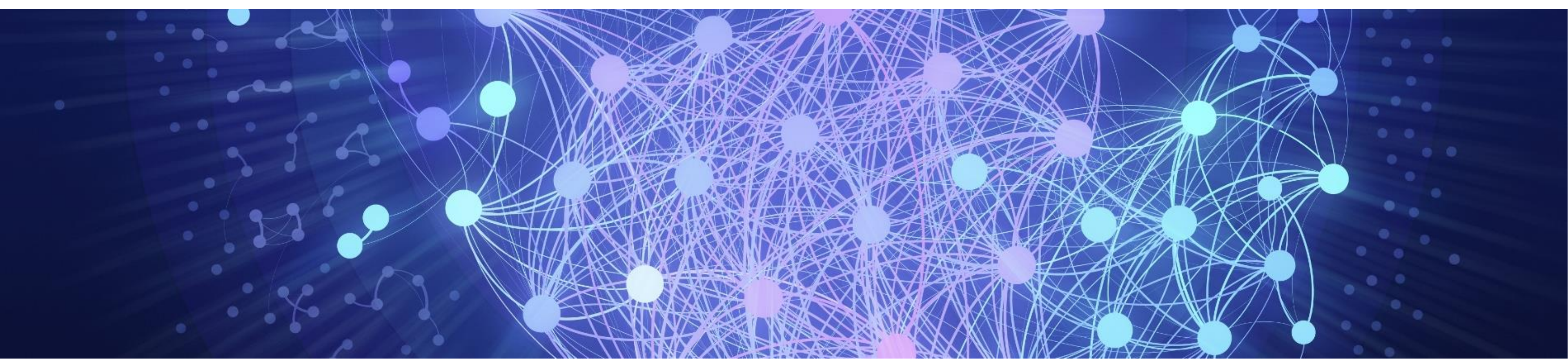
Hartree Centre
High Performance Software Engineering

Luke Mason
STFC - Hartree Centre, UK



Overview

- Introduction to the Hartree Centre
- Research Software Engineering at Hartree
- Current hardware and software trends
- Case Studies

Our mission

Transforming UK industry by accelerating the adoption of high performance computing, big data and cognitive technologies.

What we do

- **Challenge lead research**
  Collaborative R&D with academic and industrial partners

- **Platform as a service**
  Pay-as-you-go access to our compute power

- **Creating digital assets**
  License the new industry-led software applications we create with IBM Research

- **Training and skills**
  Drop in on our comprehensive programme of specialist training courses and events or design a bespoke course for your team

Our platforms

Intel platforms

Bull Sequana X1000 (840 Skylake + 840 KNL processors)

IBM big data analytics cluster | 288TB

IBM data centric platforms

IBM Power8 + NVLink + Tesla P100

IBM Power8 + Nvidia K80

Accelerated & emerging tech

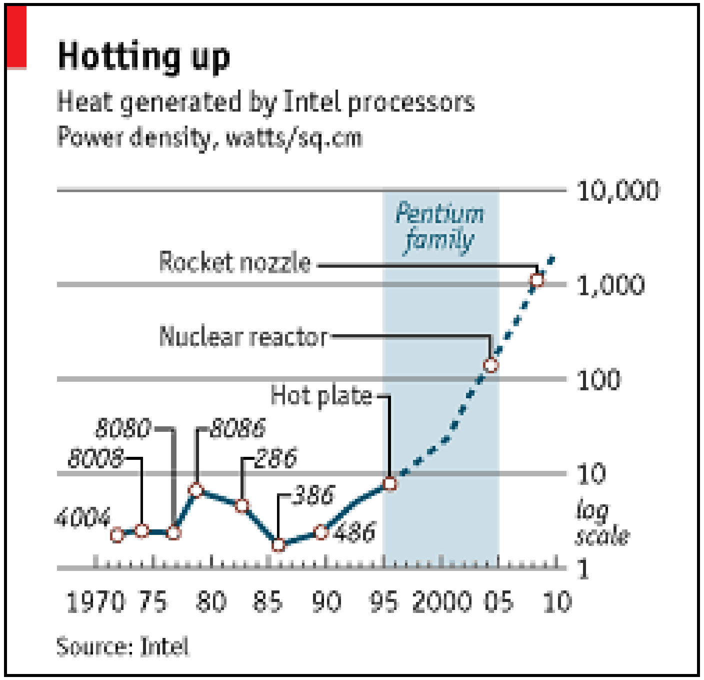
Maxeler FPGA system

ARM 64-bit platform

Clustervision novel cooling demonstrator

Software engineering at Hartree

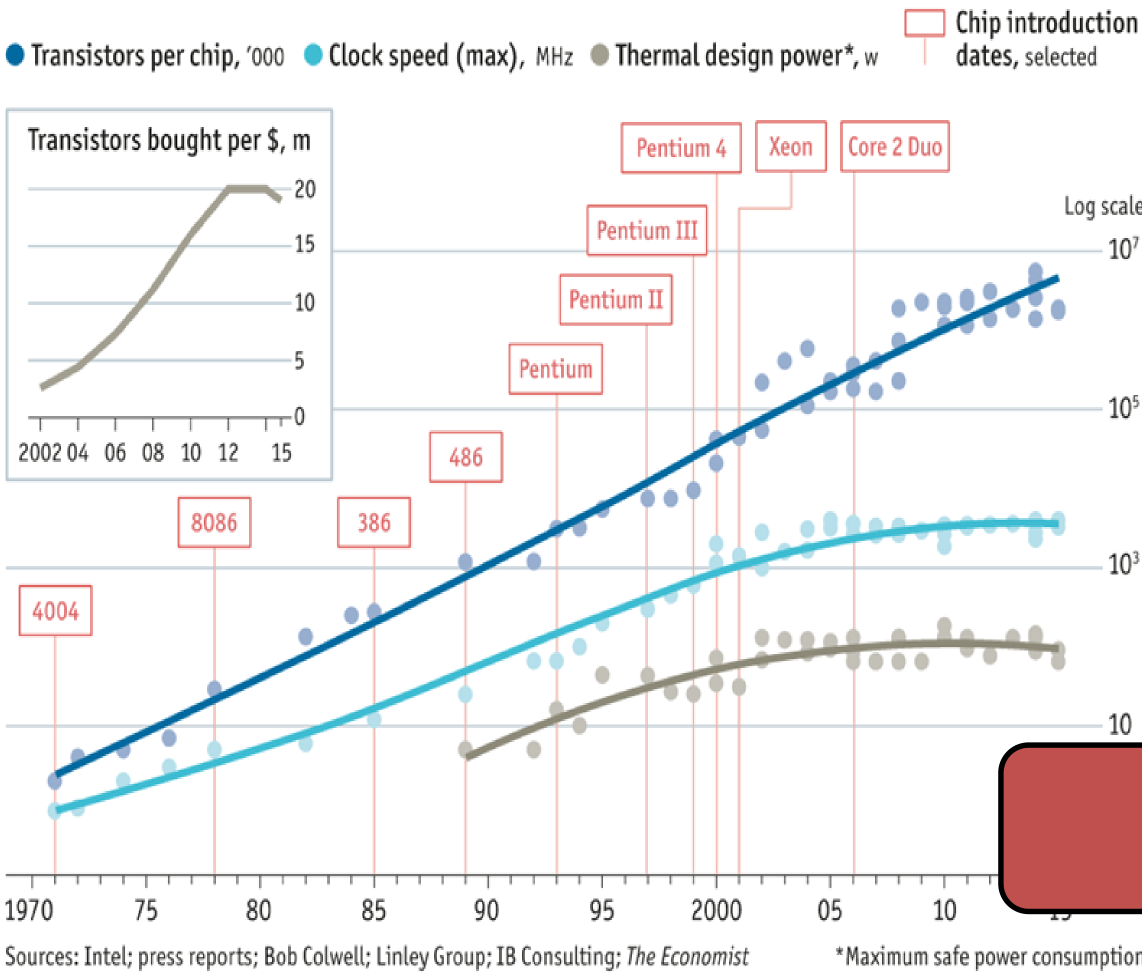
High Performance Computing Challenges



Since the 90s we know current transistor technology won't increase speed.

