The POP Centre of Excellence

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EU H2020 Centre of Excellence (CoE)

1 October 2015 – 31 March 2018

Grant Agreement No 676553

The POP Centre of Excellence

- A Centre of Excellence
  - In **P**erformance **O**ptimisation and **P**roductivity
  - Collaborative European project funded by the EU's Horizon 2020 programme
  - Ran October 2015 – March 2018
  - Will run November 2018 – October 2021 (dates awaiting confirmation)
- Providing **Free** Services within Europe
  - For academic and industrial codes and users
  - Precise understanding of **parallel** application and system behaviour
  - Across application areas, platforms and scales
  - Suggestions/support on how to rewrite code in the most productive way

The POP Team

- The POP Partners
  - Barcelona Supercomputing Center, Spain (coordinator)
  - NAG, UK
  - HLRS, Germany
  - Jülich Supercomputing Centre, Germany
  - RWTH Aachen IT Center, Germany
  - TERATEC, France
  - Versailles Saint-Quentin-en-Yvelines University, France
  - IT4Innovations National Supercomputing Center, Czech Republic
- A team with
  - Expertise in performance analysis and optimisation, along with parallel programming models and practices
  - A research and development background and a proven commitment to real academic and industrial use cases.

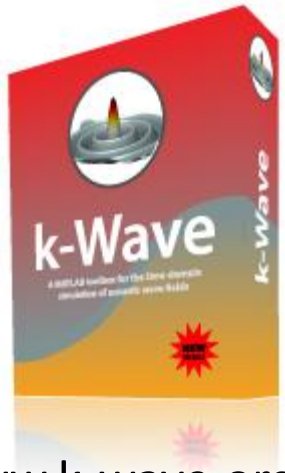
POP Tools

- A number of profiling tools are developed by POP partners
  - BSC Tools – Extrae and Paraver
  - Scalasca
- Further development of these tools will take place as part of POP, with a view to improving usability.
- The POP website is a good source of documentation on these and other useful performance tools
  - https://pop-coe.eu/further-information/learning-material

POP Services

- Performance Assessment ⇨ Report
  - Identifies any performance issues in the customer's code
  - Determines the root causes of these issues and recommends fixes
  - Typically 2 person months effort
- Proof-of-Concept ⇨ Report and Software Demonstrator
  - A follow-up to the performance assessment
  - Implements one or more of the recommendations and assesses the resulting improvement in performance
  - Up to 6 person months effort, typically 3-4 months

