

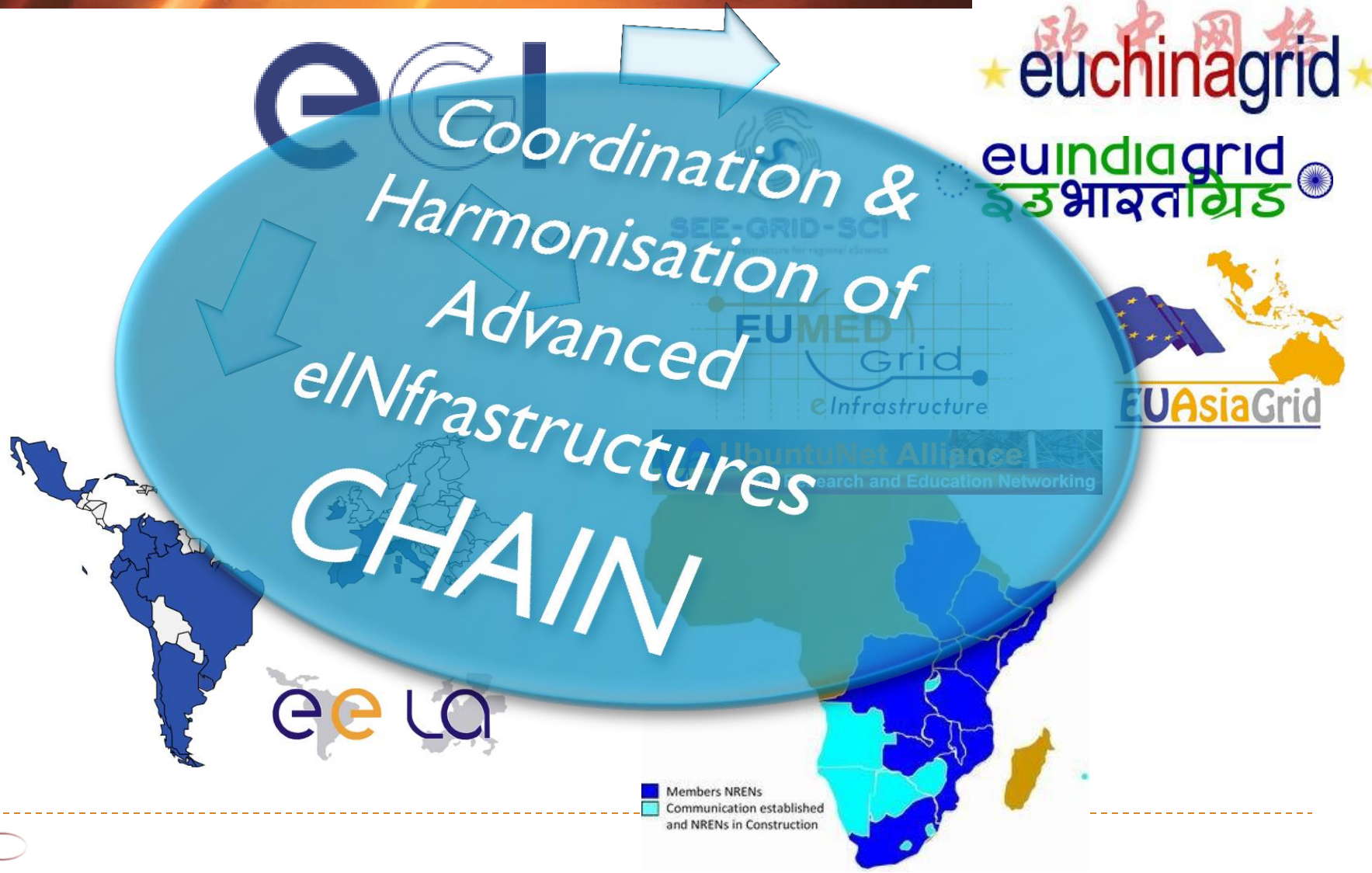
*Co-ordination & Harmonisation of Advanced e-Infrastructures
for Research and Education Data Sharing*

**Jointly exploiting data and distributed
computing eInfrastructure**

Rafael Mayo García (CIEMAT)

