ACCES:

Autonomous Characterisation and Calibration via Evolutionary Simulation

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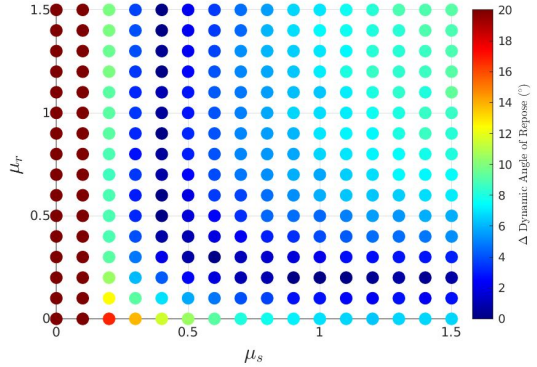
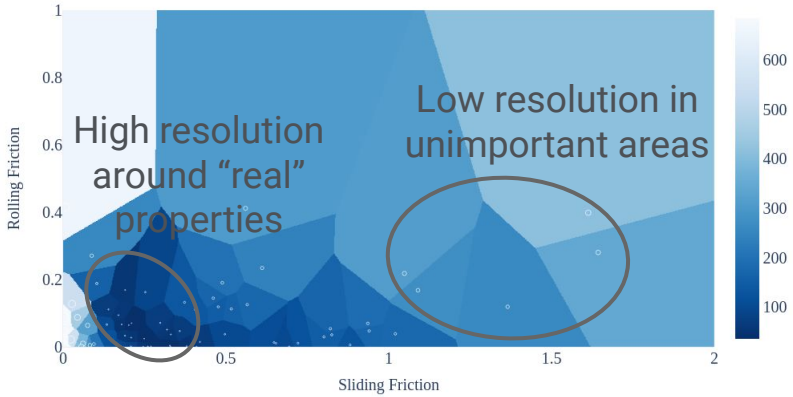
Calibrating Simulations against Experiments

Micro-macro mapping problem: what microscopic parameters do I need to match a macroscopic measurement?

- Manual calibration is tedious and error-prone
- Grid-based calibration is expensive and limited

ACCES autonomously learns the physical properties of a simulated system that reproduce an experiment, as efficiently as possible!





Modelling Calibration as an Optimisation Problem

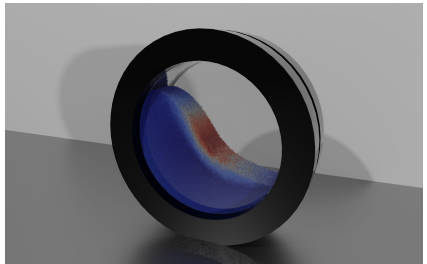
Vary

< Optimiser >

Minimise

Free parameters → Simulation → “Difference to Reality”

