PyBluIce

Modular MX Data Collection Software
for Fully Automated, High Data Rate and Long Duration Experiments

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MX Data Acquisition at GM/CA

Two ID MX Beamlines

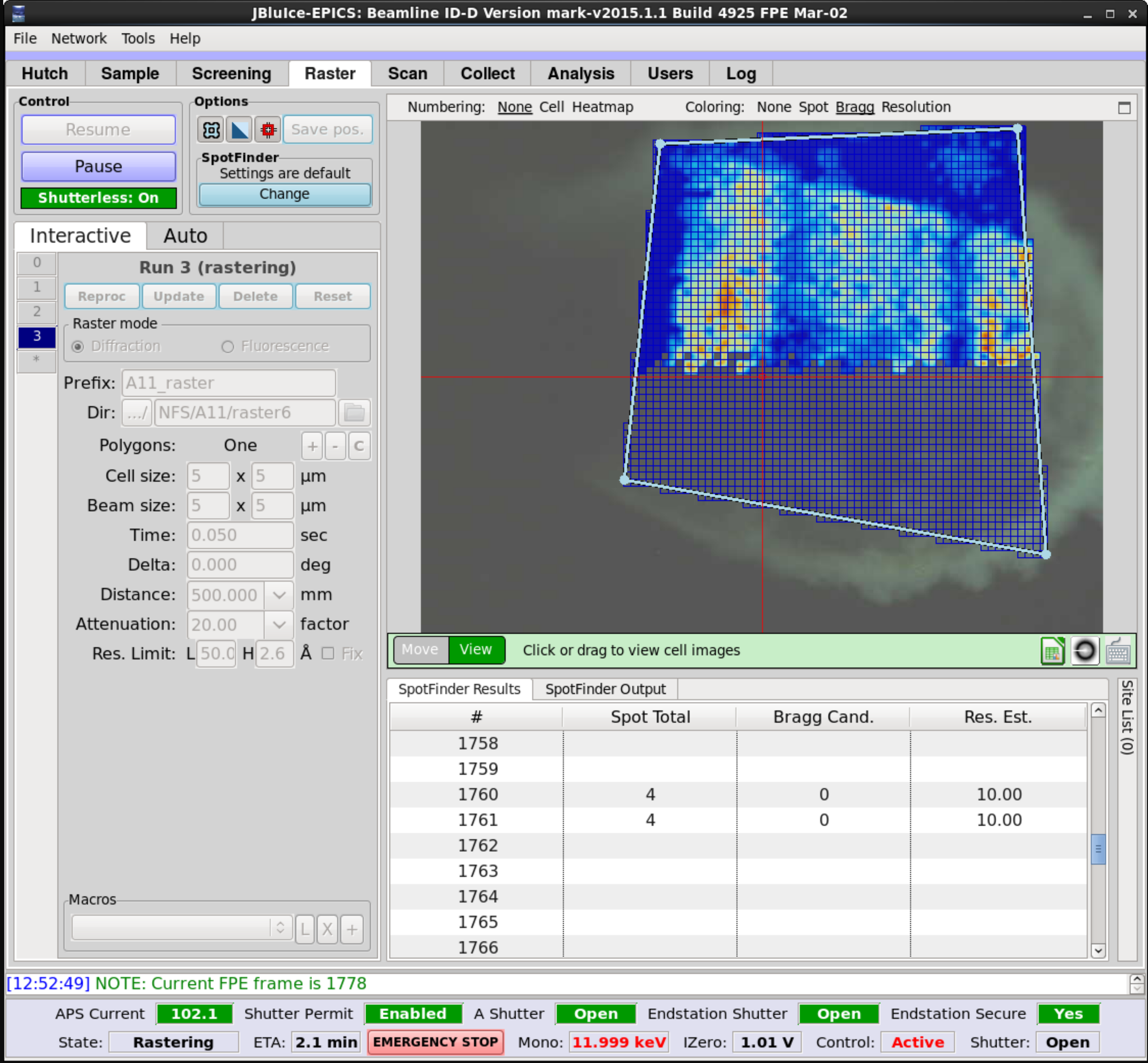
- Sector 23 at the Advanced Photon Source, Argonne National Laboratory

