

What do we do?

"The Angry Penguin", used under creative commons licence from Swantje Hess and Jannis Pohlmann.



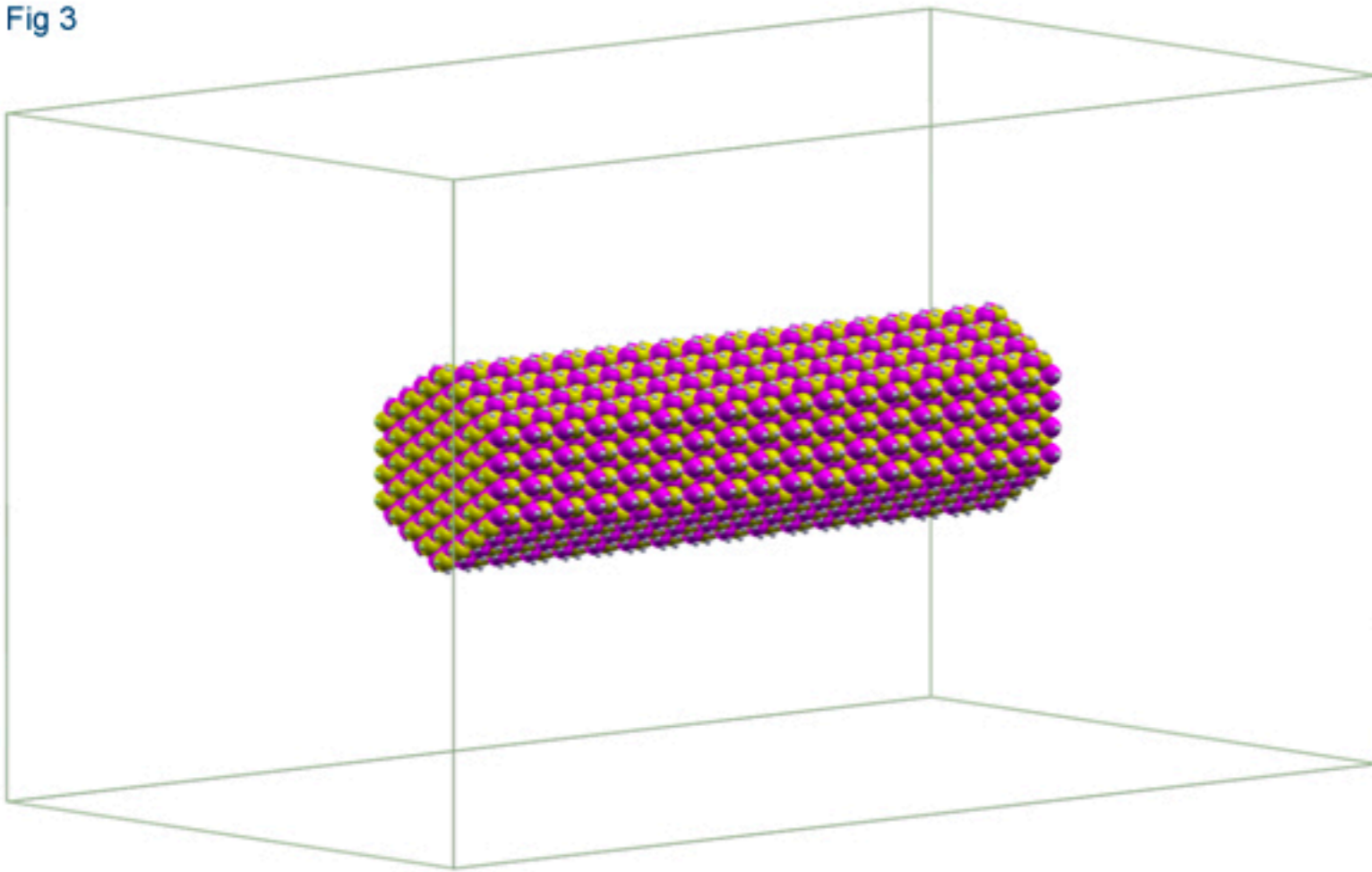
Warwick RSE

Who Are We?

