Research Software Challenges: What are they and how to tackle them

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Context

RS ==

[*EN*] research software, [*ES*] software de investigación, [*FR*] logiciel de la recherche

- (2006-...) Local context: "Mission logiciels", Computer Science Lab LIGM
  Goal: to promote **the visibility** of RS produced in the lab
  Challenges: definition, dissemination
- (2007-2013) National context in France: CNRS PLUME Project
  2nd goal: to promote the RS produced in the academic (ESR) community
  Challenges: definition, dissemination, and legal & scientific production contexts
- (2014-2018) Among other projects, PRESOFT for RS SMPs
- (2018) Question: How to take into account the RS in evaluation processes
- (2018-...) Collaboration with Tomas Recio, Profesor magistral, Univ. Nebrija
  Theoretical studies on RS, Open Science, Research Data...
  (see the final list of references)
- (2022-...) Local context: "Mission logiciels, données et science ouverte"

The goals of this presentation (1/2)

The goal of this presentation is to study and to understand some challenges that appear in the RS produced in a scientific context, and thus to propose answers to the raised questions.

We will deal with the following challenges:

- definition
- dissemination
- evaluation
- The FAIR Guiding Principles
- Borgman's conundrun challenges

And we will mention questions about legal issues and scientific policies that we have studied in the context of French research labs.

The goals of this presentation (2/2)

1. Context
2. Goals
3. Research software
   - Software or computer program
   - Challenge: the definition of Research Software
   - Challenge: a RS dissemination procedure
   - Challenge: questions about the legal & scientific production contexts
   - What means RS author?
   - Publications on RS/ RS Papers
   - Referencing and citation issues
4. On the evaluation of RS in Research
   - Evaluation contexts in Research
   - Two evaluation methods
   - CDUR for RS in Research evaluation
   - CDUR vs The FAIR Guiding Principles
   - Challenges: The RS Borgman's conundrum challenges
5. Conclusions

Concept: software or computer program as a legal object

(2010, 2015) TGD. Article vs. Logiciel : questions juridiques et de politique scientifique dans la production de logiciels
(2022) TGD, T. Recio. Research Software vs Research Data I (Definition, Conundrum)

- [EC] Directive 2009/24/EC, 23/04/2009, On the legal protection of computer programs

  For the purpose of this Directive, the term **computer program** shall include programs in any form, including those which are incorporated into hardware.

  This term also includes *preparatory design work* leading to the development of a computer program provided that the nature of the preparatory work is such that a computer program can result from it at a later stage.

- [ES] Boletín Oficial del Estado, núm. 97, de 22 de abril de 1996, Ley de Propiedad Intelectual

  Artículo 10. Los **programas de ordenador** están incluidos en la lista de las creaciones originales literarias, artísticas o científicas que son objeto de propiedad intelectual.

  Artículo 96. A los efectos de la presente Ley se entenderá por **programa de ordenador** toda secuencia de instrucciones o indicaciones destinadas a ser utilizadas, directa o indirectamente, en un sistema informático para realizar una función o una tarea o para obtener un resultado determinado [...] comprenderá también su documentación preparatoria.

- [FR] Code de la propriété intellectuelle (CPI), Article L. 112-2 :

  un **logiciel** est une œuvre de l'esprit protégée par le droit d'auteur.

  Arrêté du Ministère de l'Industrie du 22 décembre 1981 (vocabulaire de l'informatique) :
  un **logiciel** est un ensemble des programmes, procédés et règles, et éventuellement de la documentation, relatifs au fonctionnement d'un ensemble de traitement de données.

Digital object: https://fr.wikipedia.org/wiki/Logiciel

– [FR] Les séquences d'instructions, appelées programmes, ainsi que les données du logiciel sont ordinairement structurées en fichiers.

– [EN] The sequences of instructions, called programs, and data included within the software are usually structured in files.

