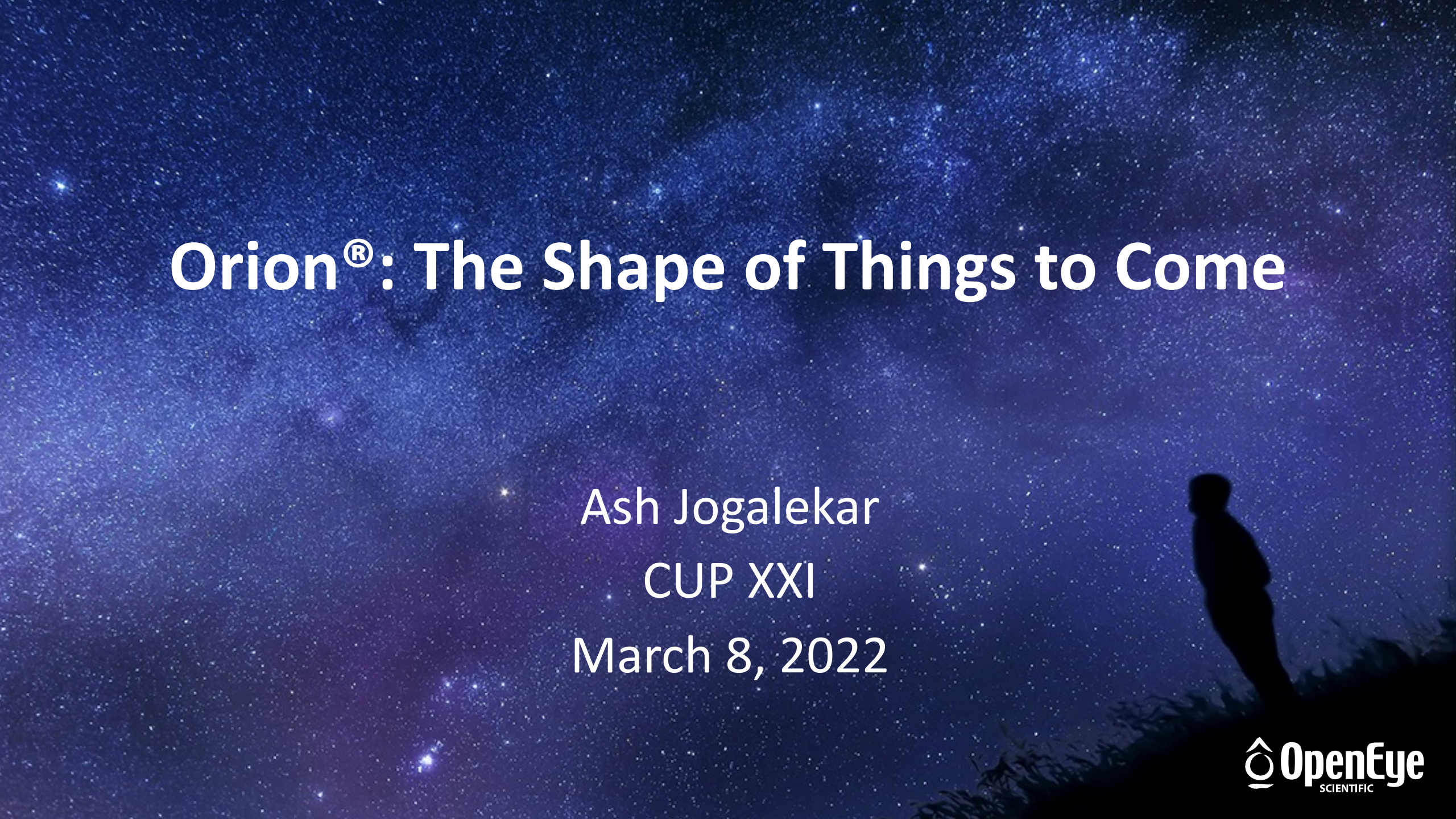
Orion®: The Shape of Things to Come

Ash Jogalekar

CUP XXI

March 8, 2022



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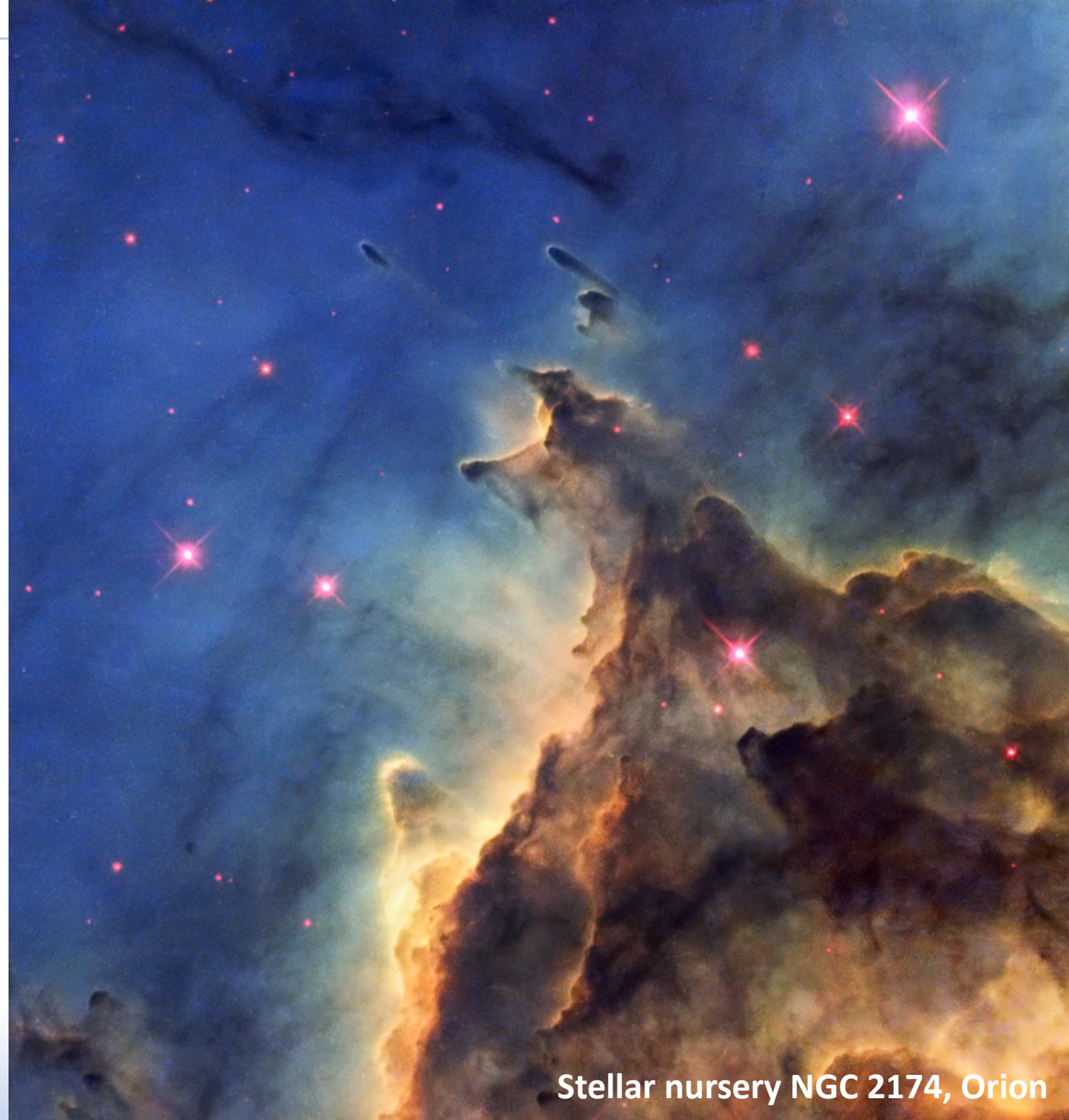
Agenda

