# NAG Update

## ExaTEPP

Adrian Tate, CEO
Numerical Algorithms Group Ltd

# Contents





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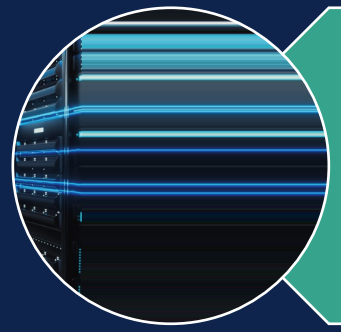
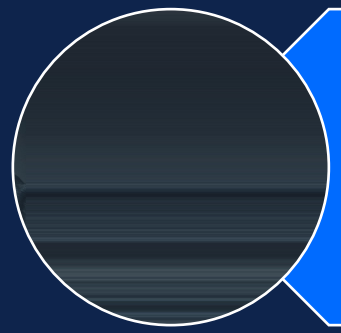
# NAG - we serve science and engineering

Exists to serve science and engineering



Provide highly technical product and services



Not-for-profit group of commercial companies



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# NAG's evolution in HPC

## 1970s

NAG was founded in 1970 with the NAG Library released shortly after in 1971

## 1980s

NAG began work on the NAG Fortran Compiler and continued to develop the NAG Library

## 1990s

A period of multiple collaborations with US national laboratories, Intel and AMD on critical numerical libraries

## 2000s

In the 2000s NAG pioneered the development of automatic differentiation tools and took on CSE support for the UK national supercomputer HECToR

## 2010s

Major International Energy client service engages NAG for major managed services contract covering HPC, Engineering and Cloud Data Management

## 2020s

NAG continues to innovate particularly around Cloud HPC and the Cost-to-Solution framework

product

service

NAG Library

AD Suite

NAG Compiler

"service"

HPC Cloud migration

Managed HPC Services

Virtual Supercomputer



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# Team NAG

## Principal Scientists

Prof. Simon McIntosh-Smith
U. Bristol

Prof. Uwe Naumann
RWTH Aachen

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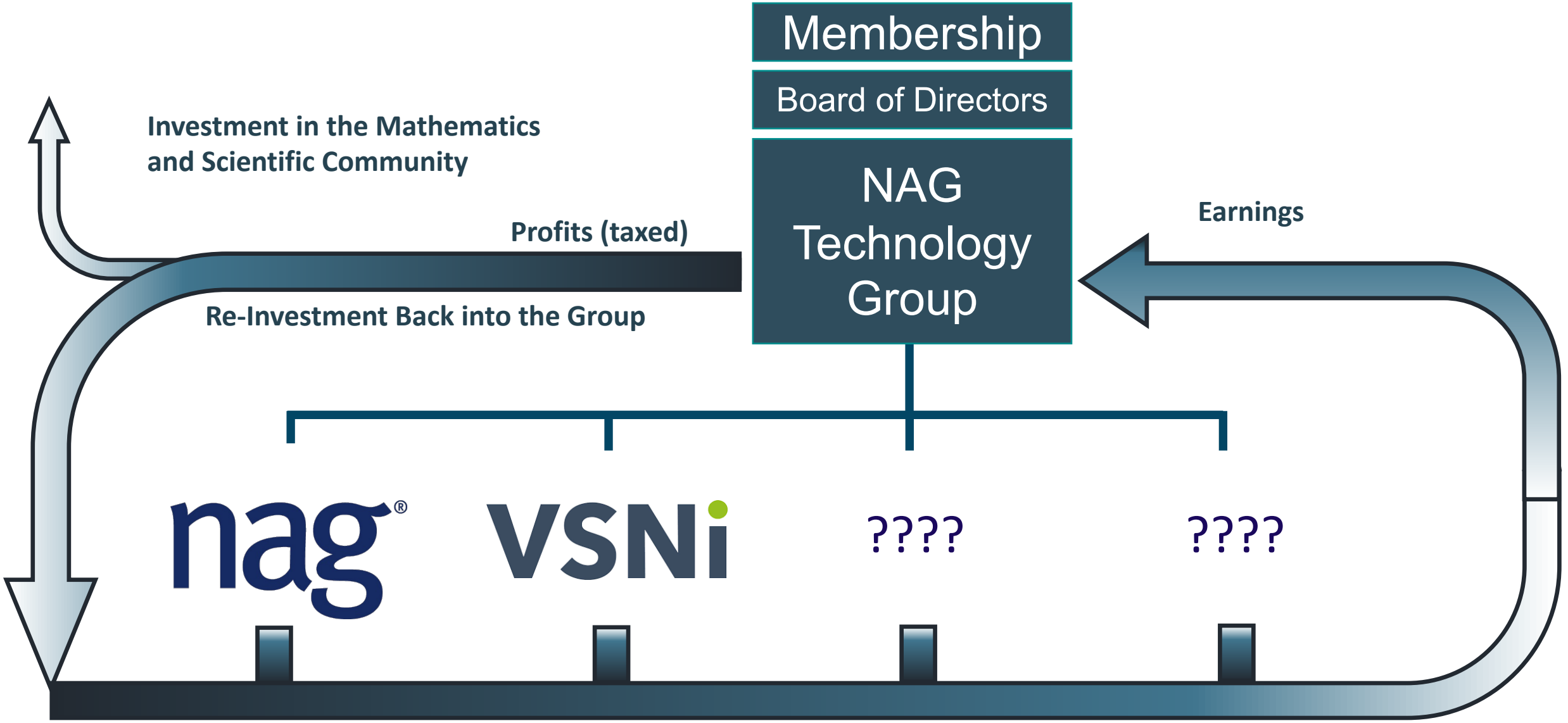
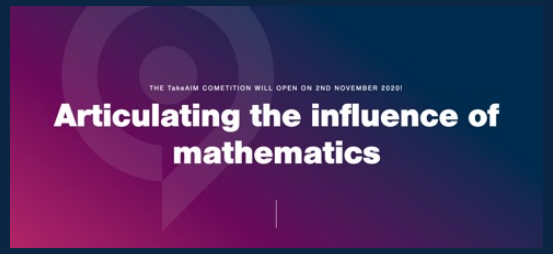
# NAG Funding the community



