





Open Science in action

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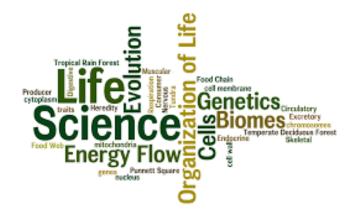
Workshop Bibliosan 2019 - Roma, 3 dicembre 2019



Concetti chiave della presentazione

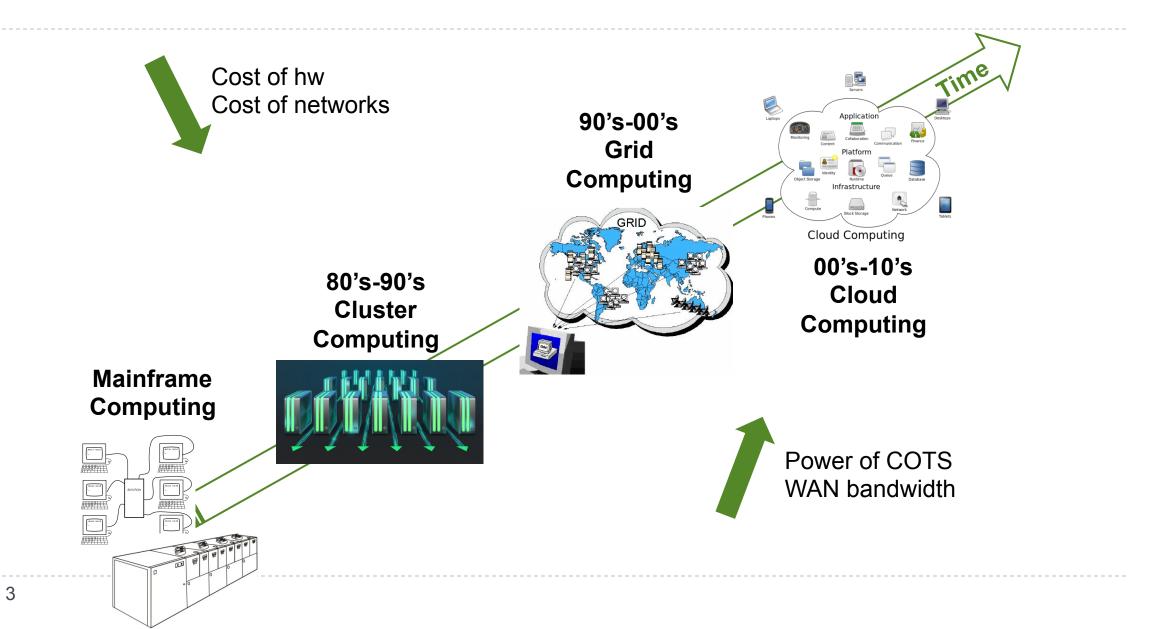




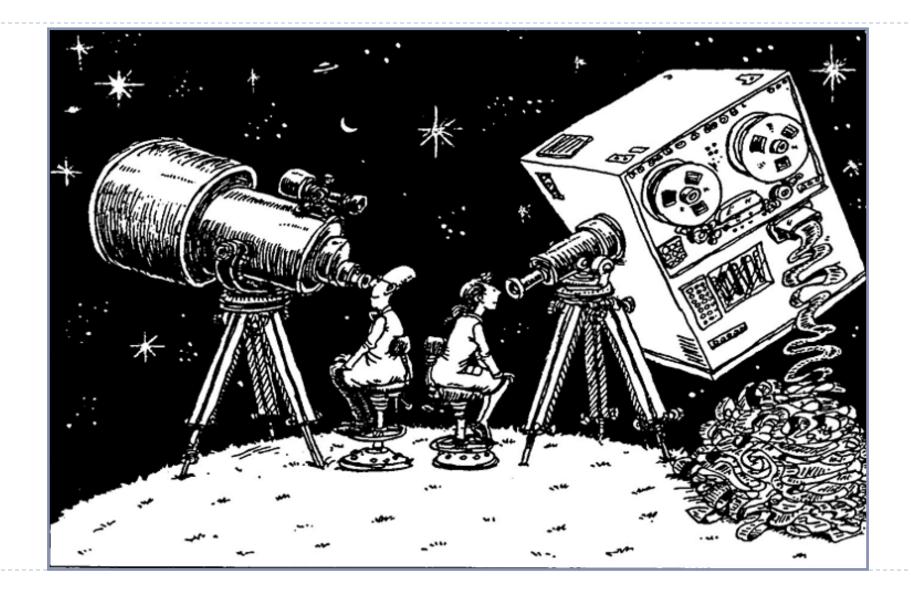




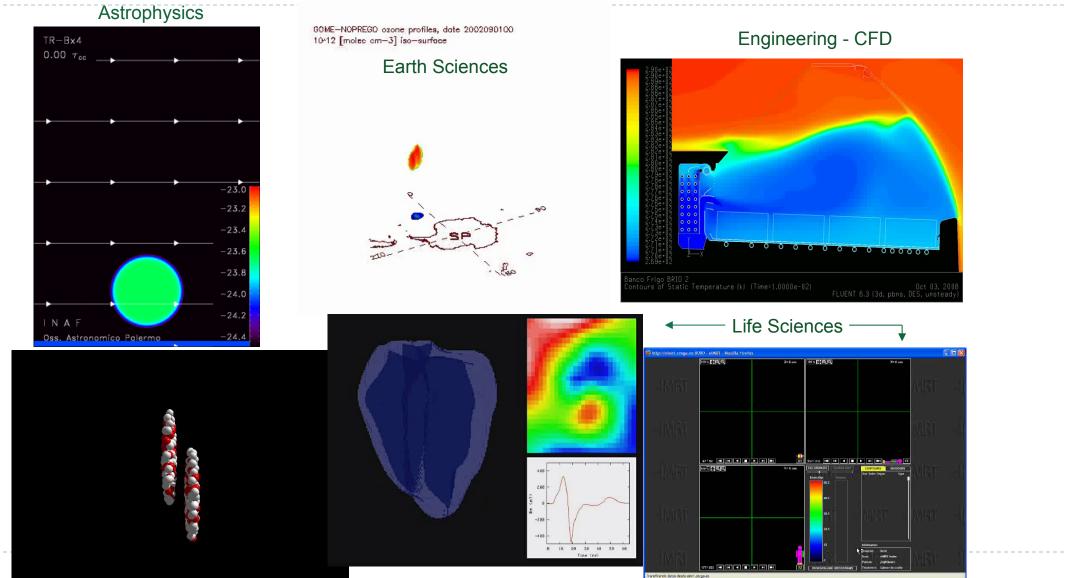
(E/Ri)voluzione del calcolo scientifico



intensive»