- Motivation
- Where we are now
- Where we are going

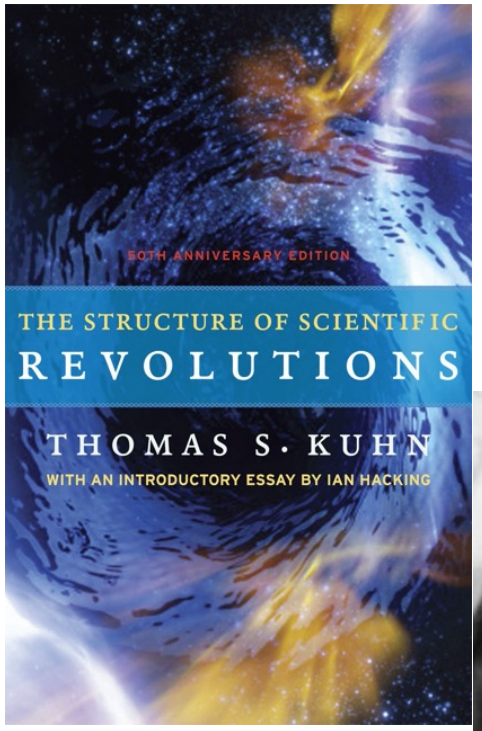


Stellar nursery NGC 2174, Orion

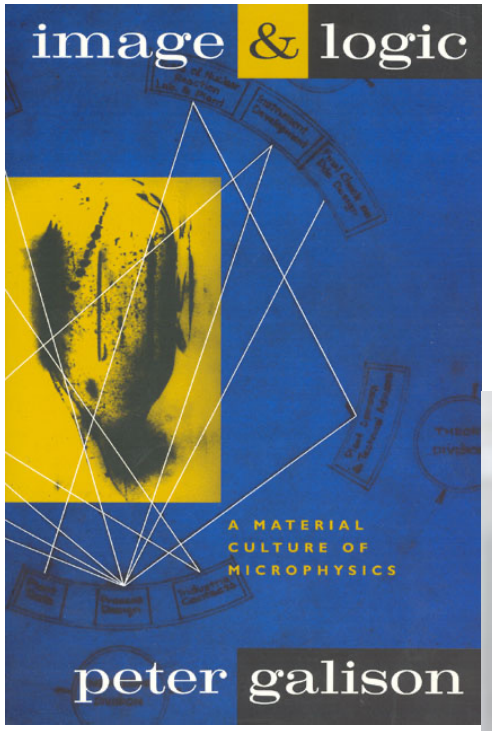
Very much alive guy quote

- “We always overestimate the change that will occur in the next two years and underestimate the change that will occur in the next twenty years.” – Bill Gates

Scientific revolutions: Ideas and tools



Quantum theory
Hydrogen bonding
Gene regulation



Spectroscopy
Crystallography
PCR

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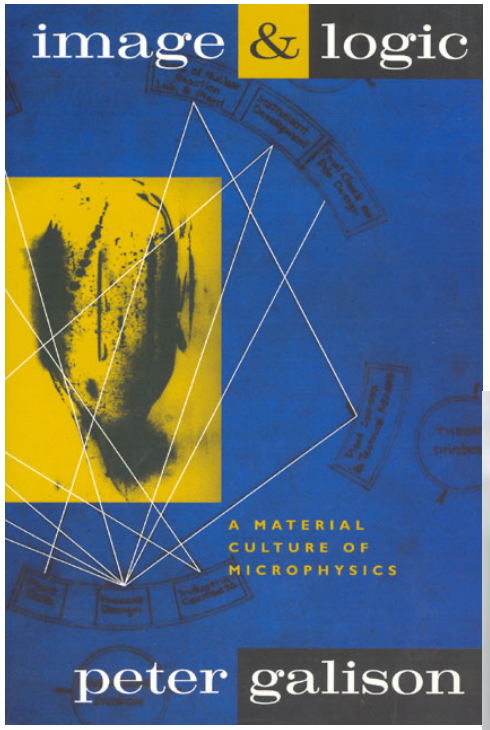
Scientific revolutions: Tools enable ideas



