COVID-19: An Unexpected Breakthrough

Discovery of a Druggable Pocket

"Oracle Cloud computing let us work at the pace required to achieve tangible results in this crisis."

—Imre Berger, Professor Biochemistry and Chemistry, University of Bristol

ORACLE for Research

University of BRISTOL

Oracle HPC Cloud Accelerated COVID-19 Research

Faster Time to Results Means More Opportunities for Discovery

As hospitals filled with severely ill patients and the world went on lockdown to try to slow the spread of the novel coronavirus in early 2020, it was self-evident that treatments and vaccines were urgently needed. Researchers around the globe, including an international team led by Professor Christiane Schaffitzel of the University of Bristol's School of Biochemistry and Professor Imre Berger of the Max Planck-Bristol Centre for Minimal Biology, shifted their focus to SARS-CoV-2. It seemed that COVID-19, the disease caused by SARS-CoV-2, was triggered by its spike protein, and Professors Schaffitzel and Berger aimed to generate that spike to help clinicians conduct serological tests.

When they used cryo-electron microscopy to perform a quality control check of their generated spike, they found something unexpected: the spike had a pocket that appeared to bind to an essential fatty acid – linoleic acid – potentially connecting the virus to its clinical symptoms of severe respiratory distress and organ inflammation. Even more exciting was the realization that if the pocket could be closed, the virus could be rendered harmless. The team had discovered a potentially druggable pocket and opened the door to the possibility of stopping COVID-19.

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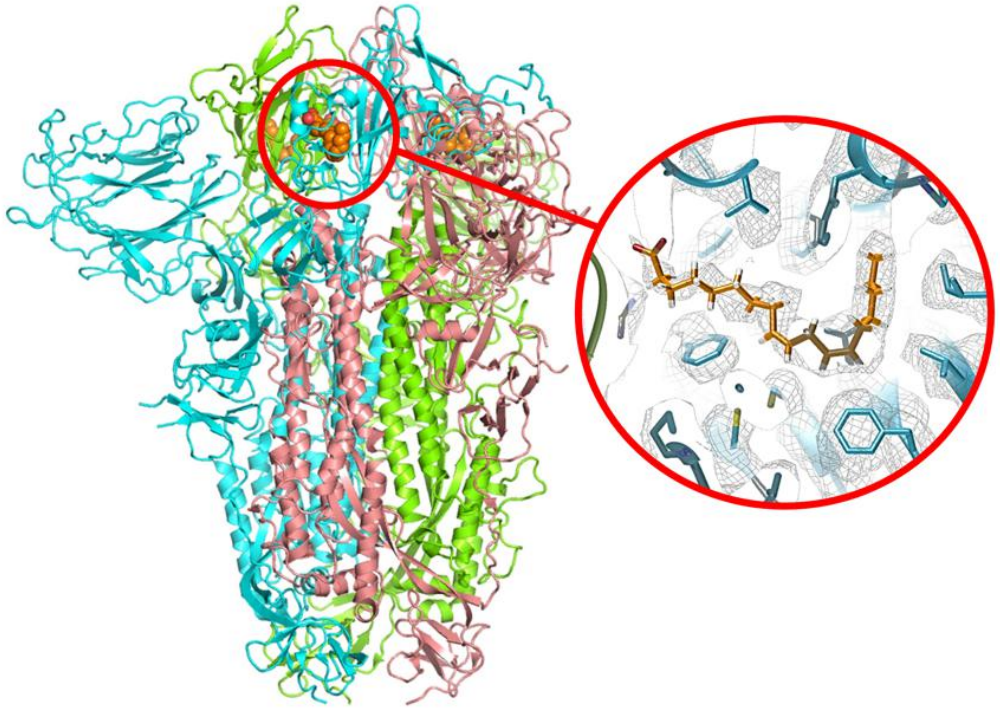

The SARS-CoV-2 spike protein captures linoleic acid, a key molecule in the body that regulates inflammation and immune response.
COURTESY OF THE UNIVERSITY OF BRISTOL

- The team led by researchers at the University of Bristol discovered that the SARS-CoV-2 spike protein binds with linoleic acid, an essential fatty acid that the human body cannot produce.
- Linoleic acid is important for regulating inflammation and immune response, and in patients with severe COVID-19 disease, linoleic acid is depleted. The discovery by the research team potentially helps explain why this is so, connecting linoleic acid, the SARS-CoV-2 virus and COVID-19.
- Even more importantly, the Bristol-led team found the “unique binding pocket” where the spike protein captures the linoleic acid, and discovered that when the SARS-CoV-2 spike protein binds with linoleic acid, it gets locked in a state that prevents it from binding to human ACE2 cell receptors – rendering it non-infectious.
- If this pocket on the spike protein can be drugged to its locked state, potentially using antiviral drugs, COVID-19 treatments will be improved and lives will be saved.
- Computational modeling of SARS-CoV-2 was critical to these discoveries. On-premise super computers needed the power of enterprise computing to process the very large data sets from the University of Bristol’s powerful cryo-electron microscope.
- The researchers leveraged Oracle’s high-performance Cloud infrastructure to develop a novel computational approach to create a 3D, high-resolution digital model that allowed them to visualize and study the spike protein molecule composition.

