Designing for Expert Use

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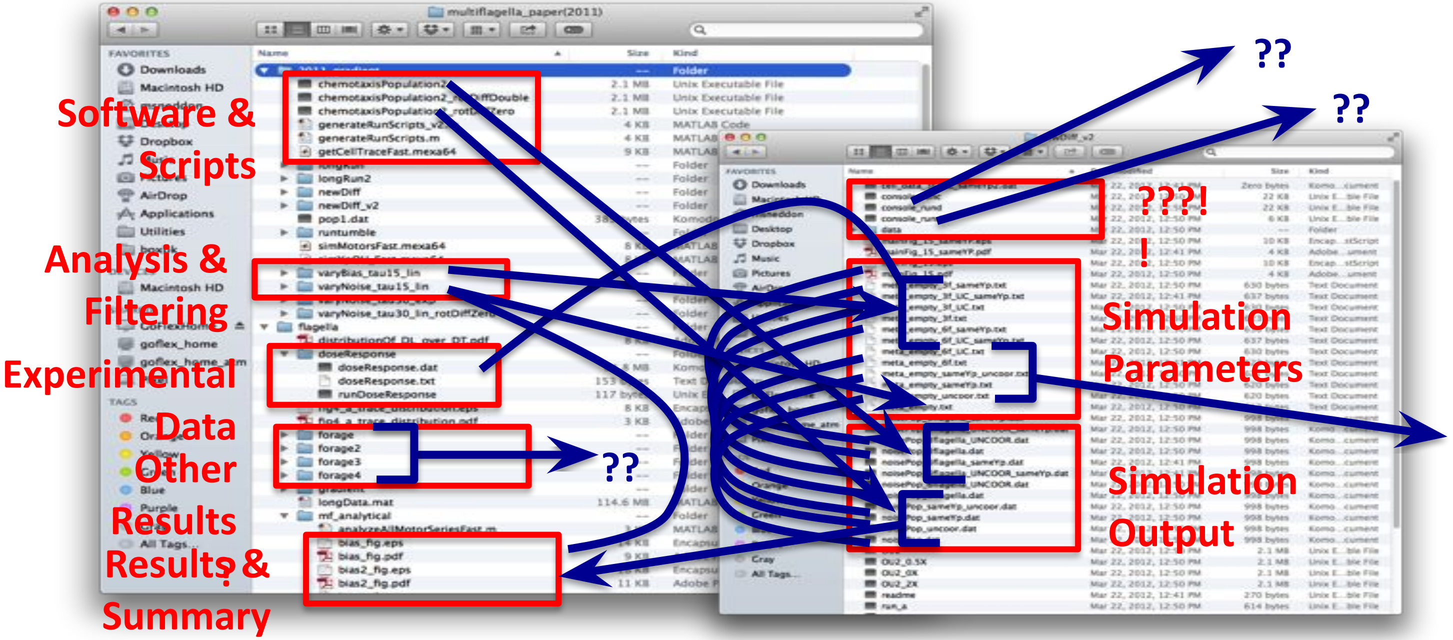
U.S. DEPARTMENT OF ENERGY | Office of Science

Why UX in the sciences?

The realities of scientific work

- Not a sequential, well defined process
- Supporting artifacts and contexts of use are not always captured by software
- Collaborations might have existing complex software stacks that need to be considered

UX research can help uncover these considerations and UX design ensures that software that take these factors into account.



Software & Scripts

Analysis & Filtering

Experimental Data

Other Results

Results & Summary Figures

Simulation Parameters

Simulation Output

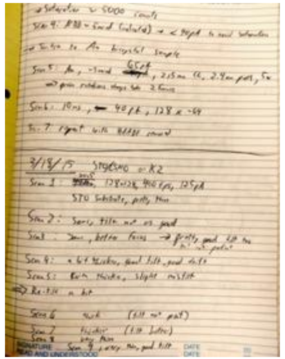
??

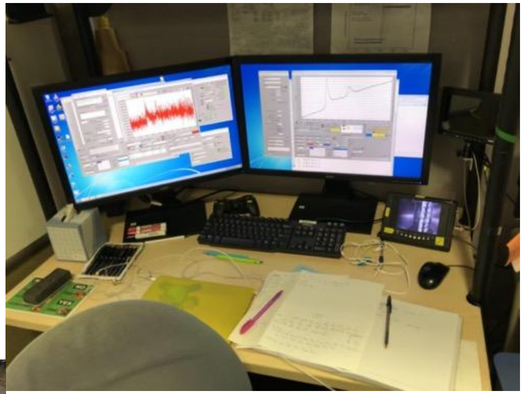
??

??

???!
!

Courtesy: Paramvir Dehal, KBase team

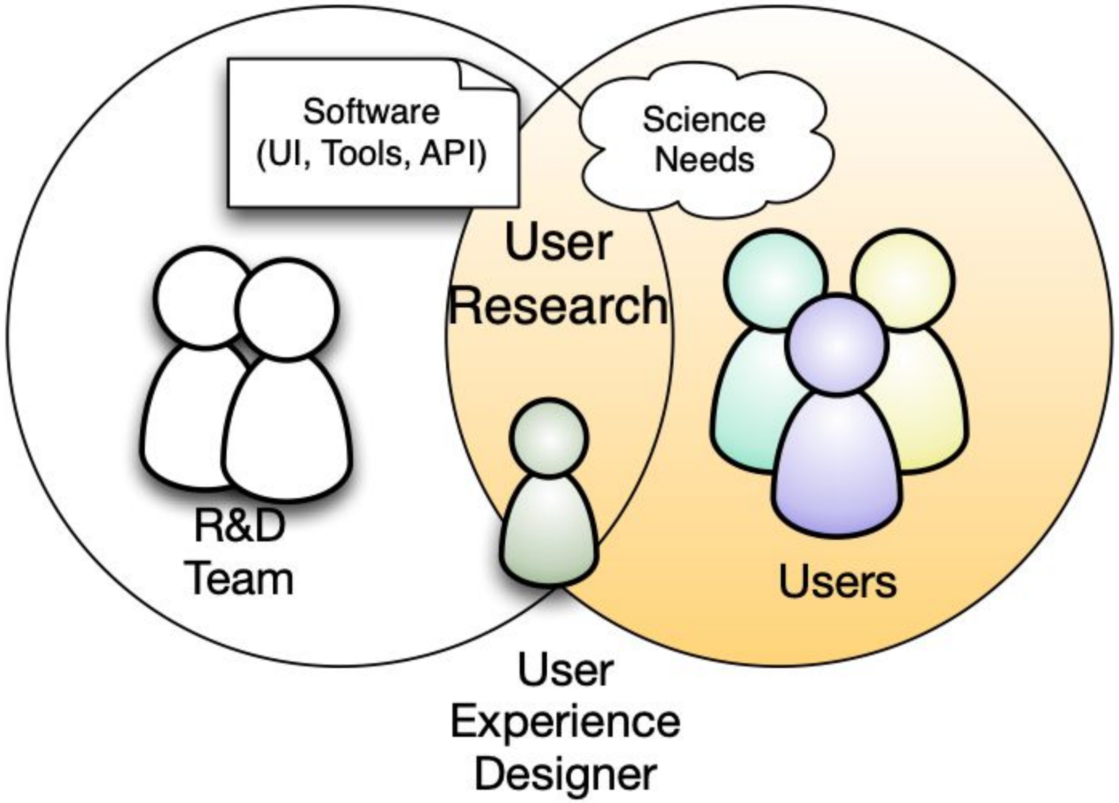




Source: Ameriflux project

Adapted from slide courtesy of Lavanya Ramakrishnan

We work as interdisciplinary teams to develop scientific software



Courtesy of Lavanya Ramakrishnan

- We work closely with application scientist to develop methods and tools to manage the data and workflows
- We use UX methods to understand user needs and convert that into concrete and actionable outputs

Developing the “right thing” is important for user adoption of new software, and the UX research and design process is essential to achieve this.

