

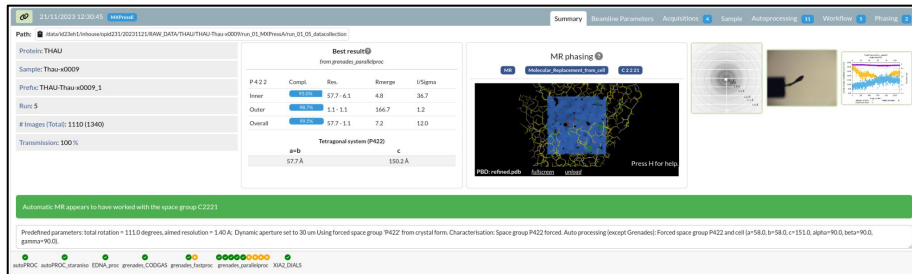
DRAC UI & Micro-frontends

NOBUGS - 27/09/2024

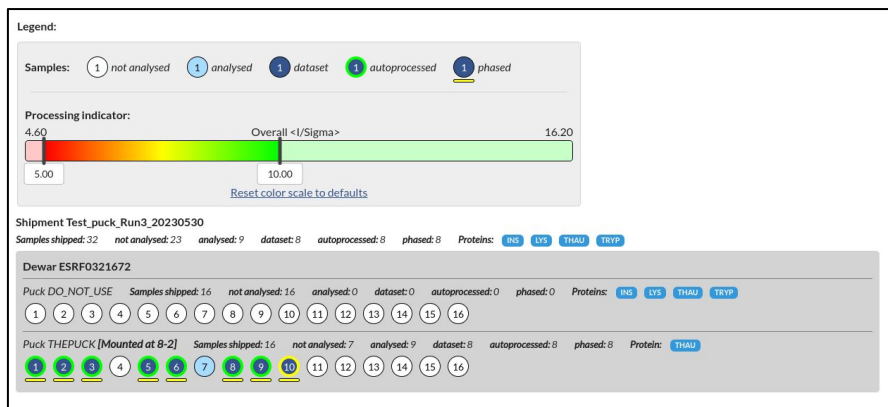
**Maël Gaonach
Marjolaine Bodin
Alex De Maria**

Starting point

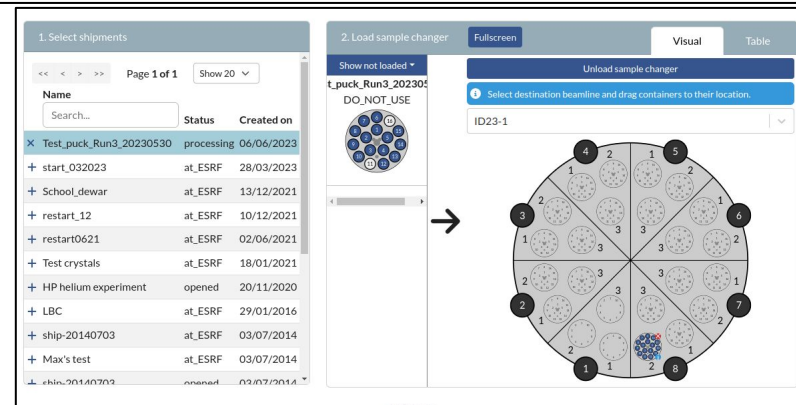
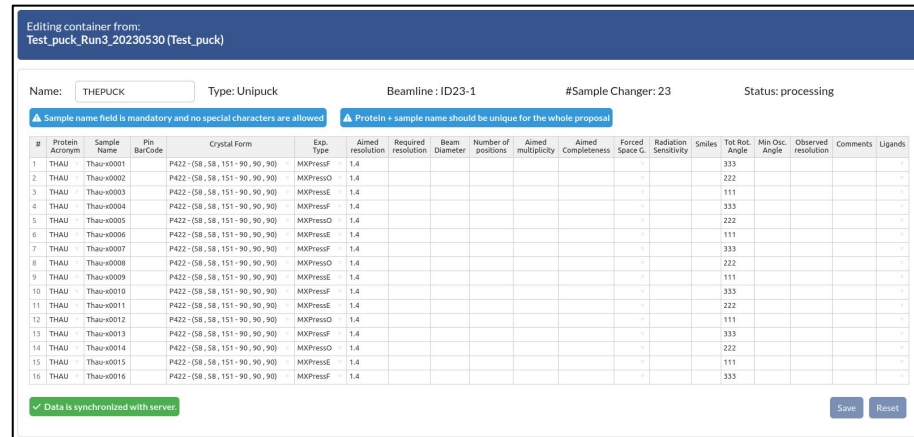
Growing amount of essential features for SB