JBluIce is written for and by GM/CA

- Tools are optimized for GM/CA capabilities

Major functions

- Raster, vector and helical collect
- Fluorescence spectrum and edge scan
- Screening
- Analysis



PyBluIce Project

PyBluIce started as a project to bring new features to JBluIce
The benefits we found led us to decide on a full rewrite to Python

The new features we need are

Long Duration Experiments	High Data Rates	Full Automation	More data collection tools
• Million cell raster • Multi-hour injector collect	• 100Hz sustained	• Optical center • Raster-based center • Multi-site strategy • Strategy-based collect	• Several collect modes • Multiple tools per mode

PyBluIce Project

PyBluIce features driving changes

- Long Duration Experiments
- High Data Rates
- Full Automation
- Independent Collect Plug-ins

Improvements needed to deliver these features

Performance

- Responsive GUI while viewing collection plans and results for million frame collections
- Viewing, processing and analysis at hours-long sustained high data rates

Modularity

- Independent collect plugins prevent too much complexity in shared components
- Complex operations need a simple interface for automation

Reliability

- Automation needs to run all day long and recover from errors

PyBluIce Project

PyBluIce features driving changes

- Long Duration Experiments
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Technical Changes Needed

Current	Change	Benefit
Java & SWT	Python3 & Qt5	Concise and efficient
EPICS & SQL	Redis	Fast, atomic, random access data passing
Single process	Thin GUI with HTTP RPC	Non-GUI load completely offloaded
Hardware abstraction simulation	Realistic beamline simulation	Interactive and automatic short & long-duration tests

Why focus on modularity?

Allow more overall complexity

- Remove specifics from shared components
- Clearly define API between components to expose shared data

Speed development

- Reduced dependencies makes changes easier

Enable a larger development team

- Scripts used by the server are short and easy to modify for new tasks
- The same API used by server components is clearly documented and accessible

Tolerate offline hardware

- Individual testing of modules eliminates unnecessary dependencies

Achieving modularity

Independent scripts

- Complex operations are moved to independent scripts with no server imports, only HTTP/Redis API usage
- Separates high-level, unique tasks from core, shared components
- Provides templates for developers to start with

Unit tests

- Enforce modularity by only starting the modules that are needed

Redis

- Passing data via organized, documented Redis DB locations makes debugging easier
- Easier to diagnose and fix broken database links instead of more complex code-based links

