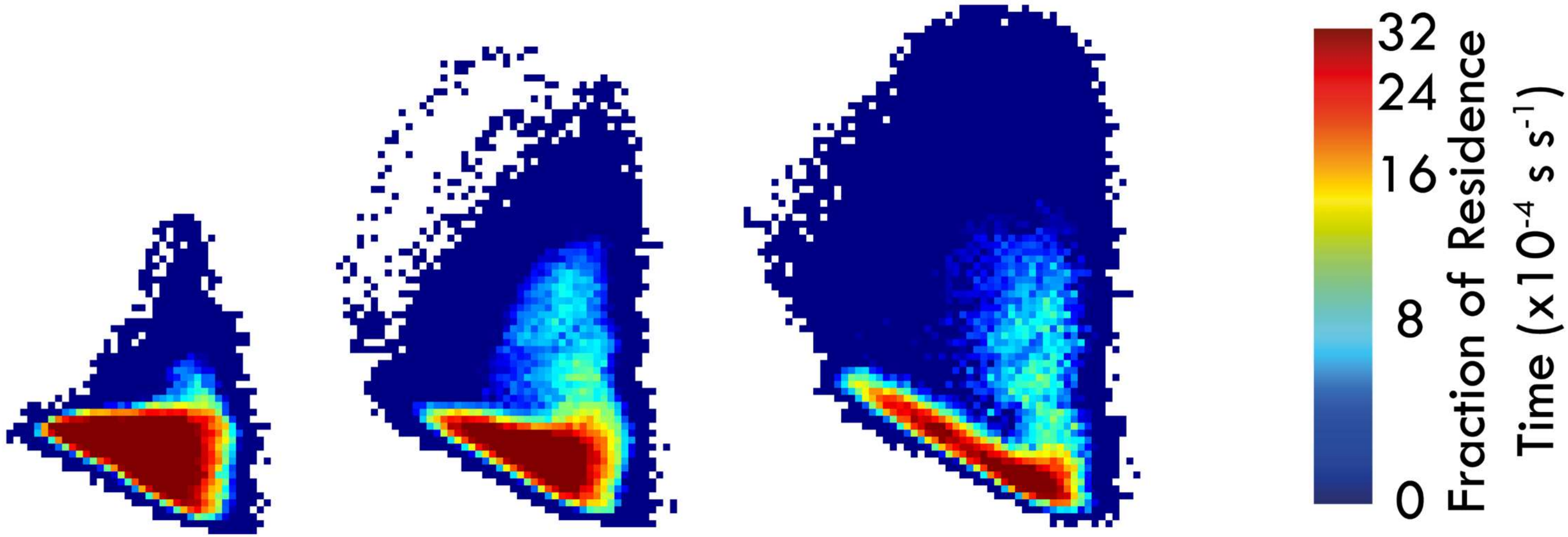


roasted coffee with an air velocity of 7.2 m s^{-1}

Larger batch → larger bed → reduced heat transfer

Results – Effect of batch size

Increasing air velocity



200g batches of green coffee
roasted coffee with an air velocity of 7.2 m s^{-1}

Higher air flow→ smaller bed → improved heat transfer

The Commercial Dilemma

Larger batch size

- Increased throughput
- Decreased heat transfer

Increased air flow

- Increased heat transfer
- Increased energy requirements

A complex optimization problem!

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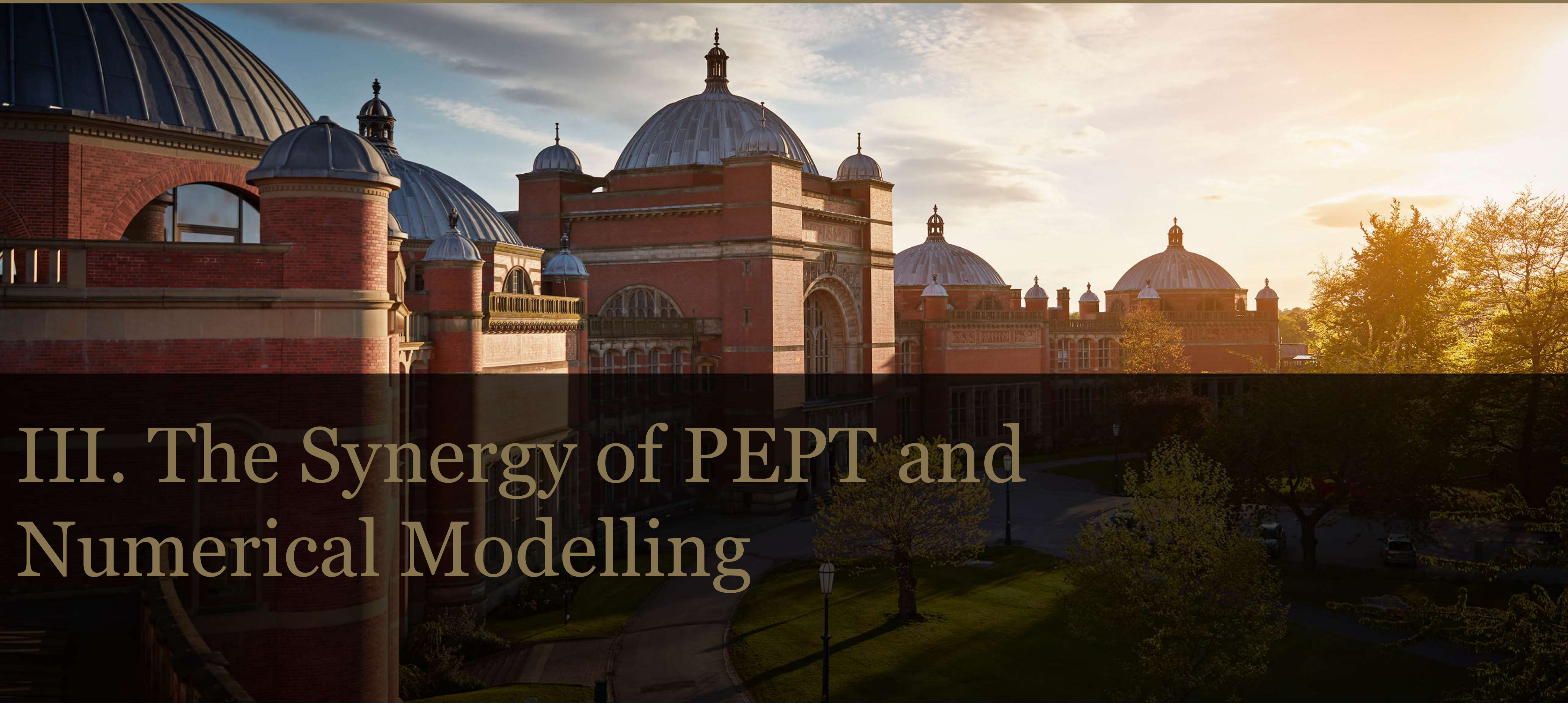


III. The Synergy of PEPT and Numerical Modelling

An Efficient Route to Optimisation

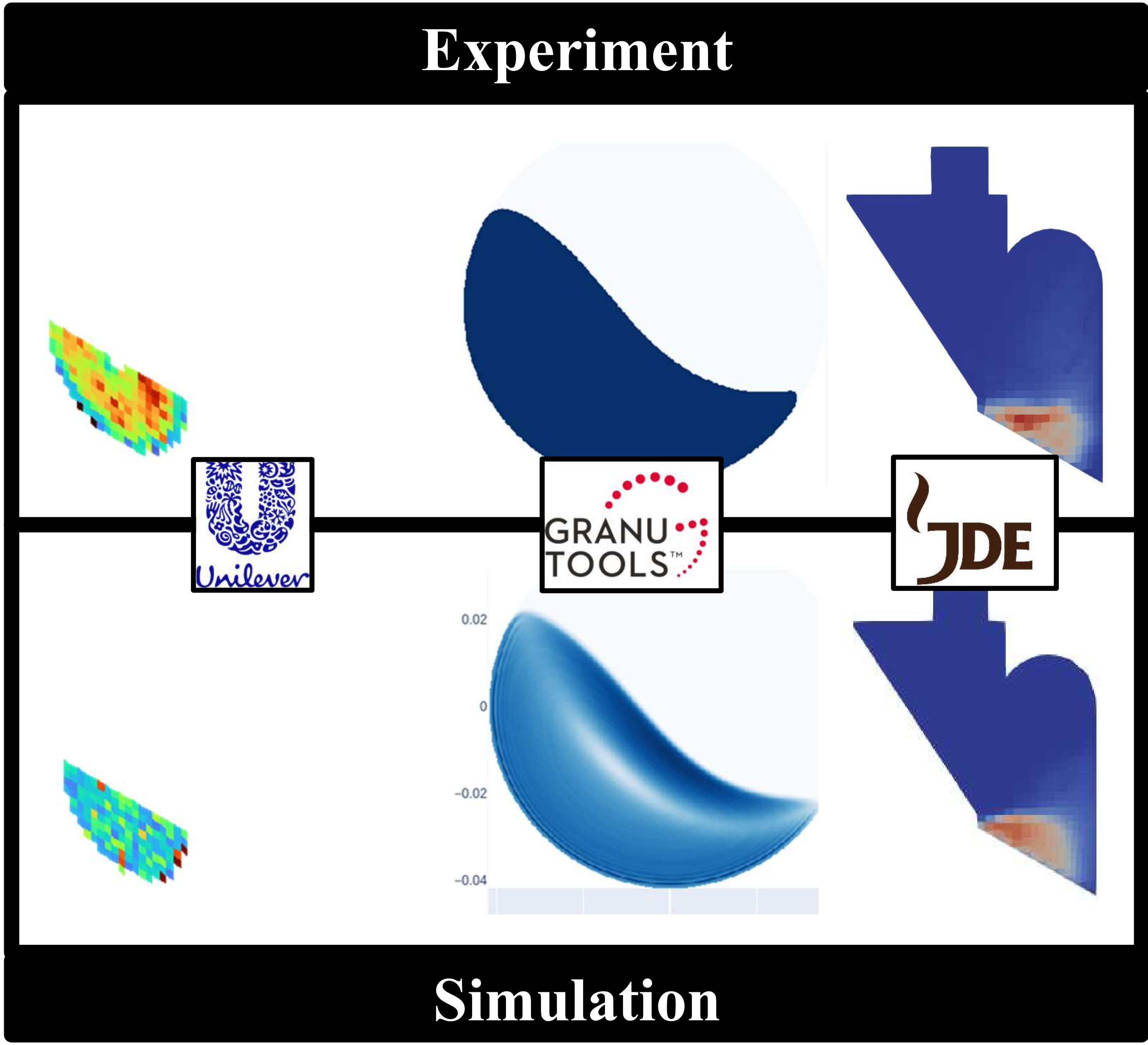
- Solving an optimisation problem requires a detailed exploration of the relevant parameter space
- (Lots of experiments!)
- Though powerful, PEPT facilities are rare, and thus oversubscribed – and the technique is costly to run

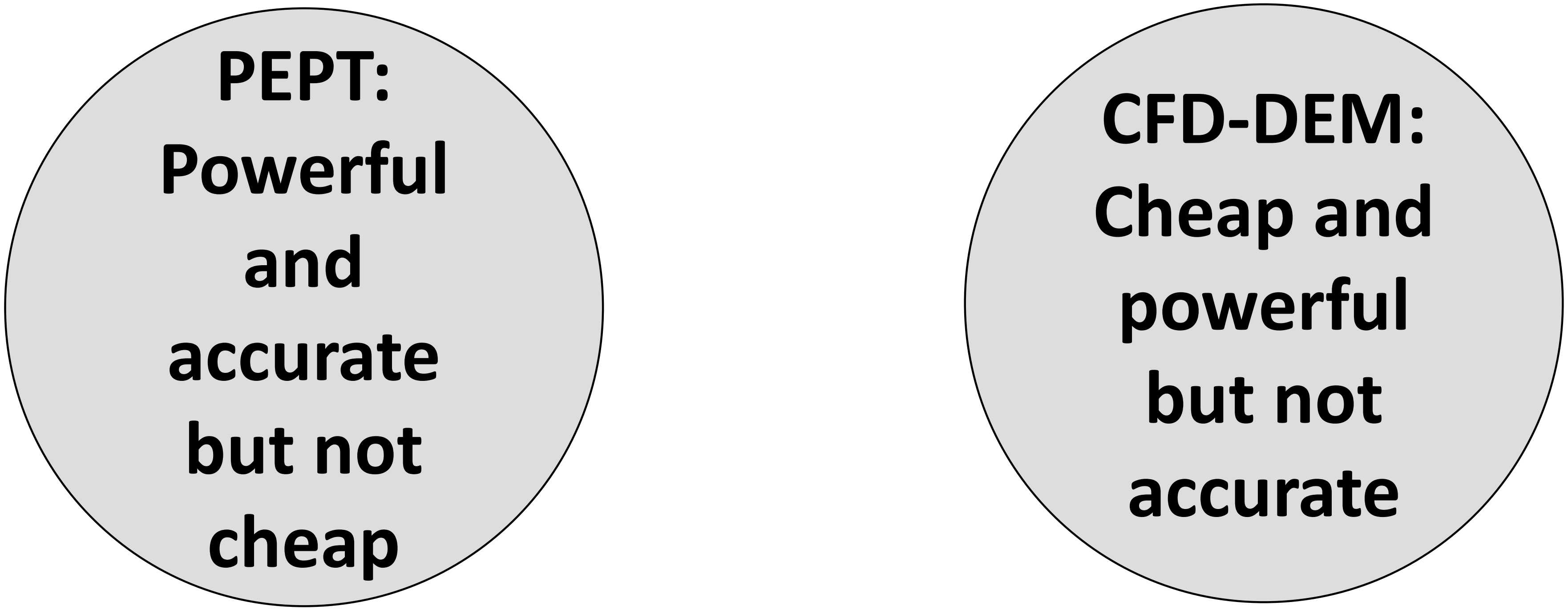
An Efficient Route to Optimisation

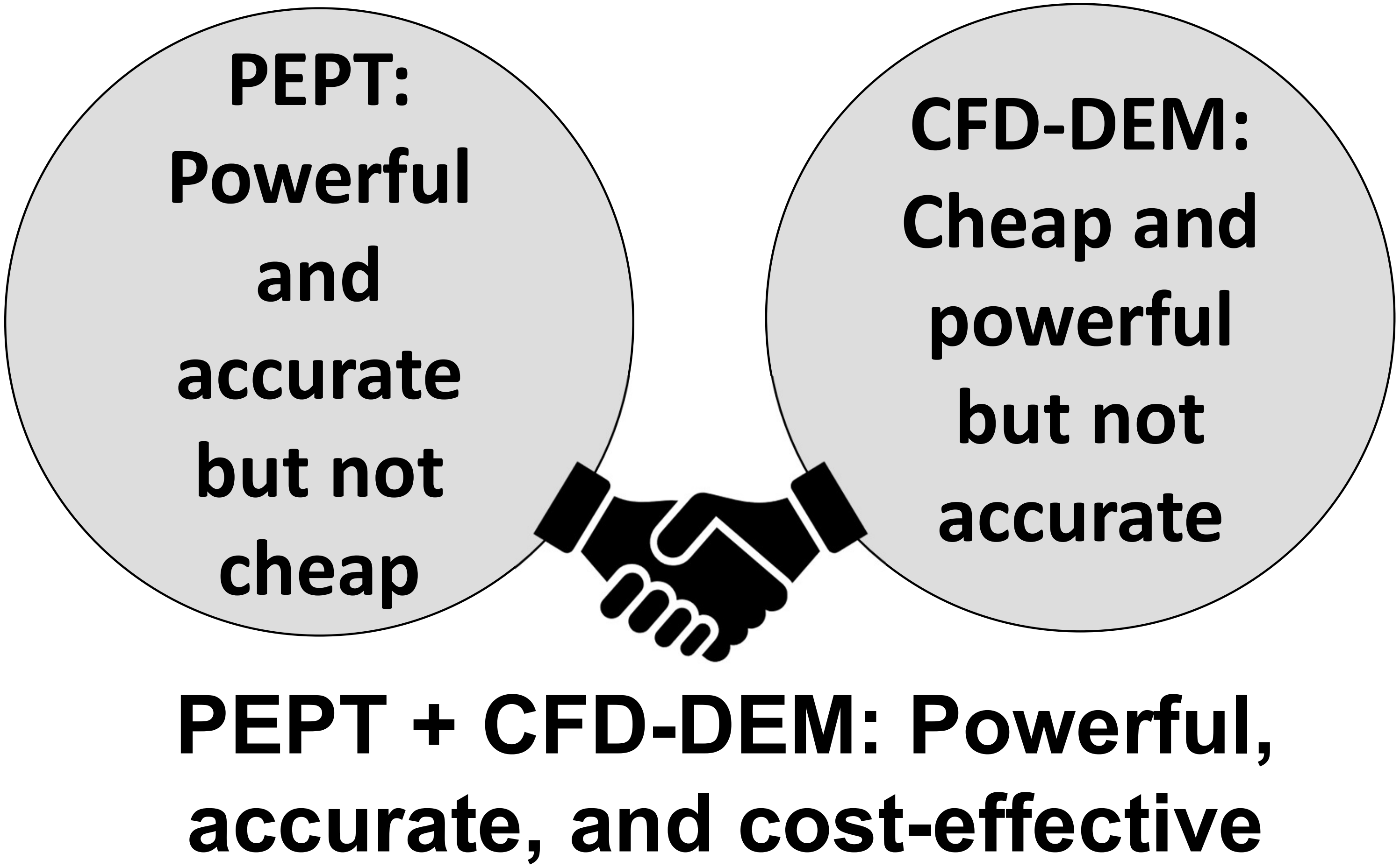
- Numerical simulations – e.g. CFD-DEM – are cheap to run and thus allow the exploration of vast parameter space
- However, as established earlier, we cannot trust them to be accurate

PEPT as a Validation Tool

- PEPT can provide **identical outputs** to DEM, MP-PIC, CFD…
- → Facilitates **detailed, multi-point comparison** between experiment and simulation, considering **local** variations in key fields **at all points in space**
- **→ Uniquely comprehensive validation**

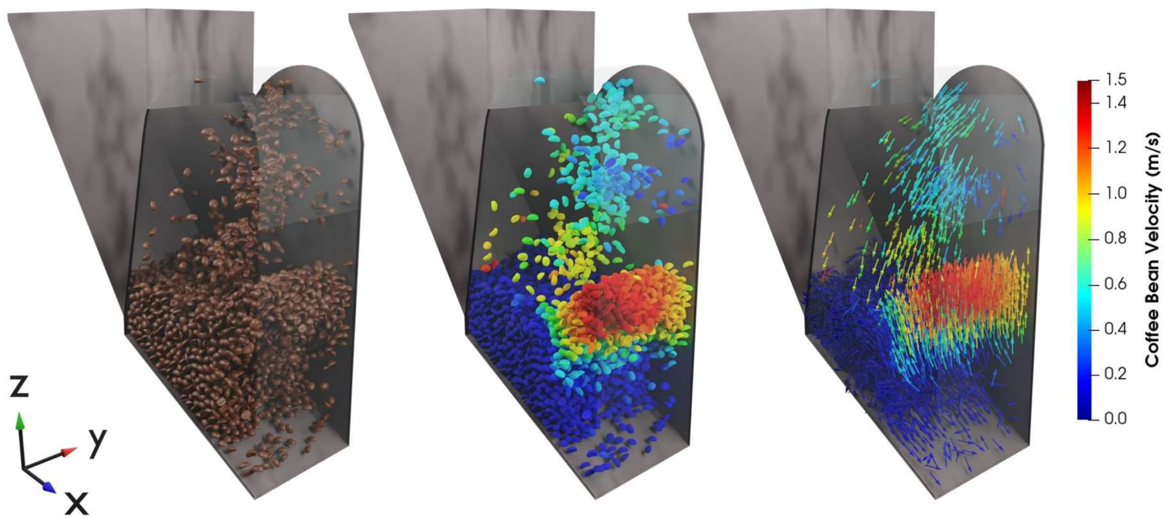



PEPT:
Powerful
and
accurate
but not
cheap
CFD-DEM:
Cheap and
powerful
but not
accurate


PEPT:
Powerful
and
accurate
but not
cheap
CFD-DEM:
Cheap and
powerful
but not
accurate
PEPT + CFD-DEM: Powerful,
accurate, and cost-effective

