PAX: Modelling Particles at Exascale

ExCALIBUR to DRI

CIUK 2025

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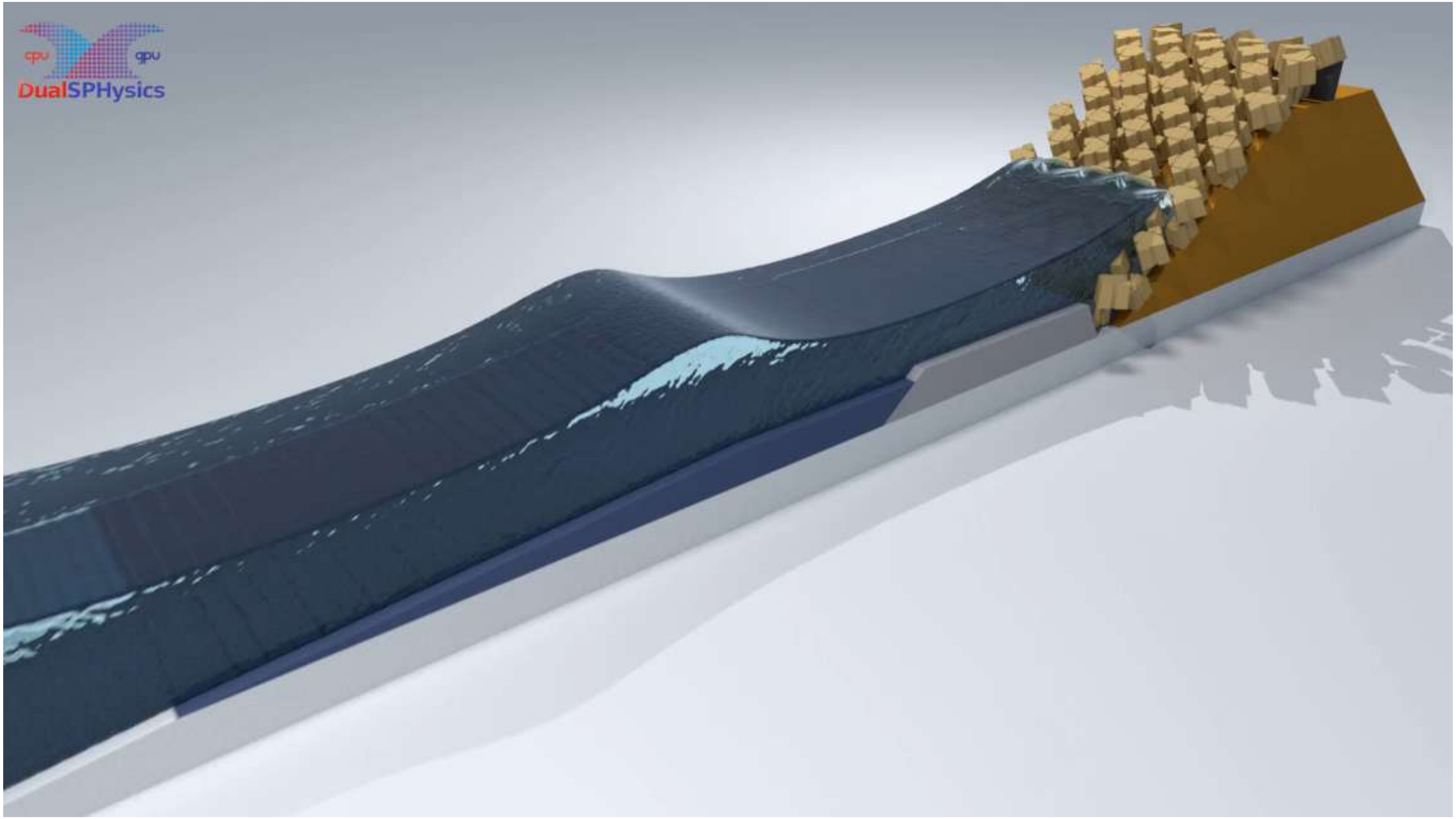
Particles At Exascale

- Aim: Deliver high-performance software for particle-based simulation methods.

