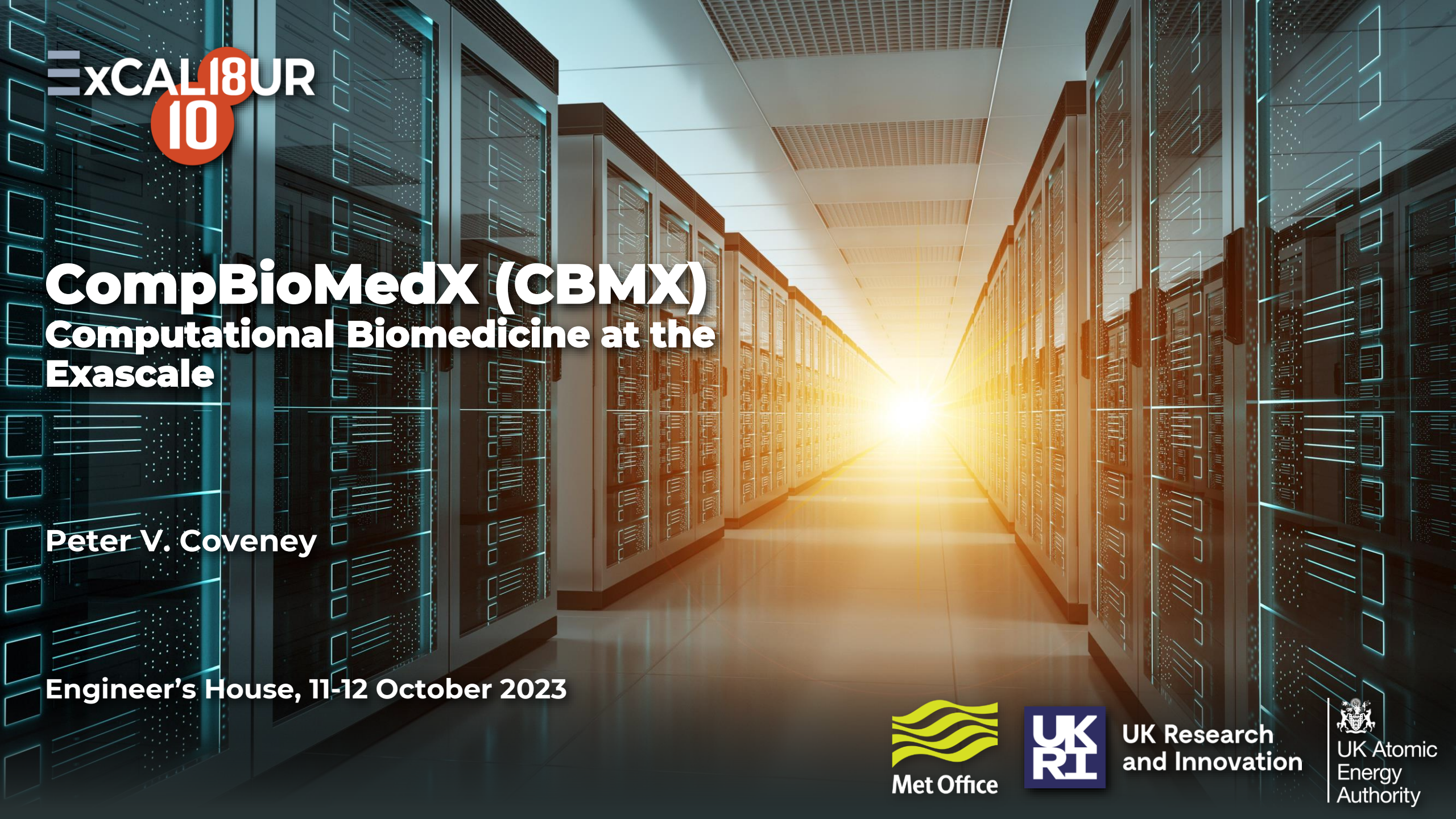


CompBioMedX (CBMX)