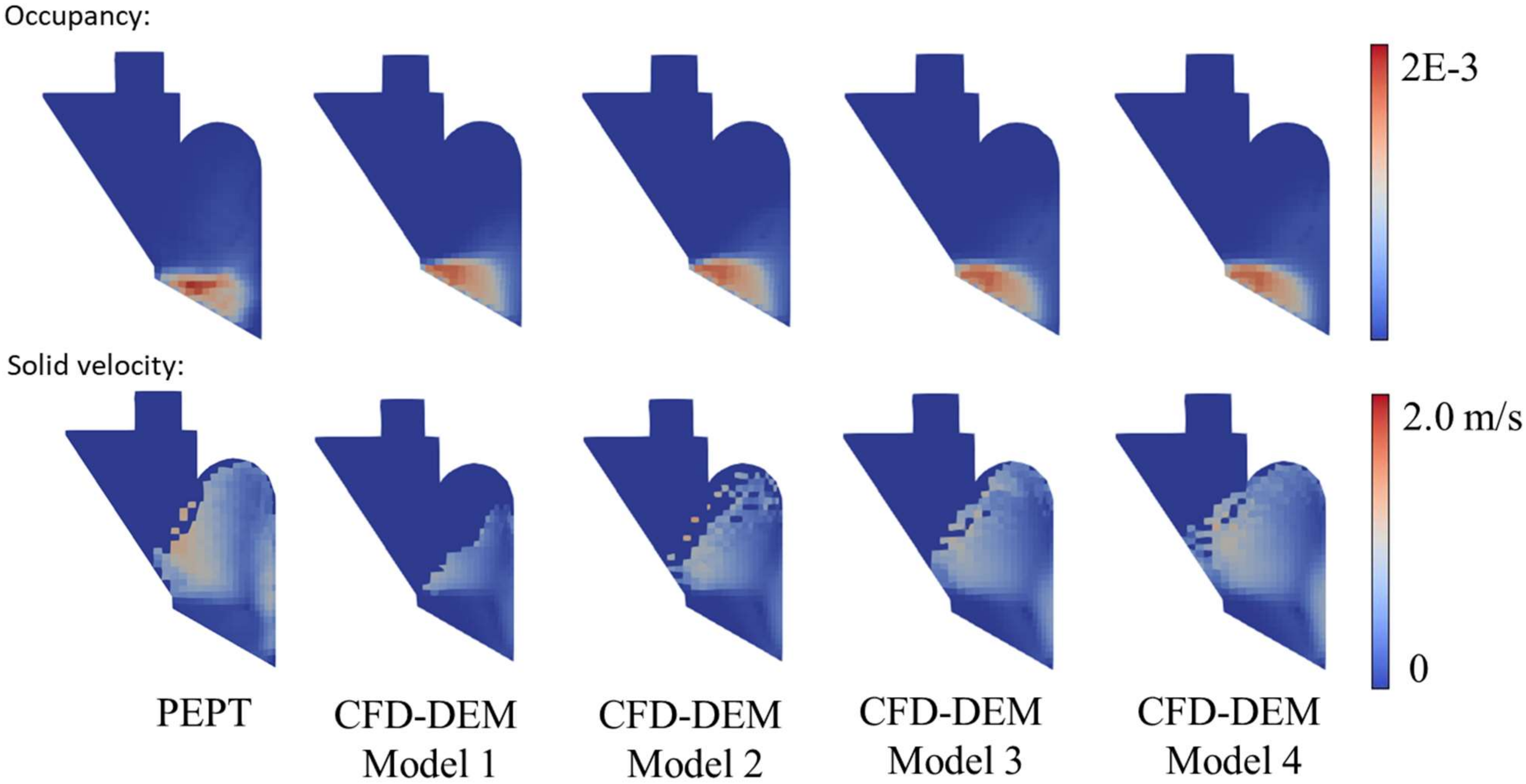
Back to our Case Study

- CFD-DEM model of roaster
- 3D velocity & occupancy fields produced **for both PEPT and CFD-DEM**
- PEPT data and CFD-DEM data discretised on **the same three-dimensional mesh**



Comparing PEPT & CFD-DEM

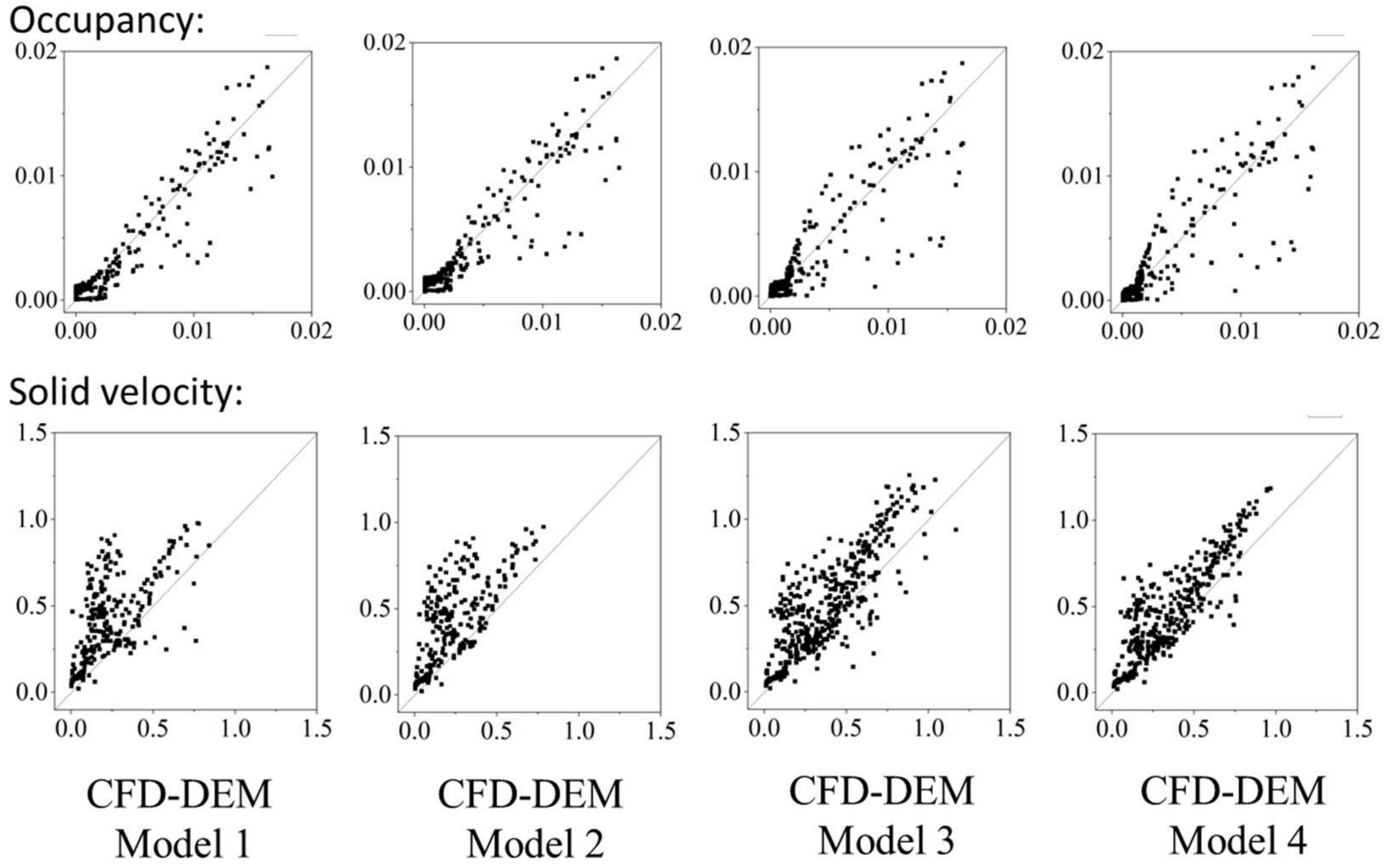
Che, **Windows-Yule**, et al. (2023). PEPT validated CFD-DEM model of aspherical particle motion in a spouted bed. *Chemical Engineering Journal*, *453*, 139689.



Cell-by-cell comparison of multiple three-dimensional fields → **detailed, highly-rigorous validation** of models used → aid model choice.

Rigorous, Quantitative Validation

Che, **Windows-Yule**, et al. (2023). PEPT validated CFD-DEM model of aspherical particle motion in a spouted bed. *Chemical Engineering Journal*, *453*, 139689.

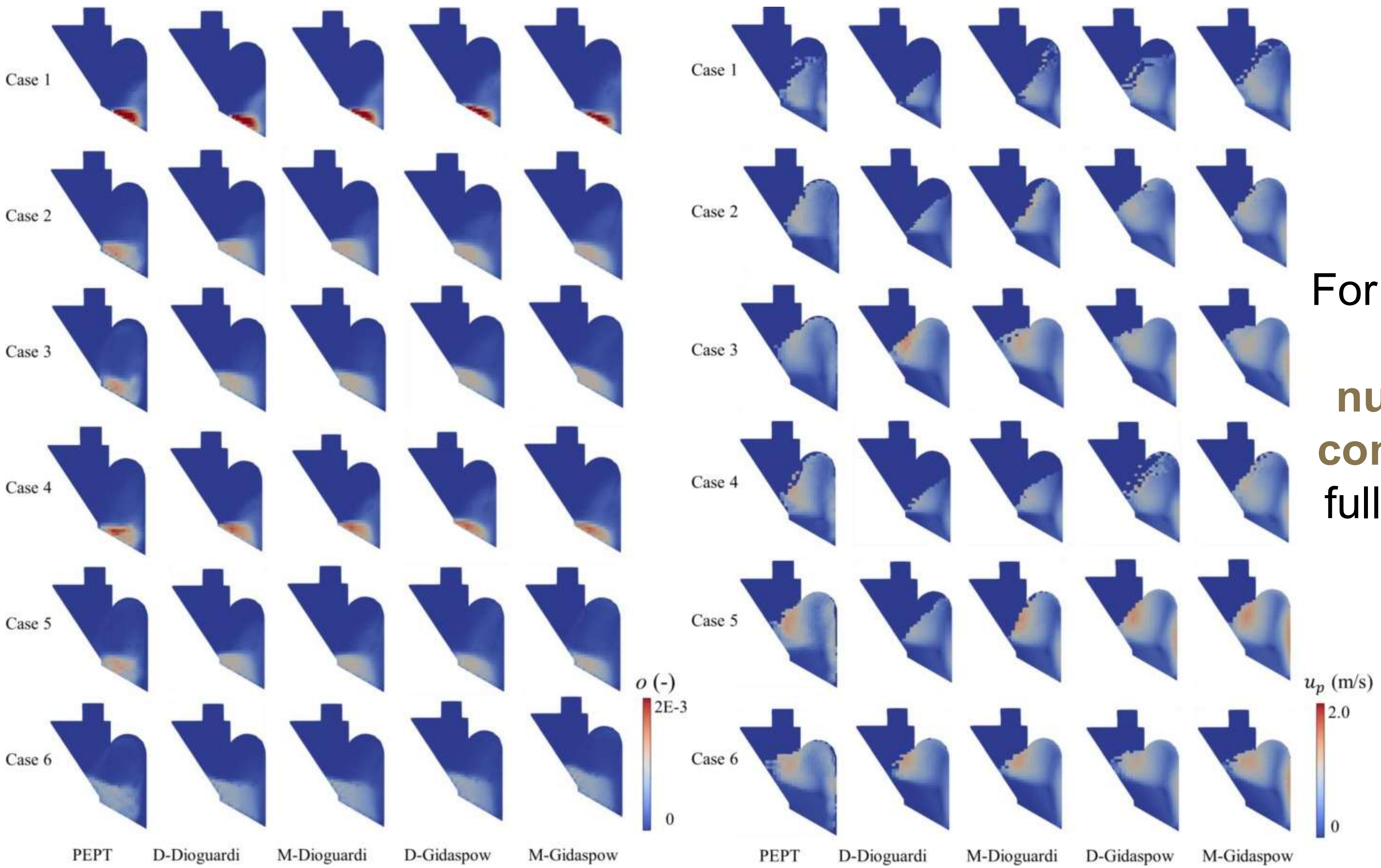


	Model 1	Model 2	Model 3	Model 4
Occupancy	0.659	0.733	0.867	0.834
Velocity	0.942	0.930	0.913	0.903

- Simulation accuracy can be **quantitatively assessed** through Pearson coefficient (or others statistical measures)
- Pearson coefficient can also be used as a **cost function** for ACCES calibration
- **→ Skip the characterisation step!**

Rigorous, Quantitative Validation

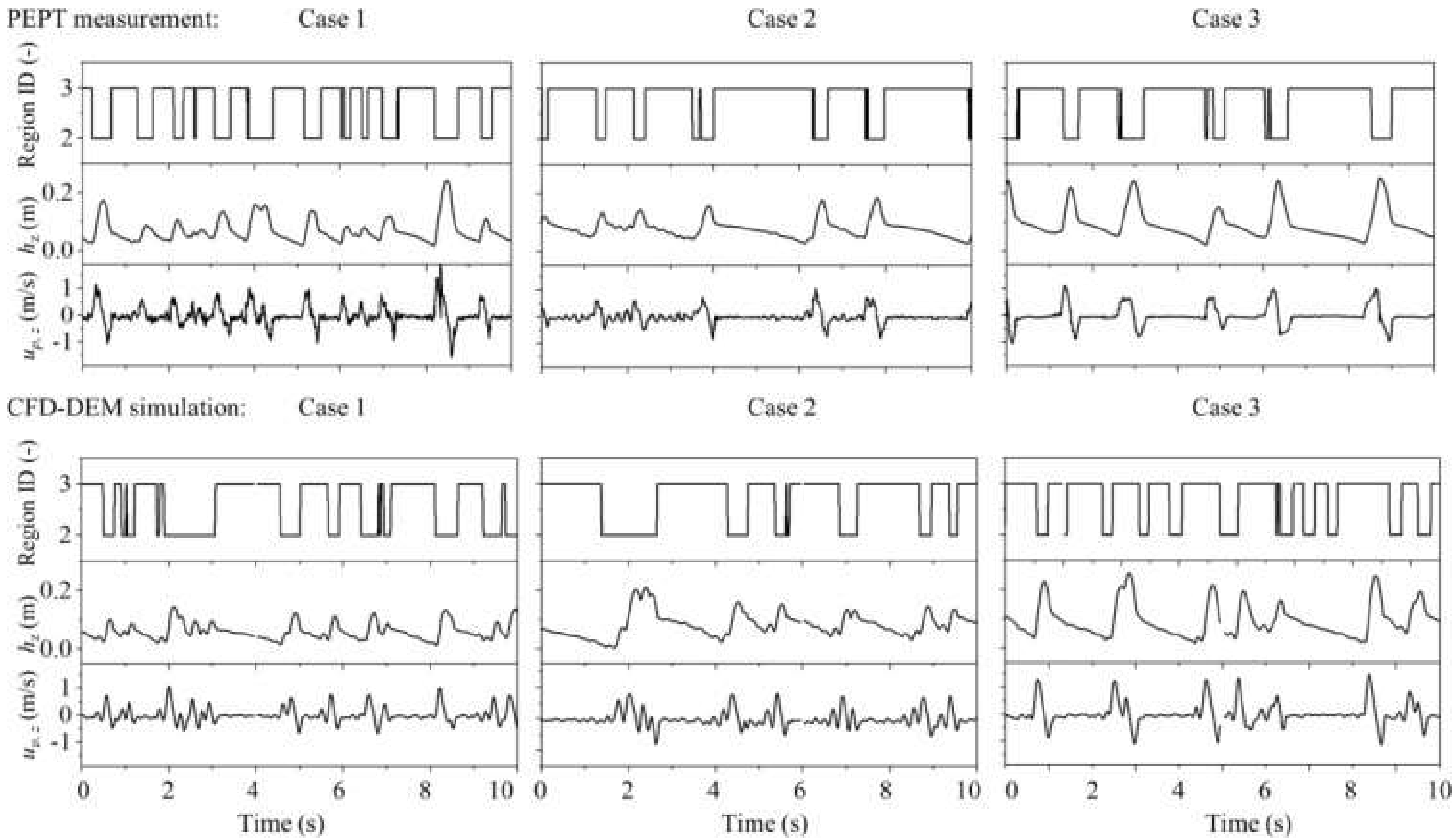
Che, **Windows-Yule**, et al. (2023). PEPT validated CFD-DEM model of aspherical particle motion in a spouted bed. *Chemical Engineering Journal*, *453*, 139689.



For further rigour, can validate under **numerous system conditions** spanning full parameter space of interest...

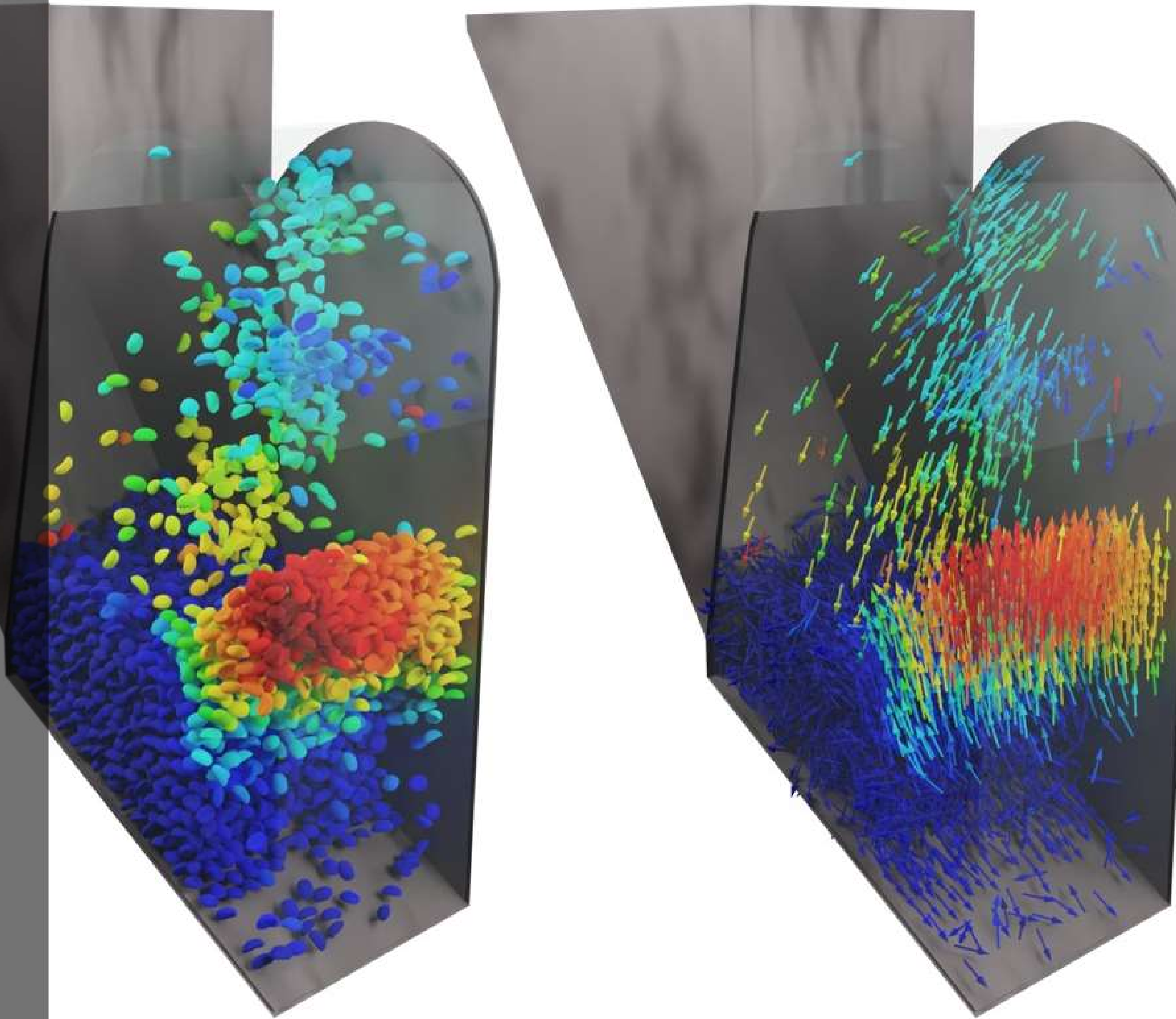
Rigorous, Quantitative Validation

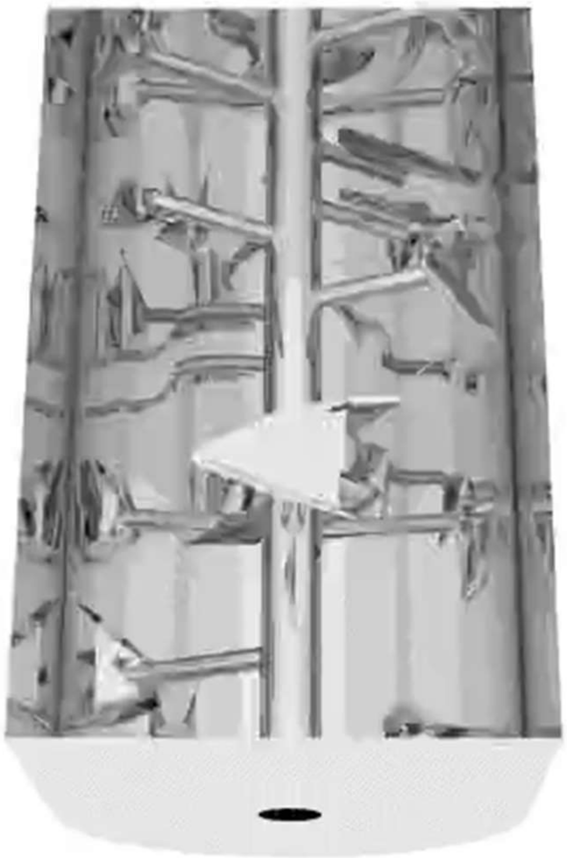
Che, **Windows-Yule**, et al. (2023). PEPT validated CFD-DEM model of aspherical particle motion in a spouted bed. *Chemical Engineering Journal*, *453*, 139689.