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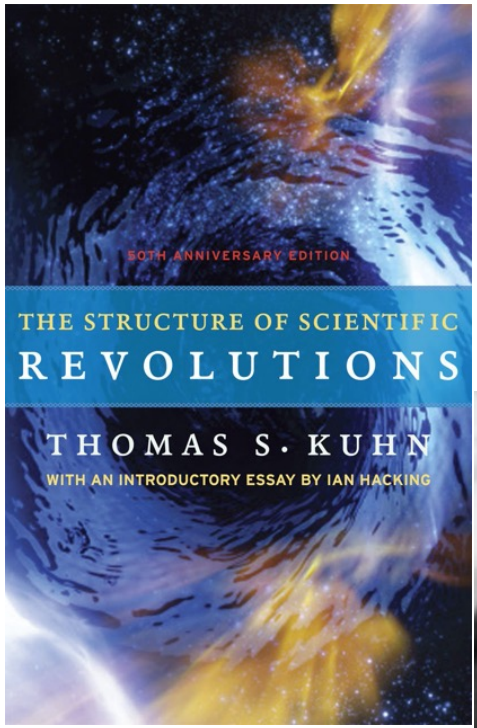

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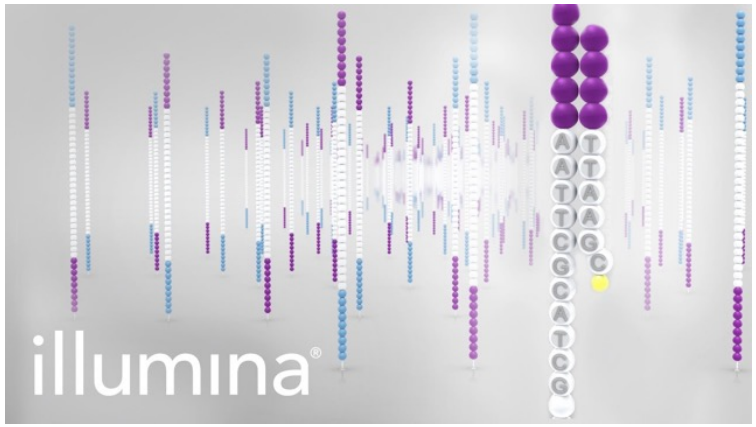
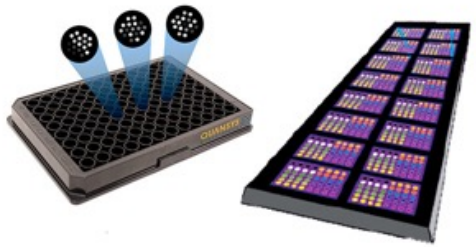
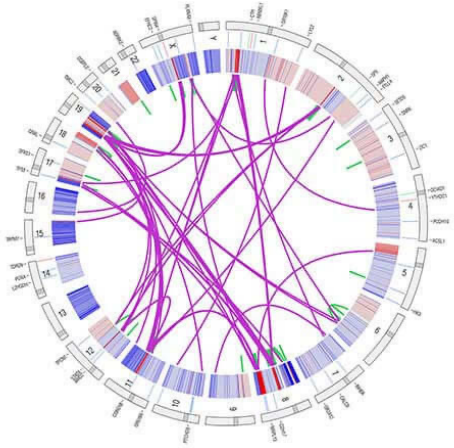
Technological revolutions: Platforms enable apps



Deep DNA sequencing
Multiplexing
OS X





Cancer genomics
GPCR drug discovery
Ridesharing

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Single platform enables multiple apps

Core technology platform

Suites of **apps** as turnkey solutions

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The Orion® Platform

Suites of **scientific** methods as turnkey solutions

- *Small Molecule* Discovery Suite
- *Antibody* Discovery Suite
- *Formulations* Suite
- *To Be Announced* Suite

Core technology platform

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Platform synergy

+

Core technology platform

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Technological convergence and Orion

Powered flight

Physics of flight (Cayley, 1849)
AND Petroleum distillation (Silliman, 1854)
AND Aluminum (Hall-Héroult process, 1886)

High-performance drug design

orion®

OpenEye Science (1997-now)
AND OpenEye Software (1997-now)
AND Cloud Technology (AWS, 2007-now)

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The Orion® *Cloud* Platform: Harnessing Programmable Hardware

Suites of **scientific** methods as turnkey solutions

- *Small Molecule* Discovery Suite
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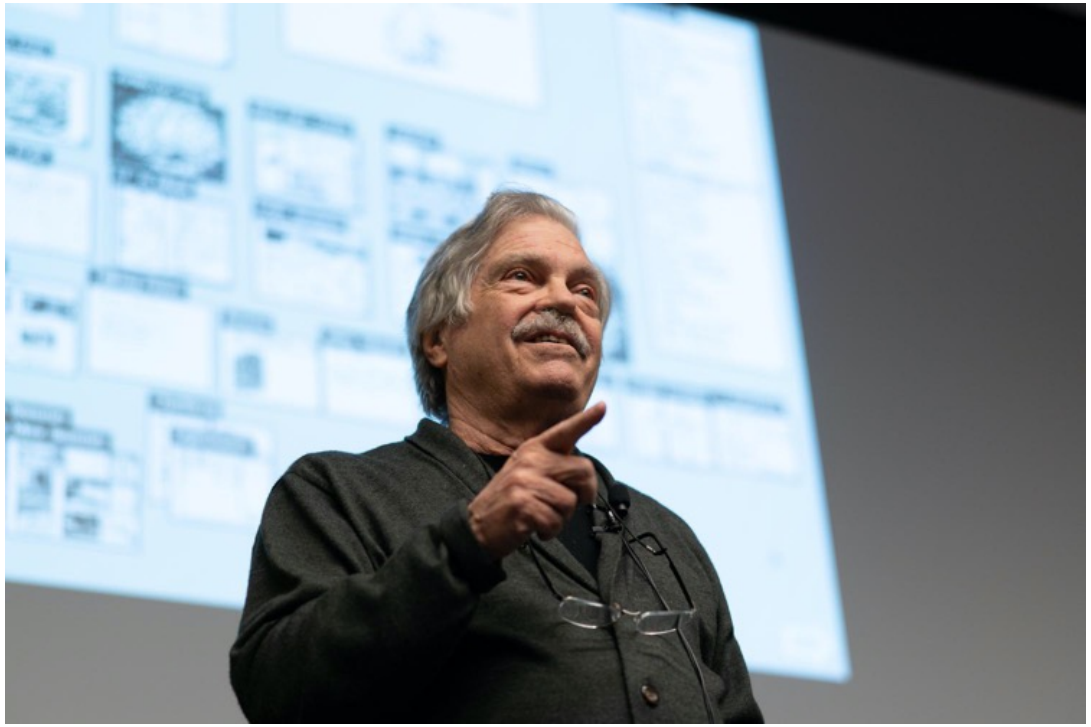
Core technology platform

The second-best solution to Alan Kay's suggestion?