Collect plug-ins

- Moving collect mode-specific code to plug-ins contains their complexity

Reliability for more complex tasks

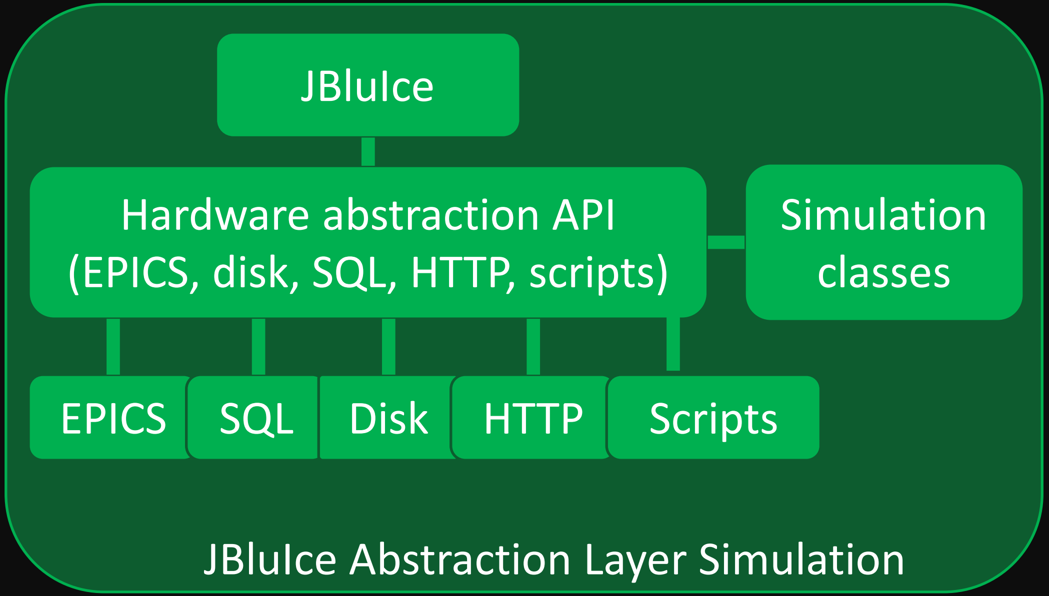
Lights-out automation

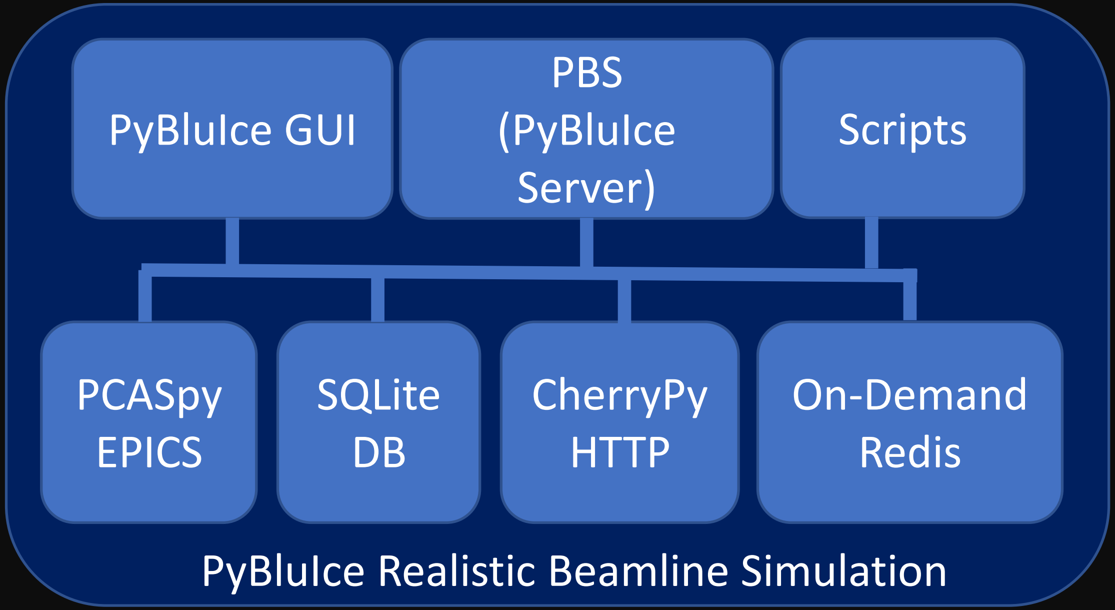
- Detect errors that occur only after repeated or certain patterns of calls
- Recover from hardware errors
- Know when to stop and prompt the user

