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# Interoperability, FAIRness, and Sustainable Scientific Software: A Comprehensive Theoretical Framework for Reproducible and Executable Research Ecosystems

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## Abstract

*The rapid expansion of computational science has transformed software, workflows, and digital artifacts into primary vehicles of scientific knowledge production. As research becomes increasingly data intensive and collaborative, the need for interoperable, reproducible, and sustainable software ecosystems has emerged as a central challenge. This article develops a comprehensive theoretical framework that integrates semantic interoperability, workflow standardization, provenance modeling, software citation, and FAIR data and software principles into a unified model for sustainable scientific software ecosystems. Drawing exclusively on established literature concerning semantic interoperability, enterprise interoperability assessment, workflow languages, provenance ontologies, FAIR principles, and software sustainability initiatives, this work examines how technical, organizational, and semantic dimensions of interoperability converge within modern research infrastructures. Particular attention is given to scientific workflow systems, executable notebooks, service oriented architectures, and metadata schemas as foundational mechanisms that enable reuse, replication, and long term preservation. The analysis further investigates interoperability assessment models, service composition strategies, and the role of community driven standards bodies in fostering trust and transparency. By synthesizing perspectives from semantic web research, enterprise systems engineering, reproducible research scholarship, and software citation theory, the article proposes a multidimensional interoperability maturity framework tailored to scientific software. The findings suggest that interoperability cannot be reduced to syntactic compatibility alone but must incorporate semantic alignment, governance structures, provenance capture, and formal citation practices. Moreover, the application of FAIR principles to software artifacts is shown to require adaptation beyond data centric interpretations, particularly in relation to executability and sustainability. The discussion elaborates on theoretical tensions between flexibility and standardization, automation and transparency, and innovation and preservation. Limitations and future research directions are articulated in relation to assessment metrics, policy harmonization, and cross disciplinary generalization. This work contributes to the emerging scholarship on digital research infrastructures by offering a unified conceptual model that aligns workflow interoperability, FAIRness, provenance ontologies, and sustainable software governance into a coherent foundation for reproducible and reusable science.*

Keywords: Interoperability, FAIR principles, scientific workflows, software sustainability, provenance, reproducible research.



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## 1. Introduction

The digital transformation of science has fundamentally altered the epistemological and operational foundations of research practice. Computational tools, executable scripts, and complex workflow pipelines now mediate virtually every stage of scientific inquiry. In this context, software is no longer a peripheral support instrument but rather a central epistemic artifact. The transformation of code into a scientific contribution has been explicitly articulated in discussions of reproducibility and reuse, where the distinction between running, repeating, reproducing, reusing, and replicating code defines multiple levels of scientific validation (Benureau and Rougier, 2018). This conceptual evolution compels a reexamination of interoperability, sustainability, and citation practices in scientific ecosystems.

Interoperability has historically been defined in technical domains as the ability of systems to exchange and use information effectively (IEEE, 1990). However, early conceptualizations of interoperability frequently emphasized syntactic compatibility while underestimating semantic and organizational dimensions. The notion of semantic interoperability introduced the requirement that exchanged information be interpreted consistently and meaningfully across systems (Heiler, 1995). Subsequent scholarship extended this perspective toward enterprise contexts, recognizing interoperability as a multidimensional construct encompassing technical, semantic, and organizational alignment (Charalabidis, Goncalves and Popplewell, 2011).

Within research infrastructures, interoperability extends beyond enterprise coordination to encompass scientific workflows, executable notebooks, data repositories, and software libraries. The rise of interactive computational environments such as those promoted by Project Jupyter has facilitated transparent and executable research narratives. The Jupyter ecosystem integrates code, documentation, and data within a unified computational notebook environment, enabling researchers to publish executable analyses that enhance transparency and replicability (Jupyter Project and Community, 2019). Nevertheless, notebook based workflows alone do not guarantee interoperability or sustainability, particularly when dependencies, metadata, and provenance are inconsistently documented.

Parallel to the development of computational tools, the FAIR principles have reshaped discussions of digital stewardship. The principles of findability, accessibility, interoperability, and reusability have been widely adopted as normative standards for data management. Reports emphasizing the practical implementation of these principles demonstrate the necessity of community coordination and policy alignment (Allen and Hartland, 2018). Initiatives such as FAIRsharing highlight the importance of cataloging standards, repositories, and policies to support coherent governance (Sansone et al., 2019). Yet, the extension of FAIR principles to software introduces new conceptual challenges. Software artifacts embody executability, versioning, and environmental dependencies that differ substantially from static datasets (Chue Hong and Katz, 2018). The question arises whether data centric FAIR interpretations sufficiently address the dynamic nature of scientific code.