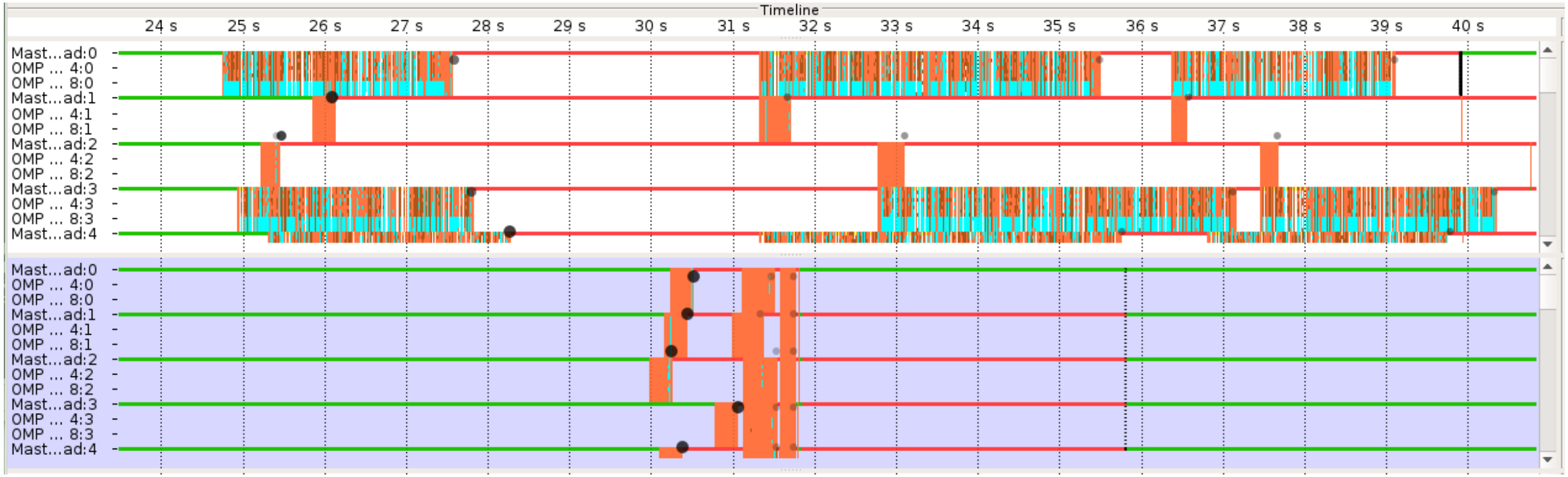
k-Wave – Brno Uni. of Technology



www.k-wave.org

- Toolbox for time domain acoustic and ultrasound simulations in complex and tissue-realistic media
- C++ code parallelised with Hybrid MPI and OpenMP (+ CUDA)
- Profiling showed that
  - 3D domain decomposition suffered from major load imbalance: exterior MPI processes, with fewer grid cells, took much longer than interior
  - OpenMP-parallelised FFTs were much less efficient for grid sizes of exterior, requiring many more small and poorly-balanced parallel loops
- Using a periodic domain with identical halo zones for each MPI rank reduced the overall runtime by a factor of 2.

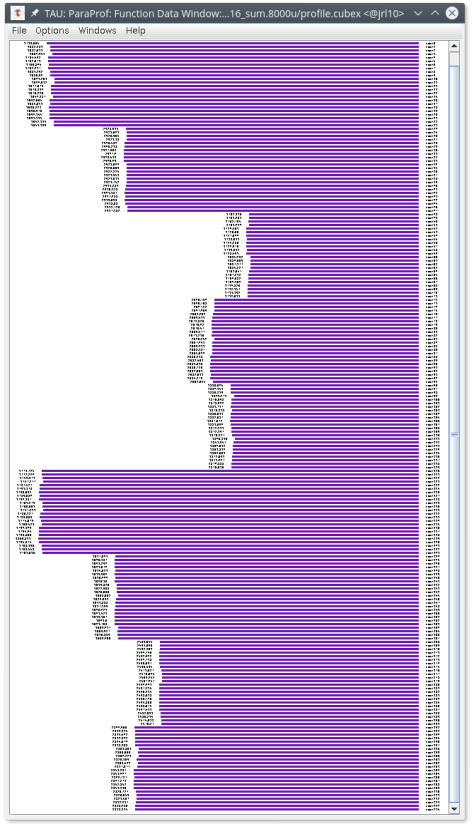
k-Wave – Brno Uni. of Technology



- Comparison time-line before (top) and after (bottom) balancing, showing exterior MPI ranks (0,3) and interior MPI ranks (1,2)
  - MPI synchronization in red; OpenMP synchronization in cyan

EPW – University of Oxford

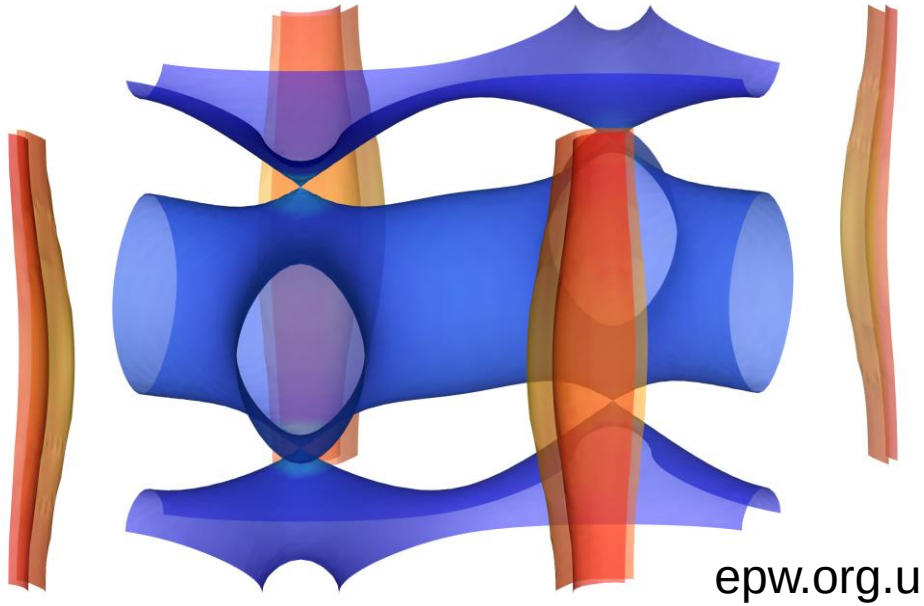
- Electron-Phonon Wannier (EPW) materials science DFT code; part of the Quantum ESPRESSO suite
- Fortran code parallelised with MPI
- Profiling showed
  - Poor load balance
  - Large variations in runtime, likely caused by I/O
  - Final stage spends a great deal of time writing output to disk



