

Quantum Enhanced Verified Exascale Computing

collaboration:

- ★ **Strathclyde**
- ★ **Durham**
- ★ **London Southbank**
- ★ **UCL**
- ★ **Warwick**

fundes and partners:



★ ExCALIBUR Cross-Cutting project:
<https://excalibur.ac.uk/projects/qevec/>
potential disruptor: quantum computing

current – NISQ* era – quantum computers
need near exascale classical to verify

⇒ challenge is to make this potential useful ⇐

[*NISQ = noisy intermediate-scale quantum]

⇒ *two use cases*: fluids sim and materials sim
systematic evaluation, identification, and
development of relevant quantum
algorithms for exascale subroutines

⇒ quantum VVUQ

⇒ methodology to apply to other use cases

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★ **Strathclyde:**

Viv Kendon (PI)

★ **Durham:**

Alastair Basden,
Stewart Clark,
Nicholas Chancellor,
Halim Kusumaatmaja

★ **London Southbank:**

John Buckeridge (KE)

★ **UCL:** Scott Woodley,

Richard Catlow,
Paul Warburton

★ **Warwick:** Animesh Datta

★ **Manchester** Steve Lind

★ **who we are** ★

- *RSEs/PDRAs in:*
 - quantum verification (Warwick – Theo Kapourniotis → NQCC)
 - quantum computing (Strathclyde – Rhonda Au-Yeung and Steph Foulds)
 - fluids simulations (Durham – Omer Rathore)
 - materials simulations (UCL – Bruno Camino)
- *related PhDs in:*
 - quantum simulations of plasma (Warwick)
 - hybrid quantum algorithms (Strathclyde – Lara Janiurek)
 - Accreditation and partition functions (Warwick – Andrew Jackson)

June 2023: **QuANDiE funded!** (Quantum Algorithms for Nonlinear Differential Equations) *Software for Quantum Computation call* funded through March 2025

QEVEC results so far:

- tutorial paper on using D-Wave for solid solutions:
Quantum computing and materials science: A practical guide to applying quantum annealing to the configurational analysis of materials
Bruno Camino, JB, PW, VK, SW, J. Appl. Phys. 133, 221102 (2023)
- quantum algorithm for core of SPH tested in 1D simulation:
Quantum algorithm for smoothed particle hydrodynamics
Rhonda Au Yeung, AW, VK, SL, Comp. Phys. Commun., 294, 108909 (2024)
- accreditation methods for quantum annealing and simulation
Accreditation of Analogue Quantum Simulators
Andrew Jackson, Theo Kapourniotis, AD, arXiv:2306.03060
- better classical algorithms:
Partition-function estimation: Quantum and quantum-inspired algorithms,
Andrew Jackson, Theo Kapourniotis, AD,
PRA 107, 012421 (2023)

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QEVEC work in progress:

in preparation:

- using D-Wave to optimise task scheduling – *Omer Rathore, AB, NC*
- (invited) review for Reports on Progress in Physics
Rhonda Au Yeung, BC, OR, VK
- using D-Wave for simulating real-world disordered materials and, review for Materials Chem – *Bruno Camino, ...*
- quantum predictor-corrector strategy *Omer Rathore, HK, NC, AB*
(use QPU to check if a costly classical solution step for $Ax = b$ is required)

current challenges ...

- viable encodings? *depends on required outputs from QPU; may lose advantage*
- training for application specialists?
enable quantum algorithm design by application experts

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QEVEC KE:

★ results made possible through KE:

bringing together a team with diverse knowledge and backgrounds

- 6-monthly team meetings focused on the science, to learn from each other and plan projects
- 3 workshops on fluid simulations (joint with CCP-QC) to collaborate with wider community [led to QuANDiE funding]
- attending PAX-HPC and SEAVEA meetings to share progress
- Scientific Applications of Quantum Computing: meeting at LSE Bankside 22nd September 2023 covering biology, chemistry and materials simulations

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