Climate DT + Quantum?

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Intro: Quantum Computing

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What is a quantum computer *not*?

A quantum computer is *not* a super-fast version of a classical computer —

It is *different*

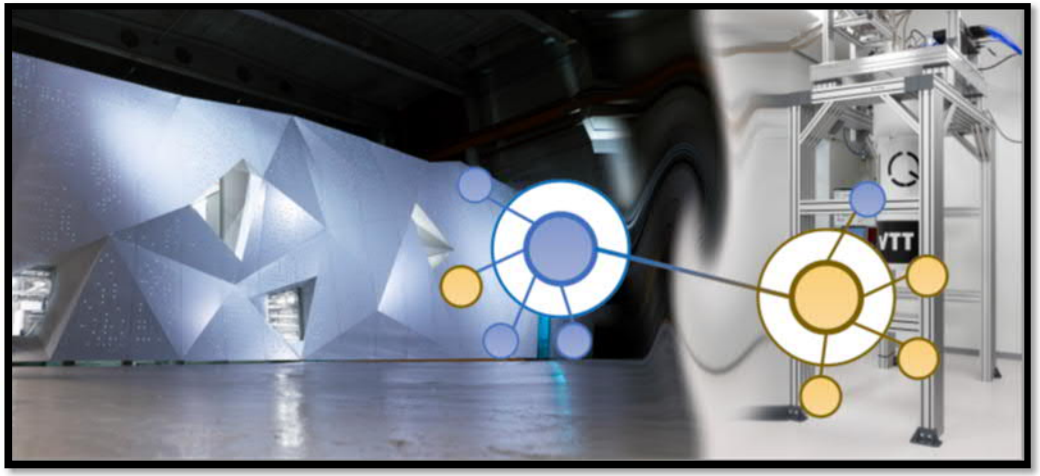
Speeds up *some* types of calculations, others not at all

Connecting supercomputers with quantum computers

High-Performance Computing + Quantum Computing (HPC+QC)

Quantum acceleration

- Quantum computers are performing computations in a **completely different manner**
- **For *some* types of calculations**, QC can potentially speed up calculations significantly
- **For most types of calculations**, QC provides *no* advantage over classical computing



LUMI and Helmi
Available for users since 2022

→ **Hybrid HPC+QC is the future!**

- Quantum computers will merge with supercomputers, *both need each other*

Intro: Climate DT

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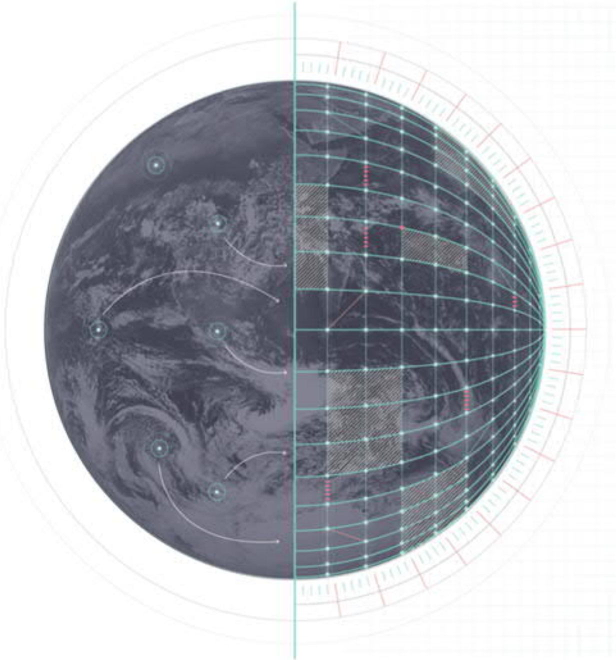

