

Workflow interoperability

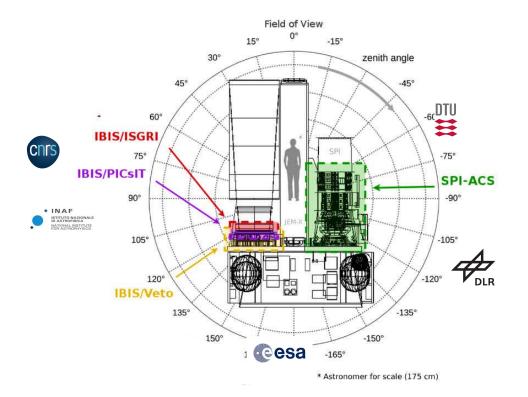
for telescope operations and time domain astronomy

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INTEGRAL space observatory Data Center, 2002+





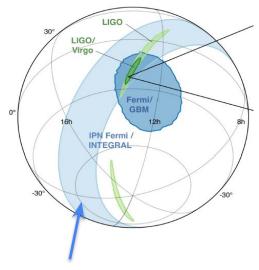
Core role of **ISDC** is to provide community with means to leverage the telescope, we:

- Consolidate and provide data, software, services.
- Perform **quick-look analysis**, especially relevant in time domain astronomy
- Keep an eye on instruments

INTEGRAL provides best results by **combining with spectral, timing information from other missions**, and to make an impact on their own, it was decided to **provide API to access** public data, instead of hiding data/workflows and sending uninformative **publications**.

This mean that we need to handle FAIR live services/APIs/workflows not just FAIR data.

Multi-messenger time-domain astronomy is collaborative



Fermi + INTEGRAL Triangulation unique multi-mission approach

VS+ 2017, LVC 2017

log(Frequency [Hz]) 12 14 24 28 []________10^{-1'} cm⁻² E² dN/dE [erg 2 Neutrino source 10^{-13} Archiva VLA Fermi-LA OVRO ASAS.SM AGILE Kanata/HONIE Swift XR1 MAGIC 10^{-14} leutrino - 7 5v Kiso/KWFC NuSTAR H.E.S.S. (UL 10^{-3} Energy [eV]

Our focus on **broad synergies** allowed us to take a leading role or contribute in some of the key recent discoveries in our domain:

- Detection of the first Gravitational Wave Light coincidence (2017)
- First detection of light emission from **high-energy neutrino source** (2018)
- Discovery of the source of mysterious **Fast Radio Burst** (2020)

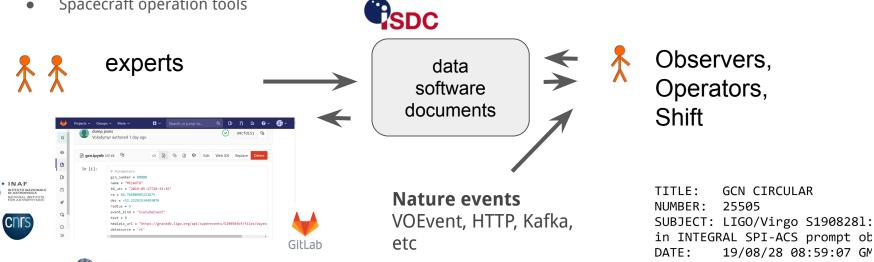
Traditional INTEGRAL transient analysis

Research, development environment lets experts develop, test, and integrate:

- data reduction
- theoretical models
- Spacecraft operation tools

Observers and Operators:

- **Find combinations** of data, adapters, statistical methods, publishers, planners
- suggest new observations
- distribute results



esa

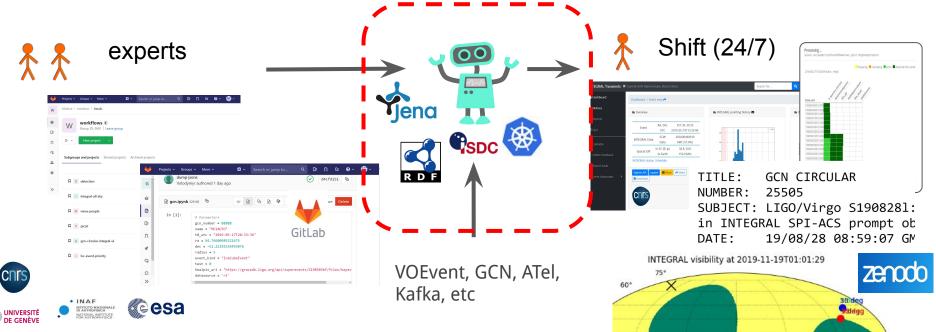
Not good enough if we want to try many combinations guickly: be exhaustive and ready for unexpected Setup automation for low latency and high-variety activity.

