Orion®: State of the U(I)nion

Ash Jogalekar
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Dead guy quote

“The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction.” – Sidney Coleman
Orion® as destination

The universe as a (alien) simulation

- Modeling
- Medicinal Chemistry
- Data Science
- Data
- Compute
- Science
Orion: From then to now and beyond

- Orion: State-of-the-art HPC platform with UI bolted on top
- Bottom-up vs top-down approach
- “Big jobs (eg. Gigadock™) sped up, small jobs (eg. interactive modeling, I/O) slowed down.” – Jonas Boström (Treeline)
Abstraction

- Matches UI and UX with personas and user problems
- Provides right level of interaction depending on needs
- Ideally, users can work at multiple levels of abstraction depending on persona
Building an industry-leading CADD interface

- Abstraction
- Molecule-centric
- Modular
- Collaborative
- Low latency
- Cloud-based
- Integrates with 3rd party software
Current Orion UI highlights

Floes

Analyze spreadsheet

Data and Folders

3D viewer
Present and future Orion UI: A blueprint

<table>
<thead>
<tr>
<th>Feature</th>
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<tbody>
<tr>
<td>Molecule-centricity (vis-à-vis floe-centricity): Elevate 3D viewer</td>
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<td>Fewer clicks, minimal to no context-switching</td>
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<td>Format-agnostic file uploads (files...datasets...collections, oh my!)</td>
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<td>More exposed functionality: editing, styling, duplication etc.</td>
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<td>3rd-party integrations</td>
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<td>Enhanced spreadsheet capabilities: annotation, multi-conformer handling etc.</td>
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<td>UI performance and latency improvements</td>
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What’s shipped and shipping soon

• 2022.3 – 2023.1
  o Shareable links
  o 2D search, potential replacement for MaaS
  o Make Receptor in Orion
  o Collections v2: Better I/O stability for large collections

• 2023.2 – beyond
  o Support for ARM instances
  o Lower latency for interactive calculations
  o Ability for users to upload their own databases
  o Improved I/O for database collections
  o Spruce and protein preparation
  o ELN and compound registry integration
  o Generative chemistry
  o Medicinal chemistry roles in Orion
2D search page (beta)
UI-based workflows: universal OE tool coverage
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Thank you

“Every great and deep difficulty bears in itself its own solution.” – Niels Bohr