The Power Wall

Processor Trends



However, human ingenuity:

- Replication
- Increased IPC
- We can put more transistors in a chip than we can afford to turn on. (e.g. clock gating)

- Increase in complexity.
- These techniques will not scale exponentially.

The Power Wall

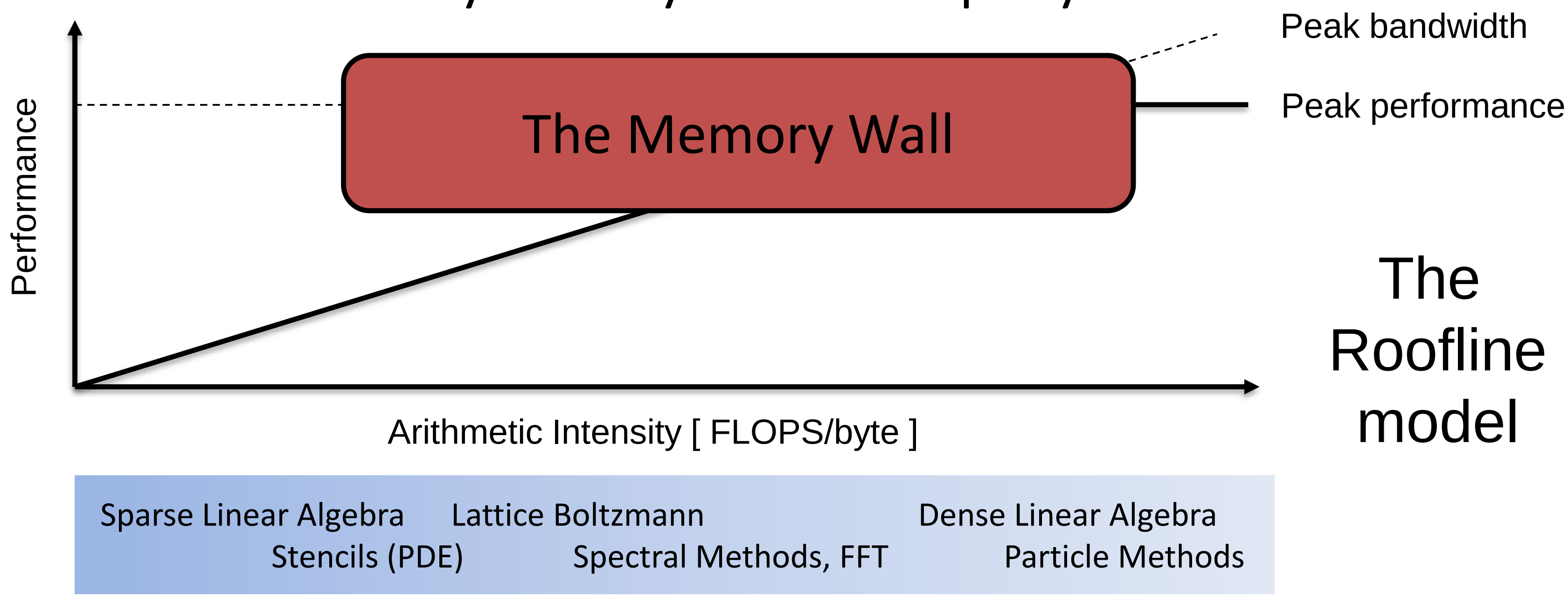
System trends

Peak FP Performance: 50% better per year

Memory Bandwidth: 24 % better per year

Interconnect : 20% better per year

Memory Latency: 4% worse per year

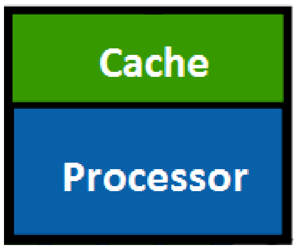


The Roofline model

[1] John McCalpin HPC machines trends (SC16)
[2] http://crd.lbl.gov/departments/computer-science/PAR/research/roofline/

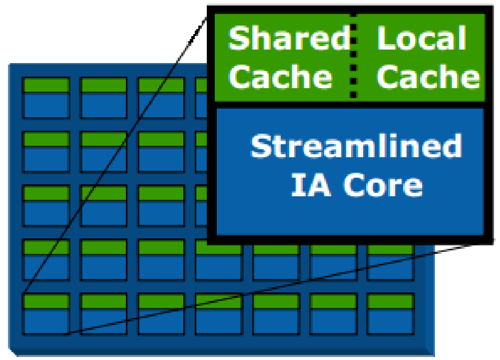
Modern and Future Architectures

Single Core Processor



Long pipelined, out-of-order execution

Many-core Processor

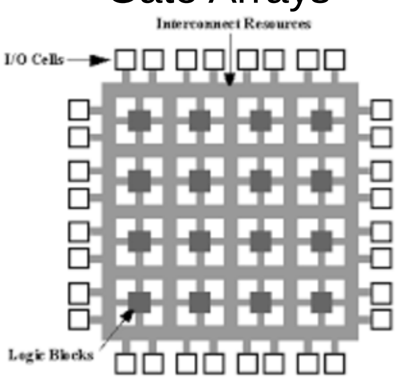


Short pipelined, cache coherent

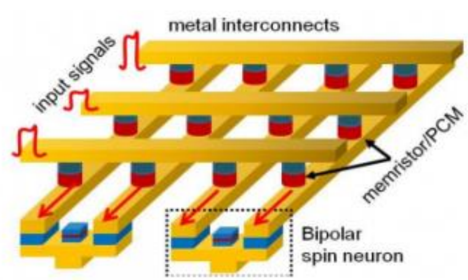
GPU

Shared instruction control, small cache

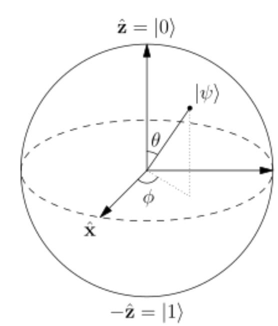
Field-Programmable Gate Arrays



Neuromorphic Computing



Quantum Computing



Software implications

- Legacy code needs to be **modernized** to benefit from newer platforms.
  - Vectorization, threading, micro-arch optimizations, accelerators...

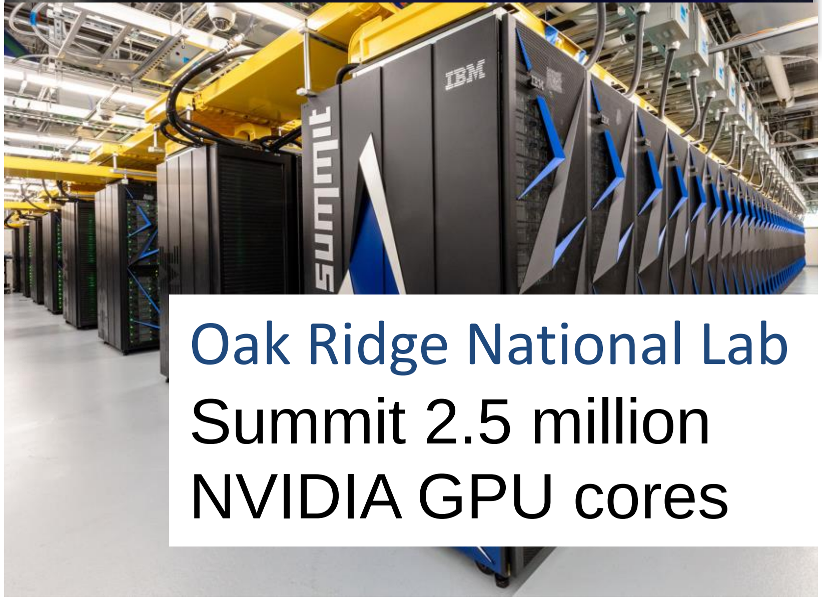
- We need to deal with the increasing complexity. Software needs good **abstractions** to efficiently **separate** the parallel and platform specific optimizations from the science domain.

