

The Orion User Interface One Year Later

Joe Moon



Scale of Orion UI and its challenges

Highlights from recent releases:

- Data handling

- 3D modeling

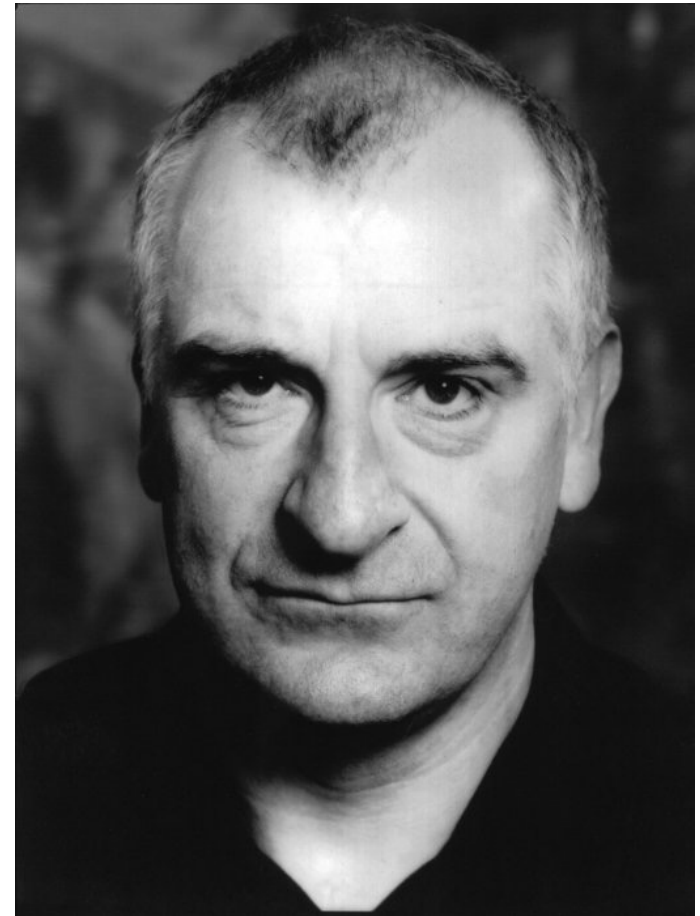
- Discussion boards

Looking forward

Orion is Big

“Space is big. You just won't believe how vastly, hugely, mind-bogglingly big it is. I mean, you may think it's a long way down the road to the chemist's, but that's just peanuts to space.” — Douglas Adams, *The Hitchhiker's Guide to the Galaxy*

“Orion is kinda big, too.” — Joe Moon, *CUP 2022*



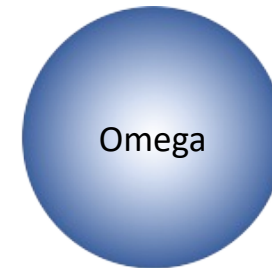
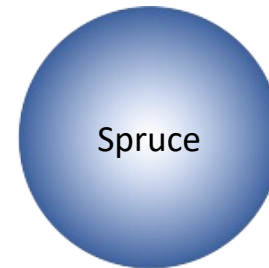
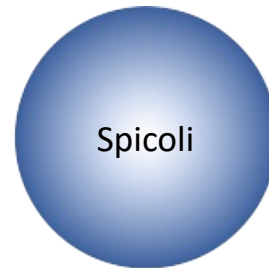
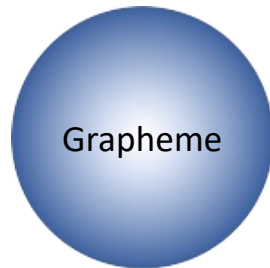
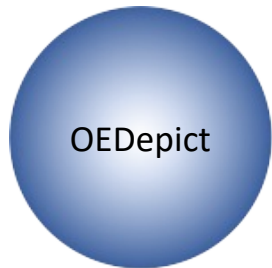
Lots of Pieces

