ACCES:

Autonomous Characterisation and Calibration via Evolutionary Simulation

EPSRC CENTRE FOR DOCTORAL TRAINING
TOPOLOGICAL DESIGN

POSITRON IMAGING CENTRE

Interactive Example

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EPSRC MAPP-funded Project

BlueBEAR HPC Service
Positron Imaging Centre
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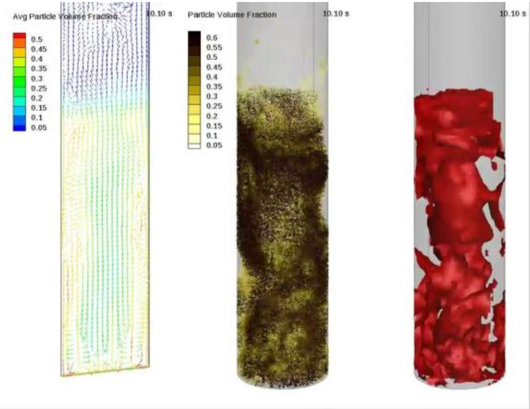
Why Simulate and Calibrate?

Interactive Example

Compared to noisy experiments, simulations offer:

- Faster results
- Cheaper modifications
- More information
- Higher accuracy



If, and only if, they are **correctly calibrated** - otherwise the outputs cannot be trusted

- Leading project with IFPRI investigating current industrial **simulation calibration strategies**. Key findings:
  - **No two companies** use the same procedure
  - **>20** instruments used… each with a 5-figure price tag

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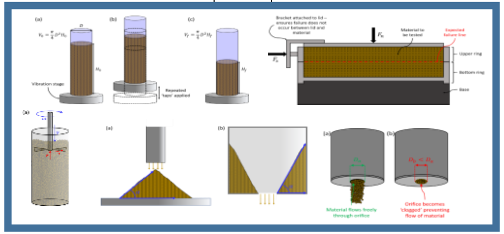
IFPRI International Fine Particle Research Institute

Conventional Calibration

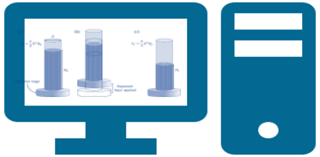
Interactive Example

1) Take material from system of interest

2) Manually measure bulk properties



3) Recreate **test systems** in Simulation Engine

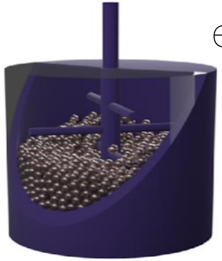


4) Use calibration simulations to **manually** infer microscopic parameters

CI φ_w HR σ_c f φ AOR ffc

μ_s ε_n τ_c μ_r μ_t E CED ε_t

5) Recreate **real system** in Simulation Engine



6) Validate against experiment

7) Repeat!

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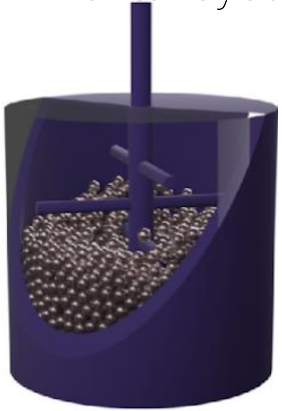
ACCES Calibration

Interactive Example

1) Run suitable set of test experiments

2) ACCES uses experimental data & a basic, uncalibrated simulation to autonomously **"learn"** the relevant parameters

3) Comprehensively validated simulation of experimental system



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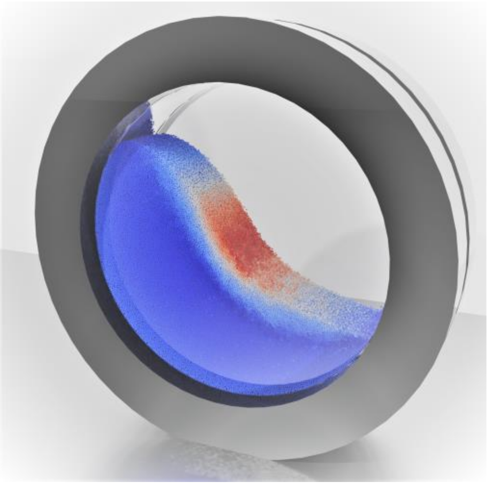
DEM Calibration as an Optimisation Problem

