Master's Thesis Defense

Development of a Data Management Architecture for the Support of Collaborative Computational Biology

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Acknowledgements

- Ed Komp—My mentor.
- Terry Clark—My advisor.
- Victor Frost—My “other” advisor.
- Heather, Jesse, Justin, Keith, Andrew—Project team members.

Presentation Overview

- Computational biology background
- Analysis of similar projects
- Design Objectives
- Implementation
- Conclusions

Computational Biology

- Small & Large data sets
  - Input: protein structure, genetic sequence
  - Output: MD simulation, BLAST
- Exponential data growth
  - New data becoming available at impressive rate
  - Curated vs. non-curated data
- Experiments can be represented as pipelines, possibly with feedback to earlier stages
- Runs frequently re-done
  - Parameter variation and re-analysis of results
  - Use of recently available data with previously used experimental configuration

Computational Biology

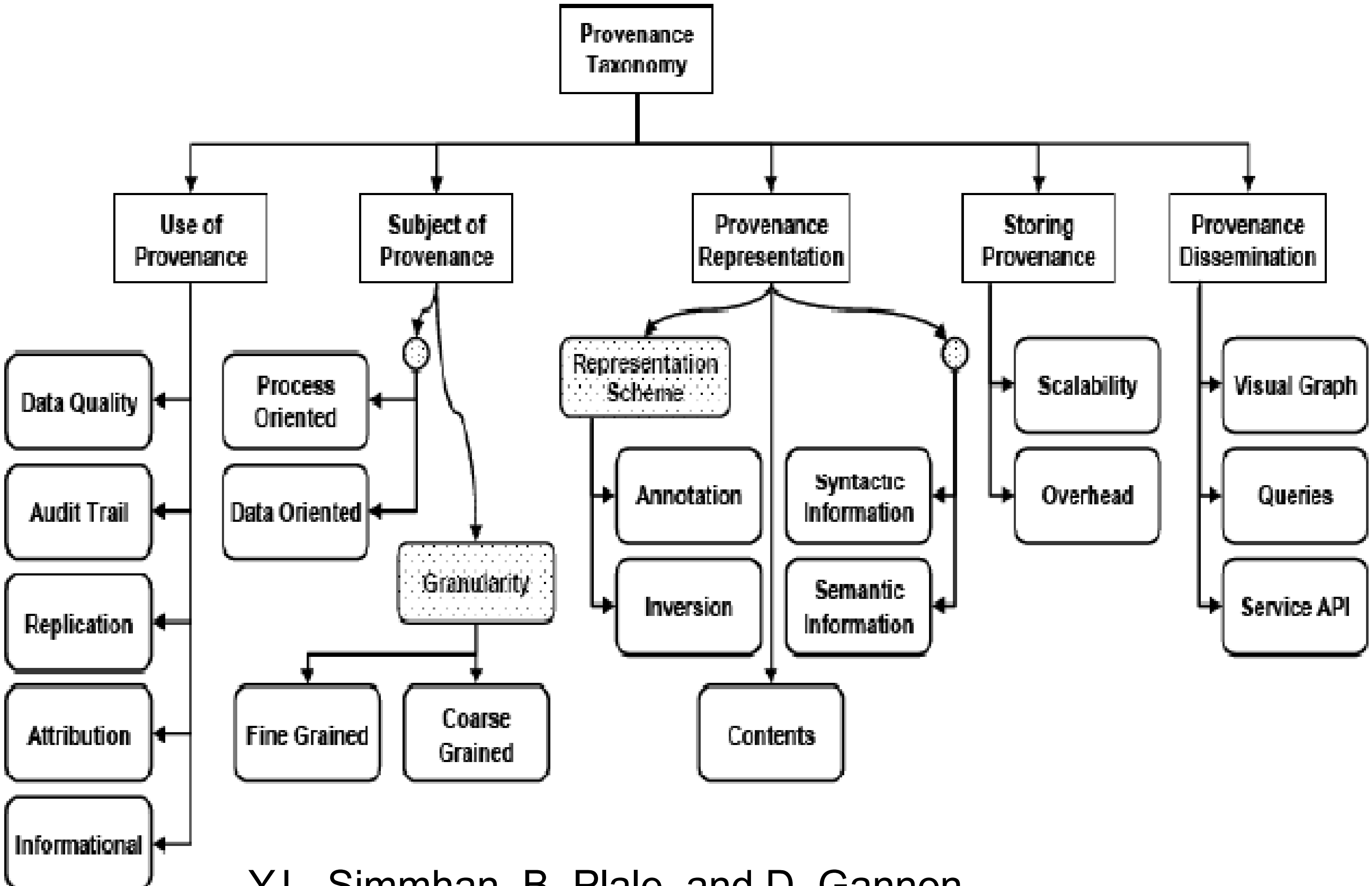
- Maintenance of provenance records required when publishing results
  - Challenging in fast-paced, high-volume environment
- Collaboration important
- Controlled information access levels
- Wet-lab techniques do not scale well
- Tools and formats used in analysis do not inherently provide integrated, end-to-end provenance trail

Why is provenance important?

