Co-ordination & Harmonisation of Advanced e-Infrastructures for Research and Education Data Sharing

Jointly exploiting data and distributed computing eInfrastructure

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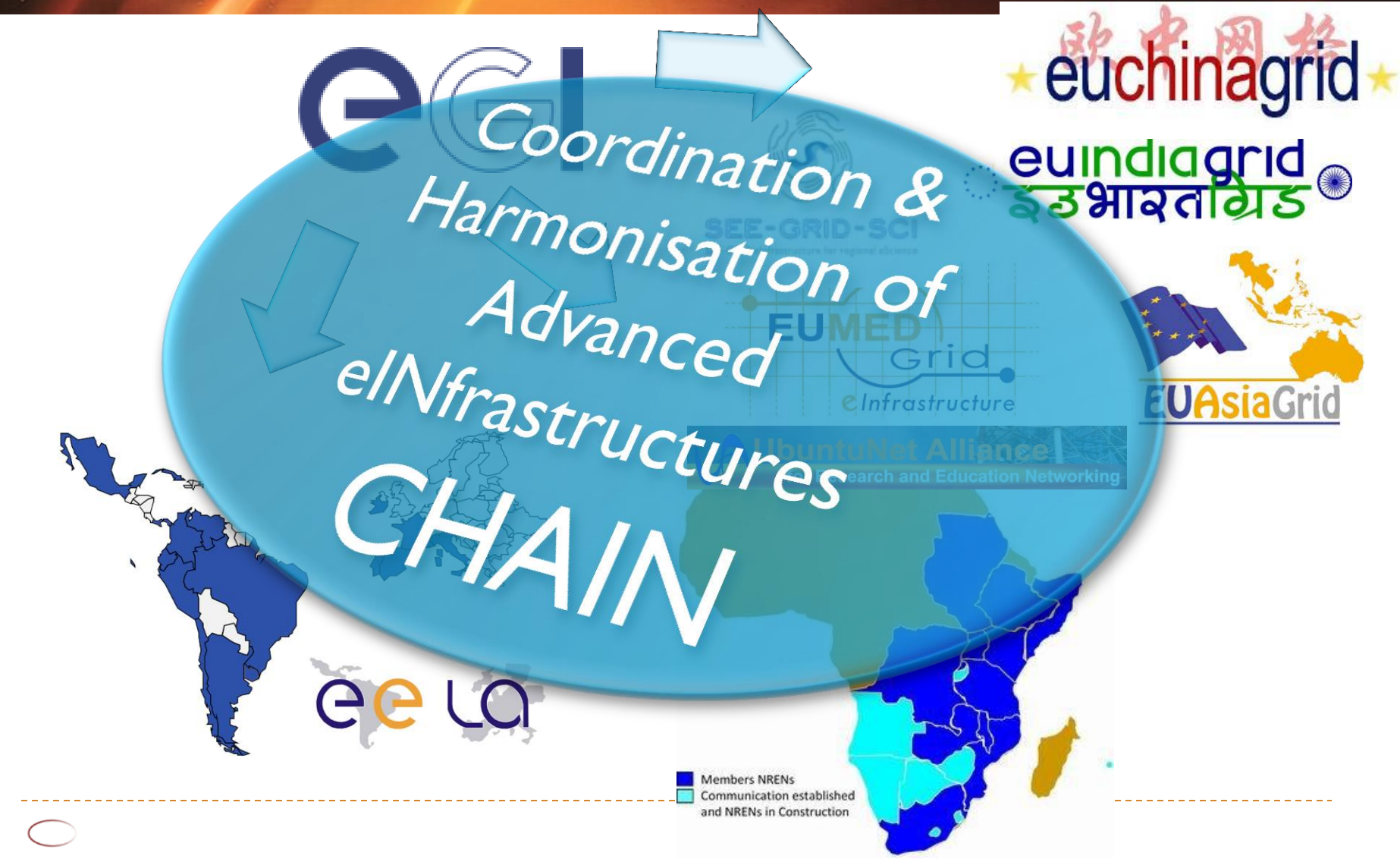
e-infrastructure

CHAIN-REDS: A legacy from CHAIN



WP4 in CHAIN-REDS

- CHAIN-REDS is an EC (306819) funded project
  - ~ 2.1 M€
  - 1 December 2012 – 30 months
- Structured in
  - WP 1 Project Management
  - WP 2 Dissemination, Training and Outreach
  - WP 3 Interoperation and coordination of e-Infrastructures
  - WP 4 Data Infrastructures
  - WP 5 Support to small groups and emerging communities

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WP4 'Data infrastructures'