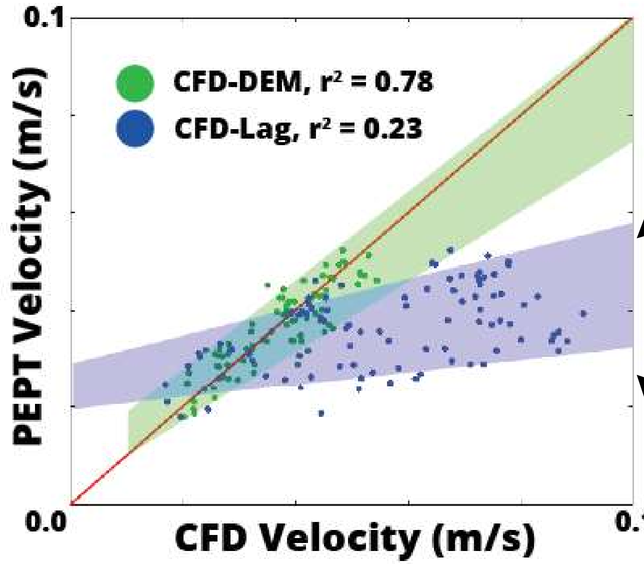


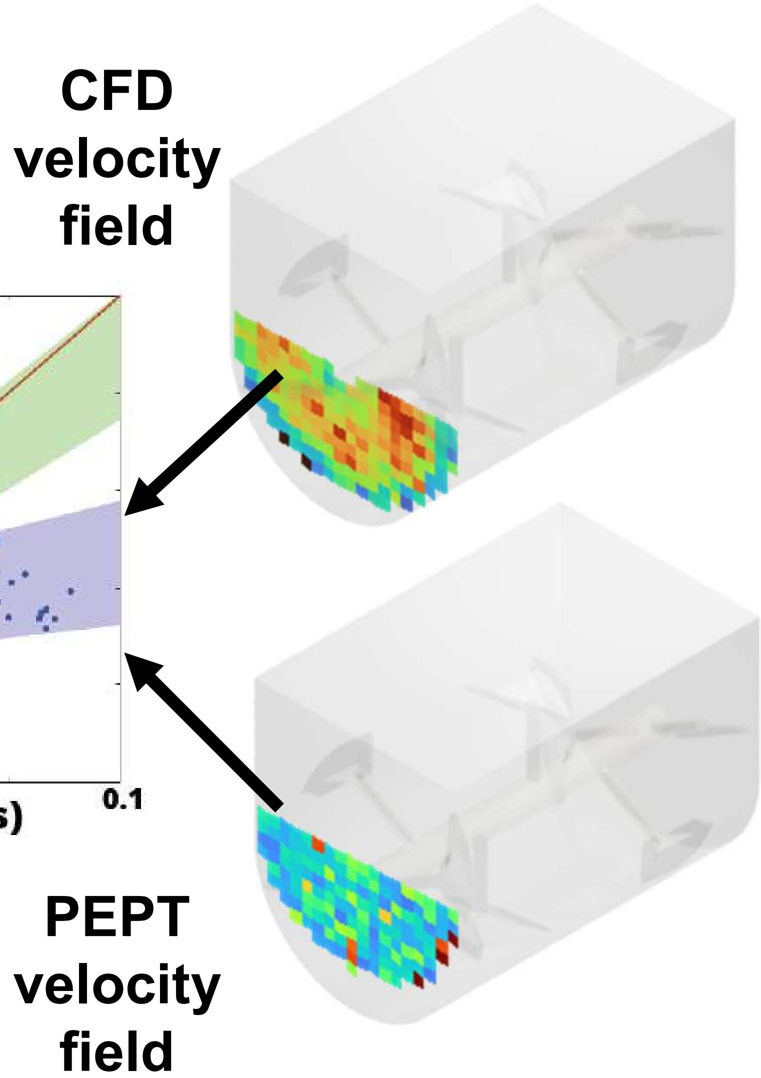
…as well as investigating a diverse array of other (**Eulerian & Lagrangian**) quantities!

End result: a **comprehensively validated** numerical model which can be used to **easily, efficiently and cheaply** gain insight into JDE’s systems.

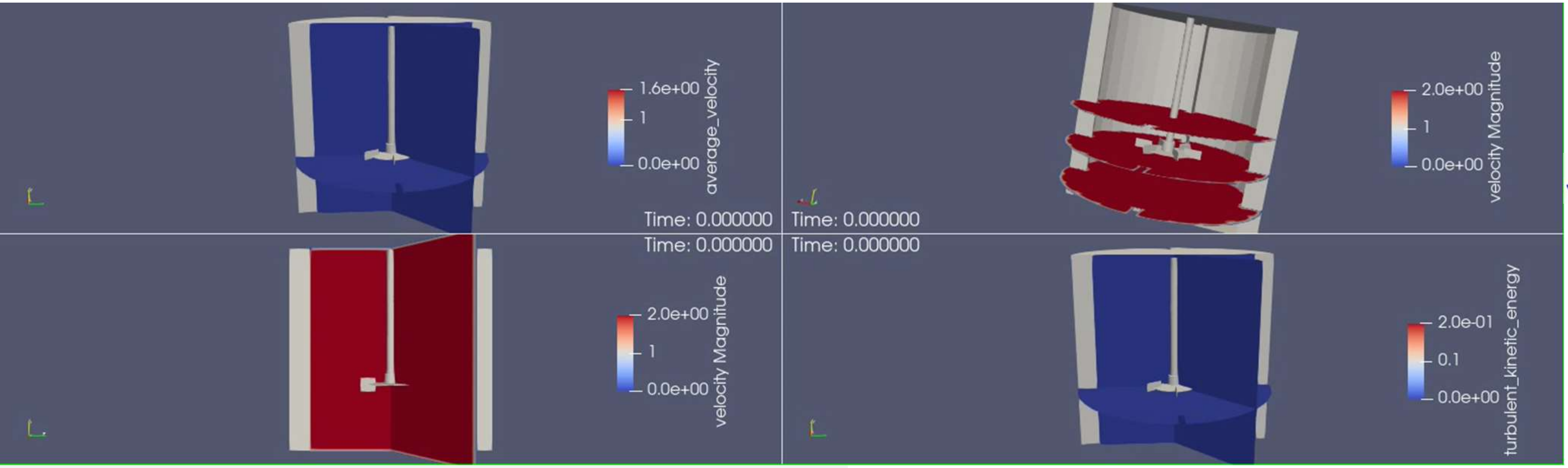








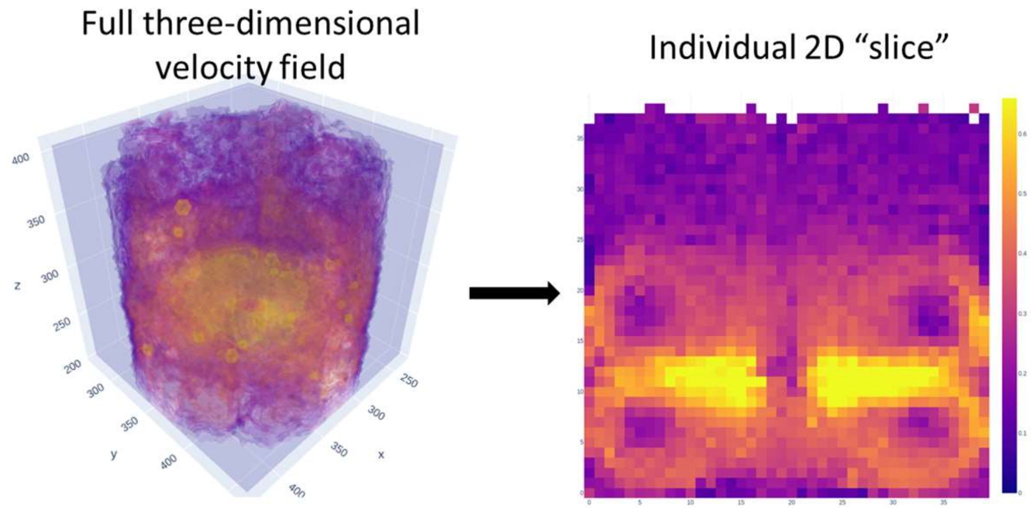
Not *just* spouted beds, not '*just*' particles



JM Johnson Matthey
Inspiring science, enhancing life

ifp Energies nouvelles

Not *just* spouted beds, not '*just*' particles



MAPP

HENRY ROYCE INSTITUTE

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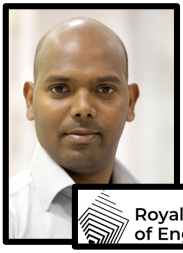
UKRI Engineering and Physical Sciences Research Council

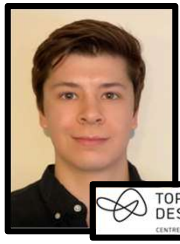
Funder Acknowledgements

Innovate UK

The Team




William Peace


Jack Sykes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Ben Jenkins


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IV. PEPT as a *Calibration* Tool

ACCES

Autonomous Calibration using Evolutionary Algorithms

- Calibration is an **infamously slow and difficult task**
  - And one too often overlooked in the literature!
- As well as simply *validating* existing algorithms, PEPT can be used to *calibrate* simulations
- Specifically, it can be used to provide detailed objectives for **evolutionary algorithms**

ACCES: Autonomous Characterisation & Calibration using Evolutionary Simulation

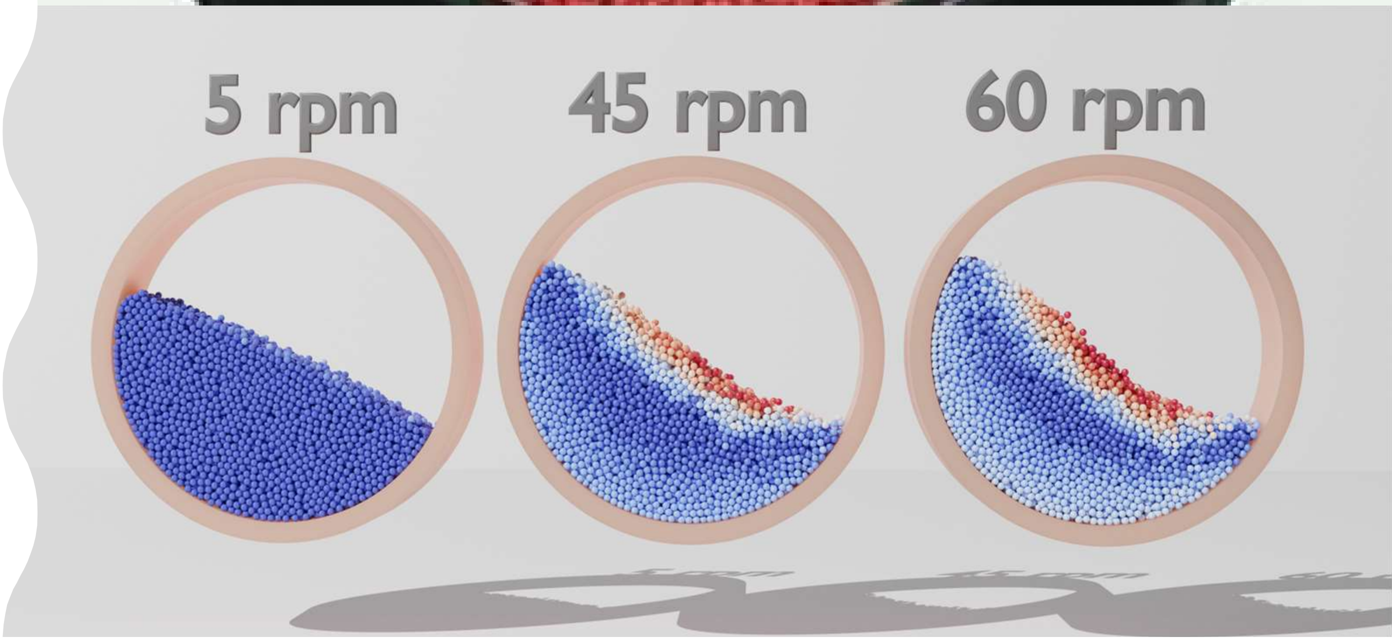
ACCES

I. Choose experimental system to model
II. Define a cost function to quantify difference between experiment & simulation
III. Choose a suitable optimiser
IV. Set goal to minimise error function (i.e. maximise agreement between simulation and experiment)
V. Iterate towards minimum (i.e. find ‘true’ DEM parameters)

I. Choosing a system

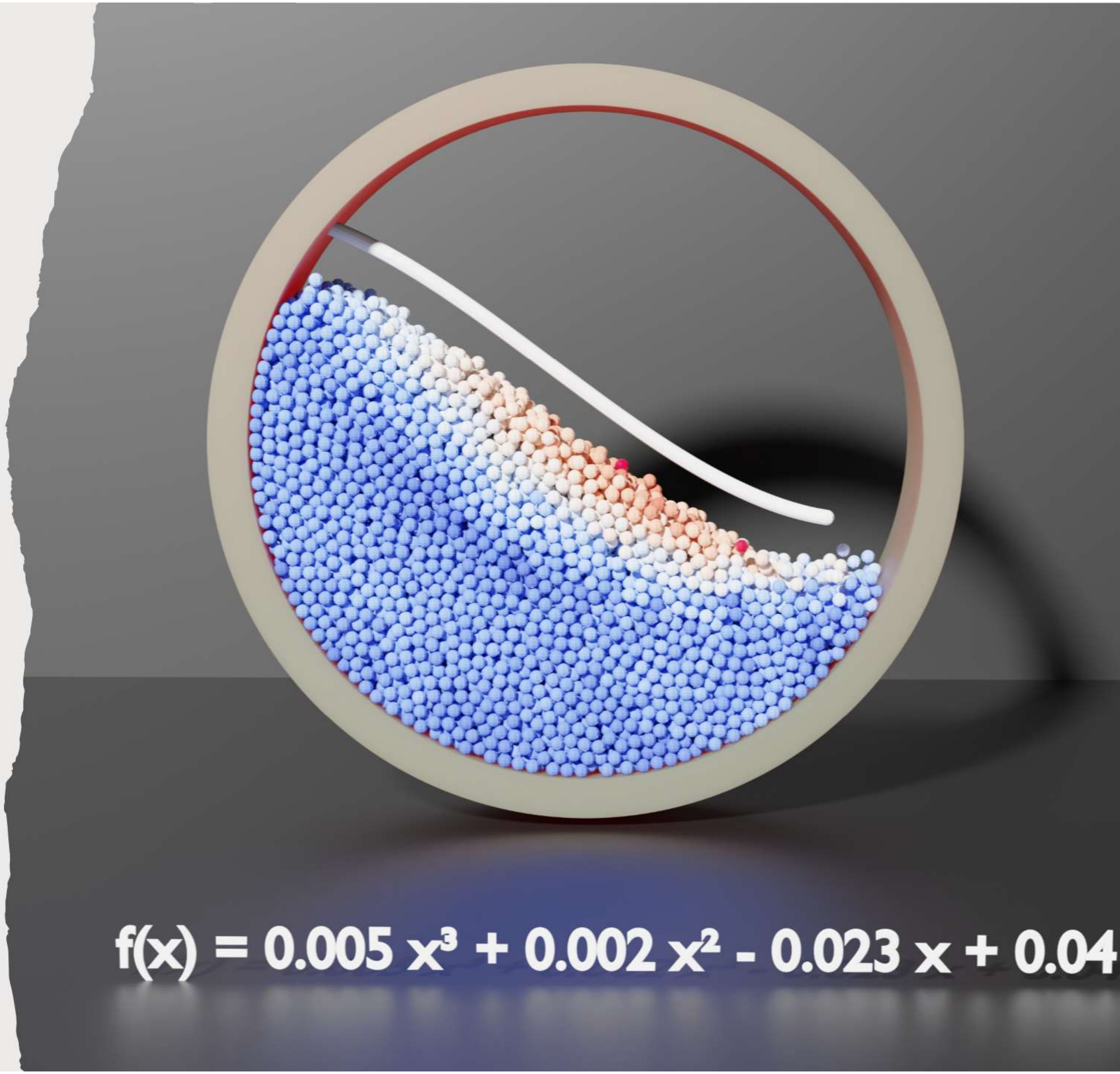
To illustrate ACCES in an accessible manner, let us consider a simple system to model: Granutools *GranuDrum*