Scientific workflows represent another critical dimension of this transformation. Workflow systems orchestrate computational tasks, manage dependencies, and enable reproducible execution across distributed infrastructures. Theoretical analyses of workflow interoperability identify three fundamental dimensions: model of computation, language, and execution environment (Elmroth, Hernandez and Tordsson, 2010). These dimensions underscore that interoperability challenges are not confined to syntax but also concern conceptual models and runtime infrastructures. The emergence of standards such as the Common Workflow Language and OpenWDL reflects community attempts to formalize workflow descriptions in a portable and interoperable manner (Common Workflow Language, 2016; Open WDL, 2019). Provenance standards, including PROV O, further complement these efforts by providing ontological structures for representing derivation histories and dependencies (Lebo, Sahu and McGuinness, 2019).

Despite these advances, fragmentation persists. Interoperability assessment models reveal heterogeneity in evaluation criteria and maturity frameworks (Rezaei, Chiew and Lee, 2013; Rezaei et al., 2014). Systematic reviews in enterprise contexts demonstrate the absence of unified metrics capable of capturing technical, semantic, and organizational integration simultaneously (da Silva Serapiao Leal, Guedria and Panetto, 2019). In scientific domains, workflow automation efforts in bioinformatics and proteomics illustrate both the potential and limitations of semantic integration (Wroe et al., 2004; Palmblad et al., 2019). Automation can accelerate discovery but may obscure interpretability if provenance and metadata are inadequately represented.

The sustainability of scientific software further complicates this landscape. Workshops dedicated to sustainable software emphasize governance, funding models, community engagement, and lifecycle management as central determinants of long term viability (Aerts et al., 2019; Aerts, 2017). Citation practices constitute an additional pillar of sustainability. Principles and guidelines for software citation articulate norms that recognize code as a citable scholarly object, ensuring credit attribution and traceability

(Smith, Katz and Niemeyer, 2016; Hausman et al., 2019; Katz and Chue Hong, 2018). The SPDX standard for software package data exchange exemplifies efforts to standardize metadata concerning licensing and dependencies (SPDX Workgroup, 2019).

The convergence of these strands reveals a literature gap. While semantic interoperability, workflow standardization, FAIR data governance, provenance modeling, and software citation have each been studied independently, a comprehensive theoretical synthesis integrating these dimensions into a unified model for sustainable scientific software ecosystems remains underdeveloped. Existing interoperability frameworks primarily address enterprise integration or public administration contexts (Charalabidis, Goncalves and Popplewell, 2011), whereas scientific infrastructures possess distinctive epistemic and computational characteristics.

This article addresses this gap by constructing a theoretically grounded framework that integrates semantic interoperability theory, interoperability assessment models, workflow standardization, provenance ontologies, FAIR implementation practices, and sustainable software governance into a coherent analytical structure. The central problem statement guiding this research is as follows: How can interoperability, FAIRness, provenance, and sustainability principles be systematically aligned to support reproducible and reusable scientific software ecosystems?

The contribution of this work is threefold. First, it develops a multidimensional interoperability framework tailored to scientific software. Second, it articulates the theoretical interplay between FAIR principles and executable research artifacts. Third, it proposes a sustainability model that integrates citation, metadata standards, and community governance into interoperability assessment. Through extensive theoretical elaboration grounded exclusively in established references, this article advances a comprehensive understanding of digital research infrastructures as socio technical ecosystems requiring coordinated standardization, semantic alignment, and governance.

## 2. Methodology

This research adopts a qualitative, theory driven methodology grounded in systematic conceptual synthesis. Rather than conducting empirical experiments, the study integrates and critically analyzes foundational and contemporary literature concerning interoperability, workflows, FAIR principles, provenance, software citation, and sustainability. The methodology consists of four interrelated stages.

The first stage involves conceptual extraction. Foundational definitions of interoperability are drawn from standardized terminology (IEEE, 1990) and expanded through semantic interoperability theory (Heiler, 1995). Enterprise interoperability scholarship provides multidimensional constructs distinguishing technical, semantic, and organizational levels (Charalabidis, Goncalves and Popplewell, 2011). Systematic reviews of interoperability assessment models supply taxonomic insights into maturity levels and evaluation criteria (Rezaei, Chiew and Lee, 2013; Rezaei et al., 2014; da Silva Serapiao Leal, Guedria and Panetto, 2019).