- Current work on Data Infrastructure can be found in the public project Deliverables
  - D4.1 Trans-continental Data Infrastructures and Data repositories
  - D4.2 Analysis of Data Infrastructures and Data repositories
  - D4.3 Use cases of the identified Data Infrastructures and Data repositories
    - It describes the CHAIN-REDS solution for data workflows
  - D4.4 Report on the development of the use cases
    - Coming soon

- Available at http://www.chain-project.eu/deliverables

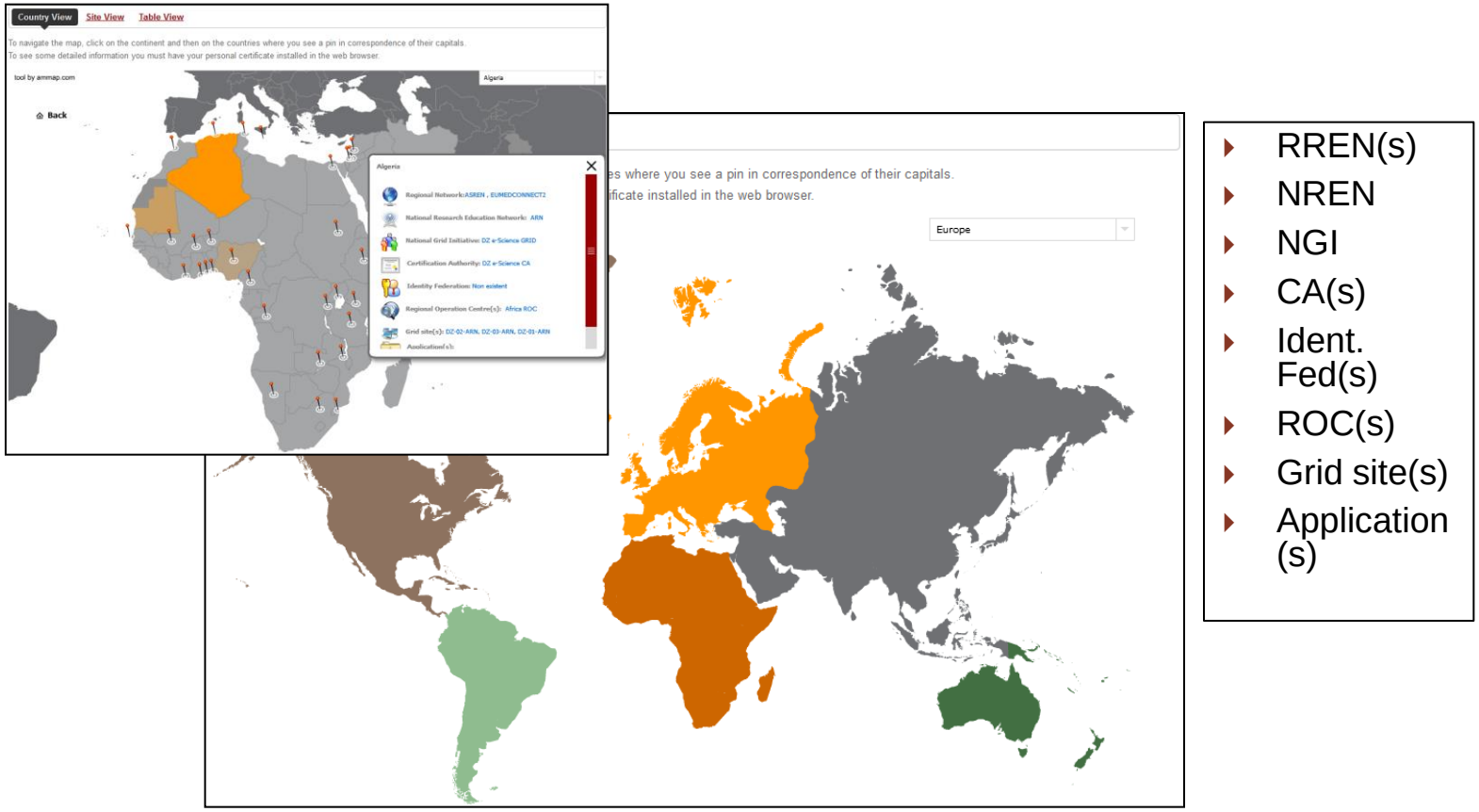
WP4 'Data infrastructures'

- Such work has been focused on scientific codes, but the developments that come afterwards can be easily applied to services of interest to the NRENs, Research Centres and Universities

  - Access to services, data, tools (IdF)
  - Semantic enriched search that allows new knowledge (SSE)
  - Friendly front-end for the execution of tasks (SG)
  - Retrieval of results and further storage of them (PID)

Knowledge Base: Infrastructure

- Extend the CHAIN-REDS Knowledge Base (BS) with Data capabilities http://www.chain-project.eu/knowledge-base



