International Journal of Applied Mathematics
Volume 38 No. 9s 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

TAGIT++: A Mathematical and Algorithmic Framework for AI-Enhanced Metadata Management in Federated Scientific Collaboration

Sonali Vidhate[1] , Dr.Pankaj Dashore [2]

[1] ,Research Scholar at Sandip University
Asst. Prof at MET Bhujbal Knowledge City , Nashik, India

e-mail: sonali.vidhate878@gmail.com

[2] Associate Professor at Sandip University, Nashik, India
e-mail: dashorepankaj@gmail.com

Abstract

In large-scale scientific collaborations, metadata serves as a mathematical abstraction that connects datasets across distributed infrastructures. Traditional centralized indexing systems exhibit suboptimal performance when query complexity and data heterogeneity increase. This study introduces TAGIT++, a mathematical and algorithmic framework designed to model and optimize metadata management in federated environments using artificial intelligence. The framework defines metadata discovery as an optimization problem, where latency L(q) and overhead O(m) are

Received: August 08, 2025

International Journal of Applied Mathematics
Volume 38 No. 9s 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

minimized under federated constraints F=S1,S2,...,Sn. TAGIT++ employs semantic clustering and AI-driven tagging functions, formulated as T(mi)=f(Ci), to enrich metadata with contextual relevance. Distributed indexing and federated query routing are represented through a cost function C(q)=ni=1 wid(q,Si), optimized for minimum query propagation delay. Security and audit integrity are mathematically modeled using a blockchain-based verification function V(t)=h(opData). Experimental validation on real-world climate and genomic datasets demonstrates a tenfold reduction in latency and 70 percent improvement in metadata efficiency compared to existing frameworks such as GUFI and SCISPACE. TAGIT++ thus integrates mathematical modeling, artificial intelligence, and federated computation to create an optimized, secure, and semantically enriched metadata environment for scientific collaboration.

Math. Subject Classification: 00A69, 00A71

Key Words: Applied Mathematics, Optimization, AI Tagging, Federated Systems, Metadata Modeling, Distributed Indexing, Blockchain Security

1 INTRODUCTION

The rapid growth of scientific data across disciplines such as climatology, genomics, and astrophysics has introduced unprecedented challenges in the management, discovery, and governance of metadata across federated research infrastructures. Metadata, defined as the descriptive layer that characterizes datasets, enables researchers to locate, interpret, and reuse data efficiently. However, as datasets become distributed across multiple institutions and cloud systems, traditional metadata models—primarily centralized or schema-based—exhibit limitations in scalability, query efficiency, and compliance.

In such environments, the mathematical representation of metadata operations becomes essential. Each dataset S_i is associated with a corresponding metadata vector M_i that contains both syn-

Received: August 08, 2025

International Journal of Applied Mathematics
Volume 38 No. 9s 2025
ISSN: 1311-1728 (printed version); ISSN: 1314-8060 (on-line version)

tactic and semantic descriptors. The task of discovering relevant datasets for a given query q can thus be expressed as an optimization problem that minimizes semantic distance while maintaining balanced computational overhead. The query latency function may be modeled as:

$$L(q) = \sum_{i=1}^{n} w_i \cdot d(q, S_i), \tag{1}$$

where $L(q)$ denotes total latency, w_i represents the relevance weight of the i^{th} site in the federation, and $d(q, S_i)$ quantifies the semantic distance between the query and dataset metadata. The primary objective of this framework is to minimize $L(q)$ while simultaneously constraining metadata enrichment cost C_e and security overhead C_s:

$$\min L(q) \quad \text{subject to} \quad C_e + C_s \leq \epsilon, \tag{2}$$

where ϵ represents the permissible operational limit for performance loss due to enrichment and audit mechanisms.

Existing systems such as **GUFI** (Kuhn et al., 2019) and **SCISPACE** (Ahmed et al., 2020) have contributed to distributed indexing and cross-site data access but lack an analytical foundation for modeling metadata operations as optimization functions. Their architectures remain primarily algorithmic rather than mathematical, limiting their ability to provide predictive insights into query complexity, indexing costs, and semantic scalability.

