CAPE-OPEN REST-API
(Whitepaper Draft Presentation/Proposal)

Content

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- Some quick notes about MQS
- What is a REST-API?
- Kubernetes
- How to adapt a REST-API to COBIA, or at least some ideas we have
- Some thoughts about parallelization, mainly MPI for now

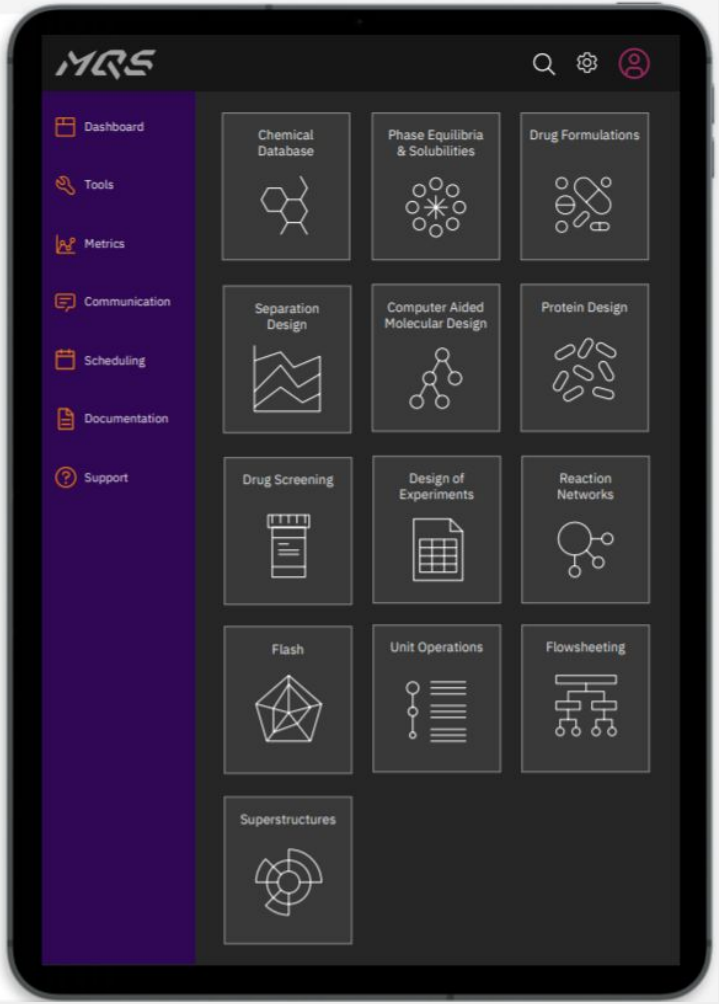
Objectives of MQS

- A multi-scale simulation platform to combine quantum chemistry and machine learning with upper-layer use-case applications
- Bottom up approach to design a software platform which makes use of distributed resources: CPUs, GPUs, FPGAs, QPUs
- API-driven software development
- Connectivity to laboratories/process plants and simulation software

A custom portfolio dashboard of industrial tools

at a flexible license price

in the cloud.



Companies and tools

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Cheméo
High Quality Chemical Properties

whitson

DWSIM

PubChem

TLK ENERGY

What is a REST-API?