- Chris Brady, Pip Grylls, Heather Ratcliffe
- CB - previously laser plasma physicist, sysadmin, contract programmer
- PG - previously astrophysics (already an RSE when arrived at Warwick)
- HR - previously astrophysics/solar physics
- Collectively
 - Physics and HPC backgrounds
 - Scientific C/C++/Fortran/Python developers
 - Data analysis/reduction

ONETEP

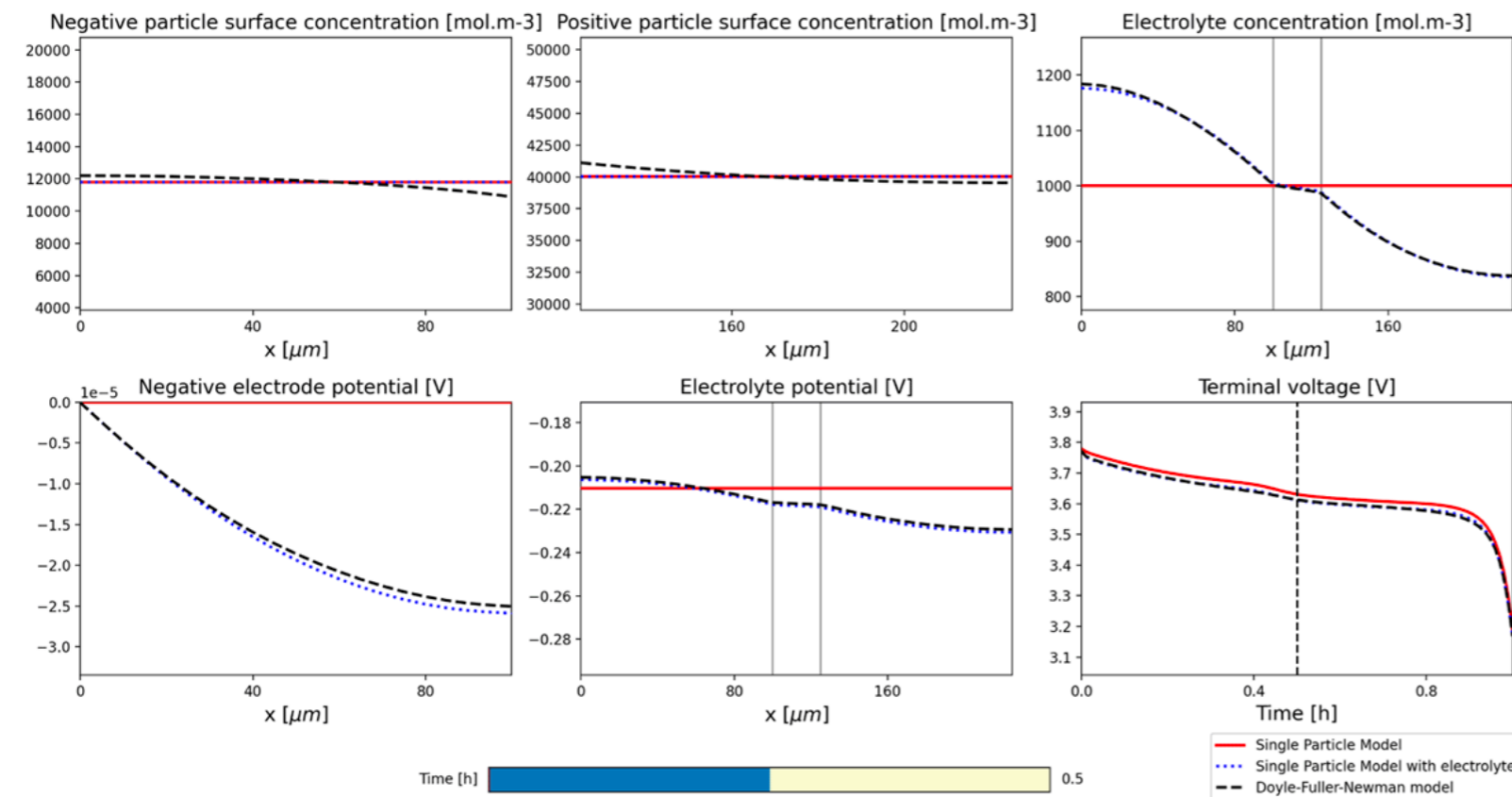