Reliable scripting interface

- All API options should be tested even if not currently in use

Reliability for more complex tasks: Realistic Simulation





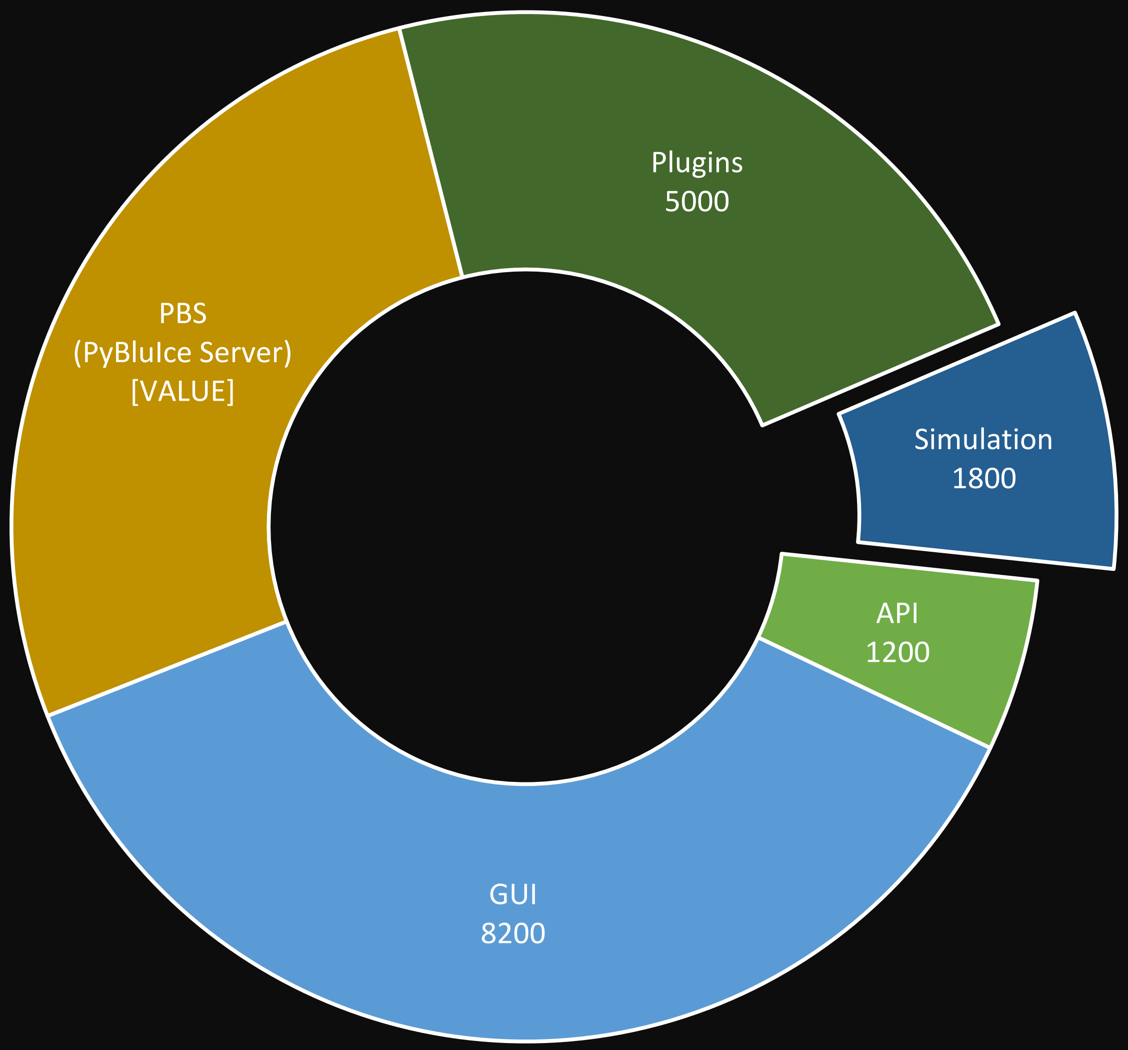
- For JBluIce we wrote an API for each type of hardware device
- This required implementing some part of each protocol e.g. SQL parsing
- High maintenance costs
- Did not achieve offline development

- Python libraries are available to simulate EPICS, SQL and HTTP
- Clients see real EPICS, Redis and HTTP servers
- Enables automated testing and offline development and debugging
- Nearly all operations are currently supported