"People who are really serious about software should make their own hardware."

- Orion on the cloud offers:
  - Cloud-native apps built from the ground up, designed for very large-scale calculations
  - Elastic, instantaneous autoscaling and parallelization
  - Unprecedented data storage and storage model designed for scale
  - Possibility for seamless integration between internal and third-party apps



2021 O'Reilly survey

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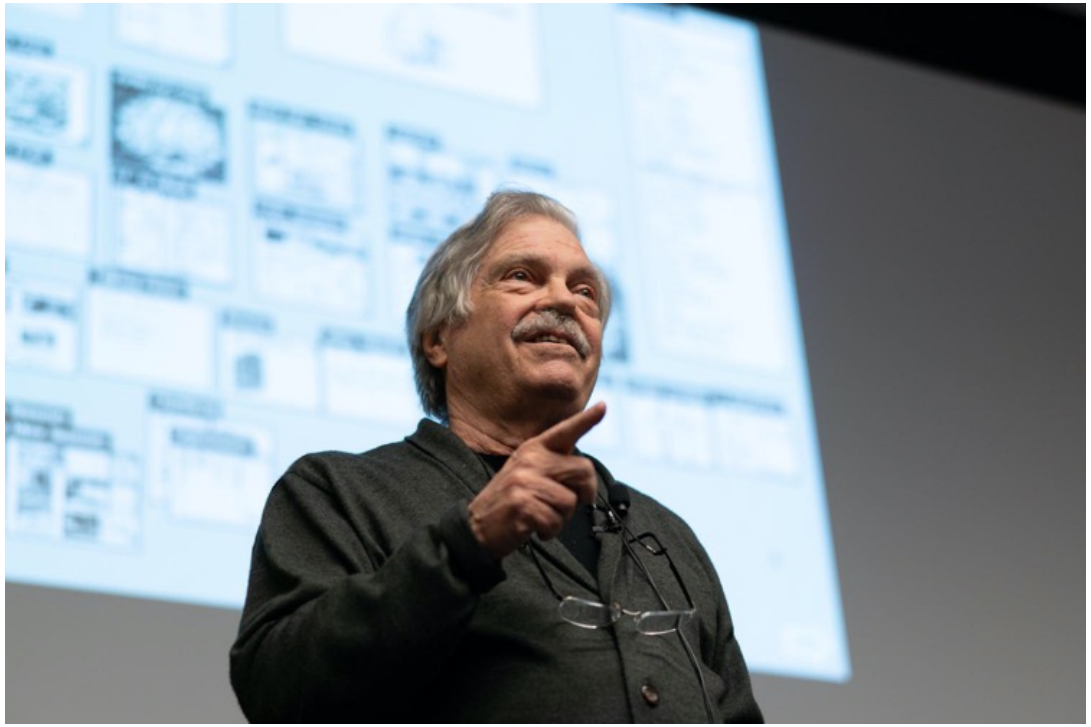
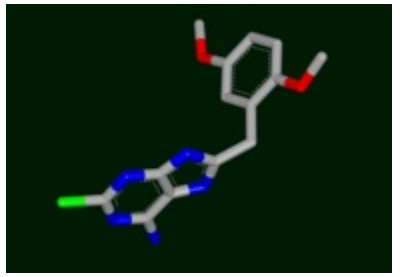


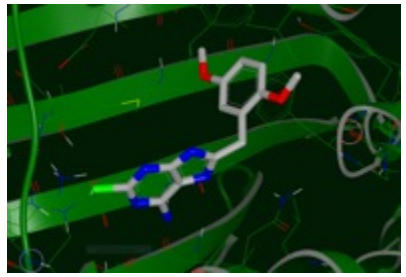
2021 O'Reilly survey

Orion®: What we do well

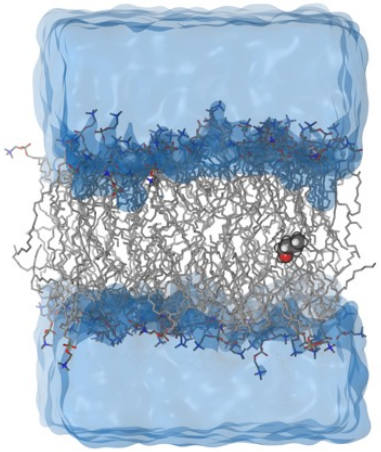
- Industry-leading OpenEye apps powered by the cloud: Gigadock, FastROCS, MaaS
- A scheduler and backend optimized for the cloud and responsive to new cloud resources
- Data models and schemas for large-scale data tailored to the cloud (eg. collections)
- Cutting-edge new science expressly built for the cloud: crystal structure prediction, non-equilibrium thermodynamics
- Leading third-party apps powered by cloud: Gaussian
- Development and editing of user-defined floes and cubes