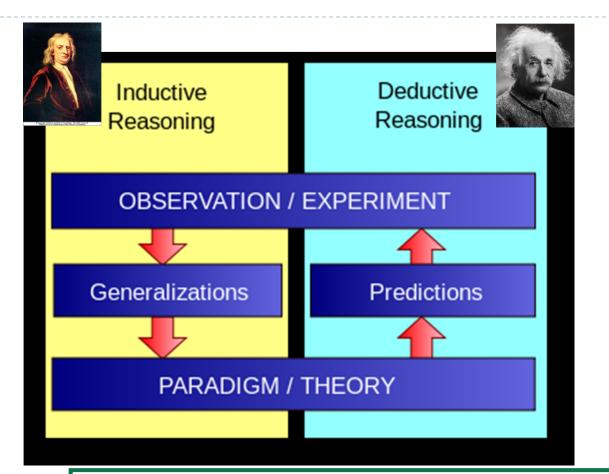


intensive»



High Energy Physics

intensive»

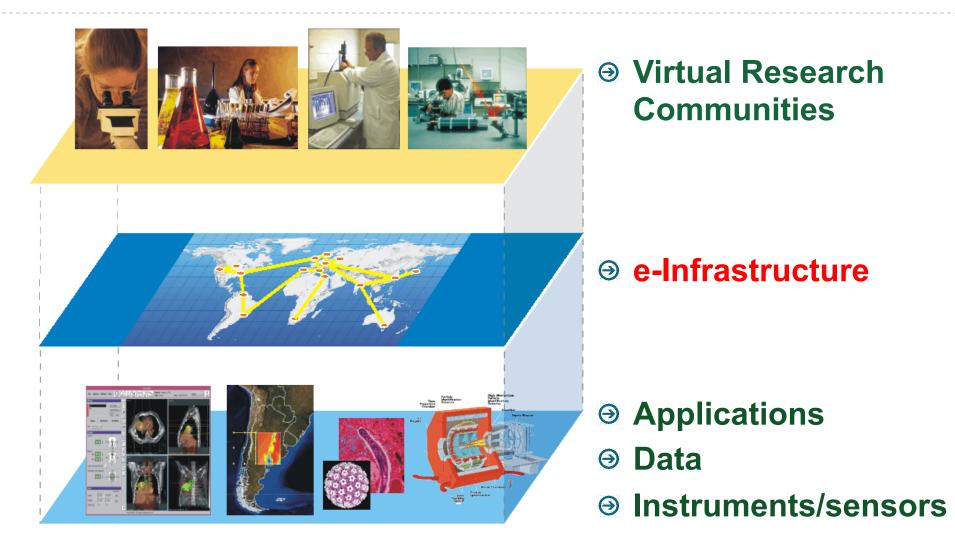


- Examples of IR:
 - Classical Mechanics
 - Newton's Gravitation Theory
- Examples of DR:
 - General Relativity
 - Standard Model of Particle Physics

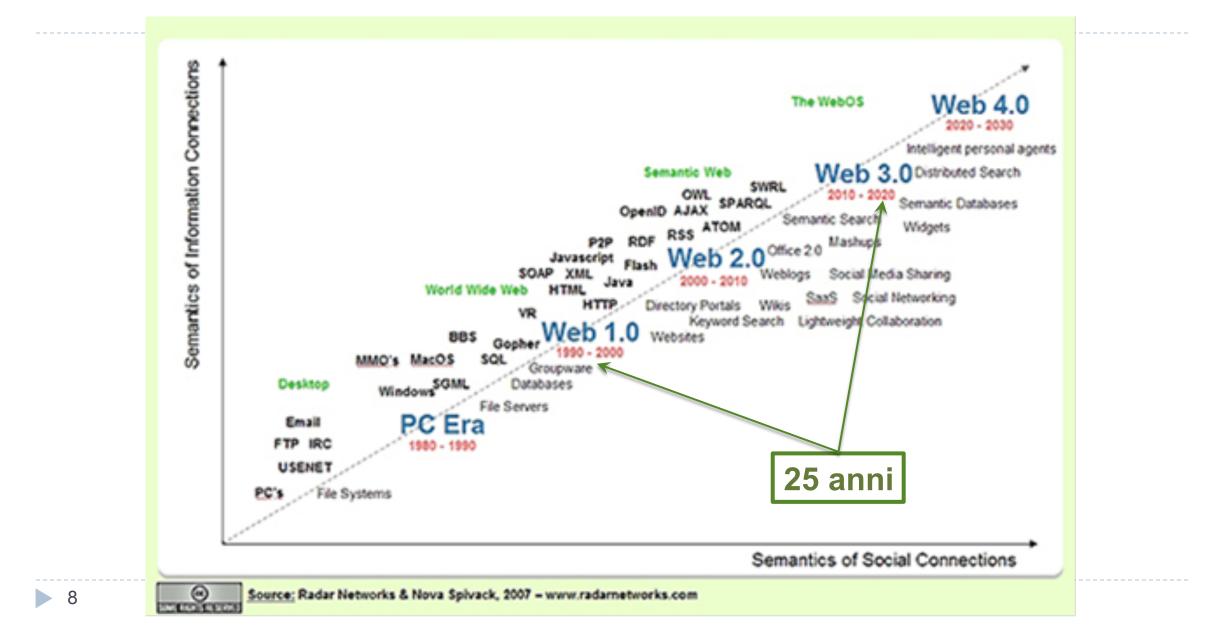
Computer simulations reconcile the inductive and deductive reasonings of the Scientific Method