- Provides context and specifications work was done in
- CS pioneer Jim Gray on provenance:

"scientific data [to] remain available forever so that other scientists can reproduce the results and do new science with the data…To understand the data, those later users need the *metadata*: (1) how the instruments were designed and built; (2) when, where, and how the data was gathered; and (3) a careful description of the processing steps that led to the derived data products that are typically used for scientific data analysis." [Gray02]

Provenance Taxonomy



Y.L. Simmhan, B. Plale, and D. Gannon
“A Survey of Data Provenance in e-Science”

Related Work

- NoteCards
  - Xerox D, LISP machine
  - Semantic network of related notes
  - Tree-like graphical browse/manipulation tool
  - Semantic network entirely user-maintained
    - Flexible, but very tedious and time-consuming
  - Search was limited to the title and content of a NoteFile
- Virtual Notebook Environment (ViNE)
- BioCoRE
- myGrid/Taverna
- Scientific Annotation Middleware (SAM)

Related Work: Shortcomings

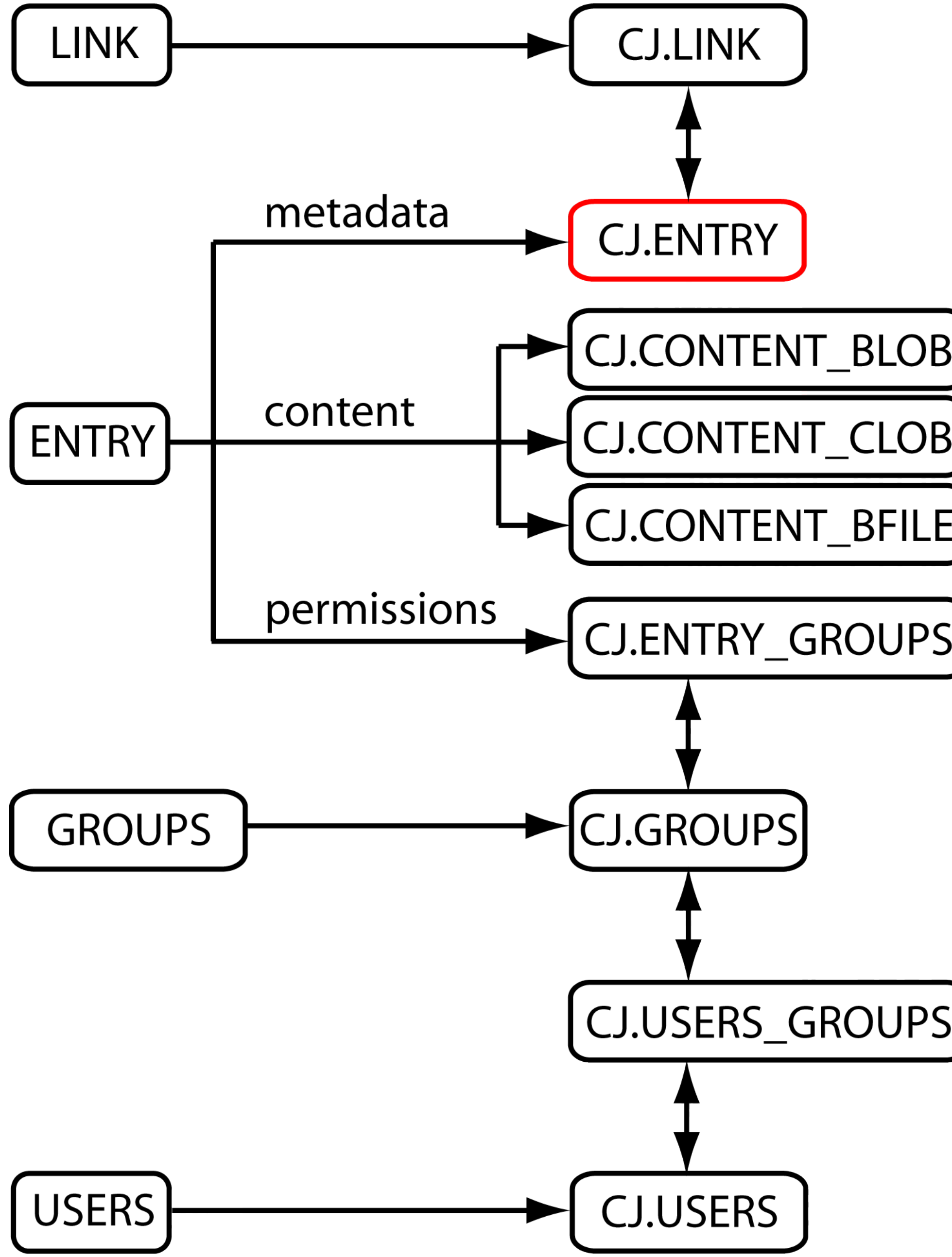
- Limited or no provenance or other meta-data management
- Concept of workflow that other users can view, import, and alter
- Collaborative features don't include managed re-use that maintains provenance trail
- Weak search capabilities result in overly cluttered user interfaces
  - Search can be used as a filter to select visible data plane in navigation tools
- Integration of secure computational facility while keeping user's rights and restrictions on usage intact

Design Objectives

- Derived from analysis of related projects
- Identified five key areas as vital in aiding computational biologists

  1) Type Hierarchy & Data Abstraction
  2) Data Storage
  3) Provenance Management
  4) Data Security
  5) Data & Provenance Search

Type Hierarchy & Data Abstraction



Type Hierarchy & Data Abstraction

- Type Hierarchy: Design Goals
  - Provide core type definitions that could be used pervasively as basis
  - Extensible by users as well as administrators
  - Allow grouping of types for “namespaces”
- Data Abstraction: Design Goals
  - Allow interaction in generic fashion
  - Enable extensive search and computational usage capability
  - Maintain or improve performance

Data Model: Entry

- Electronic journal concept as basis
- Page <==> Entry
- Visible journal entry comprised of a single top-level entry (node) with arbitrary number of related nodes
- Entry (node) is an atomic unit of information associated with a single type that may be re-used
- Entry data structure composed of meta-data + content

Data Model: Entry

1) *EntryId* (INTEGER): PK for Entry table. Positive integers for all non-core entries. 0 reserved to prevent infinite recursion of type relationships.