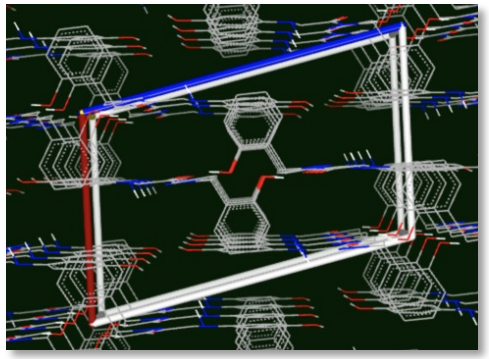
FastROCS™



Gigadock™



Membrane Permeability



CSP of drug-like molecules

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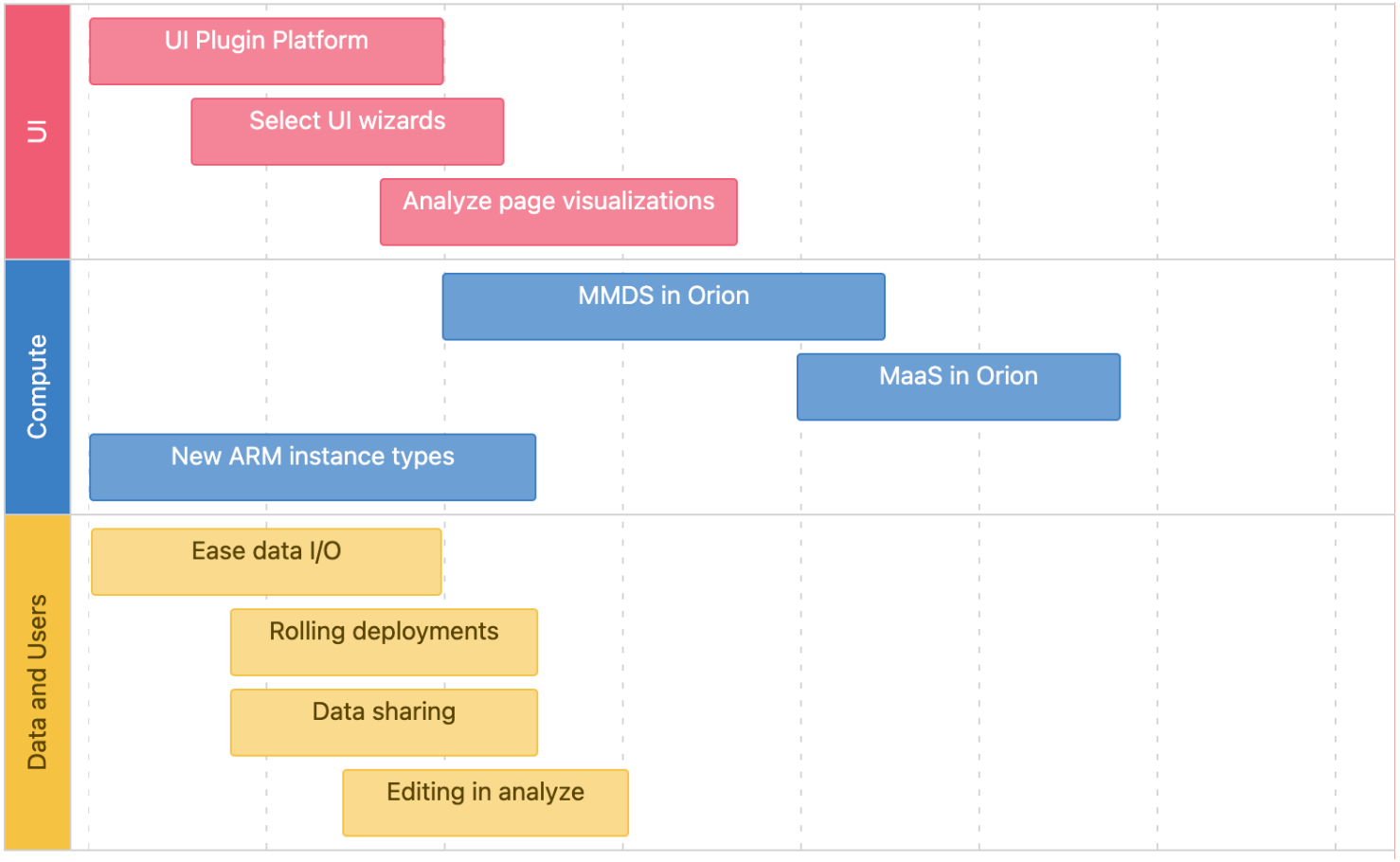
Orion®: The road ahead



Orion®: The road ahead

- Build general purpose UI for wide customer base
- Bring science services into the Orion fold
- Optimize cloud resource utilization
- Improve data and user management
- Integration and programmability