https://plato.stanford.edu/entries/scientific-method/

Evoluzione: il concetto di «e-Science»



(Ri/E)voluzione del web



(LOD)

W3C^{*} Semantic Web User interface and applications Trust Proof Unifying Logic Ontologies: OWL Rules: RIF/SWRL Querying SPARQL Taxonomies: RDFS Data interchange: RDF Syntax: XML Character Set: UNICODE Identifiers: URI

*



9





OL RE OF URI LD

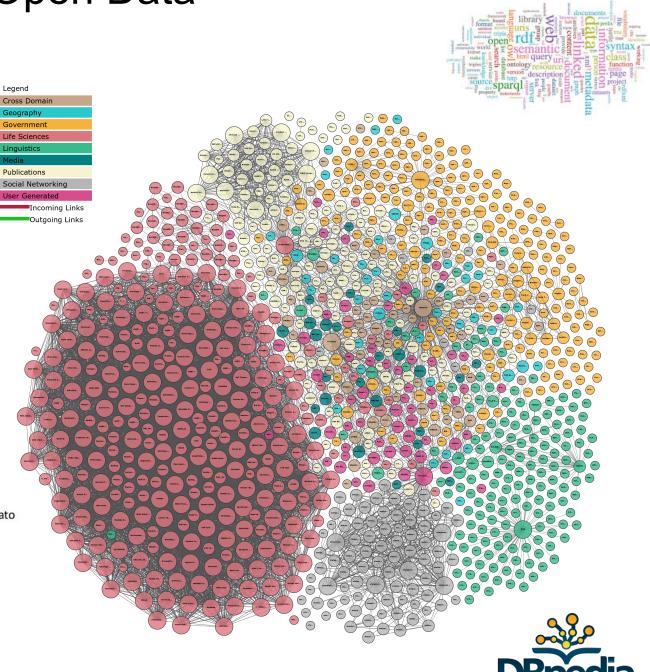
Dato disponibile sul Web in un qualsiasi formato (anche PDF) rilasciato con licenza Open

Leggibile dal calcolatore. Dati strutturati in formati proprietari (es. Excel)

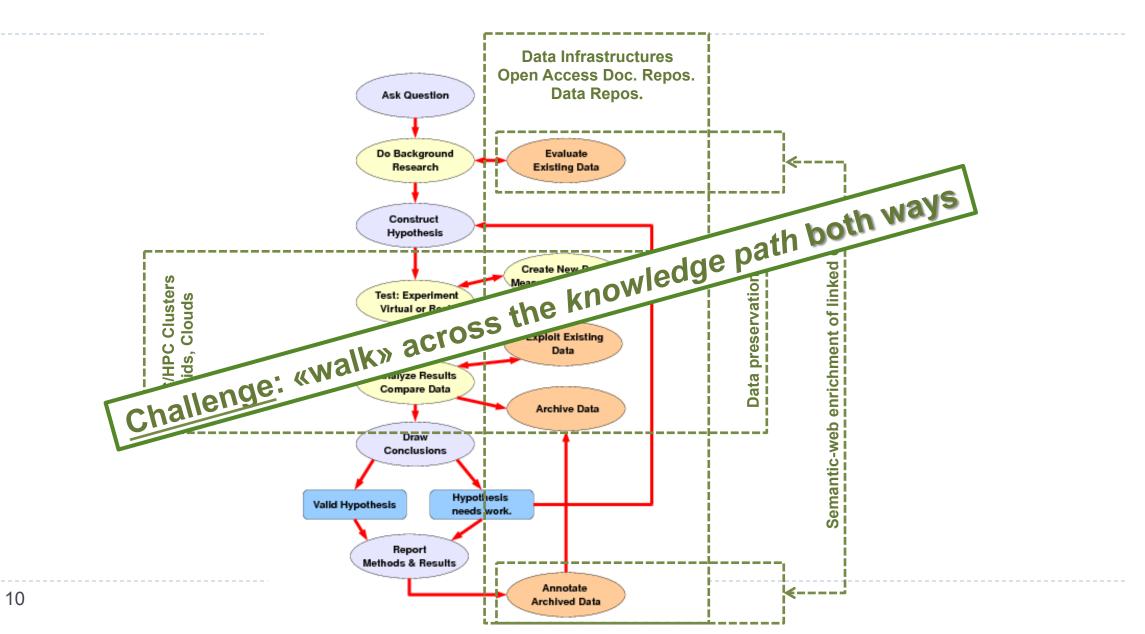
Come gli Open Data a 2 stelle ma in formato non proprietario (es. XML)