- RREN(s)
- NREN
- NGI
- CA(s)
- Ident. Fed(s)
- ROC(s)
- Grid site(s)
- Application (s)

Knowledge Base: Document, Data and Educational repositories

- ~3,200 repos
- >33 M docs

Copy | Print | Save — Search: malawi

Show 10 entries — First Previous 1 Next Last

Country	Name	Domain	Organization
Malawi	The University of Malawi Chancellor College	Multidisciplinary	The University of Malawi
Malawi	USAID CERT Educational Repository for Malawi	Multidisciplinary	Chancellor College University of Malawi
Malawi	NDR	Multidisciplinary	Malawi Library and Information Consortium

Showing 1 to 3 of 3 entries (filtered from 2,661 total entries) — First Previous 1 Next Last

Registry of Open Access Repositories (ROAR)

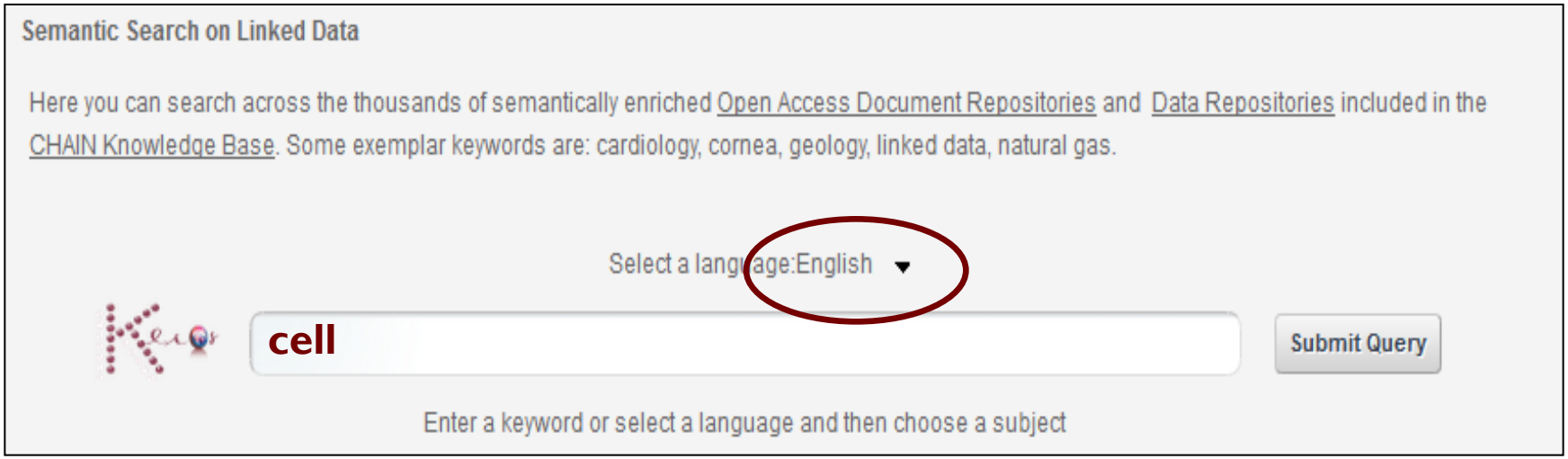
driver OpenAIRE OpenDOAR

Standards

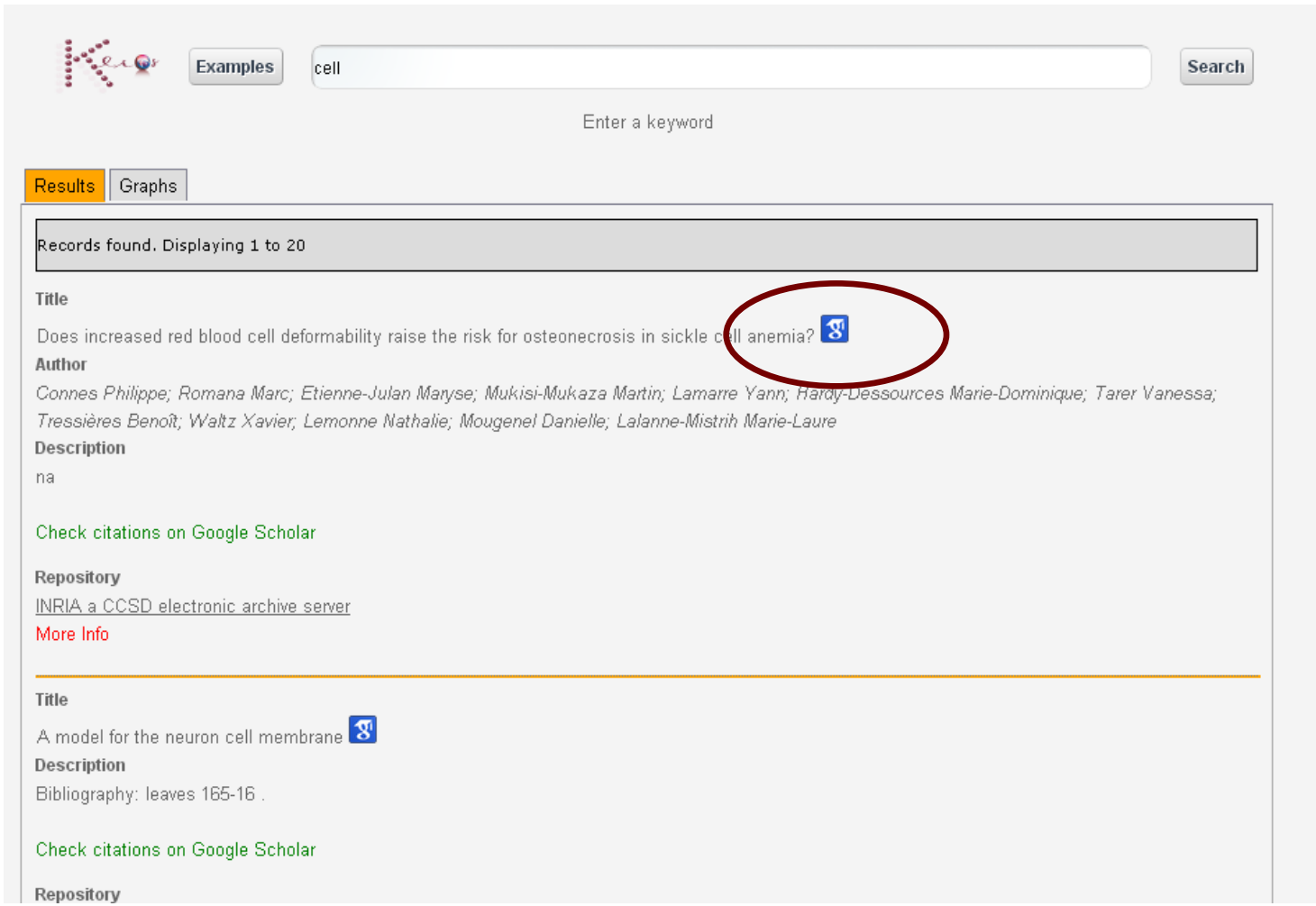
- About Open Access Data Repositories, standards have been promoted
  - OAI-PMH for metadata retrieval
  - Dublin Core as metadata schema
  - SPARQL for semantic web search
  - VOTable (XML) as potential standard for the interchange of data represented as a set of tables
  - Persistent Identifiers (PID)

OADRs and DRs

- The semantic search engine on CHAIN-REDS linked data is available
  - Allows searching among the semantically-enriched metadata coming from the OADRs and DRs included in the KB



