Entangled Worlds: Engineering, Physics, Applied Mathematics, and the Future of High-Performance Computing

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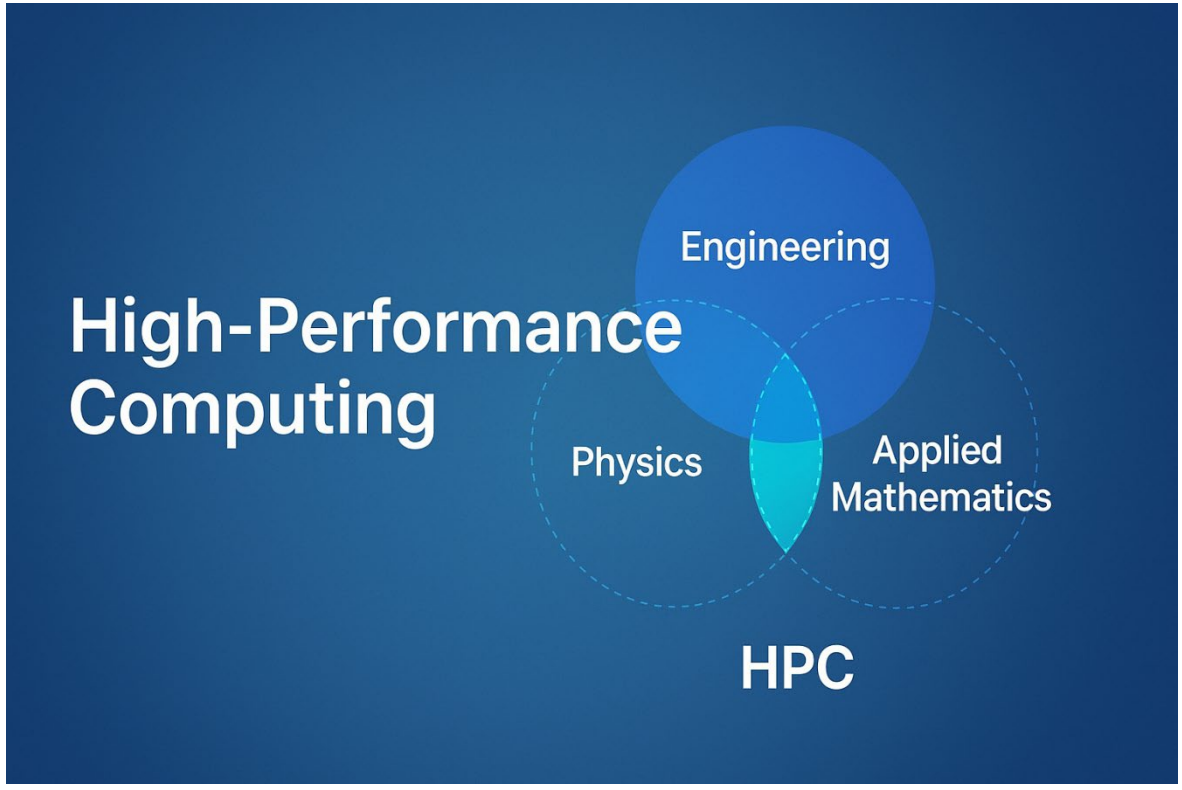
Three Worlds, One Thread

- My research spans engineering, physics and applied mathematics
- At first glance these fields look distinct
- But they share a core dependence on high-performance computing (HPC)
- This talk explores the entanglement of these disciplines through computational demands
- and how emerging technologies reshape what is possible

Computation is the bridge that unifies these domains.



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Why HPC Matters (Sits at the Centre of Modern Science?)

- Engineering simulations → **high-fidelity CFD**, structural analysis
- Physics → particle-level simulation, **detector modelling**, statistical inference
- Applied mathematics → **numerical linear algebra, PDE solving, optimisation**
- All require:
  - large-scale data movement
  - high-precision numerical stability
  - parallelisable algorithms
  - efficient memory and bandwidth usage
- Often methods developed in one solves problems in the other

They don't just overlap conceptually — they require the same computational architecture.