Discrete Element Method Simulation
e.g. GranuDrum

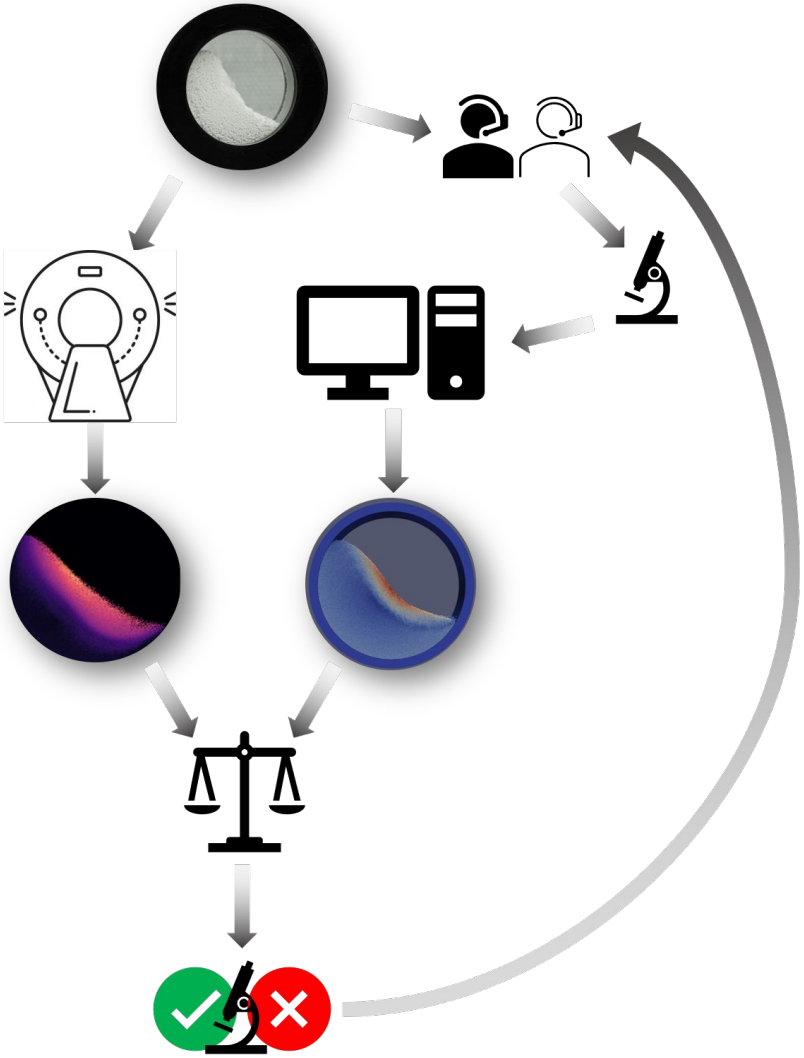


Friction, Restitution, Cohesive Energy Density, etc.

Velocity Distribution, Free Surface Shape, Residence Time, etc.

Conventional Calibration against an Experiment

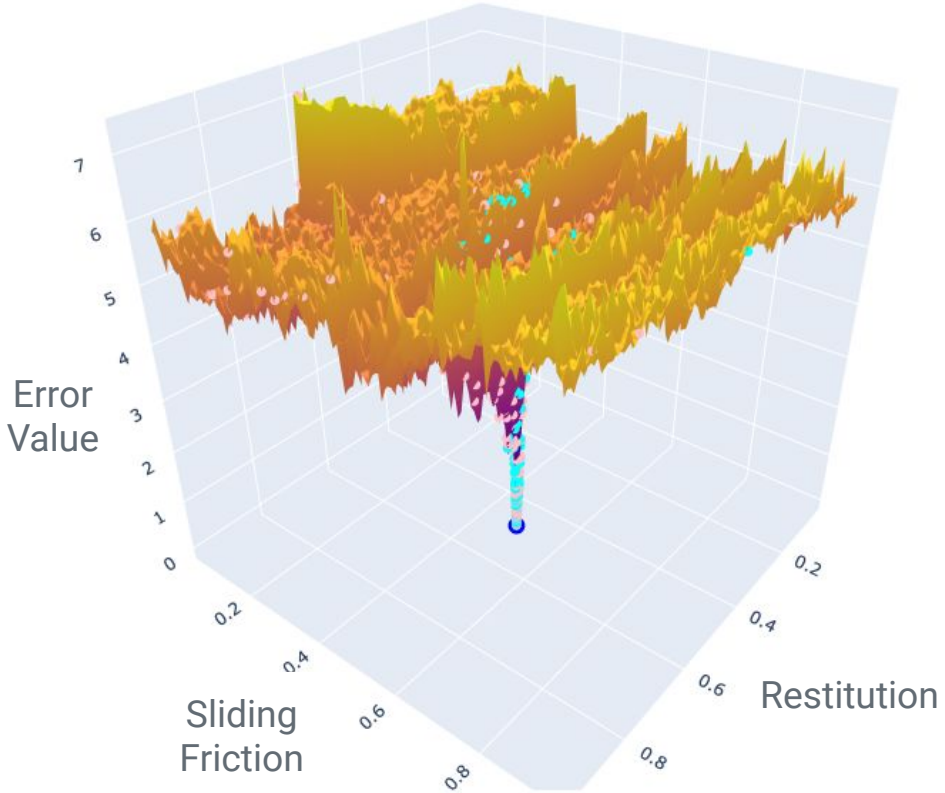
“Difference to reality”



So what does the “difference to reality” look like?

Awful.