Challenge: the definition of Research Software (1/5)

(2007) TGD. Autour de la valorisation de logiciels développés dans un laboratoire de recherche
(2009) TGD. Guide laboratoire pour recenser ses développements logiciels
(2010, 2015) TGD. Article vs. Logiciel : questions juridiques et de politique scientifique dans la production de logiciels

Un logiciel du laboratoire *est un programme utile pour faire avancer la recherche qui a été produit avec la participation d'un membre du laboratoire.*

Il arrive souvent que des publications de recherche soient associées.

- goal: research, and sometimes the RS
- a member of the lab has participated in the code writing (idem publicaciones)
- the main production is the publication, the RS is an associated object

This vision has changed a lot since 2006...

(2019) TGD, T. Recio. On the evaluation of research software: the CDUR procedure

Research software (RS) *is a well identified set of code that has been written by a well identified research team. It is software that has been built and used to produce a result published or disseminated in some article or scientific contribution.*

Each RS encloses a set of files containing the source code and the compiled code. It can also include other elements as the documentation, specifications, use cases...

Challenge: the definition of Research Software (2/5)

- [2] (1994) Partha D, David PA: Toward a new economics of science

  there may be **important positive spillovers** *across projects in the form of "learning effects" [...] including the development of computer software for performing data processing, storage, retrieval and network transmission.*

- (2007) TGD. Autour de la valorisation de logiciels développés dans un laboratoire de recherche
  (2009) TGD. Guide laboratoire pour recenser ses développements logiciels
  (2010, 2015) TGD. Article vs. Logiciel : questions juridiques et de politique scientifique dans la production de logiciels

  logiciel du laboratoire tout programme utile pour faire avancer la recherche, qui a été produit avec la participation d'un membre du laboratoire. Il arrive souvent que des publications de recherche soient associées.

- [16] (2011) Kelly D: An Analysis of Process Characteristics for Dev. Scientific Soft.

  Scientific software is defined by (1) it is developed to answer a scientific question ; (2) it relies on the close involvement of an sientific expert ; and (3) it provides data to be examined by the person who will answer that question ...

- [18] (2012) Sletholt MT, Hannay JE, et al.: What Do We Know about Scientific Soft. Development's Agile Practices?

  software developed by scientists for scientists

- [19] (2016) Hettrick S: Research Software Sustainability, Knowledge Exchange Report

  Research software is developed within academia and used for the purposes of research: to generate, process and analyse results. This includes a broad range of software, programs written by researchers for their own use.

- [10] (2018) NASA Committee: Open Source Software Policy Options for NASA Earth and Space Sciences

  Research software – that is, the software that researchers develop to aid their science...

Challenge: the definition of Research Software (3/5)

- [16] (2011) Kelly D: An Analysis of Process Characteristics for Dev. Scientific Soft.
  - **exclusion** of what can be included in other definitions:

    [...] control software whose main functioning involves the interaction with other software and hardware ; user interface software [...] ; and any generalized tool that scientists may use in support of developing and executing their software, but does not of itself answer a scientific question.

  - importance of the **correctness** of the results:

    If the software gives the wrong answer, all other qualities become irrelevant.

- (2010, 2015) TGD. Article vs. Logiciel : questions juridiques et de politique scientifique dans la production de logiciels
  - definitions don't take care about the **status** of the software:

    "project", "ended", disseminated, quality, scope, size, documented, maintained, team's internal use for an article, currently used in several labs...

(2019) TGD, T. Recio. On the evaluation of research software: the CDUR procedure

Conclusion of RS definition:

- what is done: code, software as a well identified set of files,
- who does it: author(s), but also contributors or scientific expert(s),
- to make what: research, science, that is, associated articles,
- **important:** quality and correctness of the produced scientific results.