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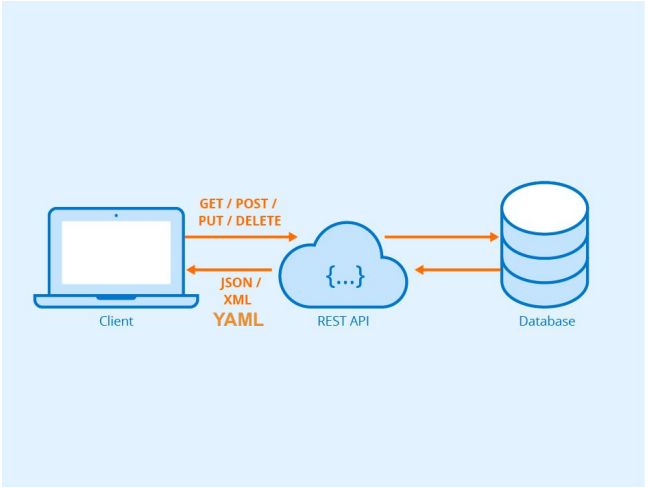
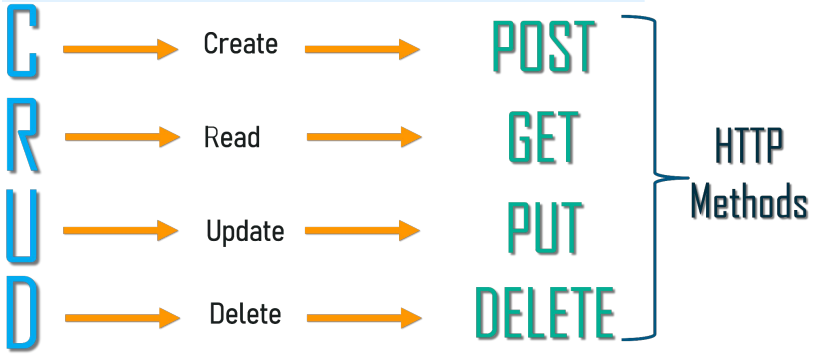
REST (Representational state transfer)

- Not a standard as CAPE-OPEN. It is an architectural style but RESTful implementations make use of standards, such as HTTP, URI, JSON, and XML.

API (Application Programming Interface)





Cybersecurity

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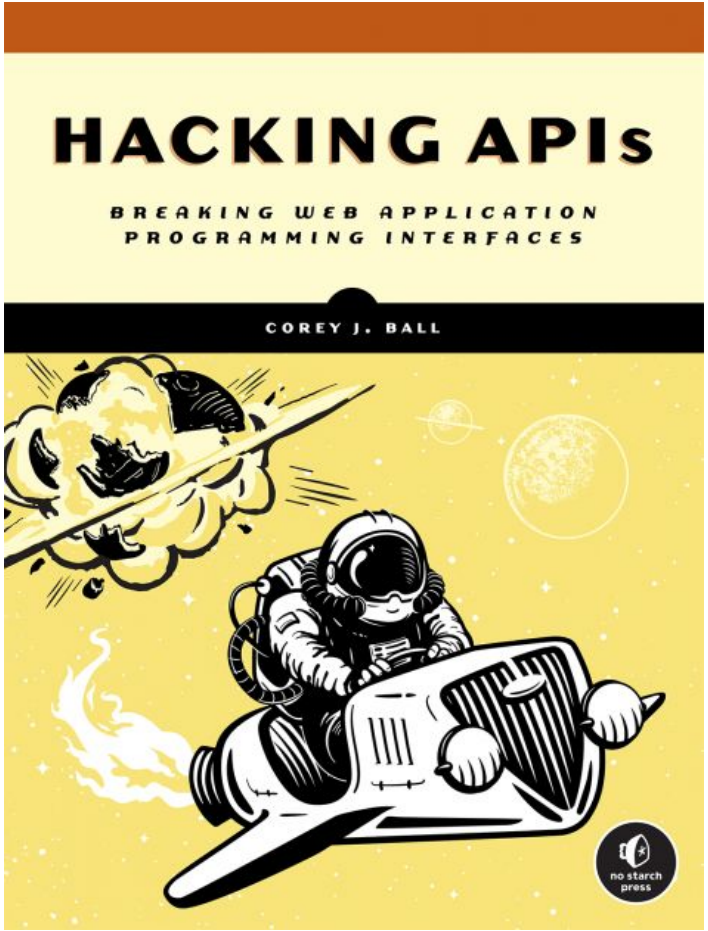

Kubernetes: Container Orchestration

“More than 75% of global organizations will be running containerized applications in production”
2022 Gartner report (https://www.gartner.com/smarterwithgartner/6-best-practices-for-creating-a-container-platform-strategy)

“Today’s researchers estimate that application programming interface (API) calls make up more than 80 percent of all web traffic.” Corey J. Ball - Hacking APIs