Lines of Code

Simulation to support all major operations adds 7% to code base

Total size is one fifth of JBluIce's 124,000 LOC



Reaching performance goals

Efficient API for offloading tasks

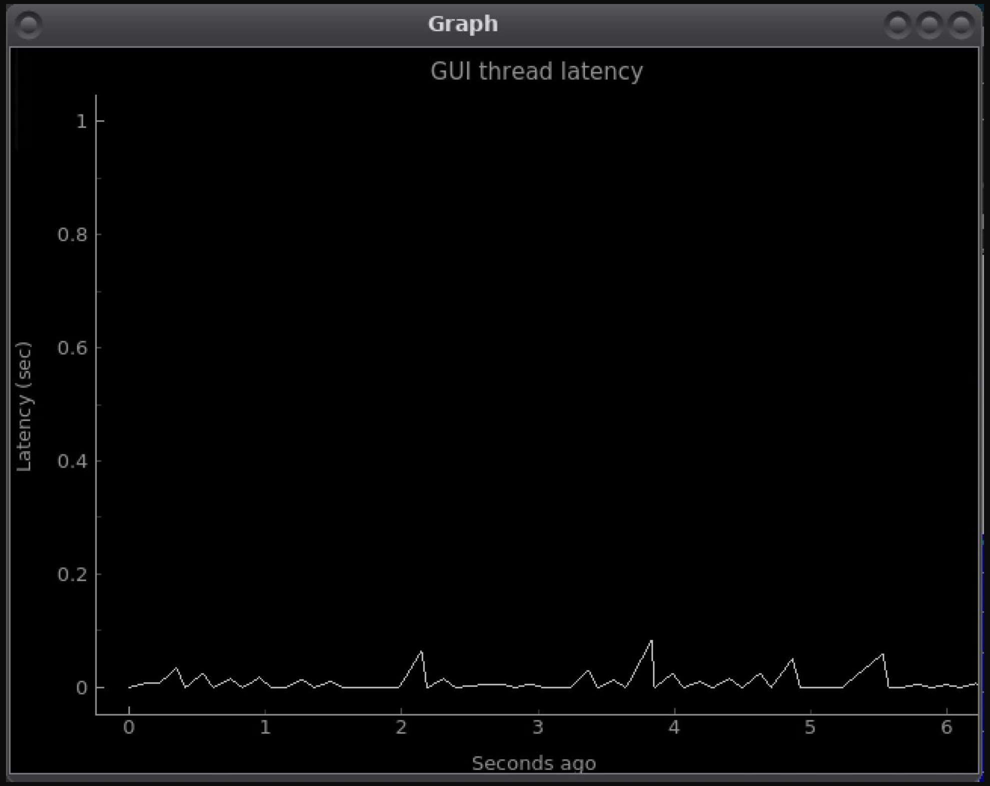
- When offloading is as easy as not, this makes keeping the GUI lean possible
- Slurm tasks also offload processing and drop their results into the database without needing to connect back to the server

High performance PyQt widgets

- pyqtgraph makes video and image viewing at high speed simple
- Lazy tables are more straightforward than in SWT

Modularity and Simulation contribute

- Concise, self-contained methods and modules make refactoring and optimization easier
- Simulation makes regular latency and resource monitoring possible offline



Built-in GUI thread latency viewer

Foundation: Redis API

```
import api.redis_api as ra
ra.run_b.delta_deg.set(0.2, id=1)
```

Setting a data collection parameter using the PyBluIce Redis API import

PyCharm integration

- Tab completion for all levels of field hierarchy
- Control+Q on fields shows their description and formatting

Synchronous, atomic, fast

- Grouping reads and writes into “pipelines” ensures atomicity
- Couple milliseconds per round trip allows for multiple calls within a GUI thread callback
- Can be combined with HTTP calls and the HTTP receiver is guaranteed to see the new values with no delay

Flexible, open

- Above can be done by any script, including external to PyBluIce
- This exposes the inner workings of the servers and makes them accessible for anyone to add on to
- Redis provides linked lists, random-access binary arrays, and other data types

Foundation: HTTP API

```
import api.redis_api as ra
import api.http_api as ha

ra.run_b.delta_deg.set(0.2, id=1)
ha.collect_runs_py(runs=1).post()
```

Starting data collection with a Redis setting followed by an HTTP call

Used for RPC

- Provides reliable parameter passing and immediate or delayed response
- ZeroMQ has protocols that are well-suited to RPC, but HTTP is sufficient, more widely known and has more tools available

Language agnostic

- Any language can either use a library or call curl
- Future web-based interfaces can directly connect to the PyBluIce servers

Auto Tab Preview

Event history

- Shows the user everything automation is doing
- Manual operations and crystal info are shown too
- Previews results: raster grids, camera snapshots, analysis summaries
- Links to full results in other tabs or external browsers
- Sorted by sample ID to include unmounted and manual mount sample events

