Quantum Computing in the Pharmaceutical Industries

Workshop Summary

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Newton Gateway to Mathematics

Quantum Computing in the Pharmaceutical Industry

Isaac Newton Institute, Cambridge

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Experts from the fields of quantum computing and the pharmaceutical industry were brought together to discuss potential applications of the former field in the latter. The aims of the day included understanding:

- the stages of drug development, where computational chemistry methods are used and their limitations;
- methods for performing computational chemistry calculations on a classical computer and how well they perform;
- the types of problems to which quantum computers are well suited and how these relate to the pharmaceutical industry;
- the current state of quantum computers and time scales on which they are developing.

Quantum Computing Landscape

Ilana Wisby and *Andy Patterson (Oxford Quantum Circuits)*

- Variety of technologies exist e.g., superconducting systems, trapped ions, photons, silicon. Each have advantages and disadvantages.
- Internal errors will remain significant in the near term but can mitigate by, for example, changing the error rate in a controlled manner and extrapolating to infer low-error results.
- Importance of bridging the gap - getting industry quantum ready, developing cross-disciplinary skills, demonstrating technology, identifying and developing end-use applications, building and developing quantum ecosystem.

Quantum Software

Steve Brierley (Riverlane)

- Quantum computers offer an exponential speed-up over classical computers for computational chemistry problems.
- Many possible applications - calculation of potential energy surfaces (for e.g., catalyst development), simulation of quantum dynamics, calculation of excited state energies (for e.g., calculating band gaps of battery materials), geometry optimisation (to find stable configurations), calculation of relativistic effects, simulation of molecular vibrations.
- Both quantum computer hardware and software are improving at exponential rate. Potential for demonstration of quantum advantage within the next few years.

Drug Discovery Pipeline

Darren Green (GlaxoSmithKline)

- Process typically takes 12-14 years. Involves identifying a target (e.g., a gene), identifying a protein, searching the compound library (with about 2 million entries) for a candidate, screening and identifying a lead, lead optimisation (making changes to molecules), testing of efficacy and safety in animals and humans. 95% failure rate at lead optimisation stage.

- Lead optimisation is a multi-objective optimisation cycle - must consider potency, safety, absorption, metabolic stability, solubility.
- Typically takes 2-7 years. 100 000s of molecules considered.
- Current challenges - predicting toxicology, modelling permeation and active transport, predicting metabolites.
- Outside drug discovery, materials and catalyst development of interest to reduce carbon footprint.

Simulation on a Classical Computer

Mike Payne (University of Cambridge)

- Biochemical simulation faces significant challenges - very high accuracy is required, and thousands or millions of configurations must be sampled.
- Some classical methods perform well in certain situations and can provide useful data.
- Full Configuration Interaction - high level of accuracy but can only consider tens of atoms.
- Empirical interatomic potential simulations - ignore quantum effects and so can be used to simulate relatively large systems. Despite approximations, can provide useful data for biochemical processes e.g., when performing optimisation, rough gradient which gives approximate descent direction can be informative.
- Density Functional Theory can also work well. Time scales linearly with system size. 2500 atoms take approximately 55 hours to simulate.
- Multiscale modelling schemes could offer advantages.

UK Funding Landscape

Roger McKinlay (Innovate UK)

- National Quantum Technologies Programme has provided approximately £400m of funding so far. Encouraged collaboration with industry.
- “Commercialising Quantum Technologies” project in Industrial Strategy Challenge Fund wave 3 - government hopefully to provide £70m over three years then rising to a total of £153m over 6 years contingent on industry funding of £205m. Includes quantum computing and simulation.
- National Quantum Computing Centre (NQCC) to be set up - suggested to be an open environment to encourage partnering with industry and to provide a testing ground.

Panel Session

Chair: Roger McKinlay

Panellists: Ilana Wisby, Andy Patterson, Steve Brierley, Darren Green, Mike Payne, Sir Peter Knight (Imperial College and *Innovate UK)*

- Follow-up on NQCC. Aim to provide a “comfort zone” for startups to share and retreat as required. Options are still being explored so input welcome.
- Desire to see industry taking long term interest and being willing to invest.
- To help businesses develop - framework for collaboration and demonstration. Assets required for hardware developers. Again, receptive to suggestions.

- Roadmap for computational chemistry demonstrations on a quantum computer - good understanding of hardware required, proof of concept demonstrations, going beyond as capabilities improve (e.g., molecular dynamics).
- Discussion of whether “critical point” in quantum computing has been reached. Have not yet seen rapid acceleration of progress as can be seen with a paradigm shift, but significant improvements have been made in, for example, the fidelity threshold required for error correction to occur.
- Consideration of whether technology or application should come first. For example, telecoms industry initially funded semiconductors for use in hearing aids, but they went on to be used far more widely. Perhaps a “quantum hearing aid” is needed.
- Importance of focussing on industry-aligned problems highlighted in order to attract investment.