Specialized data visualisation



Data quality assessment



Experiment preparation

Data Portal My Data Open Data Closed Data Feedback Log out Anonymous

Open Data / 1023-1-1000 1023-1 11/11/2023-11/11/2023 Data collected for the ISPyB Collaboration

Dataset List 439 Logbook

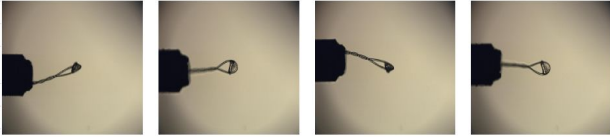
For users that want to download large volume of experimental data (>2GB), ESRF users can access the Globus service, please read the documentation for proceeding: <https://confluence.esrf.fr/display/SCKB/Globus>

Filter by samples x

Search

Date	Sample	Dataset	Definition	Files	Size	Processed	Download
11:00 14 Nov 2023	Sample-4-1-07	run_03_datacollection		22	2.3 GB	✓	Download
10:58 14 Nov 2023	Sample-4-1-07	run_02_characterisation		20	585.0 MB	✓	Download

Summary Crystallography Instrument Files 20 Metadata List

Name	run_02_characterisation [2023-11-14 10:58:26]	Resolution	1.3000423961627905 Å	
Definition		Wavelength	0.8856033875217176 Å	
Start	10:58:26 AM	Exposure Time	0.01 s	
Sample	Sample-4-1-07	Flux start	4.543246778242394e+12	
Images	4	Flux end	4.543246778242394e+12	
Transmission	100.0%	X Beam	154.46285559375 mm	
Prefix	ref-opid231_1_04d.h5	Y Beam	166.17452587499997 mm	

- diffraction_thumbnail_ref-opid231_1_0001 [2023-11-14 10:58:09] Processed
- diffraction_thumbnail_ref-opid231_1_0002 [2023-11-14 10:58:16] Processed
- diffraction_thumbnail_ref-opid231_1_0003 [2023-11-14 10:58:23] Processed
- diffraction_thumbnail_ref-opid231_1_0004 [2023-11-14 10:58:33] Processed
- characterisation [2023-11-14 10:58:57] Processed
- dozor_plot [2023-11-14 10:59:09] Processed

/data/d223eh1/inhouse/opid231/20231114/RAW_DATA/Sample-4-1-07/run_02_characterisation Download

10:56 14 Nov 2023	Sample-4-1-07	run_01_02_line		11	894.4 MB	✓	Download
10:56 14 Nov 2023	Sample-4-1-07	run_01_01_mesh		14	1.9 GB	✓	Download

+ Tons of essential features for the whole facility (including SB!)

- Data policy implementation (Raw & Processed data)
- Data download
- Electronic logbook
- DOI minting
- Sample tracking
- Reprocessing

- Limited data visualization : list of parameters, images...

- Needs to support wide variety of techniques

The ESRF Data Portal

The screenshot shows the ESRF Data Portal interface. At the top, there are navigation tabs for 'Data Portal', 'My Data', 'Open Data', and 'Closed Data'. Below this, there's a search bar and a 'Dataset List' button. A prominent orange banner provides information for users wanting to download large volumes of data. The main content area displays a table of datasets with columns for Date, Sample, Dataset, Definition, Files, Size, Processed, and Download. Two datasets are visible: 'run_03_datacollection' and 'run_02_characterisation'. Below the table, a detailed view for 'run_02_characterisation' is shown, including a 'Summary' tab and a 'Files' tab. The 'Files' tab lists several processed files, such as 'diffraction_thumbnail_ref-opid231_1_0001' and 'characterisation'. A green box highlights the 'Files' tab and its content, with a green arrow pointing from this box to a separate text box on the right. Another green box highlights the 'Summary' tab and its content, with a green arrow pointing from this box to the same text box on the right.