UbuntunetConnect 2014, Lusaka, Zambia
13-14 November 2014

CHAIN-REDS: A legacy from CHAIN



- ▶ 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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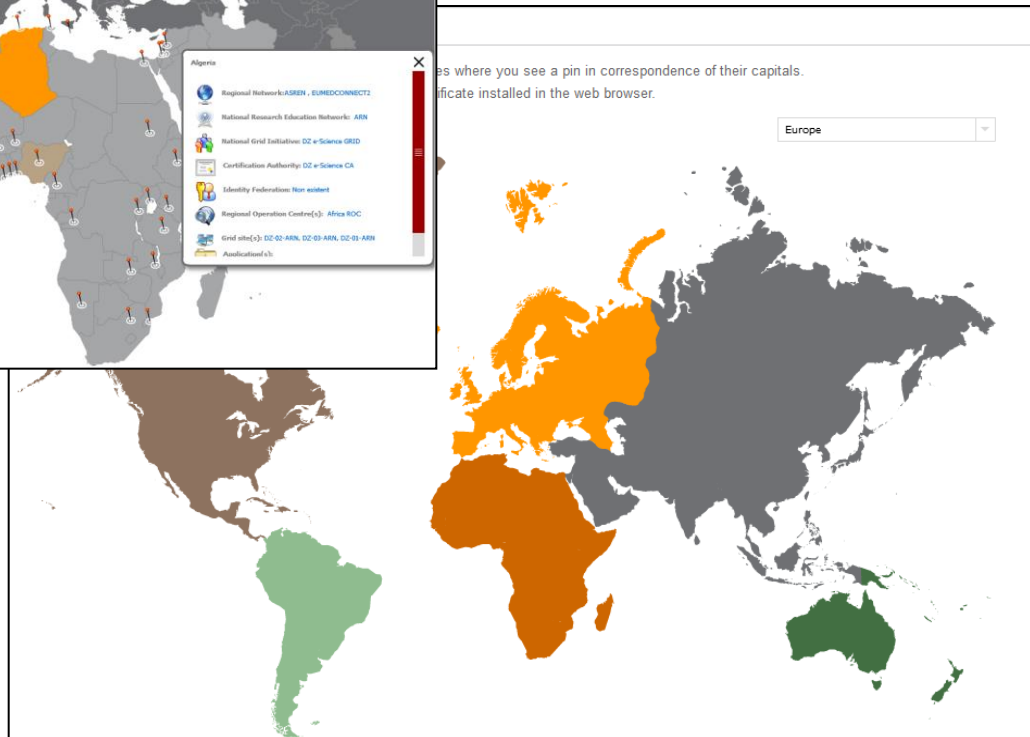
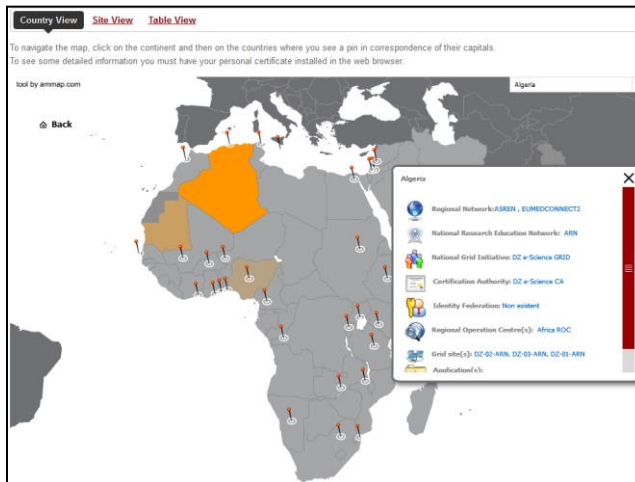


- ▶ Current work on Data Infrastructure can be found in the public project Deliverables
 - ▶ D4.1 Trans-continental Data Infrastructures and Data repositories
 - ▶ D4.2 Analysis of Data Infrastructures and Data repositories
 - ▶ D4.3 Use cases of the identified Data Infrastructures and Data repositories
 - ▶ 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>

- ▶ 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)

- ▶ 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

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)

Registry of Open Access Repositories (ROAR)



- ▶ 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)