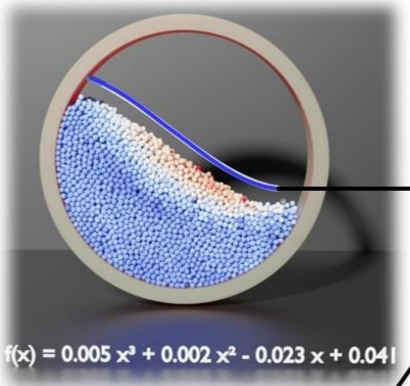
I. Choose experimental system to model
II. Define a **cost function** to quantify difference between experiment and simulation
III. Choose a suitable optimiser
IV. Set goal to minimise error function (i.e. maximum agreement between simulation and experiment)
V. Iterate towards minimum (i.e. find optimal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

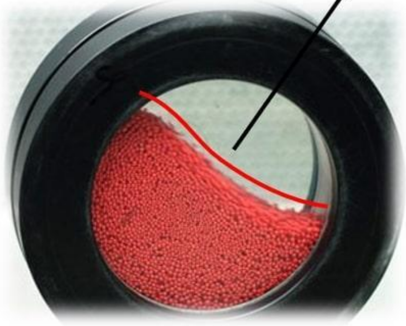
GRANUTOOLS™



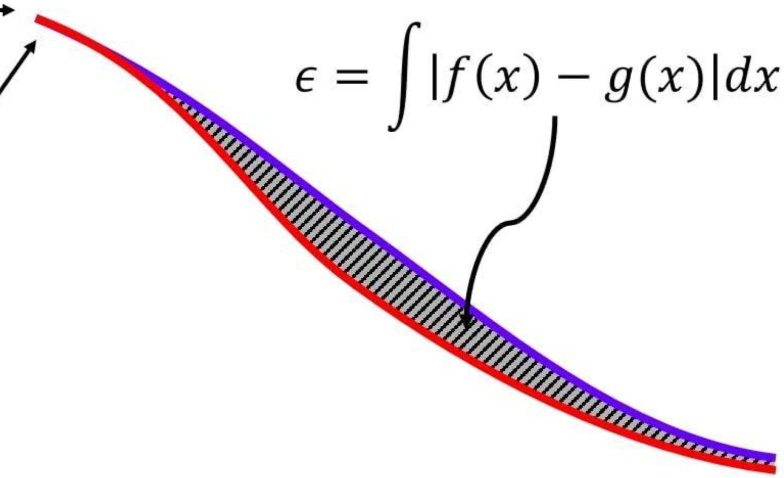
Characterising DEM Particles

Interactive Example





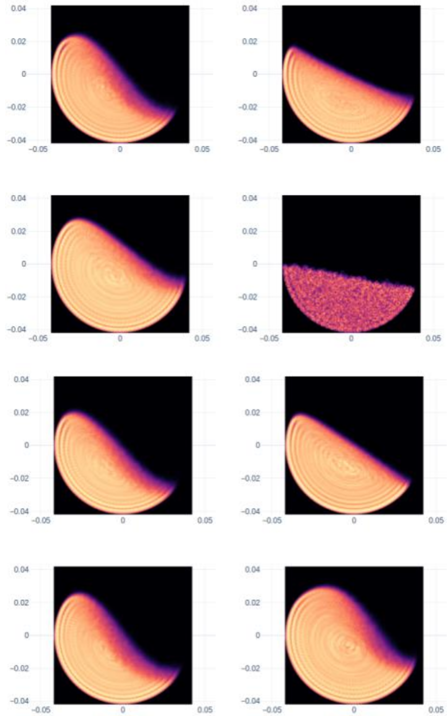
Example:
Characterisation of DEM particle friction, restitution and particle number against a GranuTools GranuDrum-imaged free surface shape.



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

The model was effectively calibrated against a single experimental data point, but was able to **reproduce other uncalibrated properties** such as velocity vector fields.