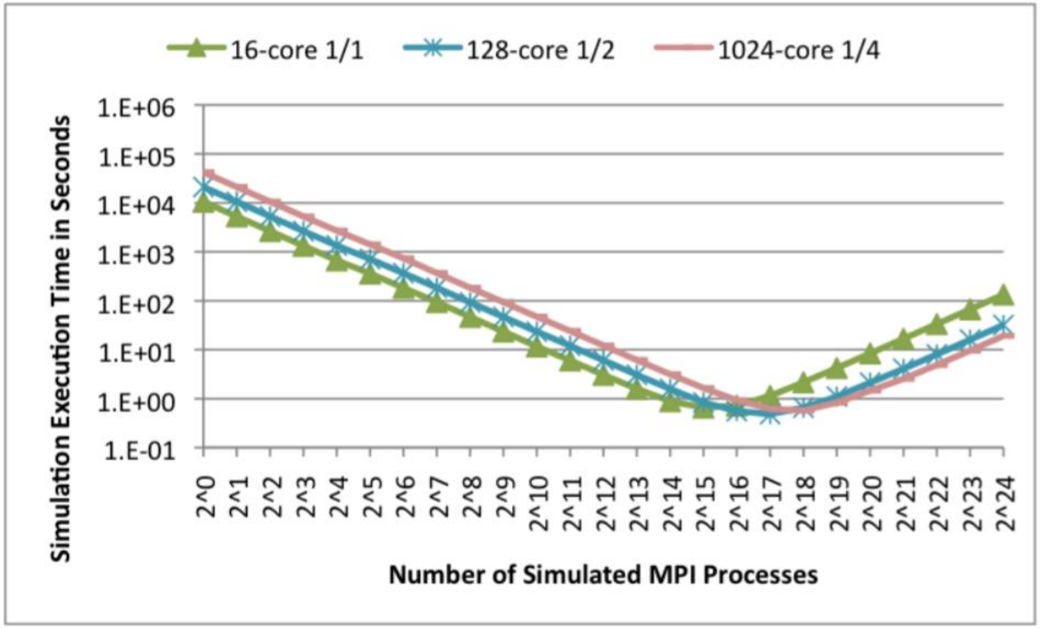
END of the Free lunch

and it is happening now...

Met Office Cray XC40
¼ million Intel Xeon cores

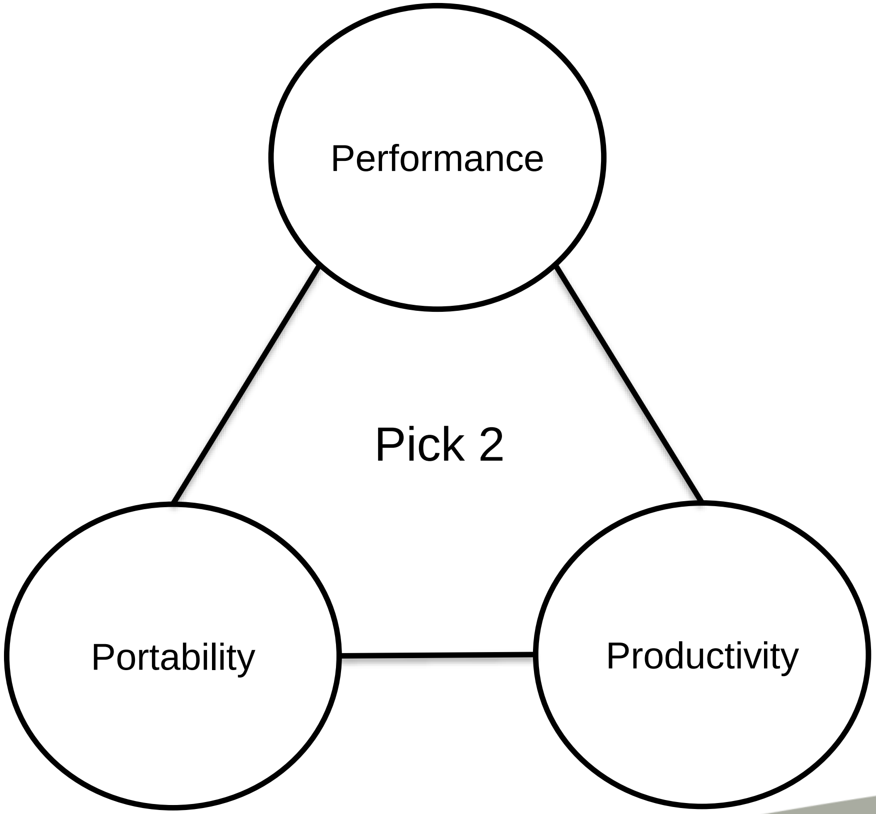
Oak Ridge National Lab
Summit 2.5 million NVIDIA GPU cores





[1] Scaling to a million cores and beyond, Christian Engelmann, Oak Ridge National Laboratory

The 3Ps Principle



Hartree Centre
Science & Technology Facilities Council

Case Study: Met Office

- **Performance:** Needs to get the results in time for forecast, ever-increasing accuracy goals for climate simulations.
- **Productivity:** hundreds of people contributing with different areas of expertise, 2 million lines of code (UM)
- **Portability:** Very risky to chose just one platform: may not be future-proofed, hardware changes more often than software, procurement negotiation disadvantage if you can only run on one architecture, ...

Difficult to compromise on one

Which design principles, parallel programming models, software abstractions and optimizations are effective for current and future HPC production software?

High Performance Software Engineering

Many open questions ...

Hartree Centre
Science & Technology Facilities Council

Software Outlook

Sue Thorne, Philippe Gambron, Andrew Taylor

Software Outlook

- Assist the CCPs and HECs in utilising
  - computational techniques, libraries, architectures (current and near-future)
  - (beyond the usual OpenMP, MPI and CUDA courses provided by the likes of ARCHER)

- Provide a horizon scan of upcoming technologies and architectures that CCPs or HECs should consider
  - CCP/HEC codes are used only to provide a realistic example of how to apply a technique or optimisation
  - Steering committee has advised that no large-scale optimisation of a CCP/HEC code should be performed by Software Outlook

Software Outlook Team (1.5 FTE)

• Luke Mason (PI)	0.2 FTE
• Sue Thorne (Co-I)	0.6 FTE
• Andrew Taylor	0.2 FTE
• Philippe Gambron	0.5 FTE

- Software Outlook Working Group

– Ben Dudson	CCP-Plasma, York
– Ed Ransley	CCP-WSI, Plymouth
– Mark Saville	CCP-EngSci, Cranfield
– Mozhgan Kabiri Chimeh	Sheffield
– Steve Crouch	Software Sustainability Institute

CoSeC
Computational Science Centre for Research Communities

Hartree Centre
Science & Technology Facilities Council

Recent Work

- Use of mixed precision reals to save energy and time
  - Online training course
- Effect of code coupling w.r.t parallel scaling
  - epubs: 1 tech. report (journal article in prep.)
- Using TAU to profile large/complex codes
  - Training course (soon to appear)
- FFT library catalogue
  - Software Outlook website
- GPU frameworks
  - On-going

LFRic & PSyclone

Rupert Ford, Andrew Porter & Sergi Siso

Hartree Centre
Science & Technology Facilities Council

The LFRic Project

- Met Office project to develop a replacement for the Unified Model
- Named in honour of Lewis Fry Richardson (first numerical weather ‘prediction’)
- Achieve good performance on current and future supercomputers

Hartree Centre
Science & Technology Facilities Council

Met Office's Unified Model

- Unified Model (UM) supports:
  - Operational forecasts at
  - Mesoscale (resolution approx. 12km → 4km → 1km)
  - Global scale (resolution approx. 17km)
  - Global and regional climate predictions (global resolution around 100km, run for 10-100 years)
  - Seasonal predictions