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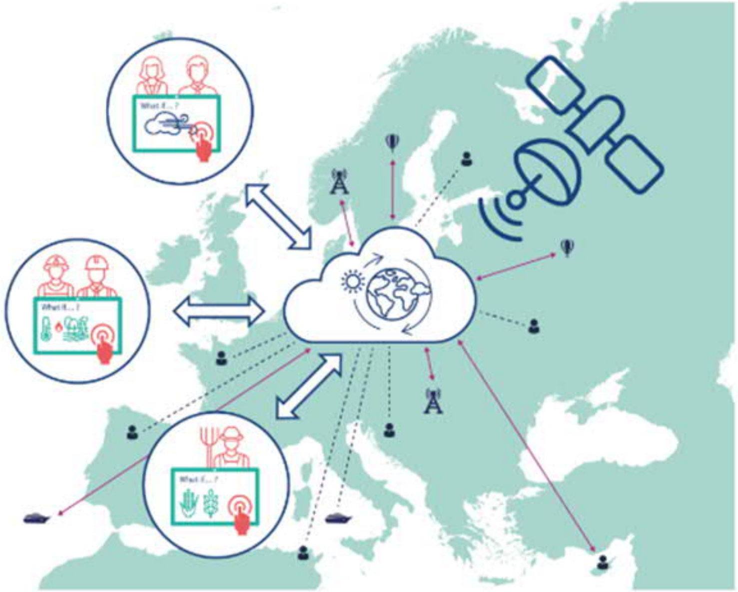
DESTINATION EARTH

Climate Change Adaptation Digital Twin to support decision making

Funded by the European Union Destination Earth implemented by ECMWF esa EUMETSAT

DESTINATION EARTH PROGRAM

- **European Commission's program developing Digital Twins (DTs) of the Earth** to support decision-making
    - Target: full digital replica of the Earth by 2030
- **Implemented by ESA, ECMWF, and EUMETSAT** through procurements
- Climate change adaptation DT is one of the first being developed
    - to **assess** the **impacts** of climate change and different adaptation strategies at **local** and **regional** levels over **multiple decades**;
    - during phase 1, multi-decadal simulations on a 5 km global mesh;
    - utilizing two climate models, IFS-FESOM/NEMO and ICON, at its core



https://digital-strategy.ec.europa.eu/en/policies/destination-earth

CLIMATE DT TEAM

Name	Organisation	Country
CSC	**CSC – IT Center for Science**	**FI**
BSC	Barcelona Supercomputing Center/Centro Nacional de Supercomputación	ES
MPI - M	Max Planck Institute for Meteorology	DE
UH	University of Helsinki	FI
AWI	Alfred Wegener Institute, Helmholtz Centre for Polar and Marine Research	DE
CNR-ISAC	Consiglio Nazionale delle Ricerche, Istituto di Scienze dell'Atmosfera e del Clima	IT
POLITO	Politecnico di Torino	IT
FMI	Finnish Meteorological Institute	FI
DWD	National Meteorological Service of Germany	DE
UFZ	Helmholtz Centre for Environmental Research	DE
UCLouvain	Université catholique de Louvain	BE
DKRZ	German Climate Computing Centre	DE
HPE	Hewlett Packard Enterprise	FR

- 13 European organizations with expertise in climate modelling, impact assessments & high performance computing