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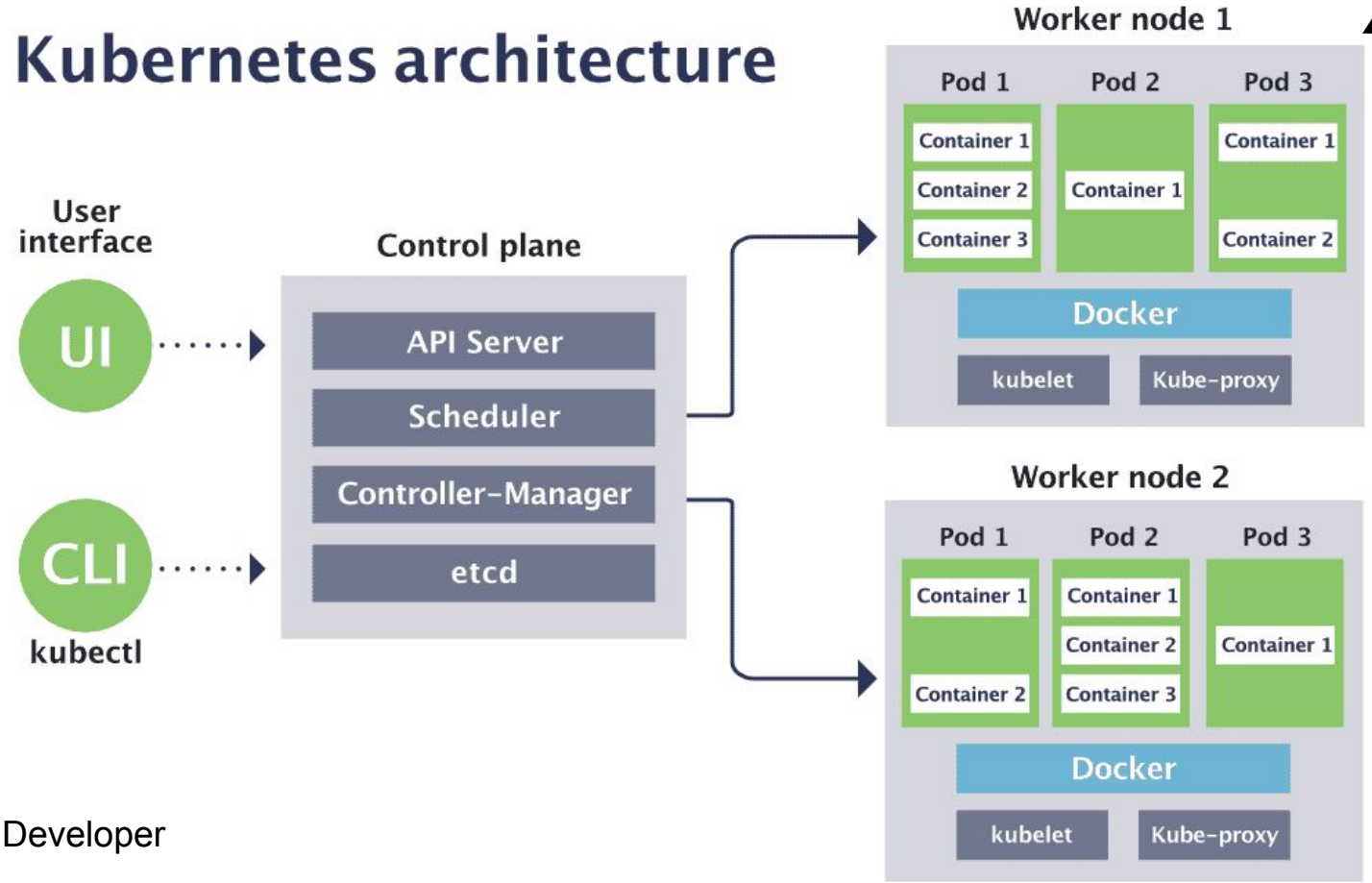
Kubernetes architecture