Date	Sample	Dataset	Definition	Files	Size	Processed	Download
11:00 14 Nov 2023	Sample-4-1-07	run_03_datacollection		22	2.3 GB	✓	Download
10:58 14 Nov 2023	Sample-4-1-07	run_02_characterisation		20	585.0 MB	✓	Download

Name	Resolution	Wavelength
run_02_characterisation [2023-11-14 10:58:26]	1.3000423961627905 Å	0.8856033875217176 Å

Start	Exposure Time
10:58:26 AM	0.01 s

Sample	Flux start	Flux end
Sample-4-1-07	4.543246778242394e+12	4.543246778242394e+12

Transmission	X Beam	Y Beam
100.0%	154.46285559375 mm	166.17452587499997 mm

Prefix	Ref	Y Beam
ref-opid231_1_004d.h5		166.17452587499997 mm

File Name	Status
diffraction_thumbnail_ref-opid231_1_0001 [2023-11-14 10:58:09]	Processed
diffraction_thumbnail_ref-opid231_1_0002 [2023-11-14 10:58:16]	Processed
diffraction_thumbnail_ref-opid231_1_0003 [2023-11-14 10:58:23]	Processed
diffraction_thumbnail_ref-opid231_1_0004 [2023-11-14 10:58:33]	Processed
characterisation [2023-11-14 10:58:57]	Processed
dozor_plot [2023-11-14 10:59:09]	Processed

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But all the data we need is already there!

**Could we federate these
features?**

How to manage the diversity?

ISPyB focuses on SB and is already too complex. It would be impossible to manage an all-techniques monolith...

We need to split up things:

Generic features

Logbook

Sample
tracking

Core features

- User management
- Proposal/session management
- General navigation
- Data fetching
- Generic visualization