2) *UserId* (INTEGER): Entry creator/owner. Joined with other tables to define permissions and search for entries.

3) *ContentTypeId* (INTEGER): References by *EntryId* the type of the information stored in this entry.

4) *Title* (VARCHAR2): Used to assign a title to an entry. *Titles* are not unique.

5) *JournalId* (INTEGER): References by *EntryId* another entry, which must be of content type journal. All journals are attached to a single root journal.

Data Model: Journal

- Collection of entries
- Entry may only be a member of a single journal
- Journals may be nested
- Multiple writers to a single journal
  - Furthers collaboration

Data Abstraction

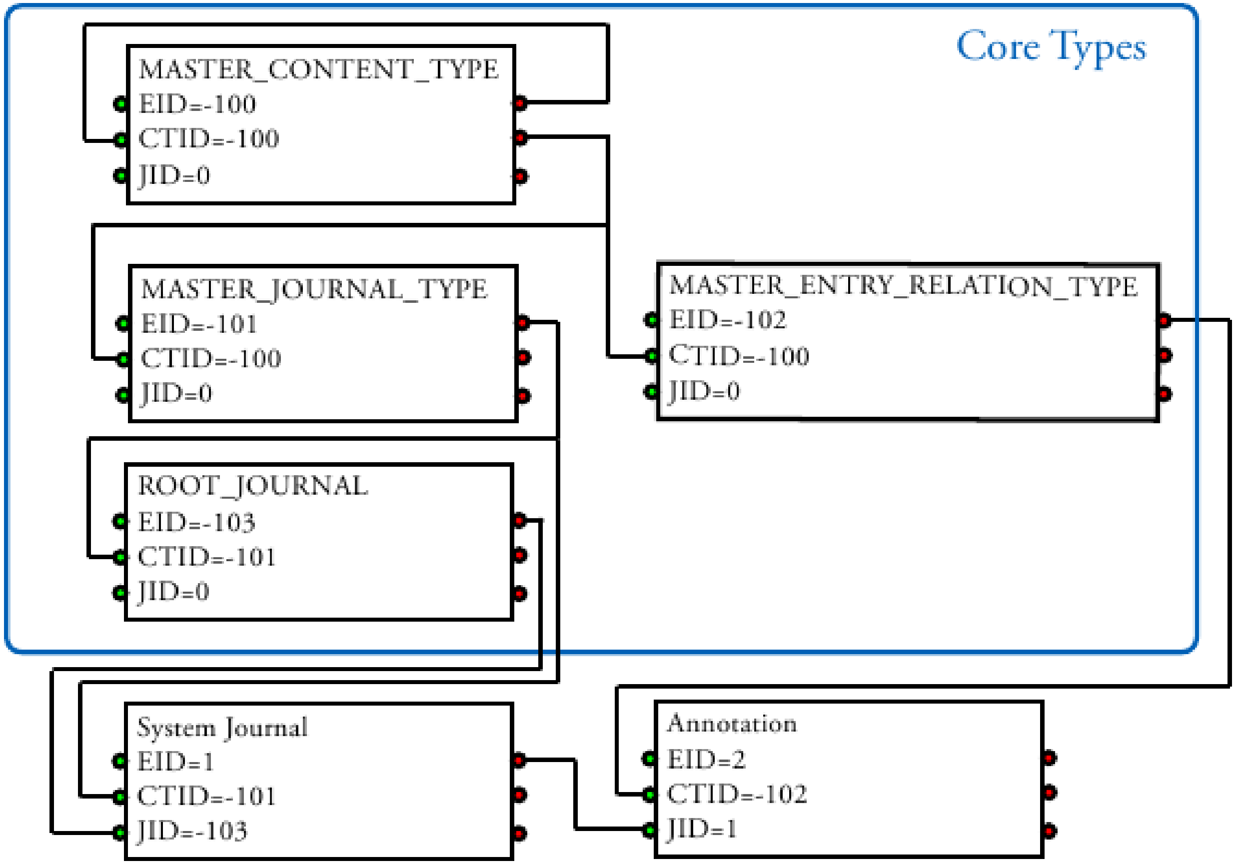
- Achieved through:
  - Extensible type hierarchy
  - Plug-in architecture
- Dissociate content from meta-data
  - High-performance
  - Pervasive, comprehensive search capability
  - Attribution provenance
- Content type & content storage type