- ▶ 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

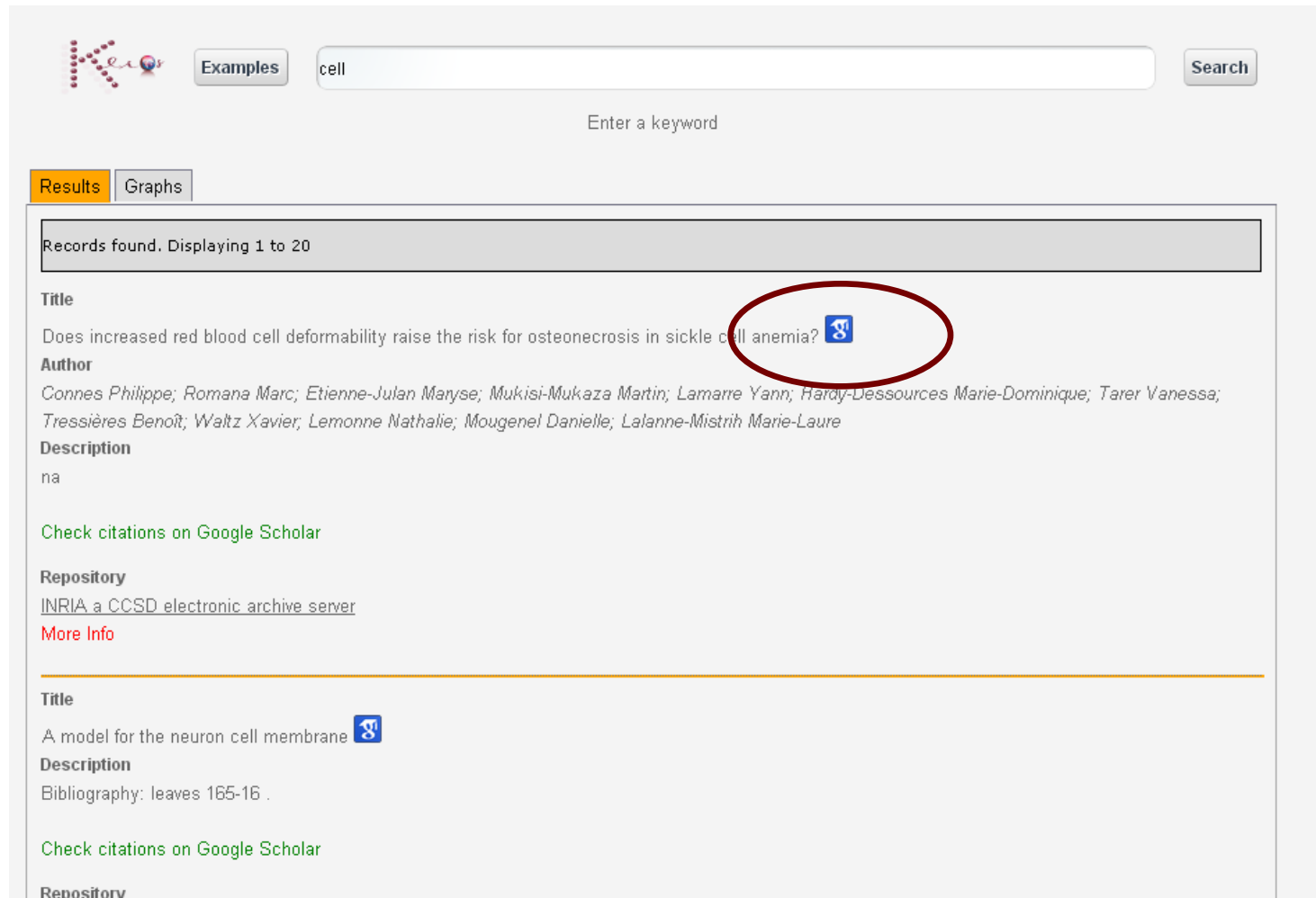
Semantic Search on Linked Data


Here you can search across the thousands of semantically enriched [Open Access Document Repositories](#) and [Data Repositories](#) included in the [CHAIN Knowledge Base](#). Some exemplar keywords are: cardiology, cornea, geology, linked data, natural gas.

Select a language: English ▼



Enter a keyword or select a language and then choose a subject




 [Examples](#) [Search](#)

Enter a keyword

[Results](#) [Graphs](#)

Records found. Displaying 1 to 20


Title
Does increased red blood cell deformability raise the risk for osteonecrosis in sickle cell anemia? 