Fig 3



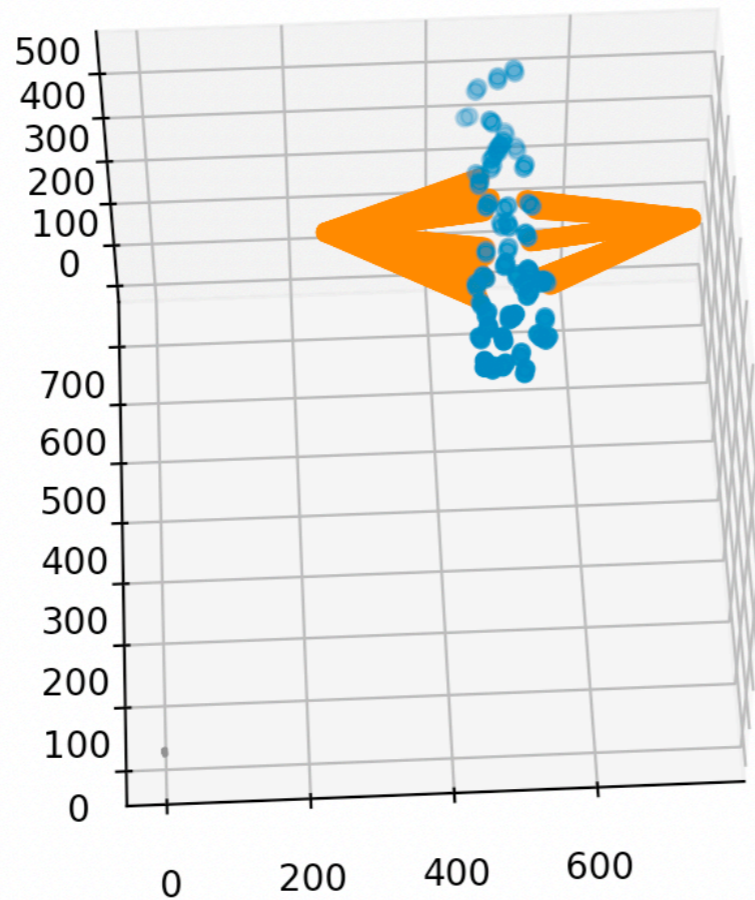
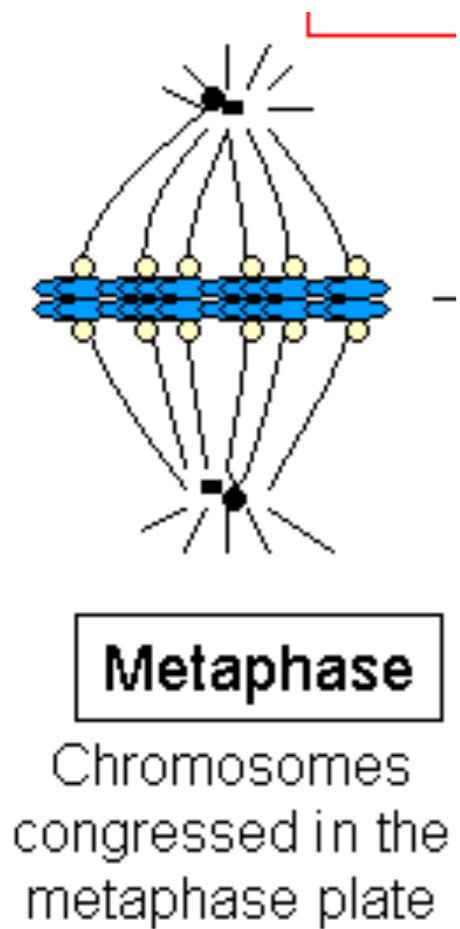
- Linear scaling density functional theory
- In parallel has sections that work by negotiating with other processors for data
- Switch to MPI one sided

pybamm-param

- Additional package for PyBaMM battery simulation tool
- Parameter optimization framework
- Architectural, design and management work (mainly)