TYPICAL EARTH SYSTEM MODEL

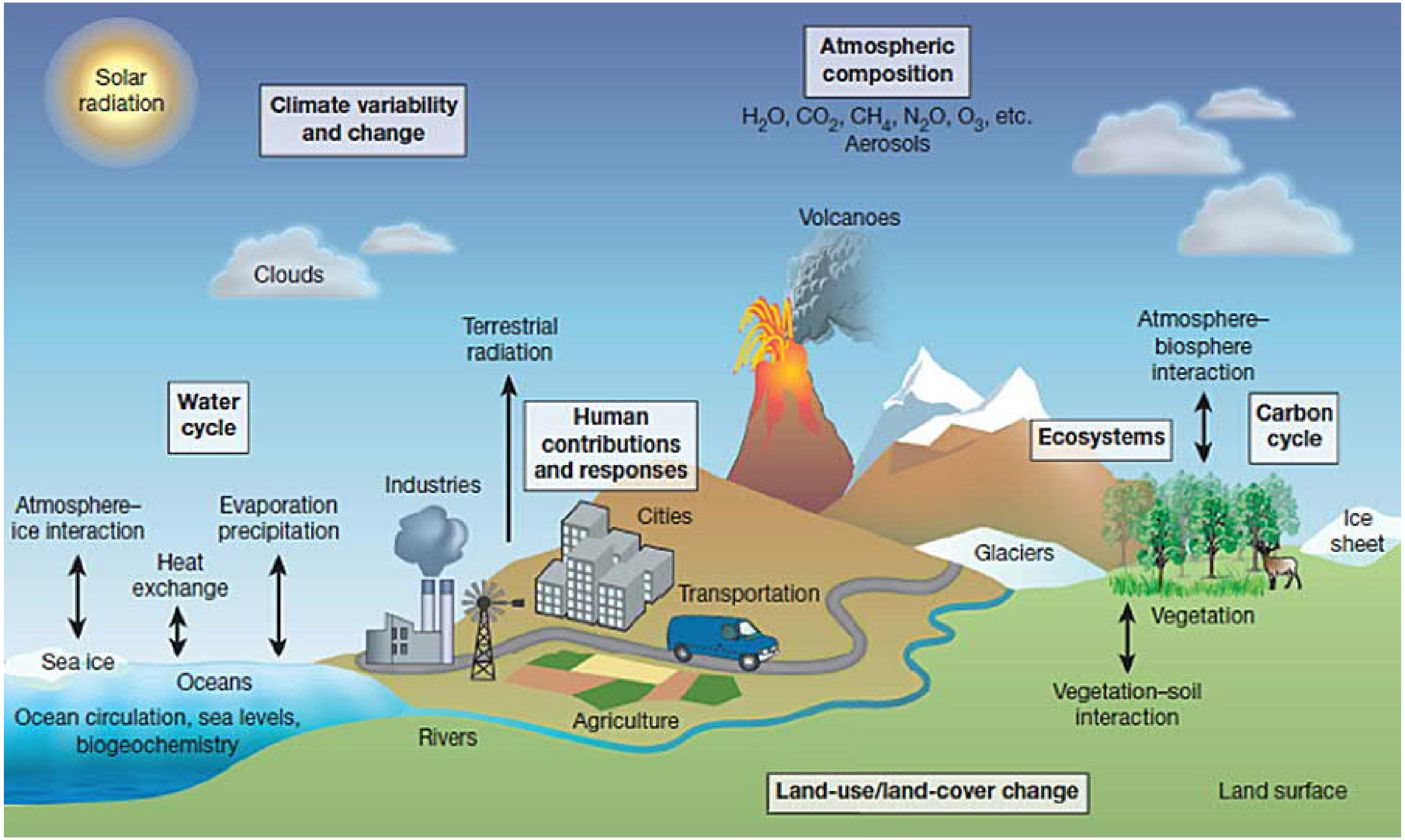


Figure from U.S. Climate Change Science Program. Strategic Plan for the Climate Change Science Program, Final Report (eds Subcommittee on Global Change Research) Figure 2.5 19 (US Climate Change Science Program, Washington DC, 2003).

MAJOR COMPONENTS OF A TYPICAL ESM

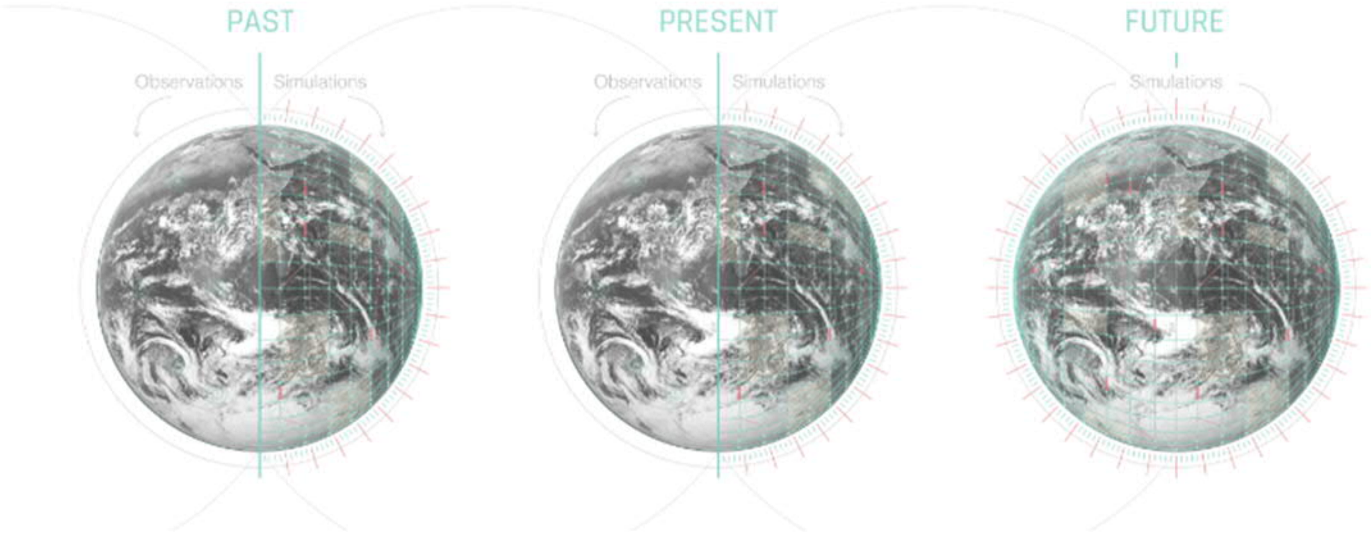
- **Atmosphere (~90%)**
- Temperature, humidity, and pressure profiles
- Wind patterns and circulation
- Radiative transfer, including solar and infrared radiation
- Cloud formation and dynamics
- Atmospheric chemistry, including greenhouse gas concentrations