"Standard" modern INTEGRAL transient analysis

Research, development environment lets experts develop, test, and integrate:

- data reduction (close to data)
- theoretical models (linked to literature)
- statistical methods (as portable as possible)
- Spacecraft operation tools

- **Find combinations** of data, adapters, statistical methods, publishers, planners
- suggest follow-up
- **distribute** standard results with public data, uploads to zenodo sandbox.

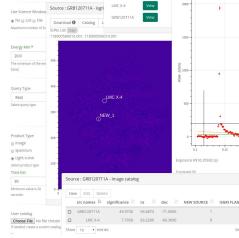


Addressing our challenges relies on FAIR Work Space



To optimize collaborative efforts, in this environment, we need robust means of **Finding**, **Accessing**, **Interoperating**, **and Reusing** our assets:

- Documents
- Data
- Software:
 - Code: scientific software which we build and distribute
 - Official instrument software (source, binary, doc, more recently containers)
 - INTEGRAL Quick Look Analysis
 - Web-based Software (services): API's and Frontends, which we provide to the community
 - Data browse interface (developed by NASA, hosted un Geneva/Versoix, since ~2002)
 - Help desk, **issue** handling and resolution
 - **Realtime data** interoperability (since 2011)
 - AstroODA online analysis (internally since before 2017, first public in 2019)
 - And all of it's backends separately
 - Multi-Messenger Transient Analysis (since 2018)
 - Various smaller API's for specific purposes



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New tools: more and more web-based data analysis

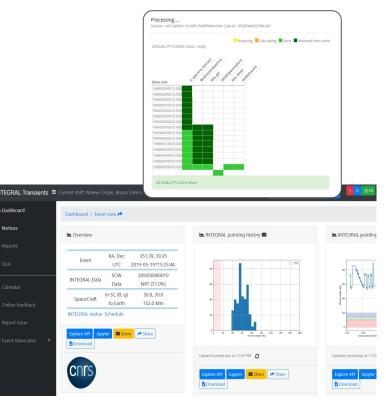
Last years, we develop and consume more and more web-based data analysis services.

In development, we:

- rely on cloud-native technologies, gitlab/github, CI/CD
- Allow domain experts to contribute easily, with code-to-service workflow
- support of right-to-replicate

Of course, we use VO services, but also many others. In reuse, we:

Strive to provide provenance, as much as possible in standard formats (like PROV-O)



https://github.com/oda-hub/ https://www.astro.unige.ch/cdci/astrooda /

Notices

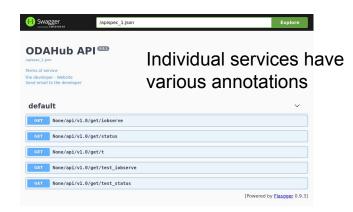
Neronov, Savchenko+ 2021, A&A in press

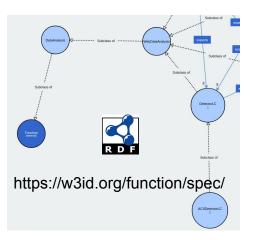
Sharing workflows is hard

It is possible to annotate and share software like data (e.g. on github or ASCL).

But this would leave too much work to actually make the software do it's thing: transform data.

Without going too ambitious, it should be possible to find a good way to describe collection of workflows (software code and software as a service), describing **software as functions**





INTEGRAL/ODA Knowledge Base (and Graph - KG)

Ontology of **processes** based on **fno** when feasible: most important to define input and output formats (types), this allows composition.

Bring some domain context by using **IVOA RDF** vocabularies for scientific terms and **concepts** and **relations** between, as much as needed by our case: a lot of specific things, some general with common terms (e.g. Crab_pulsar is a neutron star) when possible.

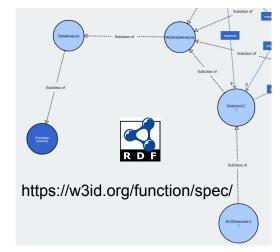
Use Dublin Core, schema.org, whenever feasible.

OWL2 and **SHACL** when possible. But also not always over-obsess over definitions, turns out sometimes ontology can be defined and enforced as KG evolves.

Simple domain-specific literature parsing ingests new events in the KG.