Single Epoch



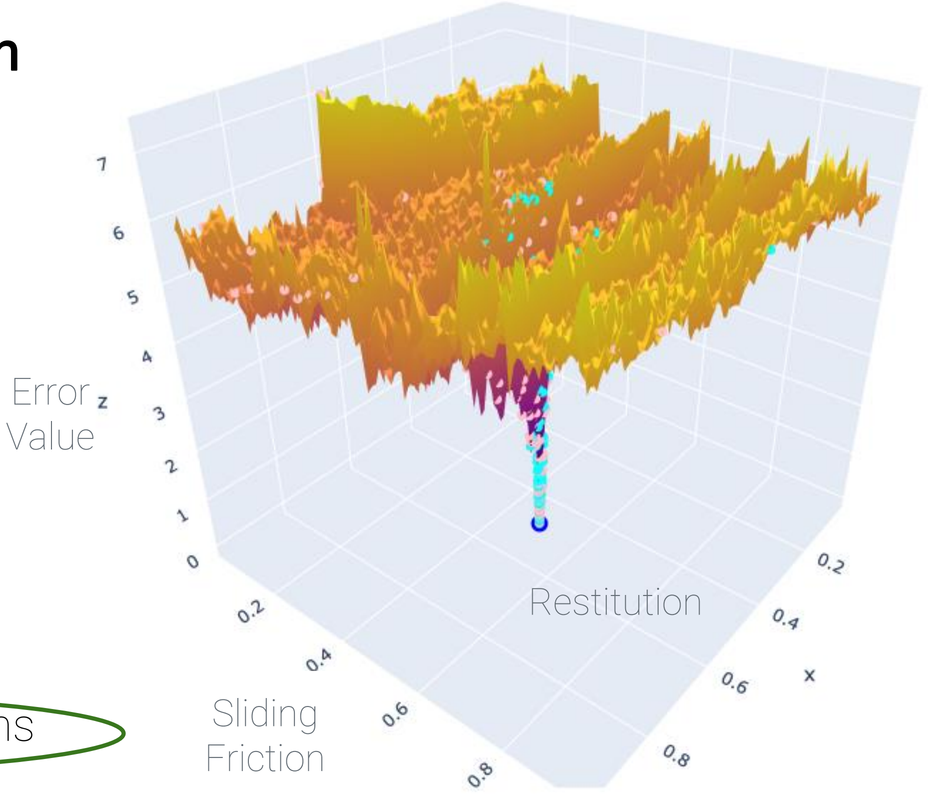
How do we optimise this?

Every function evaluation is an entire simulation run

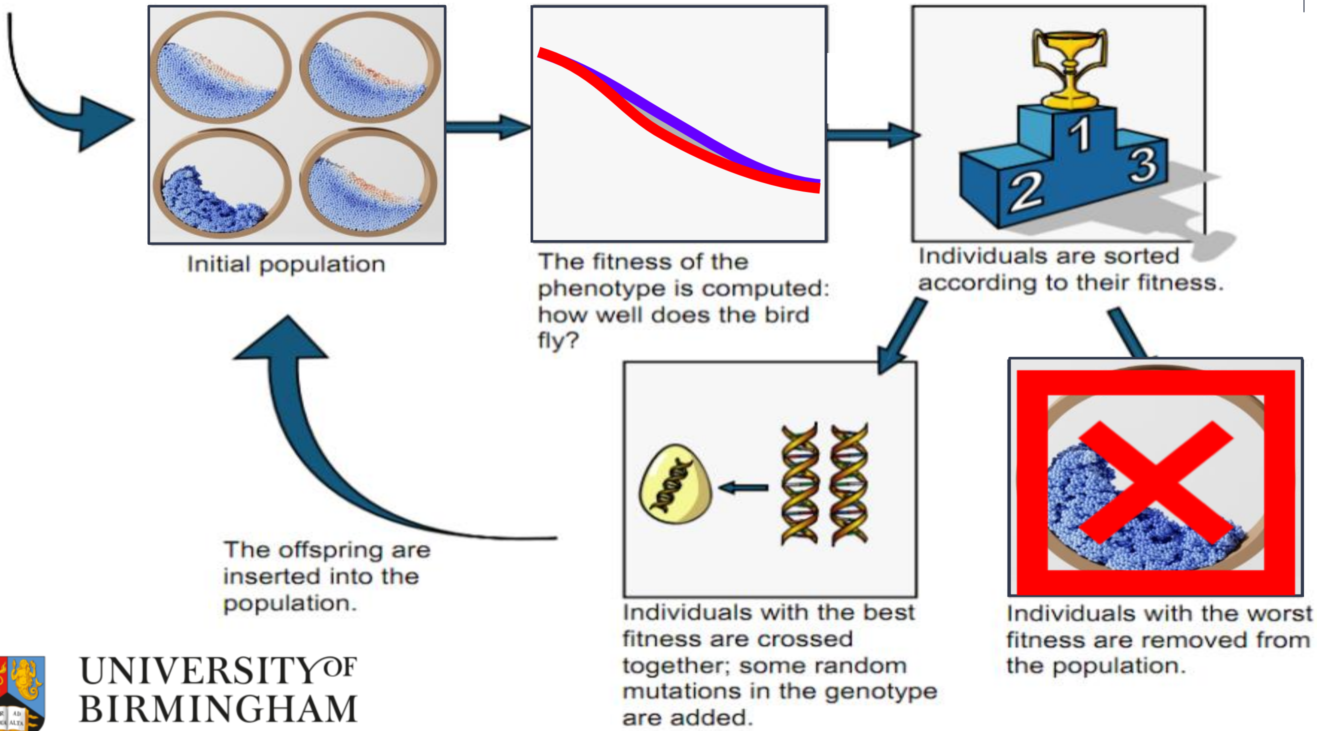
~~Gradient-based optimisers~~
- ~~10s - 100s evaluations~~