Author
Connes Philippe; Romana Marc; Etienne-Julan Maryse; Mukisi-Mukaza Martin; Lamarre Yann; Hardy-Dessources Marie-Dominique; Tarer Vanessa; Tressières Benoît; Waltz Xavier; Lemonne Nathalie; Mouguel Danielle; Lalanne-Mistrih Marie-Laure

Description
na

[Check citations on Google Scholar](#)

Repository
[INRIA a CCSD electronic archive server](#)
[More Info](#)

Title
A model for the neuron cell membrane 

Description
Bibliography: leaves 165-16 .

[Check citations on Google Scholar](#)

Repository

Results
Graphs

Filter to view a struct of Resource (max 10 Resource)

Select one or more Resources to view

[R2] Kaposi's Sarcoma-Associated Herpesvirus vFLIP and Human T Cell Lymphotropic Virus Type 1 Tax Oncogenic Proteins Activate I κ B Kinase Subunit β by Different Mechanisms Independent of the Physiological Cytokine-Induced Pathways

[R3] The metastasis-associated extracellular matrix protein Osteopontin forms transient structure in ligand interaction sites

[R4] Analysis of antigenically important residues in human influenza A virus in terms of B-cell epitopes

6 Resources Selected

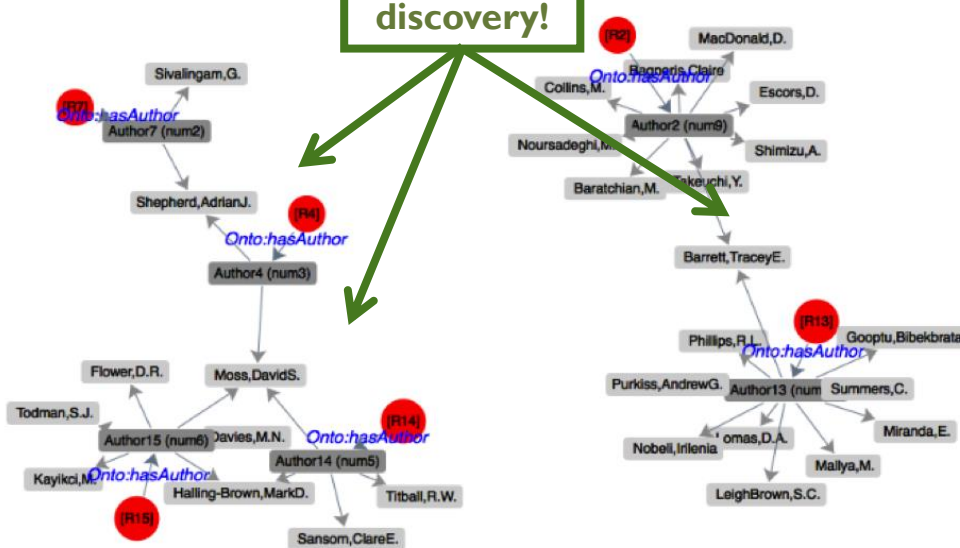
Select a Filter for visualization:

Authors

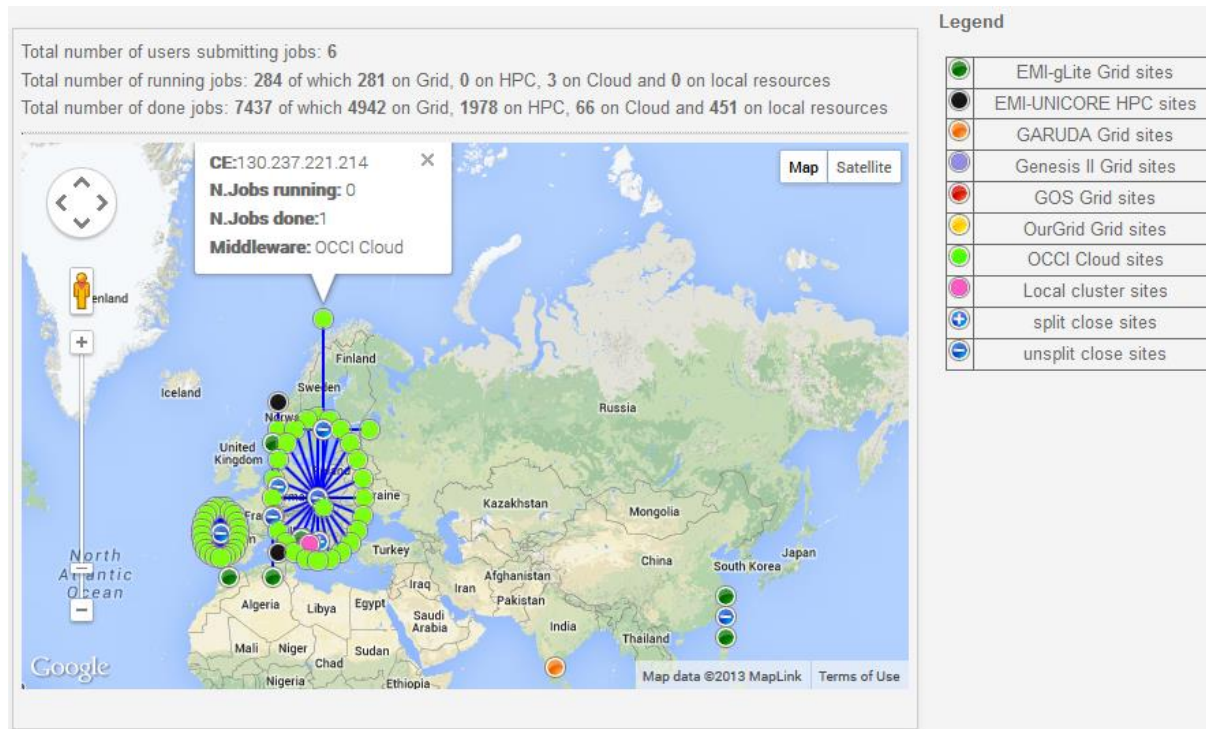
- Authors
- Subjects
- Publishers

(To clear the graph wait until the particles are firmly)

New knowledge discovery!

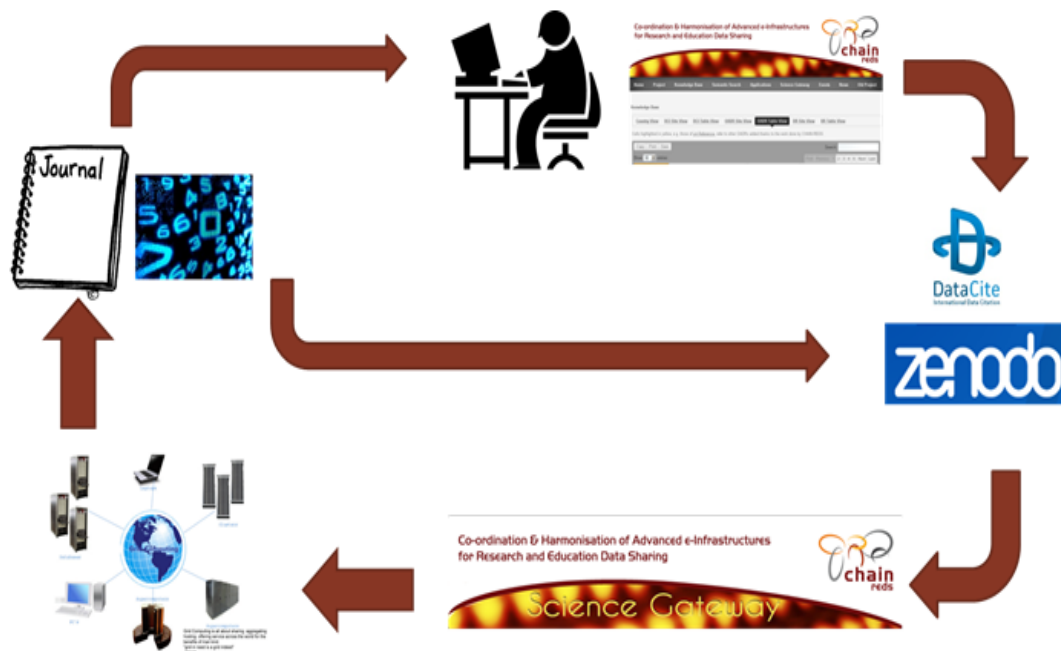


- ▶ Data Accessibility, Reproducibility and Trustworthiness (DART)
 - ▶ Based on the interoperability demo performed by CHAIN-REDS at EGITF 2013




- ▶ 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 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 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-Rudek¹, Geert K. Moortgat², Rolf Sander², Rüdiger Sörensen¹

¹Satellite Group
²Atmospheric Chemistry Division

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](#) q 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:

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

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/cm³), and σ is the absorption cross section (in cm² molecule⁻¹).