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UI/UX

“Blame Ant.” - Ant

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UI/UX

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UI/UX

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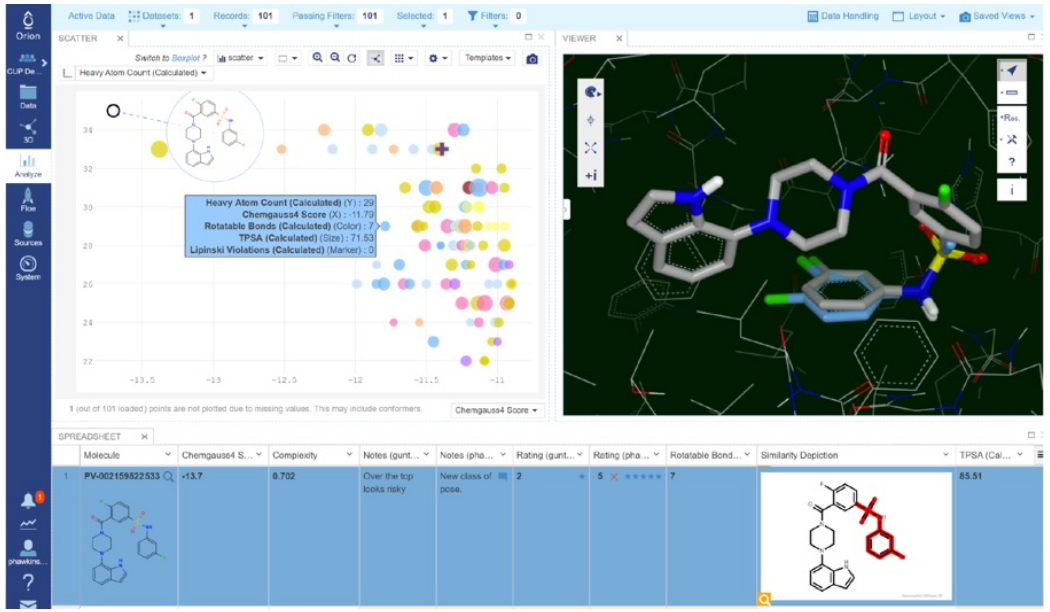
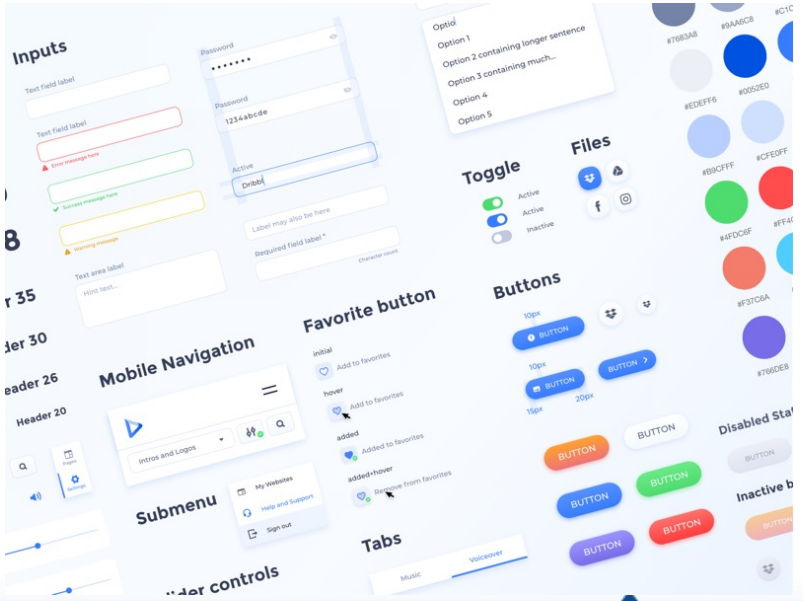
General purpose UI

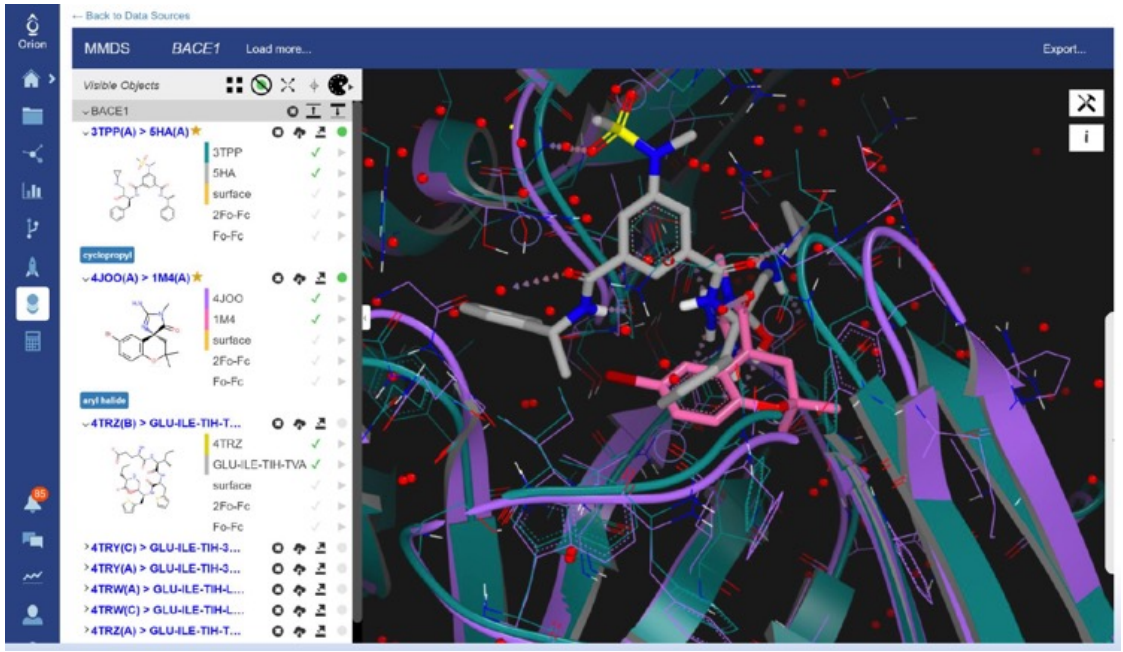
- Chemistry-centered UI ingesting data and kicking off calculations; active dataset front and center
- UI plugin platform: Enables building custom UIs for specific science applications
- Wizards for selected applications: eg. generative floes, protein prep
- Enhancements to analyze page for better control and selection of data
- UI/UX-centered design key part of process





Key science services integrated into Orion

- MMDS, MaaS and FastROCS currently unable to utilize full power of Orion compute
- MMDS in Orion: Search proteins, search ligands, compare structures (including AlphaFold), upload structures
- MaaS, FastROCS: Enhanced searching of growing vendor databases
- Services take advantage of Orion's superior existing and continued data and user management