User

Developer

Hybrid Cloud

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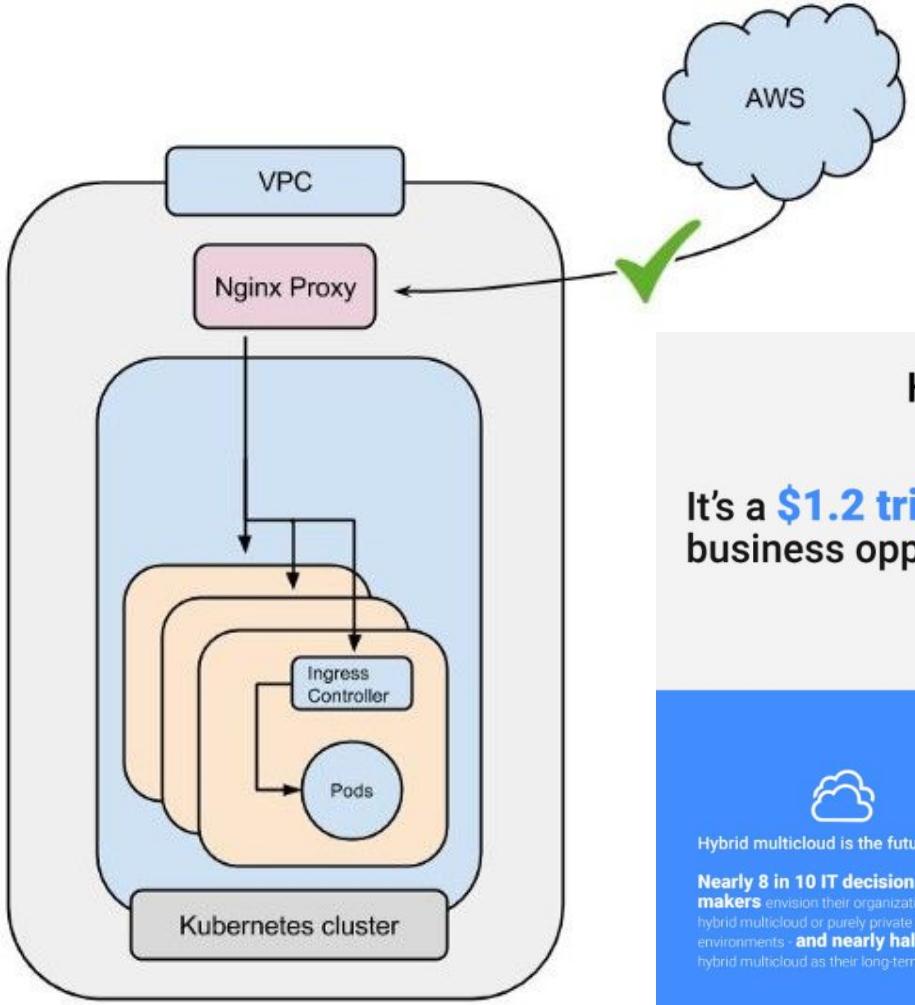
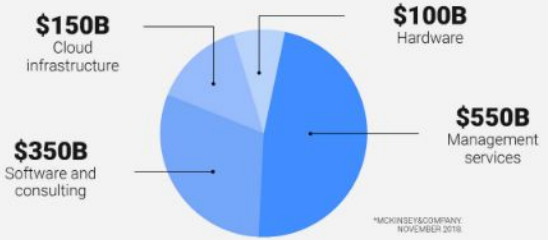


Hybrid Cloud By the Numbers

It's a **$1.2 trillion*** business opportunity



Business priorities are clear:

Hybrid multicloud is the future

Nearly 8 in 10 IT decision makers envision their organization using hybrid multicloud or purely private cloud environments - **and nearly half** see hybrid multicloud as their long-term solution.

Vendor lock-in is a huge concern

86% of IT decision makers say vendor lock-in by a cloud provider is a key concern in their purchasing decisions.

Security is number one

Nearly 6 in 10 IT decision makers rated security the #1 attribute when determining a cloud provider.