# Community Activities




UKRI Science and Technology Facilities Council

code club

STEM AMBASSADOR

ExCALIBUR 10

MANCHESTER 1824
The University of Manchester

University of BRISTOL

- U. Manchester NAG MSc Applied Mathematics
- Smith Institute TakeAim Competition
- InfoMM Centre for Doctoral Training at U. Oxford
- Fluid Dynamics Award at U. Leeds
- Founding member of Women in HPC
- AIMLAC Centre for Doctoral Training in AI/ML
- Centre for Doctoral Training in Fluid Dynamics EAB
- EXATEPP Excalibur project partner
- Bristol Award for HPC students
- PAX Excalibur project partner
- STFC Daresbury Early Career Award
- Collaboration with STFC Rutherford Appleton Laboratory
- STEM initiatives (virtual Code Club, schools program)
- EAB U. Manchester Mathematics
- EAB U. Bristol Computer Science

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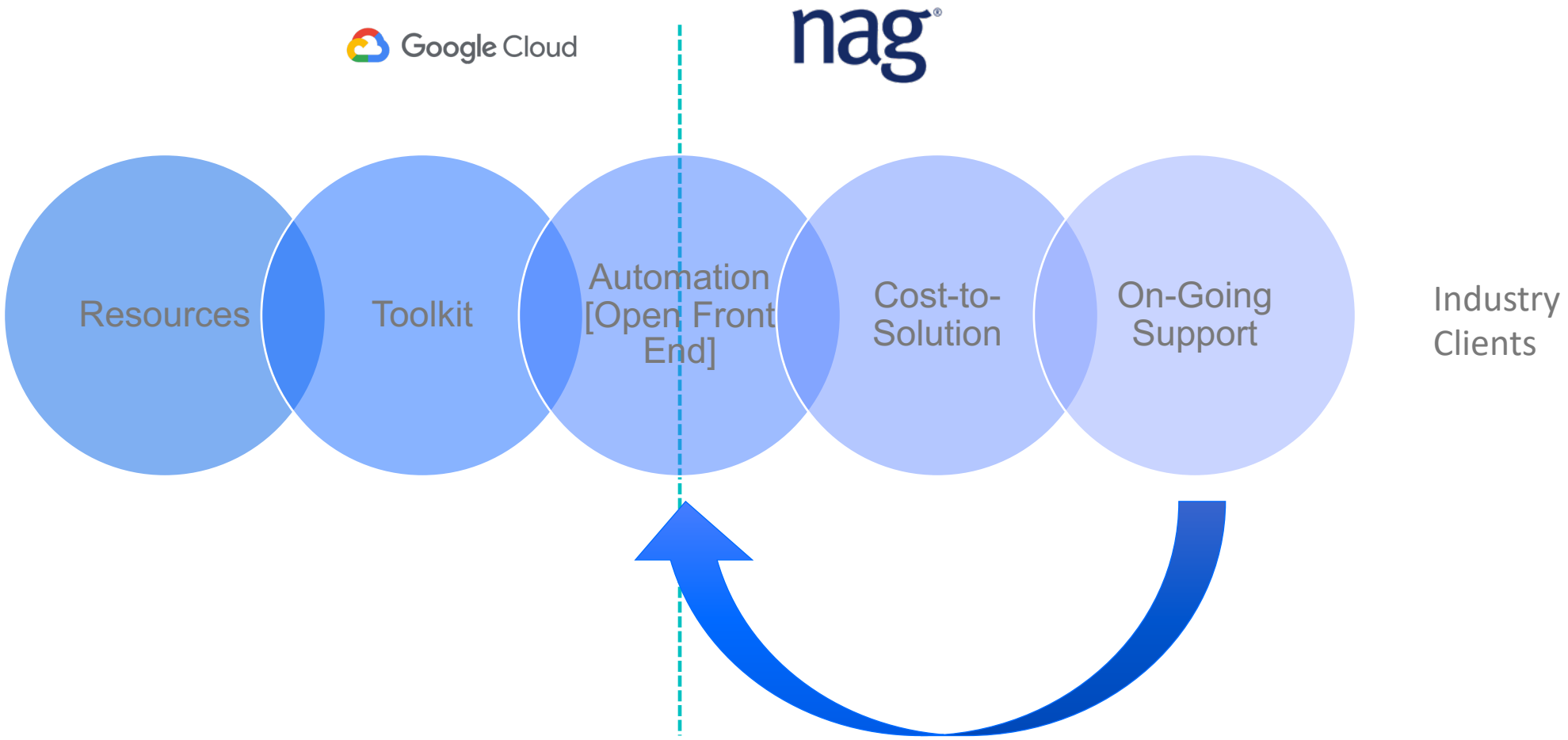
# Cloud enablement & accessibility



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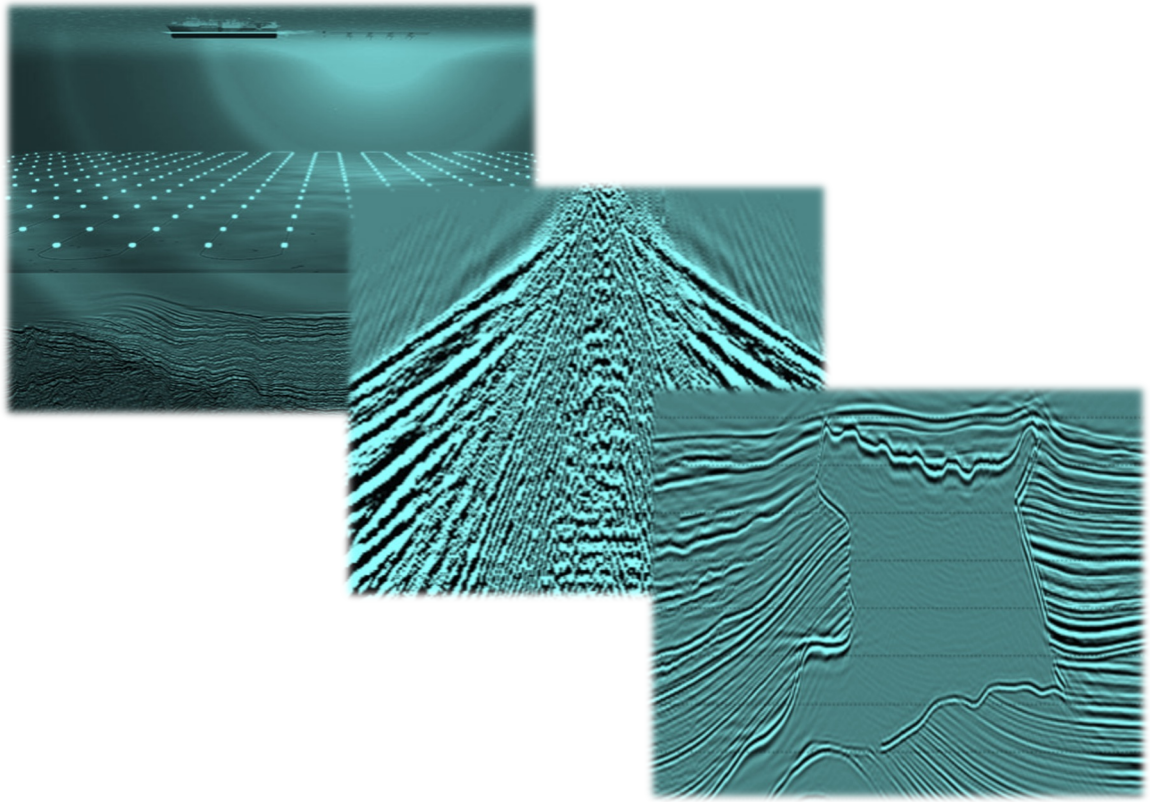
# A motivating example for Cost-to-solution