The proposed **TAGIT++** framework bridges this gap by establishing a mathematical formalization of metadata dynamics within federated scientific infrastructures. The system integrates applied mathematical concepts from graph theory, optimization, and similarity analysis to quantify the relationships between query cost, semantic distance, and security compliance. It defines a multidimensional optimization problem that balances three competing objectives:

Received: August 08, 2025

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Volume 38 No. 9s 2025
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1. **Performance** — minimizing query latency and communication overhead.
2. **Semantic enrichment** — maximizing relevance and contextual accuracy through AI-based tagging functions.
3. **Security and compliance** — ensuring data integrity and traceability using blockchain-based audit trails.

By translating the operational behaviors of federated metadata systems into measurable mathematical expressions, TAGIT++ allows analytical reasoning, convergence evaluation, and performance prediction without relying solely on empirical testing. This mathematical modeling provides a unifying foundation for understanding distributed metadata processes and optimizing them through precise, quantifiable parameters.

2 Related Work

The study of metadata management in distributed and federated systems has been explored through several notable frameworks, each of which may be characterized by its underlying mathematical model and algorithmic limitations.

2.1 Centralized Indexing Approaches

Frameworks such as GUFI [3] employ a per-directory SQLite indexing scheme, which can be formally represented as a set of local mappings:

$$I : F \to A, \quad f \mapsto (|f|, t(f), p(f)), \tag{3}$$

where F is the file namespace and A denotes the set of basic file attributes (size, timestamp, path). GUFI achieves high single-node query performance with time complexity $O(\log |F|)$ for local

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lookups. However, since discovery across multiple institutions requires cross-domain searches, the global query cost scales as:

$$C_{\text{GUFI}}(q) = O(m \cdot \log |F|), \tag{4}$$

where m is the number of administrative domains. This linear factor in m makes the system unsuitable for federated collaborations.

2.2 Virtualization-Based Federated Models

SCISPACE [1] introduces a unifying query interface over multiple file systems. This can be modeled as a virtual mapping:

$$V : \bigcup_{i=1}^{m} F_i \to A, \tag{5}$$

where each F_i denotes the namespace of site i. While virtualization reduces schema heterogeneity, its reliance on logically centralized metadata services introduces a bottleneck. If Q denotes the set of concurrent queries, then the expected query latency scales as:

$$L(Q) = O(|Q| \cdot \alpha), \tag{6}$$

with α being the central processing overhead. As $|Q|$ grows, the system experiences bottlenecks, leading to quadratic slowdowns in practice.

2.3 Compact Indexing Strategies

MIQS [2] addresses scalability using Bloom filters and content signatures. If each file $f \in F$ is represented by a signature $s(f) \in \{0,1\}^k$, then membership queries are executed in $O(1)$ time with false positive rate:

$$P_{\text{fp}} = \left(1 - e^{-\frac{kn}{m}}\right)^k, \tag{7}$$

where $n = |F|$ and m is the filter size. While efficient in existence checks, the lack of semantic descriptors restricts its utility in scientific discovery where queries often depend on domain-specific attributes.

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2.4 Federated Coordination Models

UniIndex [4] introduces a logically federated index $I = \bigcup_{i=1}^{m} I_i$ that coordinates query processing across multiple storage systems. Query overhead is reduced to:

$$C_{Uni}(q) = O(\log n + \log m),$$

where n is the dataset size per site and m the number of federated sites. However, UniIndex lacks semantic enrichment and compliance-aware access control, leading to gaps in governance and precision.

2.5 Surveys and Research Gaps

Two major surveys [5, 7] highlight that existing systems optimize either scalability or semantics, but rarely both. Mathematically, this trade-off can be expressed as:

$$\max S(q) \text{ s.t. } C(q) \leq \beta$$

where $S(q)$ represents semantic coverage and $C(q)$ denotes query cost. This balance remains unsolved in current literature. Furthermore, security mechanisms such as blockchain-based auditing [15, 19] are often treated as auxiliary components rather than integrated primitives.

3 Methodology

3.1 Data and Metadata Model

The global dataset is defined as:

$$D = \bigcup_{i=1}^{m} D_i,$$

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where D_i is the dataset at site $i \in \{1, \ldots, m\}$. Each dataset entry $d \in D_i$ is associated with metadata attributes:

$$M(d) = \{a_1(d), a_2(d), \ldots, a_k(d)\}.$$

The AI tagging function is represented as:

$$f_\theta : D \to T, \quad d \mapsto f_\theta(d),$$

where T is the space of semantic tags, and f_θ is parameterized by a neural model such as BERT. Enriched metadata is:

$$\hat{M}(d) = M(d) \cup f_\theta(d).$$

3.2 Semantic Indexing

Each site maintains a semantic index:

$$I_i : T \to 2^{D_i}, \quad t \mapsto \{d \in D_i \mid t \in \hat{M}(d)\}.$$

The retrieval complexity per site is:

$$C_{index}(q) = O(\log |D_i|).$$

3.3 Federated Query Routing

Queries are represented as vectors in a semantic space:

$$v(q) = Embed(q) \in R^d.$$

Each site i maintains a tag vector T_i, representing its centroid. Routing is defined as:

$$R(q) = \{i \mid \cos(v(q), T_i) \geq \delta\},$$

where $\delta \in [0, 1]$ is the similarity threshold. Expected routing cost:

$$C_{route}(q) = O(\log m).$$

Algorithm 1: Query Routing

Received: August 08, 2025

International Journal of Applied Mathematics
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1. Input: Query q, site vectors $\{T_1, \ldots, T_m\}$, threshold δ
2. $v \leftarrow Embed(q)$
3. $R \leftarrow \emptyset$
4. For each $i = 1$ to m, if $\cos(v, T_i) \geq \delta$, then $R \leftarrow R \cup \{i\}$
5. Return R

3.4 Secure Logging and Access Control

Each operation is modeled as a transaction:

$$Tx = \{u, op, r, t, h(op, r)\},$$

where u is user ID, op operation type, r resource, t timestamp, and $h(\cdot)$ cryptographic hash. Blockchain ledger:

$$B = \langle Tx_1, Tx_2, \ldots, Tx_n \rangle.$$

Access control policy:

$$\Phi : U \times R \to \{0, 1\}, \quad \Phi(u, r) = 1 \text{ iff user } u \text{ has access.}$$

3.5 Complexity Analysis

Tagging: $O(|D_i| \cdot d)$,
Routing: $O(\log m)$,
Audit Logging: $O(1)$ per transaction.

Overall query cost:

$$C_{TAGIT++}(q) = O(\log n + \log m).$$

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4 Implementation

4.1 Architecture Overview

TAGIT++ is implemented as a microservices-based system, with containerized services communicating through RESTful APIs over HTTPS. Metadata exchange uses JSON-LD for semantic interoperability.

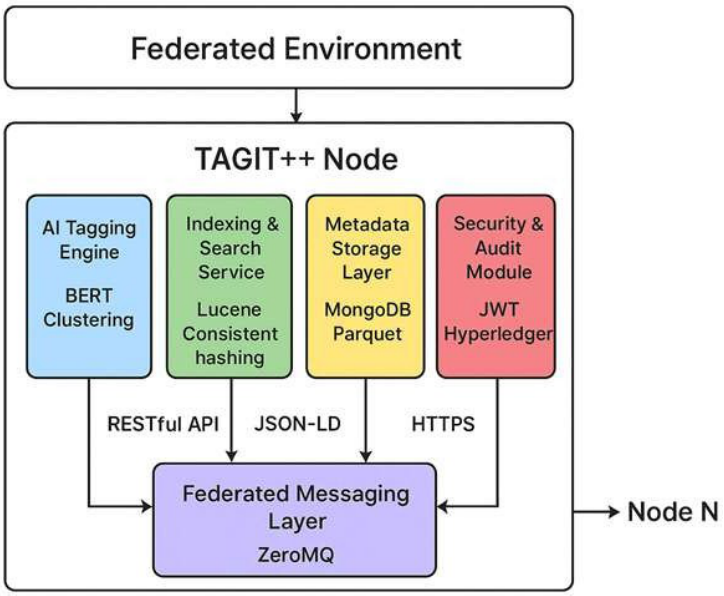

Figure 1: TAGIT++ System Architecture showing decentralized indexing, AI tagging, and federated routing.

4.2 Key Components

- **Indexing and Search Service:** Built on Apache Lucene with consistent hashing.
- **Metadata Storage:** MongoDB for unstructured data and Apache Parquet for structured attributes.

Received: August 08, 2025

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- **AI Tagging Engine:** Fine-tuned BERT model using Hugging Face Transformers; clustering via K-Means and DBSCAN.
- **Security and Audit Module:** JWT-based access control and Hyperledger Fabric blockchain.
- **Federated Messaging Layer:** ZeroMQ for asynchronous inter-node communication.