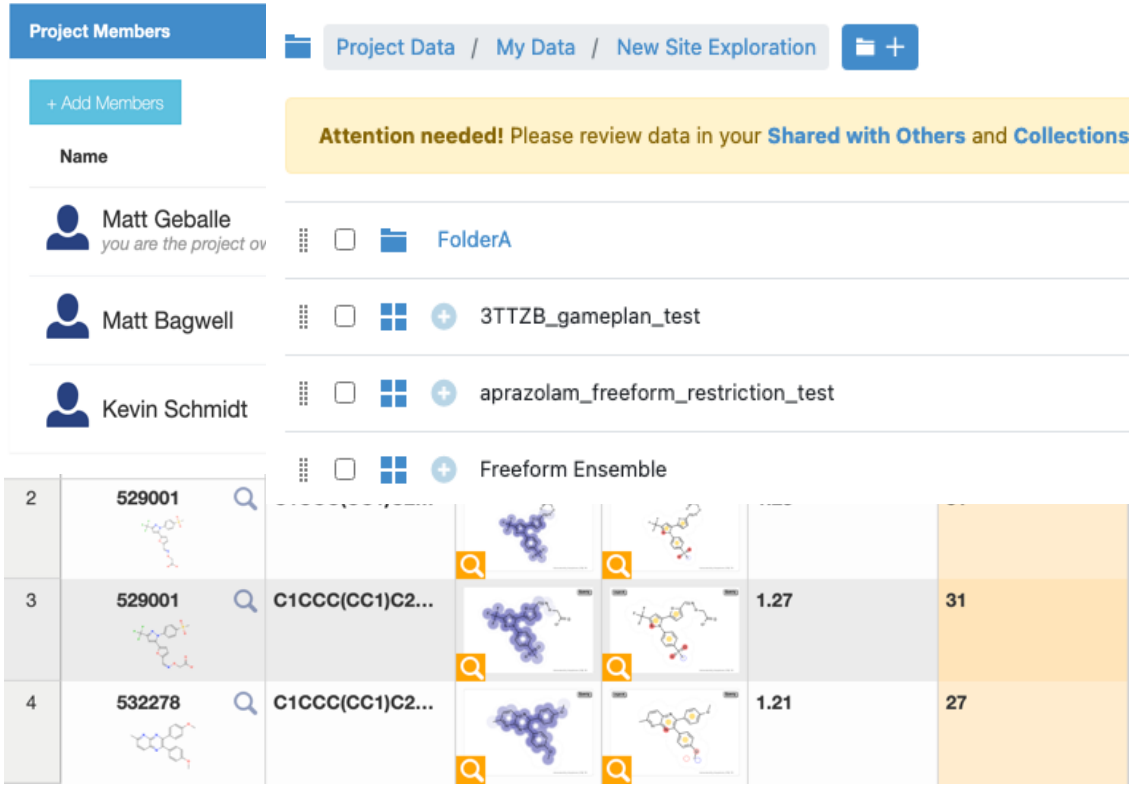


Optimize cloud resource utilization

- Improvements for running jobs, faster access to hardware, cost-savings
- Improve scheduler reliability and performance
- Better spot instance utilization, including multiple instance types simultaneously (can scale to at least 1000 GPUs)
- Utilize new instance types, including ARM and Intel C6i chips
- Cross-over to multiple AWS regions

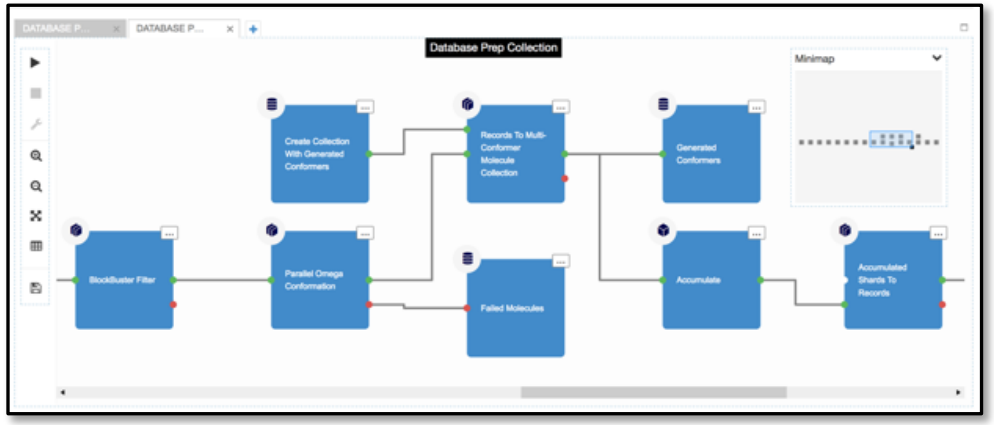
Improve data and user management

- Easing data I/O and minimizing data transfers
- Improved user management (and related data management)
- Faster and smoother rolling deployments, minimizing service disruption and downtime
- Enabling users to control access to data-rich schemas (eg. discussion boards)
- Better data sharing through links, filters, states

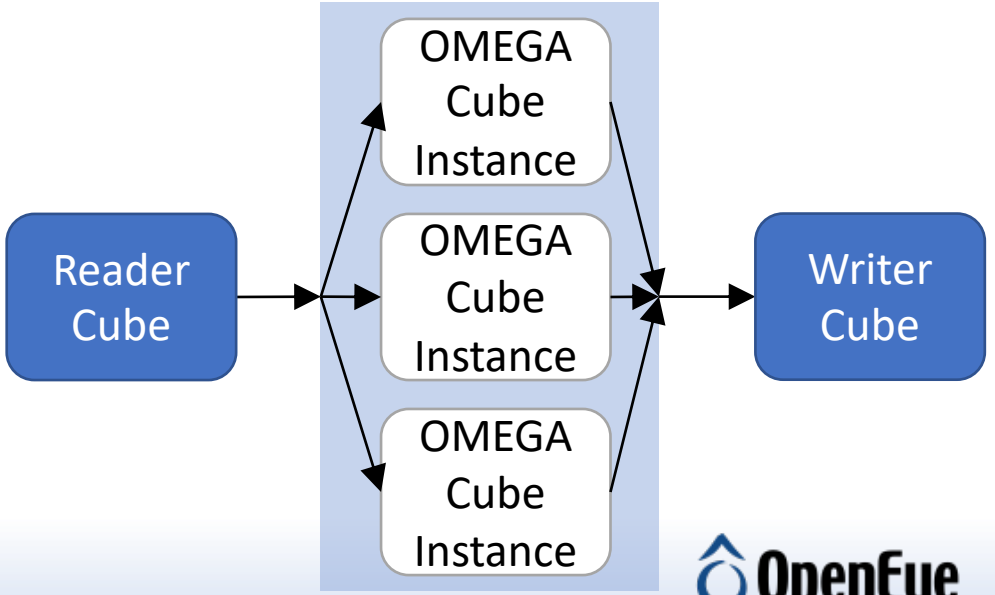


Integration and programmability

- Docker-image upload enhancements, being able to use image just to update floes and cubes
- Improvements to floe editor and cube organization. Floe classification (for next release).
- Improving floe writing UX and deployment, scaling cubes up and down in real time
- Chunk and chain floes. Mix and match cubes to enable meta-science