~~Neural networks~~
- ~~10,000+ evaluations~~

Evolutionary algorithms
- Used to be 1,000+ evaluations
- State of the art 100s evaluations



Evolutionary Optimisers



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 cost function deforms

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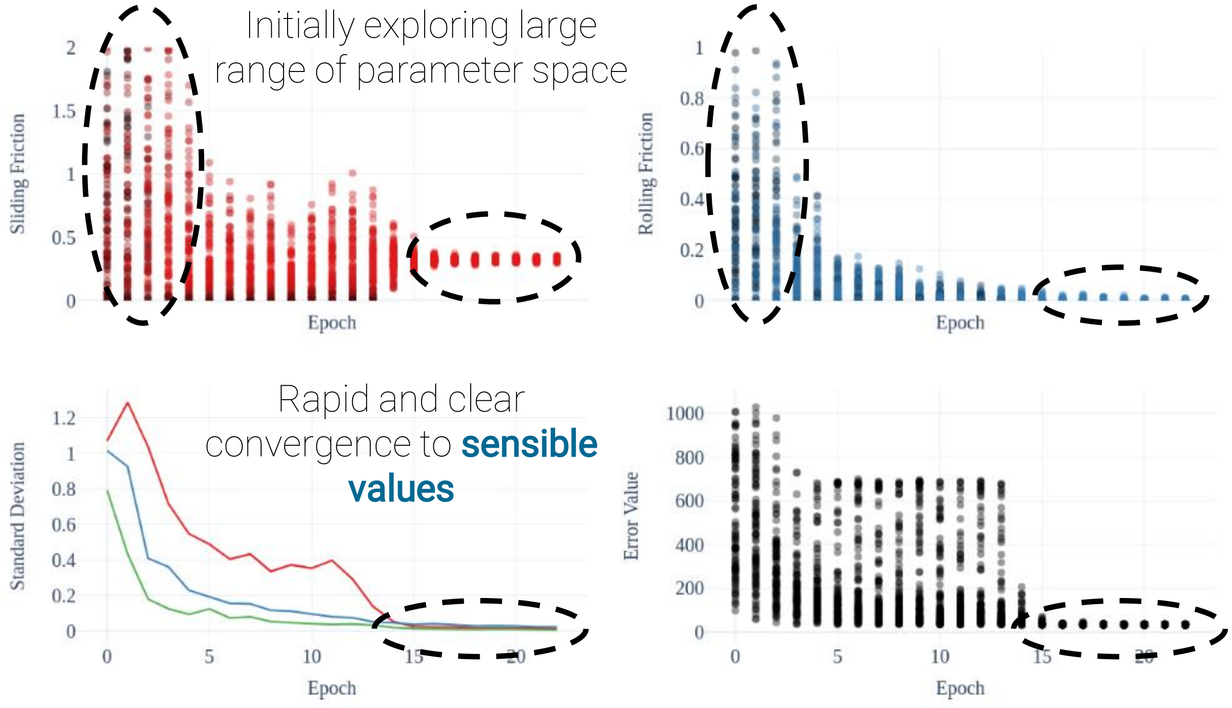
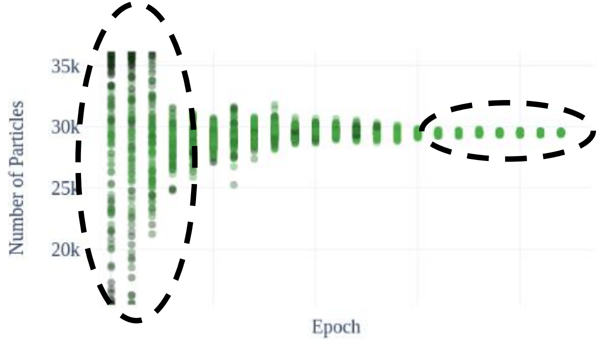
Finding Optimum Parameters