- **Ocean (~10%)**
- Sea surface temperature and salinity
- Ocean currents and circulation patterns
- Thermohaline circulation (e.g., the Gulf Stream)
- Heat and carbon dioxide uptake and release

- **Land surface**
- Surface temperature and moisture content
- Vegetation and land cover types
- Soil properties and dynamics, including moisture and nutrient content
- Land use changes and human impacts (e.g., deforestation, urbanization)

WHAT DOES THIS HAVE TO DO WITH QUANTUM?

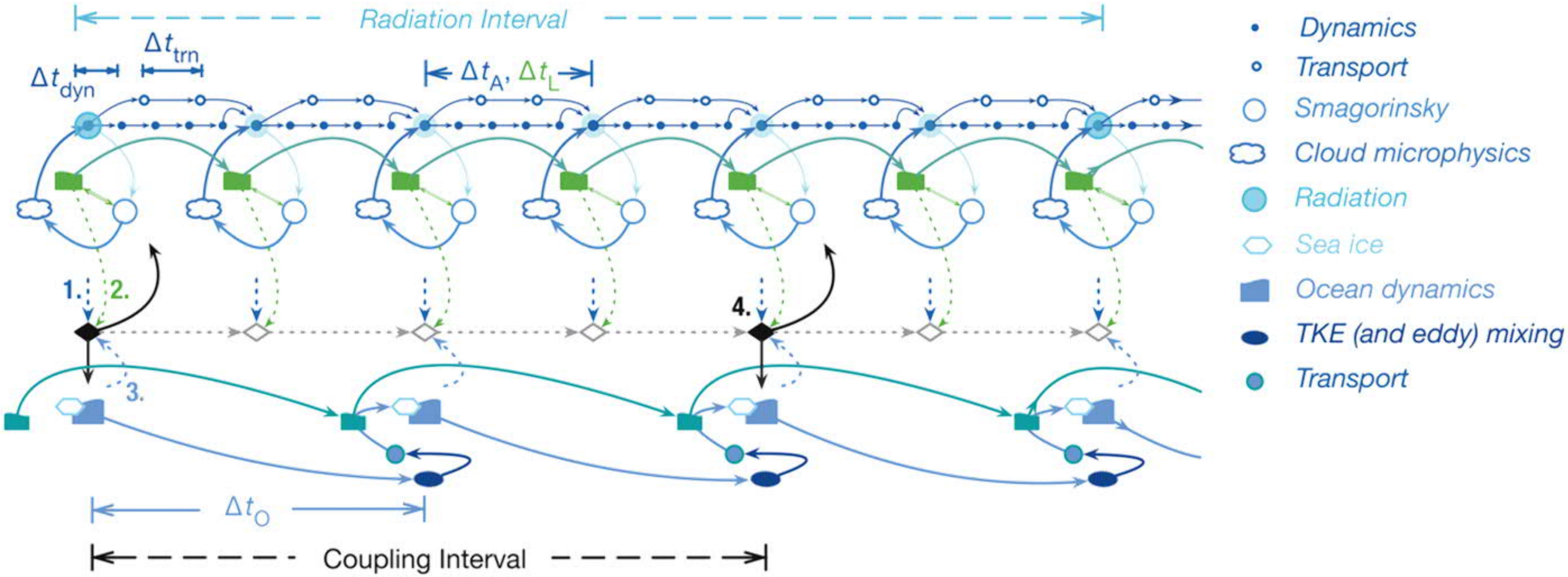
- **ClimateDT** is a new type of data-intensive **climate information system** based on high-resolution climate simulations, impact modeling and high-performance computing
- The simulations contain a plethora of **calculations** (*e.g.*, fluid dynamics) that could **potentially benefit** from **quantum** computing
- **Higher resolution** additionally exposes the simulations to **smaller scale physics and processes** (*e.g.*, clouds and atmospheric chemistry)



Climate DT + Quantum?