EPW – University of Oxford

- Original code had all MPI processes writing result to disk at the end.
- This was modified this so that only one process wrote the output.
- On 480 MPI processes, time taken to write results fell from over 7 hours to just 56 seconds: a 450-fold speed-up!

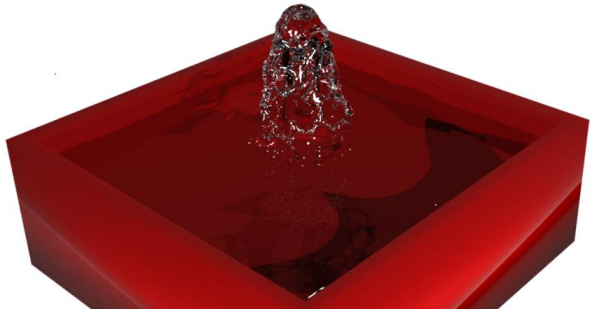
- Combined with other improvements, this enabled simulations to scale to a previously impractical 1920 MPI processes.



epw.org.uk

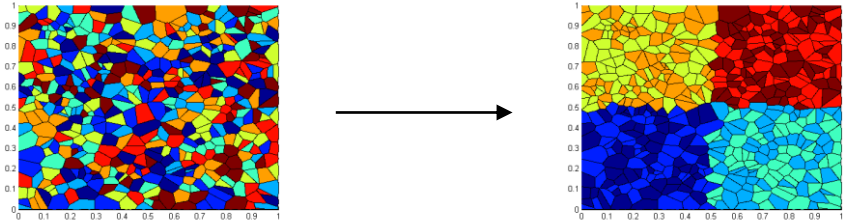
sphFluids – Stuttgart Media University

- Smoothed particle hydrodynamics code
  - C++ with OpenMP
- Profiling identified several issues
  - Definitions of variables in inner loops
  - Unnecessary operations caused by indirection in code design
  - Frequently-used non-inlined functions
  - High cache misses, which could be reduced by reordering the processing of particles
- The developers decided to completely rewrite the code based on their new knowledge, leading to an overall performance improvement of 5x - 6x.



GraGLeS2D – RWTH Aachen

- Simulation of microstructure evolution in polycrystalline materials
- After profiling, the following optimisations were implemented
  - Memory allocation library optimised for multi-threading
  - Reordering the work distribution to threads



  - Algorithmic optimisation in the convolution calculation
  - Code restructuring to enable vectorisation
- An improvement of over 10x was demonstrated for the region concerned, with an overall application speed-up of 2.5x.

Accessing POP Services

- If you're a code developer or user interested in a free performance assessment of a code, you can sign up to the service directly via the POP website.
  - Feel free to contact us first to discuss the service and what might be possible.
- Alternatively, if you're part of a service with a number of candidate codes on your systems, we'd be happy to discuss how we might work together.
- If you're hosting or know of any events which we could attend to inform people about our services, then let us know.

POP Webinars

- The service runs regular webinars on topics of interest to the community
  - Profiling and performance assessment and optimisation
  - Aspects of parallel programming
  - Let us know what you'd like us to cover!
- 30 minute presentations, then attendees' questions answered
- Recordings and the slides from all previous webinars can be found at https://pop-coe.eu/blog/tags/webinar
- The next webinar, "Hybrid parallelization performance - analysis and considerations for MPI+X applications", will be on 18th October at 2p.m. BST
  - Sign up here.

Keep in touch!

- Browse the POP website at https://pop-coe.eu and subscribe to the newsletter.
- Follow us on twitter @POP_HPC
- Subscribe to the POPHPC YouTube Channel
- Join the LinkedIn group

Performance Optimisation and Productivity

A Centre of Excellence in Computing Applications

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This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 676553.