Interactive Example

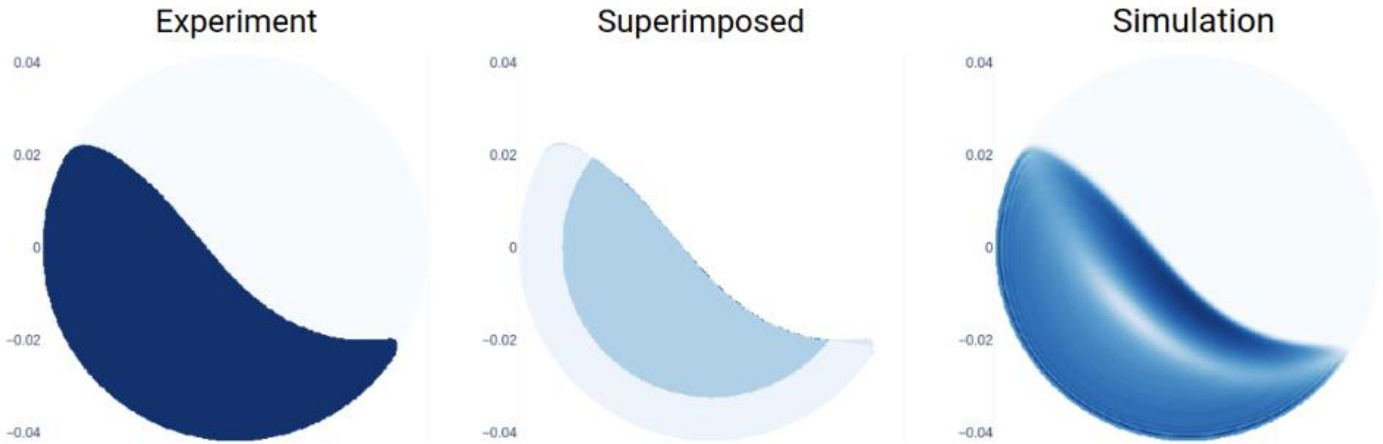




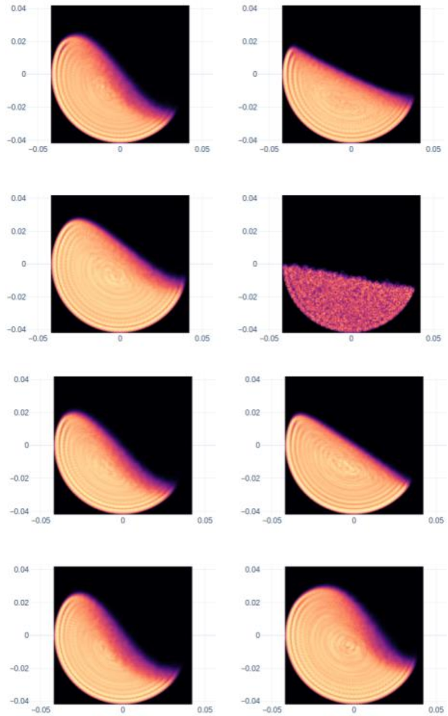
ACCES converges on the parameter values that minimise the error values.
It evolves a family of solutions in epochs (***x***-axis) towards the fittest individuals.