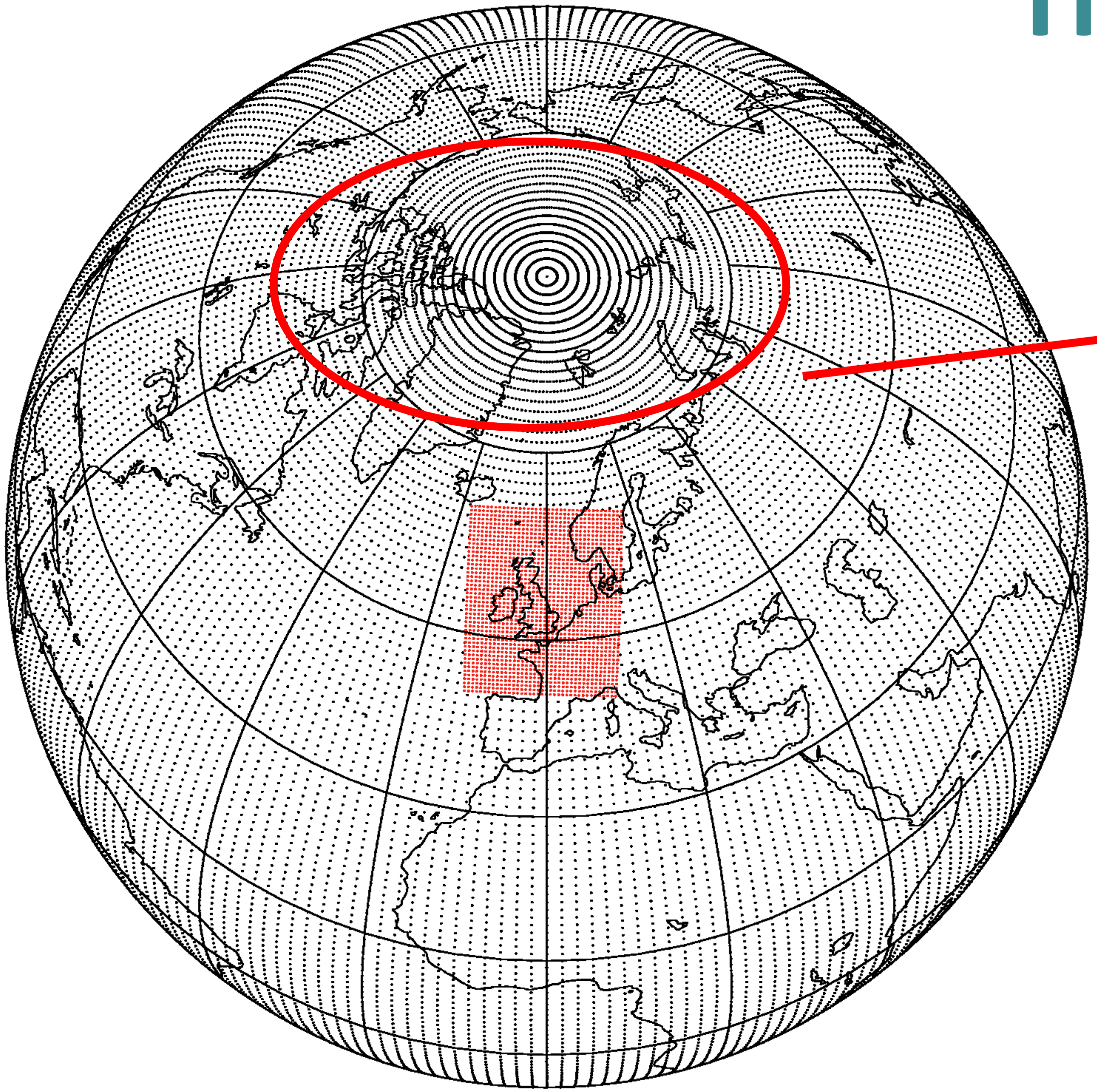
- 26 years old this year
- Unsuited to current multi-core architectures
- Limited OpenMP
- Cannot run on GPUs
- Scalability inherently limited by choice of mesh...

Hartree Centre
Science & Technology Facilities Council

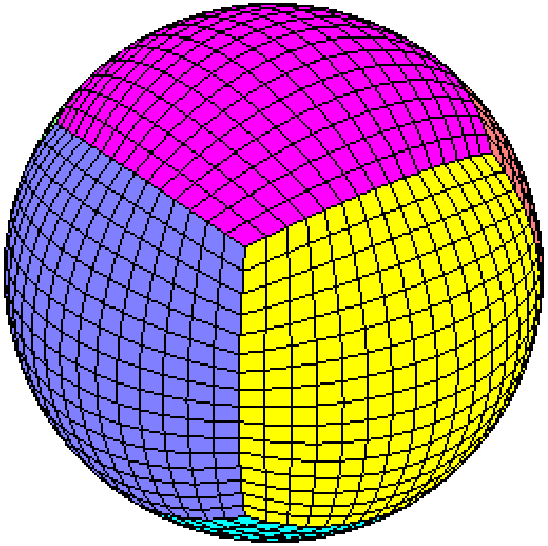

North Pole

?

The Pole Problem



- At 25km resolution, grid spacing near poles = 75m
- At 10km reduces to 12m!



Hartree Centre
Science & Technology Facilities Council

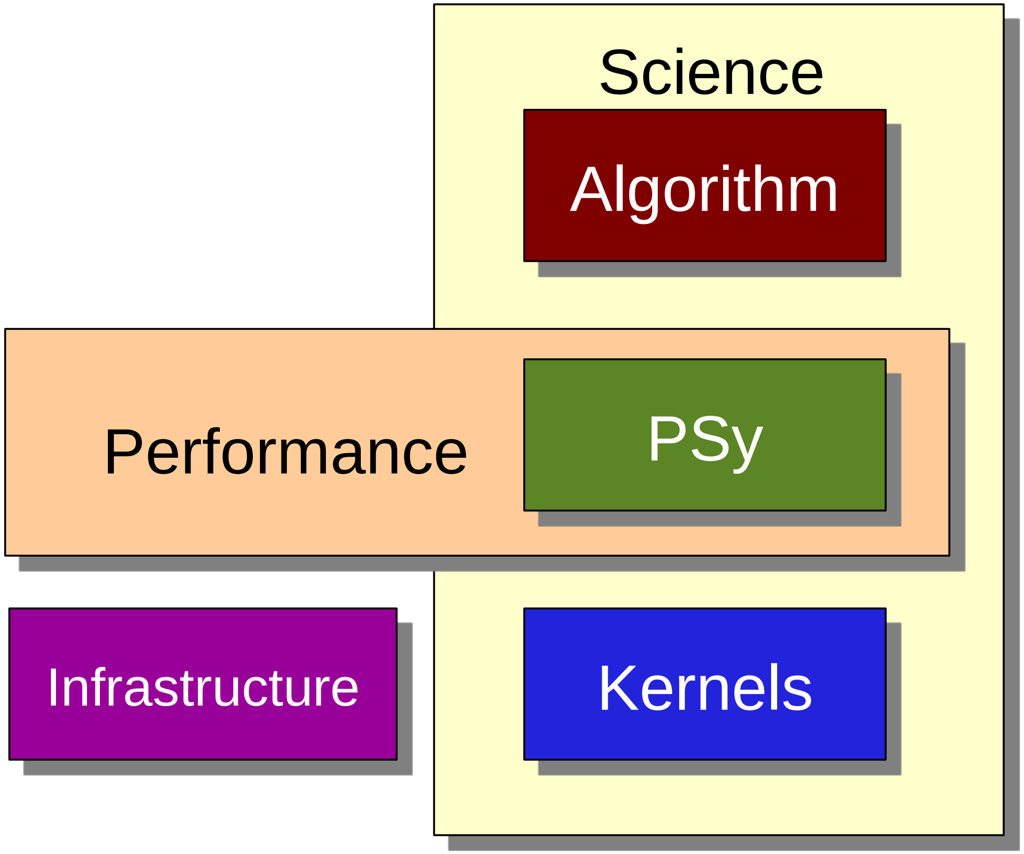
Portable Performance

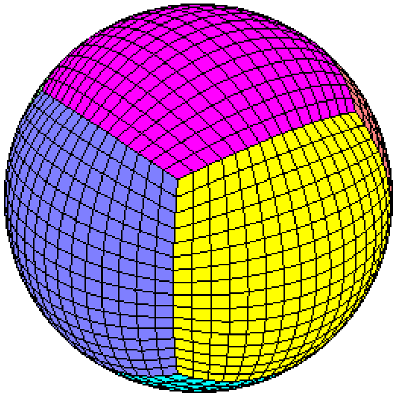
Even for traditional, CPU-based systems (let alone GPUs *etc*.) this is almost impossible to achieve, *e.g.*:

- CPU architecture: Intel, ARM, Power, SPARC...
  - micro-architectures constantly evolving
- Fortran compiler: Intel, Cray, PGI, IBM, Gnu...
  - bugs and 'features' vary from release to release

=> choices made for one architecture/compiler combination are almost certainly not optimal for other combinations
=> resort to *e.g.* pre-processing as a work around

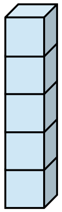
PSyclone





Algorithm layer refers to the whole model domain

Parallel System layer handles multiple levels of parallelism



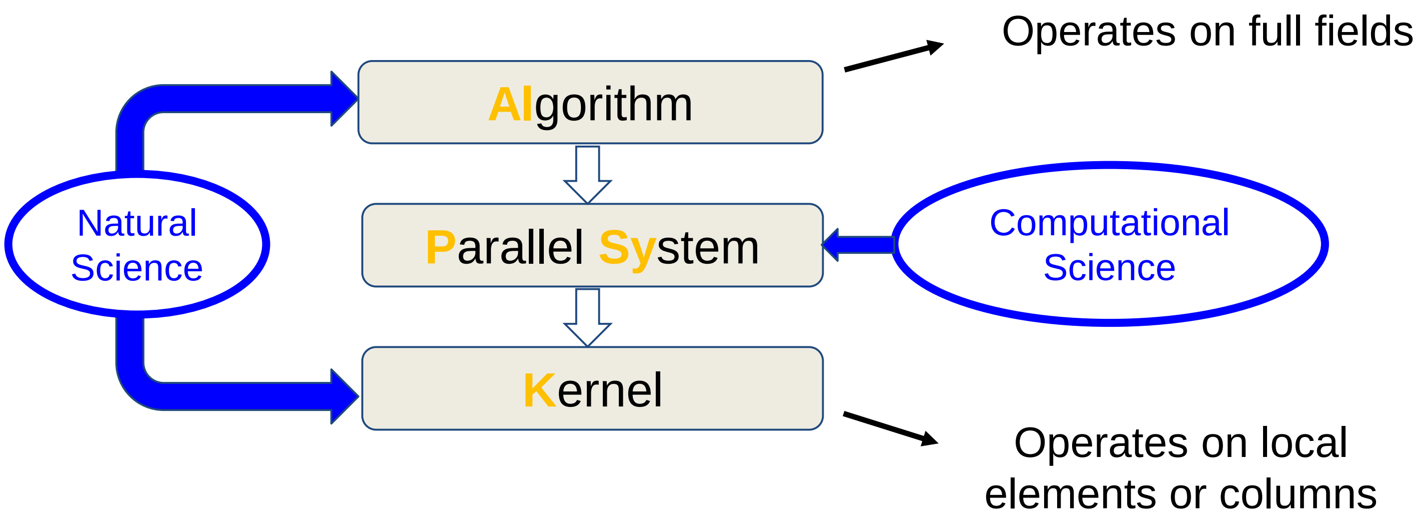
Kernels for individual columns

工合

Hartree Centre
Science & Technology Facilities Council

Domain Specific Languages: PSyclone

Embedded Fortran-to-Fortran code generation system used by the UK MetOffice next-generation weather and climate simulation model (LFRic)



Given domain-specific knowledge and information about the Algorithm and Kernels, PSyclone can generate the Parallel System layer.

EuroEXA

Xiaohu Guo, Andrew Attwood, Sergi Siso

Hartree Centre
Science & Technology Facilities Council

European project that targets to provide the template for an upcoming **Exascale system** by co-designing and implementing a petascale-level prototype with ground-breaking characteristics. Builds on top of cost-efficient architecture enabled by novel **inter-die links** and **FPGA** acceleration.

Work package 2: Applications, Co-design, Porting and Evaluation

Work package 3: System software and programming environment

Work package 5: System integration and hosting

- Containerised data centre
- Sub atmospheric cooling system
- Dense & liquid cooled
- Combination of ARM cores and Xilinx FPGA

Hartree Centre
Science & Technology Facilities Council


EUROEXA
FUNDED BY THE EUROPEAN UNION
PARTNERS
ICEOTOPE
COOLING REDEFINED
Hartree Centre
SYNELIXIS
ZeroPoint Technologies
Fraunhofer
imec
arm
neurasmus
SUPPORTERS
Schneider
JOHN SUTCH
CRANES

Quantum Computing

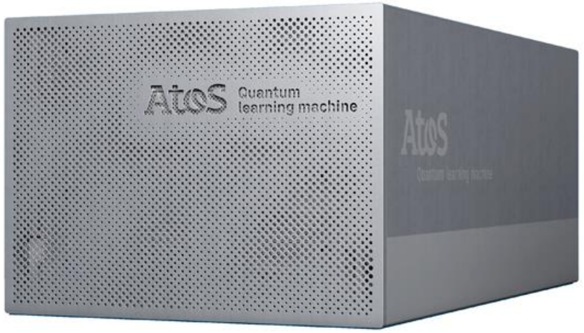
James Clark

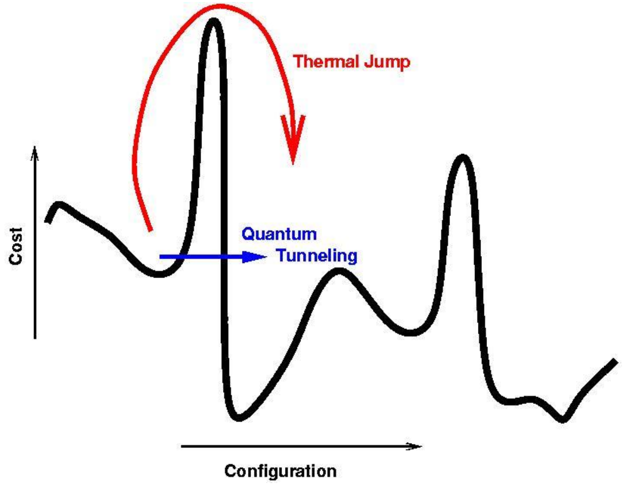
Hartree Centre
Science & Technology Facilities Council

Quantum Computing

Universal Quantum Computing

- Collaboration with Atos in quantum computing research to have the UK's first "quantum learning as a service".
- Work with academics and industry to accelerate the use of quantum computing via simulators.