- 3D Editor
- 3D Object List
- 3D Viewer
- Active Data control
- Analog Generation
- Analyze page
- Discussion Boards
- Event Notification
- FastROCS
- Filters
- Floe Editor
- Floe Launcher
- Floe Package Manager
- Floe Page
- Floe Browser
- Help Page
- Job Form
- Job Viewer
- License Disclosure
- MaaS
- Metrics Viewer
- MMDS
- Molecule Overlay
- Molecule Style Control
- Plots
- Preferences
- Project Cost Accounting
- Project Data Management
- Project Membership
- Project Summary
- Property Calculator
- Protein Edit Tools
- R-Group Calculation
- Record Search
- Regression Tool
- Scaling Group Status
- Sketcher
- Spreadsheet
- Stack Status
- Substructure Search
- Tile View
- Token Management
- Upload Tool
- User Cost Analysis
- User Management
- User Profile
- What's New

Lots of Code

```
ctrl.isParamHidden = (param) => ctrl.floeItem.getOwnerId() !== UserManager.getSelf().id  
    && param.getHidden()  
ctrl.toggleSectionExpand = (cube) => (ctrl.expandedSections[cube.getName()] = !ctrl.expandedSections[  
    cube.getName()  
    ])
```

- Orion's front end is ~300,000 lines of code
- Larger than



- 50-70 developer-years by industry standard metrics
- Built on top of 8M lines of library code
- 3 new feature requests per week – 1 new feature delivered

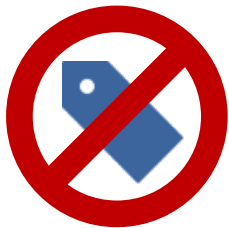
Lots of Challenges



- Complexity!
- Sending lots of data over network to/from a browser
- Splitting work between browser and servers
- Organizing and sharing data
- Complex data structures
- Communication and collaboration

Project Data v.2

- Folders instead of tags
- My Data
- Team Data
- Organization Data
- Shared Workspaces



- + Add Data
- Active Datasets
- Organization Data
- Project Data
- My Data
 - Team Data
 - Shared Spaces
- Favorite Folders
- Ideas
 - Kinases
- Trash

Search: enter a tag or resource name...

☒ Current folder ☐ All project folders

Show:

Sort by: Created: Newest First


My Data	+	-	
Analysis			
Demo			
Kinases			
非常に重要なデータ			
Peptidomimetics			
Ideas			
Copy of 7C3N AaltA-FHX A-9000 ligand 4	1 record	02/19/2022	1198614
Copy of AGS(A-501) - Cluster Heads #1	4578 records	02/14/2022	1196953
Copy of Docking output no protein	5578 records	02/14/2022	1196952
Spruce_prep_dataset (1)	3 records	02/11/2022	1195642
PFKFB3 (6-phosphofructo-2-kinase_fructose-2,6-biphosphatase 3)	25 records	02/04/2022	1193694
no_hist_complete_torscan	1 record	01/28/2022	1191508


Load more items


3D Viewer Improvements





- Selected functionality from OE Toolkits compiled for browser
- Lots of server-side calculations moved into browser
 - 3D editor
 - Surfaces, grids, protein-ligand interactions
 - Protein editing tools
- List improvements
- Faster rendering
- Support for Design Units



OpenEye



Kevin's Project



Data


3D


Analyze


Floes


Sources


System

Active Datasets 1

Filters 0/0

Records: All 4

ALL DATA

DU with primary

Dataset has hidden fields

manage

JQ1(A-201)

bl d r s

JQ1(A-201)

bl d r s

JQ1(B-201)

bl d r s

JQ1(B-201)

bl d r s

VISIBLE OBJECTS

JQ1(A-201)

bl d r s

bl JQ1(A-201)

r 4FLP(A)altA > JQ1(A-201)

P 4FLP(A)altA > JQ1(A-201)

ALL DATA

DU with primary

Dataset has hidden fields

manage

	bl	d	r	s	
★ JQ1(A-201)	bl	d	r	s	
▶ JQ1(A-201)	bl	d	r	s	
▶ JQ1(B-201)	bl	d	r	s	
▶ JQ1(B-201)	bl	d	r	s	

VISIBLE OBJECTS

Nothing here - change list mode?


The image shows a screenshot of a 3D Viewer application window. The window has a title bar at the top with the text "3D VIEWER" and a close button. Below the title bar is a menu bar with the following items: "View", "Select", "Modeling", "Tools", and "Help". Below the menu bar is a toolbar with several icons: a camera, a selection tool, a delete tool, a left arrow, a right arrow, a rotation tool, a blue arrow pointing up and to the right, a small rectangle, a red and blue circular icon, and a grey icon with a circular arrow. The main area of the window is a dark green 3D environment. In the bottom right corner, there is a small white arrow pointing left.