Example ACCES Calibration

Interactive Example



Example States

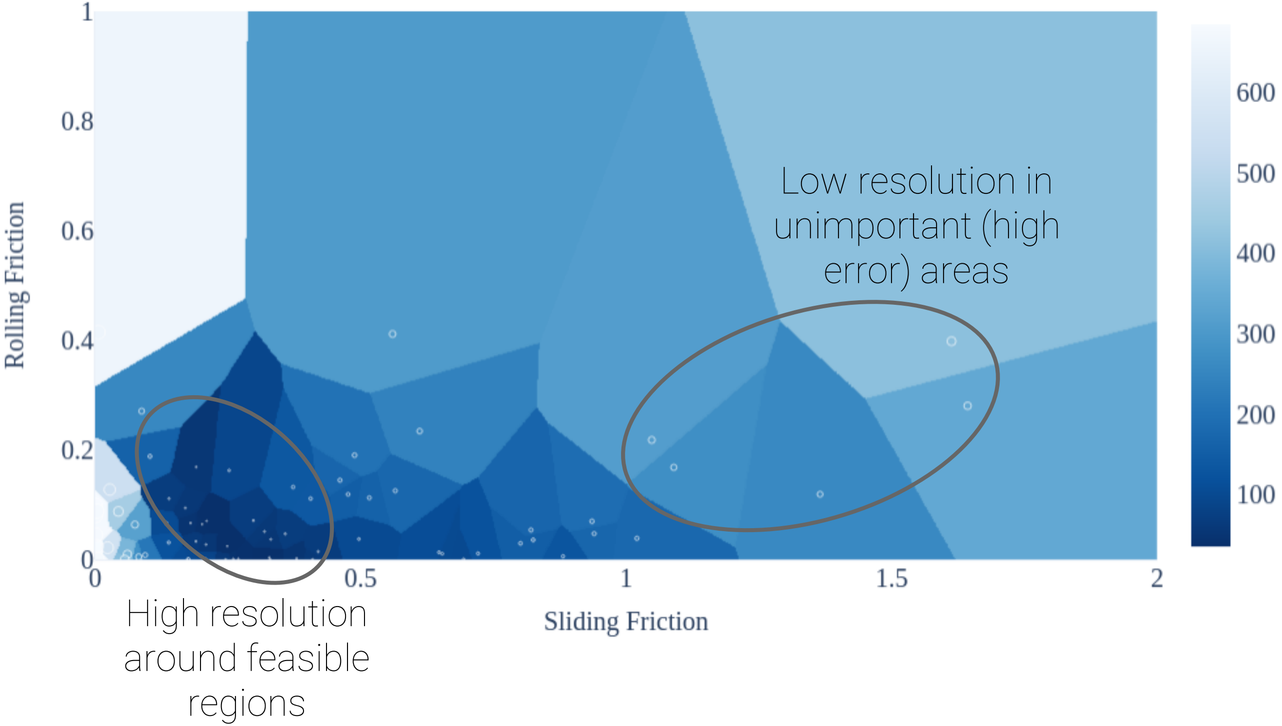


Efficient Parameter Space Exploration

Interactive Example

ACCES can calibrate virtually ***any*** parameters, in arbitrarily high dimensions

It is more precise, yet less computationally expensive than e.g. grid-based calibration



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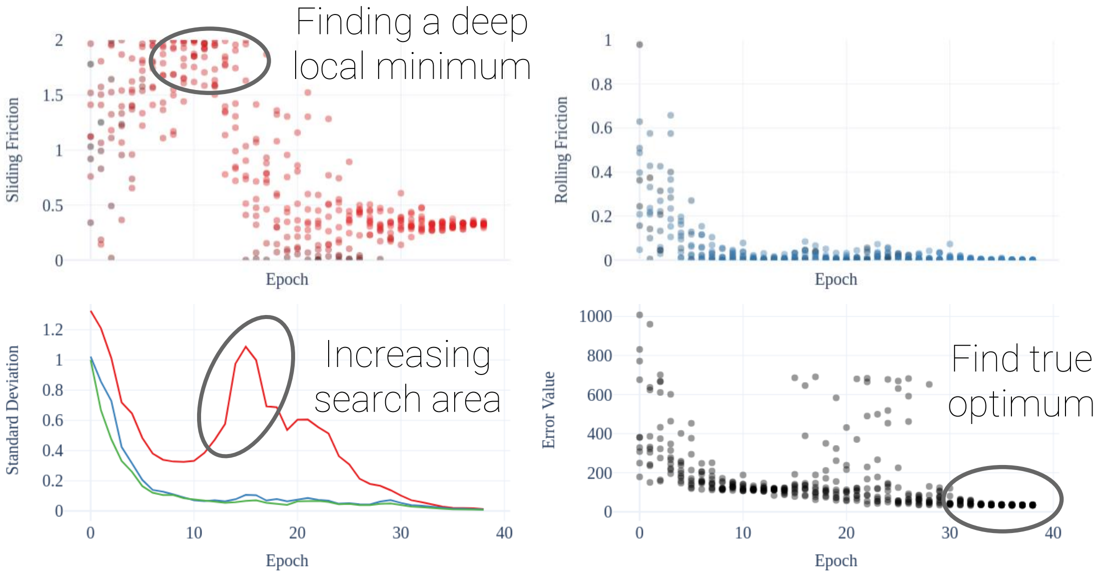
Power of *Scalable* Evolutionary Algorithms