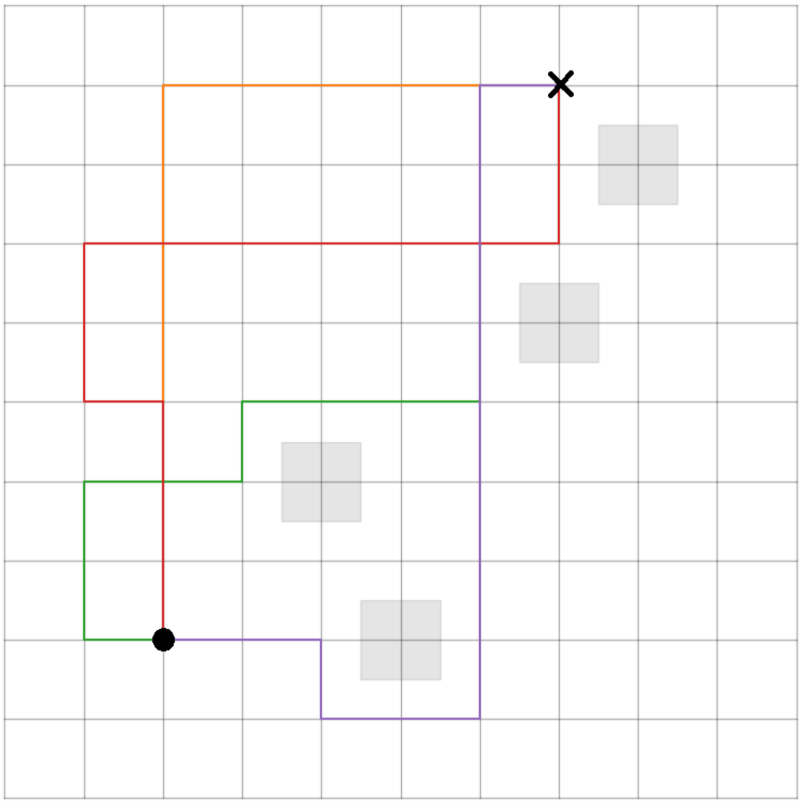
Quantum Annealing

- Multiple projects in engineering sectors using quantum annealing for optimization problems.

Ocado Technology

- Ocado is the world's largest online-only supermarket
- Ocado Technology powers Ocado.com and Morrisons.com
- International customers include Kroger (USA) and Casino (France)
- Wealth of optimization challenges
- Innovation at core of business

Candidate Generation

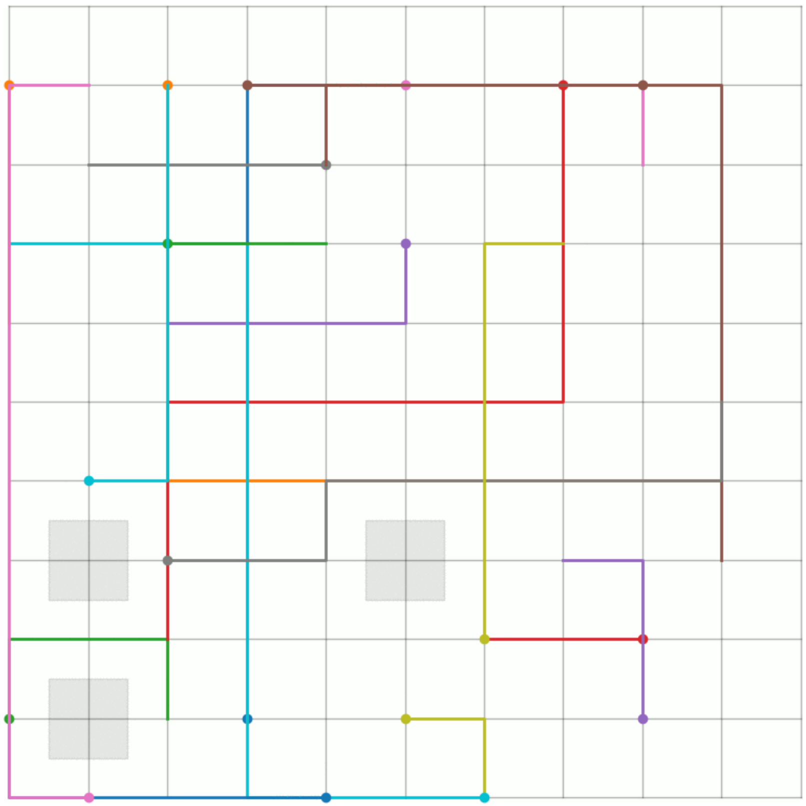


Quickly generate some candidates

N candidates per robot

Candidate generation not optimised

First Pass

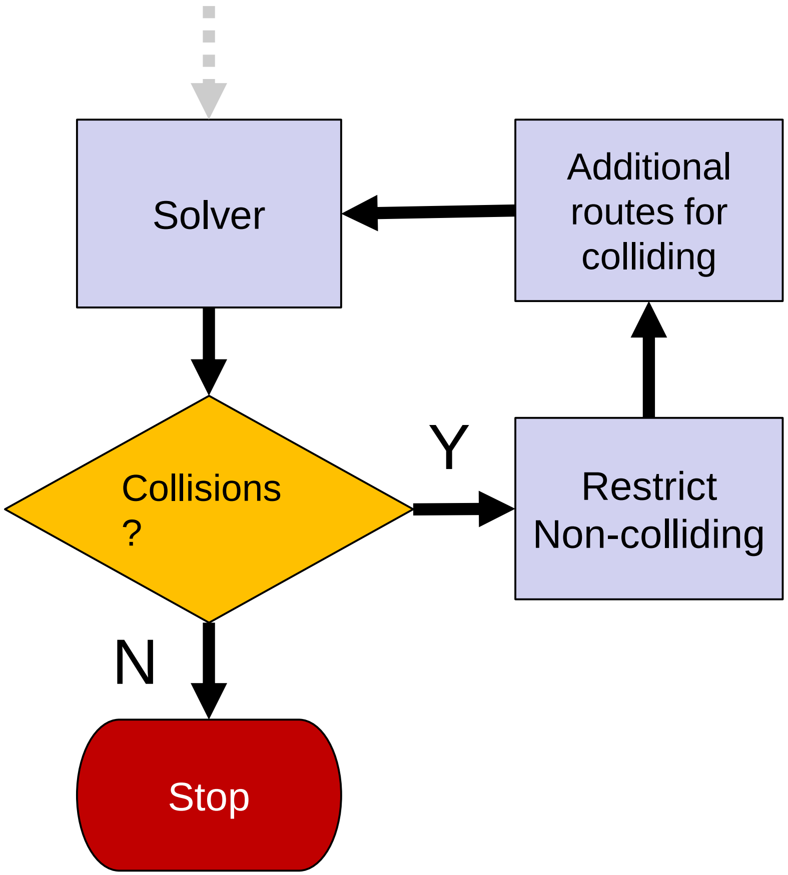


Works!

Still have collisions ✘

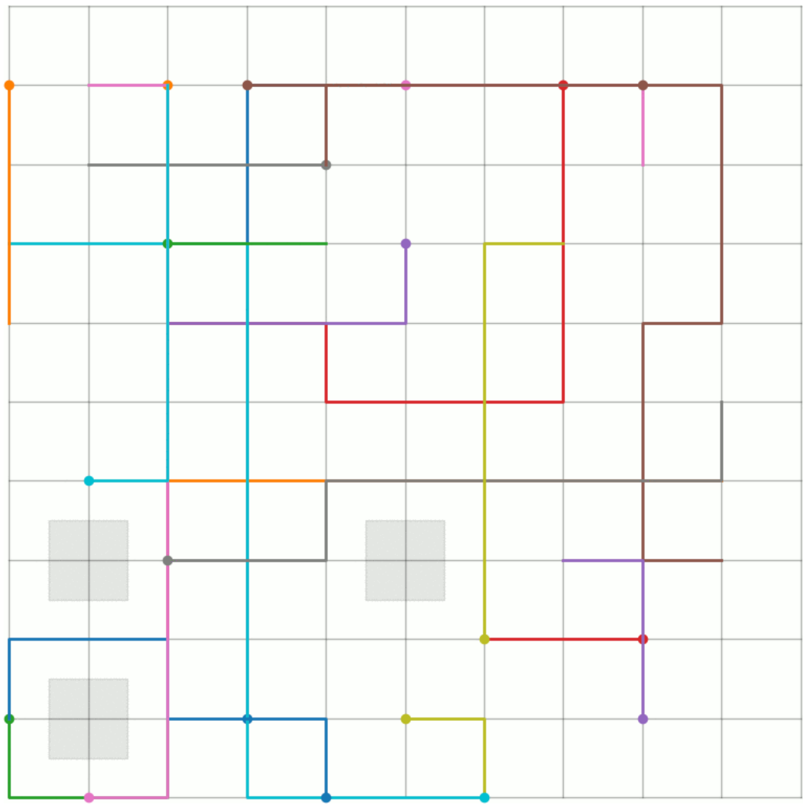
We can do better

Resolving Collisions



- Iterate with more candidates for robots that collide
- Reduce candidates for non colliding robots