- Simple
- Industrially relevant
- Diverse phenomenology



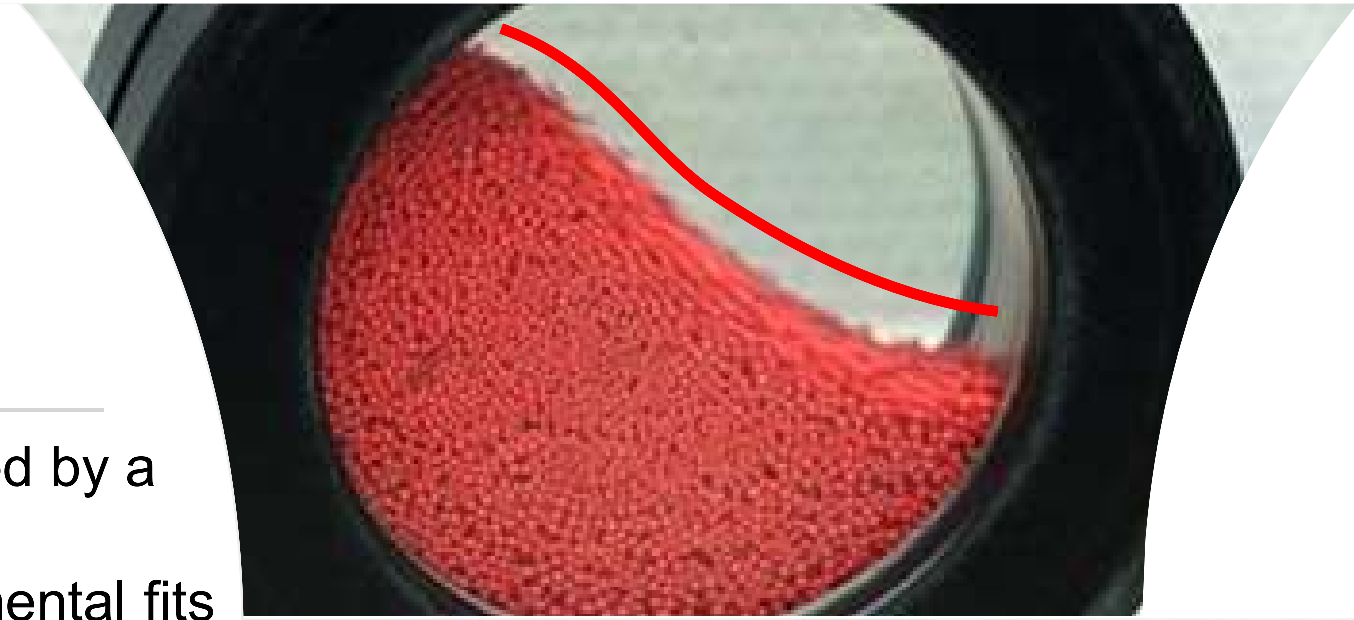
II. Defining a cost function

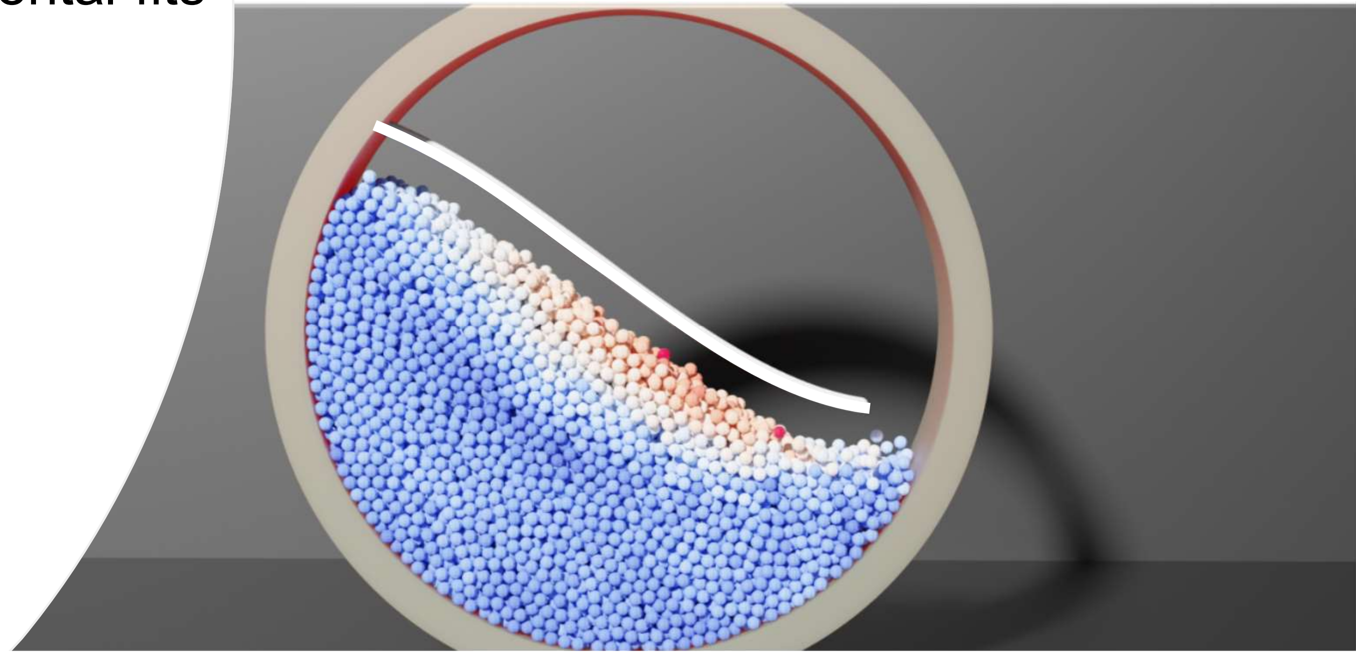
- Cost function can relate to **practically any quantity**
  - Mean system velocity
  - Velocity distribution
  - Density distribution
  - Granular temperature…
- Precise choice depends on goals of calibration
- In this example we want to obtain values for **sliding & rolling friction**
- →Free surface shape as cost function



II. Defining an error function

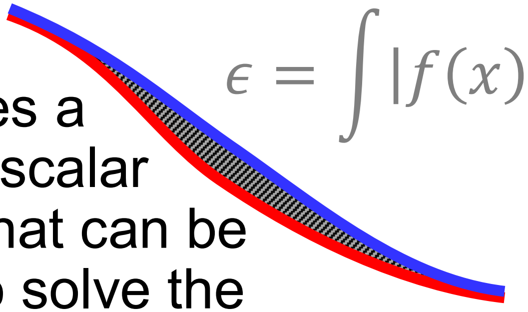
- Free surface can be characterised by a 3rd order polynomial
- Compare simulation and experimental fits





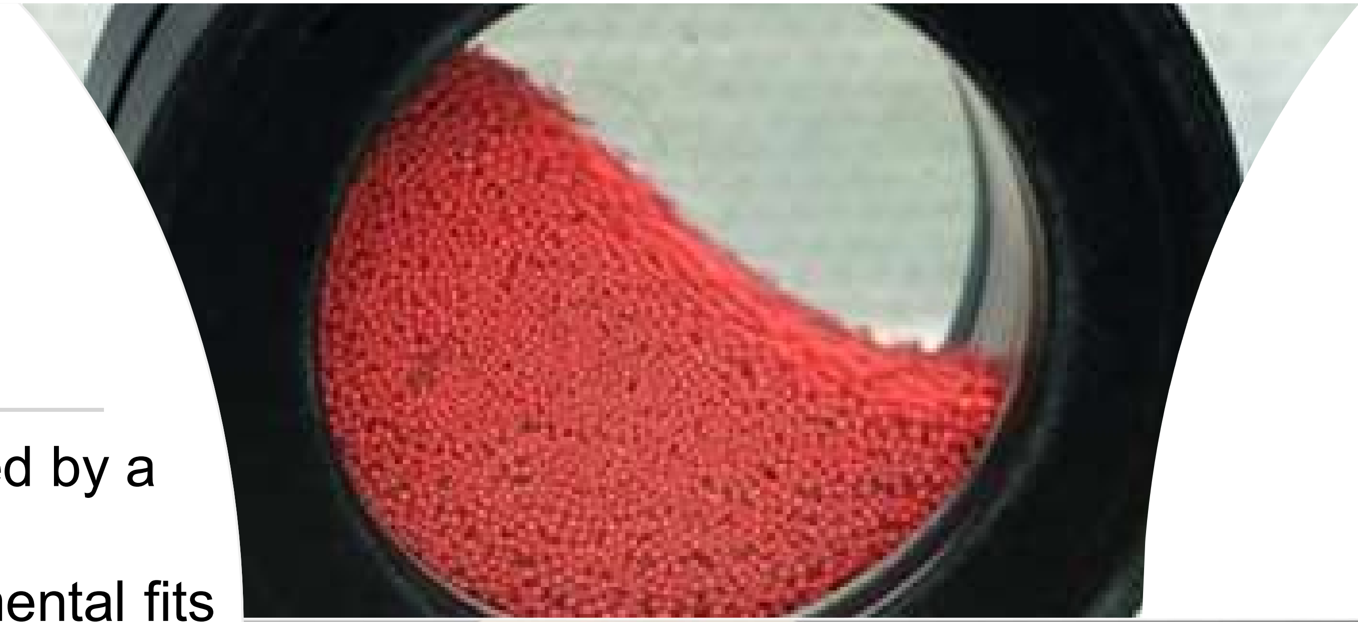
II. Defining an error function

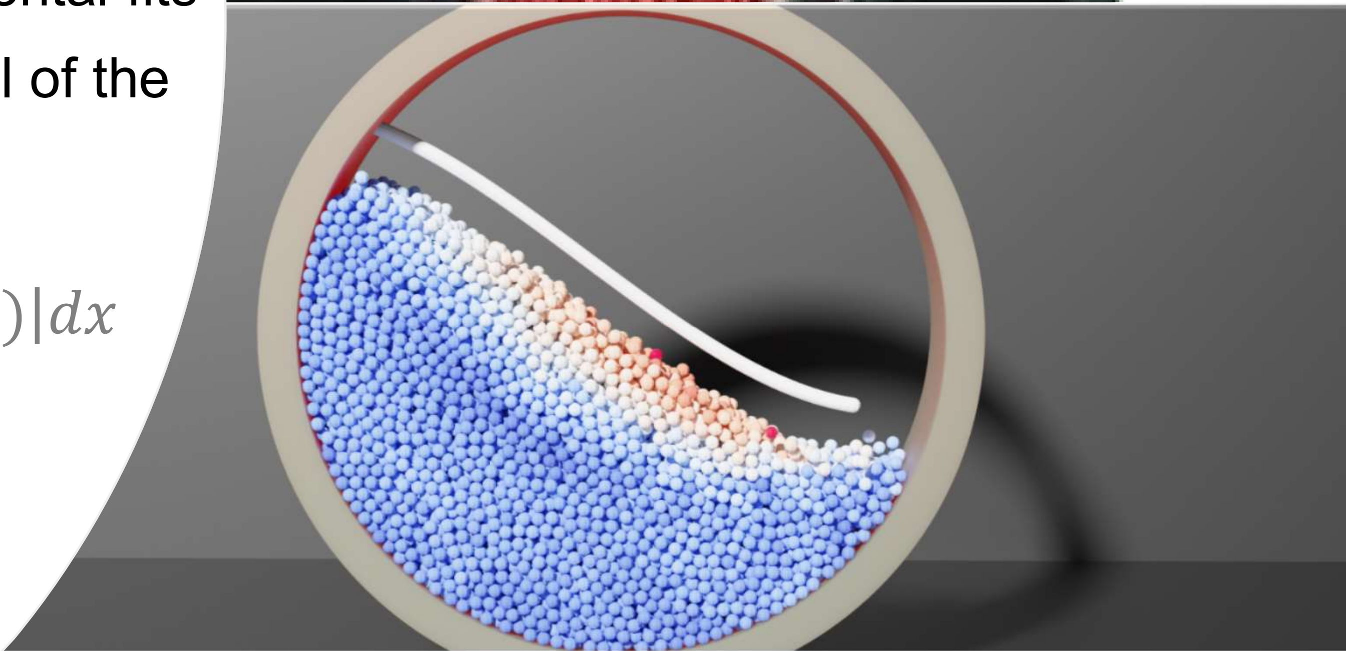
- Free surface can be characterised by a 3rd order polynomial
- Compare simulation and experimental fits
- Cost function taken as the integral of the absolute difference between the 2 polynomials



$$\epsilon = \int |f(x) - g(x)| dx$$

Provides a simple scalar value that can be used to solve the optimisation problem





Evolutionary Optimisation – How it Works

The problem with evolutionary algorithms: **lots of function evaluations**

Especially problematic when coupled to DEM

Utilise state-of-art **CMA-ES** algorithm, which adaptively changes as the spread of the function increases

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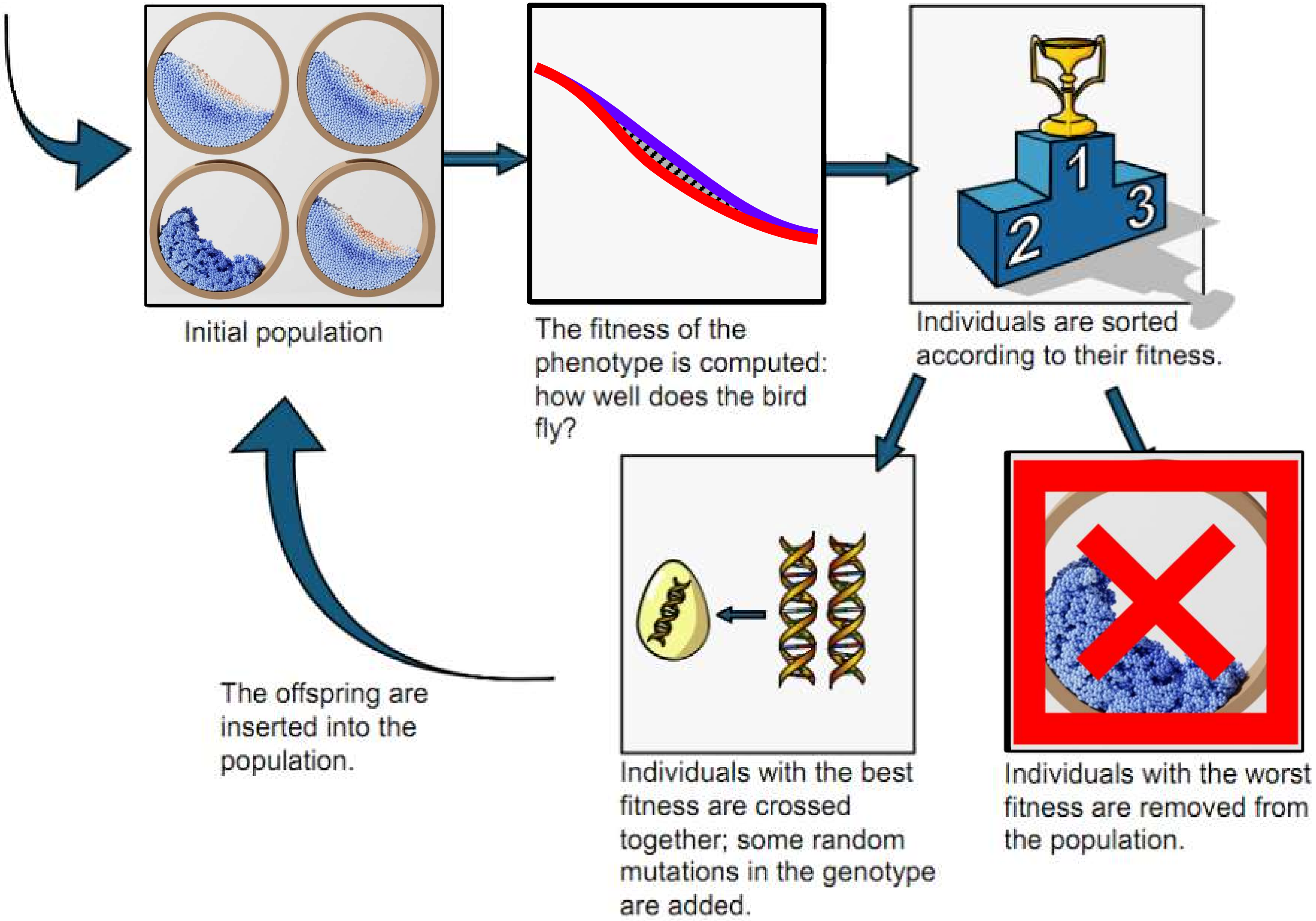
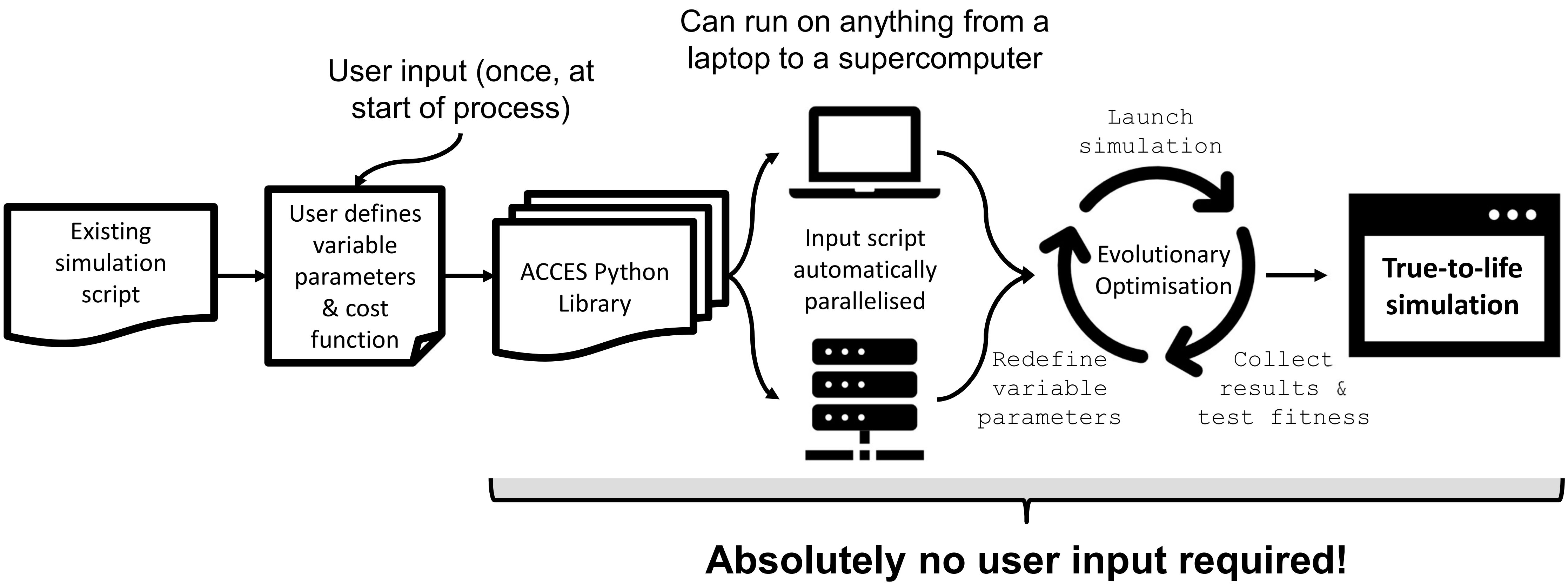


Evolutionary Optimisation – How it Works **in ACCES**



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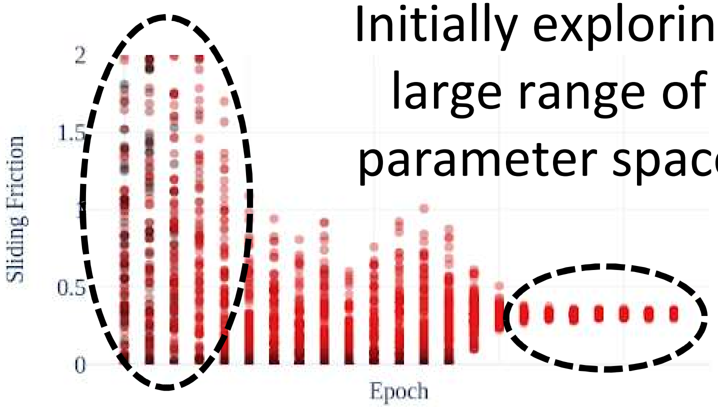
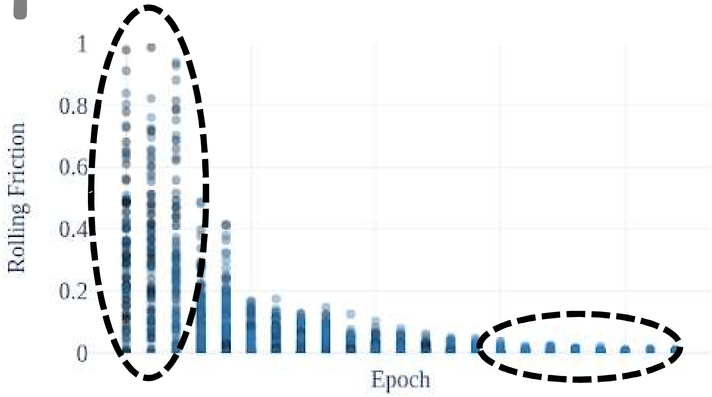
Metaprogramming (code that writes code): ACCES takes input scripts, understands them, hacks them, and modifies them to run in fault-tolerant massively parallel environments

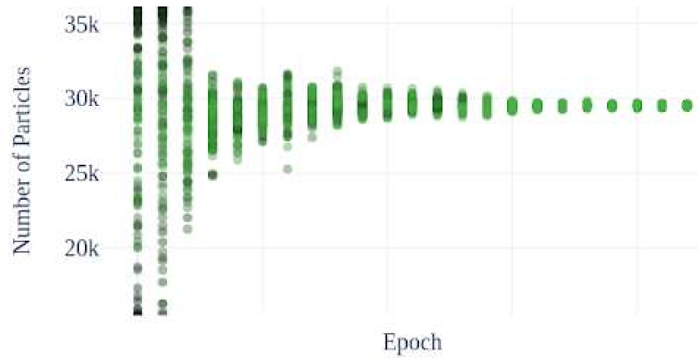
V. Iterating toward optimal parameters

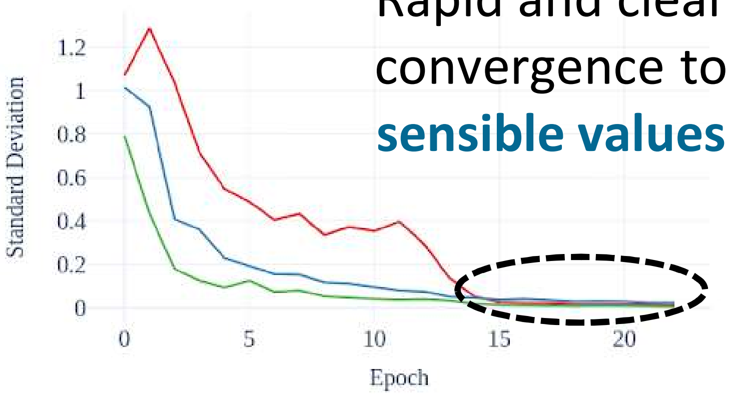
- ACCES converges on the parameter values that minimise the error values (cost function)
- It evolves a “family” of solutions in epochs (*x*-axis) towards the fittest individuals.