Type Hierarchy

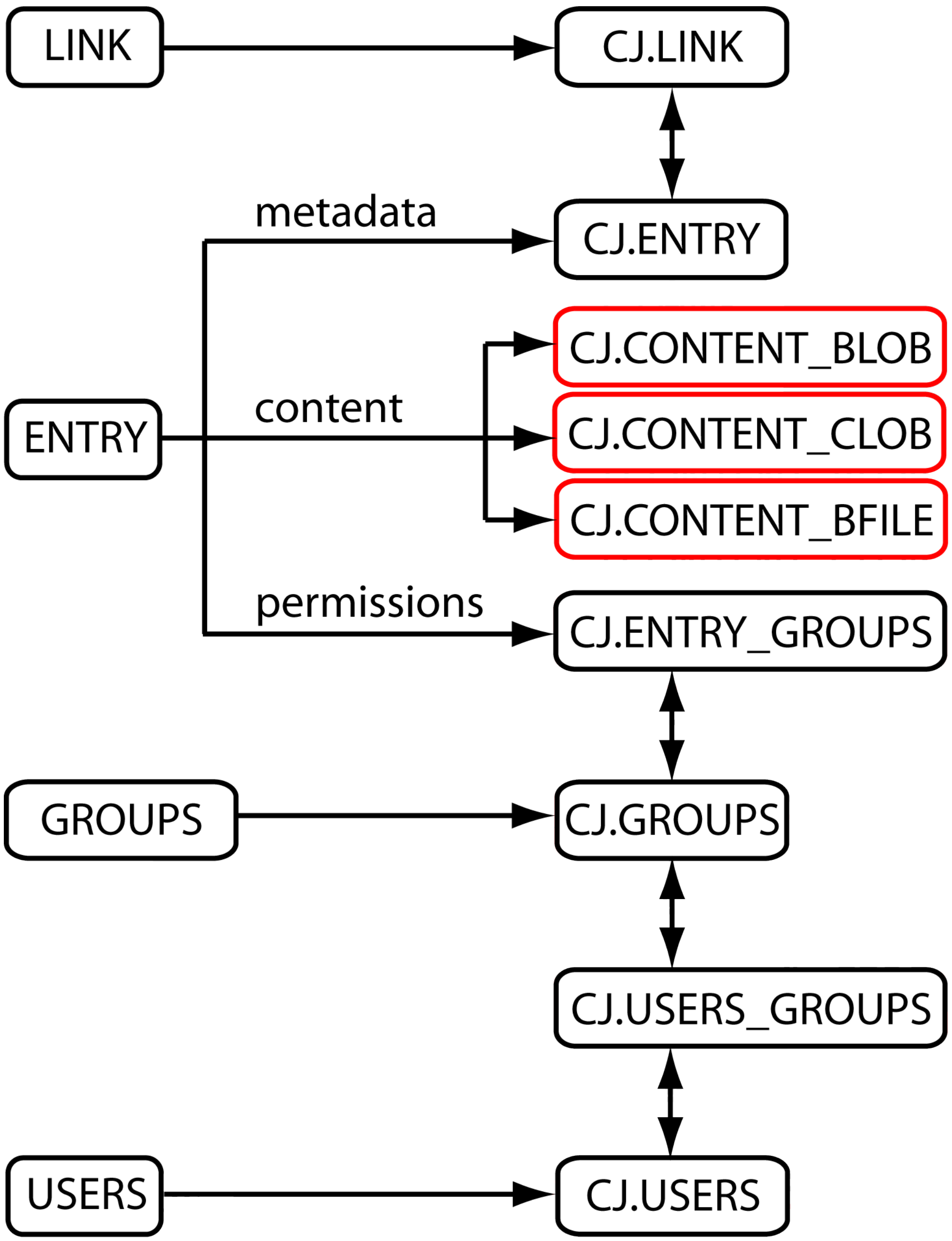
- Extensibility: Addition of new types
  - By both administrators and users
  - Aids flexibility and re-use
- Flexibility: Changes to hierarchy should not break existing infrastructure
- Robustness: Operations that compromise stability are prevented
- Data-driven, plug-in architecture reduces coupling
- No nested types: simplifies processing of an entry
- Type hierarchy stored as a collection of entries, with relationship to special “master type” entry

Type Hierarchy: Design

ENTRYID	USERID	CONTENTTYPEID	TITLE	JOURNALID
-100	CJ	-100	"MASTER_CONTENT_TYPE"	0
-101	CJ	-100	"MASTER_JOURNAL_TYPE"	0
-102	CJ	-100	"MASTER_ENTRY_RELATION_TYPE"	0
-103	CJ	-101	"ROOT_JOURNAL"	0