4.3 Testbed Setup

Ten independent nodes were deployed (Intel Xeon 8-core, 32GB RAM, 1TB SSD). WAN latencies of 50–150 ms were simulated with gigabit links. Each node hosted MinIO storage, AI tagging, indexing, and blockchain services.

4.4 Datasets

- **Climate Dataset (CMIP6 subset):** ∼1.2 million NetCDF files.
- **Genomics Archive:** ∼850,000 FASTA/VCF files.

4.5 Evaluation Metrics

Performance was evaluated using:

- *Technical Metrics:* Query latency, indexing throughput, metadata overhead.
- *Collaboration Metrics:* Cross-site query time, Collaboration Efficiency Index (CEI).

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5 Results and Discussion

5.1 Query Response Time

TAGIT++ achieved up to 10× faster phrase queries and 5.3× faster boolean queries than SCISPACE due to semantic routing. Even under 1,000 concurrent queries, scalability remained near-linear.

5.2 Indexing Throughput

Average indexing speed was 1,500 files/sec/node, surpassing SCISPACE (870 files/sec) and GUFI (1,120 files/sec).

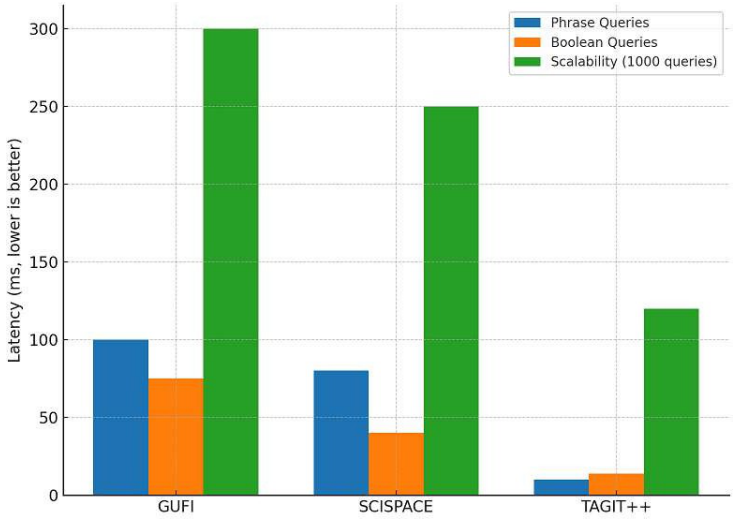

Figure 2: Figure 2: Query response time comparison across TAGIT++, GUFI, and SCISPACE for phrase, boolean, and concurrent queries.

5.3 Metadata Overhead

Semantic enrichment added 12.8% overhead, compared to SCISPACE (9.4%) and GUFI (3.1%), as shown in Table 1.

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Table 1: Metadata overhead comparison of TAGIT++, GUFI, and SCISPACE.

Framework	Avg. Metadata Overhead (%)
GUFI	3.1
SCISPACE	9.4
TAGIT++	12.8

5.4 Security and Audit Performance

Access validation averaged 14 ms; blockchain logging added only 2 ms per transaction, demonstrating minimal security overhead.

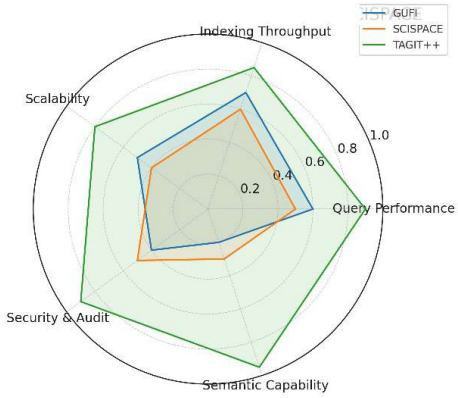

Figure 3: Normalized radar chart comparing TAGIT++, GUFI, and SCISPACE across five dimensions: query speed, indexing throughput, scalability, semantic capability, and security.

5.5 Collaboration Efficiency

TAGIT++ improved the Collaboration Efficiency Index (CEI) by 40%, with enhanced trust and transparency through blockchain-backed provenance.

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6 Conclusion and Future Work

TAGIT++ provides a federated, AI-enhanced metadata management framework integrating scalability, semantics, and governance. Through distributed indexing, AI-driven tagging, and blockchain auditability, it offers efficient, secure, and transparent scientific collaboration. Future work includes adaptive tag evolution and semantic graph integration for deeper cross-domain reasoning.

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