Come I livelli precedenti ma segue gli standard W3C (RDF e Sparql)

Come i livelli precedenti ma i dati sono collegati (Linked Data)

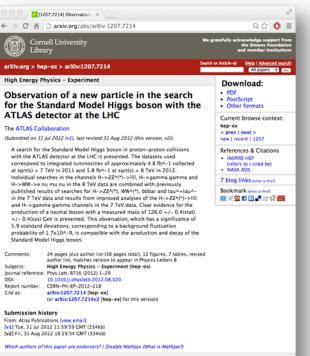


Le e-Infrastrutture, il Web 3.0 ed il Metodo Scientifico



L"output" del Metodo Scientifico

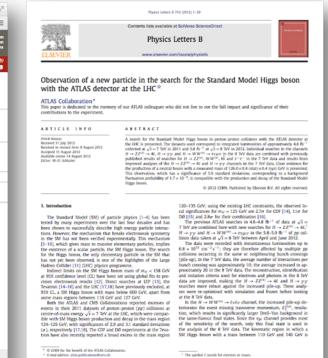
THILOSOTHICAL TRANSACTIONS: GIVING SOME COMPT OF THE PRESENT Undertakings, Studies, and Labours OF THE INGENIOUS IN MANY CONSIDERABLE PARTS OFTHE WORLD weed. Vol I. For Anno 1665, and 1666. In the SAVOY, Printed by T. N. for John Martyn at the Bell, a little with-out Temple-Bar, and Fames Alleftry in Duck-Lant, Printers to the Reyal Society.



Link back to: arXiv, form interface, contact

DOI

Cite as:



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Marked a real Scientific Revolution but. it is the same since almost 4 centuries!

I «pilastri» del Metodo Scientifico

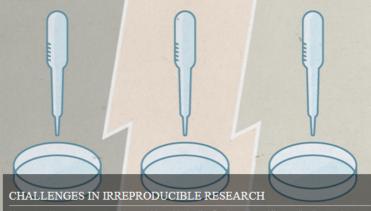
- Repeatability
 - scienza è veramente riproducibile? The closeness of agreement between independent results the same method on identical test material, under the ions (same operator, same apparatus, same labe intervals of time)
 - Affected by random error
- Reproducib
 - agreement between independent results obtained with ethod on identical test material but under different conditions (onerent operators, different apparatus, different laboratories and/or after different intervals of time)
 - Affected by systematic errors

Challenges in irreproducible research

(https://www.nature.com/collections/wjsrmrdnsm)

Search Go Advanced search Advanced search Home News & Comment Research Careers & Jobs Current Issue Archive Audio & Video For Authors Archive Specials & supplements archive Challenges in irreproducible research Find out more V X Take part in Nature Publishing Group's annual reader survey here for the chance to win a Macbook Air. Find out more V X

SPECIAL



No research paper can ever be considered to be the final word, and the replication and corroboration of research results is key to the scientific process. In studying complex entities, especially animals and human beings, the complexity of the system and of the techniques can all too easily lead to results that seem robust in the lab, and valid to editors and referees of journals, but which do not stand the test of further studies. *Nature* has published a series of articles about the worrying extent to which research results have been found wanting in this respect. The editors of *Nature* and the *Nature* life sciences research journals have also taken substantive steps to put our own houses in order, in improving the transparency and robustness of what we publish. Journals, research laboratories and institutions and funders all have an interest in tackling issues of irreproducibility. We hope that the articles contained in this collection will help.

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Perspectives and reviews

EDITORIAL See all specials

Journals unite for reproducibility

Consensus on reporting principles aims to improve biomedical research. Nature 515, 7 (8 November 2014)

Code share

Papers in Nature journals should make computer code accessible where possible. *Nature* 514, 536 (29 October 2014)

Reducing our irreproducibility

Nature 496, 398 (25 April 2013)

Further confirmation needed

A new mechanism for independently replicating research findings is one of several changes required to improve the quality of the biomedical literature. *Nature Biotechnology* **30**, 806 (10 September 2012)