OADRs and DRs



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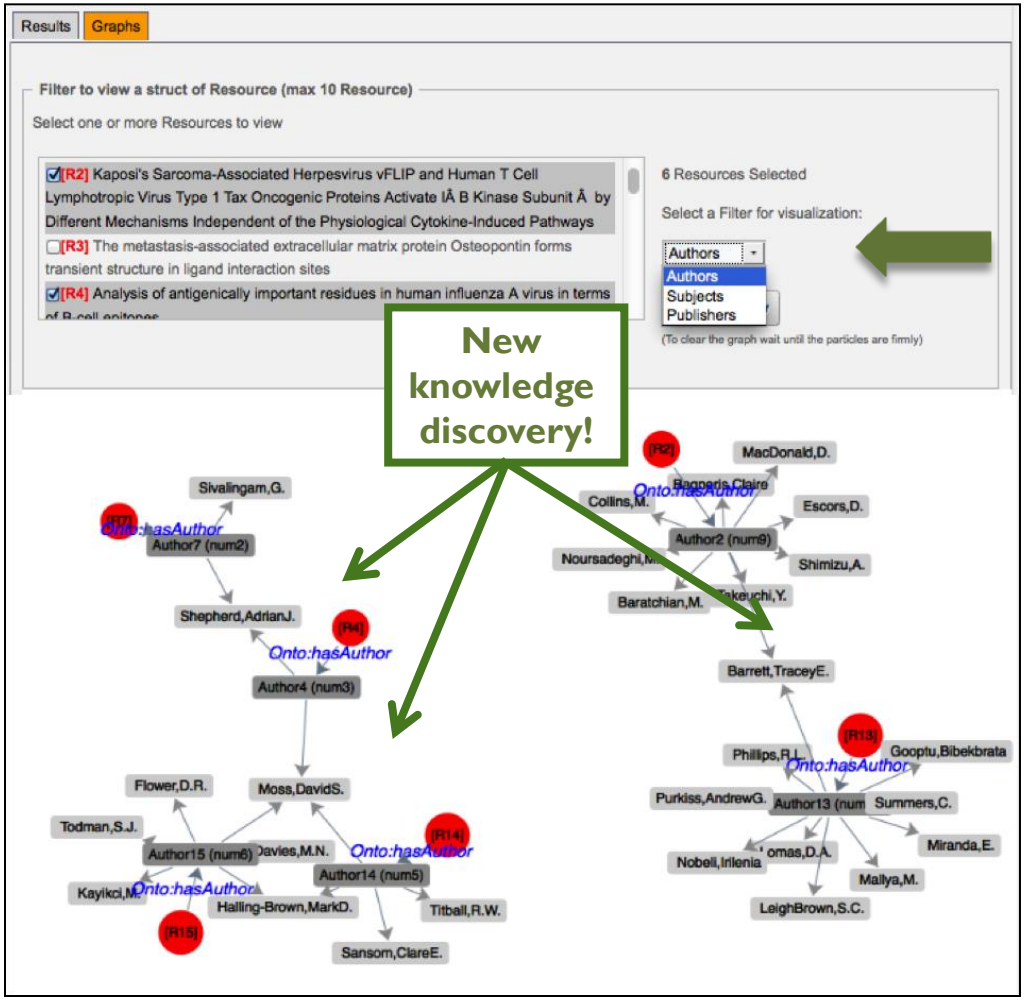
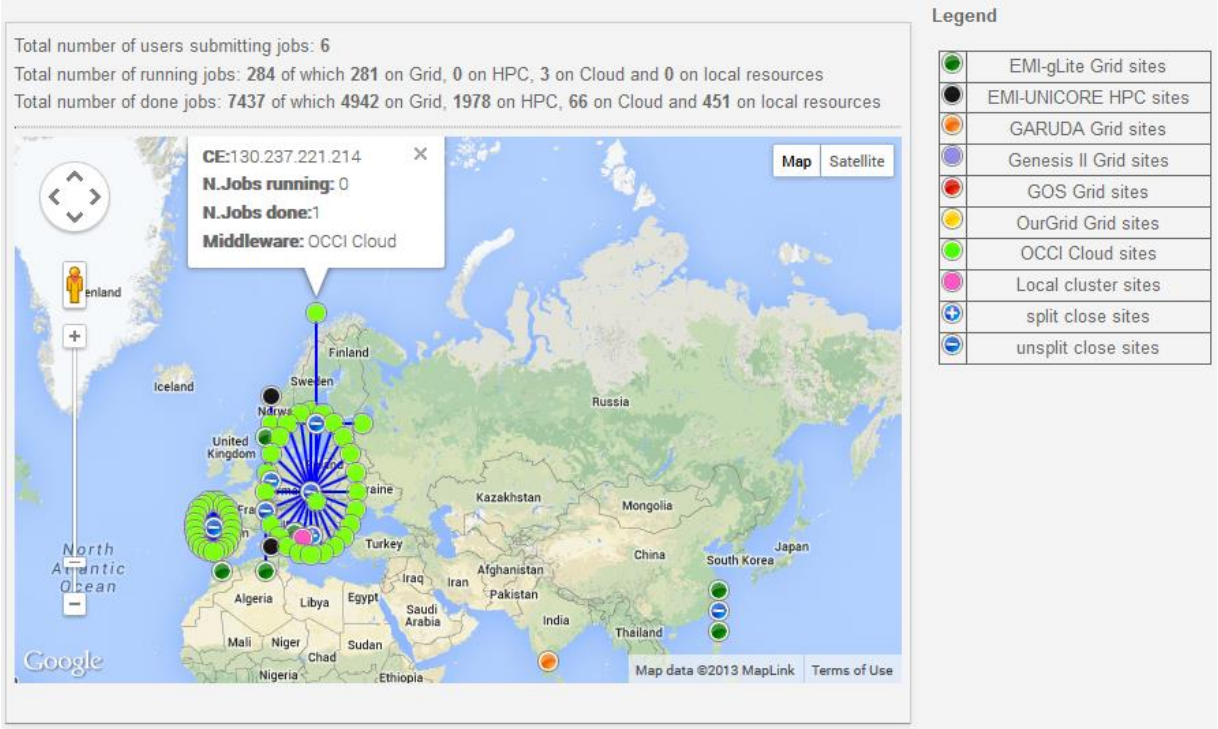


DART

- Data Accessibility, Reproducibility and Trustworthiness (DART)
  - Based on the interoperability demo performed by CHAIN-REDS at EGI TF 2013