- Particle based?
  - Engineering
  - Astrophysics

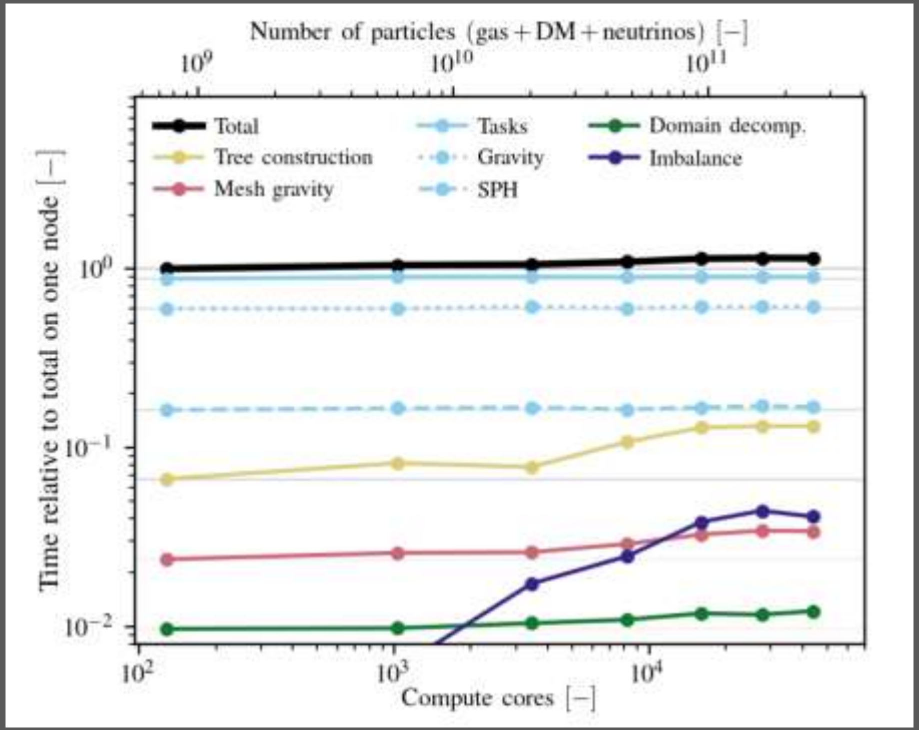
    Smoothed Particle Hydrodynamics
  - Nano-scale material design – Quantum Mechanics


cpu
gpu
DualSPHysics

Task-parallel → **Extremely scalable**

Schaller et al. (2024)
Weak scaling up to 50k threads!