Challenge: the definition of Research Software (4/5)

- **Software** is a legal concept: Directive 2009/24/EC of the European Parliament & Council 23/04/2009, https://eur-lex.europa.eu/eli/dir/2009/24/oj

- Research Data Alliance FAIR 4 Research Software (FAIR4RS) working group,
  https://www.rd-alliance.org/groups/fair-research-software-fair4rs-wg

- (2021) Gruenpeter, M. et al. Defining Research Software: a controversial discussion
  https://doi.org/10.5281/zenodo.5504016

  Research Software includes source code files, algorithms, scripts, computational workflows and executables that were created during the research process or for a research purpose. Software components (e.g., operating systems, libraries, dependencies, packages, scripts, etc.) that are used for research but were not created during or with a clear research intent should be considered software in research and not Research Software. This differentiation may vary between disciplines. The minimal requirement for achieving computational reproducibility is that all the computational components (Research Software, software used in research, documentation and hardware) used during the research are identified, described, and made accessible to the extent that is possible.

- (2022) Collège Codes sources et logiciels
  Le logiciel de recherche, un pilier de la recherche scientifique ouverte
  https://www.ouvrirlascience.fr/le-logiciel-de-recherche-un-pilier-de-la-recherche...

  Les logiciels de recherche sont développés pour répondre à des besoins spécifiques de la science. Ils sont conçus, maintenus, et utilisés par des scientifiques (chercheurs et ingénieurs) et institutions de recherche, éventuellement dans une dimension internationale. Ils peuvent découler de travaux de recherche comme ils peuvent les favoriser, notamment par des publications avant/sur/autour/avec le logiciel. Ceux-ci peuvent se formaliser de différentes façons (une plateforme, un intergiciel, un workflow ou une bibliothèque, module ou greffon d'un autre logiciel) et être ainsi en interaction dans un écosystème ou au contraire plus autonomes.

Challenge: the definition of Research Software (5/5)

Comparison framework of three definitions in ten points:

	D1-COSO	D2-RDA	D3-CDUR
Cadre d'élaboration de la formulation :			
- équipe	nationale	internationale	internationale
- nb. de personnes	?	21	2
- type de publication	article	preprint	article, avec *open peer review*
- nb. de références	2	18	22
Qualité de la formulation	faible	faible	forte
Compréhension de l'objet numérique	faible	forte	forte
Compréhension de la production scientifique	forte	forte	forte
Compréhension de l'objet juridique	faible	faible	forte
Réponses aux *conundrum challenges*	partielles	partielles	complètes
Compréhension de *données de la recherche*	faible	faible	forte

(2026) TGD, T. Recio, Research software, qui es-tu ? Une conversation scientifique et juridique sur les logiciels...

Challenge: RS dissemination

Easy to adapt to many situations, also valid for (research) data.

- Choose a name, avoid trademarks and proprietary names, associate date, version...
  Harvard, File Naming Conventions
- (*) (research team step) Establish list of authors/contributors (% participation, affiliations). Consider a Software Management Plan (2018, TGD, G. Romier, PRESOFT V3.2)
- (*) Establish the list of main functionalities.
- (*) Establish the list of included software & data components, their licences
- **Choose a licence**, have an agreement (signed) with rightholders and authors, consider FLOSS licences. Beware of licence compatibility and inheritance issues.
- Choose a website, forge, deposit for dissemination, indicate licences and how to cite the work. Use persistent identifiers (PIDs) if possible.
- (*) Archive a tar.gz or similar regularly to keep track of added functionalities.
- Inform your laboratories and head institutions (if not done in the licence step).
- Set and indicate clearly a contact address, and a citation form.
- **Distribute** your (research) software or data component.
- Inform the target scientific community. Consider Software or Data papers...

(*) To be reviewed with each new version.

(2014) TGD. Free software, Open source software, licenses. A short presentation including a procedure for research software ...
(2022) TGD, T. Recio. Research Software vs Research Data II (Dissemination, CDUR, FAIR)
(2025) TGD, T. Recio. Perceptions on the adoption of Free/Open Source Software policies by a Scientific Institution

Challenge: questions about the legal & scientific production contexts

Licences !

(2009) JL Archimbaud, TGD. Licence & copyright pour les développements de logiciels libres de laboratoires de recherche

In order to understand and to explain the bases of (French) copyright issues, the chain of decisions and the scientific policy issues related to RS we have used comparative methods with the main scientific production: the articles.