UX Design Process

RESEARCH
DESIGN
EVALUATE

Learning about how the users work, context of use, limitations of current tools

Design the experience of how the user will use the software to do their work

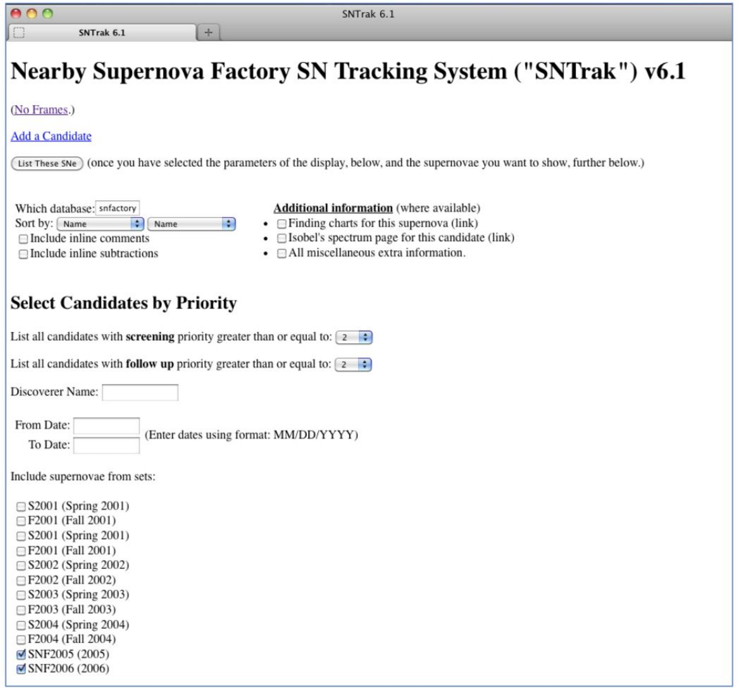
Evaluate the design through usability studies and follow-up interviews

Takeaways for Expert Use Design

RESEARCH

Understand Work Processes and Goals

SNFactory originally used a search interface as their primary data system.
What they actually needed was a tracking system.



SNTrak 6.1

Nearby Supernova Factory SN Tracking System ("SNTrak") v6.1

(No Frames.)

Add a Candidate

List These SNe (once you have selected the parameters of the display, below, and the supernovae you want to show, further below.)

Which database: snfactory
Sort by: Name Name
☐ Include inline comments
☐ Include inline subtractions

Additional information (where available)

- ☐ Finding charts for this supernova (link)
- ☐ Isobel's spectrum page for this candidate (link)
- ☐ All miscellaneous extra information.

Select Candidates by Priority

List all candidates with **screening** priority greater than or equal to: 2

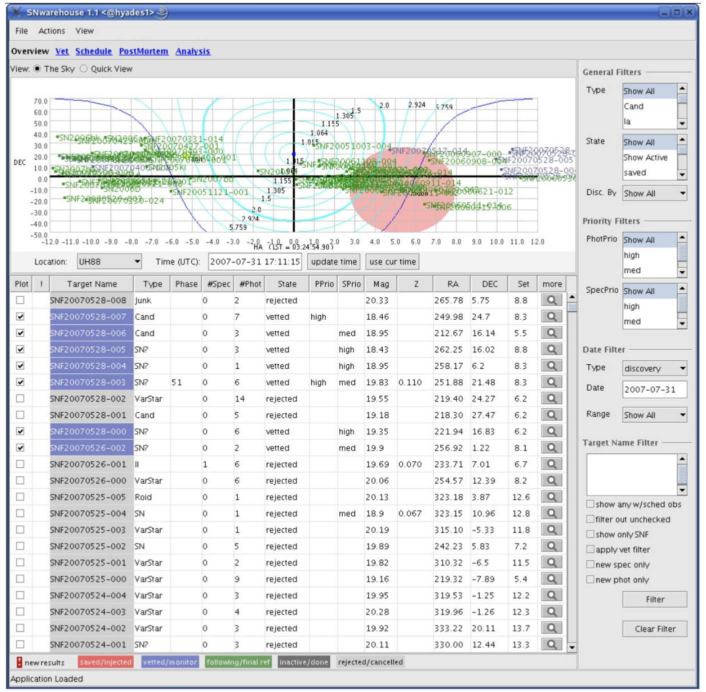
List all candidates with **follow up** priority greater than or equal to: 2

Discoverer Name:

From Date:
To Date: (Enter dates using format: MM/DD/YYYY)

Include supernovae from sets:

☐ S2001 (Spring 2001)
☐ F2001 (Fall 2001)
☐ S2001 (Spring 2001)
☐ F2001 (Fall 2001)
☐ S2002 (Spring 2002)
☐ F2002 (Fall 2002)
☐ S2003 (Spring 2003)
☐ F2003 (Fall 2003)
☐ S2004 (Spring 2004)
☐ F2004 (Fall 2004)
☑ SNF2005 (2005)
☑ SNF2006 (2006)



SNwarehouse 1.1 <@hyades1>

View: ● The Sky ○ Quick View

Location: UH88 Time (UTC): 2007-07-31 17:11:15 update time use cur time

Plot	!	Target Name	Type	Phase	#Spec	#Phot	State	PPrio	SPrio	Mag	Z	RA	DEC	Set	more
☐		SNF20070528-008	Junk		0	2	rejected			20.33		265.78	5.75	8.8	🔍
☑		SNF20070528-007	Cand		0	7	vetted	high		18.46		249.98	24.7	8.3	🔍
☑		SNF20070528-006	Cand		0	3	vetted		med	18.95		212.67	16.14	5.5	🔍
☑		SNF20070528-005	SN?		0	3	vetted		high	18.43		262.25	16.02	8.8	🔍
☑		SNF20070528-004	SN?		0	1	vetted		high	18.95		258.17	6.2	8.3	🔍
☑		SNF20070528-003	SN?	51	0	6	vetted	high	med	19.83	0.110	251.88	21.48	8.3	🔍
☐		SNF20070528-002	VarStar		0	14	rejected			19.55		219.40	24.27	6.2	🔍
☐		SNF20070528-001	Cand		0	5	rejected			19.18		218.30	27.47	6.2	🔍
☑		SNF20070528-000	SN?		0	6	vetted		high	19.35		221.94	16.83	6.2	🔍
☑		SNF20070526-002	SN?		0	2	vetted		med	19.9		256.92	1.22	8.1	🔍
☐		SNF20070526-001	II		1	6	rejected			19.69	0.070	233.71	7.01	6.7	🔍
☐		SNF20070526-000	VarStar		0	6	rejected			20.06		254.57	12.39	8.2	🔍
☐		SNF20070525-005	Roid		0	1	rejected			20.13		323.18	3.87	12.6	🔍
☐		SNF20070525-004	SN		0	1	rejected		med	18.9	0.067	323.15	10.96	12.8	🔍
☐		SNF20070525-003	VarStar		0	1	rejected			20.19		315.10	-5.33	11.8	🔍
☐		SNF20070525-002	SN		0	5	rejected			19.89		242.23	5.83	7.2	🔍
☐		SNF20070525-001	VarStar		0	2	rejected			19.82		310.32	-6.5	11.5	🔍
☐		SNF20070525-000	VarStar		0	9	rejected			19.16		219.32	-7.89	5.4	🔍
☐		SNF20070524-004	VarStar		0	3	rejected			19.95		319.53	-1.25	12.2	🔍
☐		SNF20070524-003	VarStar		0	4	rejected			20.28		319.96	-1.26	12.3	🔍
☐		SNF20070524-002	VarStar		0	3	rejected			19.92		333.22	20.11	13.7	🔍
☐		SNF20070524-001	SN?		0	3	rejected			20.11		330.00	12.44	13.3	🔍

! new results saved/injected vetted/monitor following/final ref inactive/done rejected/cancelled

Application Loaded

General Filters
Type: Show All, Cand, Ia
State: Show All, Show Active, saved
Disc. By: Show All

Priority Filters
PhotPrio: Show All, high, med
SpecPrio: Show All, high, med

Date Filter
Type: discovery
Date: 2007-07-31
Range: Show All

Target Name Filter

☐ show any w/sched obs
☐ filter out unchecked
☐ show only SNF
☐ apply vet filter
☐ new spec only
☐ new phot only

The original search style interface didn’t capture the need to track the currently active candidate supernovae.