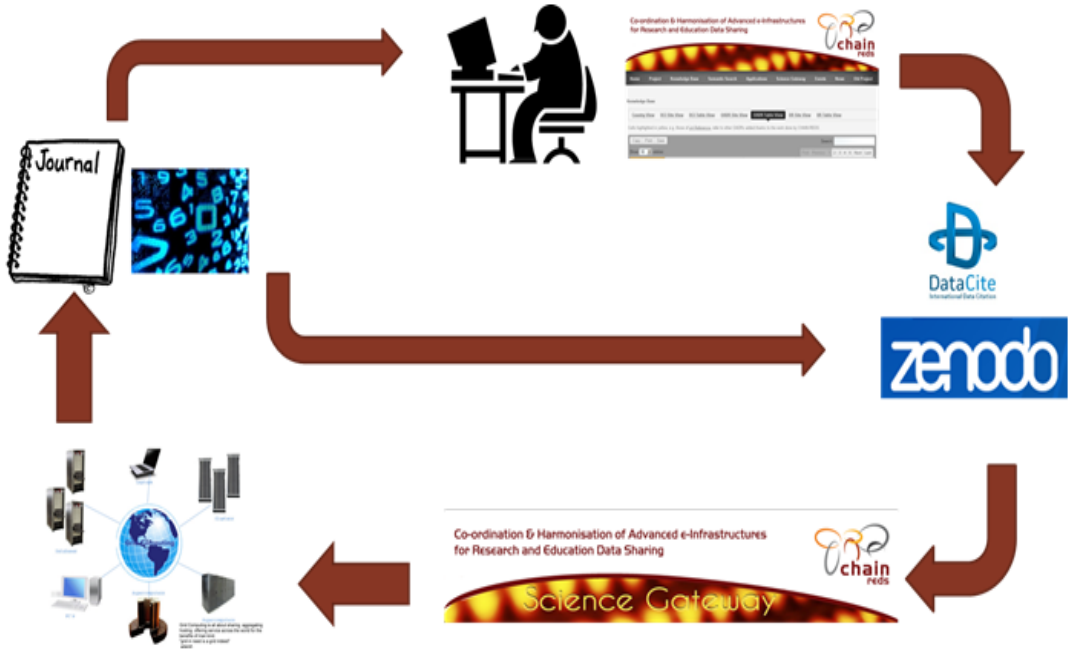


WP4 'Data infrastructures'

- Imagine an student looking for his/her record, a researcher looking for previous works or an engineer operating an NREN
  - Access to services, data, tools (IdF)
    - Login into the academia record, a scientific database or the NREN database
  - Semantic enriched search that allows new knowledge (KB/SSE)
    - Find a qualification, but know if others are available now; find similar papers; find some statistics of an NREN, but know if others are available about the ROC
  - Friendly front-end for the execution of tasks (SG)
    - A tool for analytics process of qualifications (by a Prof.), executing jobs or data network usage
  - Retrieval of results and further storage of them (PID)
    - A new digital object (the previous analysis) is uniquely identified

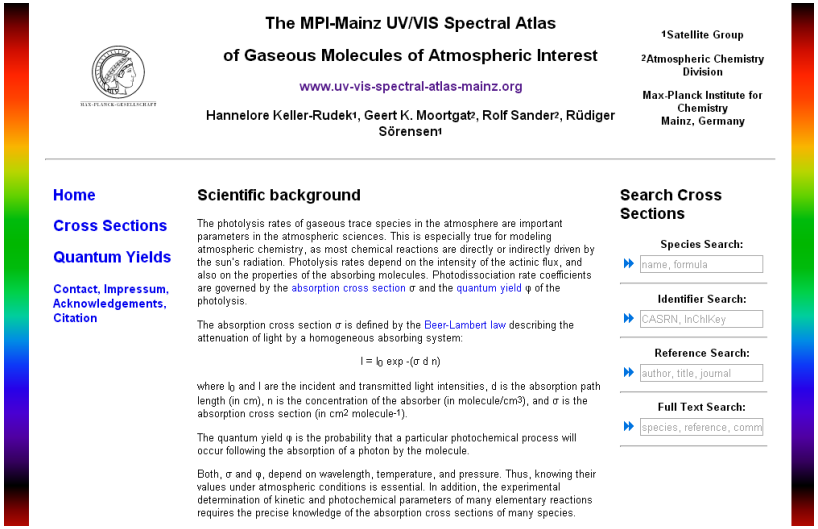
DART

- DART aims at seamlessly perform the cycle
  - Access to a document → Extraction of associated raw data → Execution of a code taking those data as input → Generation of new results → Upload of the new results and article



DART

- DART has been successfully tested using the Molon portlet
  - The MPI-Mainz UV/VIS Spectral Atlas of Gaseous Molecules of Atmospheric Interest
  - Cross sections → Molecular Absorption coefficients