Storage Architecture

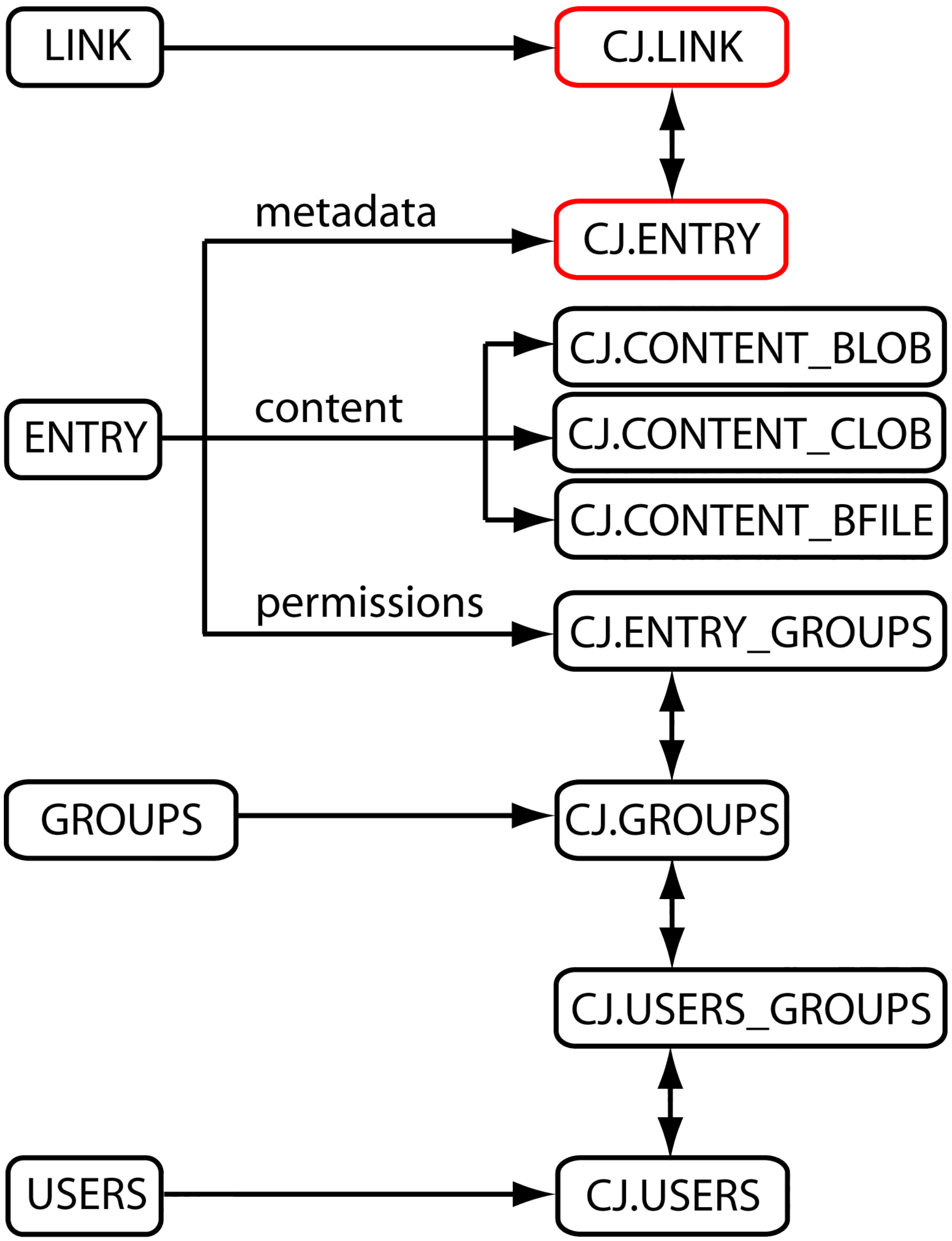


Storage Architecture

- Objectives:
  - Rapid textual & meta-data search
  - High-performance (latency and B/W) cluster-based computing
- Split "atomic" entry into meta-data and content-data
- Hybrid content-data storage: in DBMS or in cluster file system

	Latency	Volume	Searchable
CLOB	Low	Low	Yes
BLOB	Low	Low	No
BFILE	High	High	No

Provenance



LINK
CJ.LINK
metadata
CJ.ENTRY
CJ.CONTENT_BLOB
ENTRY
content
CJ.CONTENT_CLOB
CJ.CONTENT_BFILE
permissions
CJ.ENTRY_GROUPS
GROUPS
CJ.GROUPS
CJ.USERS_GROUPS
USERS
CJ.USERS

Provenance

1) Attribution
    1) Owner-only write model + link creation on copy + security model ensures attribution is maintained
2) Audit Trail
3) Data Quality
4) Informational
5) Replication

Provenance: Entry Fields

- Five Fields
  - *UserId*
  - *CreateDate*
  - *ModifyDate*
  - *CommitDate*
  - *Committed*

Provenance: Semantic Relationships

- RDF 3-tuple: <subject,predicate,object>
- Predicate defines an “IS-A” relationship
- <'Junior','son','Senior'>
  - “Junior IS A son OF Senior”
- Choice to require “IS-A” eliminates need for inverse relationship searches on “HAS-A”
- *FromEntry* **IS A** *LinkType* **OF** *ToEntry*

Provenance: Semantic Relationship Integrity Constraint

- Second stage in ensuring durability of provenance (first is secured commit)
- Extension of Resource Description Framework (RDF) 3-tuple of <subject,predicate,object>
- Depending on predicate, removal of subject or object may nullify ability to maintain definitive provenance trail
- Form 5-tuple with addition of two values describing subject's dependence on object and vice-a-versa
- Assurances of non-removal of content protected by SRIC encourages collaborative sharing and re-use of experiments & data from other users

Provenance: SRIC

- Flags:
  - *ToRequiresFrom*
  - *FromRequiresTo*

ToRequiresFrom	*FromRequiresTo*	Valid?
False	False	Yes
False	True	Yes
True	False	Yes
True	True	No

- Commit vs. SRIC – Describe how this plays out.