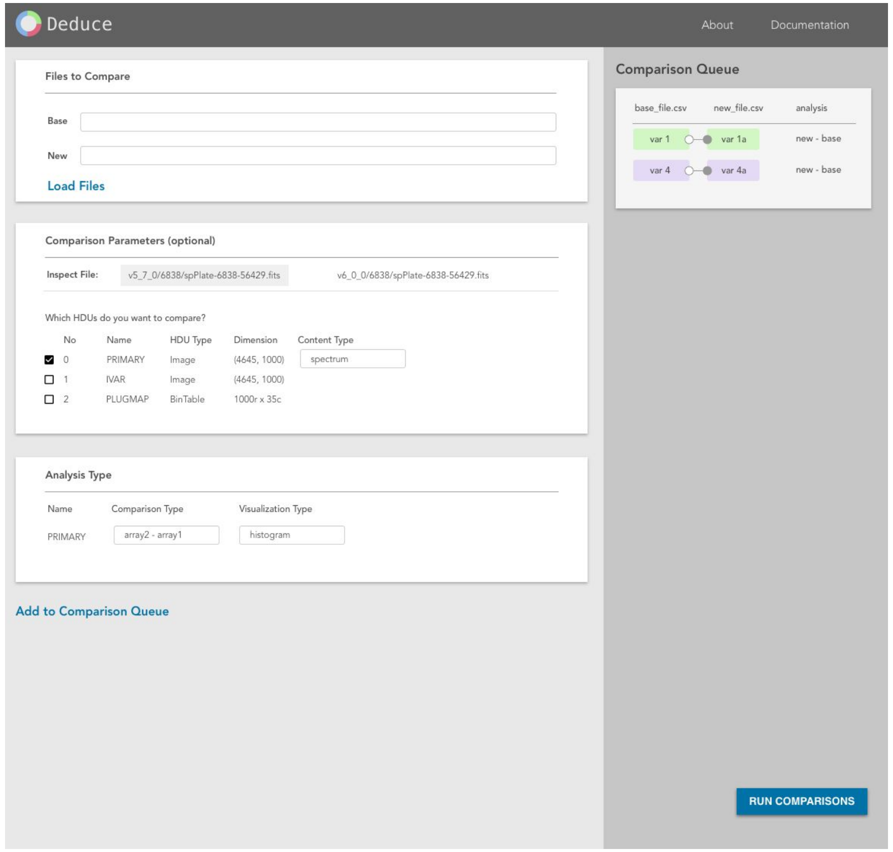
- Interviews and observations can reveal underlying workflows.
- Pay attention to “shadow systems” such as notebooks and files.

RESEARCH

Understand User Motivations and Values

“If I’m going to go to all the trouble of coding my own plugin, why would I bother using your framework?”

- There can be a tension between the time and effort needed to write code and the value you get being able to run that code at scale.
- We decided to create a visual plugin builder. This helps support exploratory work needed to understand data change and also eases some of the coding burden of developing plugins. The output script can run at scale.



Files to Compare

Base

New

Comparison Parameters (optional)

Inspect File: v5_7_0/6838/spPlate-6838-56429.fits v6_0_0/6838/spPlate-6838-56429.fits

Which HDUs do you want to compare?

	No	Name	HDU Type	Dimension	Content Type
☑	0	PRIMARY	Image	(4645, 1000)	spectrum
□	1	IVAR	Image	(4645, 1000)	
□	2	PLUGMAP	BinTable	1000r x 35c	

Analysis Type

Name	Comparison Type	Visualization Type
PRIMARY	array2 - array1	histogram

Comparison Queue

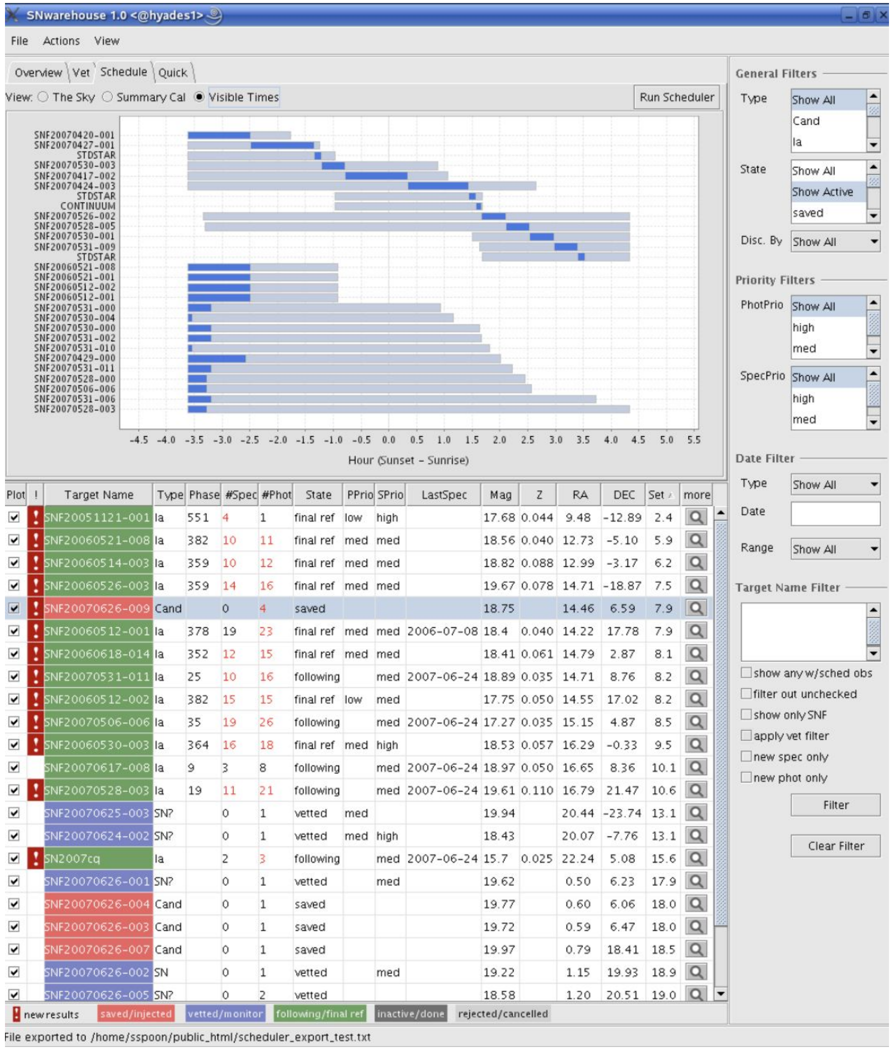
base_file.csv	new_file.csv	analysis
var 1	var 1a	new - base
var 4	var 4a	new - base

Deduce helps users understand data change across datasets. This visual plugin builder helps users define and explore data change.

DESIGN

Design for User Control

- Expert users often want to be able to override automations and tweak outputs from algorithms
- If possible, consider human in the loop scenarios before writing the algorithm



General Filters

Type: Show All / Cand / Ia

State: Show All / Show Active / saved

Disc. By: Show All

Priority Filters

PhotPrio: Show All / high / med

SpecPrio: Show All / high / med

Date Filter

Type: Show All

Date:

Range: Show All

Target Name Filter

□ show any w/sched obs
□ filter out unchecked
□ show only SNF
□ apply vet filter
□ new spec only
□ new phot only