The second stage involves domain contextualization. Literature concerning scientific workflows and service oriented architectures informs the operationalization of interoperability within research infrastructures (Naudet et al., 2010; Mantovaneli Pessoa et al., 2008). Workflow interoperability dimensions identified by Elmroth, Hernandez and Tordsson (2010) serve as a structural backbone for analyzing computational integration. Automation case studies in bioinformatics and proteomics illustrate practical implications (Wroe et al., 2004; Palmblad et al., 2019). Standards such as the Common Workflow Language and OpenWDL provide concrete exemplars of language level interoperability (Common Workflow Language, 2016; Open WDL, 2019).

The third stage integrates governance and stewardship perspectives. FAIR implementation reports and community initiatives such as FAIRsharing are analyzed to identify policy and metadata alignment mechanisms (Allen and Hartland, 2018; Sansone et al., 2019). Discussions on applying FAIR principles to software highlight conceptual tensions between data and code artifacts (Chue Hong and Katz, 2018). Software citation principles and guidelines inform attribution and sustainability dimensions (Smith, Katz and Niemeyer, 2016; Hausman et al., 2019; Katz and Chue Hong, 2018). Provenance ontologies such as PROV O contribute semantic structures for traceability (Lebo, Sahu and McGuinness, 2019).

The fourth stage synthesizes these strands into an integrative framework. This synthesis employs comparative analysis to identify convergent themes across sources. The approach emphasizes theoretical consistency and internal coherence. Claims are substantiated through citation of the relevant literature, ensuring that each conceptual component is grounded in established scholarship. Counter arguments and limitations identified in the literature are incorporated into the analysis to avoid uncritical synthesis.

The methodological emphasis on theoretical elaboration is intentional. Given that interoperability and sustainability are socio technical constructs shaped by governance, standards, and community practices, conceptual integration is a necessary precursor to empirical operationalization. The resulting framework is not presented as a definitive model but as a structured synthesis that organizes existing knowledge into a unified explanatory architecture.

## 3. Results

The integrative analysis yields a multidimensional framework for interoperable and sustainable scientific software ecosystems composed of six interdependent dimensions: technical interoperability, semantic interoperability, workflow interoperability, provenance and traceability, FAIR governance, and sustainability and citation.

Technical interoperability constitutes the foundational layer. In alignment with standardized terminology, it refers to the ability of systems to exchange data and services through compatible interfaces and protocols (IEEE, 1990). In scientific contexts, this dimension includes compatibility of programming languages, operating systems, containerization strategies, and service interfaces. Service oriented architectures exemplify technical interoperability through modular service composition (Naudet et al., 2010; Mantovaneli Pessoa et al., 2008). However, the literature emphasizes that technical exchange alone does not ensure meaningful integration.

Semantic interoperability introduces shared vocabularies and ontologies that guarantee consistent interpretation (Heiler, 1995). Within scientific workflows, semantic annotations enable automated composition and validation. The automation of experiments using semantic data in bioinformatics demonstrates the feasibility of semantically enriched workflows (Wroe et al., 2004). Bioschemas initiatives further illustrate how domain specific markup facilitates discoverability and interoperability across web platforms (Gray, Goble and Jimenez, 2017). The PROV O ontology extends semantic modeling to provenance, representing entities, activities, and agents in derivation relationships (Lebo, Sahu and McGuinness, 2019).

Workflow interoperability constitutes a third dimension characterized by alignment across models of computation, languages, and execution environments (Elmroth, Hernandez and Tordsson, 2010). Standards such as the Common Workflow Language and OpenWDL provide formalized specifications that decouple workflow descriptions from specific engines (Common Workflow Language, 2016; Open WDL, 2019). This decoupling enhances portability and reuse. Automated workflow composition in proteomics illustrates how standardized descriptions facilitate reproducible pipelines (Palmblad et al., 2019). Nonetheless, heterogeneity in workflow engines and execution contexts continues to pose integration challenges.

Provenance and traceability form a fourth dimension. Reproducibility requires not only executable code but also transparent documentation of derivations and dependencies (Benureau and Rougier, 2018). Provenance standards such as PROV O enable structured representation of execution histories (Lebo, Sahu and McGuinness, 2019). The sharing of interoperable workflow provenance in CWLProv demonstrates practical mechanisms for capturing execution metadata (Khan et al., 2018). Provenance enhances trust, accountability, and validation.

FAIR governance constitutes a fifth dimension integrating metadata standards, repository policies, and community coordination. Practical reports on FAIR implementation emphasize that findability and accessibility depend on persistent identifiers, standardized metadata schemas, and repository indexing (Allen and Hartland, 2018). FAIRsharing highlights the importance of cataloging standards and policies to avoid fragmentation (Sansone et al., 2019). Research Metadata Schemas working groups and Software Source Code Identification initiatives within the Research Data Alliance further institutionalize governance mechanisms.