Global path config

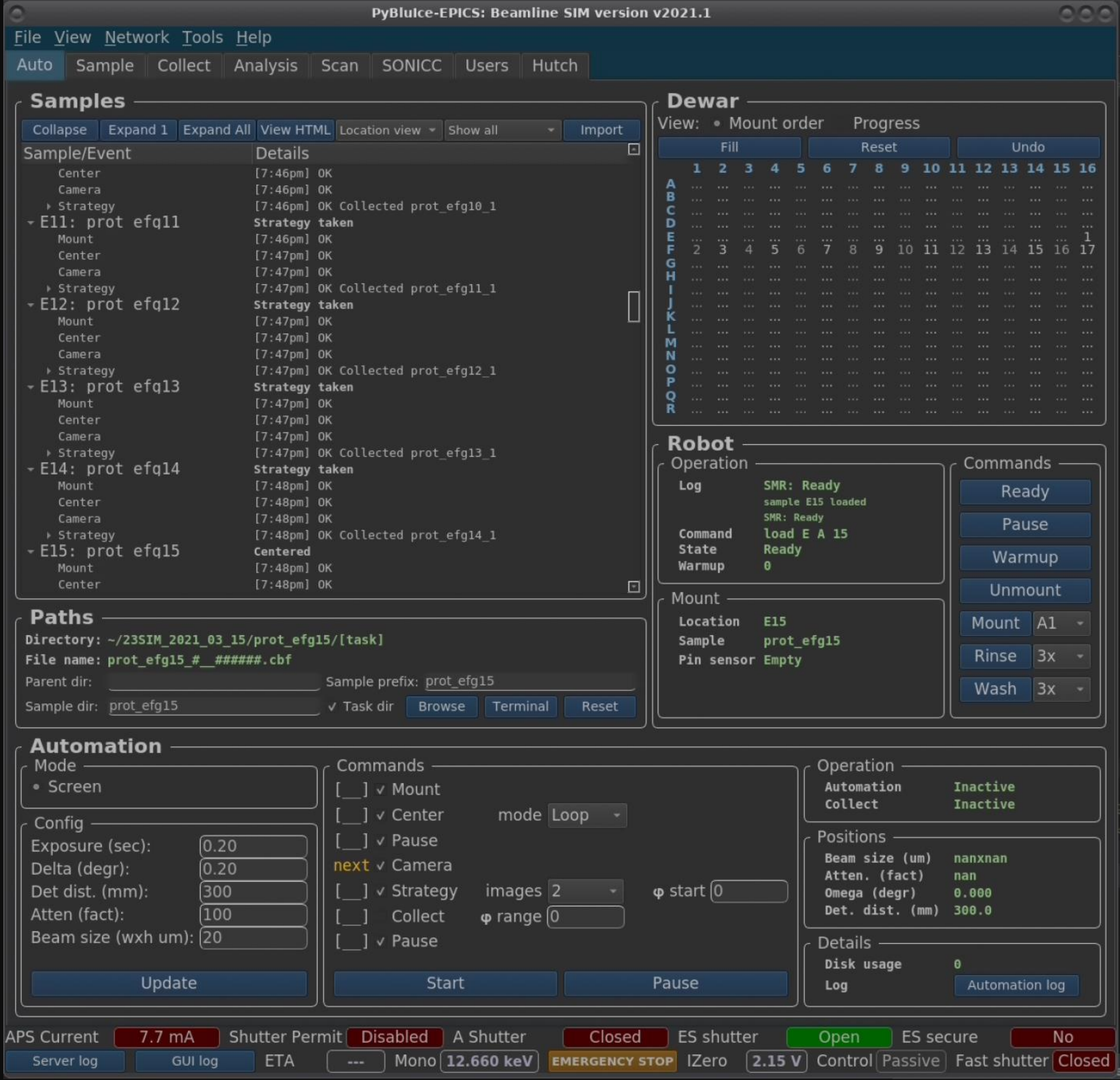
- In automatic mode, operations need a way to determine an output path

Automation queue

- In screening mode, the queue is fixed
- Future modes may allow arbitrary user editing of the queue

Ergonomics

- Compact mode for laptops and large text mode for certain large monitors
- Optional dark mode can reduce eye strain
- Resizable and pop-out widgets make zooming in easy