Plot	!	Target Name	Type	Phase	#Spec	#Phot	State	PPrio	SPrio	LastSpec	Mag	Z	RA	DEC	Set	more
☑	!	SNF20051121-001	Ia	551	4	1	final ref	low	high		17.68	0.044	9.48	-12.89	2.4	🔍
☑	!	SNF20060521-008	Ia	382	10	11	final ref	med	med		18.56	0.040	12.73	-5.10	5.9	🔍
☑	!	SNF20060514-003	Ia	359	10	12	final ref	med	med		18.82	0.088	12.99	-3.17	6.2	🔍
☑	!	SNF20060526-003	Ia	359	14	16	final ref	med	med		19.67	0.078	14.71	-18.87	7.5	🔍
☑	!	SNF20070626-009	Cand		0	4	saved				18.75		14.46	6.59	7.9	🔍
☑	!	SNF20060512-001	Ia	378	19	23	final ref	med	med	2006-07-08	18.4	0.040	14.22	17.78	7.9	🔍
☑	!	SNF20060618-014	Ia	352	12	15	final ref	med	med		18.41	0.061	14.79	2.87	8.1	🔍
☑	!	SNF20070531-011	Ia	25	10	16	following		med	2007-06-24	18.89	0.035	14.71	8.76	8.2	🔍
☑	!	SNF20060512-002	Ia	382	15	15	final ref	low	med		17.75	0.050	14.55	17.02	8.2	🔍
☑	!	SNF20070506-006	Ia	35	19	26	following		med	2007-06-24	17.27	0.035	15.15	4.87	8.5	🔍
☑	!	SNF20060530-003	Ia	364	16	18	final ref	med	high		18.53	0.057	16.29	-0.33	9.5	🔍
☑		SNF20070617-008	Ia	9	3	8	following		med	2007-06-24	18.97	0.050	16.65	8.36	10.1	🔍
☑	!	SNF20070528-003	Ia	19	11	21	following		med	2007-06-24	19.61	0.110	16.79	21.47	10.6	🔍
☑		SNF20070625-003	SN?		0	1	vetted	med			19.94		20.44	-23.74	13.1	🔍
☑		SNF20070624-002	SN?		0	1	vetted	med	high		18.43		20.07	-7.76	13.1	🔍
☑	!	SN2007cq	Ia		2	3	following		med	2007-06-24	15.7	0.025	22.24	5.08	15.6	🔍
☑		SNF20070626-001	SN?		0	1	vetted		med		19.62		0.50	6.23	17.9	🔍
☑		SNF20070626-004	Cand		0	1	saved				19.77		0.60	6.06	18.0	🔍
☑		SNF20070626-003	Cand		0	1	saved				19.72		0.59	6.47	18.0	🔍
☑		SNF20070626-007	Cand		0	1	saved				19.97		0.79	18.41	18.5	🔍
☑		SNF20070626-002	SN		0	1	vetted		med		19.22		1.15	19.93	18.9	🔍
☑		SNF20070626-005	SN?		0	2	vetted				18.58		1.20	20.51	19.0	🔍

! new results   saved/injected   vetted/monitor   following/final ref   inactive/done   rejected/cancelled

File exported to /home/sspoon/public_html/scheduler_export_test.txt

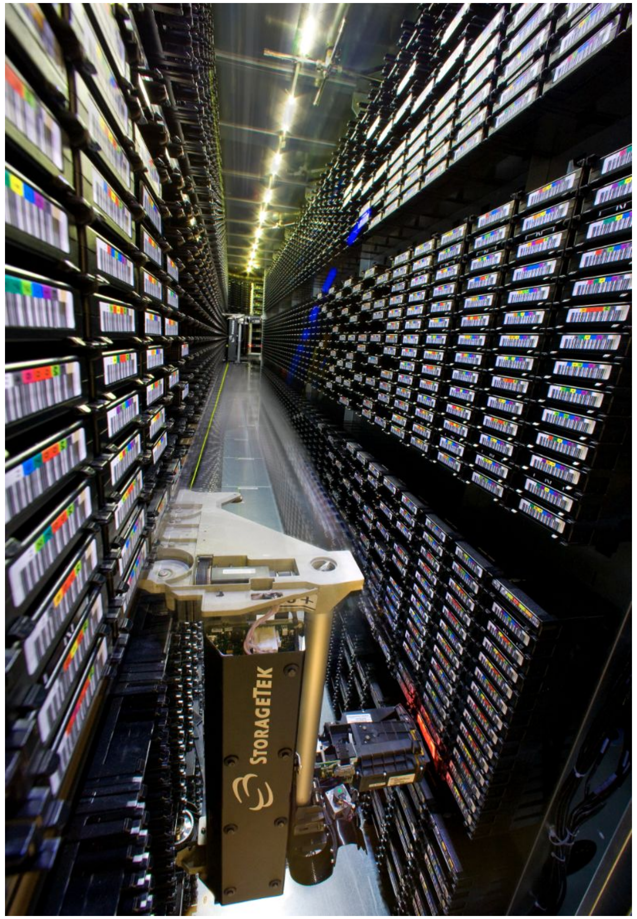
The scheduling algorithm didn’t take into account the desire to be able to tweak the schedule afterward.

DESIGN

Design for Transparency

“You had no way of telling that if I try to open this file, whether it will open in a fraction of a second or whether it will take five minutes, because it is running off to tape and doing this thing for me.”

Algorithms and abstractions are useful but can’t be black boxes. Expert users want to know what to expect.

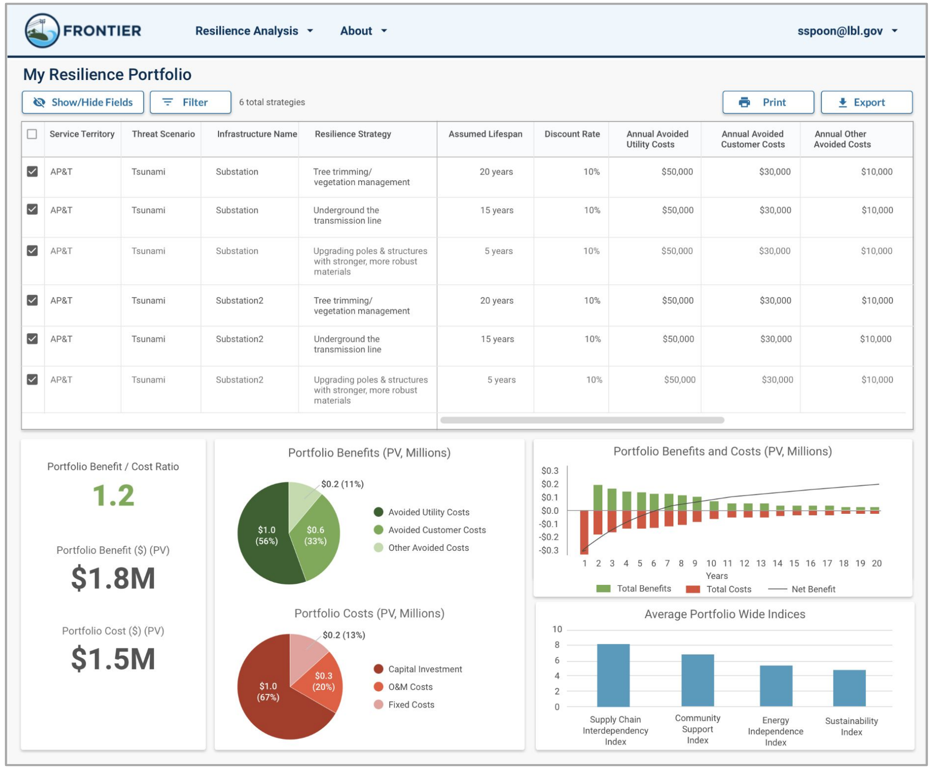


Accessing data from archival storage takes longer than data on disk. The design shouldn’t abstract away this type of information.

DESIGN

Design for Efficiency

- Scientific users want to be able to do their jobs efficiently and without errors.
- Efficiency looks different depending on the purpose and goals at hand
- UI level takeaways for the data overview pattern:
    - **Design for data density.** Minimize what needs to be held in working memory to make a decision.
    - **Don’t display more data than is needed.** Improve signal to noise by hiding ancillary information in secondary layers.



