

**SESAME**  
**an Experiment Management System for**  
**Biomolecular NMR**

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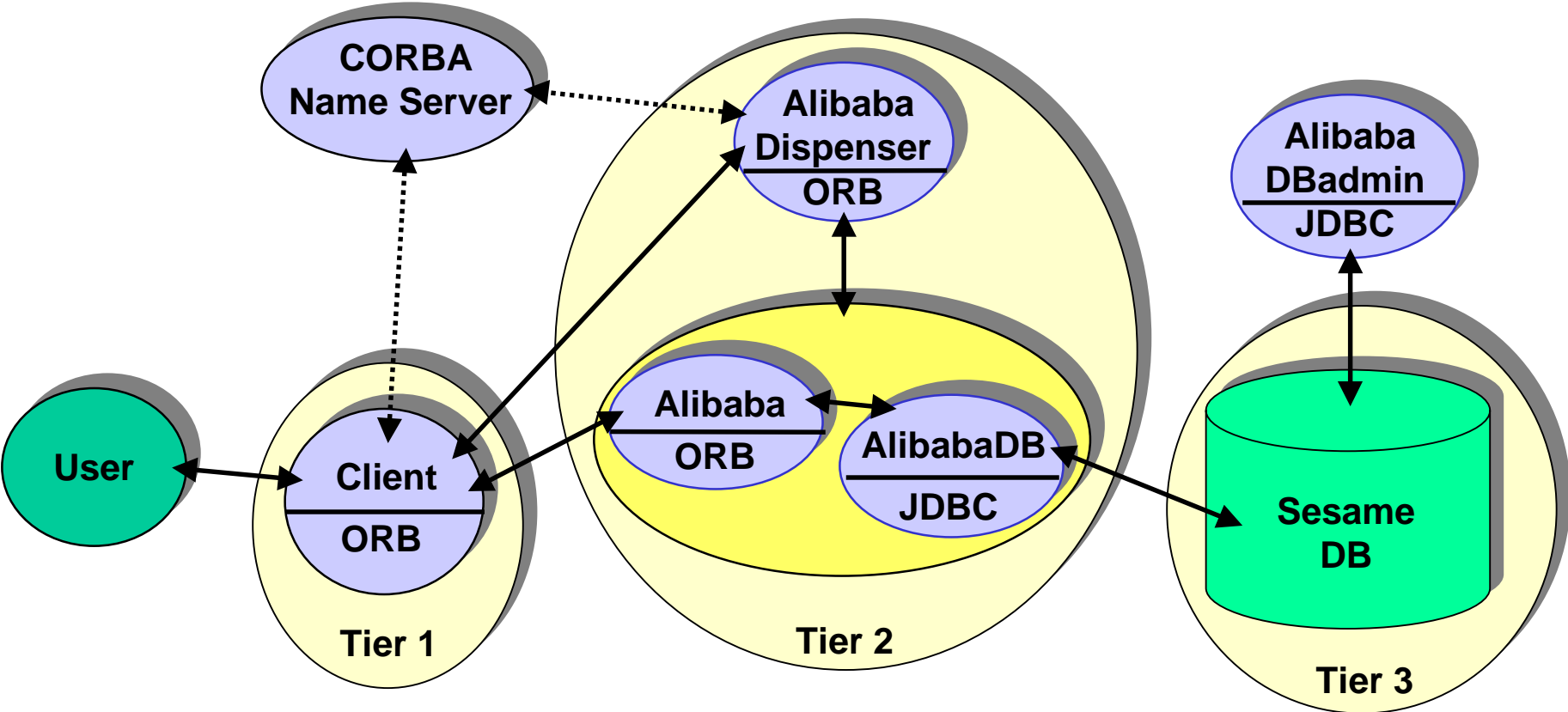
# Introduction

A computing infrastructure has been designed (Sesame), following the client/server paradigm, to assist in managing and linking individual steps in a biomolecular NMR project and to allow remote collaborations and/or expert help at various stages. The Sesame software package consists of a *framework*, which supports secure interactions among the three tiers of the system (the *client*, *server*, and *database* tiers), and *application modules*, which carry out specific tasks. The framework utilizes commercial software packages and industry standards; the database tier employs a commercial database management system. Each Sesame application module consists of a simple user interface in the client tier, one or more application packages in the server tier, and relevant defined objects represented in the centralized database. For security, access to stored data is controlled by privileges.