- Noisy, non-smooth
- Many local minima, false optimums



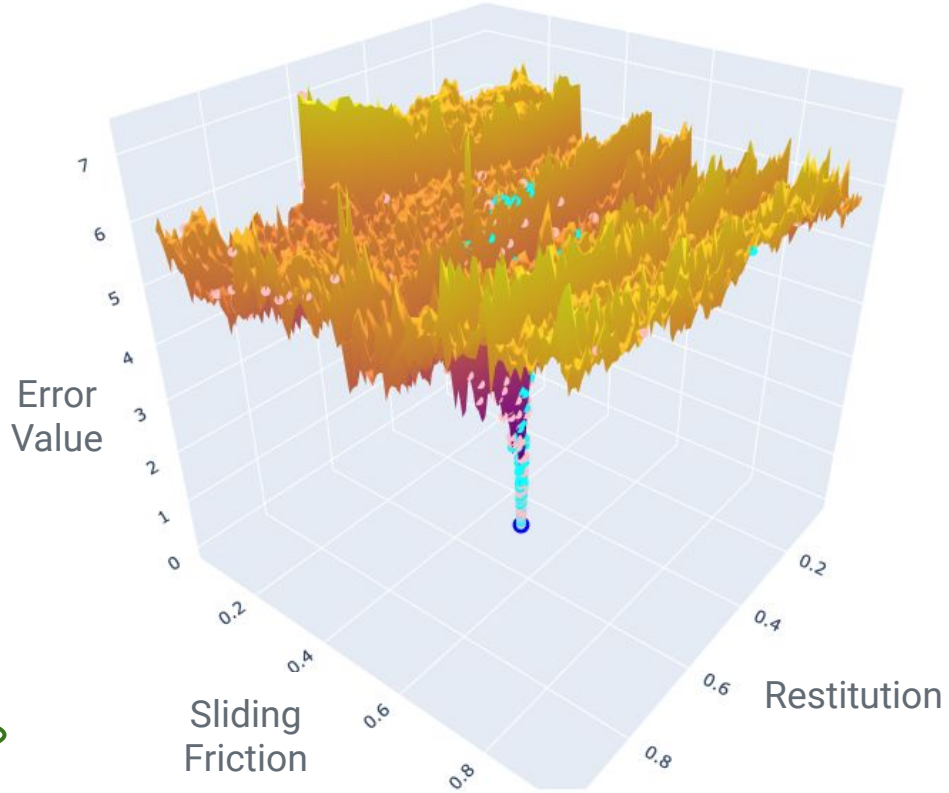
What can optimise that?! Efficiently too, please

Every function evaluation is an entire simulation run

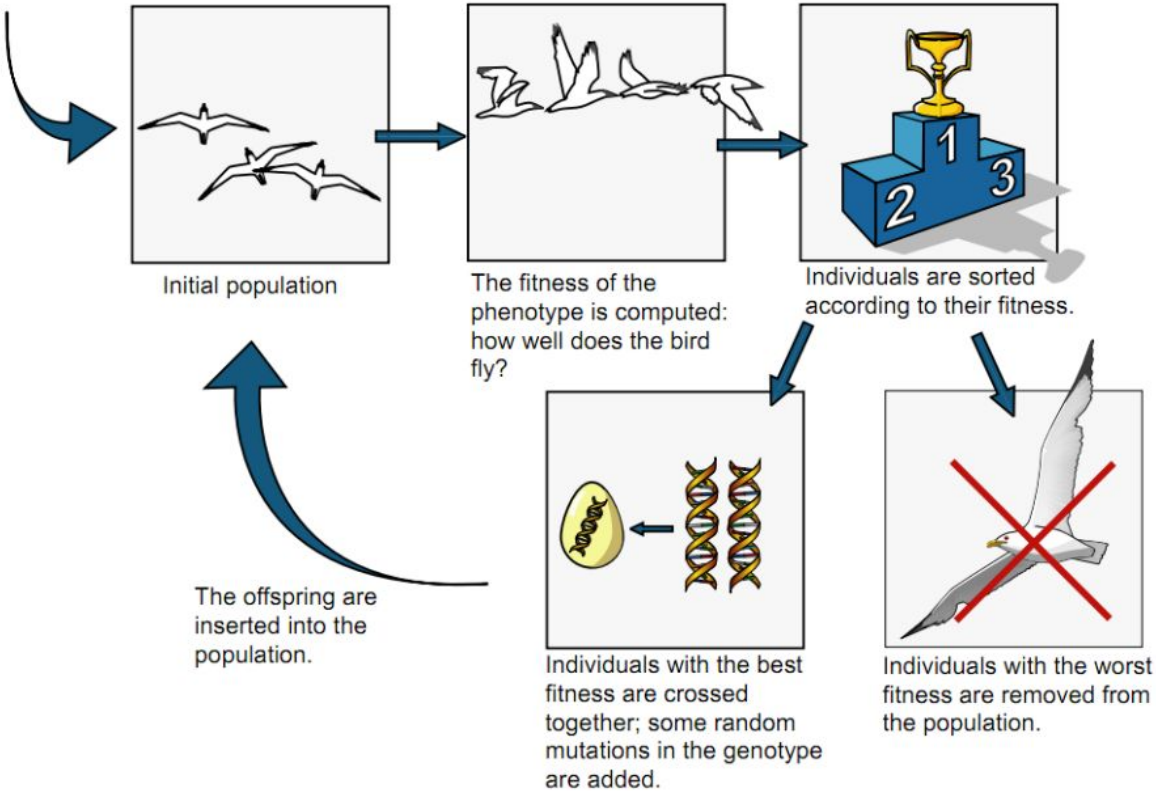
~~Gradient-based optimisers~~
- 10s - 100s evaluations