Quantum perspective on climate modelling

Time-stepping in a climate model (Hohenegger *et al., Geosci. Model Dev.* 2023)



- There is roughly a 1:30 ratio between the shortest and longest time steps
- The wall-time for computing the individual time-steps range from the **subsecond regime** to around 10 s on the LUMI supercomputer

Quantum perspective on climate modelling

Some observations om the present Climate DT workflows

- Amount of data is huge
- Already with a grid resolution of 10 km, the total number of grid points representing the atmosphere is in the hundreds of millions
- Each grid point has several associated variables:
  - air density, temperature, wind speed, humidity, *etc*.

We can now identify two main challenges that hamper direct adoption of QC

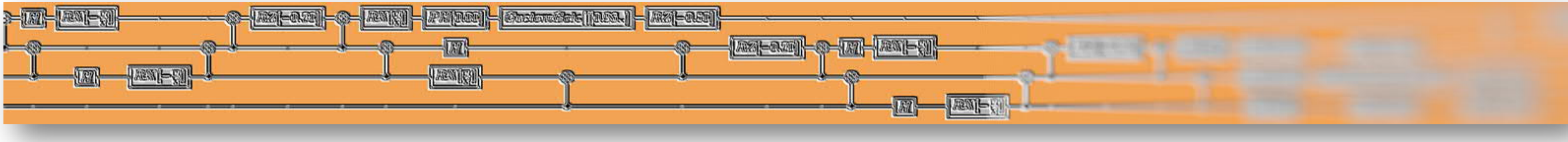
1. "Big data" problem
2. Short wall-time for individual calculations

1. “Big data” problem

- Climate models work on a large amount of data Both as input and output
- These “big data” problems are not directly suitable for quantum computers
- QC is good with problems with a *moderate* amount of both input and output variables
- The **relation** between input and output should be a **highly complex equation** that can be solved efficiently by some quantum algorithm
    - QC typically excels at problems with a **large potential solution *space***, but only a small set or even **a single solution**
    - Additionally, the input parameters need to be of the same order of magnitude as the number of qubits of the quantum computer

2. Need to solve sufficiently complex problems in very short time

- For quantum advantage (measured by time-to-solution), QCs need to solve **sufficiently complex algorithms**
  - Algorithms have to be **sufficiently deep**, *i.e.*, the number of basic operations needs to be high