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

Both, σ and q , 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:
▶

Identifier Search:
▶

Reference Search:
▶

Full Text Search:
▶

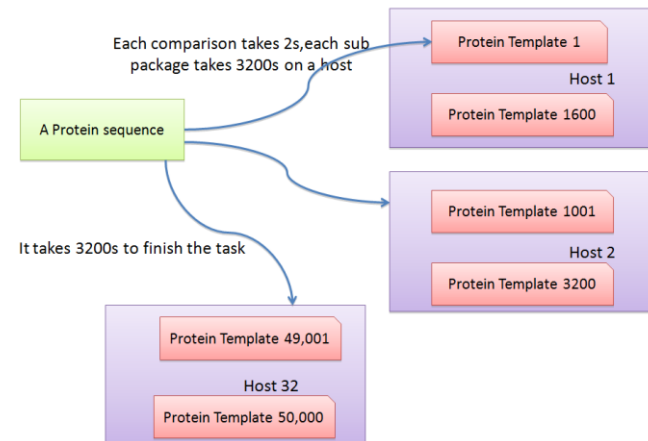
- ▶ African Population and Health Research Centre
 - ▶ Societal health and well-being
 - ▶ 60 projects
 - ▶ 60 papers
 - ▶ 150 fellows trained
 - ▶ 18 donors and 51 partners
 - ▶ Assignment of PIDs to the wide plethora of datasets that APHRC manages and curates
 - ▶ These data sets are widely used in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



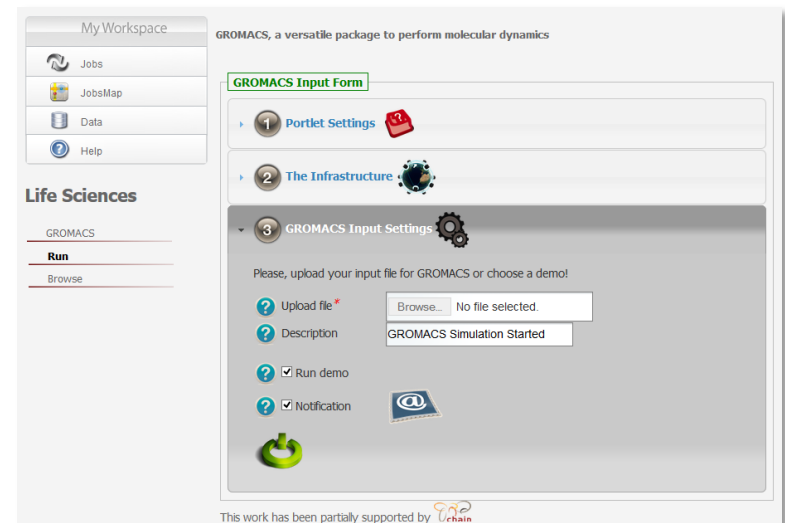
- ▶ Latin American Giant Observatory
 - ▶ Astroparticle domain
 - ▶ Cosmic rays effects on three different phenomena
 - ▶ Water Cherenkov Detectors in 9 Latin American countries
 - ▶ Fully DART based
 - ▶ Corsika code (SG)
 - ▶ LAGO data repositories and raw data
 - ▶ PID assignment



- ▶ 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



- ▶ 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



The screenshot shows a web-based interface for GROMACS. On the left, there is a sidebar with a 'My Workspace' section containing 'Jobs', 'JobsMap', 'Data', and 'Help'. Below this is a 'Life Sciences' section with 'GROMACS', 'Run', and 'Browse' options. The main content area is titled 'GROMACS, a versatile package to perform molecular dynamics' and features a 'GROMACS Input Form'. This form has three numbered steps: 1. Portlet Settings, 2. The Infrastructure, and 3. GROMACS Input Settings. The third step is expanded, showing options to 'Upload file', 'Description', 'Run demo', and 'Notification'. A 'Browse...' button is next to the 'Upload file' option, and a 'GROMACS Simulation Started' message is visible. At the bottom, there is a small logo and the text 'This work has been partially supported by'.