My Resilience Portfolio

6 total strategies

□	Service Territory	Threat Scenario	Infrastructure Name	Resilience Strategy	Assumed Lifespan	Discount Rate	Annual Avoided Utility Costs	Annual Avoided Customer Costs	Annual Other Avoided Costs
☑	AP&T	Tsunami	Substation	Tree trimming/ vegetation management	20 years	10%	$50,000	$30,000	$10,000
☑	AP&T	Tsunami	Substation	Underground the transmission line	15 years	10%	$50,000	$30,000	$10,000
☑	AP&T	Tsunami	Substation	Upgrading poles & structures with stronger, more robust materials	5 years	10%	$50,000	$30,000	$10,000
☑	AP&T	Tsunami	Substation2	Tree trimming/ vegetation management	20 years	10%	$50,000	$30,000	$10,000
☑	AP&T	Tsunami	Substation2	Underground the transmission line	15 years	10%	$50,000	$30,000	$10,000
☑	AP&T	Tsunami	Substation2	Upgrading poles & structures with stronger, more robust materials	5 years	10%	$50,000	$30,000	$10,000

Portfolio Benefit / Cost Ratio
1.2

Portfolio Benefit ($) (PV)
$1.8M

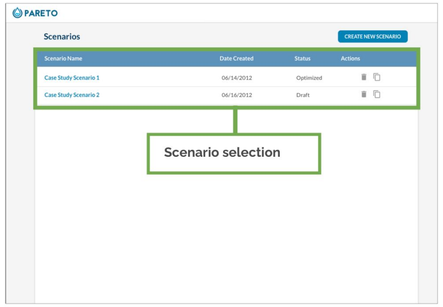
Portfolio Cost ($) (PV)
$1.5M

Example of a data overview pattern

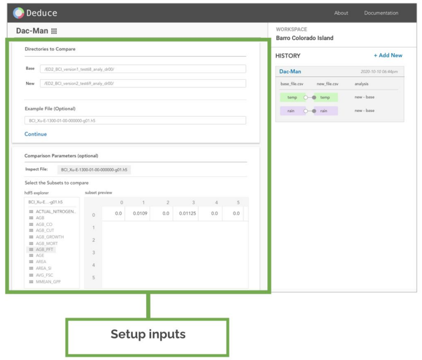
STRUDEL: Scientific software Research for User experience, Design, Engagement, and Learning

Towards developing a comprehensive UX framework for the sciences.

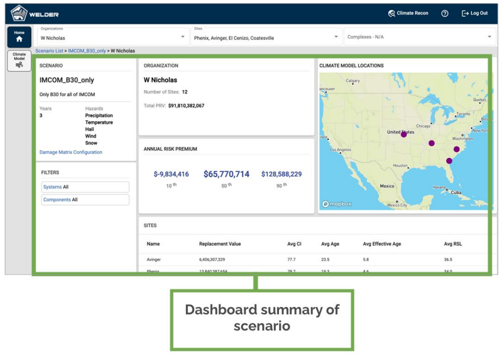
Motivation: user interfaces across the sciences have many common parts



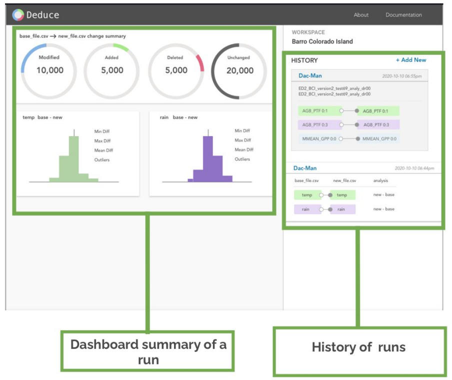
Scenario selection



Setup inputs

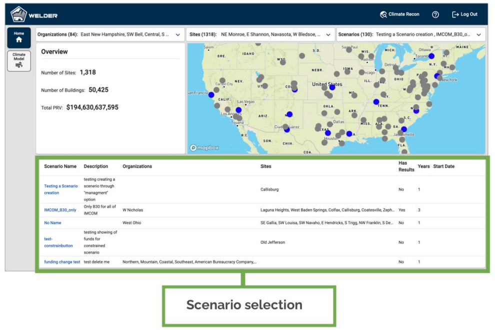


Dashboard summary of scenario

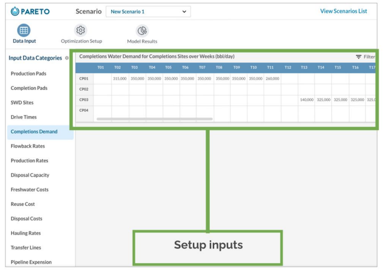


Dashboard summary of a run

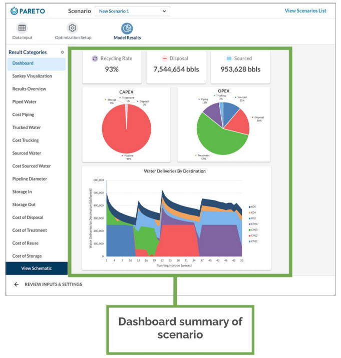
History of runs



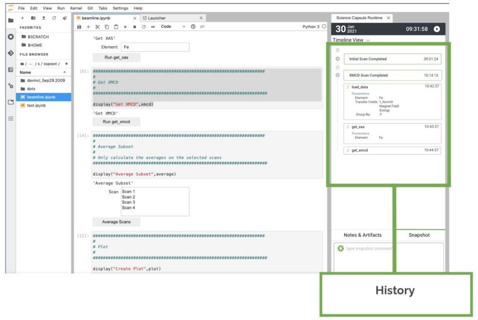
Scenario selection



Setup inputs



Dashboard summary of scenario



History

Scenario Selection

Select Input

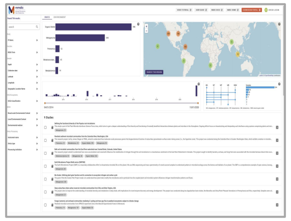
Dashboard Summary

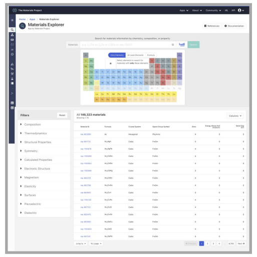
History

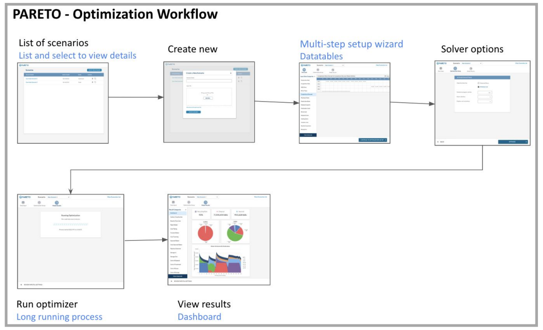
How can we empower scientific users to develop their own UIs while leveraging our learnings of how to create good scientific UIs?

STRUDEL: Develop a design system for scientific software

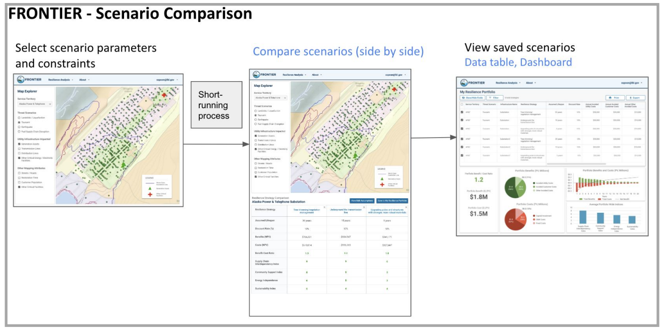
Science Project Artifacts







PARETO - Optimization Workflow



FRONTIER - Scenario Comparison

Select scenario parameters and constraints
Short-running process
Compare scenarios (side by side)
View saved scenarios
Data table, Dashboard

Science Software Characteristics

Users	Science Domain
Software Intent	Software Lifespan
Software Team	Software Stack
Main Scenarios / Workflows	Data Types

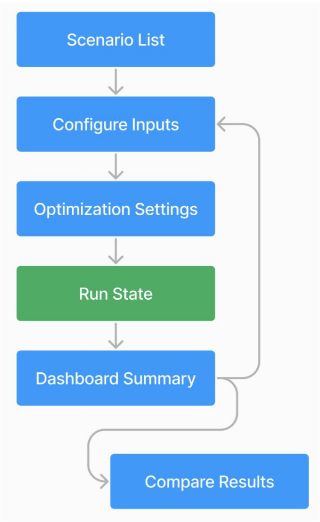
Design System

A collection of reusable components that can be assembled to build a UI

Components

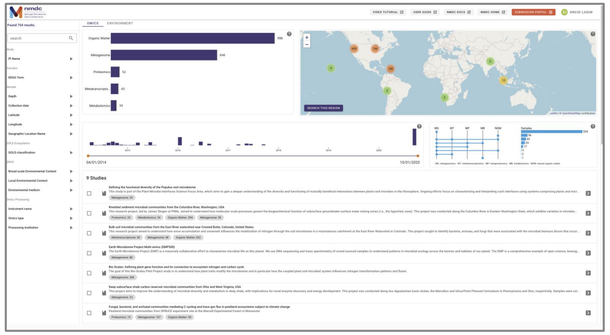
Layouts

UI Flows



Design System Guidelines & Implementation

Towards Generalized Page Layout Templates



Found 754 results.