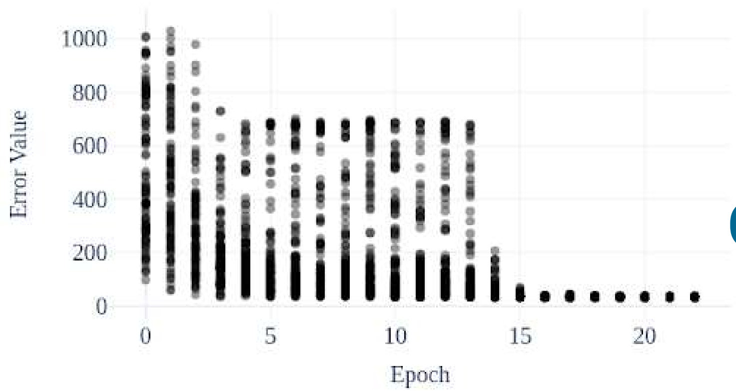
Initially exploring large range of parameter space







Rapid and clear convergence to **sensible values**



“Family size” of 100 (100 simulations per “epoch”)

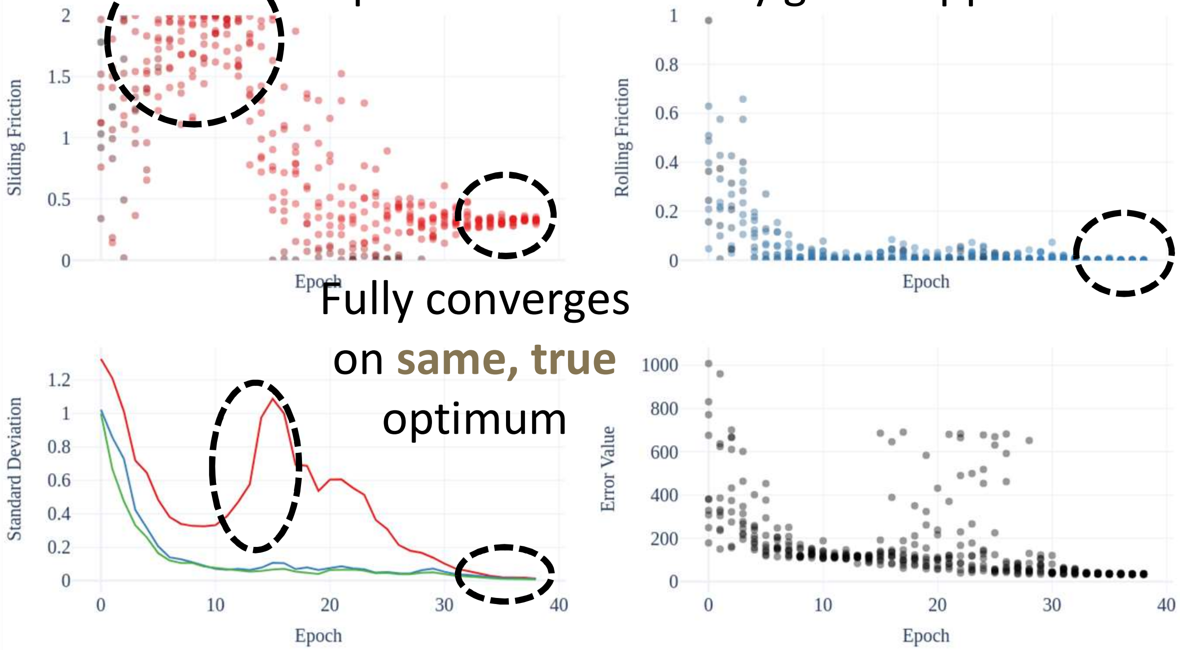
Convergence in under 20 epochs!

V. Iterating toward optimal parameters

- What if I don't have 100 CPUs handy?
- "Family size" can be varied at will.
- Larger: more global search, fewer epochs
- Smaller: fewer simulations per epoch, more epochs
- → Fully scalable from HPC to Laptop
- **Can still autonomously "escape" false minima and reach true parameter values**

Same problem, **1/10th family size**

"Deep" local minimum – gradient-based optimiser would likely get "trapped"



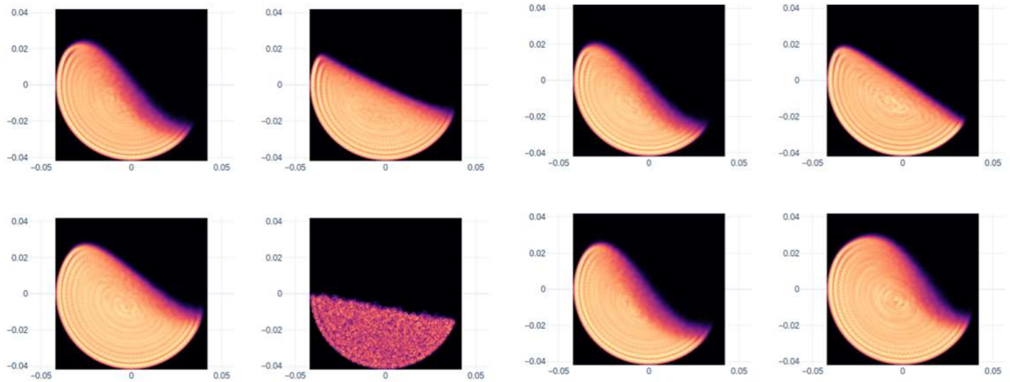
Fully converges on **same, true** optimum

ACCES autonomously increases search area

Convergence in <40 epochs (<400 evaluations) with 2 free parameters

C.f. ANNs & other optimisers for which 10,000 evaluations **per parameter** would be considered good!

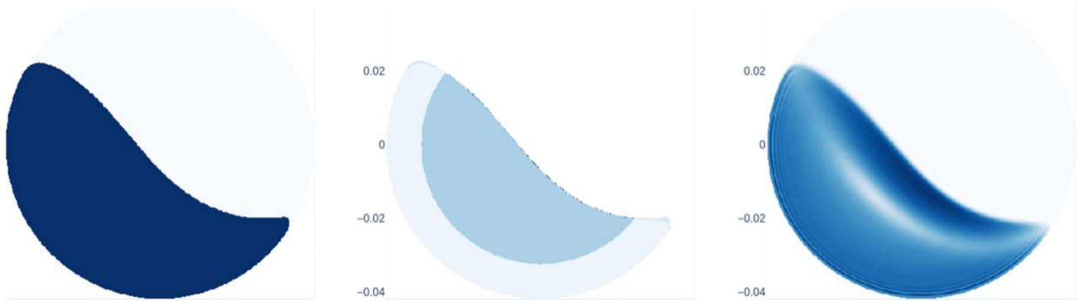
Early guesses



Converged solution

Error of less than $4\ \mathrm{mm}^2$

Experiment | Superimposed | Simulation



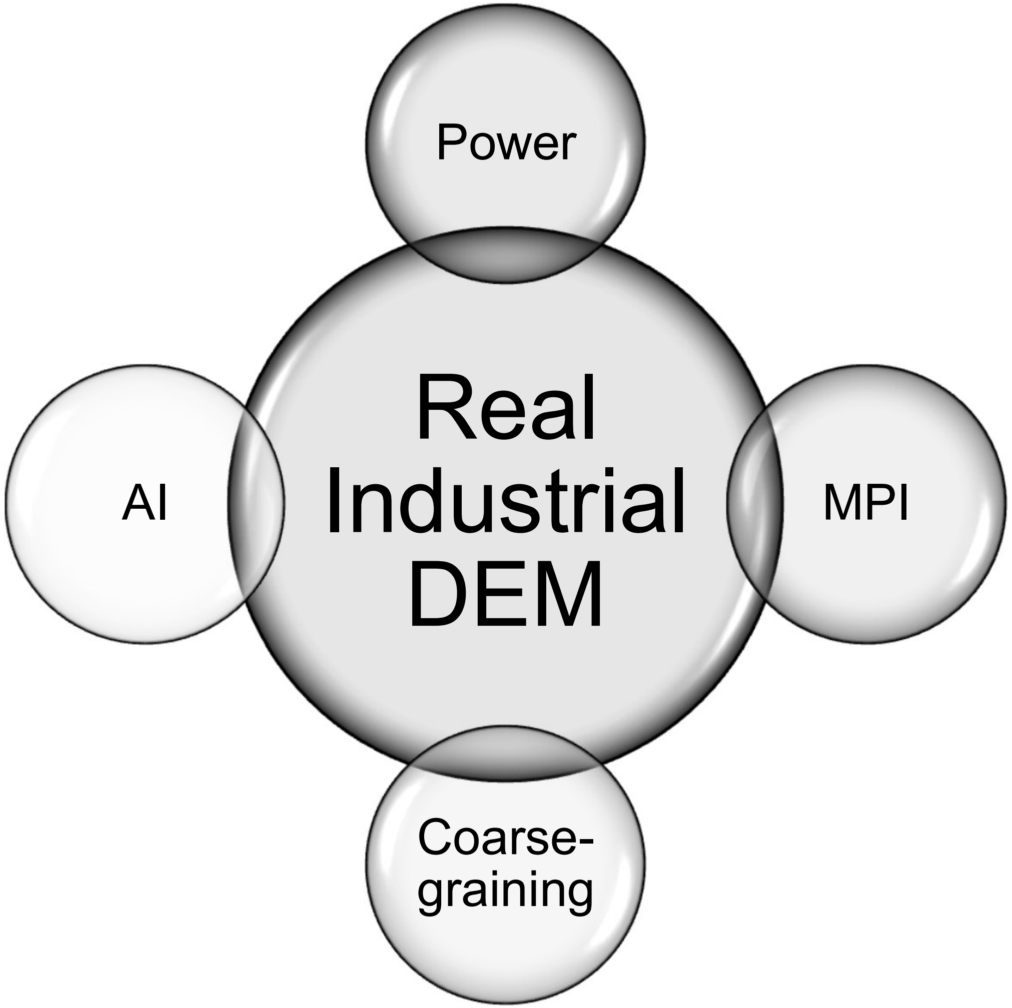
Example solution

Summary

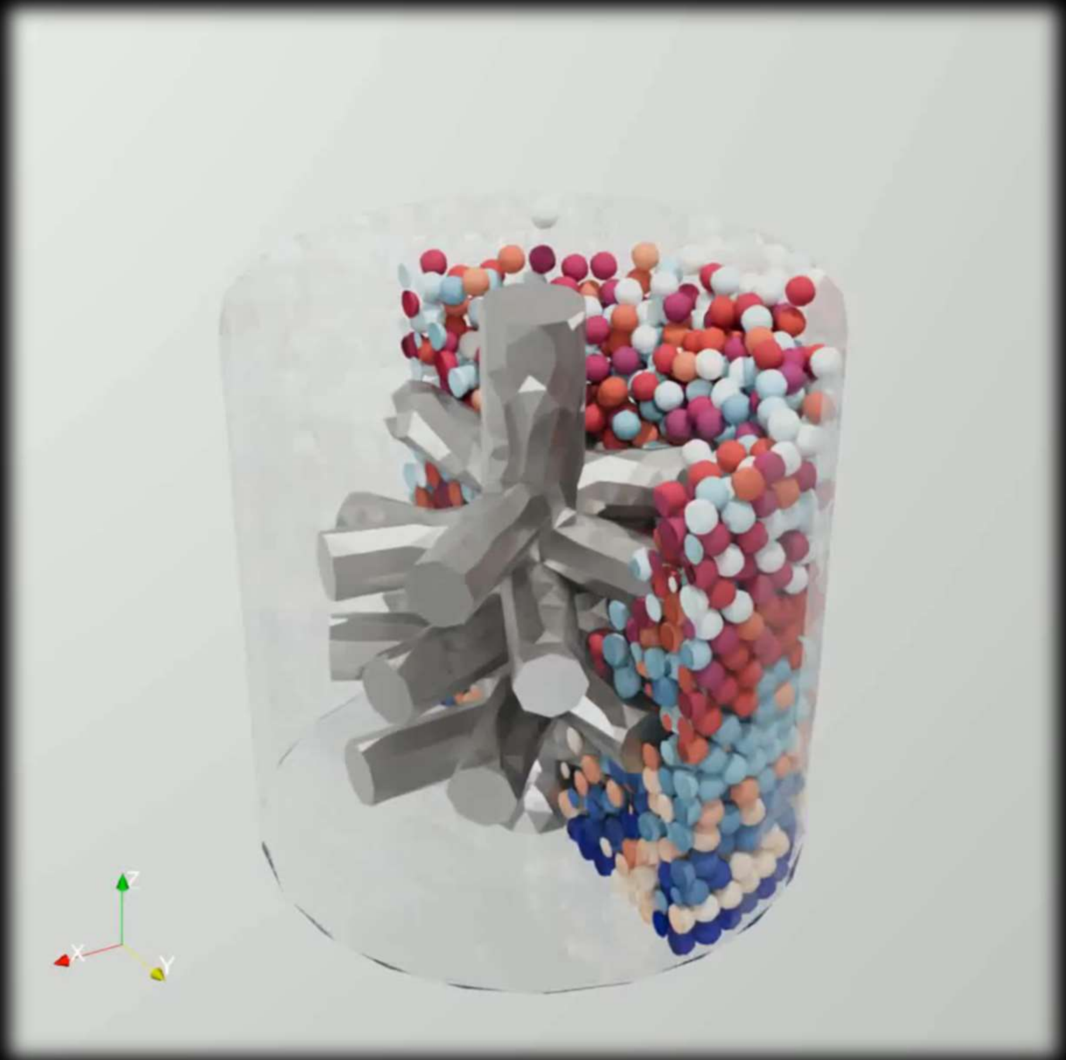
- PEPT facilitates the detailed, 3D imaging of particulate, fluid, and multiphase media, even in large, opaque systems.
- Diverse array of quantities extracted from PEPT facilitates deep insight into the internal dynamics of both scientific and industrial systems
- Synergy between PEPT and numerical methods facilitates an optimal mix of *efficiency* and *accuracy* not achievable using either methodology in isolation

Why is this talk timely?

- DEM is nothing new *but* recent advances in **computational power**, our ability to **parallelise** code, techniques for **upscaling** simulations, and advances in **AI** combined mean that today I can do things with DEM that at the start of my career I could only **dream of**
- Specifically, things like **this:**



"Evolving" the optimal design for a unit operation



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I. Evolutionary Algorithms as a Calibration Tool:

ACCES

Autonomous **C**haracterisation & **C**alibration using **E**volutionary **S**imulation (**ACCES**)

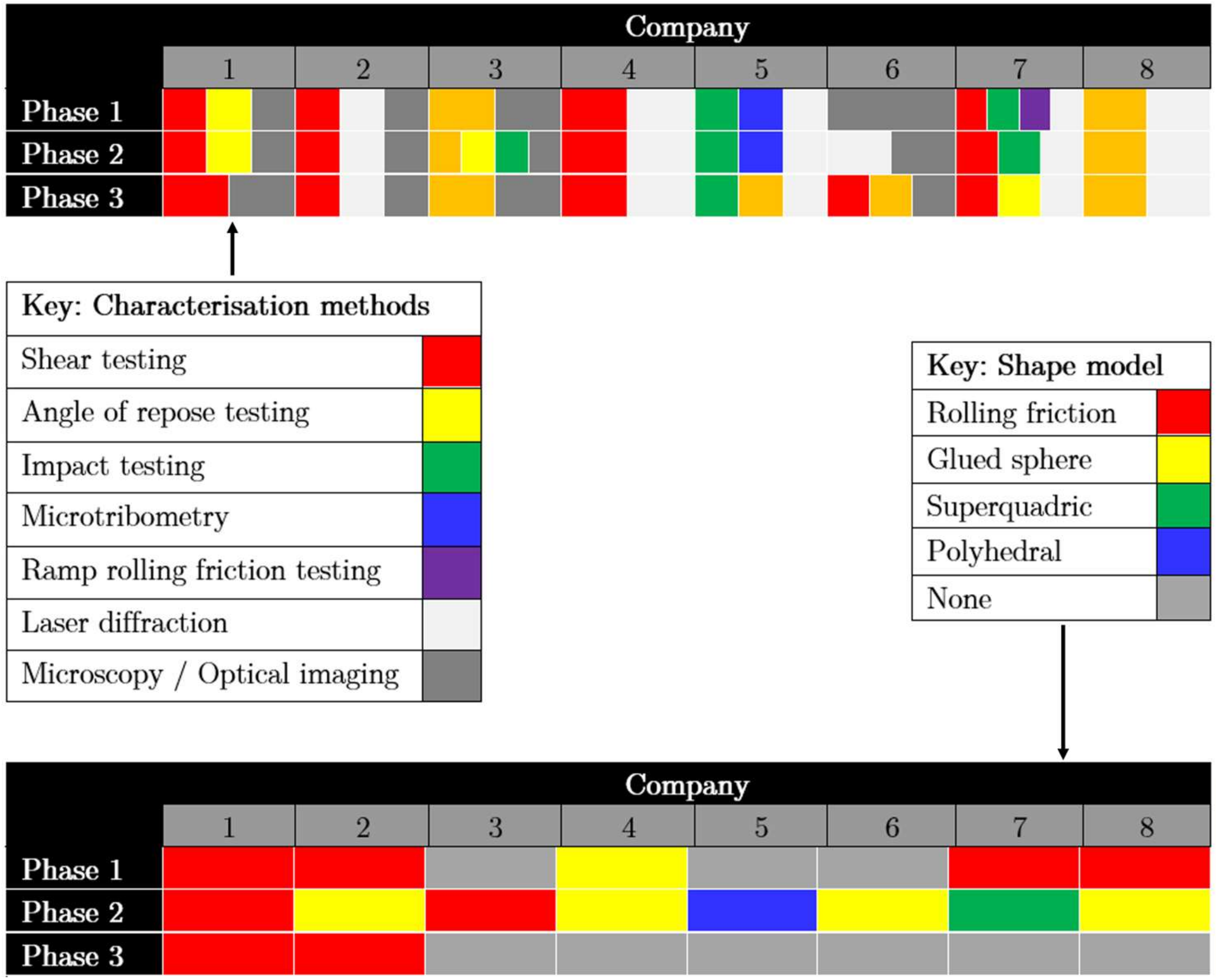
Real-world motivation: the need for a better method of calibration

IFPRI
International Fine Particle Research Institute

- Leading a 5-year project with IFPRI to investigate current industrial DEM characterisation/calibration strategies
- Detailed interviews with 8 (now 12) multinational companies who use DEM, spanning Agriculture, Chemical, FMCG, Food, & Pharmaceutical sectors
- **Goal: to determine a "gold standard" methodology for the calibration of DEM simulations**

Real-world motivation: the need for a better method of calibration

IFPRI
International Fine Particle Research Institute



- **No two companies** adopted the same procedures, equipment, or geometric models
- Most produced **different values for *same materials***
- The result?