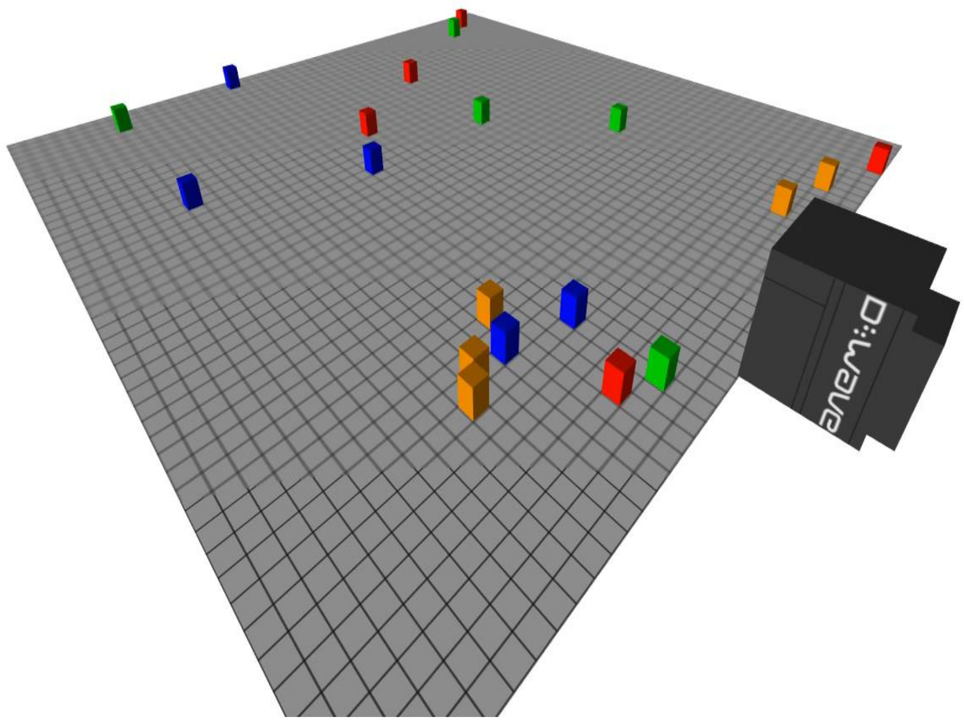
Resolving Collisions



- Iterate with more candidates for robots that collide
- Reduce candidates for non colliding robots
- No more collisions!

Hartree Centre
Science & Technology Facilities Council

Summary



- Hybrid quantum & classical computation

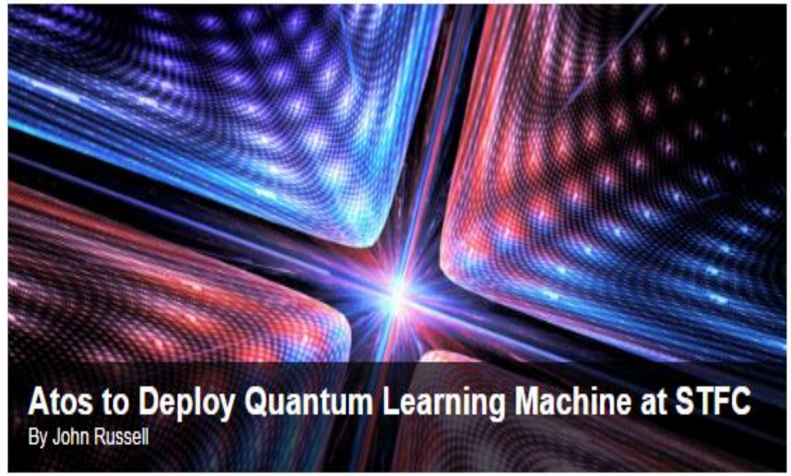
- After considering trans-Atlantic communication, quantum approach starts to become competitive

The Future

HPC wire

Since 1987 - Covering the Fastest Computers in the World and the People Who Run Them

- Home
- Technologies
- Sectors
- AI/ML/DL
- Exascale
- Specials
- Resource Library
- Events
- Job Bank
- About
- Solution Channels



February 6, 2019

The UK's Science and Technology Facilities Council (STFC) and Atos yesterday announced a collaboration to deploy an Atos Quantum Learning Machine at STFC Hartree Center. It is noteworthy that Atos has chosen an appliance approach to delivering a complete quantum training environment. This contrasts with the prevailing approach by quantum tech providers to rely on web-delivered access to their simulators. This is the first AQLM deployment the UK.