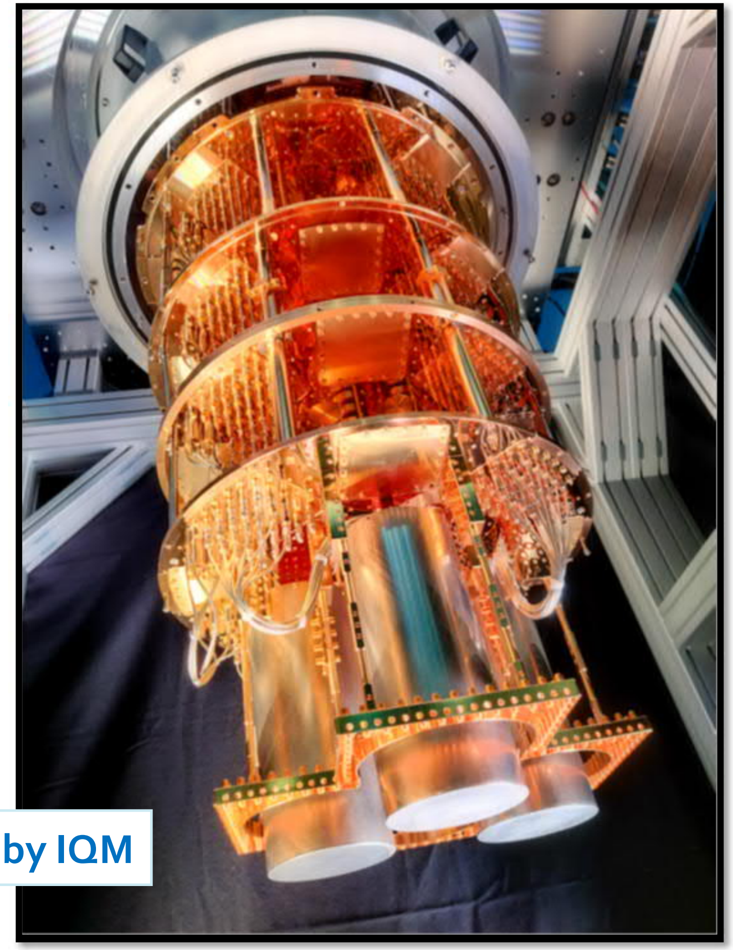


  - In practice, this means that **single *useful* quantum calculations** will take on the order of **seconds to complete** (minimum)
    - Individual variational circuits are faster, but the wall-time to solution is much longer, as several iterations are needed
  - On the other hand, *already now*, the shortest individual time-steps in Climate DT take < 1 s, and the longest ~10 s
  - The aim of Climate DT is to speed up the individual time-steps by a factor of one hundred

→ **Quantum computers cannot speed these up further**, as they are already faster than the fastest useful QC calculation

So what then?

- At a first glance, climate models seem to be rather unsuitable for quantum acceleration…
- For **quantum advantage**, we need to consider the problem from a broader perspective
  - Attempting to make quantum versions of present classical algos and their inherent approximations **will not work**
- **In the medium-term**, advantage can only be found by approaching the problem from new angles, utilising the unique features of QC
- **In the long-term**, when (fault-tolerant) Quantum Processing Units (QPUs) are integrated onto the same chip as classical processing, they might be able to work as co-processors executing useful tasks on subsecond time-scales
  - We cannot just wait-and-see whether and when this happens



Quantum computer by IQM

Computational fluid dynamics (CFD)

A large part of current workflows are in effect CFD

- Direct connection to solving linear systems of equations
- Thus, the Harrow, Hassidim, and Lloyd (**HHL**) quantum algorithm (and its refinements) have the potential to speed up also CFD

- As noted by Lapworth (2022) classical algos on supercomputers are highly efficient at solving matrix equations by, *e.g.*, side-stepping the need for matrix inversions
- Quantum algorithms do not need to, even *should not* rely an the same approximations as classical algorithms!
  - For example, HHL and the Quantum Singular Value Transformation (QSVT) can efficiently perform direct matrix inversions → no need to circumvent the problem anymore

Enhancing machine learning

Use of machine learning (ML) and artificial intelligence (AI) is increasing also in climate modelling and digital twins of the Earth

- For CFD, a promising approach is to decrease the grid size without losing accuracy, by using ML for interpolation

Quantum machine learning (QML) has potential advantages

- Need to remember that classical ML is immensely powerful
- Instead of speed-up, advantage from doing things *differently*
  - *Potential* to get by with less training data, or getting more accurate models by adding quantum layers to a neural network

Missing ingredients in the model – “forced approximations”

Some physical/chemical/dynamical processes are left out because they are too expensive to model

- Quantum computing could reduce the computational complexity sufficiently to include more parameters and additional physics in the models

Atmospheric chemistry

- Accurate modelling of atmospheric chemistry would be highly beneficial

  ”climate models indicate at least a 30% uncertainty in aerosol direct forcing and 100% uncertainty in indirect forcing due to aerosol–cloud interactions”, Li *et al.* (2020)

- **Highly challenging to model**: radicals, multireference, photochemistry, …
  - **Scales exponentially** with the size of the problem in the limit of sufficient accuracy
  - **Perfect problem for quantum computers!**

Summary and musings

In their present form, digital twins of the climate are largely not amenable to quantum acceleration

- large amounts of input and output data
- short wall-time of the individual time steps

Still, quantum computers have the potential to enhance climate digital twins through:

- smart use of quantum algorithms
- enhancing machine learning
- introducing missing physics and chemistry to the models

We need to start making the workflows quantum-ready

- **A truly multidisciplinary problem**: combine knowledge of mathematics, quantum physics, and computer science **with the application field!**
- **Crucial for HPC and quantum to work together**
    - Identify the problems that are a bottleneck due to slowness/low accuracy on classical HPC
    - **Figure out how to quantum-accelerate:** *very hard, very rewarding!*

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