> Seismic data is like doing an ultrasound of the earth

Webinar: “Solving the Cost-to-Solution Puzzle”

HPC High-performance computing

## Reverse Time Migration



# The Azure HPC & AI Collaboration Centre


- Microsoft Azure launched the Azure HPC & AI Collaboration Centre program to develop and share best practices with the HPC and AI communities.
- NAG was an active member of the collaboration.
- The Collaboration Centre program was delivered in partnership with NVIDIA

HPC High-performance computing

# Collaboration Opportunities

- Because of our special status, NAG does not need complex collaboration agreements
- If there is mutual interest, we can work together
- Fund direct “research sprints” ourselves
- No big-company bureaucracy or onboarding
- Especially interested in PINNs and surrogate models



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# Exascale and beyond



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# Machine performance through my career

12 TeraFlop/s

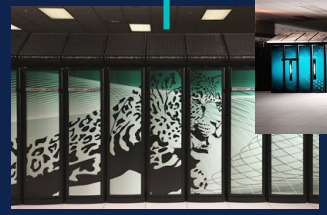
Free Lunch era

1 PetaFlop

First GPU Super

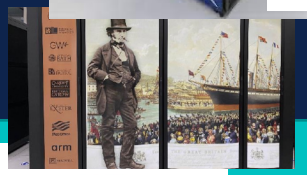
Exascale era

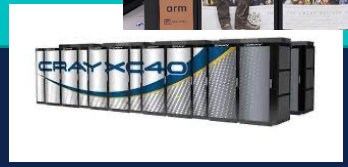
1.194 exaFLOP










**University of Manchester**
- HPC consultant

**Cray**
- Software Engineer

**Cray**
- Technical Lead
- Principal Engineer

**Cray**
- CTO Office

**Cray**
- Director of Cray EMEA Research Lab

**NAG**
- CEO



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# Exascale Computing

- My career was spent trying to solve the Exascale challenge, Petascale was a warning sign



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# 2008 was the end of road…

- It is 2008
- Cray's biggest ever installation and potentially one of fastest in world
- At installation MTBF is 3 hours
- HPL run required 24 hours to complete
- This was the first production petaflop
- Warning sign for what was coming
- Machines and software would have to be completely different



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# Exascale Computing

- My career was spent trying to solve the Exascale challenge, Petascale was a warning sign
- Exascale computing began in about 2007 at “townhalls”
  - More’s law was ending (free lunch)
  - Next-gen machines would not fit in power budget
  - Software had been massively neglected
  - Wider machines with more dist. parallel would not work
  - MTBF of such machines was becoming a nightmare
- USA govnt spent over $3B on Exascale (Fastforward, CORAL, CORAL-2, ECP)
- To USA, the benefits outweigh the costs in getting there



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# View 1) Exascale Computing is “done”

- GPUs, faster interconnects, enormous investment in SW, upskilling
- Frontier – HPL at over 1 EF
- The “next” Exascale is not Zettascale but AI
- The ECP is about to close down
- Job is done, we can all move on and get excited by AI
- USA saved the world (again!)



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# View 2) Exascale is meaningless

- NAG clients have never cared about Exascale
- FSI – play with whatever works but production is a different beast (limited GPU usage)
- O&G - good use of GPUs but the workloads are very challenging and *workflows* even more so
- Large Industry - talent availability is squeezing them
- Portability has not been solved by ECP or anything else
- Clients are spending more maintaining their codes than before Exascale
- Therefore, Exascale software development was a failure
- “Trickle down economics” does not work in Supercomputing
- How much was spent and what was achieved?