9 Studies

□ **Defining the functional diversity of the Populus root microbiome**
This study is part of the Plant-Microbe Interfaces Science Focus Area, which aims to gain a deeper understanding of the diversity and functioning of mutually beneficial interactions between plants and microbes in the rhizosphere. Ongoing efforts focus on characterizing and interpreting such interfaces using systems comprising plants and micr...
Metagenome: 29

□ **Riverbed sediment microbial communities from the Columbia River, Washington, USA**
This research project, led by James Stegen at PNNL, aimed to understand how molecular-scale processes govern the biogeochemical function of subsurface groundwater-surface water mixing zones (i.e., the hyporheic zone). This project was conducted along the Columbia River in Eastern Washington State, which exhibits variation in microbio...
Proteomics: 33 Metabolomics: 34 Organic Matter: 294 Metagenome: 50

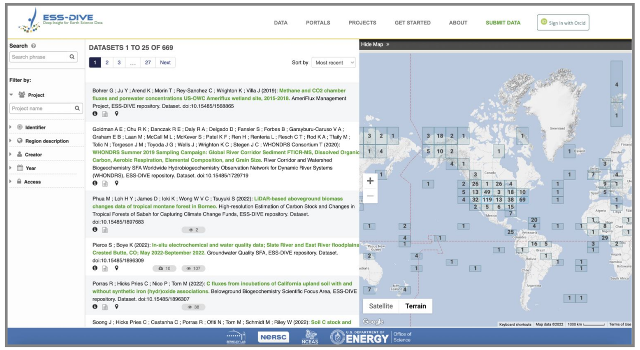
□ **Bulk soil microbial communities from the East River watershed near Crested Butte, Colorado, United States**
This research project aimed to understand how snow accumulation and snowmelt influences the mobilization of nitrogen through the soil microbiome in a mountainous catchment at the East River Watershed in Colorado. This project sought to identify bacteria, archaea, and fungi that were associated with the microbial biomass bloom that occur...
Metatranscriptome: 45 Metagenome: 48 Organic Matter: 652

□ **Earth Microbiome Project Multi-omics (EMP500)**
The Earth Microbiome Project (EMP) is a massively collaborative effort to characterize microbial life on this planet. We use DNA sequencing and mass spectrometry of crowd-sourced samples to understand patterns in microbial ecology across the biomes and habitats of our planet. The EMP is a comprehensive example of open science, leverag...
Metagenome: 80

□ **Bio-Scales: Defining plant gene function and its connection to ecosystem nitrogen and carbon cycle**
The goal of this Bio-Scales Pilot Project study is to understand how plant traits modify the microbiome and in particular how the coupled plant-soil-microbial system influences nitrogen transformation patterns and fluxes.
Metagenome: 206

□ **Deep subsurface shale carbon reservoir microbial communities from Ohio and West Virginia, USA**
This project aims to improve the understanding of microbial diversity and metabolism in deep shale, with implications for novel enzyme discovery and energy development. This project was conducted along two Appalachian basin shales, the Marcellus and Utica/Point Pleasant formations in Pennsylvania and Ohio, respectively. Samples were col...
Metagenome: 23

□ **Fungal, bacterial, and archaeal communities mediating C cycling and trace gas flux in peatland ecosystems subject to climate change**
Peatland microbial communities from SPRUCE experiment site at the Marcell Experimental Forest in Minnesota
Proteomics: 19 Metagenome: 107 Organic Matter: 50



DATASETS 1 TO 25 OF 669

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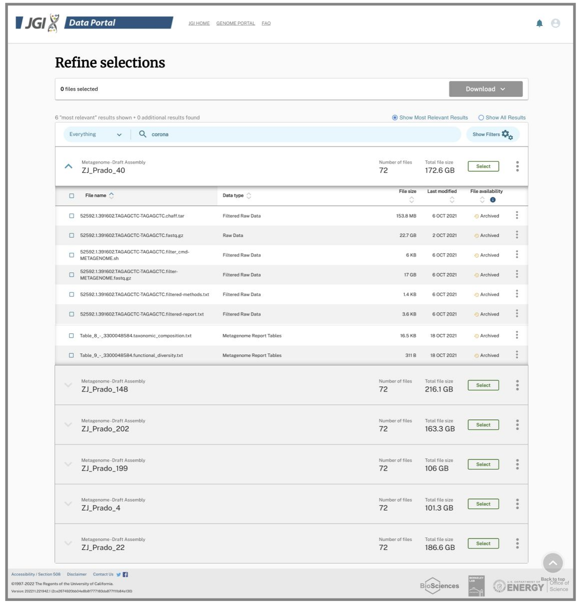

Refine selections

0 files selected

6 "most relevant" results shown + 0 additional results found

● Show Most Relevant Results ○ Show All Results

Everything corona

Metagenome - Draft Assembly
ZJ_Prado_40
Number of files 72
Total file size 172.6 GB

□	File name	Data type	File size	Last modified	File availability
□	52592.1.391602.TAGAGCTC-TAGAGCTC.chaff.tar	Filtered Raw Data	153.8 MB	6 OCT 2021	Archived
□	52592.1.391602.TAGAGCTC-TAGAGCTC.fastq.gz	Raw Data	22.7 GB	2 OCT 2021	Archived
□	52592.1.391602.TAGAGCTC-TAGAGCTC.filter_cmd-METAGENOME.sh	Filtered Raw Data	6 KB	6 OCT 2021	Archived
□	52592.1.391602.TAGAGCTC-TAGAGCTC.filter-METAGENOME.fastq.gz	Filtered Raw Data	17 GB	6 OCT 2021	Archived
□	52592.1.391602.TAGAGCTC-TAGAGCTC.filtered-methods.txt	Filtered Raw Data	1.4 KB	6 OCT 2021	Archived
□	52592.1.391602.TAGAGCTC-TAGAGCTC.filtered-report.txt	Filtered Raw Data	3.6 KB	6 OCT 2021	Archived
□	Table_8_-_3300048584.taxonomic_composition.txt	Metagenome Report Tables	16.5 KB	18 OCT 2021	Archived
□	Table_9_-_3300048584.functional_diversity.txt	Metagenome Report Tables	311 B	18 OCT 2021	Archived

	Number of files	Total file size
Metagenome - Draft Assembly ZJ_Prado_148	72	216.1 GB
Metagenome - Draft Assembly ZJ_Prado_202	72	163.3 GB
Metagenome - Draft Assembly ZJ_Prado_199	72	106 GB
Metagenome - Draft Assembly ZJ_Prado_4	72	101.3 GB
Metagenome - Draft Assembly ZJ_Prado_22	72	186.6 GB

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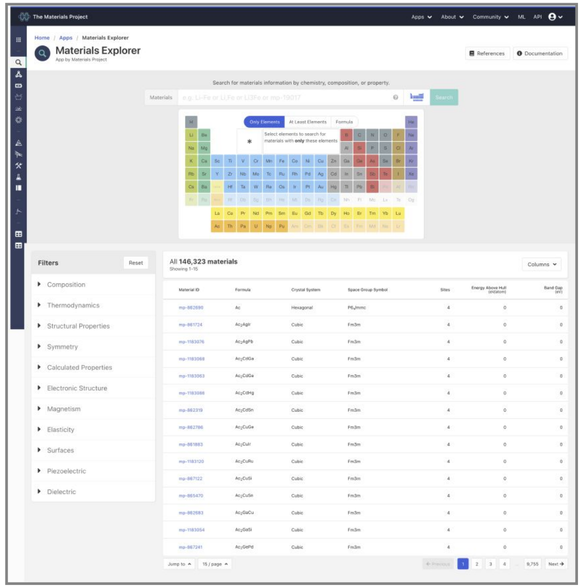
Version: 202211.221942.1 (2ce2674920bb04e8b8f777183da877f11b84a130)