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

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

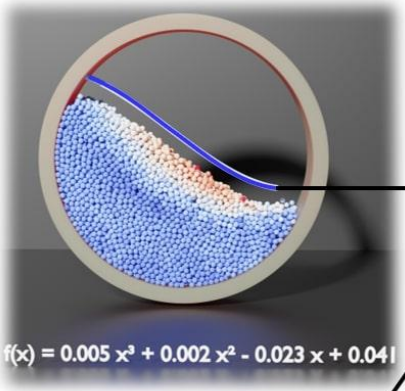


Evolutionary Optimisers

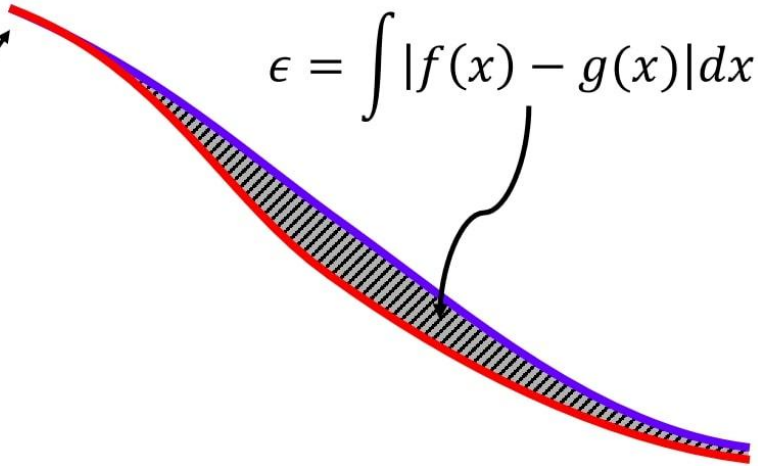


- CMA-ES consistently succeeds in global, gradient-free benchmarks [1]
- Uses among the fewest function evaluations, ~ 100 per parameter

