

Introductory Remarks & Discussion: Federated Systems

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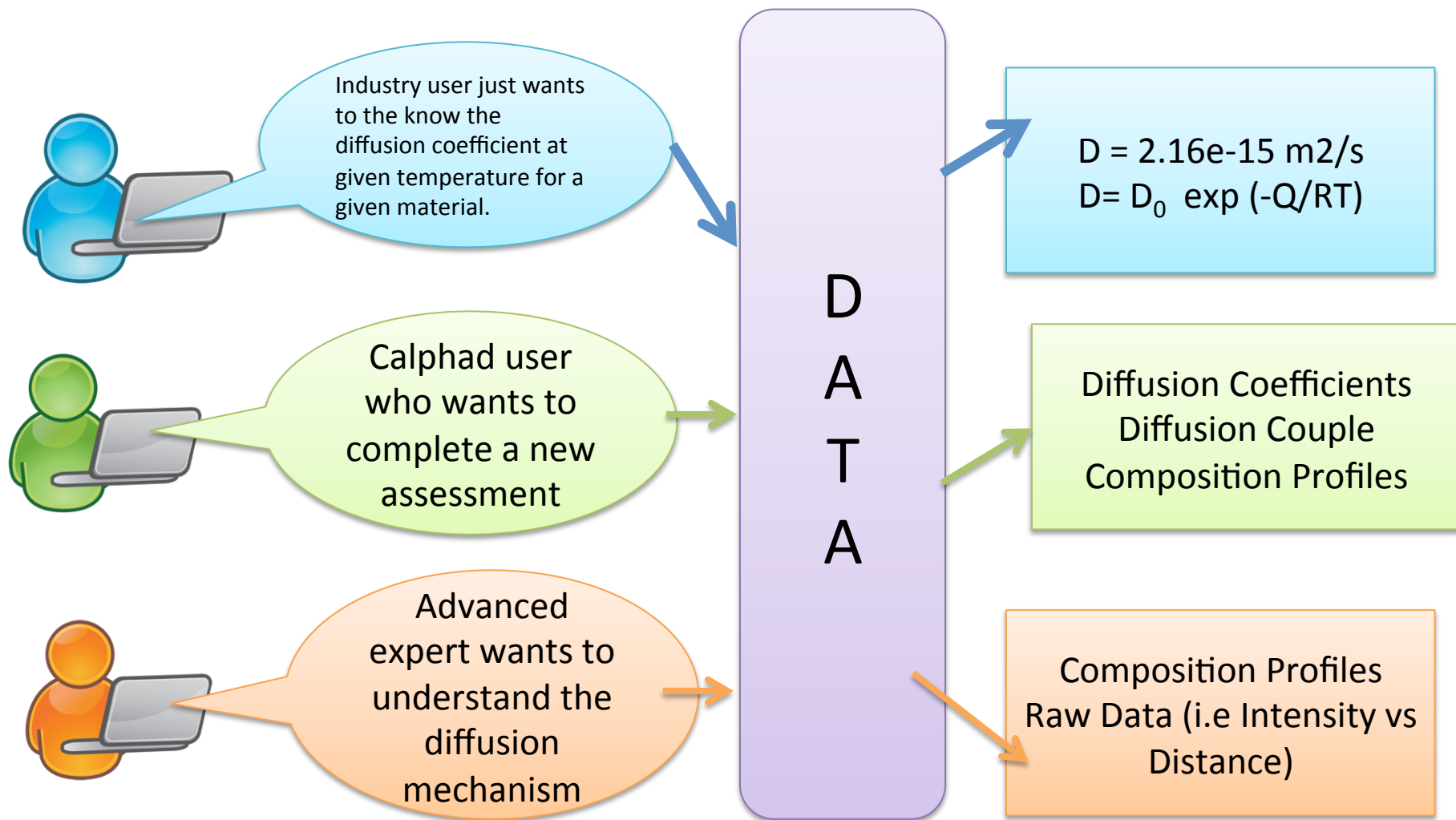
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NIST Diffusion & CHiMaD CALPHAD Workshops

Gaithersberg, MD April 29-30, 2014

End Users: Different Types of Diffusion Data Needs



Federated Data System:

What is it & Why consider implementing?