## Sesame can be expanded to support all phases of high-throughput structure - function studies

Task	Sesame module
<p>target selection</p> <p>cloning</p> <p>expression plasmid management</p> <p>protein expression, purification</p> <p>preparation of NMR sample, conditions</p> <p>request for and scheduling of data collection time</p> <p>data collection protocol</p> <p>data sets acquired and processed</p> <p>extraction of peak heights and couplings</p> <p>assignments of peaks</p> <p>analysis of secondary structure, hydrogen exchange constraint and structure determination, refinement</p> <p>solution structures and their validation</p> <p>functional investigations</p> <p>results to data banks</p>	<p>Ouroborus</p> <p>Lamp</p> <p>Jar</p> <p>Sand</p> <p>Camel</p>

# 3 - tier Sesame architecture



**CORBA**    common object request broker architecture  
**ORB**        object request broker  
**JDBC**        provides the capability to access databases from Java  
**DB**            database

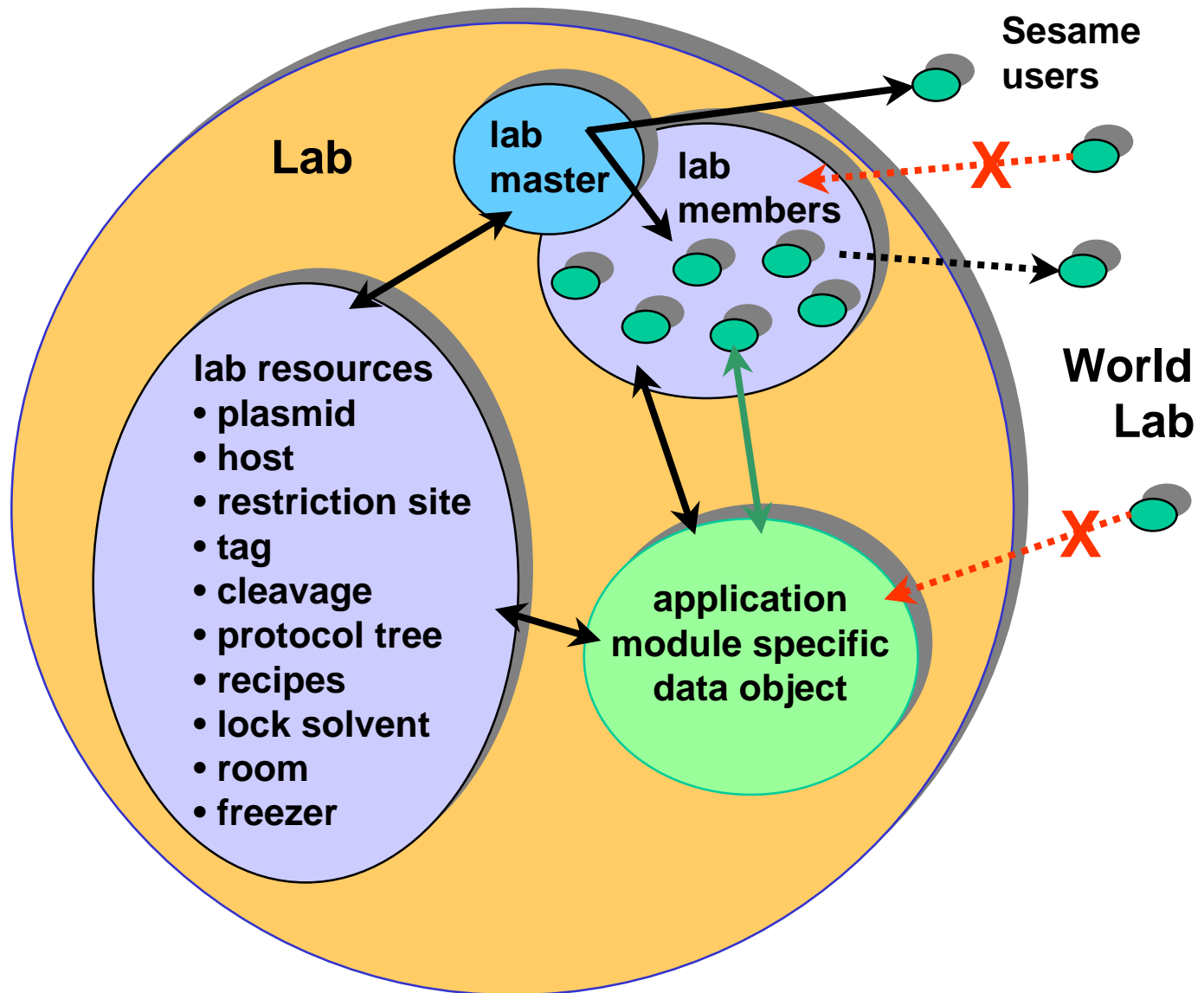