Specialized features

MX
visualization

Cryo EM/ET
visualization

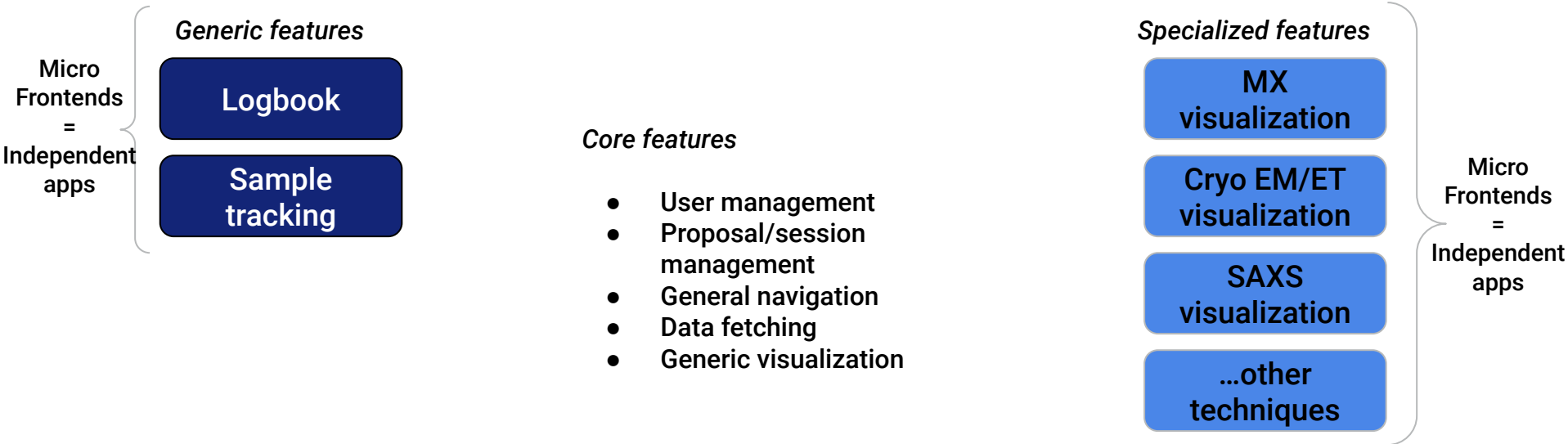
SAXS
visualization

...other
techniques

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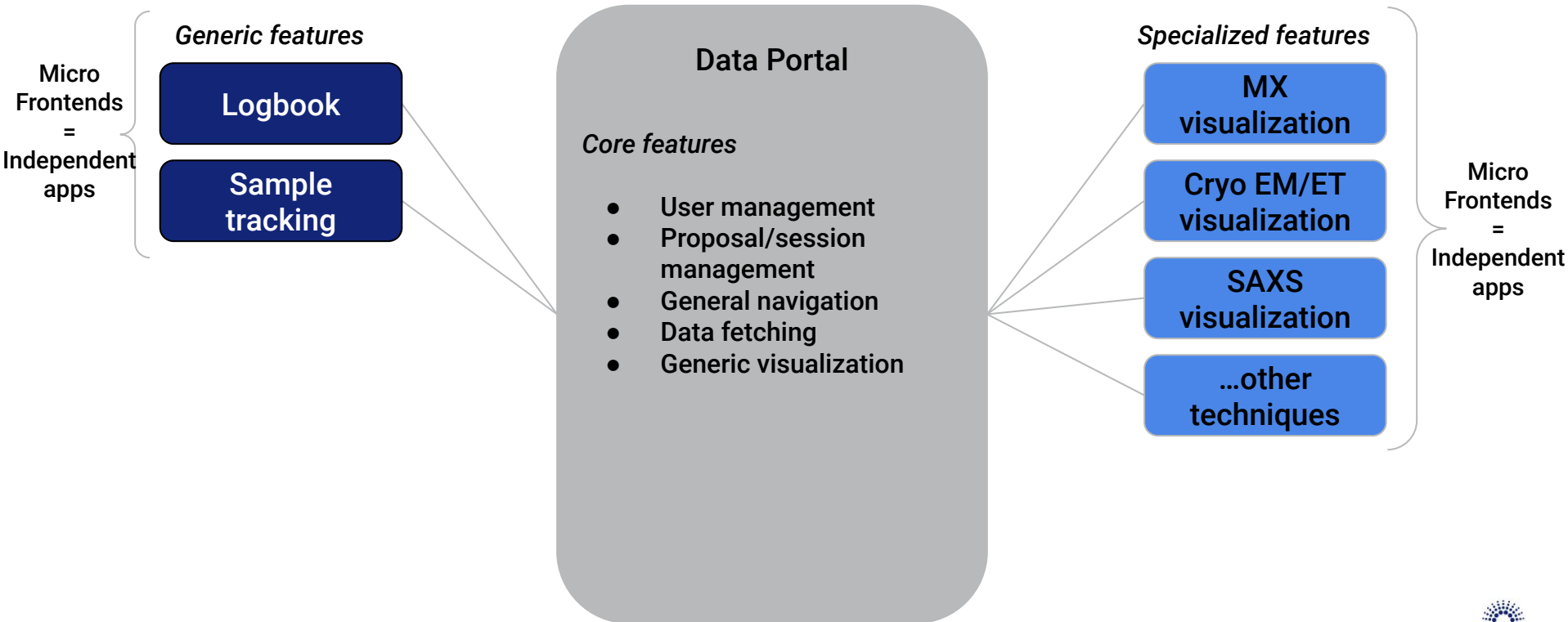
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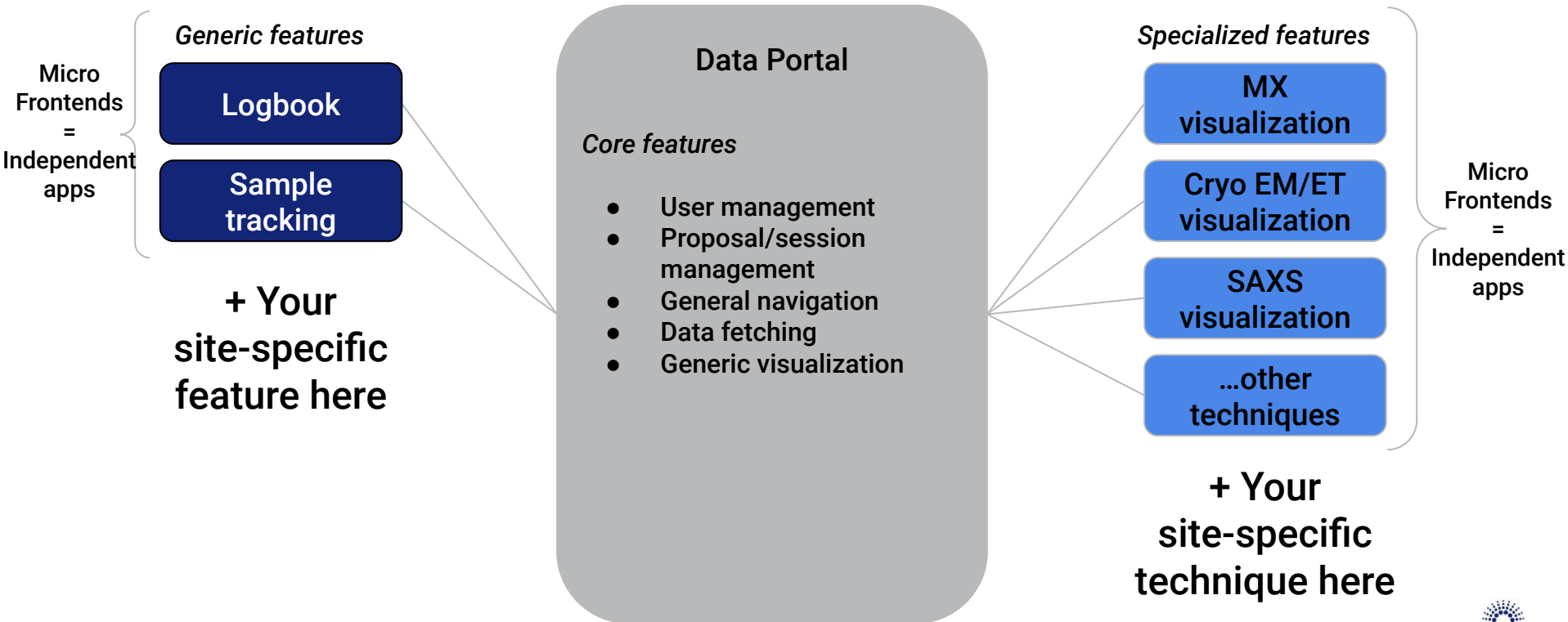
We need to split up things:



How to manage the diversity?

ISPyB focuses on SB and is already too complex. It would be impossible to manage an all-techniques monolith...

We need to split up things:



We can load the appropriate app depending on the session...

This screenshot shows the 'Data Portal' interface. The top navigation bar includes 'Data Portal', 'Data', 'Logistics', 'Instruments', 'My selection', 'Examples', 'My Jobs', and 'Admin'. A search bar is located on the right. The main content area features a sidebar with filters for 'Data type' (Investigations, Data collections, Documents) and 'Filter by' (Public data, Embargoed data, My data, Instrument). The central part of the page displays a table of investigations with the following columns: Instrument, Start, Title, A-Form, Samples, Datasets, Files, Release, DOI, and Logbook. The table lists several entries, including 'Data collected for the ISPyB Collaboration', 'Redox reactions between FeCO3 and H2O in the deep mantle', and 'Phase contrast imaging of saline spray ice'.

Portal

This includes all the portal features previously mentioned

CryoET

MX

This screenshot shows the 'Data Portal' interface for a CryoET experiment. The top navigation bar includes 'Data Portal', 'Data', 'Logistics', 'Instruments', 'My selection', 'Examples', 'My Jobs', and 'Admin'. The main content area features a sidebar with filters for 'Investigation' (Experiment, Statistics, Datasets, Logbook, Prepare) and 'Datasets' (View as: List, Summary). The central part of the page displays a 'Sample' section with a dropdown menu for 'Insectcells-leica-g2-2_Position_1_test4' and 'Position_1,2'. Below this, there is a table for 'Angles' with columns for 'total', 'step', and 'range'. The main content area shows a 'Non-aligned micrographs movie' with a video player and a 'Speed: 10 frames per second' control. The bottom of the page features logos for 'ESRF' and 'CORE REAL'.