Jacob Kegerreis
2022

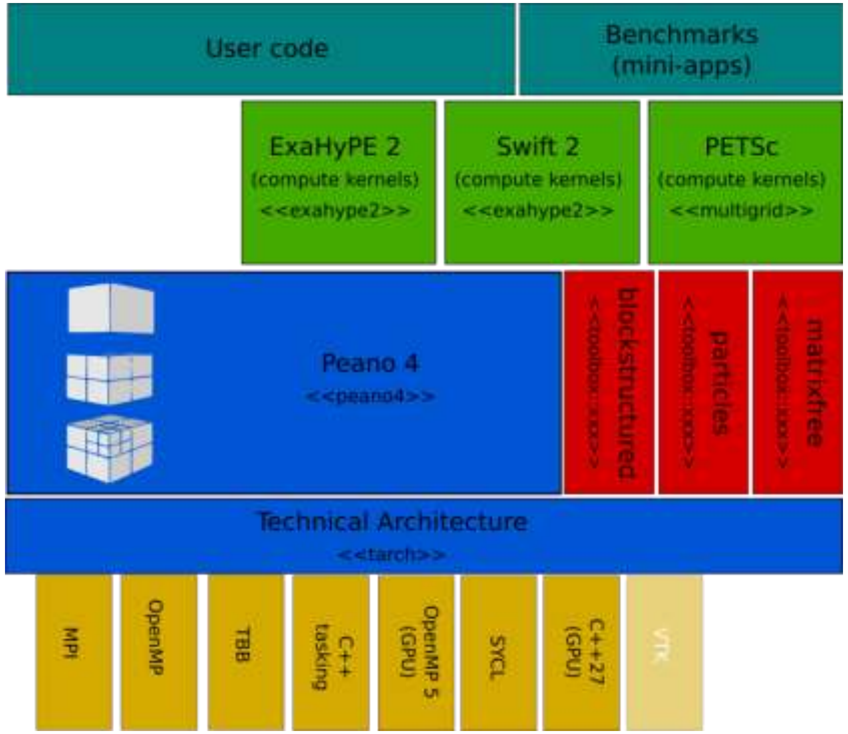


- SWIFT is established as one of the most scalable CPU solvers for Astrophysics
- Can simulate planetary collisions, and give us a much better understanding of our universe
- SWIFT has literally been used to create digital twins, of the universe! (EAGLE & FLAMINGO models)
- Only 10-15% loss of efficiency on COSMA8

SWIFT 2: Towards Exascale Smoothed Particle Hydrodynamics with Task Parallelism and the Peano4 Framework Engine

Peano4 provides parallelisation, domain decomposition, optimization

Exchanges underlying engine of SWIFT
(http://www.peano-framework.org)


User code
Benchmarks (mini-apps)
ExaHyPE 2 (compute kernels) <<exahype2>>
Swift 2 (compute kernels) <<exahype2>>
PETSc (compute kernels) <<multigrid>>
Peano 4 <<peano4>>
blockstructured <<toolbox::xxx>>
particles <<toolbox::xxx>>
matrixfree <<toolbox::xxx>>
Technical Architecture <<tarch>>
MPI
OpenMP
TBB
C++ tasking
OpenMP 5 (GPU)
SYCL
C++27 (GPU)
VTK

PAX Successes:

- Exploit task parallelism performance benefits
- Leave the hard part (software complexity, task dependency graphs, data layout, synchronisation) to compiler
- Separation of concerns: Clean split between physics, parallelisation, memory layout…

Quantum Mechanics with CASTEP

CASTEP

Materials Modelling

Predict material properties, e.g. hardness, colour, interactions

Superconductors, drugs, jet fuel, jelly… etc.

Quantum Mechanics is hard

Lots of interdependence - data and operations

Challenging to parallelise well

Widely used

2000 academic research groups worldwide.

Over 500 industrial sites, including Sony, Toyota, Pfizer, Astra Zeneca.