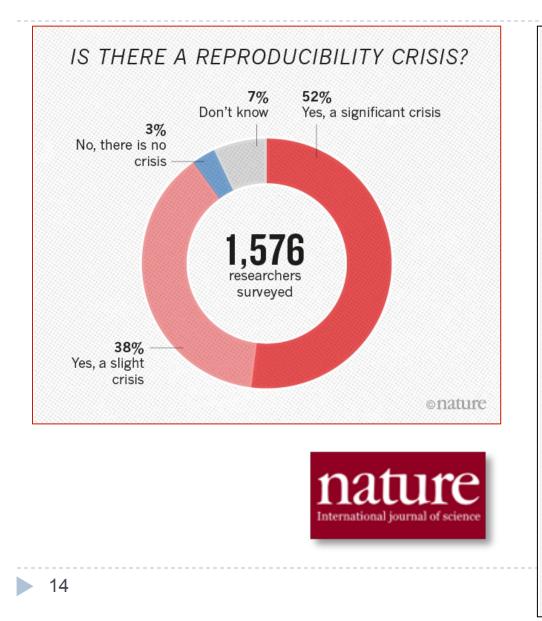
Error prone

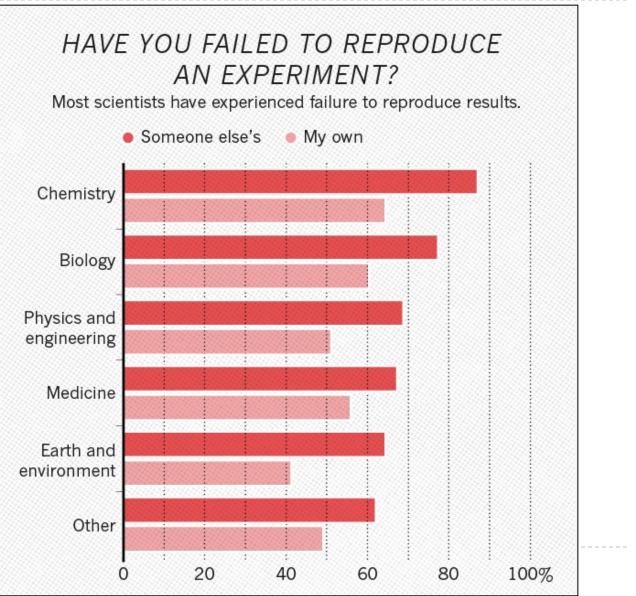
Biologists must realize the pitfalls of work on massive amounts of data. Nature 487, 406 (26 July 2012)

Must try harder

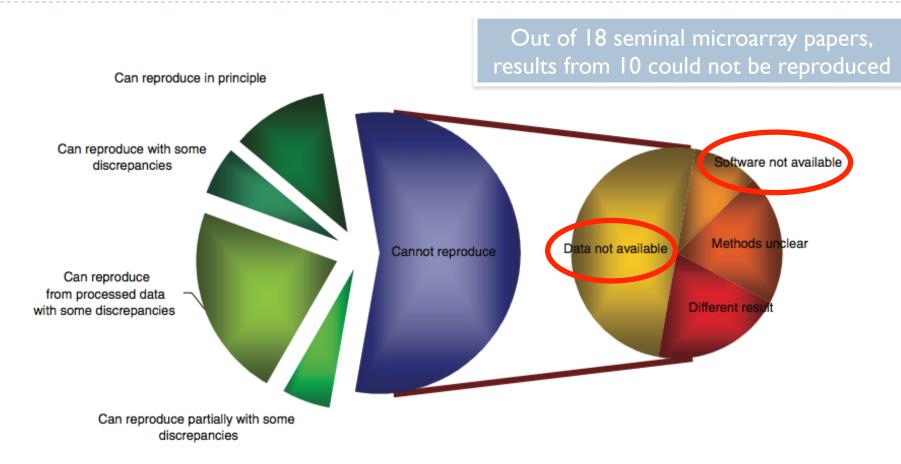
Too many sloppy mistakes are creeping into scientific papers. Lab heads must look more rigorously at the data — and at themselves. Nature 483, 509 (29 March 2012)

La «crisi di riproducibilità»



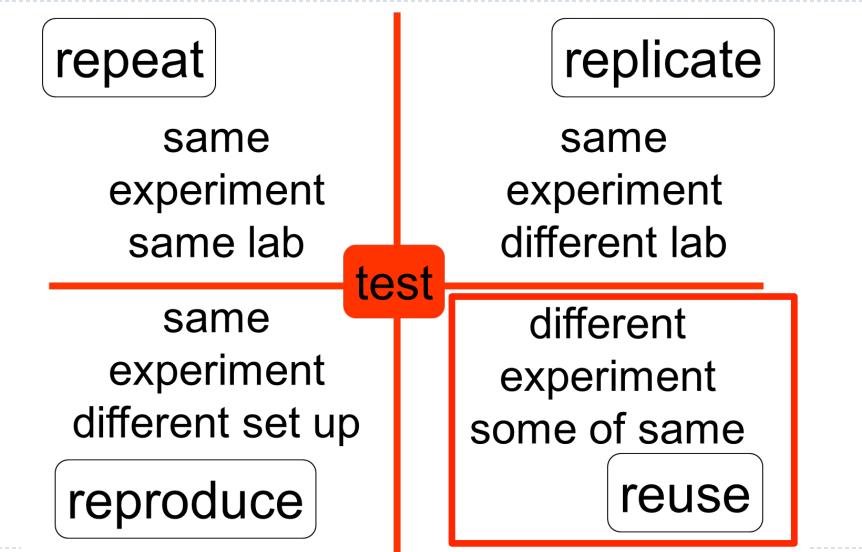


Le ragioni della «crisi di riproducibilità»



- 1. Ioannidis et al., 2009. Repeatability of published microarray gene expression analyses. Nature Genetics 41: 14
- 2. Science publishing: The trouble with retractions http://www.nature.com/news/2011/111005/full/478026a.html
- 3. Bjorn Brembs: Open Access and the looming crisis in science https://theconversation.com/open-access-and-the-looming-crisis-in-science-14950

Evoluzione: la ripetibilità e la riproducibilità non sono tutto...



Drummond C Replicability is not Reproducibility: Nor is it Good Science, online Peng RD, Reproducible Research in Computational Science Science 2 Dec 2011: 1226-1227.

La «rivoluzione» della Scienza Aperta

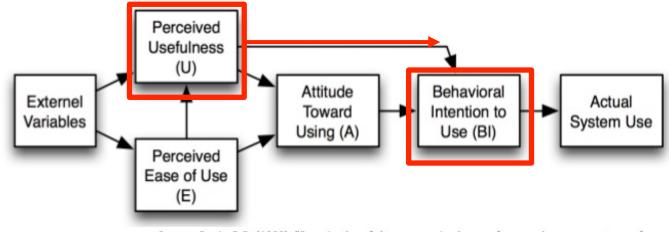
(http://book.openingscience.org 10.1787/5jrs2f963zs1-en)

http://dx.doi.org/

- "Open Science refers to a scientific culture that is characterized by its openness. Scientists <u>share results</u> almost immediately and with a very wide audience"
- "Open science is a means and not an end in itself and it is much more than just open access to publications or data; <u>it includes many</u> <u>aspects and stages of research processes</u> thus enabling full reproducibility and re-usability of scientific results."