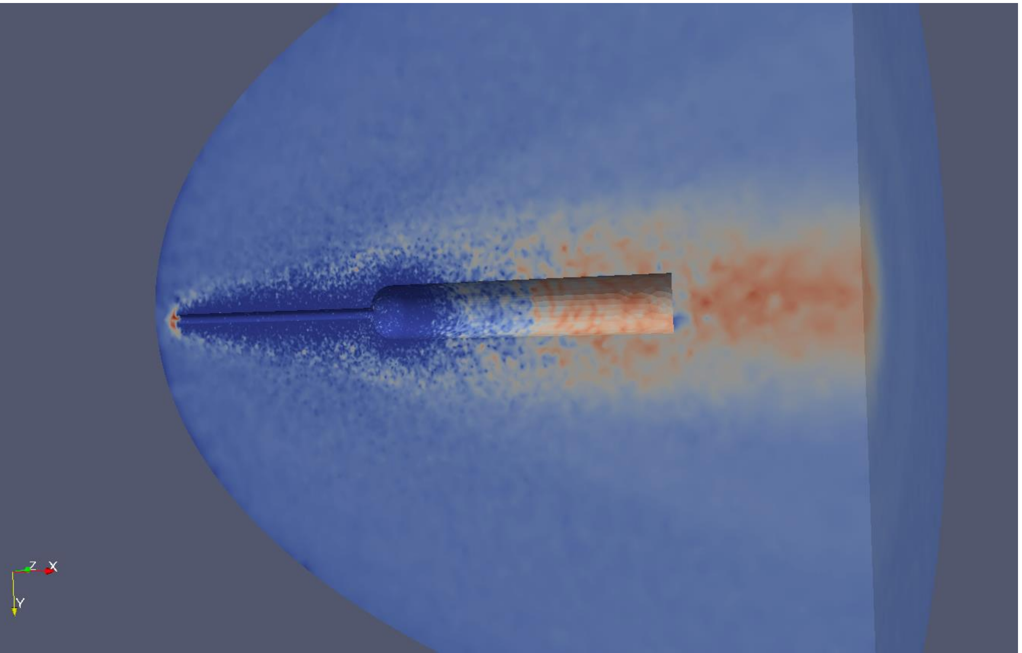
Short Case Studies

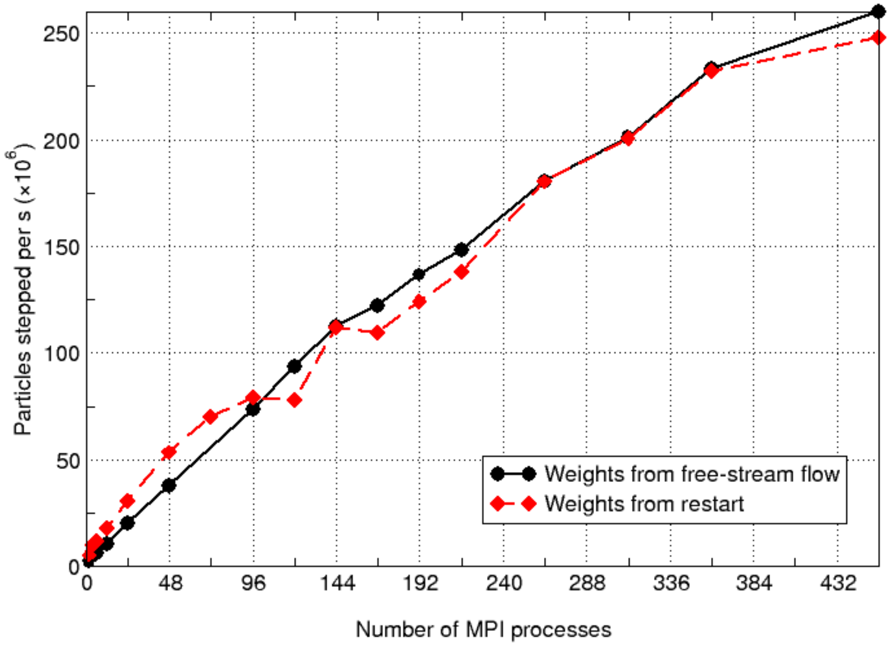
Hartree Centre
Science & Technology Facilities Council

Software Parallelization and Optimization

- Serial performance optimizations.
- Distributed-memory parallelism with MPI.
- Shared-memory parallelism.
- GPGPU Programming.

Example: Direct Simulation Monte Carlo (for rarified gas flows)

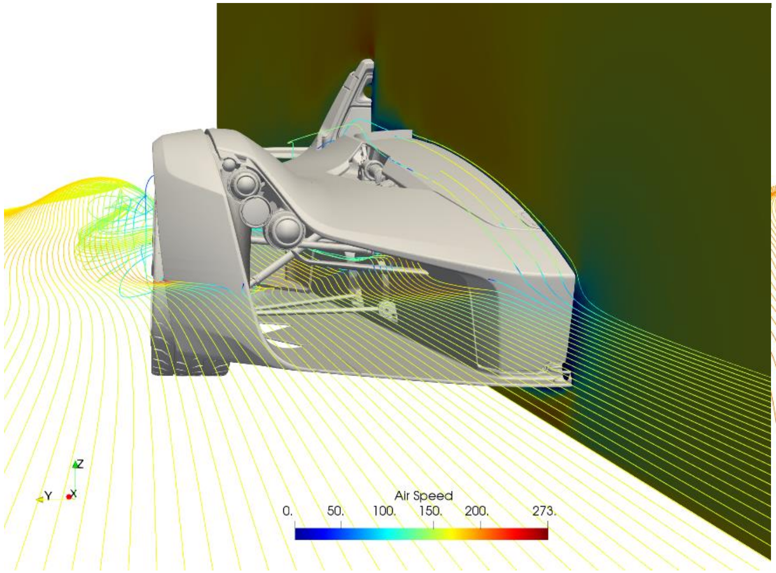


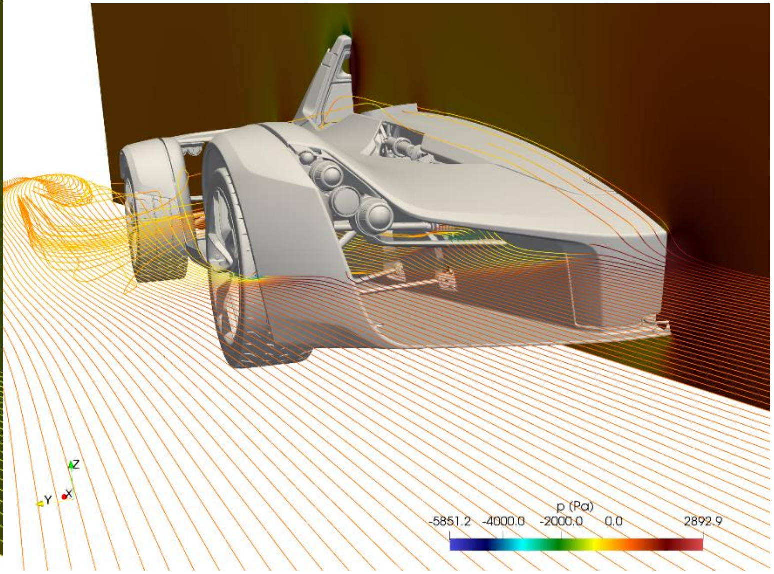


PRACE (Partnership for Advanced Computing in Europe)

Currently undertaking an industrial collaboration Briggs Automotive Company:

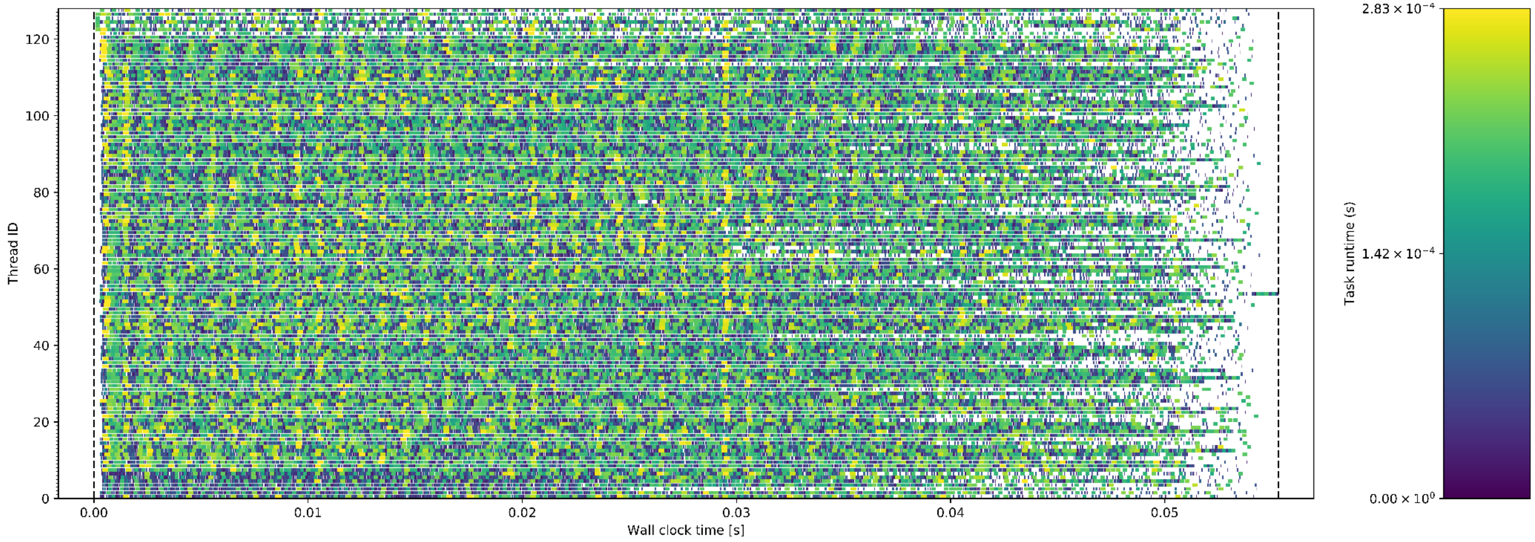
- Involves analysing and improving the design of the BAC Mono single-seat sports car using large-scale CFD computations.





Novel parallel programing paradigms: task-based parallelism

Asynchronous programming model which encapsulates parallel computation into **tasks** and defines the **dependencies** between them. A runtime system takes the responsibility to **schedule** the tasks appropriately to the underlying hardware.



Thank you

Luke Mason
Luke.mason@stfc.ac.uk

Hartree Centre
Science & Technology Facilities Council

Find out more:

hartree@stfc.ac.uk
hartree.stfc.ac.uk
/company/stfc-hartree-centre
@hartreecentre