We Need Good Vibes

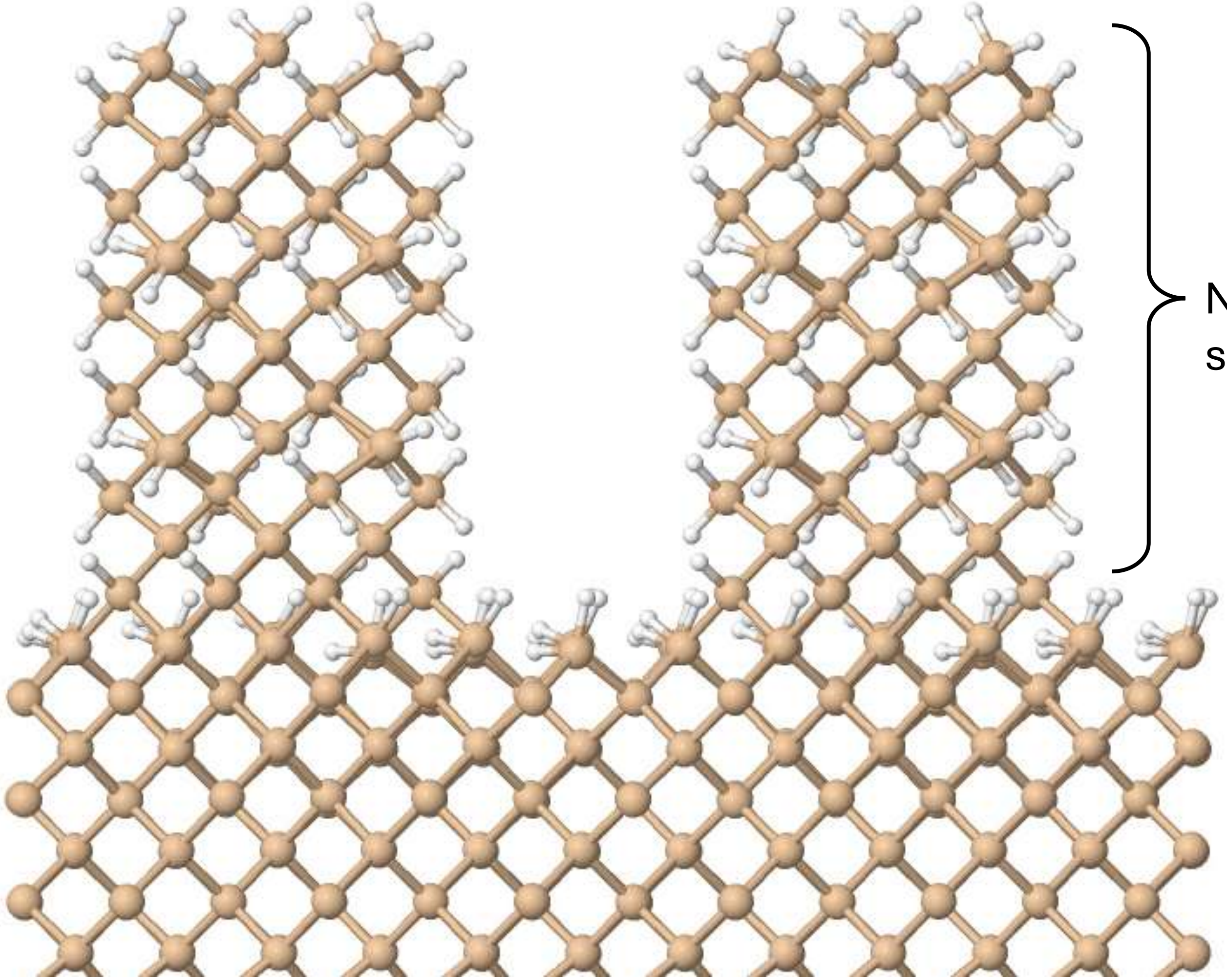
➔ Thermoelectric materials convert heat into electricity

  ➔ Many uses

  ➔ Too inefficient

Vibrations carry heat: Bad!

Tune the vibrations!