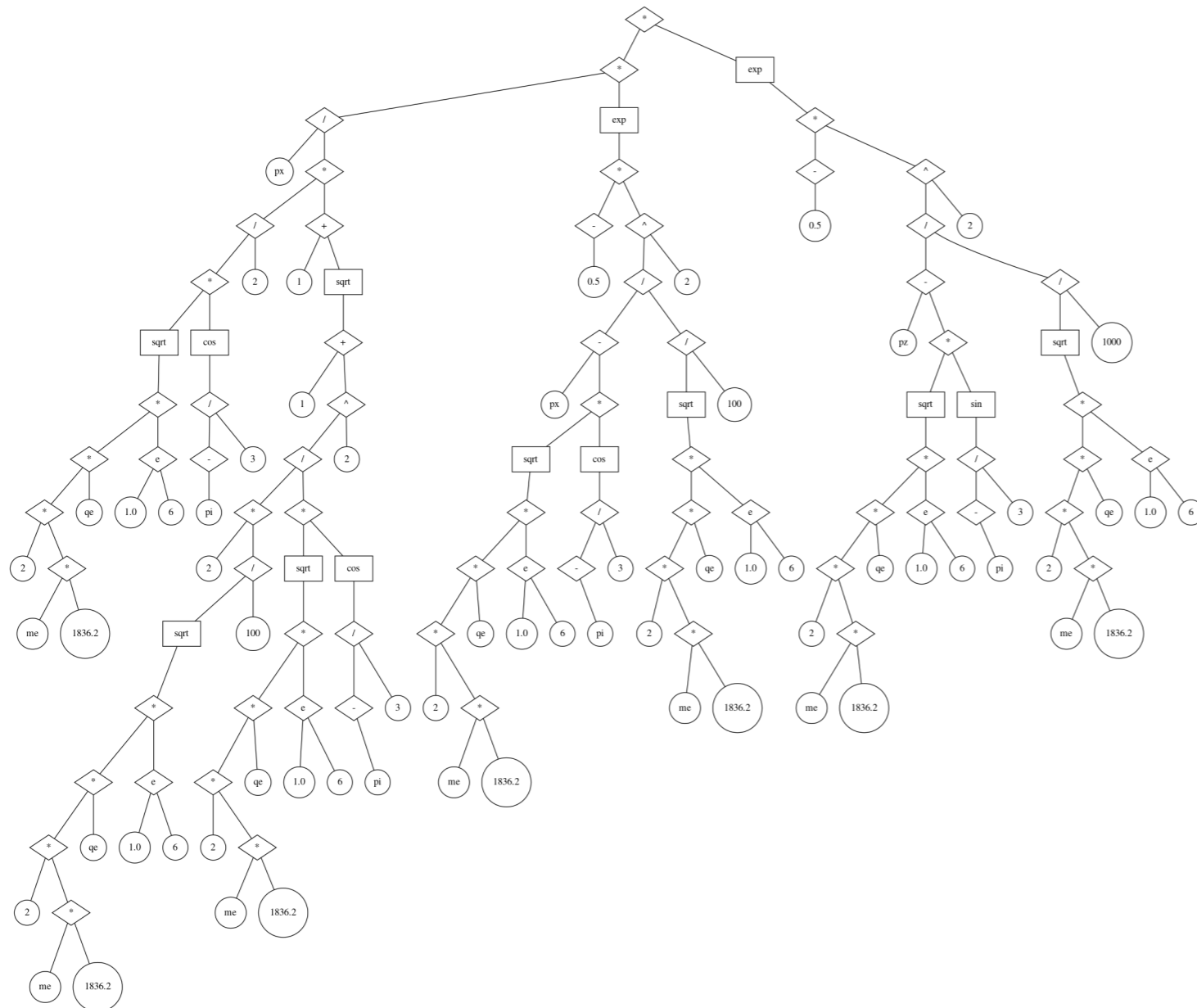
Metaphase Simulation



- Scratch written MD(ish) simulation of the metaphase of mitosis
- Not a good fit to off the shelf MD packages (because of the ish)
- Complete new C++ code