Source: Davis, F. D. (1989), "Perceived usefulness, perceived ease of use, and user acceptance of information technology", MIS Quarterly 13(3): 319–340



La «mutazione» dei dati: i principi FAIR

(https://www.force11.org/group/fairgroup/fairprinciples)

 "One of the grand challenges of data-intensive science is to facilitate knowledge discovery by assisting humans and machines in their discovery of, access to, integration and analysis of, task-appropriate scientific data and their associated algorithms and workflows." Research data have to be

• Findable:

- F1. (meta)data are assigned a globally unique and eternally persistent identifier
- F2. data are described with rich metadata
- F3. (meta)data are registered or indexed in a searchable resource.
- F4. metadata specify the data identifier

• Accessible:

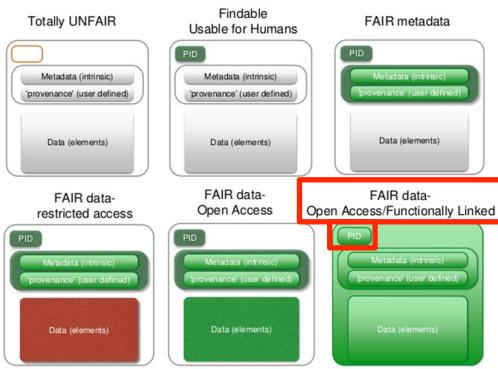
- A1 (meta)data are retrievable by their identifier using a standardized communications protocol
- A1.1 the protocol is open, free, and universally implementable
- A1.2 the protocol allows for an authentication and authorization procedure, where necessary
- A2 metadata are accessible, even when the data are no longer available

Interoperable:

- I1. (meta)data use a <u>formal, accessible, shared, and broadly applicable language</u> for knowledge representation
- I2. (meta)data use vocabularies that follow FAIR principles
- I3. (meta)data include gualified references to other (meta)data

• Reusable:

- R1. meta(data) have a <u>plurality of accurate and relevant attributes</u>
- R1.1. (meta)data are released with a clear and accessible data usage license
- ¹⁹ R1.2. (meta)data are associated with their provenance
 - R1.3. (meta)data meet domain-relevant community standards



Evoluzione (\rightarrow complessità): approccio multidisciplinare a...

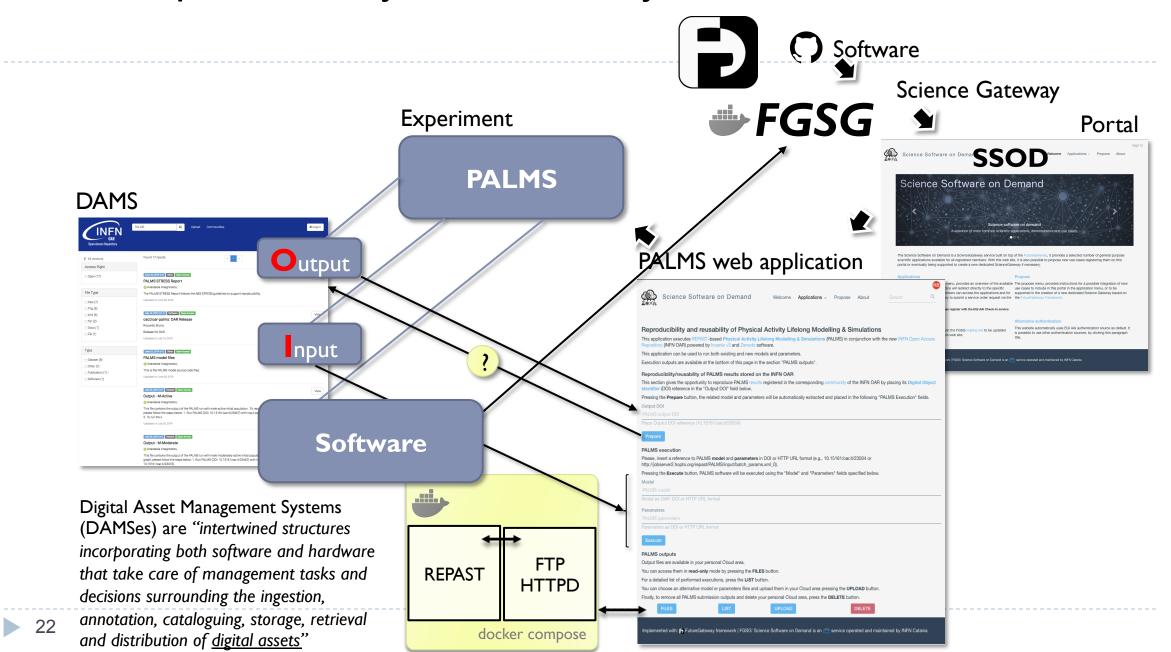




OK, tutto molto interessante...