Documents, **analysis results**, especially **workflow** executions, ingested and annotated.

Human actors are explicit focus of the KG.



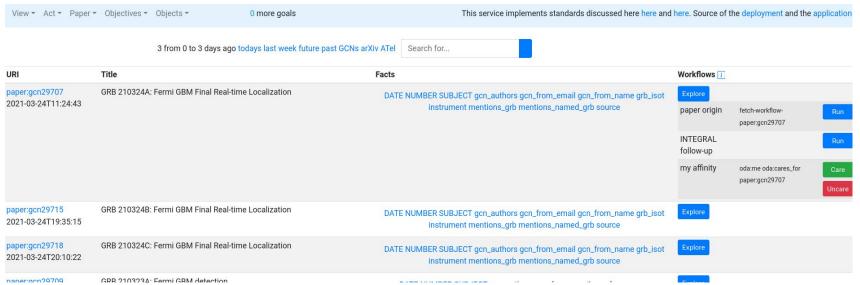
ODA Computational "Experiments"

Since KG contains records of workflows, with I/O types, and data, it is easy to run computational "**experiments**": combine workflows with data and see what it gives.

Processes that do compositions, and **objective measures** are also registered workflows.

Real classes of compositions:

- "Act on new paper or observation report"
- "Act on new software or data": re-do analysis of a "test case", ensuring assumptions about instruments cross-calibration use case
- **"Act on new observation":** testing assumptions about physical reality try to find unexpected
- "Act on new platform or time moment": make sure platform runs smoothly and is sane



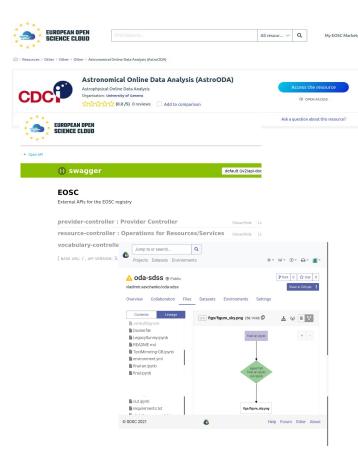
Growing federated service discovery landscape

EOSC allows to publish and annotate service offerings, helping **live service interoperability**.

ESA currently actively develops similar approach to scientific asset stewardship: **ESA DataLabs** (and we are involved in it as early adopters), with a **science application (~workflow) discovery hub.**

Swiss Data Science Center (SDSC) addresses some of the keys needs valuable for further developments, and has a **Knowledge Graph**, so we could interoperate with it.

We have an active project with **SDSC** to automatically derive workflows annotations in **RDF** from tracking **astroquery** interactions.



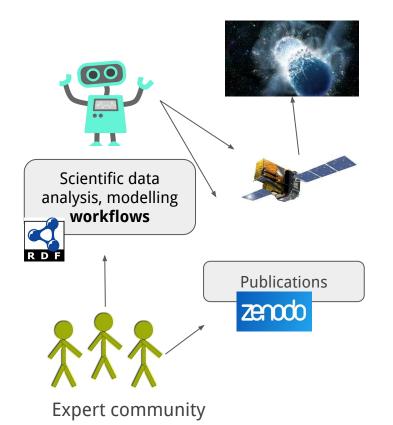
Summary

- Time domain astronomy and telescope operations really rely on "**keeping in touch**" with instruments, space, technologies.
- Growing number of tools, many of them federated, benefits from more structured annotation, enabling automated coordination and composition of data and operations on data.
- Seems like RDF (despite a number of difficulties) is not a bad way to describe and share this rather diverse assert collection.

Problems, Questions

- Dealing with diversity of languages
 - Keep consistent own world(s) of facts
- Developing ontology is hard. More tools are needed
 - we relied on "just ingesting" and then frequent refactoring, by specifying reasoning rules. It becomes part of the natural graph evolution. But more tools are needed to support this workflow.
- Defining what is authoritative claim
 - Who has a right to make propositions/claims? There are mechanisms with named graphs. We also tried RDF*.
 - Atomic Data restriction on RDF can be useful
- How to adequately share it
- All these mitigations make the **KG very verbose**.
 - Trying to use different graph views and subset to deal with it

Workflow standards let researchers build the system



- Workflow standards foster understandable, usable publishing of Findable Accessible Interoperable Reusable methods
- Workflows can offert **adapters for data formats**
- Deriving **data**, **result provenance**
 - explain data
 - trace history
 - credit and blame creators



Provenance RDF PROV-O