Interactive Example

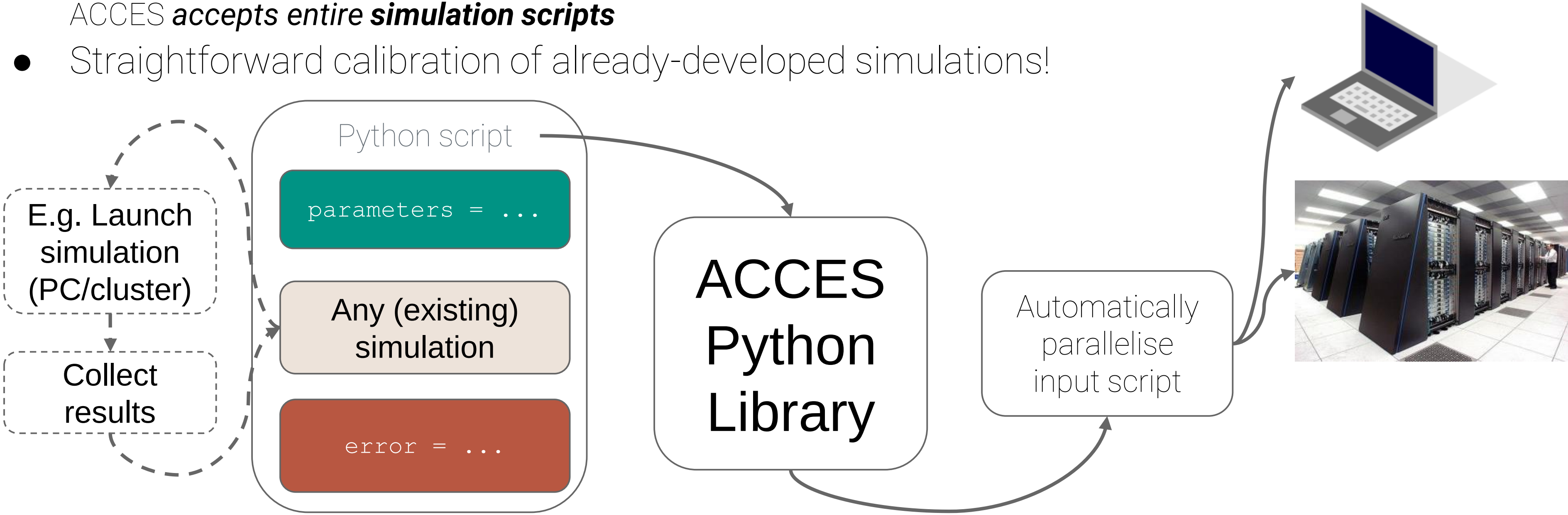
- ACCES robustly handles tough calibration problems
- It can naturally “escape” deep false optimums
- The only free parameter is the family size - the number of simulations run per epoch
- Larger family size - more global search, fewer epochs needed, more parallel computation
- Smaller family size - fewer simulations, more epochs needed



Minimally-Invasive, Scalable Optimisation

Interactive Example

- As opposed to classic optimisation frameworks which need the simulation to be rewritten inside a function, ACCES ***accepts entire simulation scripts***
- Straightforward calibration of already-developed simulations!



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Thank you!

Interactive Example

The ACCES framework would not have been possible without the continuous support and help from a great Birmingham team:

- **Dr. Kit Windows-Yule**, supervisor
- **Andrei Leonard Nicusan**, collaborator & lead ACCES developer
- **Dominik Werner**, collaborator & DEM hero

Interested? Email me at:

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Dr. Kit Windows-Yule

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