The «Reproducibility & Reusability Platform» - overview

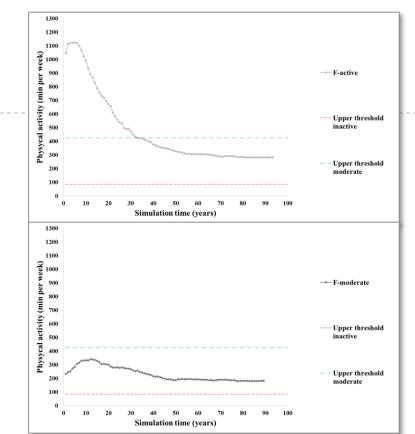


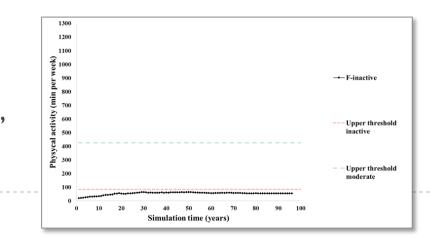
RRP ingredients: PALM simulations

- Physical Activity Lifelong Modelling & Simulations
 - Is an agent based micro-simulation that predicts the lifelong physical activity behaviour of a population taking into account individual characteristics and their effect on physical activity over time
 - Produces individual and aggregated quantitative outputs for quality of life and health conditions related costs

The software

- Uses REPAST [1], a «de facto» standard open source agentbased modeling and simulation platform
- A specific dockerhub image exists for PALMS executions (osabuoun/repast) [2]
- Two inputs necessary: model file (REPAST) and a parameters' file





RRP ingredients: The FutureGateway Framework

futuregatewayframework.github.io

INFN software project aiming to build secure and reliable Science Gateways [1]

Three core components:

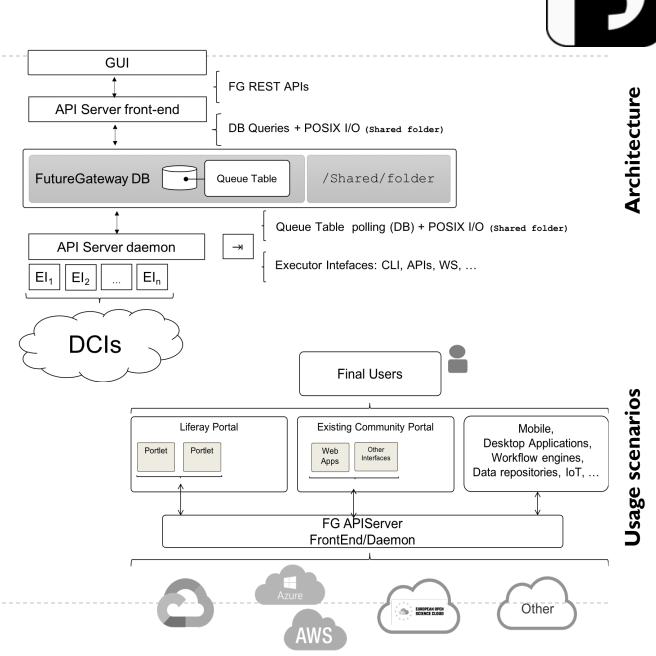
 Database, APIServer front-end, APIServer daemon + Executor Interfaces

The framework:

- Core components are enriched with a suite of tools, APIs and installation + maintenance scripts
- Open Source code available on GitHub

Targets:

 Desktop and Mobile applications, Workflow Engines, IoT and Open Science

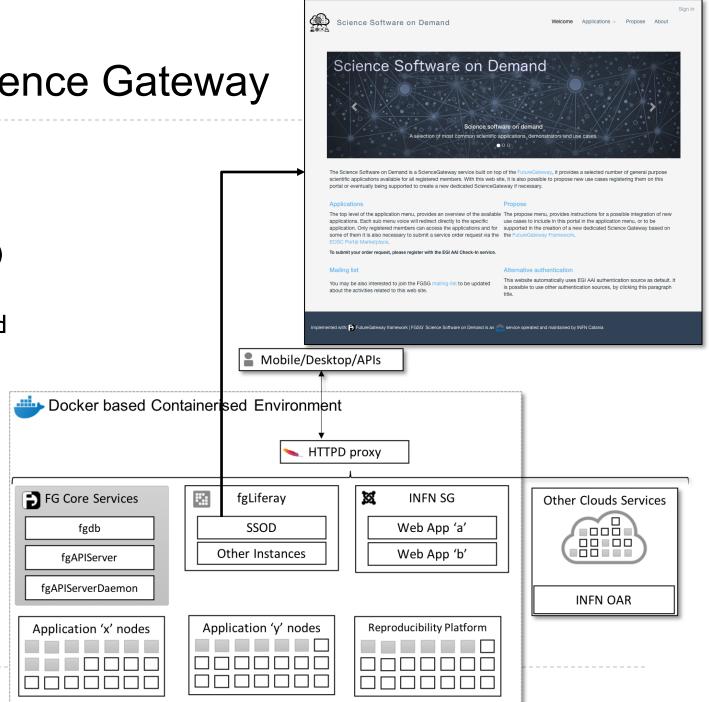


RRP ingredients: FGSG – FutureGateway based Science Gateway

Fully docker containerised environment built in the context of the EOSC-hub project [1], to provide a General purposes Science Gateway: the EGI [2] **Science Software on Demand** (SSOD) [3]

- The system allows to dynamically instantiate and destroy docker containers (it supports docker compose as well as docker swarm)
- FG core services + SSOD service

- SSOD service powered by an enterprise portal framework (Liferay)
 - One section dedicated to the **Reproducibility** & Reusability Platform
 - The platform exploits the FutureGateway and the INFN Open Access Repository