This screenshot shows the 'Data Portal' interface for an MX experiment. The top navigation bar includes 'Data Portal', 'Experiments', 'Samples', 'Publications', 'Logistics', 'Beamline', 'My selection', 'My Jobs', and 'Manager'. The main content area features a sidebar with filters for 'Experiment session' (Statistics, Datasets, Logbook, Prepare) and 'View as' (List, Summary). The central part of the page displays a 'Sample' section with a dropdown menu for 'Sample-4-1-01'. Below this, there is a 'View as' section with a dropdown menu for 'MX' and a 'Filter by type' section with a dropdown menu for 'Automesh'. The main content area shows a 'Data collection' section with a dropdown menu for 'Sample-4-1-01' and a 'Best auto processing' section with a dropdown menu for 'From gnomixs_parallelMicroscopic system (P2)'. The central part of the page displays a grid of plots and analysis tools, including 'Automesh', 'Mesh', 'Line', 'Characterisation', 'Diffraction', 'Data collection', and 'Best auto processing'. The bottom of the page features logos for 'ESRF' and 'CORE REAL'.

... Or mix them together

portal

MX

CryoET

The screenshot displays the Data Portal interface. At the top, there's a navigation bar with 'Data Portal', 'Data', 'Logistics', 'Instruments', 'My selection', 'Advanced', 'My jobs', and 'Admin'. Below this, a 'Selected datasets' section shows a list of items. The main content area is divided into two panels. The top panel, titled 'datacollection 14/11/2023 11:00:23', shows a summary of the data collection with various plots and a table of parameters. The bottom panel, titled 'Apof-q3 g1 homo-apof-q3072023_Position_1/Position_1 06/07/2023 15:58:51', shows 'Raw data', 'Motion correction', and 'CTF' sections with corresponding plots and tables.

datacollection 14/11/2023 11:00:23

Start time	14/11/2023 11:00:23
Workfile	
Profile	ap221_w1_1_306435
Beam #	
# Images	800
Transmission	1.0 %

Orthorhombic system (P222)

Comp	Min. low	Max. high	Range	Unit	σ(I) / cov
a	42.7	45.7	3.0	Å	3.52 / 1.00
b	1.1	1.2	0.1	Å	1.1 / 0.7
c	43.7	43.7	0.0	Å	1.0 / -

Apof-q3 g1 homo-apof-q3072023_Position_1/Position_1 06/07/2023 15:58:51

Raw data

Dose initial	0.0
Dose per frame	0.5
Images count	6
Magnification	64000
Sampling rate	1.25
Tilt angle	-9.0

Motion correction

Average motion	3.0
Frame dose	-1.0
Frame range	6
Total dose	-1.0
Total motion	18.2

CTF

Angle	30.93
Correlation	0.011196
Defocus u	33923.26
Defocus v	34461.25
Estimated b factor	-5.26
Resolution limit	19.011

These could be the same sample/protein analysed with different techniques on the same page.

Or fallback to a default 'generic' viewer

The screenshot shows the ESRF Data Portal interface. The top navigation bar includes 'Data Portal', 'Data', 'Logistics', 'Instruments', and 'Admin'. A search bar is present with the text 'Search in data portal...'. The user is identified as 'Maël GAONACH'. The breadcrumb trail is 'Home / HG-94 / ID21 / 26/07/2019 - 06/02/2017 / Datasets'. The left sidebar contains navigation options: 'Investigation' (Experiment, Statistics, Datasets (16), Logbook, Prepare), and 'Datasets' (Filter by sample: Type sample name). The main content area displays a list of datasets for 'ultramarine'. The first dataset, 'dataset_RAD', is highlighted with a pink box. It shows a plot of 'differential absorption' vs 'energy, eV'. Below the plot are 'Explore' and 'Download' buttons. A callout box with a pink border and a pink arrow pointing to the plot area contains the text: 'XANES : No viewer for this technique => fallback to default 'generic' viewer'. Below this, another dataset 'dataset_33' is visible, showing multiple XANES spectra plots. The bottom of the page shows 'dataset_32'.