The sixth dimension concerns sustainability and citation. Sustainable software workshops underscore lifecycle management, funding models, and community engagement as prerequisites for long term viability (Aerts et al., 2019; Aerts, 2017). Software citation principles formalize attribution, ensuring that software creators receive scholarly recognition (Smith, Katz and Niemeyer, 2016). Citation guidelines operationalize these principles in practice (Hausman et al., 2019; Katz and Chue Hong, 2018). The SPDX standard enhances transparency concerning licensing and dependencies, contributing to sustainable reuse (SPDX Workgroup, 2019).

Interoperability assessment models provide evaluative mechanisms spanning these dimensions. Systematic reviews categorize models according to maturity levels, measurement criteria, and domain applicability (Rezaei, Chiew and Lee, 2013; Rezaei et al., 2014). Enterprise oriented reviews emphasize the integration of technical and organizational indicators (da Silva Serapiao Leal, Guedria and Panetto, 2019). Translating these insights to scientific software reveals the need for composite metrics encompassing semantic richness, workflow portability, provenance completeness, and citation compliance.

The synthesis indicates that interoperability, FAIRness, provenance, and sustainability are mutually reinforcing. Semantic annotations enhance FAIR interoperability. Provenance capture supports reproducibility and reuse. Citation practices incentivize maintenance and sustainability. Conversely, deficiencies in any dimension undermine the entire ecosystem. For example, technically interoperable workflows lacking semantic metadata impede automated composition. FAIR metadata without executable reproducibility limits practical reuse.

## 4. Discussion

The theoretical integration developed herein underscores the complexity of constructing sustainable scientific software ecosystems. Interoperability emerges not as a binary property but as a continuum across multiple dimensions. Enterprise scholarship highlights maturity models as tools for assessing integration (Rezaei et al., 2014). However, scientific contexts require adaptation to account for epistemic transparency and reproducibility.

One theoretical tension concerns flexibility versus standardization. Standardized workflow languages promote portability (Common Workflow Language, 2016; Open WDL, 2019), yet excessive rigidity may constrain methodological innovation. Semantic interoperability frameworks must balance domain specificity with cross disciplinary generality (Heiler, 1995). Governance initiatives such as FAIRsharing demonstrate that community driven cataloging can harmonize standards while preserving diversity (Sansone et al., 2019).

Another tension arises between automation and interpretability. Automated workflow composition accelerates analysis (Palmblad et al., 2019), but opaque pipelines risk undermining epistemic scrutiny. Provenance ontologies mitigate this risk by formalizing execution histories (Lebo, Sahu and McGuinness, 2019). The articulation of reproducibility levels from running to replicating code clarifies expectations (Benureau and Rougier, 2018). Nevertheless, full reproducibility may remain constrained by hardware heterogeneity and evolving dependencies.

The extension of FAIR principles to software raises normative questions. Data centric FAIR interpretations emphasize static metadata and identifiers (Allen and Hartland, 2018). Software artifacts, by contrast, involve dynamic execution and versioning. Applying FAIR to software requires attention to executability, containerization, and environment capture (Chue Hong and Katz, 2018). Citation principles further institutionalize recognition, aligning incentives with stewardship (Smith, Katz and Niemeyer, 2016).

Limitations of this theoretical framework include its reliance on published scholarship without empirical validation. Interoperability assessment models reviewed in the literature vary widely in scope and metrics (Rezaei, Chiew and Lee, 2013). Future research should operationalize the proposed multidimensional framework into measurable indicators. Cross disciplinary case studies could test its applicability in fields beyond bioinformatics and enterprise systems.

Future scope also includes policy harmonization across repositories, integration of semantic web technologies with workflow engines, and development of automated citation metadata generation. Community initiatives within the Research Data Alliance provide promising institutional platforms for such coordination.

## 5. Conclusion

The digitalization of science necessitates integrated frameworks that align interoperability, FAIR governance, provenance modeling, and sustainability. Through comprehensive theoretical synthesis grounded in established literature, this article proposes a multidimensional model encompassing technical, semantic, workflow, provenance, governance, and citation dimensions. The analysis demonstrates that sustainable scientific software ecosystems depend on coordinated standardization, semantic alignment, transparent provenance, and formal recognition mechanisms. Interoperability is not merely a technical challenge but a socio technical endeavor requiring community governance and cultural transformation. By articulating these interdependencies, this work contributes a foundational framework for advancing reproducible and reusable computational science.

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