Home / Apps / Materials Explorer

Materials Explorer
App by Materials Project

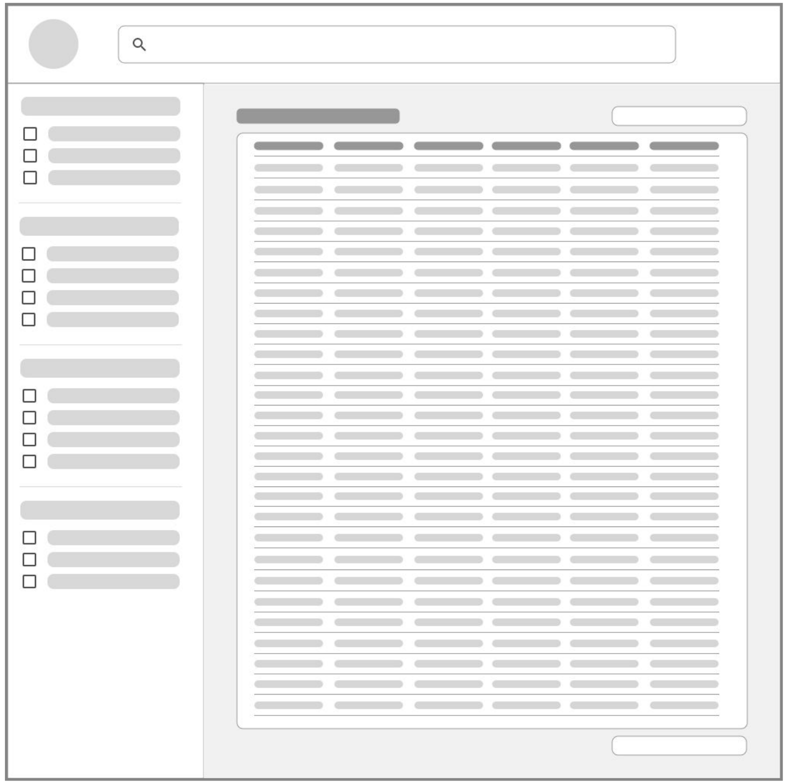
Search for materials information by chemistry, composition, or property.

Select elements to search for materials with **only** these elements

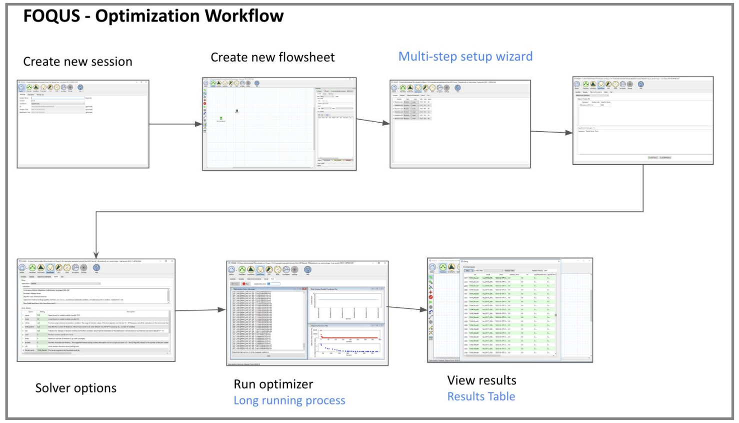
All **146,323 materials**
Showing 1-15

Material ID	Formula	Crystal System	Space Group Symbol	Sites	Energy Above Hull (eV/atom)	Band Gap (eV)
mp-862690	Ac	Hexagonal	$P6_3/mmc$	4	0	0
mp-861724	Ac_2AgIr	Cubic	Fm3m	4	0	0
mp-1183076	Ac_2AgPb	Cubic	Fm3m	4	0	0
mp-1183068	Ac_2CdGa	Cubic	Fm3m	4	0	0
mp-1183063	Ac_2CdGe	Cubic	Fm3m	4	0	0
mp-1183088	Ac_2CdHg	Cubic	Fm3m	4	0	0
mp-862319	Ac_2CdSn	Cubic	Fm3m	4	0	0
mp-862786	Ac_2CuGe	Cubic	Fm3m	4	0	0
mp-861883	Ac_2CuIr	Cubic	Fm3m	4	0	0
mp-1183120	Ac_2CuRu	Cubic	Fm3m	4	0	0
mp-867122	Ac_2CuSi	Cubic	Fm3m	4	0	0
mp-865470	Ac_2CuSn	Cubic	Fm3m	4	0	0
mp-862683	Ac_2GaCu	Cubic	Fm3m	4	0	0
mp-1183054	Ac_2GaSi	Cubic	Fm3m	4	0	0
mp-867241	Ac_2GePd	Cubic	Fm3m	4	0	0

Generalized Data Portal Layout



Towards Generalized UI Flow Patterns


FOQUS - Optimization Workflow

Create new session

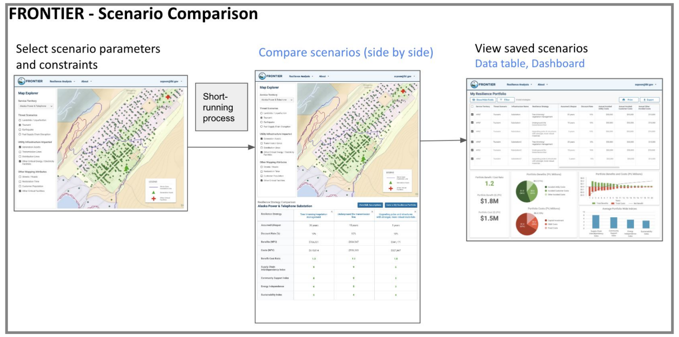
Create new flowsheet

Multi-step setup wizard

Solver options

Run optimizer
Long running process

View results
Results Table

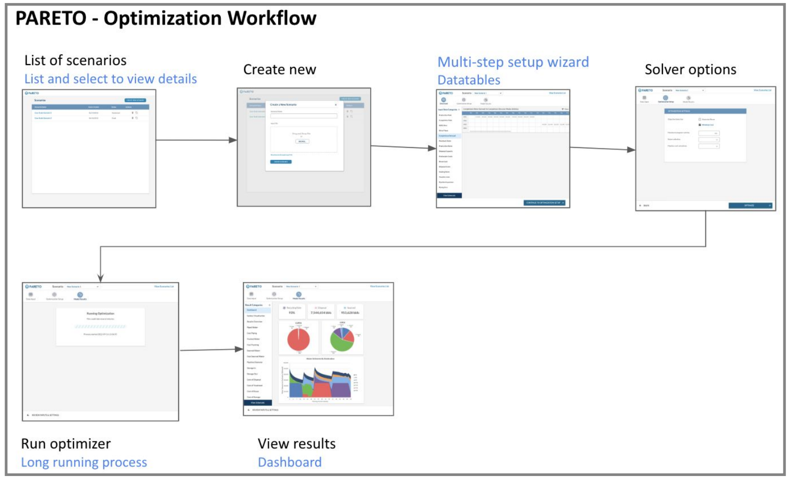

FRONTIER - Scenario Comparison

Select scenario parameters and constraints

Short-running process

Compare scenarios (side by side)