portal

**XANES : No viewer for this technique
=> fallback to default 'generic' viewer**

Implementation

<https://gitlab.esrf.fr/icat/data-portal>

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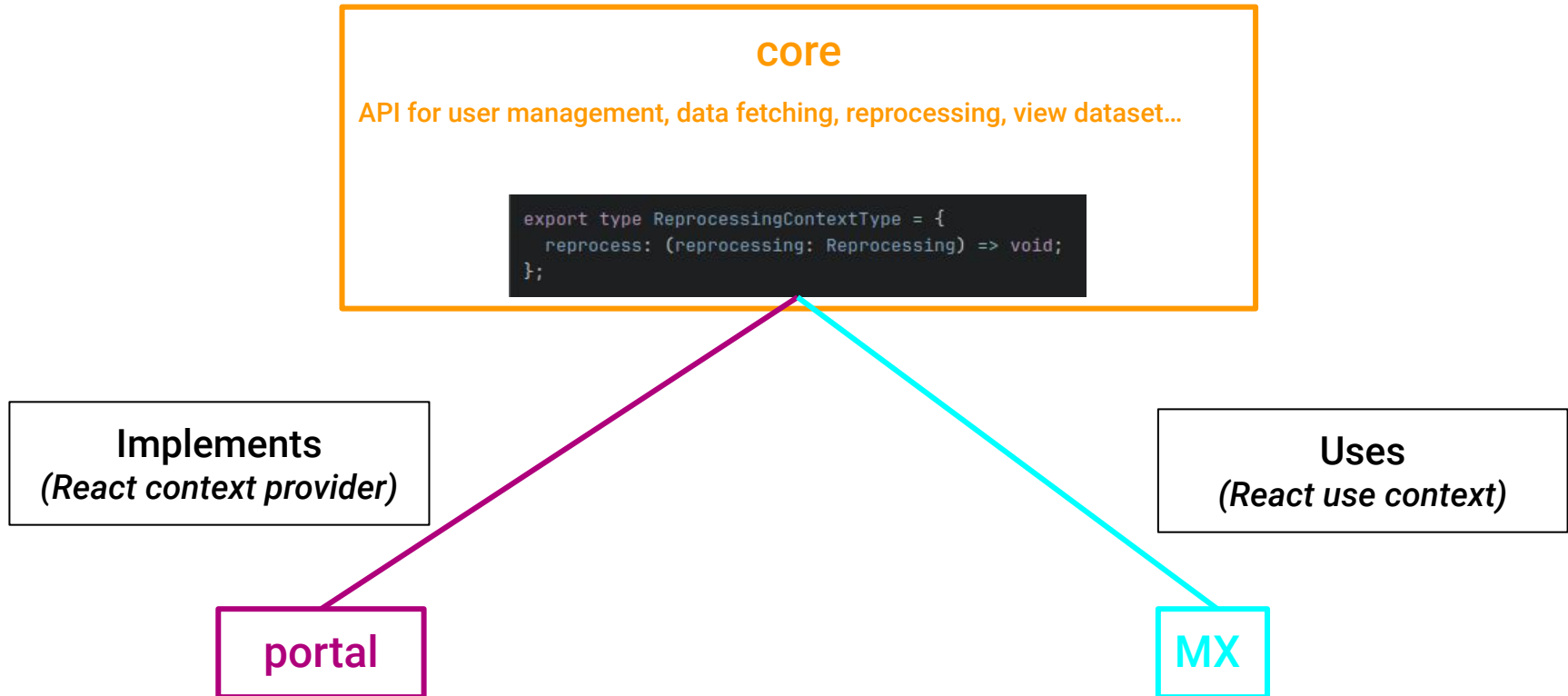
portal

```
export const investigationViewers: InvestigationViewerDefinition[] = [
  {
    date: '*',
    beamline: 'CM01',
    component: (props: any) => (
      <RemoteComponent component=CryoETInvestigationViewer {...props} />
    ),
  },
  {
    date: '24/10/2023',
    beamline: /^(ID23.*|ID30.*)$/,
    component: (props: any) => (
      <RemoteComponent component=MXInvestigationViewer {...props} />
    ),
  },
  {
    date: '*',
    beamline: 'BM29',
    component: (props: any) => <GenericInvestigationViewer {...props} />,
  },
],
```

```
remotes: {
  sessionViewer: process.env.VITE_FEDERATION_SESSION_VIEWER_URL,
  logistics: process.env.VITE_FEDERATION_LOGISTICS_URL,
  cryoet: process.env.VITE_FEDERATION_CRYOET_URL,
  mx: process.env.VITE_FEDERATION_MX_URL,
  remoteDatasetViewerApp:
    process.env.VITE_FEDERATION_DATASET_VIEWER_URL,
  logbook: process.env.VITE_FEDERATION_LOGBOOK_URL,
},
```

Micro-frontends are independents but can work together

<https://gitlab.esrf.fr/icat/data-portal>



Thank you!