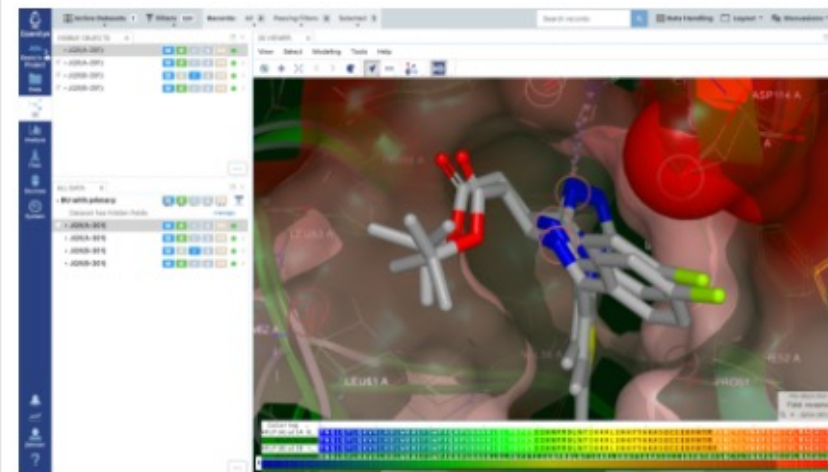
Discussion Boards

- Allow multi-way discussions about modeling sessions
- Pictures, links, rich text
- Provide links to live data
- Can be shared with team members

Joe Moon 02/28/2022 01:26 PM


Edit 

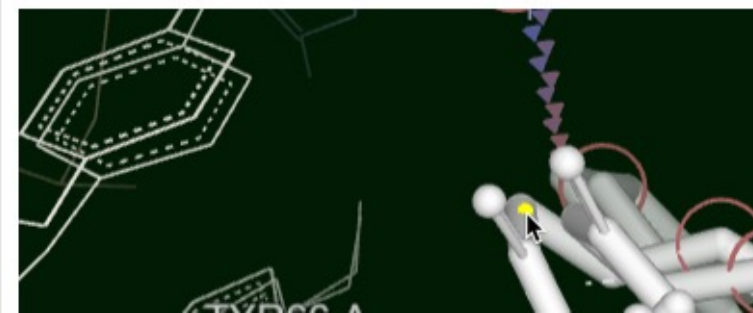
 [Main active site view](#) showing superposition of two monomers. There are multiple unsatisfied H-bond interactions here. Ignore the markers on the cysteine SH.



Joe Moon 02/28/2022 01:31 PM

Edit 

The  [bottom of the pocket](#) has two leucines, a valine, and two tyrosines, so is pretty hydrophobic.



+ Add Data

Search: du with enter a tag or resource name...

☒ Current folder ☐ All project folders

Show:

Sort by: Created: Newest First



- Active Datasets
- Organization Data
- Project Data
- My Data
- Team Data
- Shared Spaces
- Favorite Folders
- Trash

Team Data

Results for datasets containing text "du with":

			DU with NucleicAcids	1 record	10/18/2021	Kevin Schmidt	1168089		
			Folder: Team Data						
			DU with primary	4 records	11/09/2020	Kevin Schmidt	576408		
			Folder: Team Data/For Joe						

Complexity Issue

- How to add lots of new features without increasing complexity?
- Can new features go in their own place?
- Split Orion
 - Core Orion – Data Management, Analysis, 3D, Flores
 - Everything else – Gallery of apps
- UI plugin system
 - Apps are somewhat uniform
 - Don't interact with each other or the core

Looking Forward

- Ash will discuss the Orion roadmap later this morning
- Plug-in system to expand Orion
- Make the Orion user experience best in class
- Lots of changes underway to make that happen
- We welcome feedback!

A full-page background image of a starry night sky. The Milky Way galaxy is visible as a dense band of stars stretching across the upper half of the frame. In the lower right corner, the dark silhouette of a person stands on a grassy hill, looking up at the stars.

Thank You

The End