Common Computational Requirements Across Fields

- **Numerical Intensity:**
  - Dense linear algebra
  - Solvers with large iterative loops
  - Floating-point heavy workloads
- **Parallelism:**
  - Communicative intensive workloads
  - Embarrassingly parallel workloads (sometimes)
  - Domain decomposition
- **Low-Latency, High-Bandwidth Data Movement:**
  - Memory bandwidth is frequently the true bottleneck
  - Many algorithms saturate memory channels long before using full FLOP capability

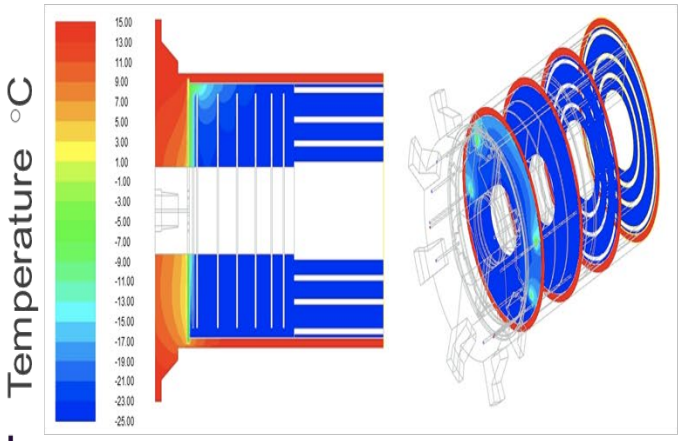
Memory Bandwidth: The Quiet Constraint

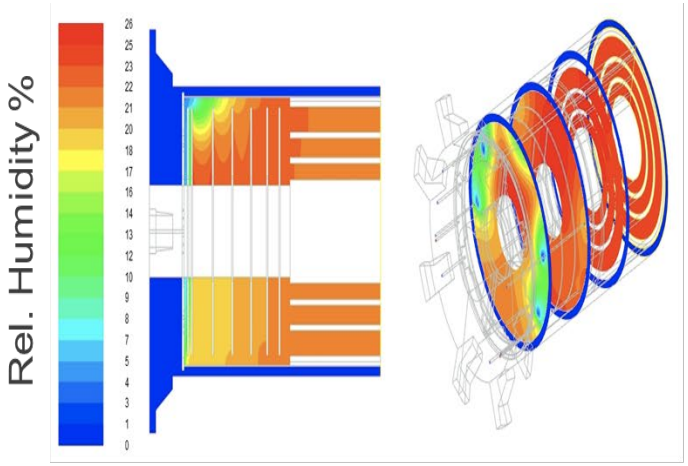
- In your research domains:
  - CFD → bandwidth-bound stencils and sparse matrices
  - Physics simulations → streaming large state vectors
  - Applied math → vector operations dominating compute

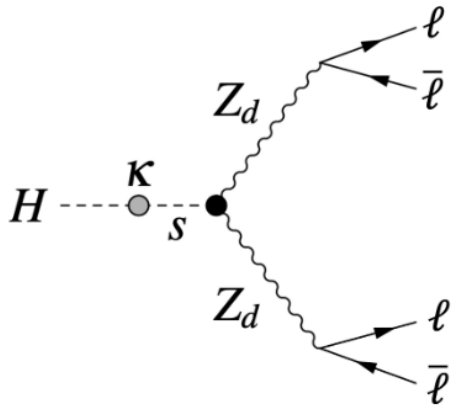
- Modern GPUs offer *massive FLOP capacity*, but performance can stall due to *insufficient data throughput*

Improving FLOPs alone does not guarantee performance; bandwidth determines scalability.