Collect Tab Preview

Raster plug-in is shown

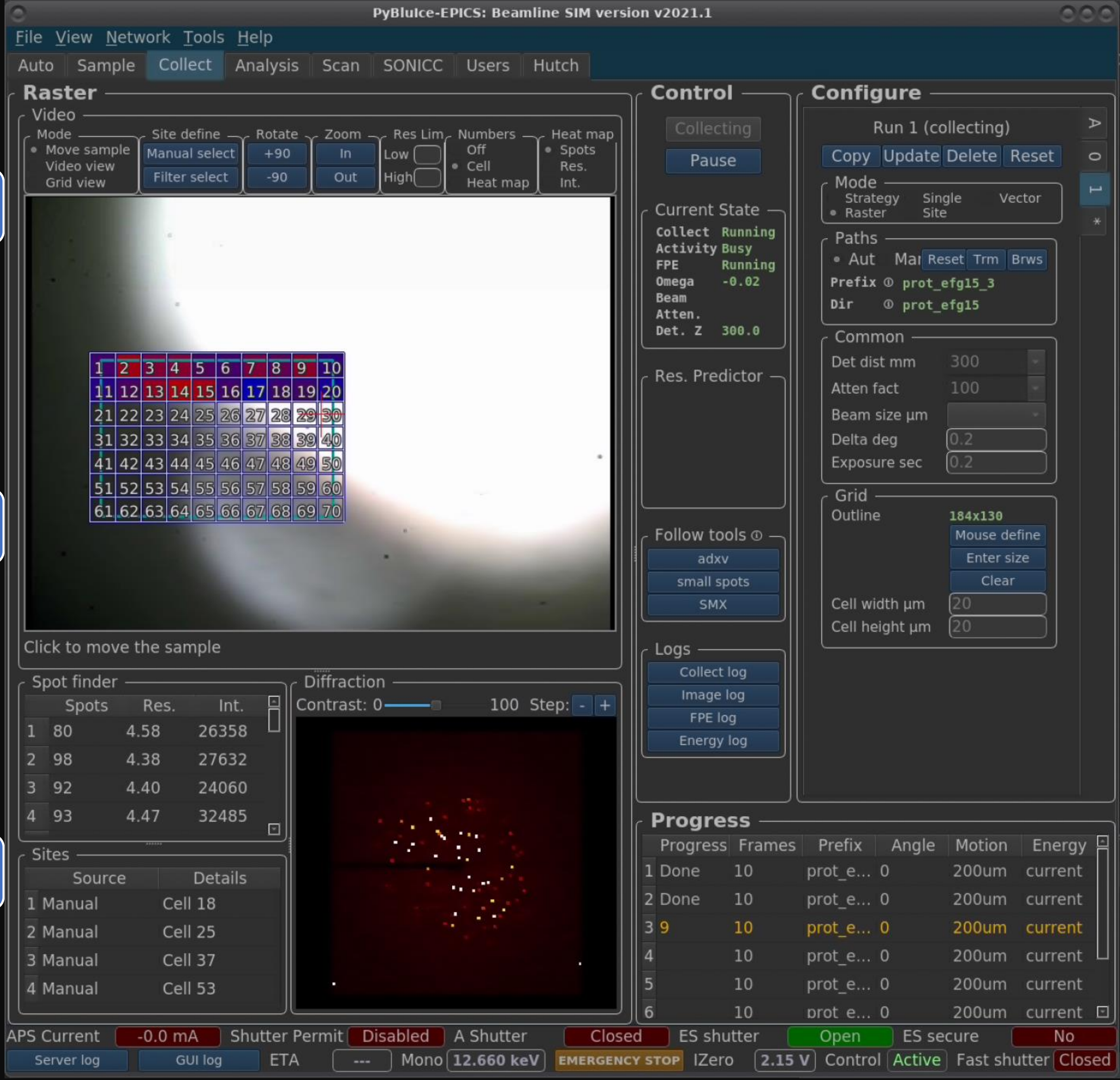
- Collect mode is selected at the top of each run
- Each plug-in:
  - Generates run field widgets
  - Calculates collect commands shown at bottom right
  - Generates widgets on the left half of the tab, though basic widgets like video view have standard versions

10Hz small-spots image viewer

- Server reads image paths from an image “stream”, which is a Redis List that clients watch the length of and read only new items from
- Images are processed at up to 10Hz, and results are saved to another Redis stream in raw binary format with numpy
- Redis+Python+numpy make these steps simple to write and debug
- Processing makes single-pixel spots visible even at the small size shown (algorithm is by David Kissick @ GM/CA)

Shared collect site list

- Site list is a Redis hash of JSON strings
- This is a trade-off making debugging easy, especially with external scripts that may manipulate the list
- Raster mode stores sites in the list, and site mode uses them to collect



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