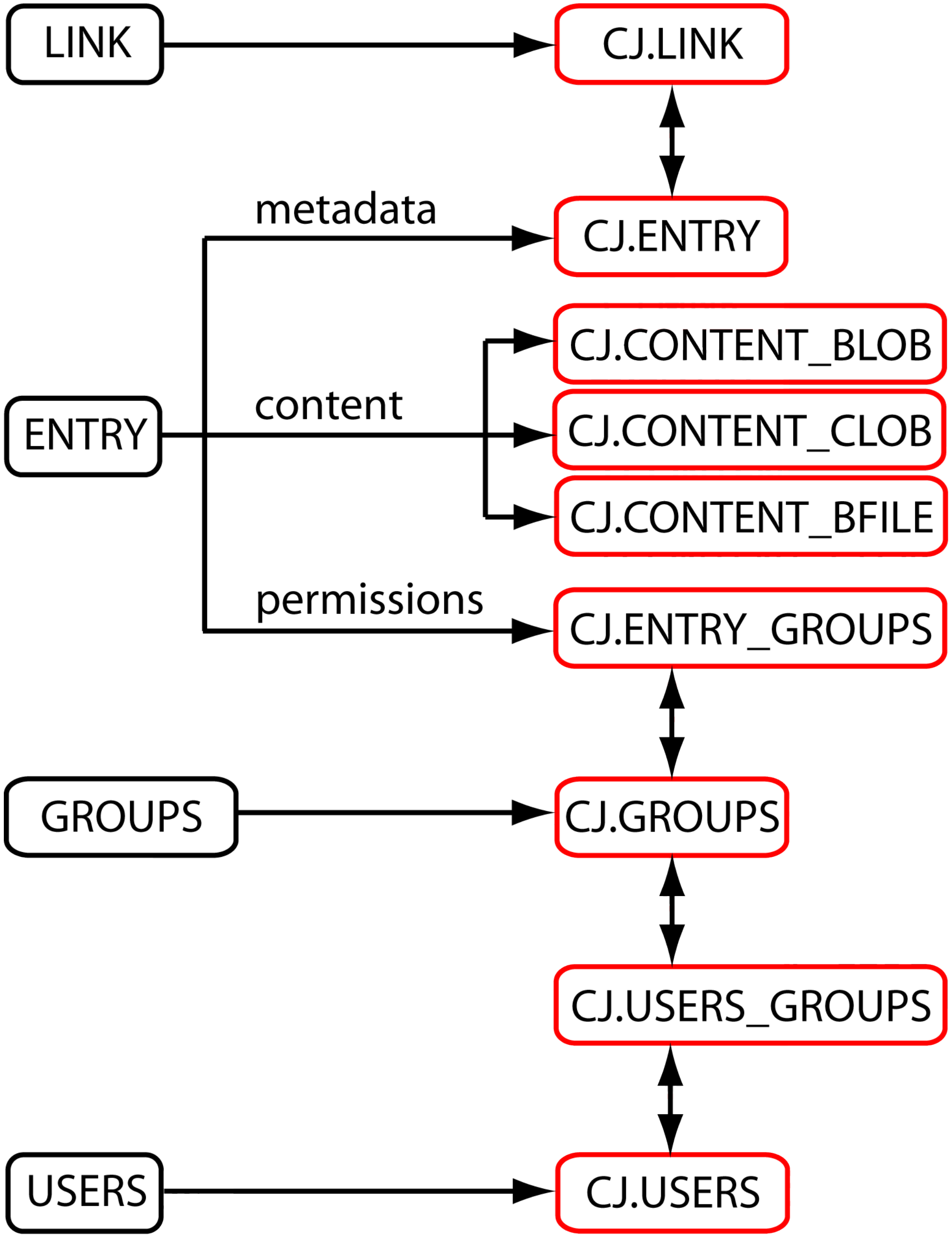
Provenance: Collection & Usage

- Two collection techniques:
  - Automatic: Done via DB triggers, Ex: create, update, commit of an entry
  - API: Done via BCJ plug-ins, Ex: input to and output from experiment, textual annotations
- Used by navigators and tools
  - Provide relevant information while reducing clutter
  - Filtering by author, create/modify/commit date, deprecated flag, rating, hidden, categorization by content types
  - Related entry view in navigator
- Open interface via views rather than purely functional interface
  - Allows complex join queries to be performed

Provenance: Conclusions

- Automated provenance management framework vital
- Eliminates burdensome folder-file management scheme to maintain association between input, experiment, and output
- Ensures attribution information is maintained from inception through multiple iterations and ending in the successful conclusion of work
- Non-repudiation assured
- Extended RDF 3-tuple encourages sharing and re-use among collaborators

Search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GROUPS
CJ.GROUPS
CJ.USERS_GROUPS
USERS
CJ.USERS