The MPI-Mainz UV/VIS Spectral Atlas

of Gaseous Molecules of Atmospheric Interest

www.uv-vis-spectral-atlas-mainz.org

Hannelore Keller-Rudek[1], Geert K. Moortgat[2], Rolf Sander[2], Rüdiger Sörensen[1]

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Max-Planck Institute for Chemistry
Mainz, Germany

Home

Cross Sections

Quantum Yields

Contact, Impressum, Acknowledgements, Citation

Scientific background

The photolysis rates of gaseous trace species in the atmosphere are important parameters in the atmospheric sciences. This is especially true for modeling atmospheric chemistry, as most chemical reactions are directly or indirectly driven by the sun's radiation. Photolysis rates depend on the intensity of the actinic flux, and also on the properties of the absorbing molecules. Photodissociation rate coefficients are governed by the absorption cross section σ and the quantum yield φ of the photolysis.

The absorption cross section σ is defined by the Beer-Lambert law describing the attenuation of light by a homogeneous absorbing system:

$$I = I_0 \exp -(\sigma\, d\, n)$$

where I_0 and I are the incident and transmitted light intensities, d is the absorption path length (in cm), n is the concentration of the absorber (in molecule/cm^3), and σ is the absorption cross section (in cm^2 molecule^{-1}).

The quantum yield φ is the probability that a particular photochemical process will occur following the absorption of a photon by the molecule.

Both, σ and φ, depend on wavelength, temperature, and pressure. Thus, knowing their values under atmospheric conditions is essential. In addition, the experimental determination of kinetic and photochemical parameters of many elementary reactions requires the precise knowledge of the absorption cross sections of many species.

Search Cross Sections

Species Search:
name, formula

Identifier Search:
CASRN, InChIKey

Reference Search:
author, title, journal

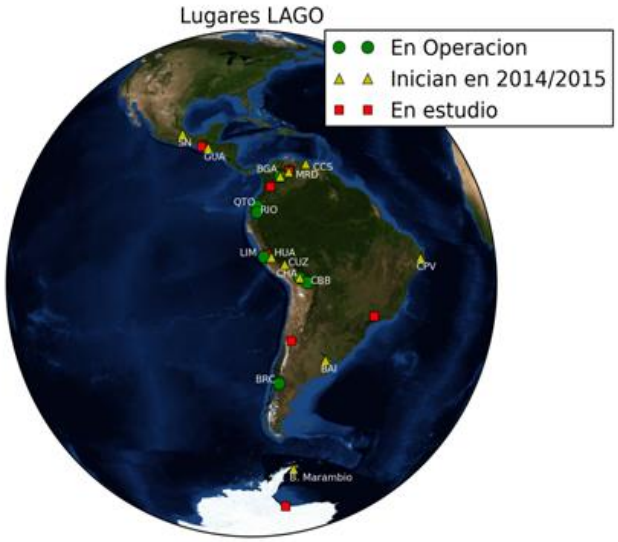
Full Text Search:
species, reference, comm

APHRC (Africa)

- African Population and Health Research Centre
  - Societal health and well-being
    - 60 projects
    - 60 papers
    - 150 fellows trained
    - 18 donors and 51 partners
  - Assignment of PIDs to the wide plethora of datasets that APHRC manages and curates
  - These data sets are widely used in African countries
    - PID will allow a much better exploitation of them

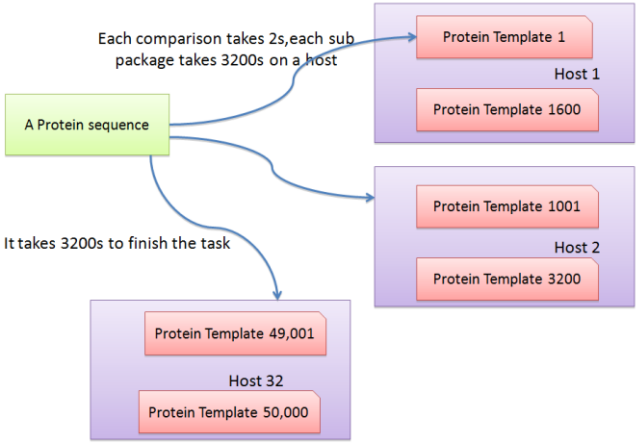
LAGO (LA)

- Latin American Giant Observatory
  - Astroparticle domain
    - Cosmic rays effects on three different phenomena
  - Water Cherenkov Detectors in 9 Latin American countries
  - Fully DART based
    - Corsika code (SG)
    - LAGO data repositories and raw data
    - PID assignment