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# JAGUAR - CRAY XT5 QC 2.3 GHZ

| | |
|---|---|
| **Site:** | DOE/SC/Oak Ridge National Laboratory |
| **System URL:** | http://www.nccs.gov/computing-resources/jaguar/ |
| **Manufacturer:** | Cray/HPE |
| **Cores:** | 150,152 |
| **Processor:** | Opteron Quad Core 4C 2.3GHz |
| **Interconnect:** | XT4 Internal Interconnect |
| **Installation Year:** | 2008 |
| **Performance** | |
| **Linpack Performance (Rmax)** | 1,059.00 TFlop/s |
| **Theoretical Peak (Rpeak)** | 1,[illegible]40 TFlop/s |
| **Nmax** | 4,712,799 |
| **Power Consumption** | |
| **Power:** | 6,950.00 kW (Submitted) |
| **Software** | |
| **Operating System:** | CNL |

RANKING

| List | Rank | System | Vendor | Total Cores | Rmax (GFlop/s) | Rpeak (GFlop/s) | Power (kW) |
|---|---|---|---|---|---|---|---|
| 06/2009 | 2 | Cray XT5 QC 2.3 GHz | Cray/HPE | 150,152 | 1,059.00 | 1,381.40 | 6,950.00 |

# FRONTIER - HPE CRAY EX235A, AMD OPTIMIZED 3RD GENERATION EPYC 64C 2GHZ, AMD INSTINCT MI250X, SLINGSHOT-11

| | |
|---|---|
| **Site:** | DOE/SC/Oak Ridge National Laboratory |
| **System URL:** | https://www.olcf.ornl.gov/frontier/ |
| **Manufacturer:** | HPE |
| **Cores:** | 8,699,904 |
| **Processor:** | AMD Optimized 3rd Generation EPYC 64C 2GHz |
| **Interconnect:** | Slingshot-11 |
| **Installation Year:** | 2021 |
| **Performance** | |
| **Linpack Performance (Rmax)** | 1,194.00 PF[illegible]p/s |
| **Theoretical Peak (Rpeak)** | 1,679.82 [illegible]Flop/s |
| **Nmax** | 24,219,648 |
| **HPCG [TFlop/s]** | 14,054.0 |
| **Power Consumption** | |
| **Power:** | 22,703.00 kW (Submitted) |
| **Power Measurement Level:** | 1 |
| **Software** | |
| **Operating System:** | HPE Cray OS |

RANKING

| List | Rank | System | Vendor | Total Cores | Rmax (PFlop/s) | Rpeak (PFlop/s) | Power (kW) |
|---|---|---|---|---|---|---|---|
| 06/2023 | 1 | HPE Cray EX235a, AMD Optimized 3rd Generation EPYC | HPE | 8,699,904 | 1,194.00 | 1,679.[illegible]2 | 22,703.00 |

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128x flops
3x the power
~40x improvement
Cost = >$3B

RANKING

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|---|---|---|---|---|---|---|---|
| 06/2023 | 1 | HPE Cray EX235a, AMD Optimized 3rd Generation EPYC | HPE | 8,699,904 | 1,194.00 | 1,679.8 | 22,703.00 |

# View 2) Exascale is meaningless

- For the >$3B spent on Exascale, what improvements in portability and available to clients?
- SYCL, Kokkos, openACC, openMP, oneAPI and all good advancements
- However, clients report spending more on code maintenance now than 10 years ago
- Trickle-down economics of HPC not working here
- “workflows” are what clients care about not ”codes”
- Industry clients do not have the talent to keep things in-house (cloud becomes attractive for this reason alone)



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# Reality is always more nuanced

- Real ROI of Exascale is impossible to calculate
- US Exascale was good to ride the coat-tails of
- To the UK, cost of achieving Exascale did not outweigh the risks of getting there (same in the EU)
- In the UK, our investment is tiny so ROI will be great
- For our future programmes – Industry benefits are essential part of ROI
- How long before general HPC users are running at Exascale?
- When will codes be really portable? This problem has not been solved by the Exascale or ECP



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# Beyond Exascale

- The new Exascale is AI
- Rather – convergence of HPC and AI
- Is this harder or easier than Exascale?
- Harder as the challenges transcend technology
- Challenges
  - Pace of innovation
  - Mismatch between AI and Academia
  - No mathematical foundations
  - Driven by industry not govnt.



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# How can NAG help in ExaTEPP

# How NAG can help in ExaTEPP

- Connection with Industrial HPC
- Community, Network and Education
- Collaboration on PINNs or Bayesian Machine Learning
- Software engineering is the key, robustness
- Tuning and Library development
- Exotic architecture kernel / library development (.e.g dataflow)
- Cloud HPC accessibility
- Benchmarking suites
- Fortran Compiler, standard parallel fortran



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# Thank you

## Any Questions?



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