Computational Biomedicine at the Exascale

Peter V. Coveney

Engineer's House, 11-12 October 2023

Met Office

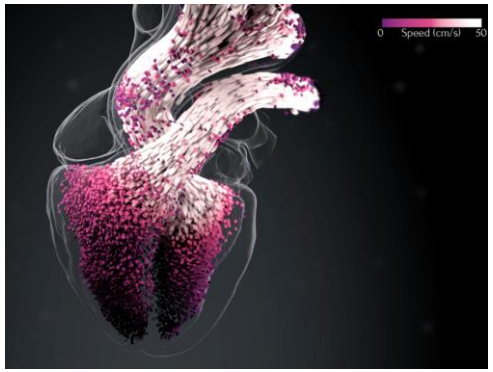
UKRI UK Research and Innovation

UK Atomic Energy Authority

Project Overview

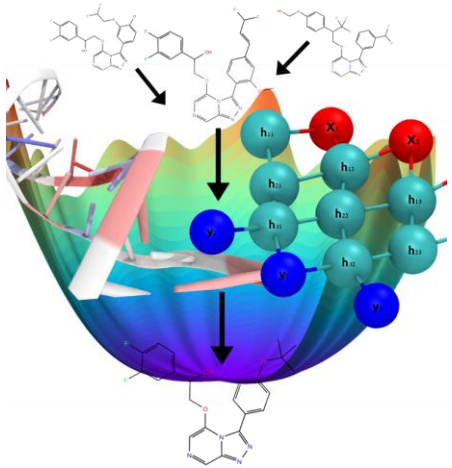
Key areas of computational biomedicine

Digital Twin of Human



Cardiac Simulations

Vascular Modelling



Accelerated Drug Discovery and Personalised Medicine

Participants and partners

UCL
Brunel University London
University of Oxford
Rutgers
evotec
Atos
Cancer Research UK
University of Southampton
NHS University Hospital Southampton NHS Foundation Trust
Universidade Federal de Juiz de Fora
arm
AMD
DiRAC
NVIDIA
AstraZeneca
SURF
Dassault Systèmes
Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften
Science Museum
Oxford University Hospitals NHS Trust
NIHR National Institute for Health Research
Barcelona Supercomputing Center Centro Nacional de Supercomputación
ExCALIBUR

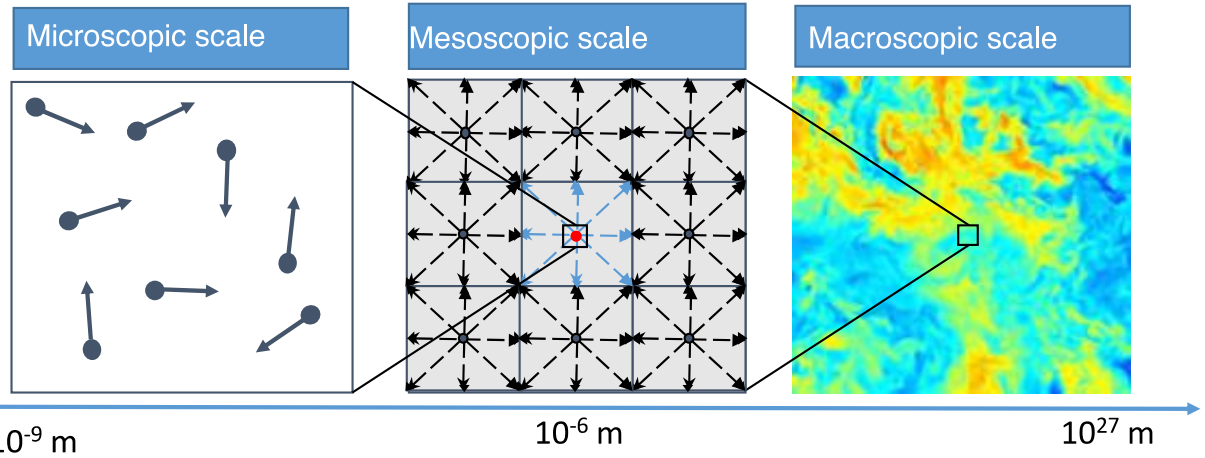
Project Status

HemeLB meet Frontier

- Lattice Boltzmann solver
- Massively paralleled high-performance code
- Available on both CPU and GPU (CUDA/Hipified)
- Designed for sparse geometry, ideal for hemodynamics simulations

The world's only exascale machine. Access to it, a pathway that has gone via Titan, BlueWaters, and then Summit.