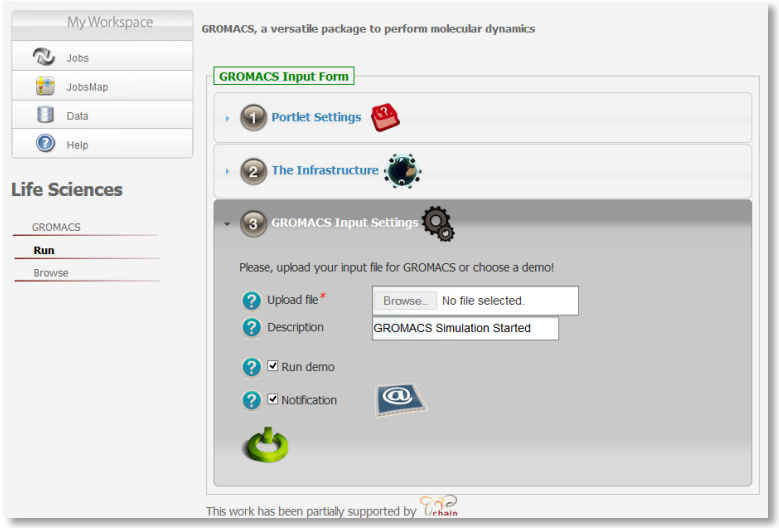
TreeThreader (China)

- Life processes at the molecular level
  - TreeThreader code developed at CAS
  - Citizen science (cas@home) and cloud computing
    - 6 millions of CPU hours/year
    - 15,000 CPU hours/month with the CHAIN-REDS cloud nodes
  - Unique front-end for the submission of jobs
    - Running in China and Europe



GROMACS (India)

- Molecular dynamics domain
  - Worldwide used application
  - CHAIN-REDS has provided a new MPI-enabled version
  - Available via the CHAIN-REDS SG running on sites in India, Arab region, Latin America and Europe
  - Training activities on the way

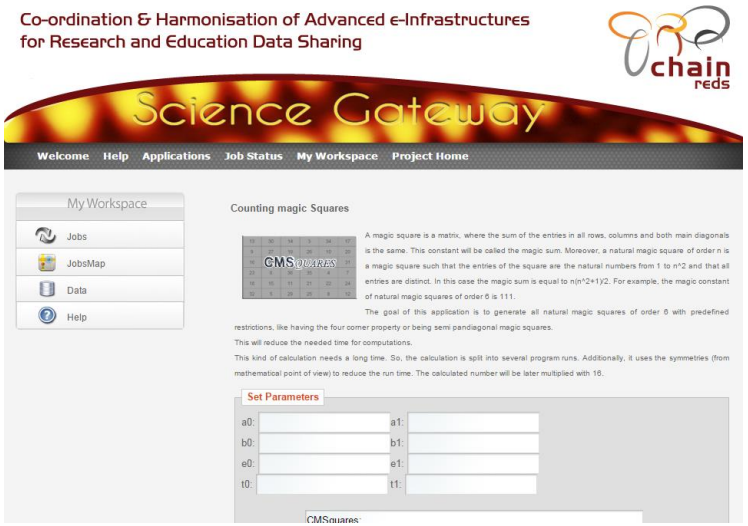


ABINIT (Arab region)

- *Ab initio* calculations on quantum chemistry and Physics of materials domains
  - Worldwide used application
  - CHAIN-REDS has provided a new MPI-enabled version
  - Available via the CHAIN-REDS and the Tunisian SGs
  - Running on sites in the Arab region, Africa, Latin America and Europe
  - Training activities on the way

CMSquares (Arab region)

- Mathematical solutions to find magic squares
  - Example of the so-called "long tail" of users, i.e. those not belonging to big organizations/experiments
  - Available via the CHAIN-REDS SG
  - Mostly used in Jordan
  - Running on sites in the Arab region and Europe



Conclusions

- CHAIN-REDS is targeting scientific communities with a worldwide presence
- Regional use cases are in a good shape to become real success stories
- CHAIN-REDS has been working on developing tools with exploit current data capabilities
  - Knowledge Base
  - Semantic Web Enrichment
  - Semantic Search Engine
  - Science Gateway

Conclusions

- CHAIN-REDS has developed the Data Accessibility, Reproducibility and Trustworthiness (DART) challenge

- DART intends to easily reproduce the whole computing process devoted to either perform or reproduce a (previous) complete research
  - Look for available data and references
  - Used them as input data on a multiplatform application
  - Execute that application seamlessly
  - Retrieve the results and stored them with a Persistent Identifier

Conclusions

- DART concept can be easily adapted to other academic purposes
  - NREN
  - Research groups
  - University Secretariat
  - Administrative tools

- A DART video can be found at the CHAIN-REDS webpage

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Thank you

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