According to Data from IBM and MORNING CONSULT

Cloud Infrastructure and Industry 4.0

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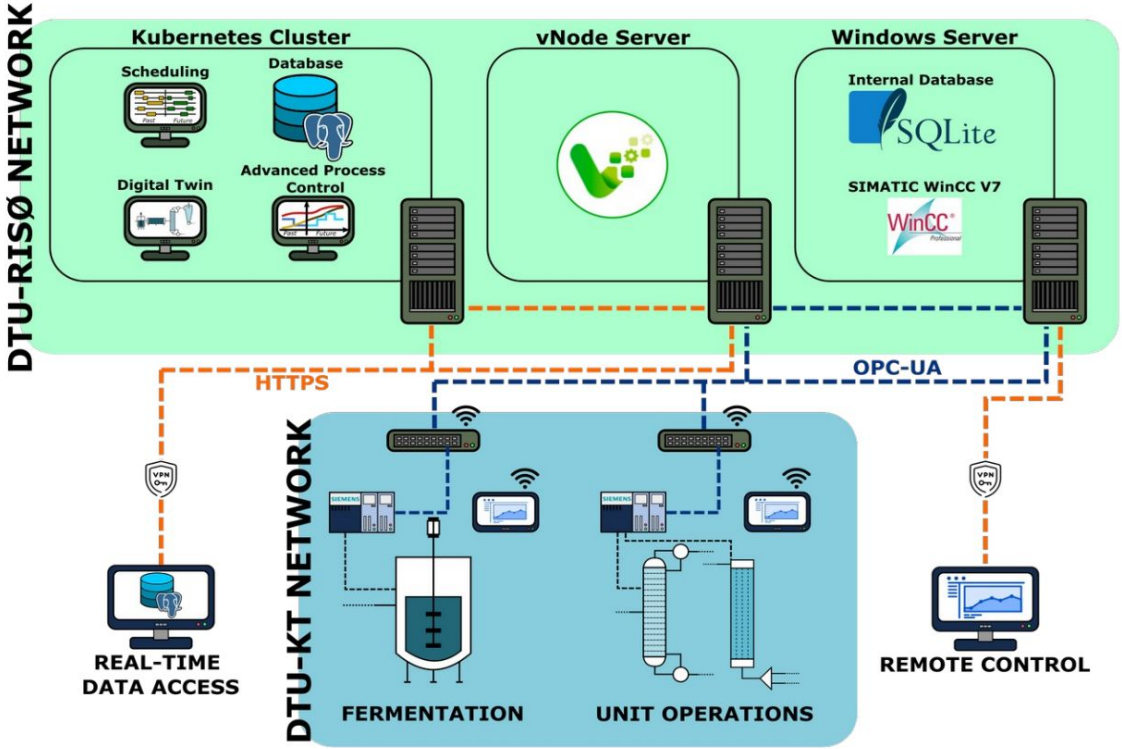

M. Jones et al.; Pilot Plant 4.0: A Review of Digitalization Efforts of the Chemical and Biochemical Engineering Department at the Technical University of Denmark (DTU); https://doi.org/10.1016/B978-0-323-85159-6.50254-2

CAPE-OPEN

A set of definitions (types) and protocols (interfaces/methods) for integrating applications

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Process Modelling Components (PMCs)

- Narrow, well-defined function such as the computation of physical properties, the simulation of a particular unit operation, or the numerical solution of certain types of mathematical problems arising in process simulation or optimization
- Unit operation, a numerical solver, a thermodynamic server, a physical property database, etc.

Process Modelling Environments (PMEs)

- PMEs with their own modelling languages (e.g. gPROMS ModelBuilder v5.0, Modelica or GAMS)
- PMEs based on a general-purpose language such as Python or Julia (e.g. Pyomo, DAE Tools or Jump)
- Equation-orientated and modular environments (gPROMS, PRO/II, ASPEN HYSYS)

M. Jones; “Design and Optimisation of Oleochemical Processes”, PhD Thesis; https://orbit.dtu.dk/en/publications/design-and-optimisation-of-oleochemical-processes

CAPE-OPEN <-> REST-API

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Process Modelling Components (PMCs)

Individual containers orchestrated

- Unit operation, a numerical solver, a thermodynamic server, a physical property database, etc.