Case Insight (ATLAS ITk CFD Models)



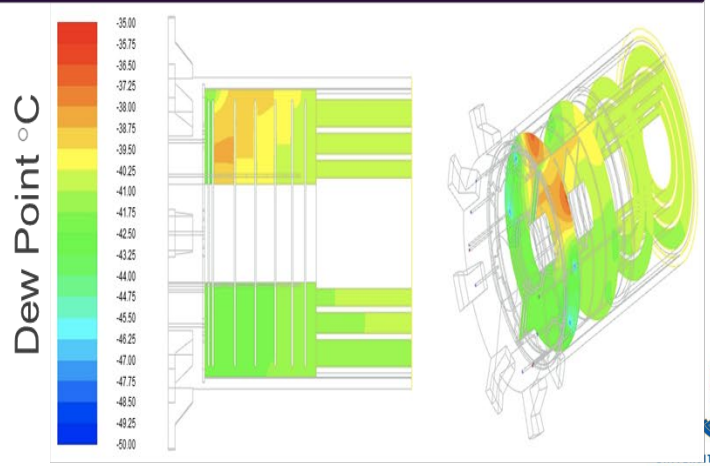




The Dew point was calculated using a the Bögel modification of the Magnus formula:

$$\gamma_m(T,RH) = ln\left(\frac{RH}{100}e^{\left(b-\frac{T}{d}\right)\left(\frac{T}{c+T}\right)}\right)$$

$$T_{dp} = \frac{c\gamma_m(T,RH)}{b-\gamma_m(T,RH)}$$



Three years of solver (algorithm) refinements by the software developer = double the discretisation (mesh) density

GPU Advances

- Tensor cores, mixed precision, sparsity acceleration
- Implications for my research areas:
  - Engineering: high-resolution real-time simulations
  - Physics: larger/faster data analysis/processing
  - Applied math: rewriting solvers to leverage tensorised operations
- “AI GPUs” – started (and continues) as *general-purpose scientific accelerators*

AI as Accelerator

- Surrogate models for CFD and physics simulations
- AI-guided optimisation and uncertainty quantification
- Neural operators enabling PDE solving without discretisation
- AI accelerates *pre-processing*, *post-processing*, and sometimes replaces expensive compute entirely (highly debated)

My view: AI expands—not replaces—classical HPC.

Emerging Questions: Is it Valuable? Does it help us find new phenomena?

Emerging View (amongst a minority): the true value of AI will be felt most in scientific applications and not in LLMs

Quantum Frontier

- Relevance (for me):
  - Engineering: optimisation, materials modelling, faster PDE/ODE solvers?
  - Physics: native quantum simulation, quantum sensing
  - Applied math: solving linear systems, eigenvalue problems
- Hybrid HPC + quantum workflows emerging
- Current limitations: error correction, noise = size of solvable problems
- But useful small-scale algorithms are beginning to appear – Lattice Boltzmann Method for CFD?

The next computation paradigm may be hybrid classical-quantum systems.

Democratisation of HPC

- Cloud-based HPC, national compute centres, GPU clusters shared across institutions
- Containerised workflows make HPC portable
- Open-source frameworks lower the barrier of entry
- More researchers can now:
  - run large-scale simulations
  - share reproducible pipelines
  - collaborate across geographic and institutional boundaries

Democratised HPC accelerates scientific progress across all fields.

Where These Worlds Meet

- Traditional boundaries
- Engineering: high-fidelity simulation and analysis
- Physics: data-intensive modelling and computation
- Applied Mathematics: developing/optimising numerical methods
- No longer the case:
  - adoption of data-driven and surrogate modelling in engineering.
  - (more) efficient numerical solvers – faster engineering solutions.
  - …..

- Unifying Thread: HPC as the foundation enabling precise modelling, better algorithms, and deeper insight.

Future Outlook: Entangled Progress

- Where the fields converge: Hardware innovation → GPUs → AI accelerators → quantum hybrids
- Algorithmic innovation → faster solvers
- Broader access to HPC → enabling more researchers, more innovation
- Interdisciplinary research will not be optional — it will be essential
- Engineering + Physics + Applied Mathematics + HPC = A unified scientific ecosystem
- My research operates at this nexus
- How advances in computation empower discovery across domains