Nano-structures

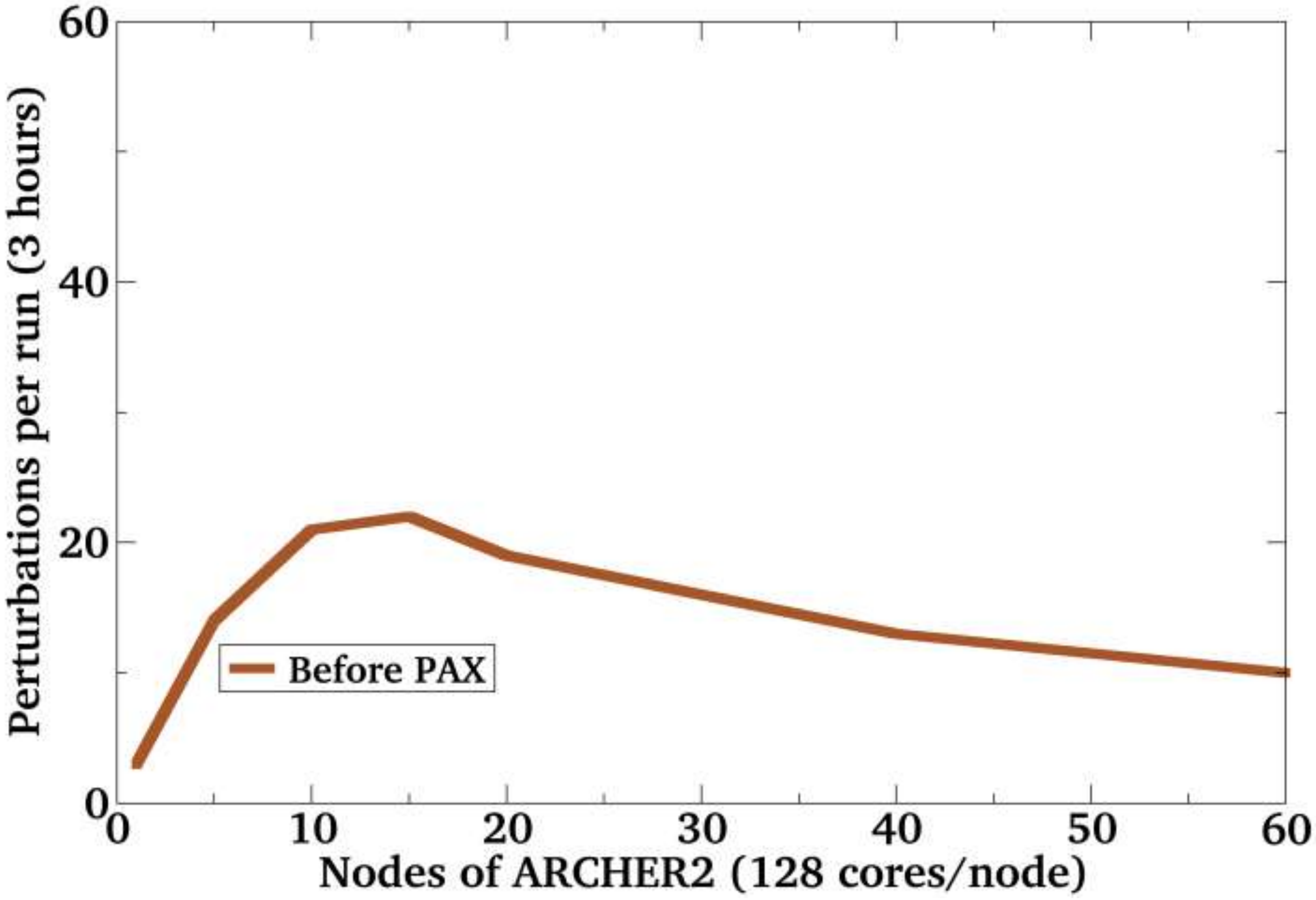
Membrane

Before PAX – Bad vibes

- Need to understand how design affects the vibrations.