What: Data Federation Architecture

Unified access to information about disparate, geographically distributed data sources

Why:

- ✧ Retain proprietary control & competitive edge
- ✧ Cultivate a culture of data sharing
- ✧ Leverage investment
- ✧ Encourage collaboration & partnership → innovation

Federated Data Repositories: Key Elements

- Focus on end user data needs
- Use with range of types of content
- Adopt common framework
 - storage repository platform
 - exchangeable metadata and data formats
 - query and discovery service overlay
 - federation/search mediator

Storage Repository Platform

NIST DSpace repository platform

- easy to install and use
- generic, agnostic, & standards-based
- Adaptable for future needs



Free, open software

Capabilities

- link to files
- support simple & customizable metadata
- browse & search
- customize with own tools
- **compatible with other repository systems**
- **export metadata (and data, if desired)**
- **assign persistent identifiers for data**
- **attach license for data use**



Repository Platform: Sample Entry

(repositories, disciplines, industries) (data, models, integration, etc.)
NIST File Repositories → NIST Data File Repositories → CALPHAD Assessments

CALPHAD Assessments

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[Al-Cr-Ni Diffusion Mobilities in Gamma Prime and B2](#)
Campbell, C.E. (2013-02-11)
This work presents the assessment of the diffusion mobilities in both the γ' (Ni₃Al-L12) and B2 phases in the Ni-Al-Cr system utilizing the phenomenological model developed by Helander and Agren. Available experimental ...

[Ni-Al-Cr system Thermodynamic Re-Assessment of the Ternary System Al-Cr-Ni](#)
Dupin, N.; Ansara, I.; Sundman, B. (2013-01-31)
A re-assessment of the ternary system Al-Cr-Ni following Dupin's thesis work using a single energy function for the gamma and gamma prime phases is presented taking into account experimental liquidus temperatures. ...

[Ag-Al Functional Description](#)
Du, Zetang; Jing, Zhan-Peng; Li, Changrong; Niu, Chunji (2013-01-31)
The energy expressions for GP zones in the Al-Ag binary system, including the ϵ -state and the δ -ones, are established by combining the essential Gibbs energy for the matrix alloy with the Int energy and the ...

Data Citation:
Al-Cr-Ni Diffusion Mobilities in Gamma Prime and B2
Campbell, C.E.
<http://hdl.handle.net/11115/51>

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Publication Citation:
Campbell, C.E. "Assessment of the diffusion mobilities in the gamma prime and B2 phases in the Ni-Al-Cr system," *Acta Mater.* 2008,56:4277. [http://dx.doi.org/10.1016/S0364-5916\(0\)00049-9](http://dx.doi.org/10.1016/S0364-5916(0)00049-9) Data: <http://hdl.handle.net/11115/51>

Related Work:
Dupin, N.; Ansara, I.; Sundman, B. "Thermodynamic Re-Assessment of the Ternary System Al-Cr-Ni" CALPHAD 2001,25:279. Publication: [http://dx.doi.org/10.1016/S0364-5916\(0\)00049-9](http://dx.doi.org/10.1016/S0364-5916(0)00049-9) Data: <http://hdl.handle.net/11115/51>

Similar Work:
Zhang, L.; Du, Y.; Chen, Q.; Steinbach, I. "Atomic mobilities and diffusivities in the fcc, L12 and B2 phases of the Ni-Al system," *International Journal of Materials Research*, 2010:1461. <http://dx.doi.org/10.3139/146.110428>

Abstract:
This work presents the assessment of the diffusion mobilities in both the γ' (Ni₃Al-L12) and B2 (NiAl) phases in the Ni-Al-Cr system utilizing the phenomenological model developed by Helander and Agren. Available experimental tracer diffusivity, interdiffusion coefficients and activation energies were evaluated and then used to optimize the composition- and temperature-dependent diffusion mobilities. For both the B2 and γ' phases, the assessed diffusion mobility descriptions reproduce the Arrhenius temperature dependence for the Ni, Al and Cr tracer diffusivities and interdiffusion coefficients. The assessment reproduces the strong composition dependence of the diffusivities in the B2 phase observed experimentally. The measured composition dependences of the diffusivities in the γ' phase are also replicated by the present mobility descriptions. The assessed mobility descriptions are validated by comparing calculated and measured composition profiles for a variety of Ni-Al and Ni-Al-Cr diffusion couples, including B2/B2, γ' (fcc)/ γ' and γ' /B2 couples.