(2009) TGD. Guide laboratoire pour recenser ses développements logiciels
(2010, 2015) TGD. Article vs. Logiciel : questions juridiques et de politique scientifique dans la production de logiciels

Aspects légaux		
	Article	**Logiciel**
Droit auteur	droits moraux, droits patrimoniaux	droits moraux réduits droits pat. dévolus à l'employeur
Œuvre	article	code source, code objet, doc., ...
Auteurs	signataires, même %	notion complexe, pb. légal, établir % de participation
Propriétaires	auteurs, même % cession des droits	tutelles en général, mais dépend du régime salarié, des contrats, ...
Dates	soumission, publication	matériel de conception, versions
Évolution	œuvre indépendante	œuvre indépendante ? il faut revoir auteurs, dates, lic., ...
Travaux préc.	références, citations	briques : compatibilité, héritage lic.
Diffusion	éditeur, web	web, forges, besoin de licence
Droits	lire, citer, ne pas copier	lire, ne pas utiliser, ..., besoin lic.
Licences	droits et obligations, CC (web)	droits et obligations, libres, propriétaires

Aspects relatifs à la politique scientifique		
	Article	**Logiciel**
Définition (L, T)	ok	à définir
Signature (C, T)	ok, déf. par tutelles	à définir (copyright) associer les laboratoires
Références (L, T)	HAL	PLUME
Liste des œuvres (L, T)	document à jour	document inconnu, PLUME peut être utile
Libre accès (C, L, T, CSI)	politique (+/-) ok, dépôt ok (HAL)	politique (lic.) à définir, dépôt à établir
Validation (C, L, T, CSI)	procédure *referee*, reproductibilité	à définir, validé au sens PLUME
Qualité/évaluation (C, L, T, CSI)	nb. citations	articles associés, attirer utilisateurs, contrats
Motivation (C, L, T, CSI)	recherche, article	recherche, pas le logiciel
Objet (C, L, T, CSI)	scientifique	3D : scientifique, potentiel de transf. de tech., obj. industriel

(2010) https://doi.org/10.5281/zenodo.7063153

(2015) https://doi.org/10.48556/SIF.1024.5.119, https://doi.org/10.5281/zenodo.18993

Most of the references included at the end of the talk deal with legal and scientific policies

Concept: RS authors

(2010, 2015) TGD. Article vs. Logiciel : questions juridiques et de politique scientifique dans la production de logiciels

What means RS author?

- legal concept: the author writes the code
- scientific concept: expert contributions, maybe no writing code

  without the scientific expert, the RS will not exist
- maybe other contributions:

  documentation, bug fixing, test, maintenance, translations...

(2019) TGD, T. Recio. On the evaluation of research software: the CDUR procedure

Definition of a RS author:

- in the article we select three rôles (limits can be fuzzy):
  - (i) RS leader,
  - (ii) main or important contributor (code writing),
  - (iii) minor contributor (code writing or other contribution).

Persons with no code writing can be assigned with some **participation percentage** of code writing by the team.

Publications on RS / RS Papers

On the current situation regarding RS papers, some may have *software peer review*.

- Journal of Open Research Software (JORS)
- The Journal of Open Source Software (JOSS)
- Research Ideas and Outcomes (RIO)
- Software Impacts
- SoftwareX
- also: (2010) Image Processing On Line Journal (IPOL), see, for example,
  P. Monasse, Extraction of the Level Lines of a Bilinear Image, IPOL 2019,
  article + RS + data: https://www.ipol.im/pub/art/2019/269/

See N. Chue Hong list at Software Sustainability Institute (SSI)

https://www.software.ac.uk/resources/guides/which-journals-should-i-publish-my-software

France, CNRS PLUME Project (2006-2013), https://doi.org/10.5281/zenodo.2591473:

- publication of RELIER "RS description cards", with links to articles,
  stats: 358 RS in French, where 116 also presented in English
- publication of "validated softw. cards in the sense of PLUME", stats: 96 RS out of 406
- no *software peer review*
- **theme classification, keywords, search interfaces**

Referencing and citation issues

(2019) TGD, T. Recio. On the evaluation of research software: the CDUR procedure

[39] (2013) Pontille D, Torny D: La manufacture de l'évaluation scientifique ...