View saved scenarios
Data table, Dashboard


PARETO - Optimization Workflow

List of scenarios
List and select to view details

Create new

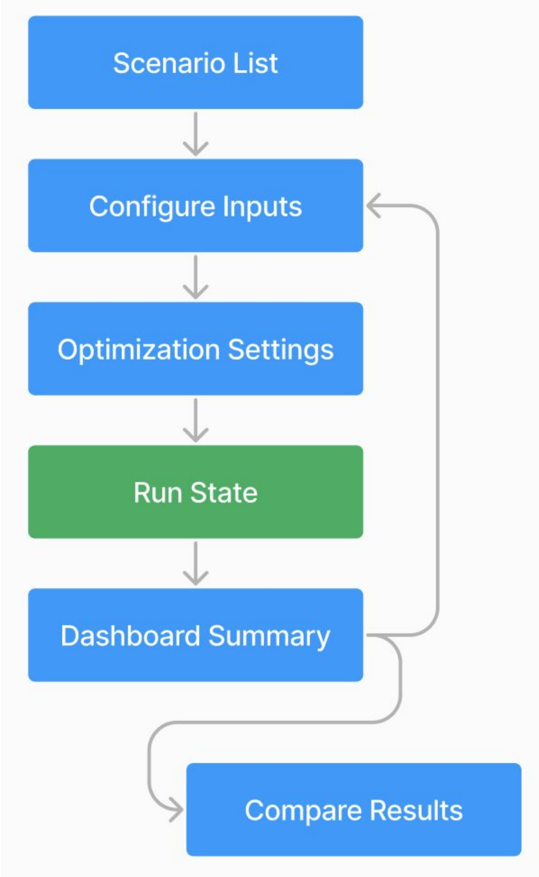
Multi-step setup wizard
Datatables

Solver options

Run optimizer
Long running process

View results
Dashboard

Generalized Optimization UI Flow



Scientific Software Dimensions

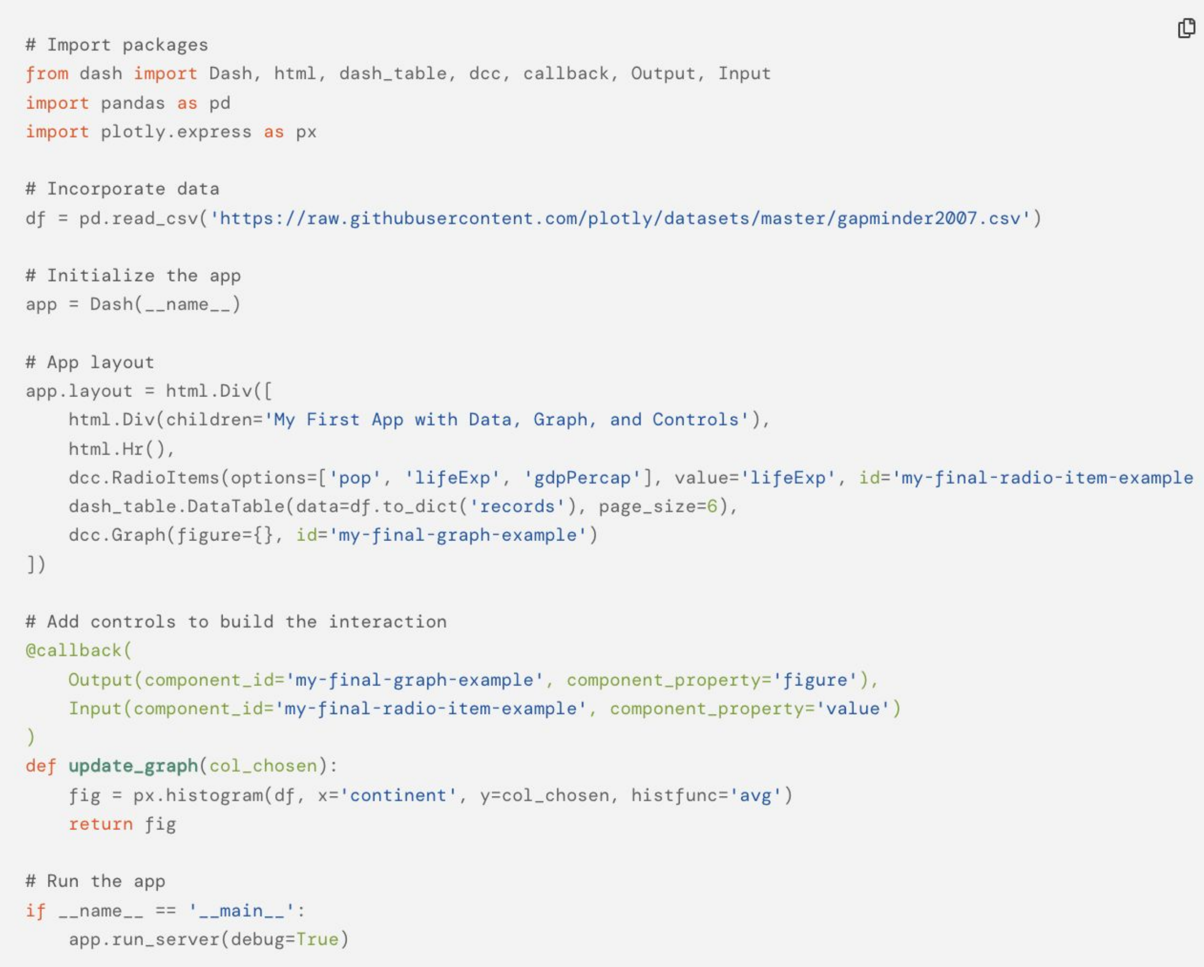
Subset of the dimensions and projects we are exploring

Project	Users	Domain	Main Scenarios	Software Lifespan	Software Team	Technical Stack
DARK ENERGY SPECTROSCOPIC INSTRUMENT	< 1000, internal collaborators	astrophysics	real time data taking	finite, the length of the survey	domain science developers (staff, postdocs, students)	bokeh
The Materials Project	>200,000, the general material science community	material science	exploring material info	ongoing	domain science developers (staff, postdocs, students)	plotly | Dash

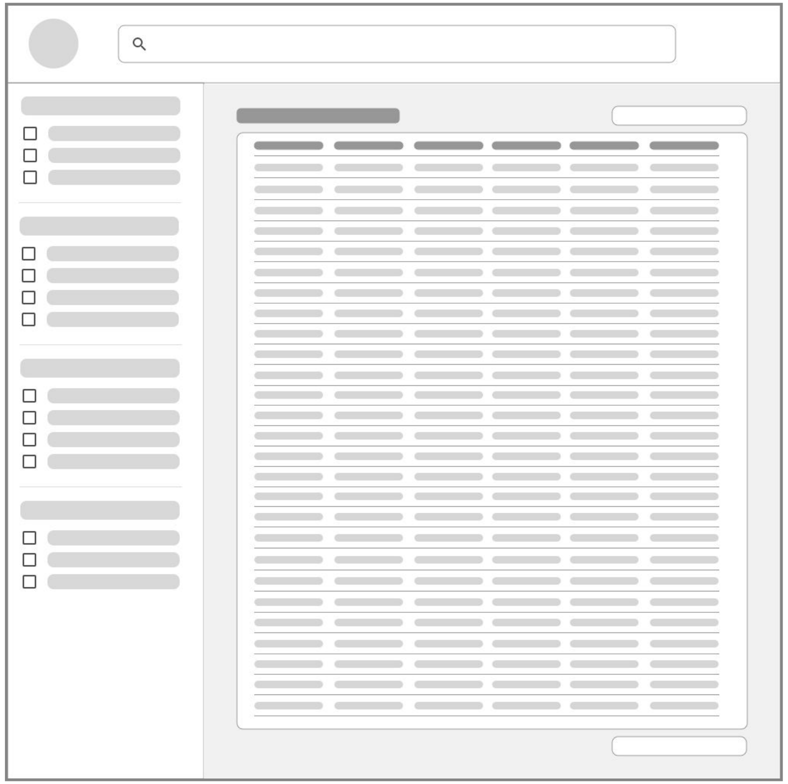
The decision to use "low code" technical stacks for both projects was based on the software team makeup

Towards A Design System Implementation

Investigate composing layouts and UI flows in python with a “low code” implementation of the design system.



```
# Import packages
from dash import Dash, html, dash_table, dcc, callback, Output, Input
import pandas as pd
import plotly.express as px

# Incorporate data
df = pd.read_csv('https://raw.githubusercontent.com/plotly/datasets/master/gapminder2007.csv')

# Initialize the app
app = Dash(__name__)

# App layout
app.layout = html.Div([
    html.Div(children='My First App with Data, Graph, and Controls'),
    html.Hr(),
    dcc.RadioItems(options=['pop', 'lifeExp', 'gdpPercap'], value='lifeExp', id='my-final-radio-item-example
    dash_table.DataTable(data=df.to_dict('records'), page_size=6),
    dcc.Graph(figure={}, id='my-final-graph-example')
])

# Add controls to build the interaction
@callback(
    Output(component_id='my-final-graph-example', component_property='figure'),
    Input(component_id='my-final-radio-item-example', component_property='value')
)
def update_graph(col_chosen):
    fig = px.histogram(df, x='continent', y=col_chosen, histfunc='avg')
    return fig

# Run the app
if __name__ == '__main__':
    app.run_server(debug=True)
```



Acknowledgements

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Questions? Contact me at sspoon@lbl.gov