Files in this item

Name	Size	Format	Description
exp-b2.zip	9.374Kb	application/zip	Experimental data for NiAl B2 phase
exp-ni3al.zip	9.619Kb	application/zip	Experimental diffusion data files for Ni3Al
alcrni-mob-NIST-0 ...	57.23Kb	application/txt	Diffusion mobility description for Ni-Al-Cr using N. Dupin thermodynamics (CALPHAD 2001)
Re-assessment-112 ...	237.1Kb	PDF	Explanation of revision of assessed diffusion mobility descriptions

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Data files

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Federated data repository system

- ✧ Low-maintenance storage & access for data
- ✧ Standards-based to ensure interoperability
- ✧ Compatibility with commercial & opensource DBs
- ✧ Easy metadata export to Federation Mediator
- ✧ Public/private efforts while protecting privacy

Federated systems

- Challenges of Coordination
 - Multiple sub-communities
 - Communication of strategy, process, & resources
 - Short time frames, rapidly moving research & accelerated industrial enterprises
- Potentials for Opportunities
 - Foundation for building on rich, diverse community
 - Connector to increasingly powerful set of tools
 - Teams of scientific partnerships for innovation



Calphad user
who wants to
complete a new
assessment

University
Content*
Tools
Facilities

Society
Content*
Tools
Facilities

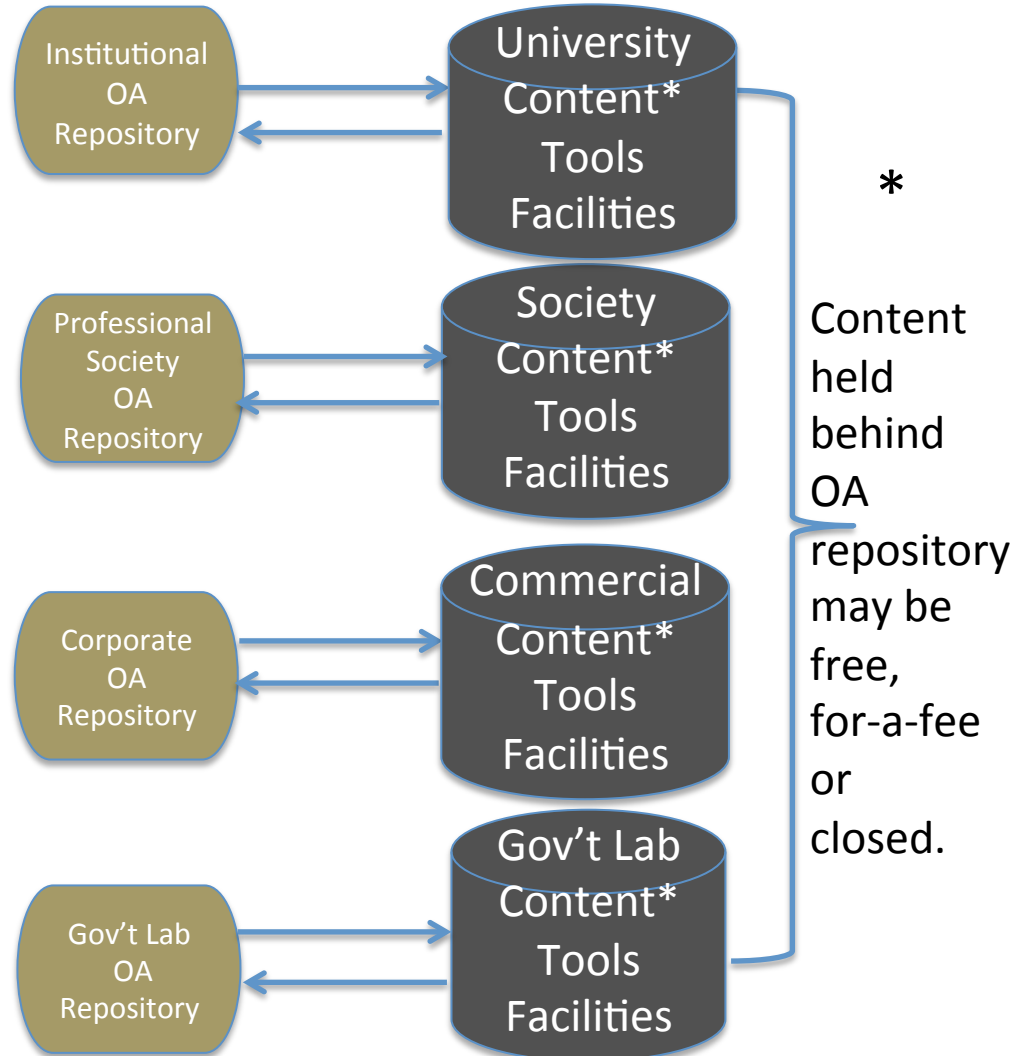
Commercial
Content*
Tools
Facilities

Gov't Lab
Content*
Tools
Facilities

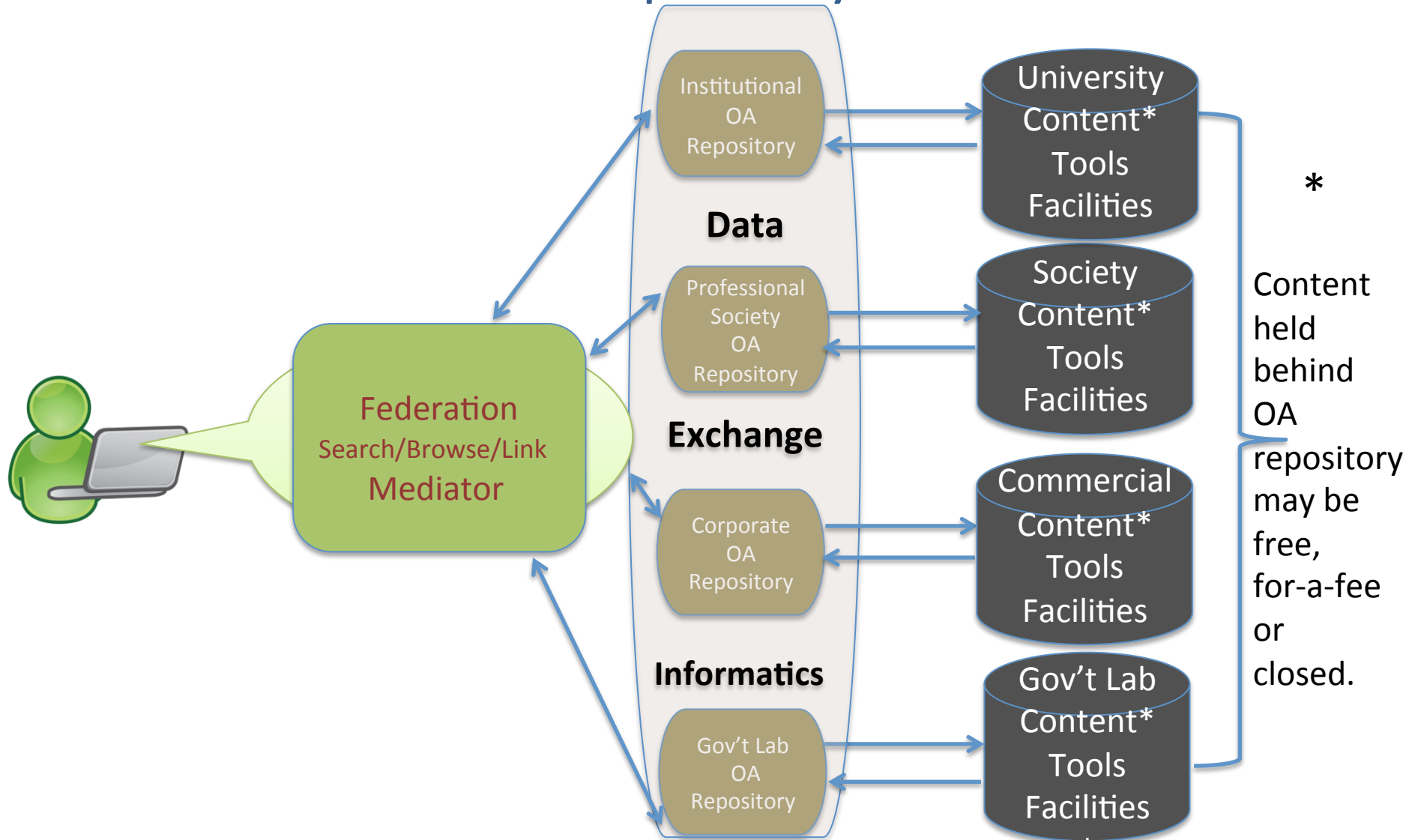
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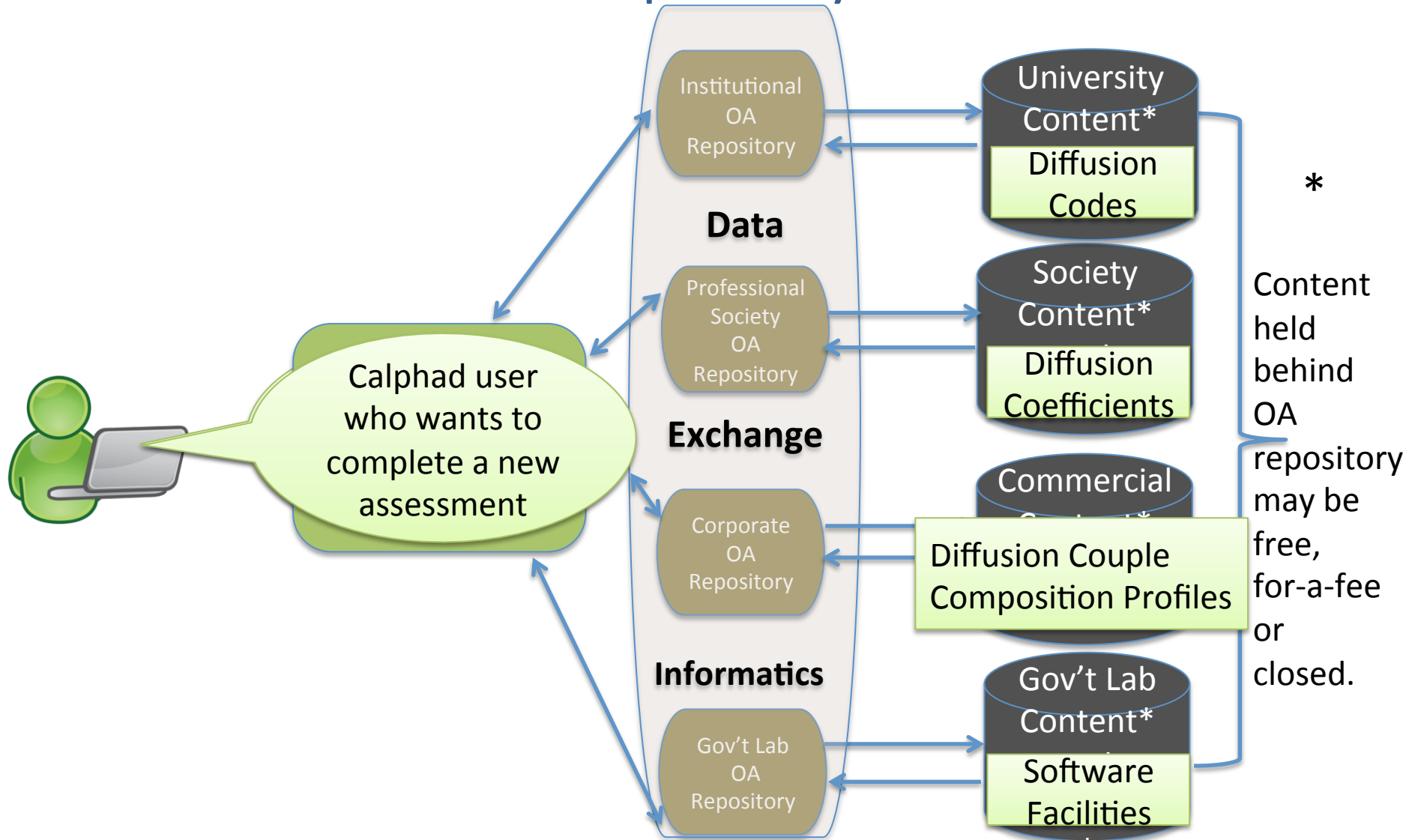
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assessment



Federated Repository Architecture



Federated Repository Architecture



Federated Repository Architecture

Discussion:

Could federated systems help or hinder your work?

How?



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Common metadata & data practices?

Who could do what?

Should/Where to begin?