> *[...] the difference between reference and citation: the act of reference is the responsibility of a given author while the citation is a new property, possibly calculable, of the source text. According to P. Wouters (1999), this reversal has radically altered the practice of referral and has literally created a new "culture of citation".*

A reference **sets** title, author(s), date, and identifies RS as a scientific object.

The article considers three different types of reference:

- the one related to the RS paper (maybe with *software peer review*),
- the one related to a classic research article describing the RS,
- a "reference": author(s), RS title, short description, version, date, url.

Remarks:

- There can be several references associated to a RS.
- There are more complete identifications: metadata, CITATION files...
- Software Citation Group, Software Citation Implementation Working Group...

Plan

Evaluation contexts in Research

Research evaluation contexts appear all along the research life:

- PhD, recruitment, career evolution,
- articles, publications, *peer review*
- participation to conferences, workshops, (selection)
- project funding: call answer, stages, end of the project
- setting collaboration networks, usually in an international context

In general, the first evaluation coming into play: **self evaluation**.

Any dissemination has its own goals and a target public:

- this result will be in a preprint or a journal article?
- this project will be funded? should I ask it this year?
- these researches will collaborate in this project or publication?
- the decisions evolve in time, following research evolution, but also when facing a new evaluation settings, for example I need more articles...

Two evaluation methods

(2019) TGD, T. Recio. On the evaluation of research software: the CDUR procedure

Roughly speaking, there are two evaluation methods:

[8] (2016) Mårtensson P, Fors U, et al.: Evaluating research: A multidisciplinary approach to assessing research practice and quality (62 references)

- the **quality** method: what criteria?
- the **quantity** method, with indicators, metrics: which ones?
  - impact factor metrics should be used with careful attention [11, 39, 51, 52, 53, 54]
- *the social factor*

  [55] (1999) Martin U: Computers, Reasoning and Mathematical Practice

  [...] the community's "social knowledge":
  the methods of checking the proof are social rather than formal.

See the "EC Expert reports" [9, 11]:

- plenty of recommandations, do take into account RS
- [9] Open Science Career Assessment Matrix (OS-CAM)
- [11] how to establish evaluation commitees

CDUR Protocol(s): Research evaluation and RS

(2019) TGD, T. Recio. On the evaluation of research software: the CDUR procedure
(2022) TGD, T. Recio. Research Software vs Research Data II (Dissemination, CDUR, FAIR)

Designed to help evaluated researchers, evaluation committees, decision makers...
also valid for (research) data.

(C) Citation measure if RS is well identified as a research output:
good citation form, but also metadata, best citation practices...
Legal point: authors, affiliations, % of participation

(D) Dissemination best dissemination practices, in agreement with
the scientific policy of the evaluation context
Policy point: Open Science, **legal point:** licences

(U) Use "software aspects" **of RS**: correct results, facilitate reuse, good softw.
practices: doc, test, install, up to read the code, launch RS...
Reproducibility point: validation of scientific results

(R) Research "research aspects": quality of the scientific work, proposed and coded
algorithms & data structures, related publications, collaborations...
Research point: impact

Flexibility of application: each decision maker or evaluation committee **sets its own CDUR protocol** adapted to the evaluation context and goals.

CDUR vs The FAIR Guiding Principles

(2022) TGD, T. Recio. Research Software vs Research Data II (Dissemination, CDUR, FAIR)

(2023) TGD, T. Recio. How to achieve FAIRER research data by studying evaluation assessment protocols, Open Science FAIR