Real-world motivation: the need for a better method of calibration

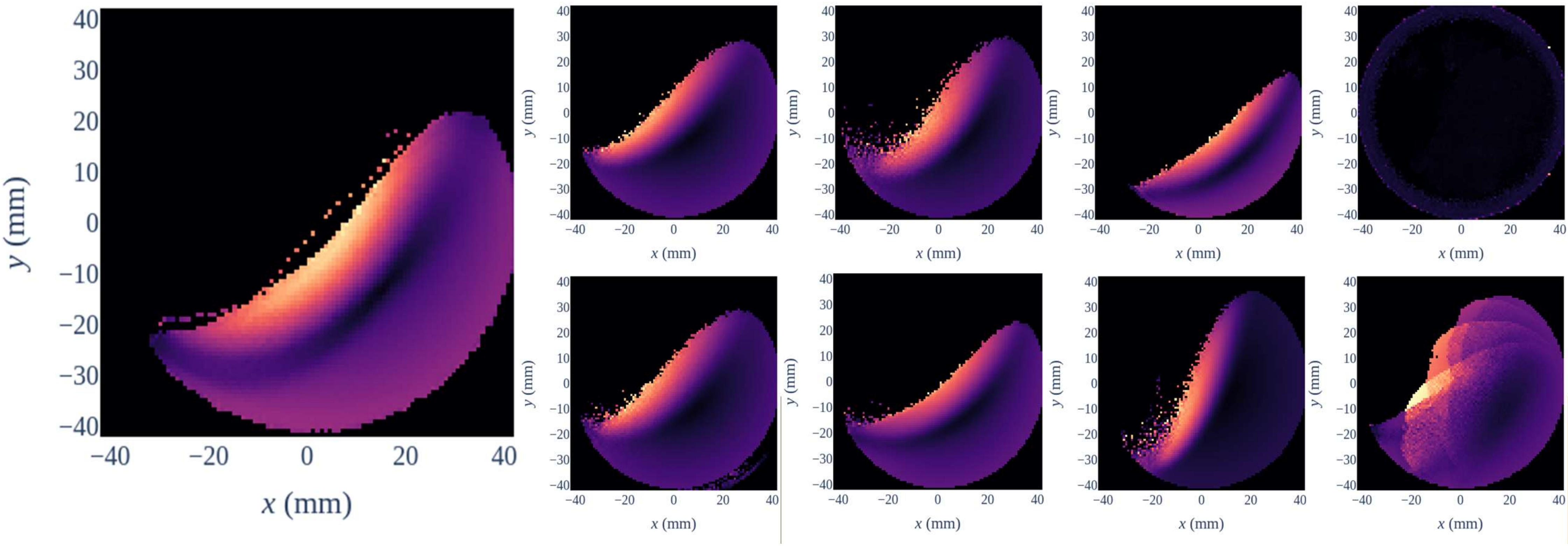
International Fine Particle Research Institute

Real, experimental PEPT data (more on this later)

Close, but no cigar

Not even close

Physically impossible!

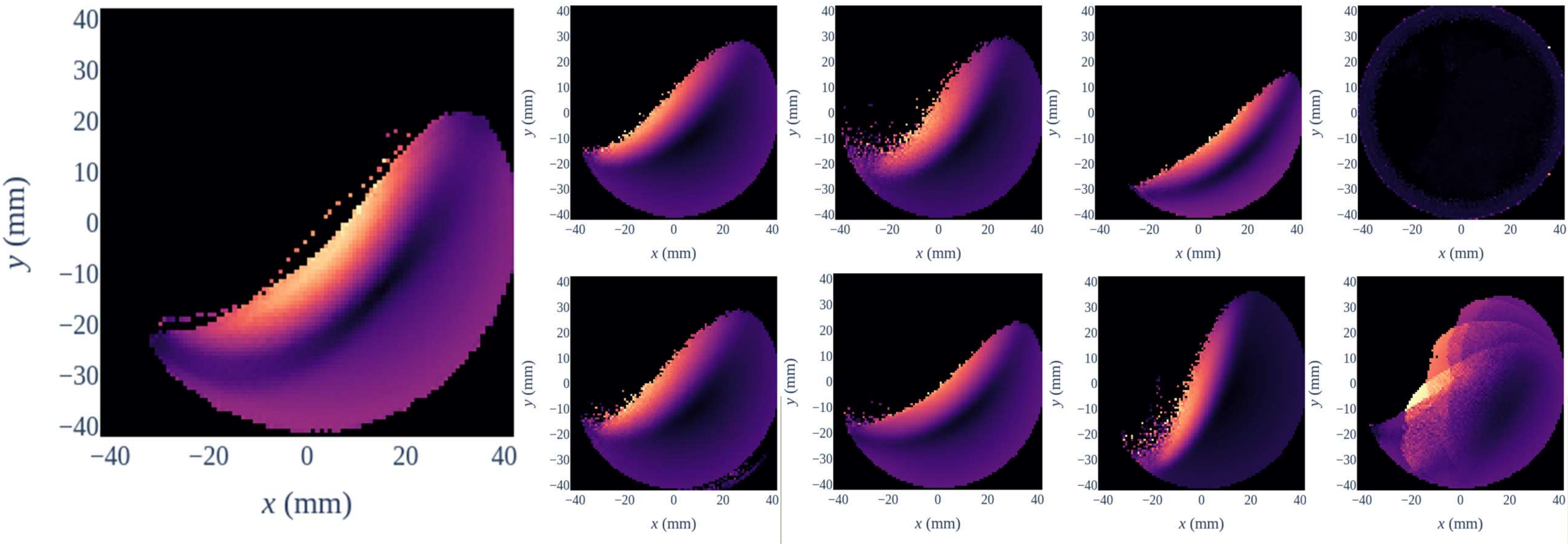


Real-world motivation: the need for a better method of calibration

IFPRI
International Fine Particle Research Institute

The scary part(s):

1) These are *real methods* used by *real companies*



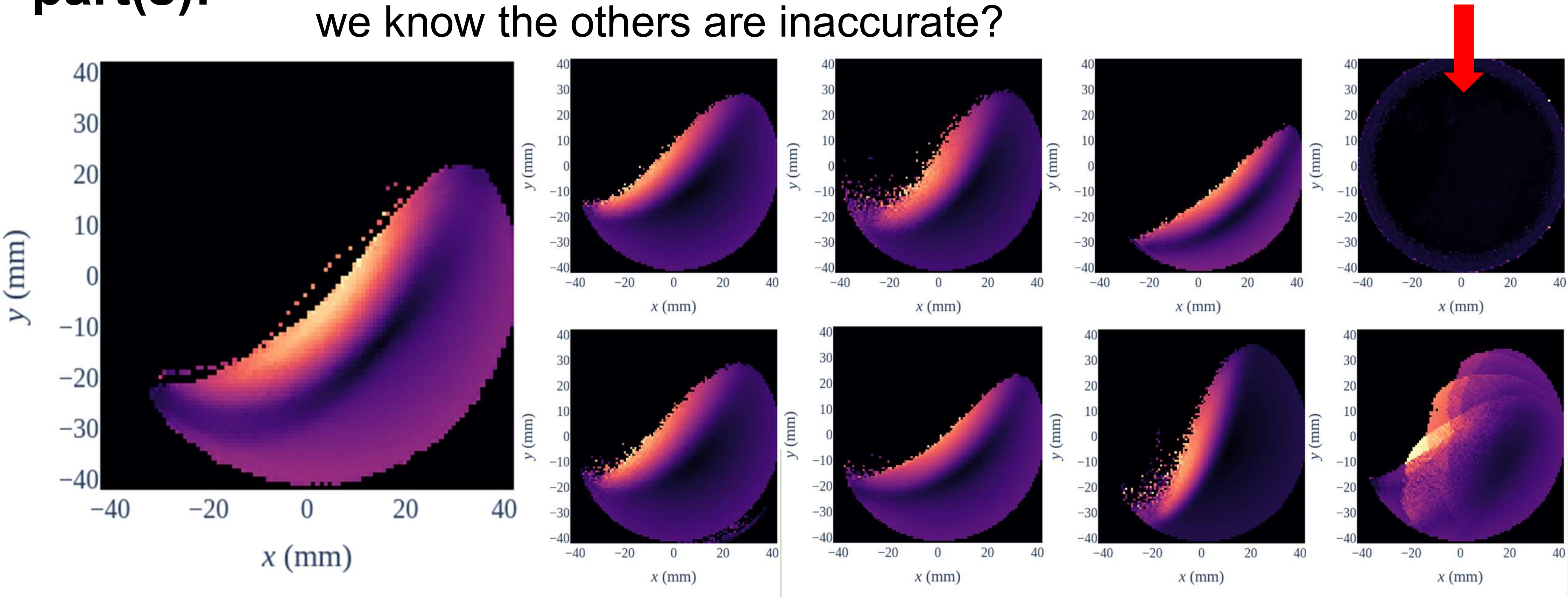
Real-world motivation: the need for a better method of calibration

IFPRI
International Fine Particle Research Institute

The scary part(s):

2) While a sensible operator will re-try these…

…without a technique like PEPT, how would we know the others are inaccurate?

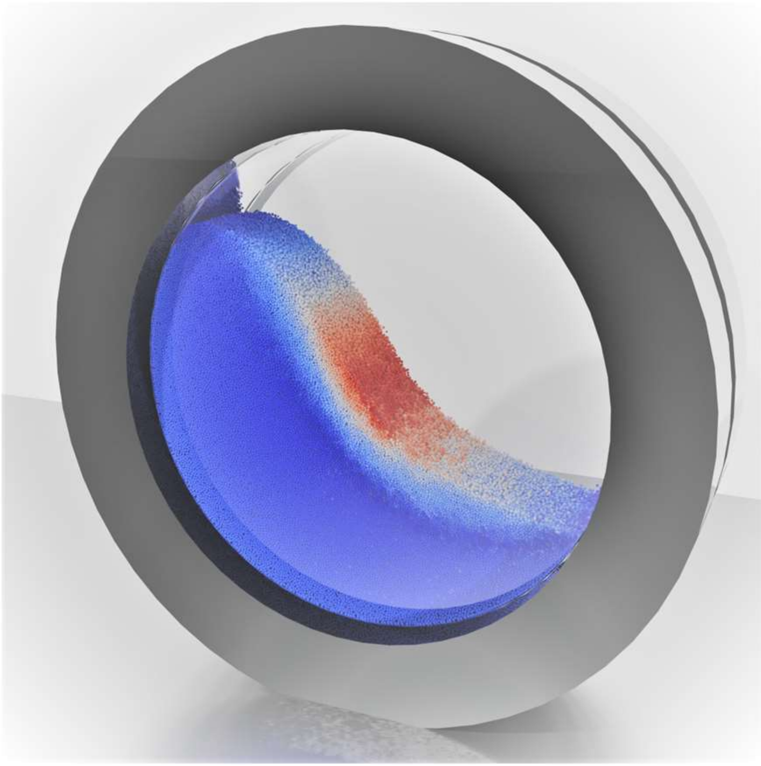


Real-world motivation: the need for a better method of calibration

IFPRI
International Fine Particle Research Institute

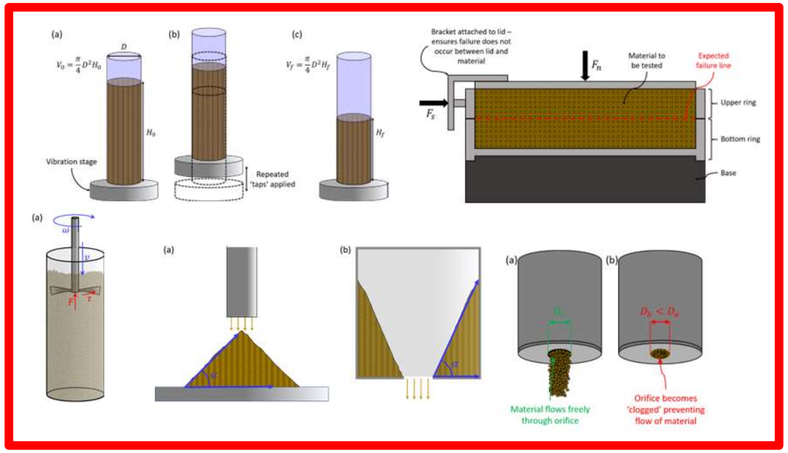
The scary part(s):

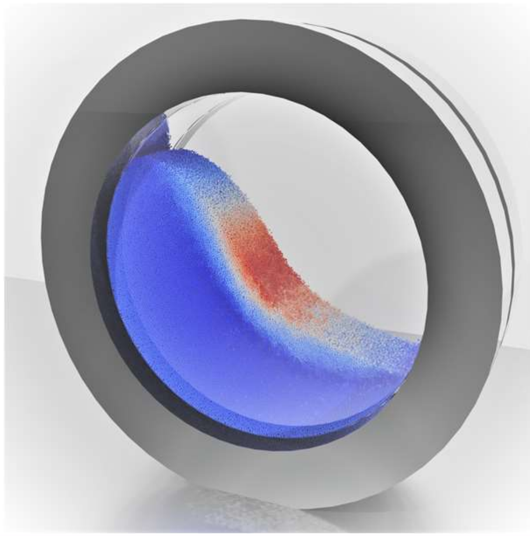
3) This is for a relatively *simple, single-phase system* containing only *spherical particles.* How will these methods stand up for more complex cases?

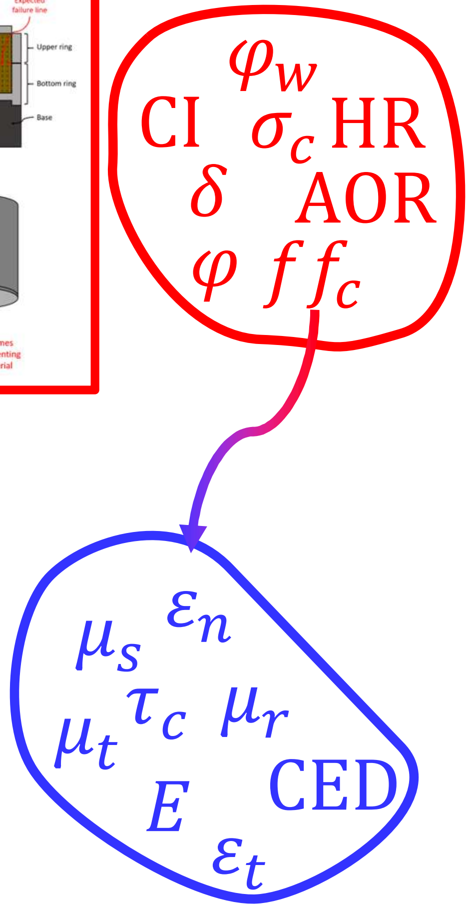


Problem statement

- Particles' **bulk** properties are quick and easy to measure using easily-available equipment and standardised procedures.
- Measurement of particles' **microscopic** properties… is none of the above
- **→ We need a quick, easy and reliable way to map bulk measurements to microscopic properties**



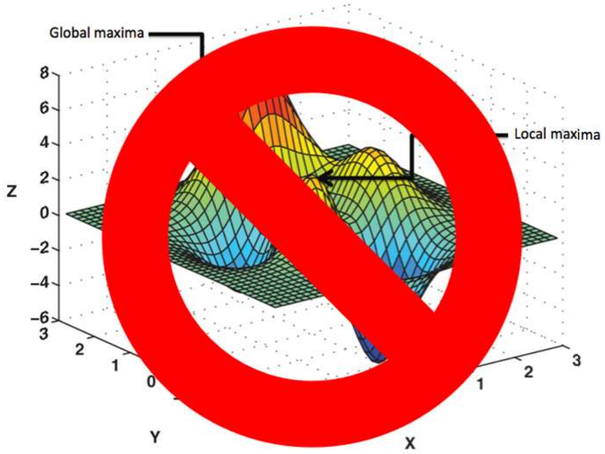




III. Choosing an Optimiser

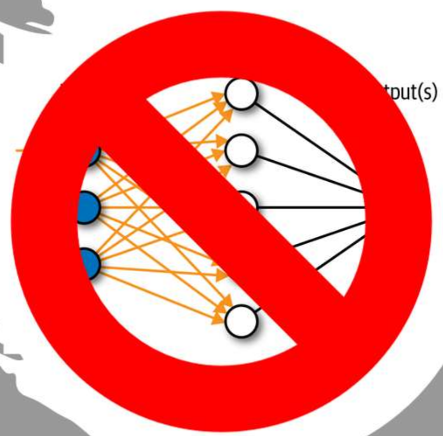
Error function can be **very non-convex** (local minima) and **very non-smooth** (lots of "jiggle") → cannot trust gradient!

→ Evolutionary algorithms are the only logical choice for calibration-by-optimisation

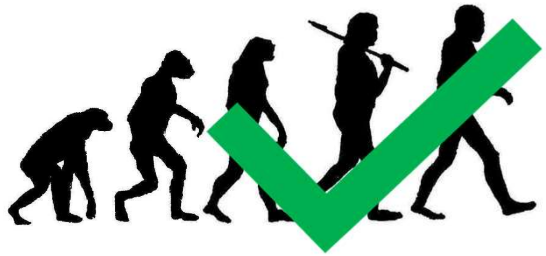


Gradient-based optimisers

ANNs

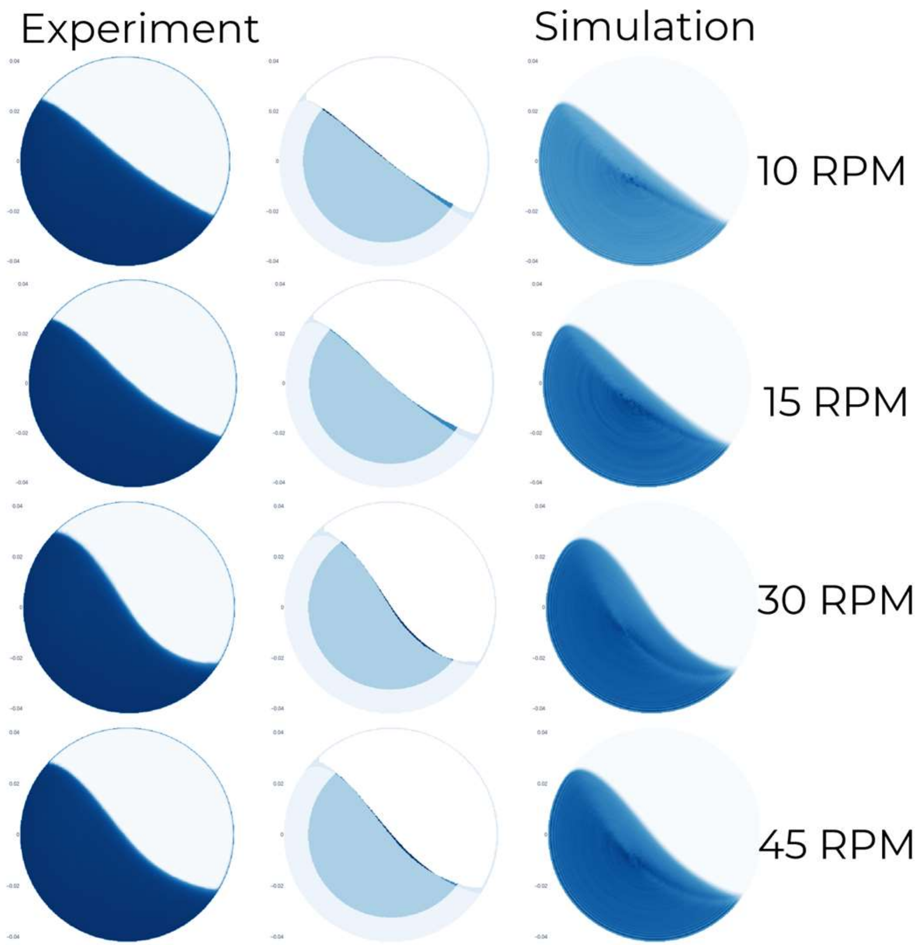


Evolutionary Algorithms



Calibrating Multiple Parameters

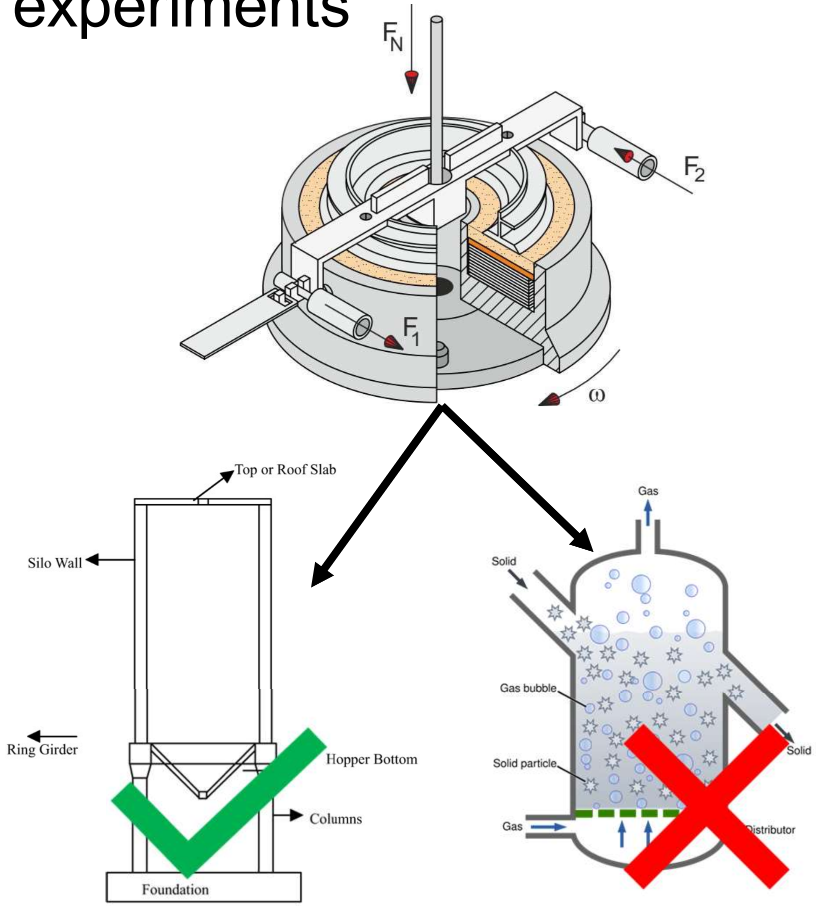
- Mathematically, to solve for **N unknowns** we need **N closure relations**
- → Calibrating 5 parameters against a single measurement is **ill-defined**
- But this does not mean we need 5 instruments!
- E.g. a GranuDrum's free surface shape can be fitted by a 3rd order polynomial → 3 outputs!
- ACCES can calibrate against **multiple measurements** – e.g. GranuDrums at different RPMs, Shear Cells, FT4…
- → Drum can (hypothetically) calibrate $3N$ parameters by running at N distinct RPM