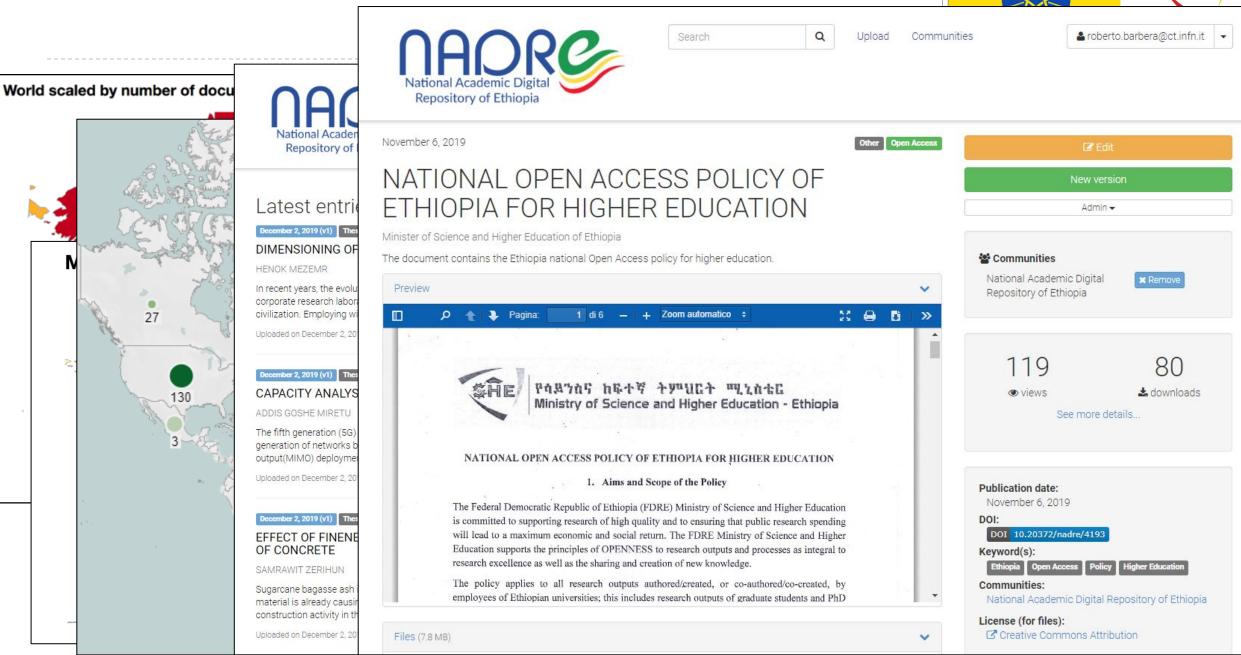
RRP ingredients: the INFN Open Access Repository (OAR)

- INFN joined the Plan S [1] initiative to promote open access
- INFN OAR is a DAMS hosted at INFN Catania
 [2] running on a dedicated kubernetes cluster
- It uses the **ZENOO** [3] open source software for DAMSes
- PALMS input, output, software and papers files are registered with DataCite DOIs (linked to
 iDORCID profiles of authors)
- INFN OAR allows to define references among registered DOIs and supports DOI versioning
- Software used by FGSG to run PALMS simulations is published as well on the INFN OAR (linked from GitHub)

	Open Access Repository	PALMS Q. Uploed Comm	munities ●Log in
e Identity P	ア All versions Access Right	Found 17 results.	< 1 > Sort by: Best match = (asc. •)
····· 🏰 !	Copen (17)	June 26, 2019 (v1) Other Open Access PALMS STRESS Report	View
	File Type	O Anastasia Anagnostou; The PALMS STRESS Report follows the ABS STRESS guide the ABS STRES	auidelines to support reproducibility.
	□ Xlsx (7)	Uploaded on June 26, 2019	
	□ Png (6) □ Xml (6) □ Tar (2) □ Docx (1) □ Zip (1)	Joby 16, 2019 (v1.1) Software Open Access osct/oar-palms: OAR Release Riccardo Bruno; Release for OAR Uploaded on July 16, 2019	 Open Access O Embargoed Access
	Type Dataset (8) Other (7) Publication (1) + Software (1)	June 25, 2019 (r1) Other Open Access PALMS model files Anastasia Anagnostou; This is the PALMS model source code files. Uploaded on June 26, 2019	 Restricted Access Closed Access
%eduGAIN	Jay 20, 2019 (r)1 Detailed View Output - M-Active Anastasia Anagnostou; This file contains the output of the PALMS run with male active initial population. To reproduce the physical activity trajectory graph, please follow the steps below: 1. Run PALMS (DOI: 10.15161/oar.it/23467) with input parameters M-Active (DOI: 10.15161/oar.it/23477). To run the s Uploaded on July 20, 2019 View Output - M-Moderate Anastasia Anagnostou; This file contains the output of the PALMS run with male moderately active initial population. To reproduce the physical activity trajectory graph, please follow the steps below: 1. Run PALMS (DOI: 10.15161/oar.it/23467) with input parameters M-Active (DOI: 10.15161/oar.it/23477). Image: State of the steps below: 1. Run PALMS run with male moderately active initial population. To reproduce the physical activity trajectory graph, please follow the steps below: 1. Run PALMS (DOI: 10.15161/oar.it/23467) with input parameters M-Moderately (DOI: 10.15161/oar.it/23473).		
Input DOIs MODEL PARAMETERS		docker comp REPAST	

<u>https://www.coalition-s.org</u>
 <u>https://www.openaccessrepository.it</u>
 https://github.com/zenodo/zenodo

Evoluzione «per contagio»: NADRE



Sommario e conclusioni

- The PALMS use case demonstrates Open Science in action
- The R&R Platform developed for PALMS can be easily reused to implement other use cases
- The INFN OAR and the R&R Platform are open to any interested communities
- FutureGateway is a mature product successfully used by:
 - Web, Desktop and Mobile Applications, Workflow engines, IoT and Open Science demonstrators
- Investigations are in progress to extend this work to a more general and widely adoptable solution

Grazie !