CDUR [2,7]	**The FAIR Guiding Principles** [1]
(C) Citation: The RD is well identified, involving issues concerning: - citation form or reference - metadata (including PIDs)	**To be Findable:** F1. (meta)data are assigned a globally unique and persistent identifier F2. data are described with rich metadata (defined by R1 below) F3. metadata clearly and explicitly include the identifier of the data it describes **To be Interoperable:** I3. (meta)data include qualified references to other (meta)data **To be Reusable:** R1.2. (meta)data are associated with detailed provenance
(D) Dissemination: The RD is well disseminated, involving issues concerning: - list of included components - RD licence - RD deposit	**To be Findable:** F4. (meta)data are registered or indexed in a searchable resource **To be 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 **To be Reusable:** R1.1. (meta)data are released with a clear and accessible data usage license
(U) Use: The RD facilitates its reuse, involving issues like: - documentation, tutorials, examples... - reproducibility and replicability issues	**To be Interoperable:** I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation I2. (meta)data use vocabularies that follow FAIR principles **To be Reusable:** R1. meta(data) are richly described with a plurality of accurate and relevant attributes R1.3. (meta)data meet domain-relevant community standards
(R) Research: Measures the impact of the RD related scientific work	Not applicable

Table 1. Relationships between the FAIR principles and the CDUR evaluation protocols.

Borgman's conundrum challenges for RS + How? + Where?

Answers inform policy makers and research funders

(1997) National Research Council. Bits of Power: Issues in Global Access to Scientific Data
(2012) Christine L. Borgman. The conundrum of sharing research data.
(2022) TGD, T. Recio. Research Software vs Research Data I (Definition, Conundrum)
(2024) TGD, T. Recio. The Conundrum Challenges for Research Software in Open Science

Which RS to be shared? It is a Team decision about the RS to be shared, which version, in which form, and when. This may be a complex decision:

which components, which versions to share, to share early versions or not, experimental branches or not...

By whom? The RS production Team who is involved in the development, its documentation, its maintenance... and that has decided to share & disseminate the RS

How? Following a dissemination procedure like the one proposed here

Where? The RS can be shared in repositories like Zenodo, in forges like GitHub, or in institutional repositories, in web pages (personal, project...)

With whom? Each scientific communication act has its own target public, initially it can be the one of the associated publications, but there is maybe some interdisciplinary value, so...

(2012) *... intended users may vary from researchers within a narrow specialty to the general public...*

Under what conditions? The licence gives the RS sharing conditions

Why, and to what effects? to answer funding demands (institution, project funding...), to follow Open Sciences policies and/or best practices, for validation and reproduction of published results... research evaluation...

(1997) **The value of data lies in their use.**

Conclusions

We have built a framework to study Research Software, to understand and to explain some challenges that appear in their production in a scientific context, mainly regarding their definition, dissemination, and evaluation.

We have proposed some solutions for these challenges, as for example the CDUR evaluation protocols, and complete answers to the *Borgman's conundrun challenges*.

Our goal is to provide elements of reflection to contribute to the construction of the Open Science landscape. **To advance** in the improvement and adoption of best Open Science practices, and, in particular, of best RS practices,

it is necessary to change and develop evaluation methods.

Expected consequences, in agreement with [11] (2019) Guédon JC, Jubb M, et al. *"world brain vision"*:

- maximize: RS visibility, accessibility and usability,
- support and expand range of contributions (equity, diversity, inclusivity criteria),
- support community building, and
- promote high-quality research with heightened integrity...

... but also to increase transparency in RS evaluation methods and to contribute to strengthen the RS pillars: (2020) J. Cohen et al., The four pillars of research software engineering

[4] (2016) Howison J, Bullard J: Software in the scientific literature (p.15):

Clearly, a policy is only as good as its enforcement.

Sincere thanks to...

- Tomas Recio, https://personales.unican.es/reciot/
- Jeremy Cohen, Peter Schmidt, and the STEP-UP team of the STEP-UP project, https://step-up.ac.uk/about/team/
  https://step-up.ac.uk/events/20260617-seminar/
- Sofía Miñano and Carlos Gavidia-Calderón for "Charlas RSE en español", https://charlas-rse-espanol.github.io/
- my research lab, the LIGM,
  https://ligm.univ-eiffel.fr
- Peter Schmidt for *"Code for Thought"* podcasts
  https://codeforthought.buzzsprout.com/
- and to you, listening here...

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100%
Open access

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