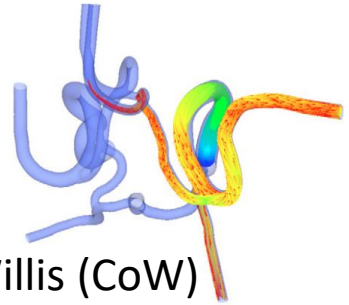
The lattice Boltzmann method



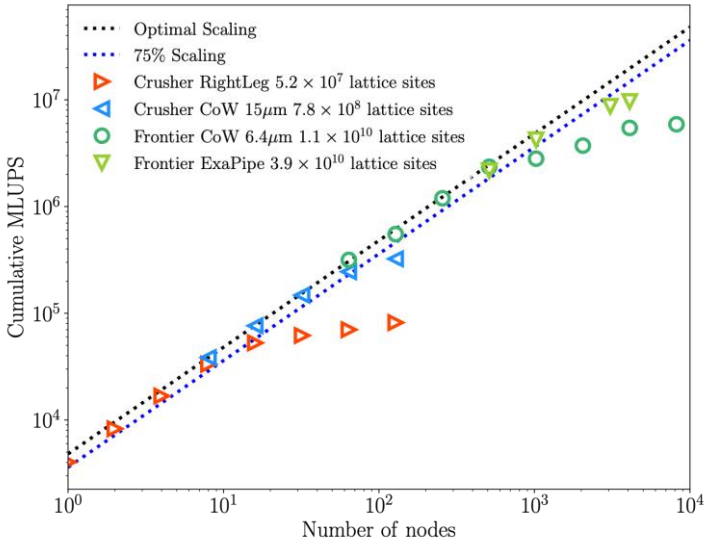
Frontier strong scaling plots

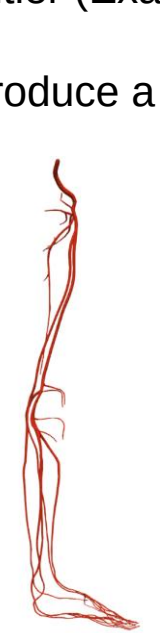
Full-human scale simulation requirements

- 140 billion lattice sites (1.4×10^{10})
- Full deployment on Frontier (Exascale computing)
- A few cardio cycles to produce a high-fidelity simulation

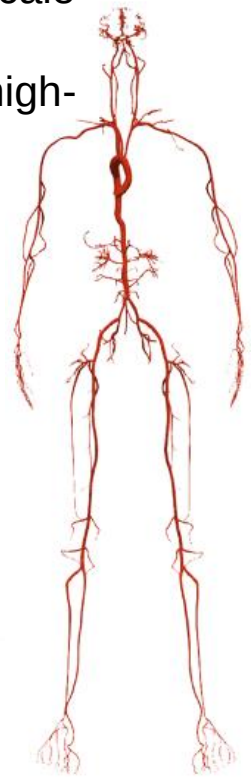


Circle of Willis (CoW)





Human Right leg



Full-human scale arterial system

Project Status

HemeLB_GPU: Towards a platform agnostic HemeLB_GPU from CUDA to HIP and oneAPI

HemeLB_GPU code – Port to oneAPI

- Single HemeLB collision-streaming CUDA kernel ported to **Intel's oneAPI** (SYCL/DPC++)
- Ongoing efforts to port the full code to **oneAPI**
  - Deploy HemeLB_GPU on NVIDIA, AMD and Intel GPUs
- **Preparing for Aurora** (ALCF's forthcoming exascale system)

Data **P**arallel C++ **C**ompatibility **T**ool

Port to oneAPI approach:

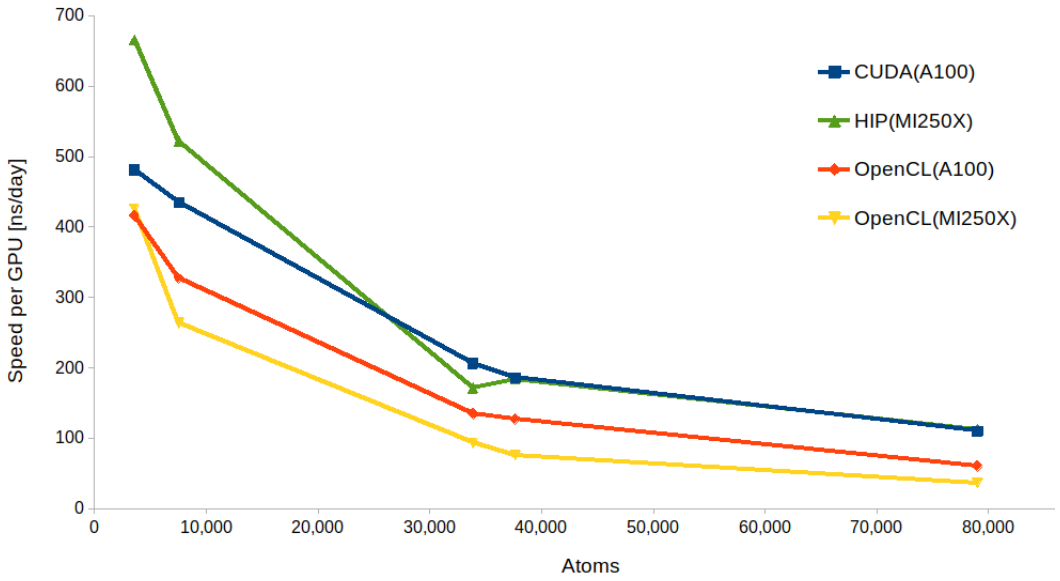
- **Both with Intel DCPT Porting tool**
  - Testing on Sunspot (**ALCF** - 2x Intel Xeon CPU Max Series (Sapphire Rapids) and 6x Intel Data Center GPU Max Series (codename Ponte Vecchio or PVC).
  - Compiles – Unstable... Debugging... Step by step approach - Focus on Initialisation and then one kernel at a time...
- **Using factor based approach**
  - Factor out the CUDA-specific parts of the code into back-ends:
  - Working for CUDA, HIP
  - **SYCL/DPC++ up and running on Frontier (OLCF)**
    - Unstable on Sunspot... Debugging in progress...