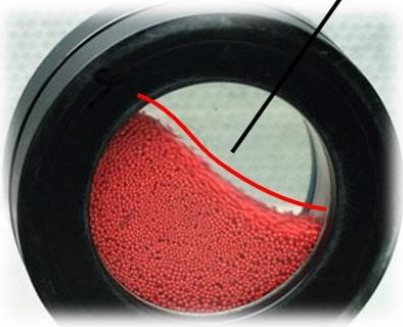
Characterising DEM Particles



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

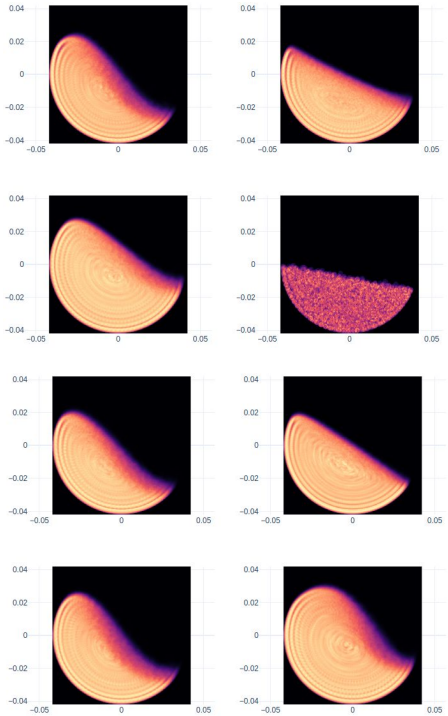


$$\epsilon = \int |f(x) - g(x)| dx$$

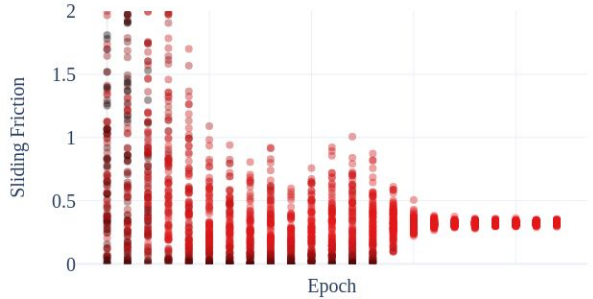


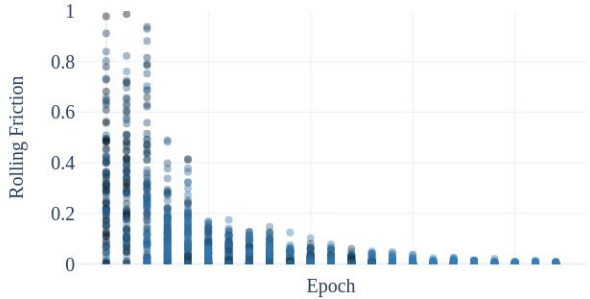
The model was effectively calibrated against a single experimental data point, but was able to **reproduce other uncalibrated properties** such as velocity vector fields.

