Scale of Orion UI and its challenges

Highlights from recent releases:
  Data handling
  3D modeling
  Discussion boards

Looking forward
“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

OpenEye
Lots of Code

- 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
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
Discussion Boards

- Allow multi-way discussions about modeling sessions
- Pictures, links, rich text
- Provide links to live data
- Can be shared with team members
Search: **du with** enter a tag or resource name...

- Current folder
- All project folders

**Results for datasets containing text “du with”:**

- **DU with NucleicAcids**
  - Folder: Team Data
  - 1 record
  - 10/18/2021
  - Kevin Schmidt
  - 1168089

- **DU with primary**
  - Folder: Team Data/For Joe
  - 4 records
  - 11/09/2020
  - Kevin Schmidt
  - 576408
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, Floes
  • 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!
Thank You

The End