- Single source files – Reduce code duplication
- Simplifies code maintenance

Project Status

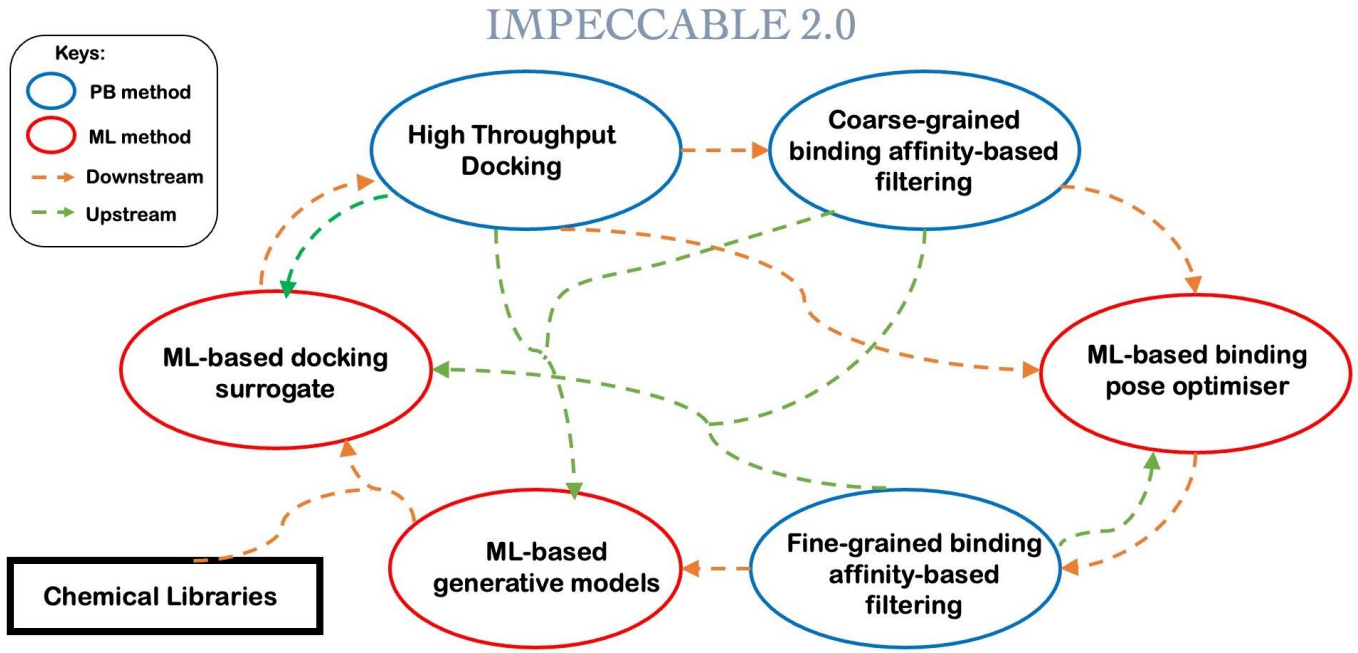
Accelerated Drug Discovery and Personalised Medicine

TIES benchmarks on exascale testbed systems



Performance comparison of TIES running on Polaris (A100) and Crusher (MI250X). All speed tests are performed with OpenMM 7.7.

IMPECCABLE 2.0 Workflow - Accelerating COVID-19 drug discovery



Physics and machine learning based methods are used symbiotically to test drugs with required accuracy and efficiency.

Current Challenges

- **Technical challenges:**

Implementation Challenge:
Full implementation of NAMD on Frontier
- Alchemical kernel not working on GPUs of Frontier (yet)
- Need one “srun” command for each task to a single GPU
- The number of “srun” commands in one submission is limited

Implementation of complex and heterogeneous workflow
- Workload: Task mix varies over campaign
- Tasks: Run for varying duration

- **People barrier:** There is an insufficient number of people available in UK with the right training and skills.

- **Funding barrier:** There is insufficient funding available to sustain the threadbare efforts which we are currently undertaking.

Algorithm Challenge: HemeLB – it is challenging to resolve high Reynolds number blood flows coupling sparse geometry interacting with hemodynamic solver

Computing Challenge: Current status of Frontier is not fully stabilised yet (jobs may fail randomly after long queue)

Storage Challenge: Exascale computing is storage demanding (lack of storage space may lead to failure in running exascale jobs)