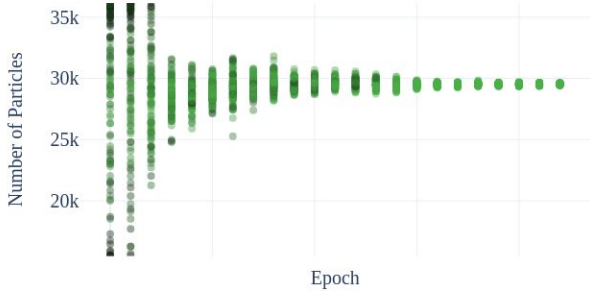
Single Epoch

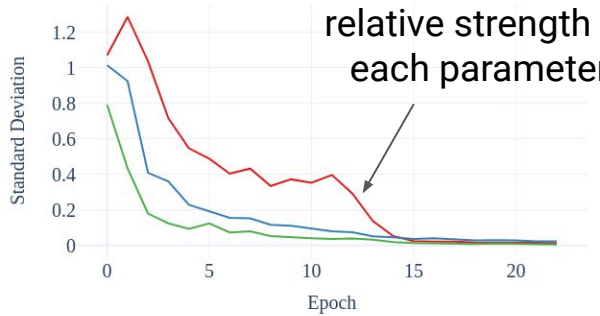


Finding Optimum Parameters

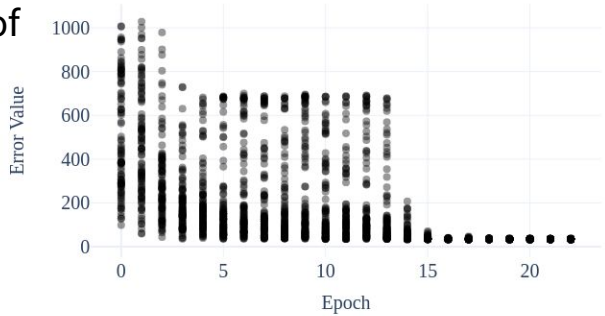








A measure of the relative strength of each parameter

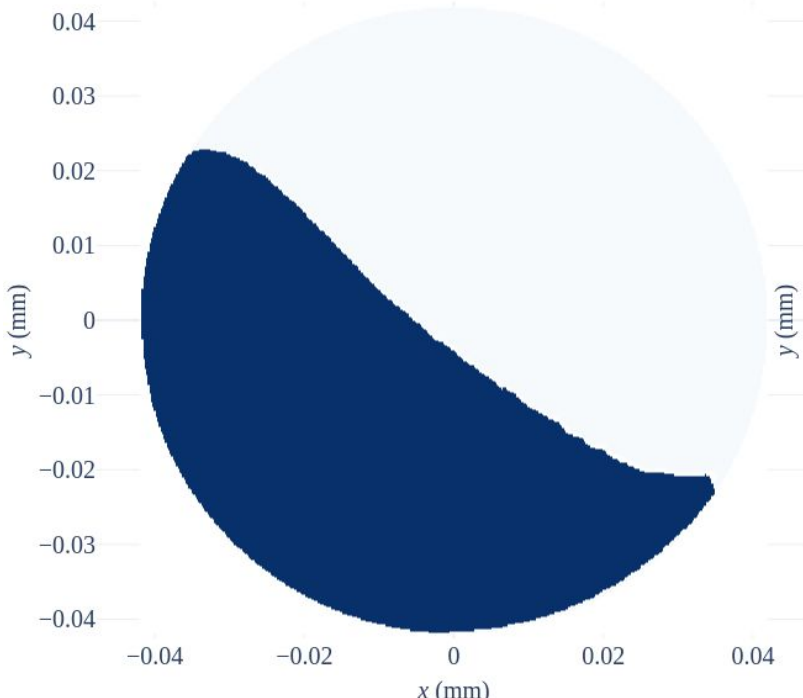


ACCES converges on the parameter values that minimise the error values.

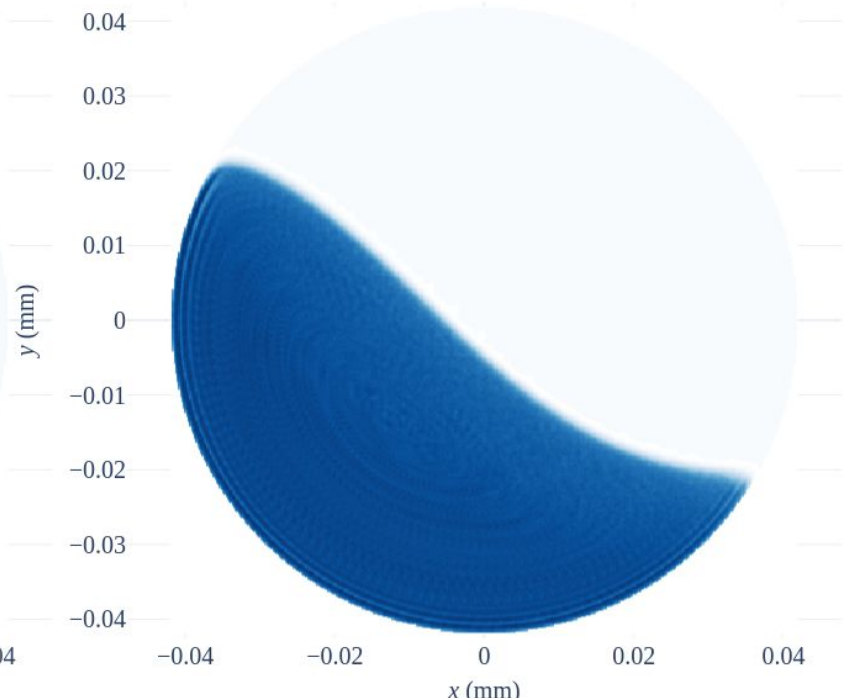
It evolves a family of solutions in epochs (*x*-axis) towards the fittest individuals.