Parallel OMEGA Cube



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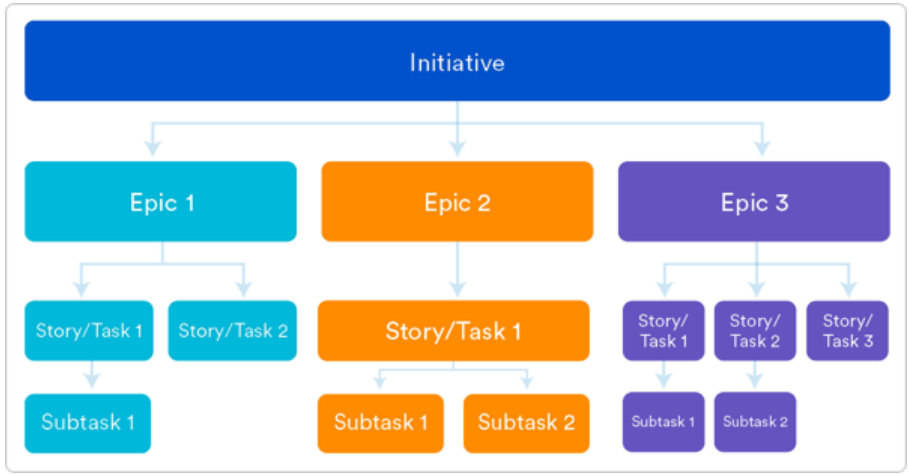
The how: People and processes

"Plans are worthless, but planning is everything." – Dwight Eisenhower

- Build formal product team: technical product manager, product designer
- Put agile process in place: sprints, demos, triage, user research
- Involve all stakeholders: users, application scientists, customer support, sales, marketing
- Use product North Star to prioritize features
- Most importantly…



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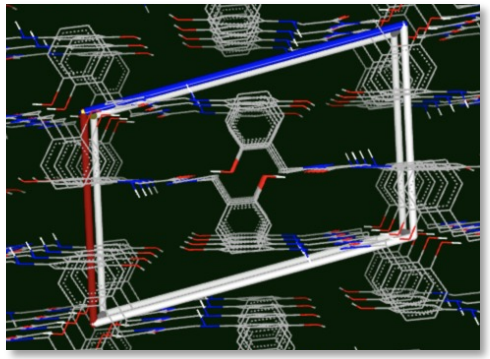
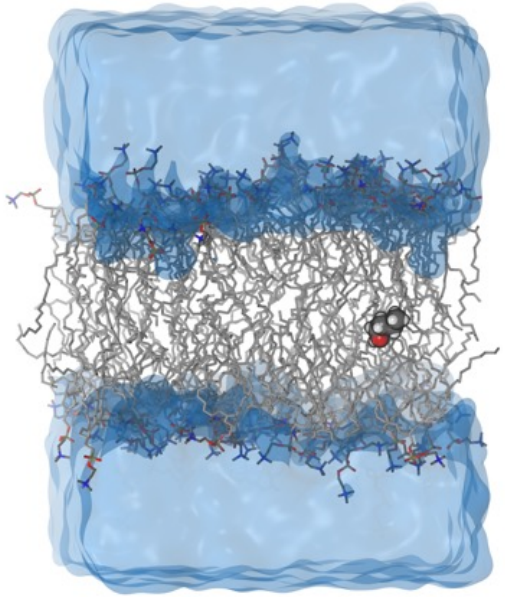
A hub for exciting science and model development

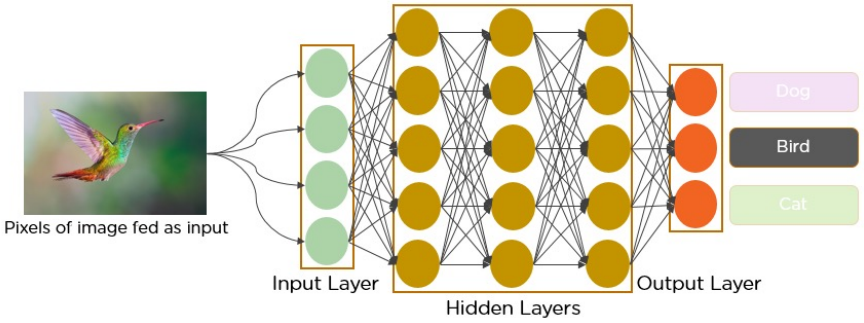
Gaussian 16



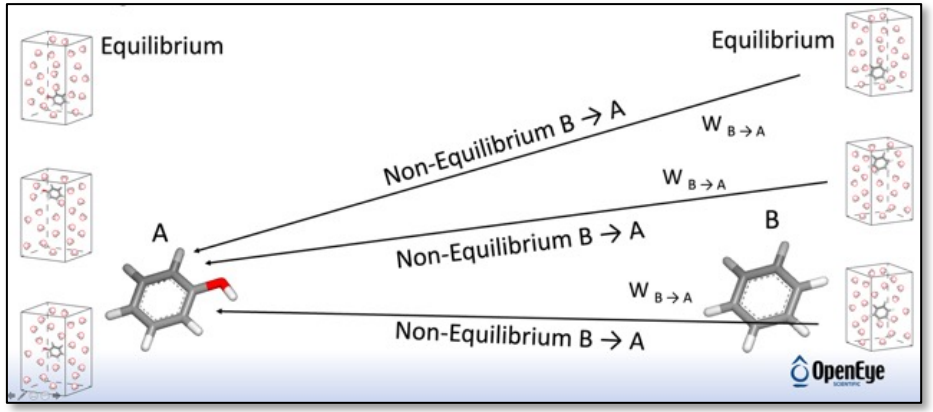
Crystal-structure prediction



Membrane Permeability modeling with MD and WestPA



Machine learning and model validation



MD-based Relative BFE prediction via NES

WESTPA

Your Method Here

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Orion as destination, not just resource

Data

Compute

Science

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Modeling

Medicinal Chemistry

Data Science

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- Matt Geballe
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