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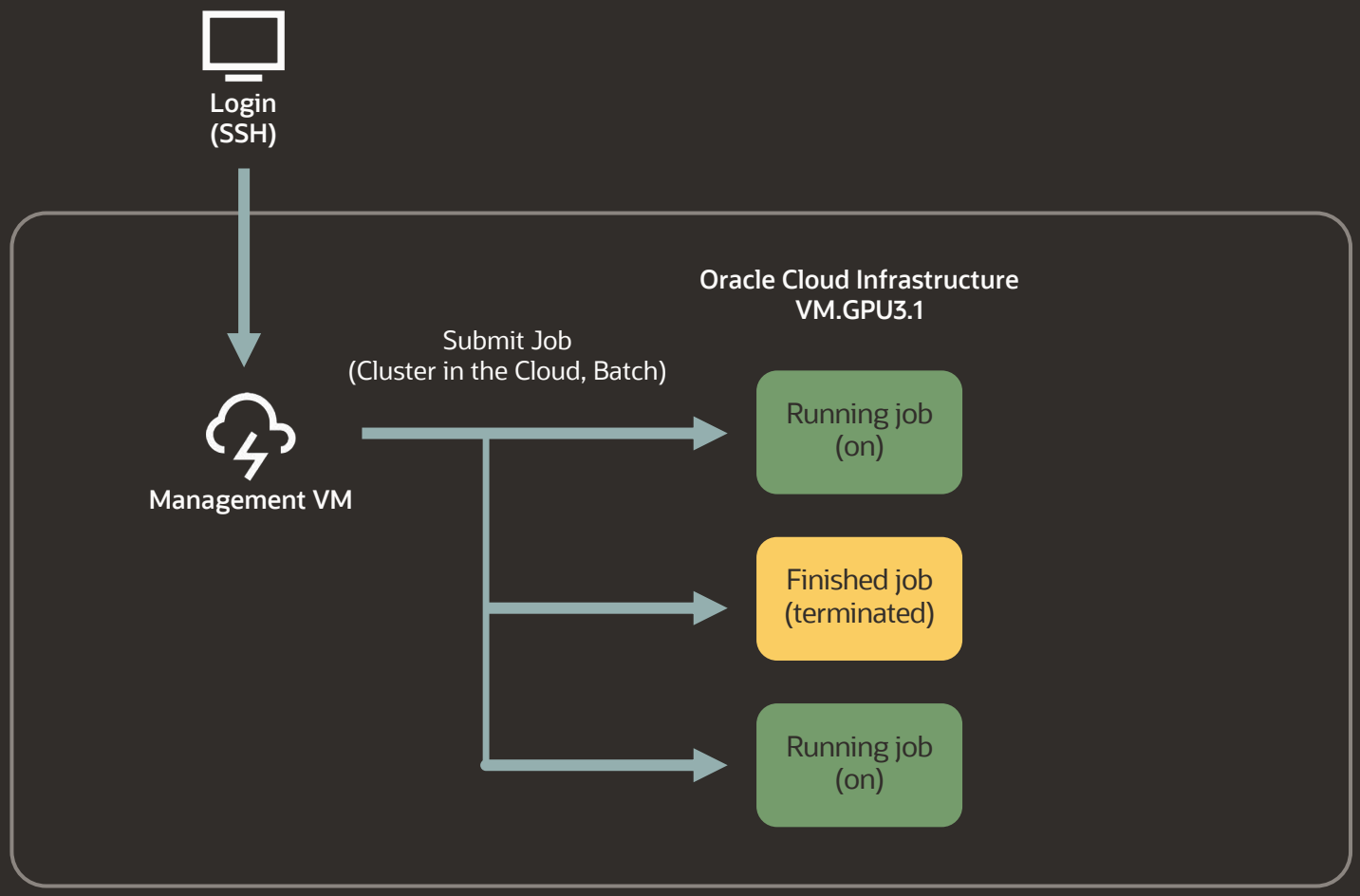
Oracle Cloud Architecture in Cluster in the Cloud



OCI Performance Characteristics

- Best suited to heterogeneous high-throughput tasks
- Pipelines needing different node type(s) for different parts
- Can be much more specific than the average on-premise cluster
- Always have access to the latest hardware
- Nodes are only switched on and paid for while jobs are running
- Nodes are switched off automatically when idle
- Great for teaching clusters

Timing

- Full system test ~ 20 minutes on Oracle
  - Create cluster from scratch
  - Submit job
  - Run job
  - Tear down whole cluster
- Job submit → job start: < 2-3 minutes