Calibrated Simulation

Experimental Photo

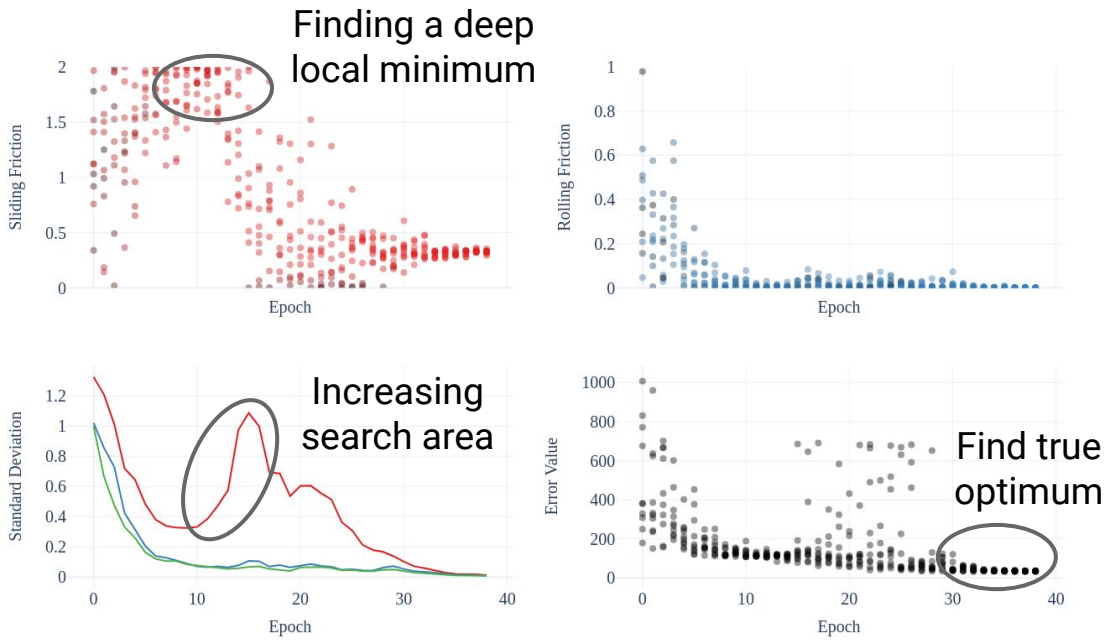


Calibrated Simulation



Power of (Scalable) Evolutionary Algorithms

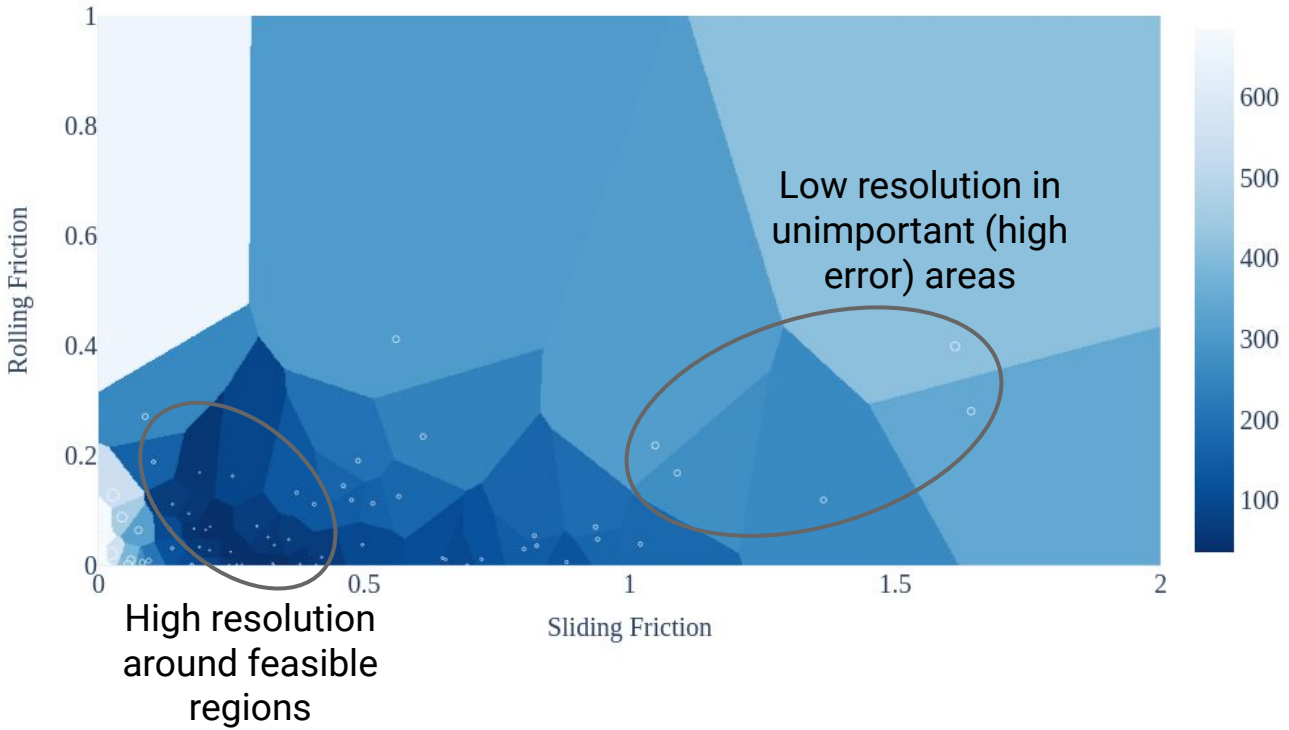
- ACCES robustly handles tough calibration problems
- It can naturally “escape” deep false optimums
- The only free parameter is the family size - the number of simulations run per epoch
- Larger family size - more global search, fewer epochs needed, more parallel computation
- Smaller family size -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