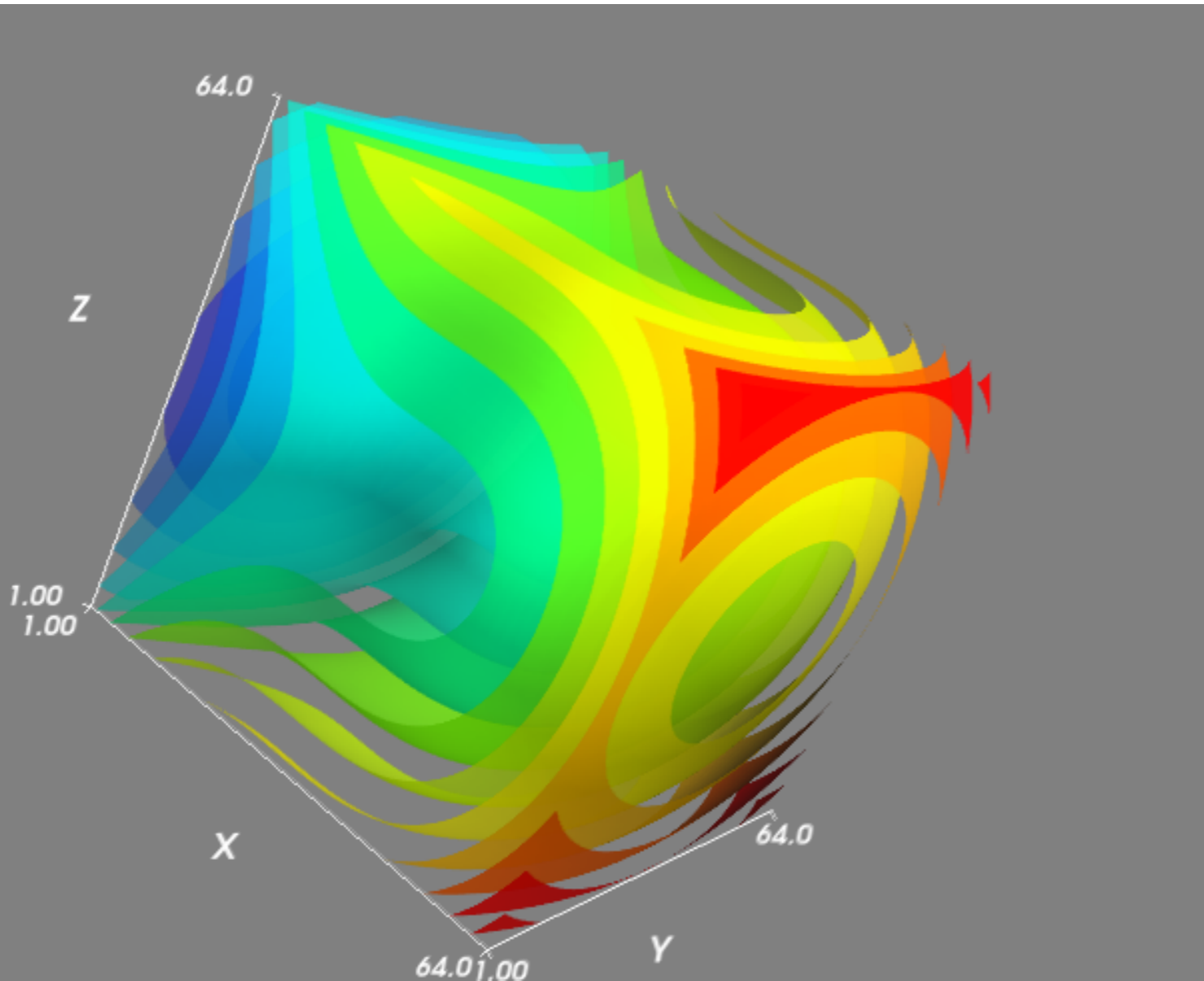
EPOCH

EPOCH



- We applied for ARCHER eCSE funding
- Improved data structures
- Enhanced maths expression parser
- <https://github.com/csbrady-warwick/EIS-2>

PX913



- PX913 -
“Introduction to scientific software development”
- Taught as part of Heterogeneous Systems DTC this year about 30% of attendees are not Hetsys

Training

- Various generally available training courses
 - Accelerating Python, Introduction to Software Engineering
 - HPC For Data Science
 - Advanced topics in MPI
 - Everything in between
- Delivered out of term time
 - 1-2 sessions in Easter and Christmas Breaks and at end of Summer holiday

Other things

- General support through bugzilla, by email and in person
- Weekly drop-in sessions
- [https://warwick.ac.uk/research/rtp/sc/
user_support/research-computing-drop-in/](https://warwick.ac.uk/research/rtp/sc/user_support/research-computing-drop-in/)
- Members of national and international committees on “things”