Process Modelling Environments (PMEs)

Communication between REST-APIs

- PMEs based on a general-purpose language such as Python or Julia (e.g. Pyomo or Jump)

M. Jones; “Design and Optimisation of Oleochemical Processes”, PhD Thesis; https://orbit.dtu.dk/en/publications/design-and-optimisation-of-oleochemical-processes

Kubeflow

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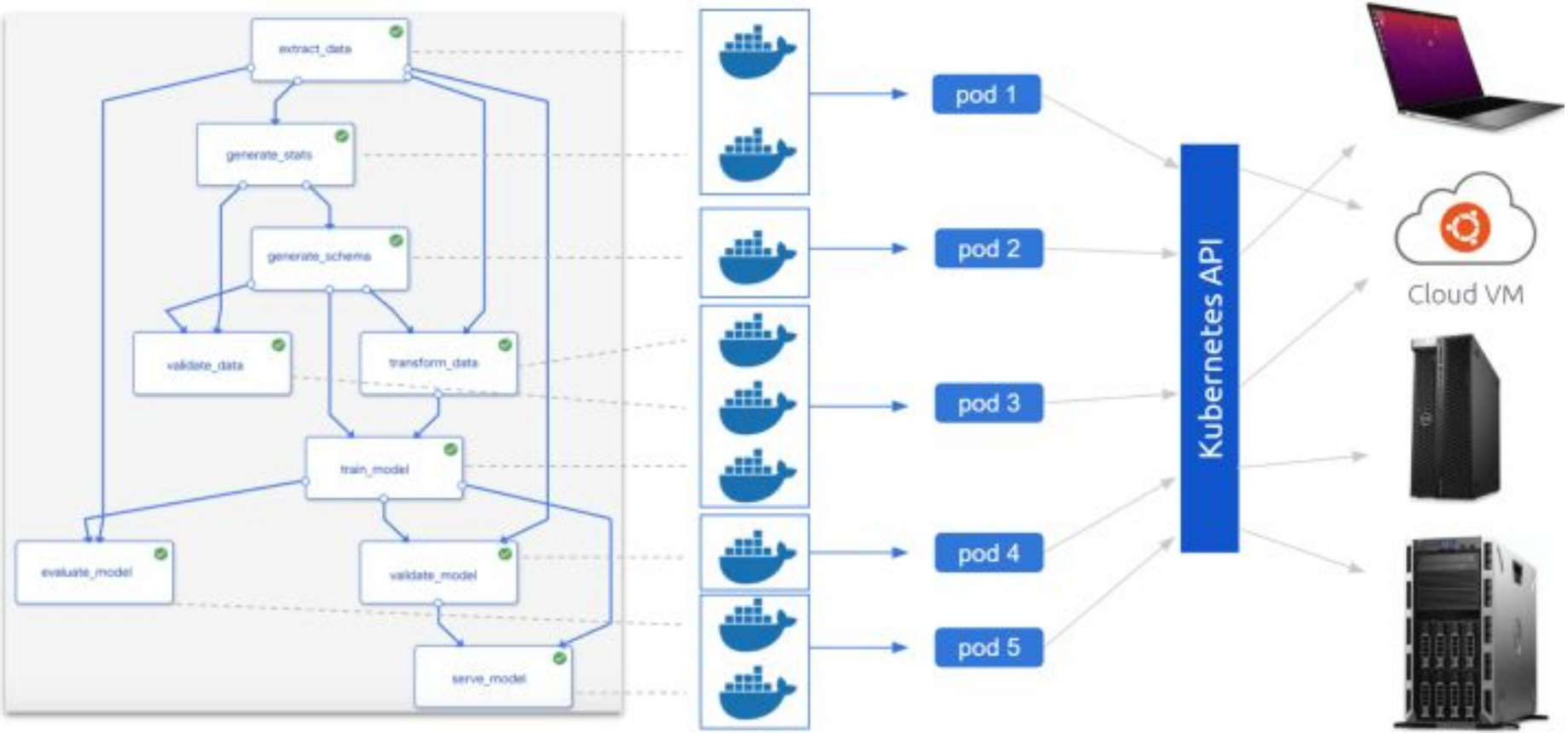