Efficient Parameter Space Exploration

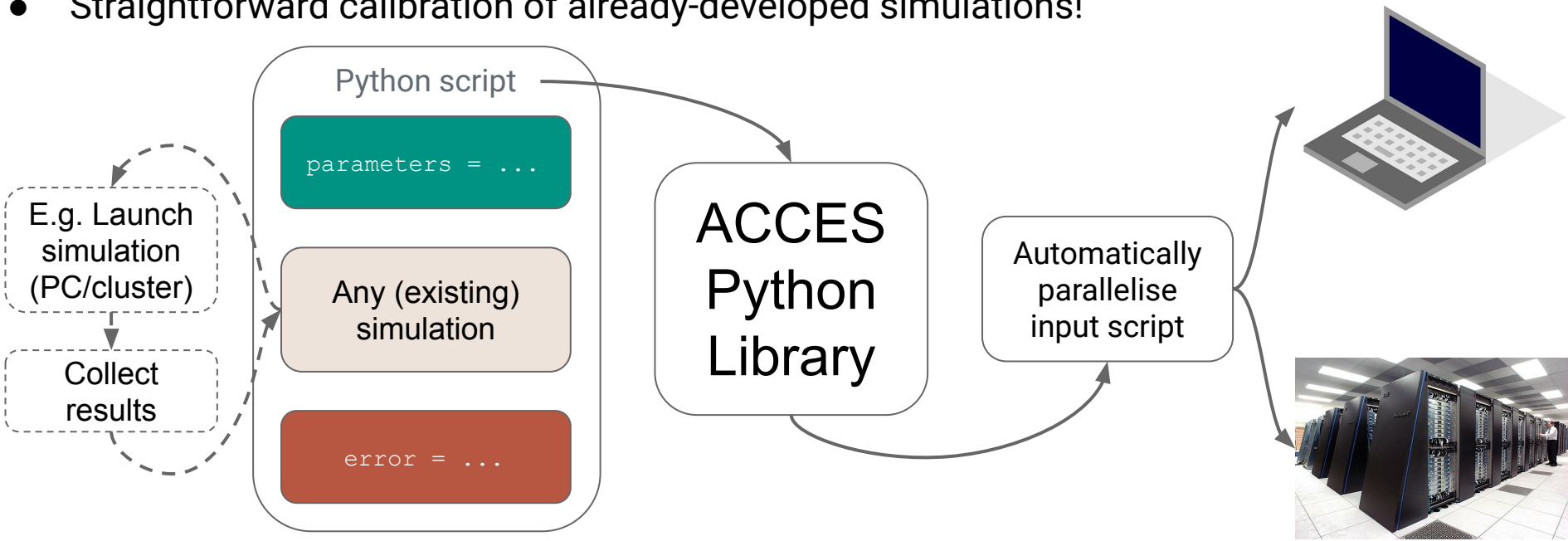
ACCES can calibrate virtually *any* parameters, in arbitrarily high dimensions

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



Minimally-Invasive, Scalable Optimisation

- 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!



Thank you!

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

- Dr. Kit Windows-Yule, supervisor
- Dominik Werner, collaborator & DEM hero
- Jack Sykes
- Matthew Herald
- Owen Jones-Salkey