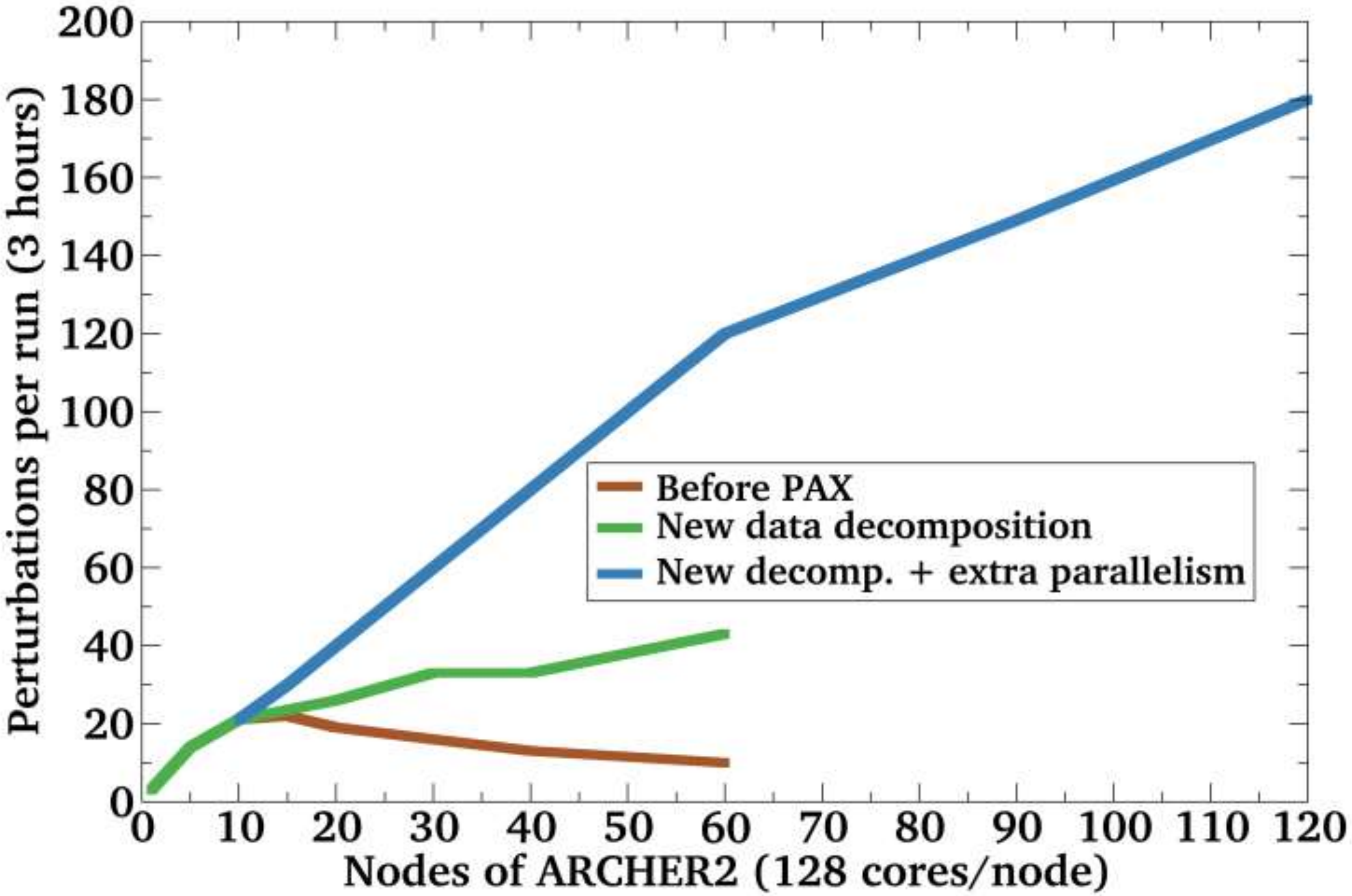
- Best performance:
  - 16 Nodes
  - 4 days / per structure

- Optimising design:
  - Impractically slow



After PAX – Better Vibes

- Reworked Parallelisation
  - New data decomposition
  - Task based parallelism
- Best performance:
  - 120(+?) Nodes
  - 10 hours / per structure
- Optimising design:
  - More practical



Improvements now available to all CASTEP users!

Acknowledgements

- Everyone involved in PAX, particularly:
  - Mladen Ivkovic and Abouzied Nasar for providing slides on SWIFT.
  - Matt Smith, CASTEP parallel decomposition.
  - Tobias Weinzierl, Benedict Rogers, George Fourtakis and Phil Hasnip
  - Scott Woodley (PI for PAX project)

Thank you for your attention!