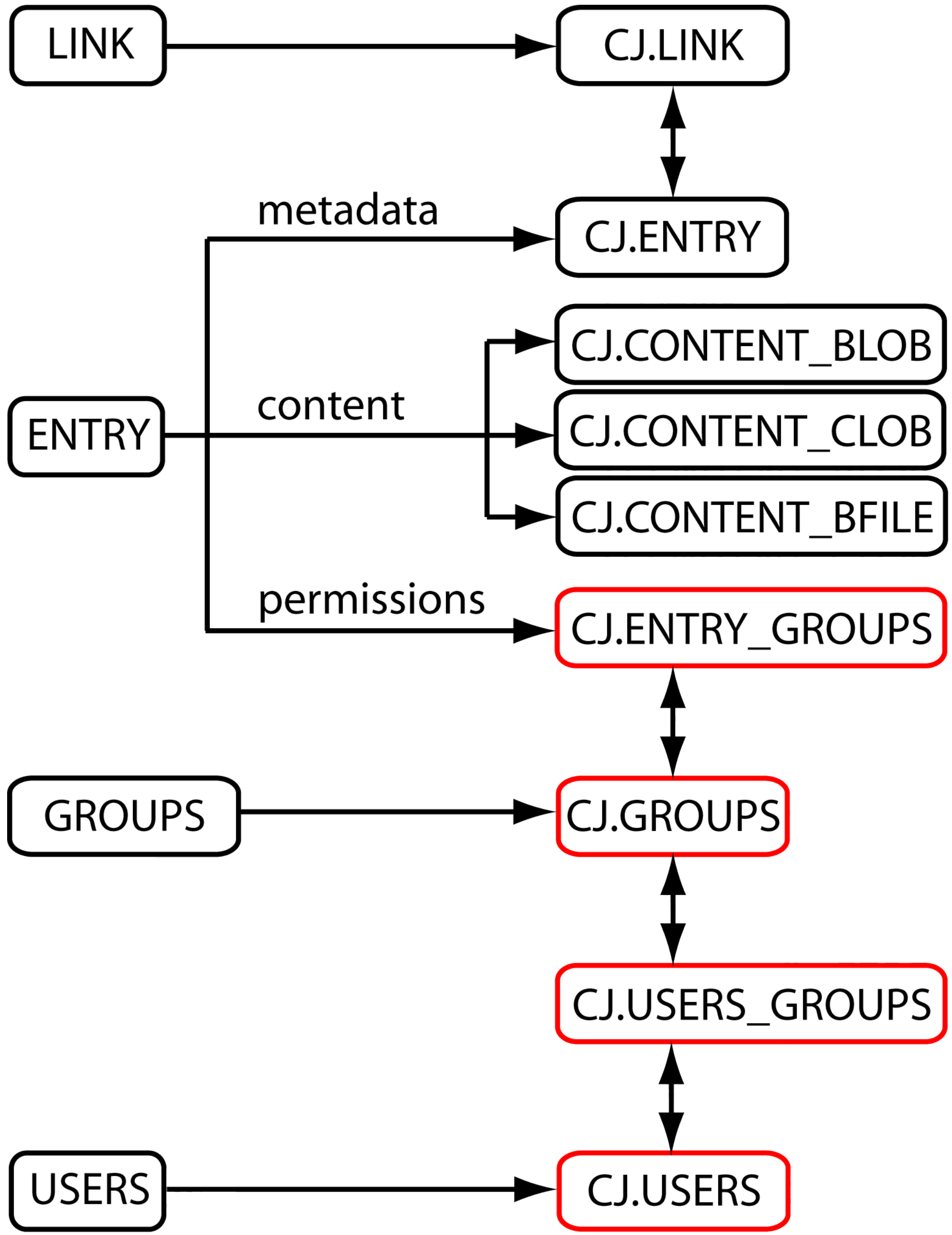
Search

- Pervasive: Fundamental activity
- Data and provenance
- Anything that user can access should be query-able
  - Content
  - Meta-Data
  - Combined content + meta-data query
- Used by navigators to define and refine presentation
- Used by workflow and experiment editors to find available and appropriate blocks and resources
- Sorting

Search: “Helper” Fields

- Four additional meta-data fields to assist search
  - *ContentLastAccessDate*
  - *Deprecated*
  - *Hidden*
  - *Rating*

Security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Security

- Coarse- vs. fine-grained
- Permission inheritance
- Goals
  - Create secure, private workspace for individuals
  - Encourage collaboration through the ability to selectively share information via find-grained access controls
  - Maintain the integrity of all provenance information collected

Security

- Actors: Users and Groups
- Group-based access control
  - Each user a member of one or more groups
  - Each group contains zero or more users
  - Each entry associated with one or more groups granted read-only access
- Read/Write Permission Levels
  - Owner-only write permission

Security

- "Commit" concept
  - Prior to commit, owner free to alter content
  - Committing entry locks content to prevent further writing
  - Meta-data fields affecting provenance also locked
  - First stage in ensuring durability of provenance (second step is SRIC)

Security: Metadata

- Two categories of metadata field access levels:
  - System-controlled, and
  - User-controlled
- Triggers used on entry metadata fields rather than functional interface
  - Maximize available information for search
  - hasEssentialDependents
- Delete compromise of strict rules