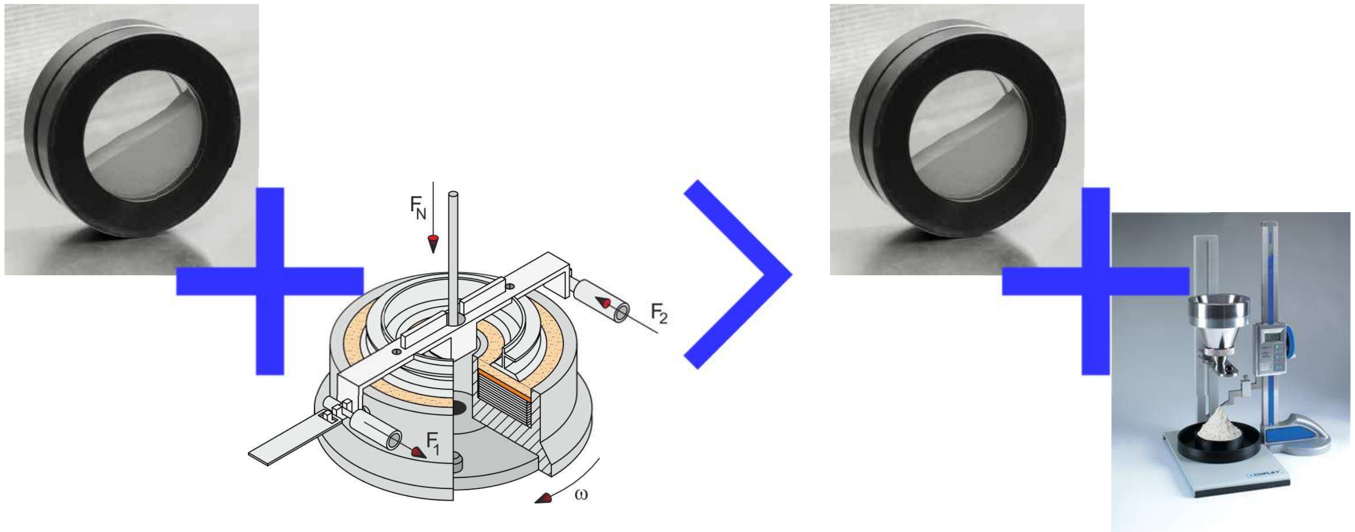


Final thought on ACCES: A tool is only as good as its user

- Easy to make ACCES seem “too good to be true”
- In reality, though the **process** is fully automated, **human intelligence is still required** in the **initial design** of calibration experiments

  ACCES can only work with what we give it!
- IFPRI project has highlighted importance of:
  1) Matching the calibration device to the “real” system
  2) When using multiple tools, choosing **distinct** tools





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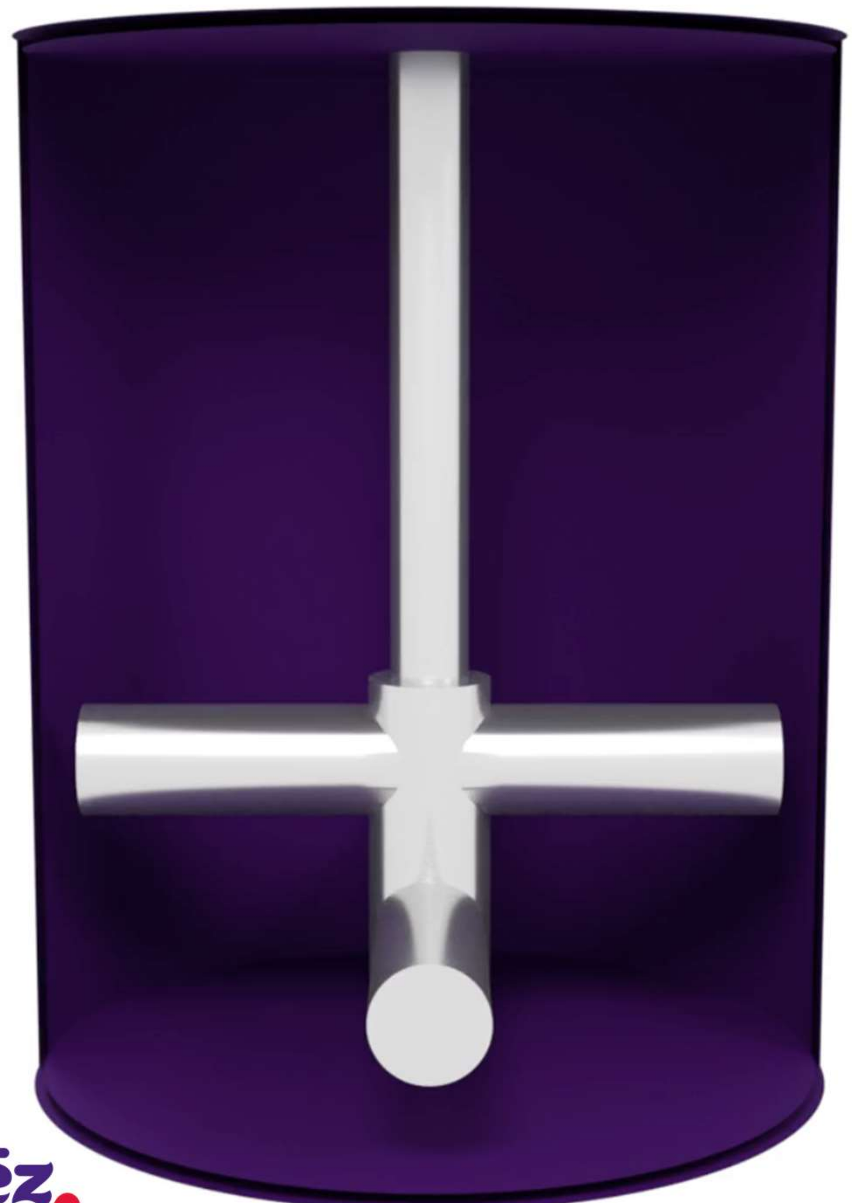
II. Evolutionary Algorithms as an Optimisation Tool:

Highly-Autonomous Rapid Prototyping for Particle-handling Processes (HARPPP)

Beyond calibration

- We have used ACCES to perfectly calibrate a simulation of (say) a mill
- So what next?
- For industry, typically:
  - Improve efficiency
  - Improve productivity
  - Reduce waste
  - → Improve green credentials
  - → Increase profit
- In other words, we have optimised **calibration**, now we want to optimise the **system itself**



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Optimising a Mill

Two main options:

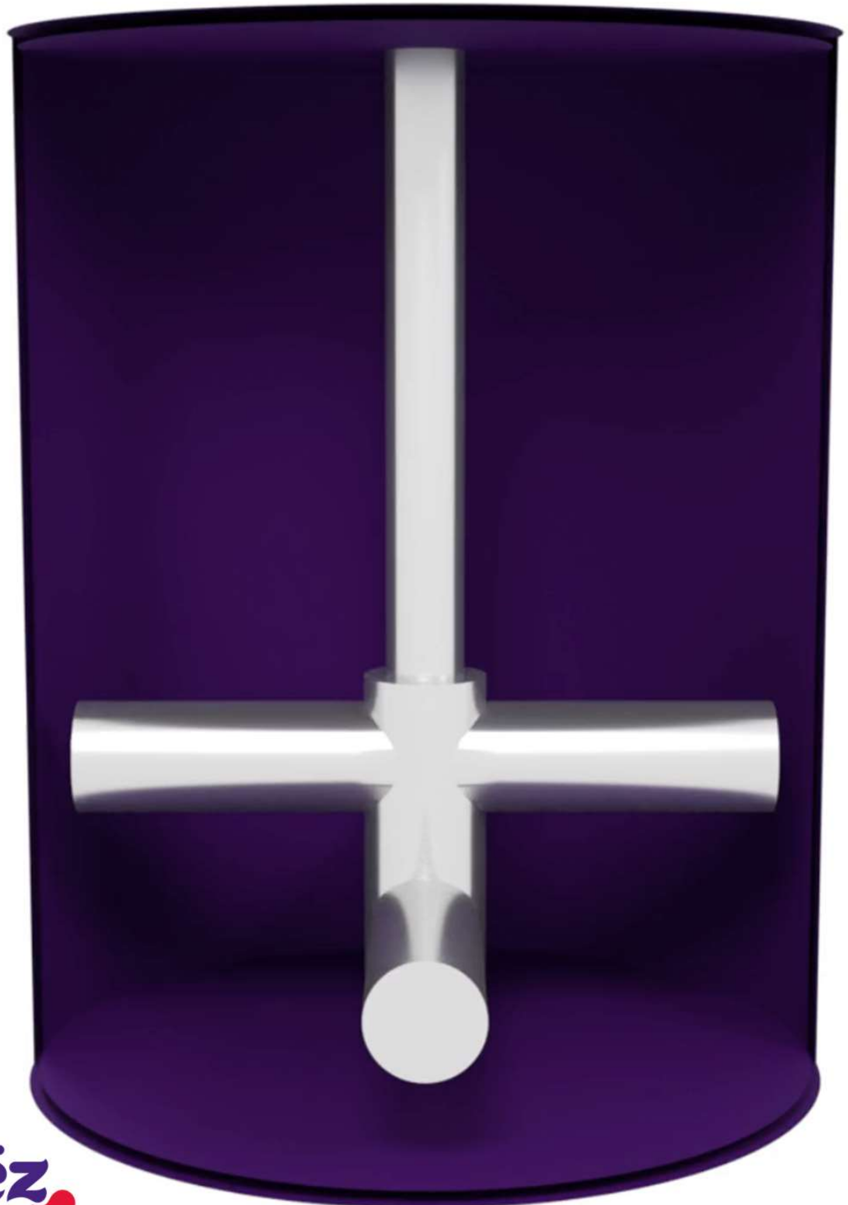
1. Optimise *process parameters* (e.g. attritor RPM, fill level…)

(Relatively) simple, easy to achieve both in "real life" and in simulation.

2. Optimise *geometry*

Highly costly in real life. Time-consuming, labour-intensive and "hit and miss" both in real life & DEM.

Can we 1) remove the element of chance and 2) remove the need for human input?



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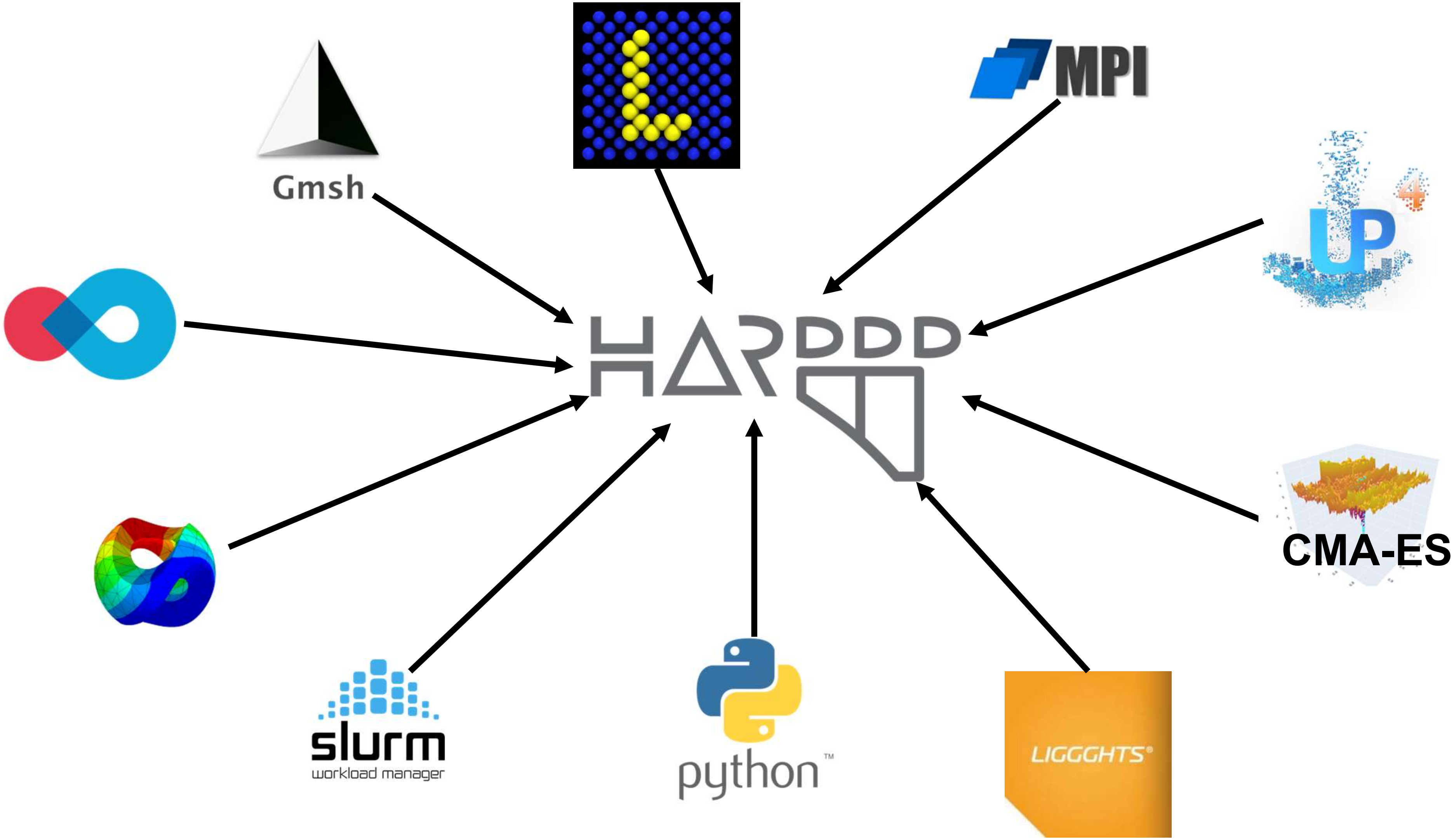
Highly Autonomous Rapid Prototyping for Particulate Processes (HARPPP)

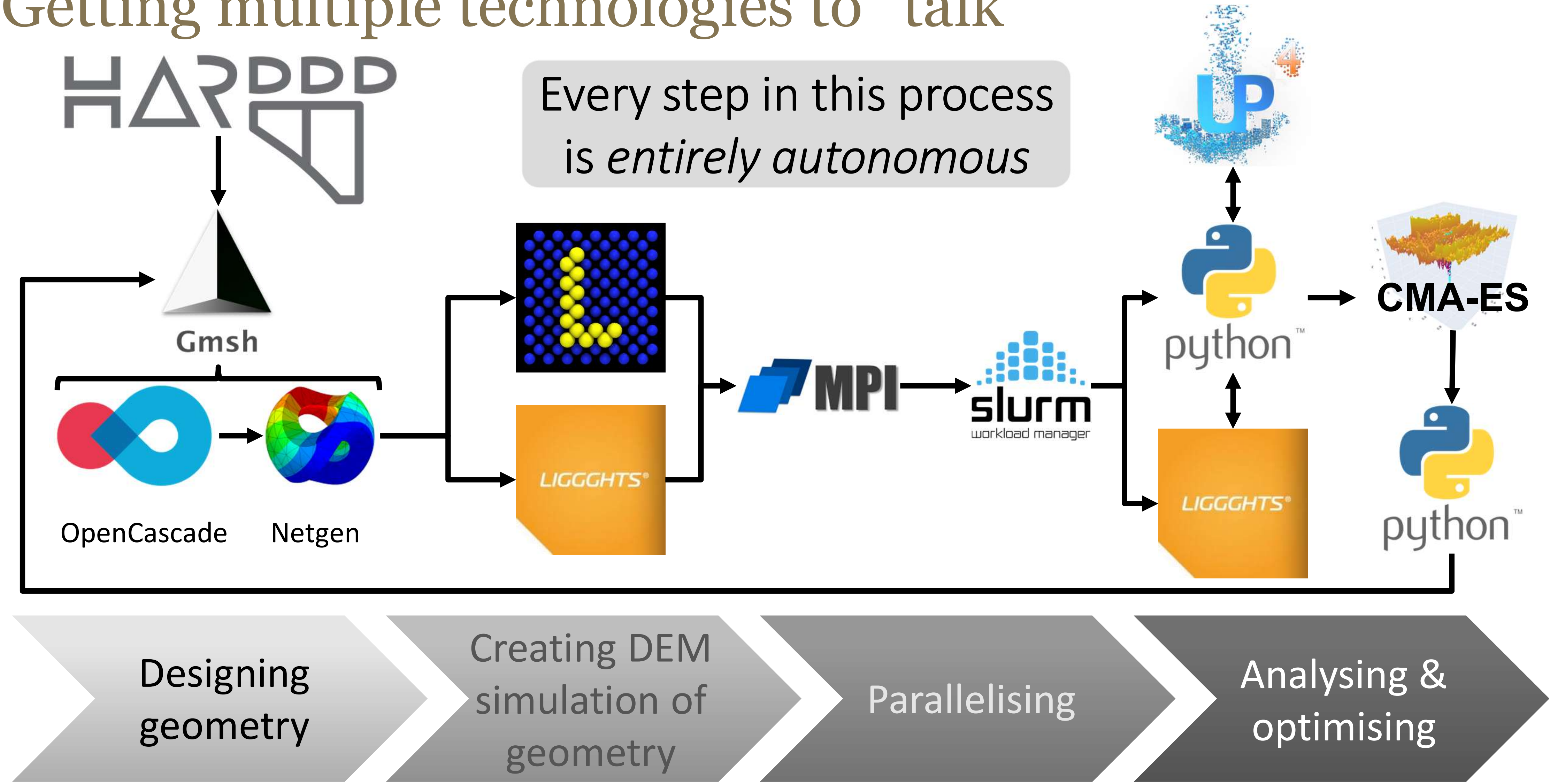
- Applying the evolutionary approach of ACCES to “real” optimisation
- Metaprogramming allows not only alteration of simulation scripts, but also **the autonomous design and implementation of entirely novel geometries**
- *Not* a simple task!