Covalent

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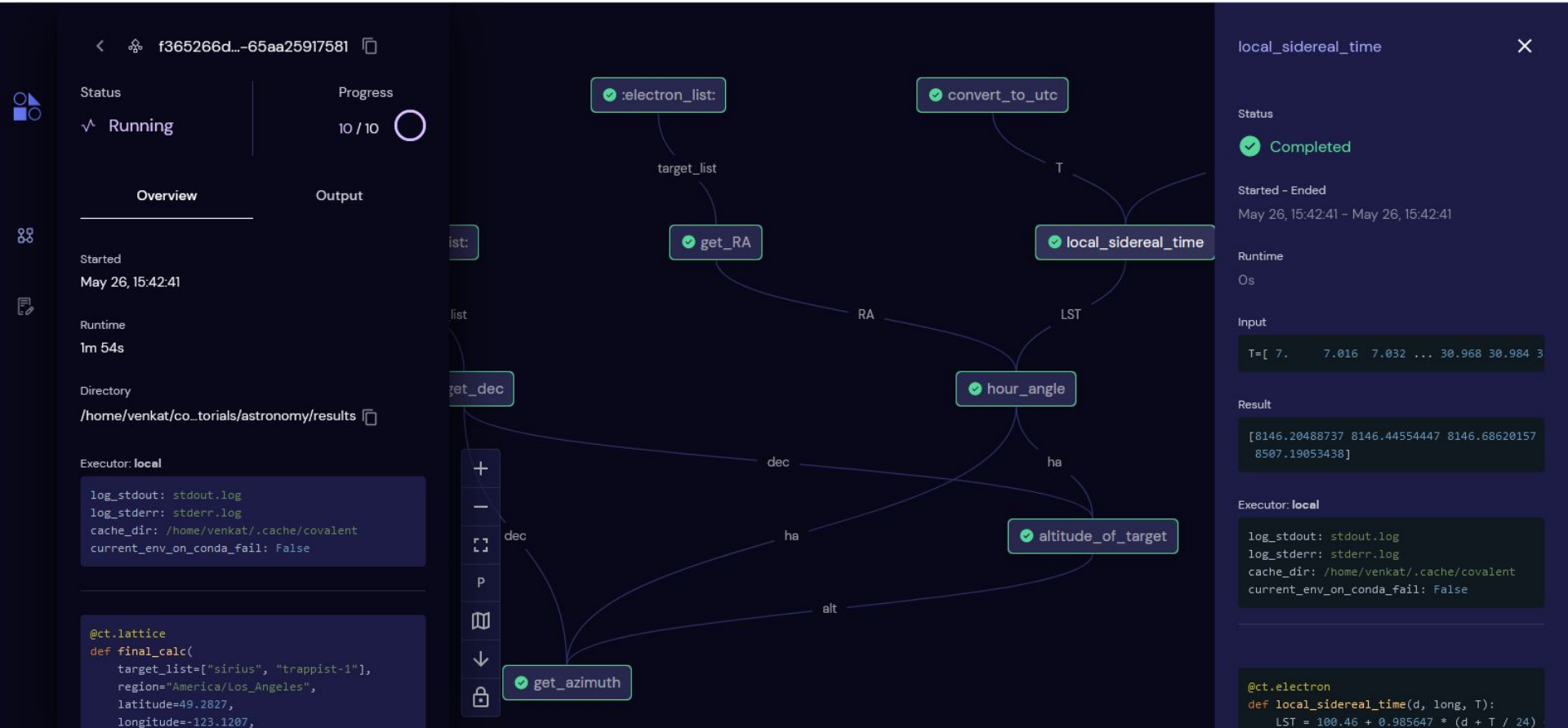

MQS REST-API adapted to CAPE-OPEN and COBIA

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- Thermodynamic and Physical Properties interface specification
- Wrapping COBIA (C++) with Python combined with good practice of REST-API design
- Publish OpenAPI Specification (OAS) conforming OpenAPI definition
- Integration/connection with COFE, DWSIM and other CAPE-OPEN compatible environments/components in a hybrid cloud setup

High Performance Computing (HPC)

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Research | Open Access | Published: 22 February 2021

Container orchestration on HPC systems through Kubernetes

Naweiluo Zhou ✉, Yiannis Georgiou, Marcin Pospieszny, Li Zhong, Huan Zhou, Christoph Niethammer, Branislav Pejak, Oskar Marko & Dennis Hoppe

Journal of Cloud Computing **10**, Article number: 16 (2021) | Cite this article

Conferences > 2017 IEEE International Confe...

Integrating MPI with Docker for HPC

Publisher: IEEE Cite This PDF

Maximilien de Bayser ; Renato Cerqueira **All Authors**

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for Lab Technicians & Researchers

High Performance Computing
for Engineers & Researchers

https://mqs.dk/workshops.html

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