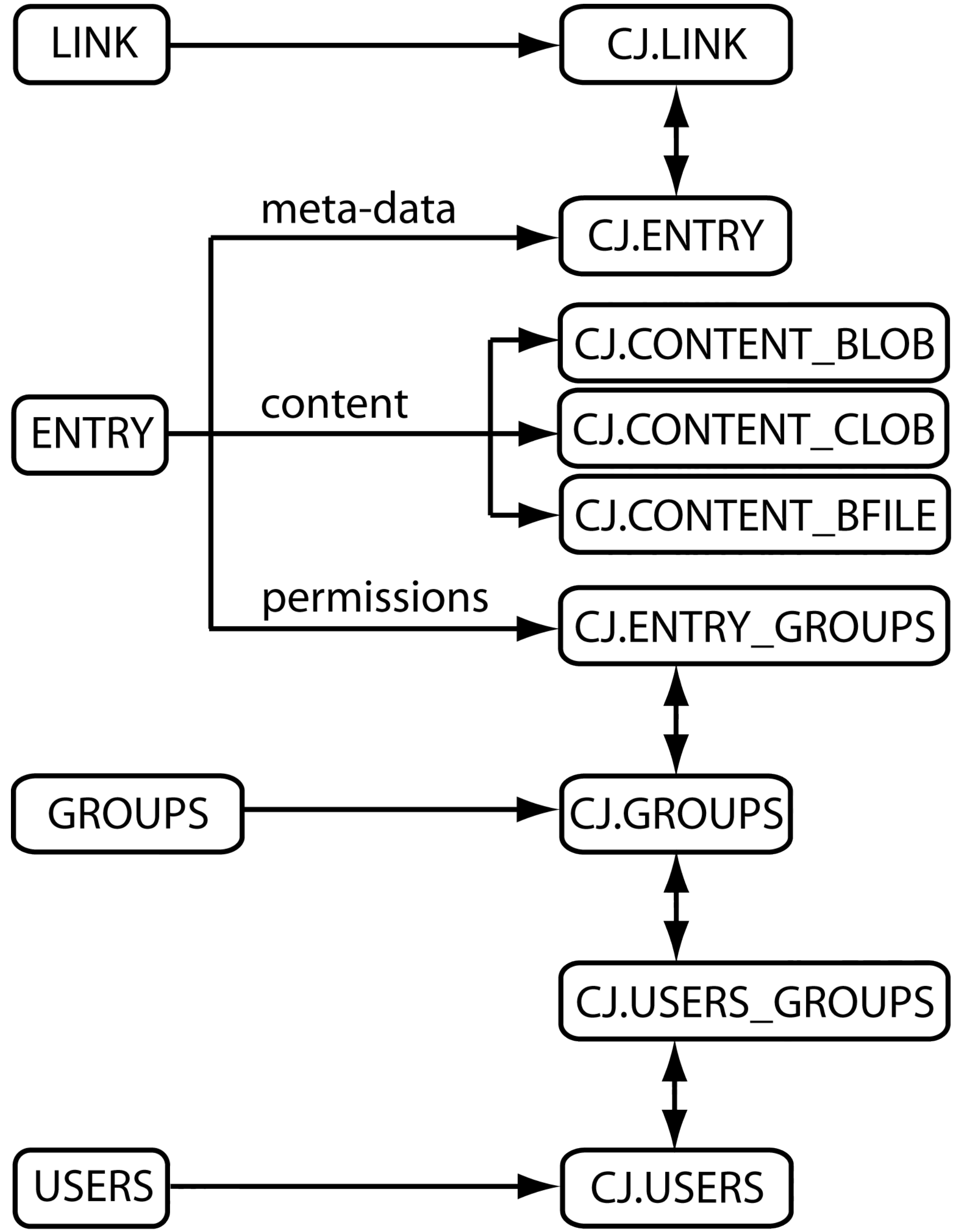
	System-Controlled	
	Fixed at Creation	Fixed at Commit
EntryId	Yes	X
UserId	Yes	X
CreateDate	Yes	X
ModifyDate	No	Yes
CommitDate	No	Yes
ContentLastAccessDate	No	No

	User-Controlled	
	Fixed at Creation	Fixed at Commit
Commited	No	Yes*
ContentTypeId	No	Yes
Deprecated	No	No
Hidden	No	No
JournalId	No	No
Rating	No	No
SystemGenerated	Yes	No
Title	No	No

Security: BFILE

- Separate cluster FS created
  - Can only be accessed by 'oracle' and special user to submit PBS jobs
- Mode bits altered when an entry is (un)committed so that FS reflects meta-data
  - Uses triggers to Java Stored Procedures (JSP)
  - UNIX permissions of 660 and 440
  - Immediate deletion

Summary & Conclusions



Summary

- BCJ represents a comprehensive solution
- Areas addressed
  1) Type Hierarchy & Data Abstraction
  2) Data Storage
  3) Provenance Management
  4) Data Security
  5) Data & Provenance Search

Summary

- Type Hieararchy
  - Four core entries, three master types
  - Data decomposition: atomic unit of information: the entry
  - Each entry associated with a single type
  - Not a hierarchy, single master type, eases addition of new types
  - Journal as organizational structure
- Provenance
  - All five types of provenance can be collected
  - Collection through automated means (triggers or API) along with user-friendly tooling eliminates manual processes

Summary

- Storage
  - Global, shared workspace provides area for collaboration
- Security
  - Flexible, efficient, tools simplify use, enables powerful search and cluster-based computing while ensuring integrity of provenance
  - SRIC extension of RDF 5-tuple

Conclusions

- Crafting a comprehensive solution is not only time consuming but also challenging
- End-product is vastly superior at lowering level of effort necessary to produce relevant biological research while maintaining vital provenance information
- Pervasive use of search & filters simplifies access to basic information while retaining complex search capabilities

Future Work

- SRIC
  - Link deletion strategy
  - Split ownership of link end-points
  - Owner of (very large) content linked-to by another user wants to delete the content
- Deployment needs to be simplified
- SRIC concept could be made extensible through the *LinkType Entry*
- Integrate SRIC into DBMS

Questions

- Wow! We made it to the end.
- Contact: lfeagan@us.ibm.com