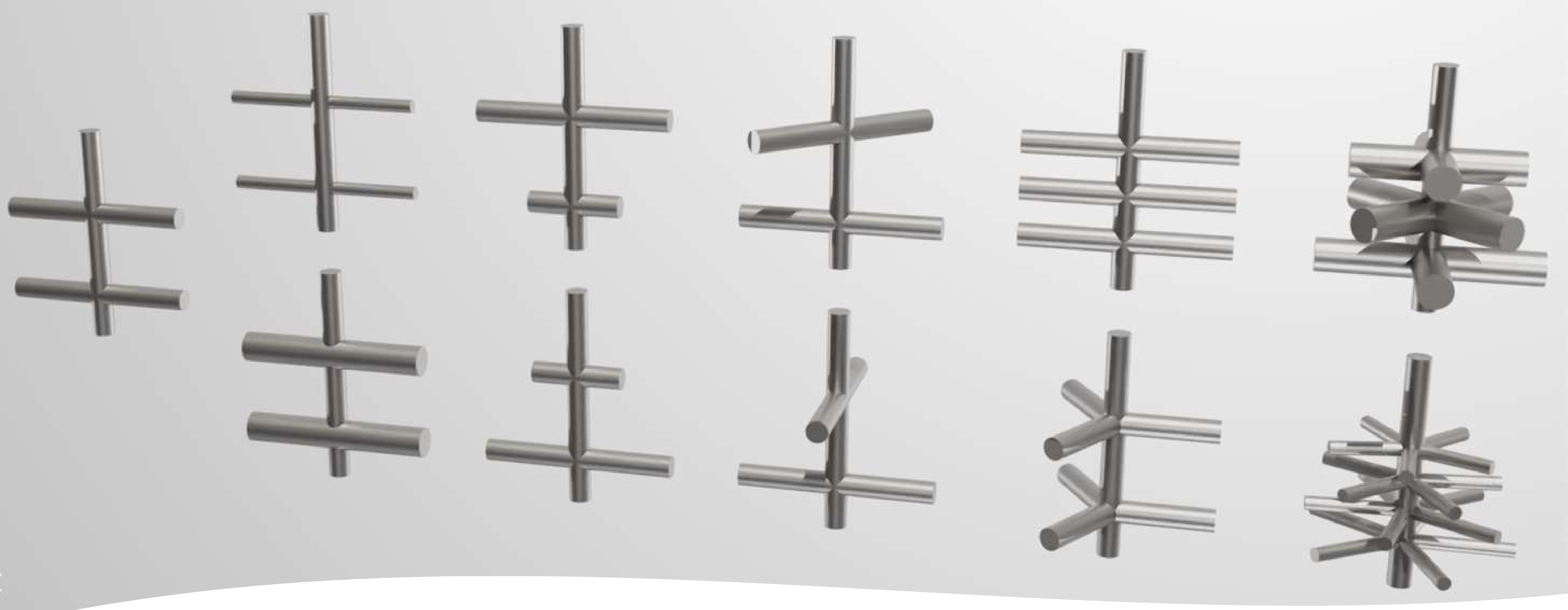
Getting multiple technologies to "talk"



Getting multiple technologies to "talk"

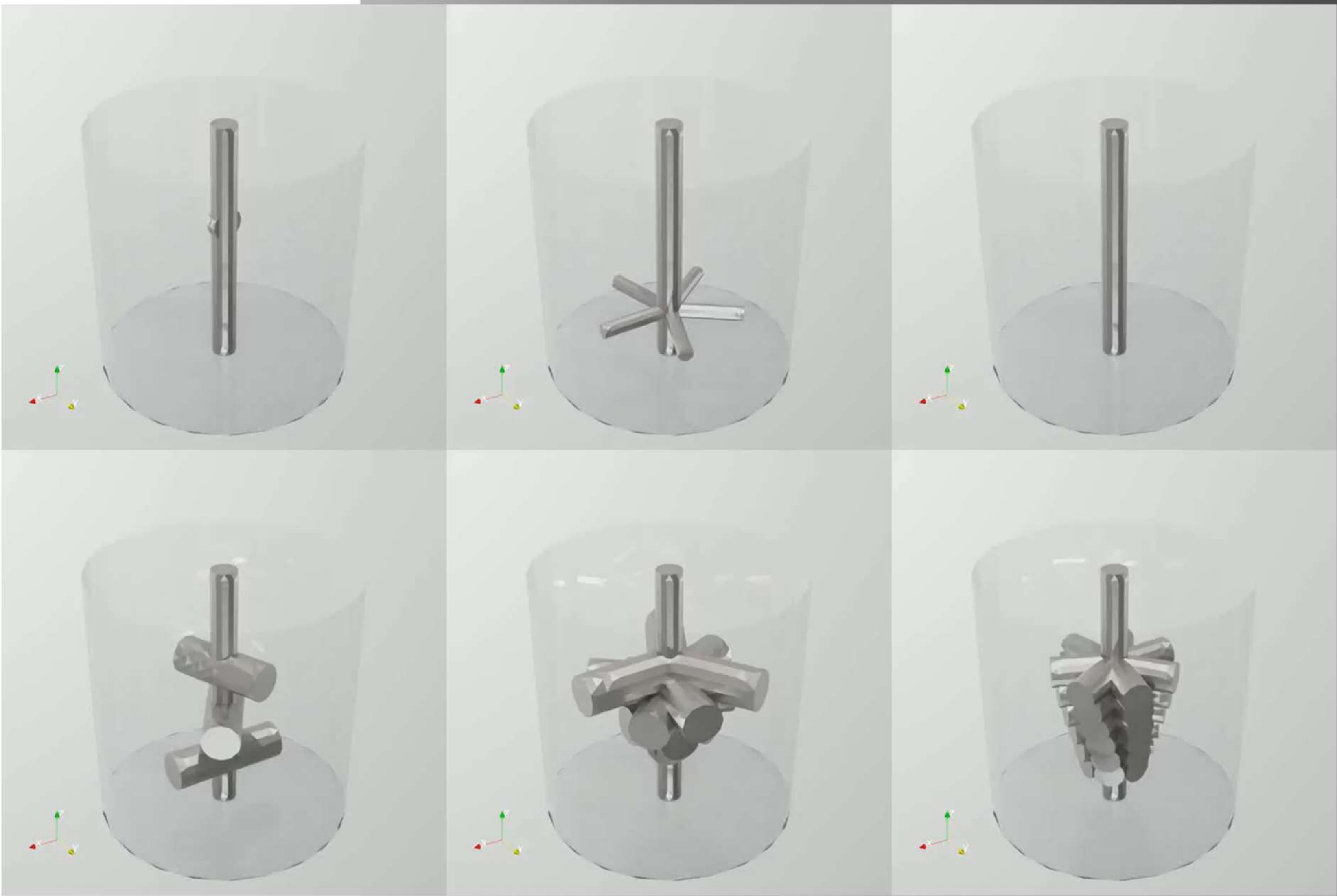
Every step in this process is *entirely autonomous*





Case Study

- Optimising a simple attritor mill
- Give HARPPP the ability to vary **pin length, pin diameter, pin number (horizontal and vertical), and pin angle**
- Set goal to minimise power draw → **reduced energy costs, "greener", more sustainable process**



What went wrong?

- Technically, **nothing**
- HARPPP did exactly what we requested and **perfectly minimised power draw**
- Nonetheless, it is decidedly *not* a good mill!
- Take home point: need to thoughtfully define our objective

What went wrong?

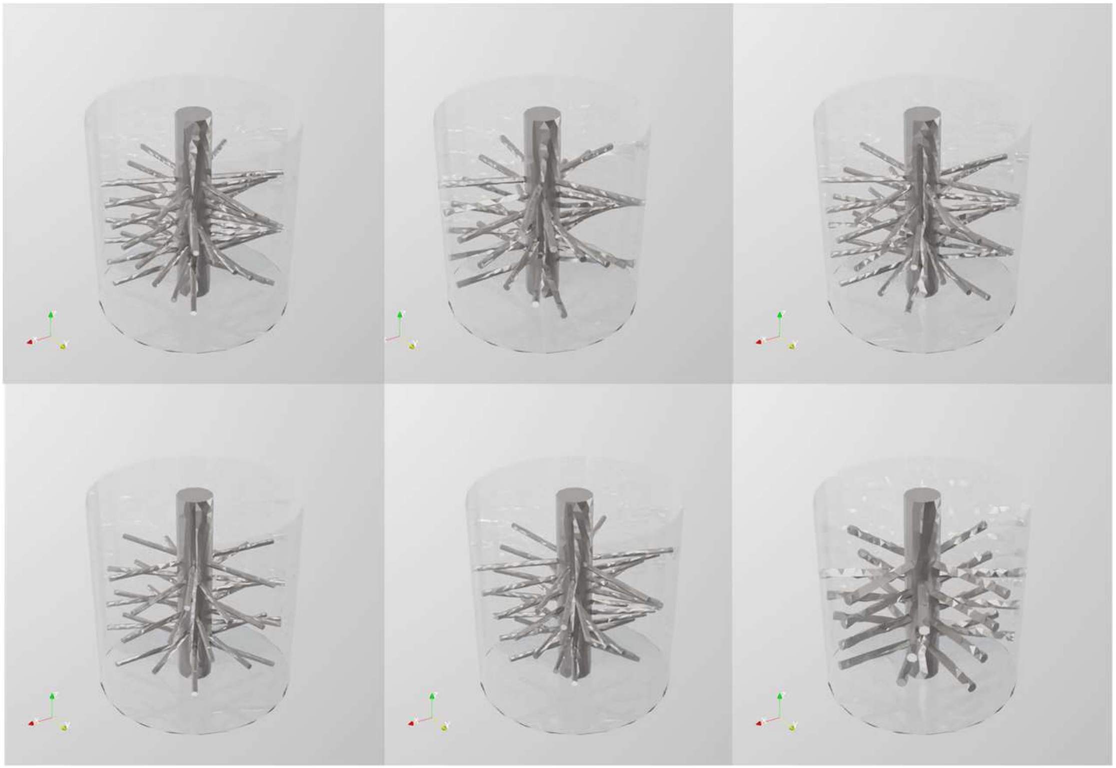
- Luckily, HARPPP is capable of **multi-objective optimization**
- Can thus define a more intelligent goal, for example minimize power draw (Objective 1) whilst maintaining a minimum mean pair stress energy (Objective 2)

Results

For different mill geometries, operating conditions and particle properties tested, **energy savings of between 24% and 40%** achieved compared to base model, whilst producing the **same or greater** average pair stress energy

Can we learn from the machines?

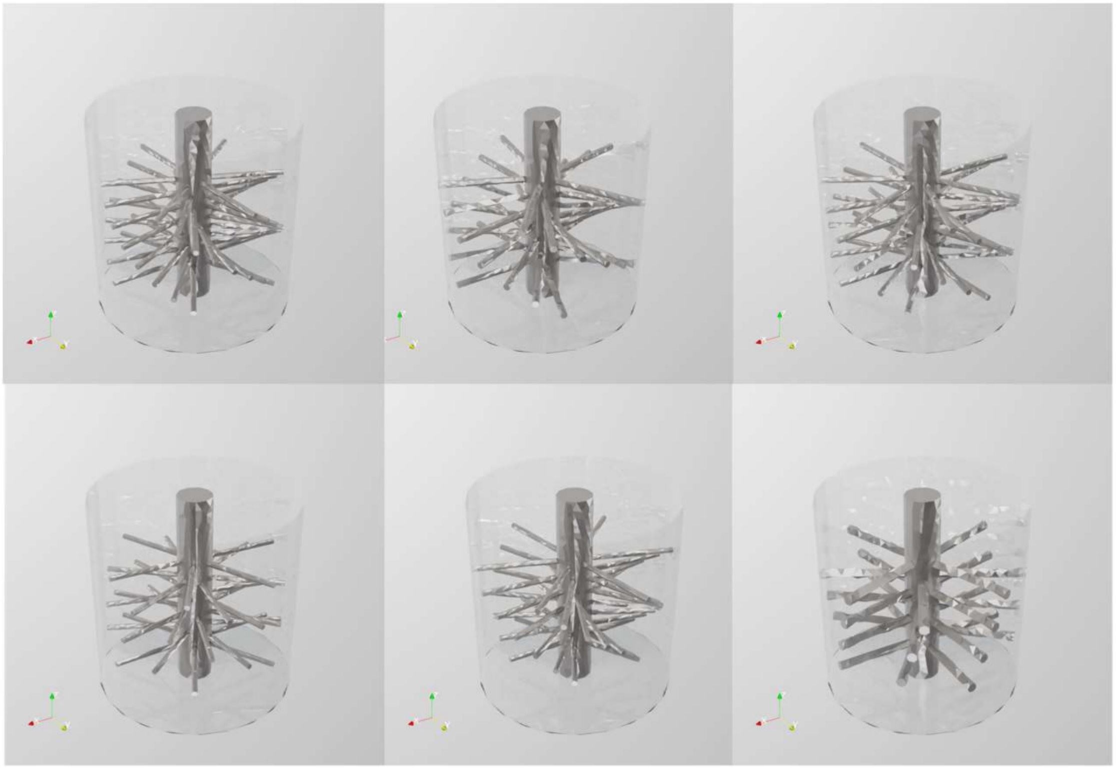
- In later stages of evolution, majority of attritors show certain commonalities, namely **large numbers of long, thin, staggered pins**
- Indeed, these features remain robust even with mills and particles at different scales!
- Does this suggest some key design principles that we can learn from HARPPP?



Can we learn from the machines?

Possible interpretations:

1. Long pins → value fairly obvious!
2. Thin pins → minimise propensity to simply “push” particles → remove interactions which cause power draw without inducing collision or shear
3. Large numbers of closely-packed, staggered pins → redirect particle motion → improve axial transport, induce “chaos”

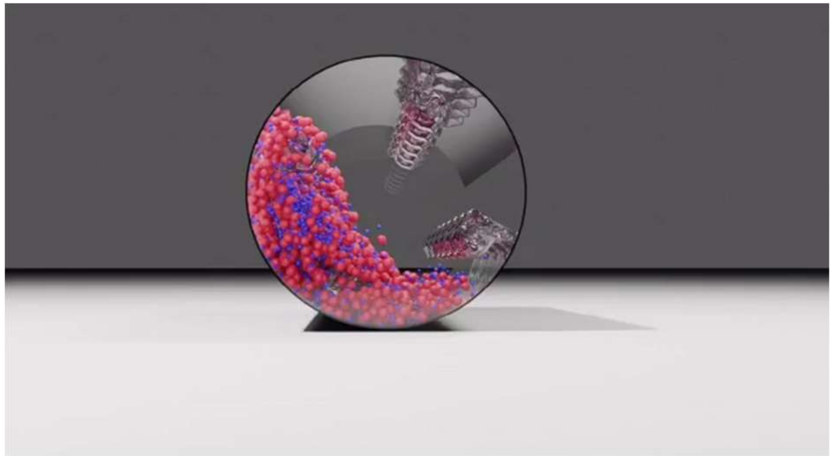


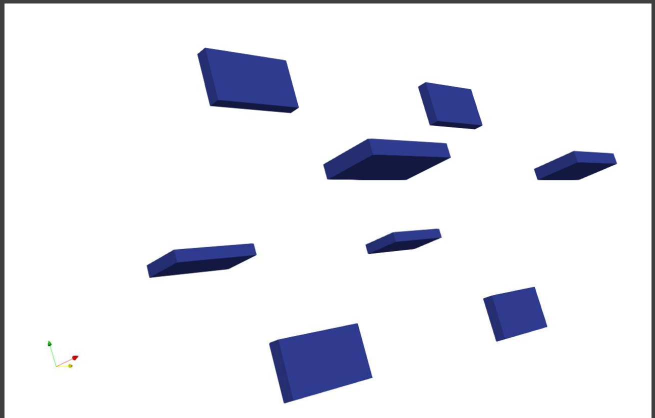
Only the tip of the iceberg

- A good proof of concept, but still relatively simple.
- Many additional factors which can be included:
  - Lower-bound on pin size to ensure robustness?
  - More complex goals – specific force *distribution*? Optimise both collision and shear?
  - More complex geometric variations?
  - …
- User can define arbitrary number of objectives & constraints dependent on their system, and their goals.
- HARPPP can also, of course, optimise much more than just mills!

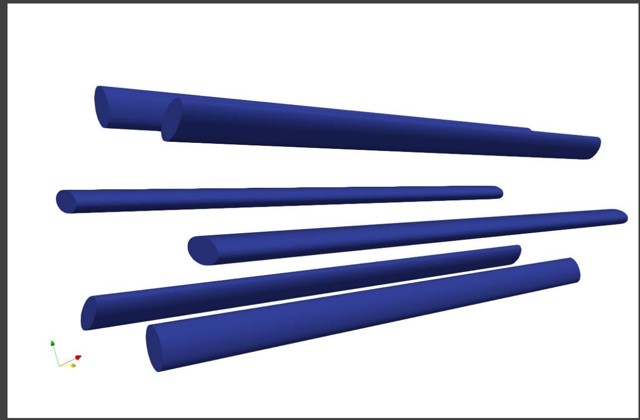
Not just mills…

- Rotating drum system with particles of differing size & density
- In standard form, significant segregation
- **Goal: design baffles to optimize mixing**

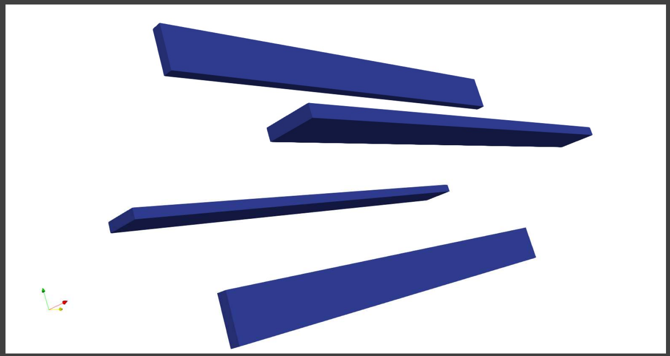




Optimise width, thickness,
number and axial position

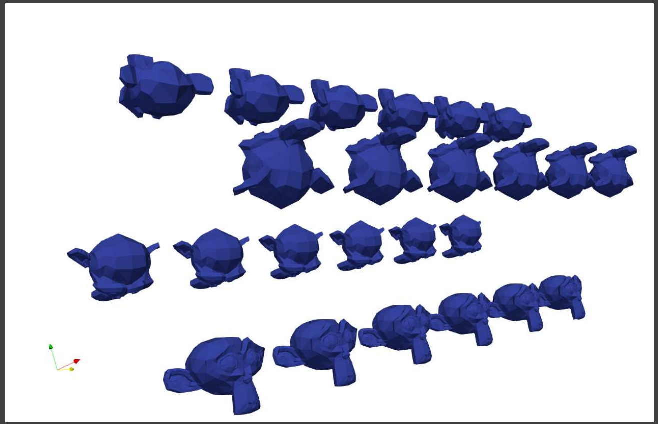


Optimise width, thickness,
number radial position & shape

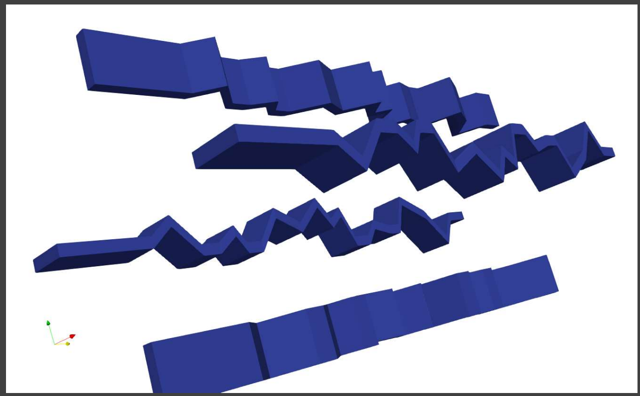


Optimise width and thickness,
constrain number and shape

Optimise size, number & position
constrain shape to monkey



Optimise width, thickness, &
local angle



Optimising Mixing

- Significant segregation in base model (Case 1)
- Marked improvement in Case 2, but geometric constraint and/or radial constraint prevents full optimization
- Case 3 achieves near-perfect mixing

Case 1 — Base Model: M = 0.80

Case 2 — Monkeys: M = 0.96

Case 3 — Rods: M = 0.99