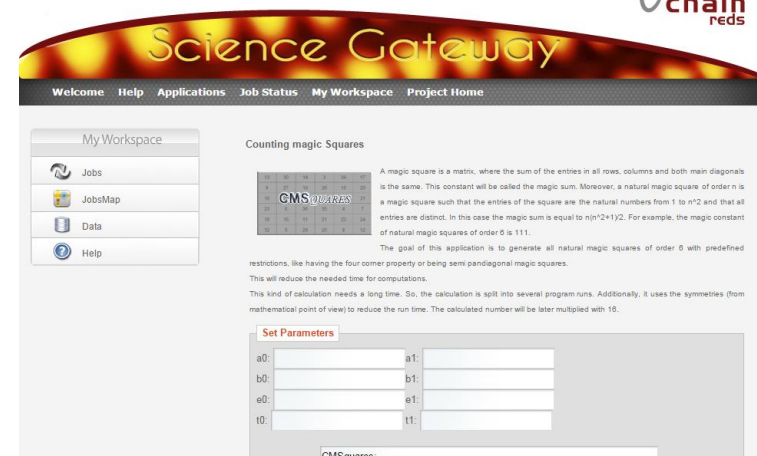
- ▶ *Ab initio* calculations on quantum chemistry and Physics of materials domains
 - ▶ Worldwide used application
 - ▶ CHAIN-REDS has provided a new MPI-enabled version
 - ▶ Available via the CHAIN-REDS and the Tunisian SGs
 - ▶ Running on sites in the Arab region, Africa, Latin America and Europe
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



The screenshot shows the ABINIT website interface. At the top, there is a navigation bar with links for Home, Applications, DZ e-Science Grid, and About. Below this, there is a sidebar with a list of applications including Sequential, Parallel, Octave, Gromacs, R-Statistic, and Abinit. The main content area features a section titled 'Abinit' with a description: 'ABINIT is a package whose main program that allows to find:'. Below this, there is a list of capabilities: 'The total energy', 'Charge density', 'Electronic structure of systems made of electrons and nuclei (molecules and periodic solids)', 'Density Functional Theory (DFT)', 'Pseudopotentials', and 'Planewave or wavelet basis'. There is also a 'Sign-in to RUN' button and a small diagram illustrating the computational process. At the bottom of the page, there are logos for ASREN, chain reds, and INF.

- ▶ 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

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



The screenshot shows the Science Gateway interface for the CMSSquares application. At the top, there is a navigation bar with links for Welcome, Help, Applications, Job Status, My Workspace, and Project Home. Below this is a "My Workspace" sidebar with icons for Jobs, JobsMap, Data, and Help. The main content area is titled "Counting magic Squares" and contains a 6x6 grid of numbers labeled "CMSSQUARES". To the right of the grid is a text description of a magic square and the application's goal. Below the text is a "Set Parameters" section with input fields for a0, b0, e0, t0, a1, b1, e1, and t1.

Science Gateway

Welcome Help Applications Job Status My Workspace Project Home

My Workspace

- Jobs
- JobsMap
- Data
- Help

Counting magic Squares

A magic square is a matrix, where the sum of the entries in all rows, columns and both main diagonals is the same. This constant will be called the magic sum. Moreover, a natural magic square of order n is a magic square such that the entries of the square are the natural numbers from 1 to n^2 and that all entries are distinct. In this case the magic sum is equal to $n(n^2+1)/2$. For example, the magic constant of natural magic squares of order 6 is 111.

The goal of this application is to generate all natural magic squares of order n with predefined restrictions, like having the four corner property or being semi pandiagonal magic squares.

This will reduce the needed time for computations.

This kind of calculation needs a long time. So, the calculation is split into several program runs. Additionally, it uses the symmetries (from mathematical point of view) to reduce the run time. The calculated number will be later multiplied with 16.

Set Parameters

a0:	<input type="text"/>	a1:	<input type="text"/>
b0:	<input type="text"/>	b1:	<input type="text"/>
e0:	<input type="text"/>	e1:	<input type="text"/>
t0:	<input type="text"/>	t1:	<input type="text"/>

CMSSquares

- ▶ 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

- ▶ 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

- ▶ 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

*Co-ordination & Harmonisation of Advanced e-Infrastructures
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Thank you

www.chain-project.eu
proj-office@chain-project.eu