## Labs in Sesame

*Lab* members share common resources, while the data attributed to a given lab is visible to all lab members and only to them. Lab data cannot be made visible to the world. Data ownership supercedes the lab for critical operations, such as *update* or *delete*. Every user can form a lab (becoming a lab-master); however, the virtual labs are usually the same as the physical labs. A user can join a lab only if he is invited by the *lab-master*. An invitation can be accepted, in which case the invited user becomes a member of a lab, or it can be refused. Lab members can resign from a lab at any time. In addition, the lab-master can remove any of the members at his discretion. The lab-master also maintains the lab resources. Non-lab members cannot get access to a particular lab's data. The users even don't have knowledge about the existence of other labs in the system.

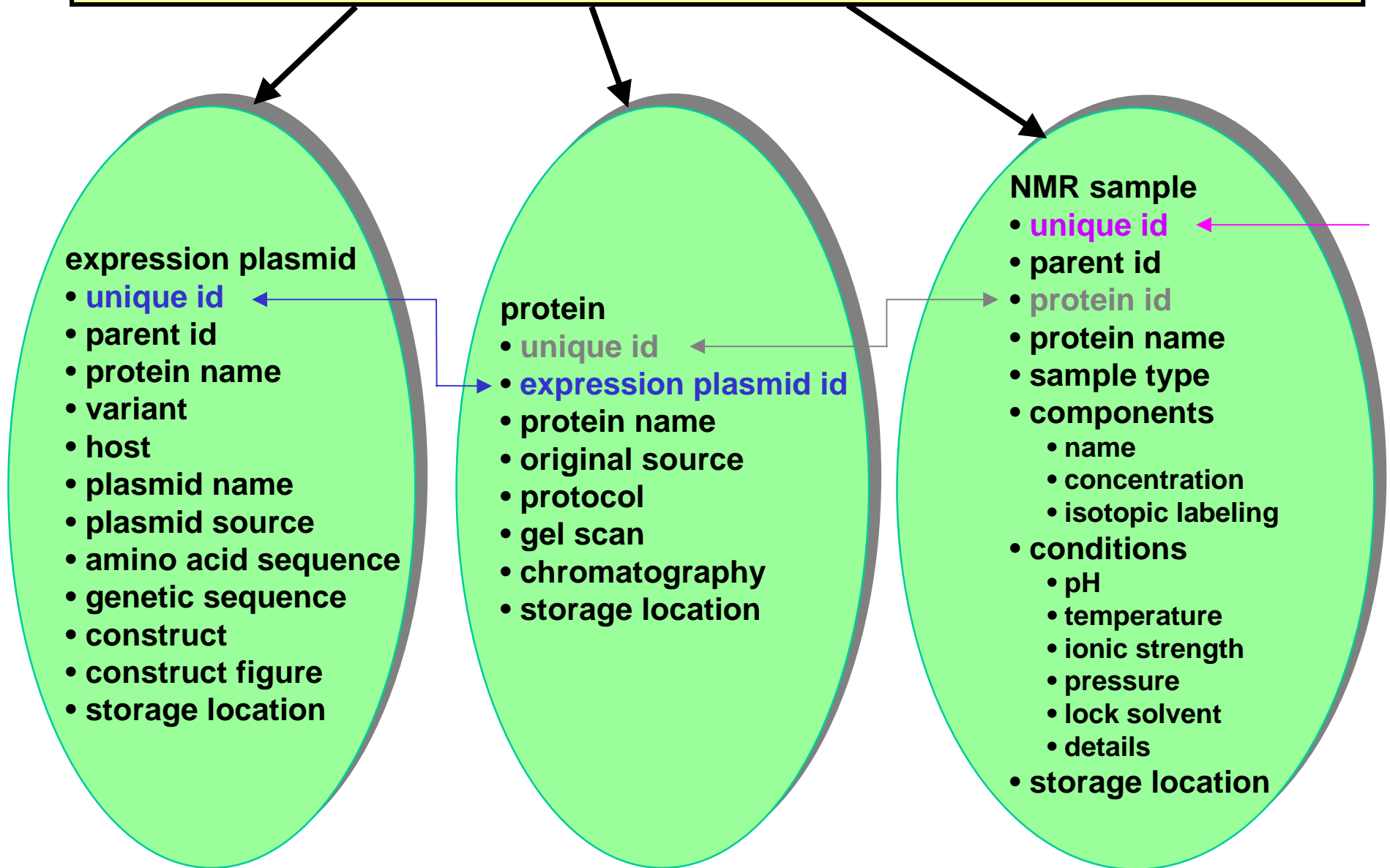
The lab related Sesame application modules are:

- [Ouroborus](#), designed to manage expression plasmids made for producing proteins
- [Lamp](#), describes expression and purification of proteins and organizes storage
- [Jar](#), designed to manage NMR samples

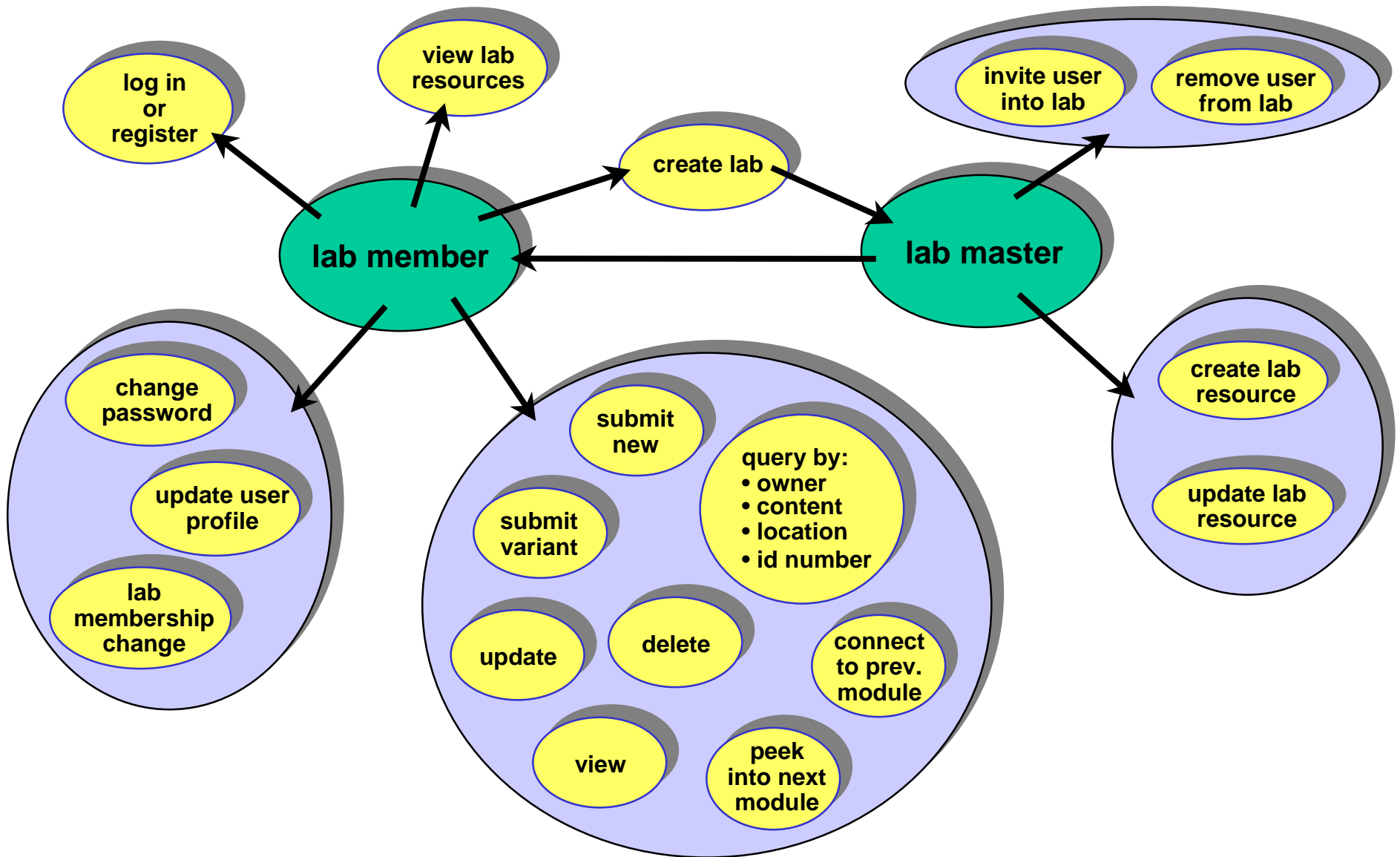
# Lab data objects



# Ouroboros, Lamp and Jar data objects



# Lab methods

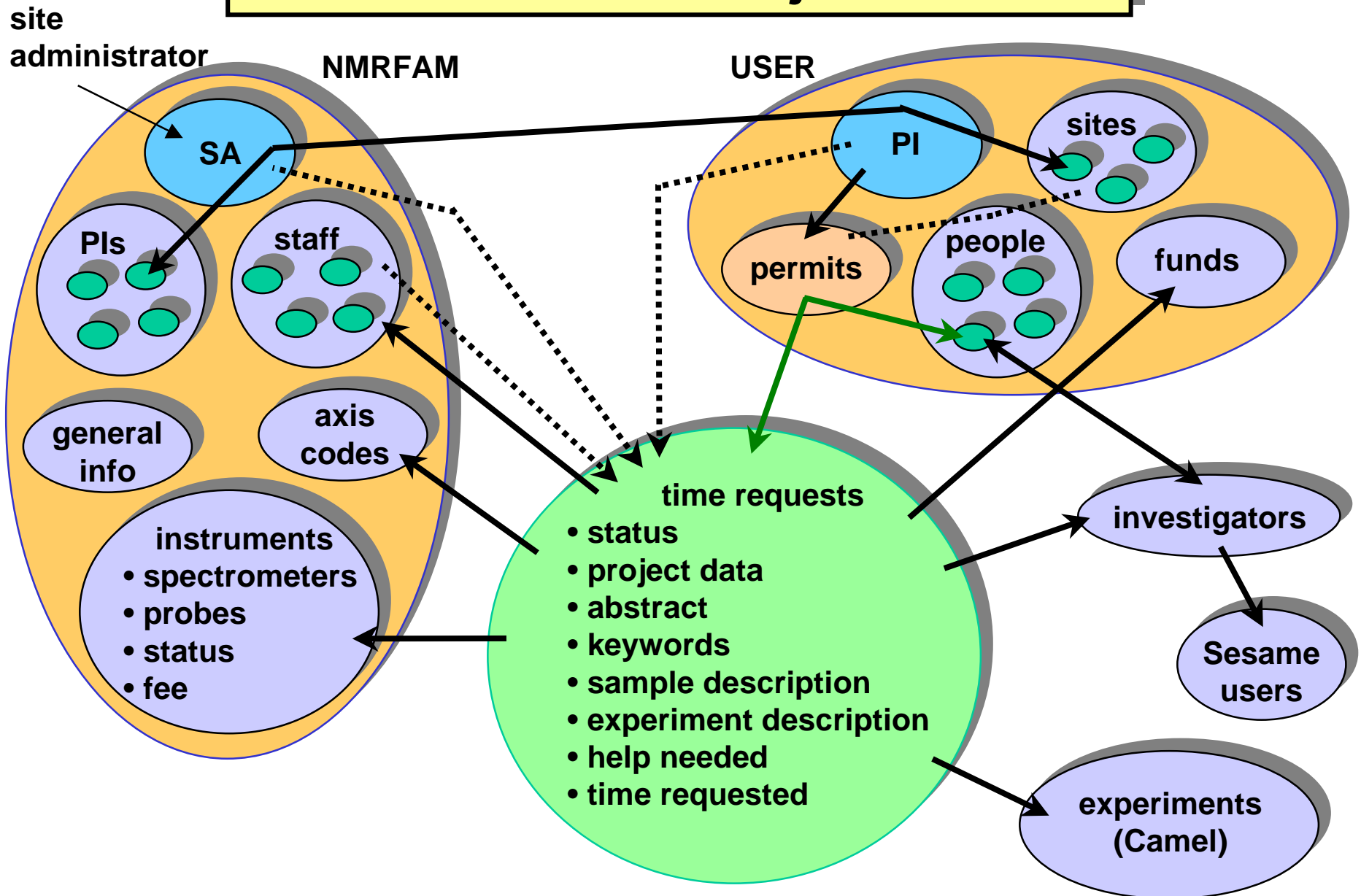


## Sites in Sesame

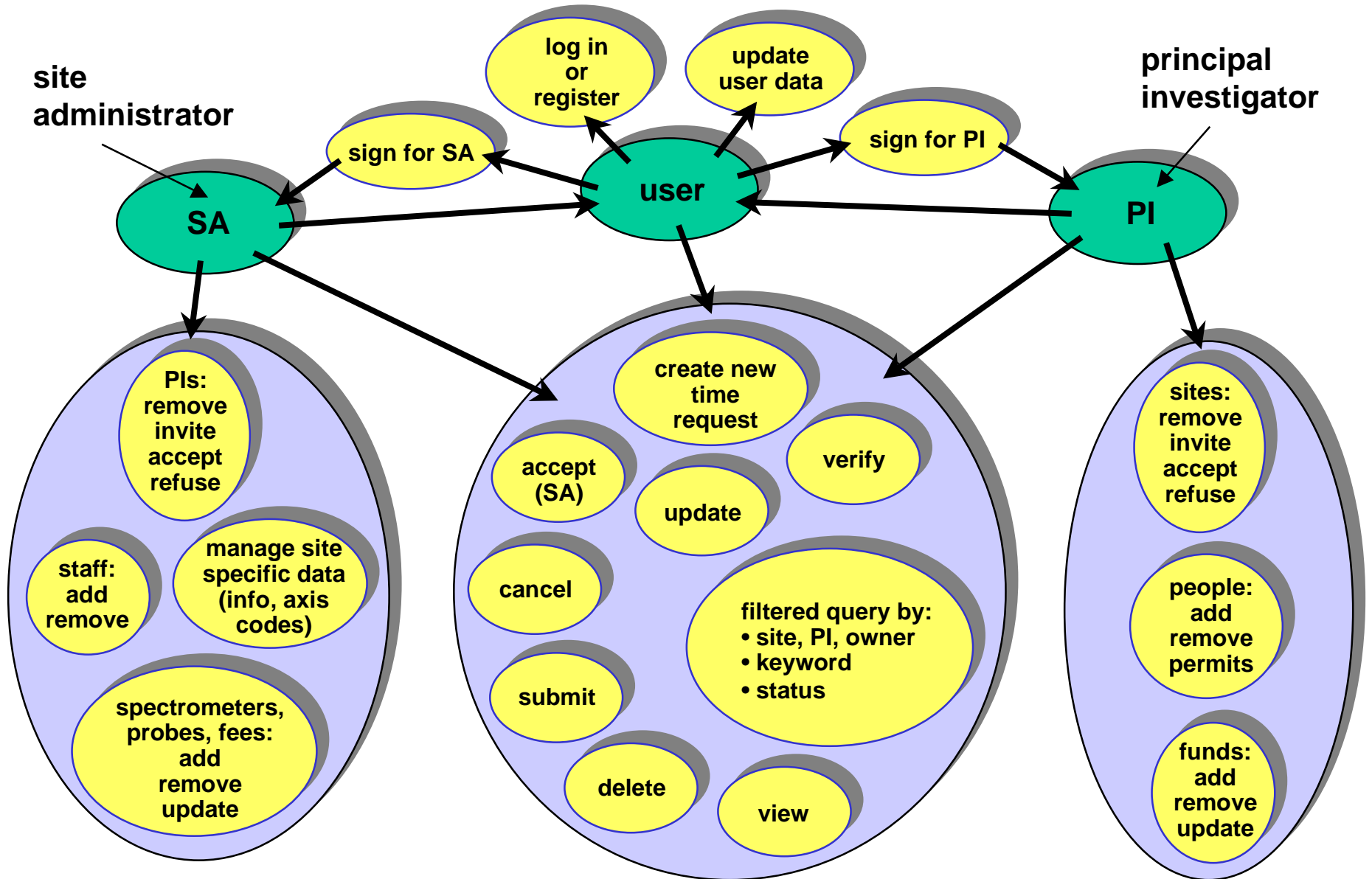
To properly service a diverse national user base, an instrumentation facility must have the capability to efficiently obtain requests from users for access to its instrumentation. Additionally, there is a need for obtaining information from users in turn for the purpose of generating activity reports to its granting agency. Finally, there is the need for a method of tracking instrument usage in order to maximize the efficient use of limited resources as well as gauging the equitability of allocated time throughout the user base.

The [Sand](#) application module is a facility time request system that provides multiple levels of access and functionality to users, principal investigators and site administrators while providing complete security of data throughout.

# Sand data objects



# Sand methods

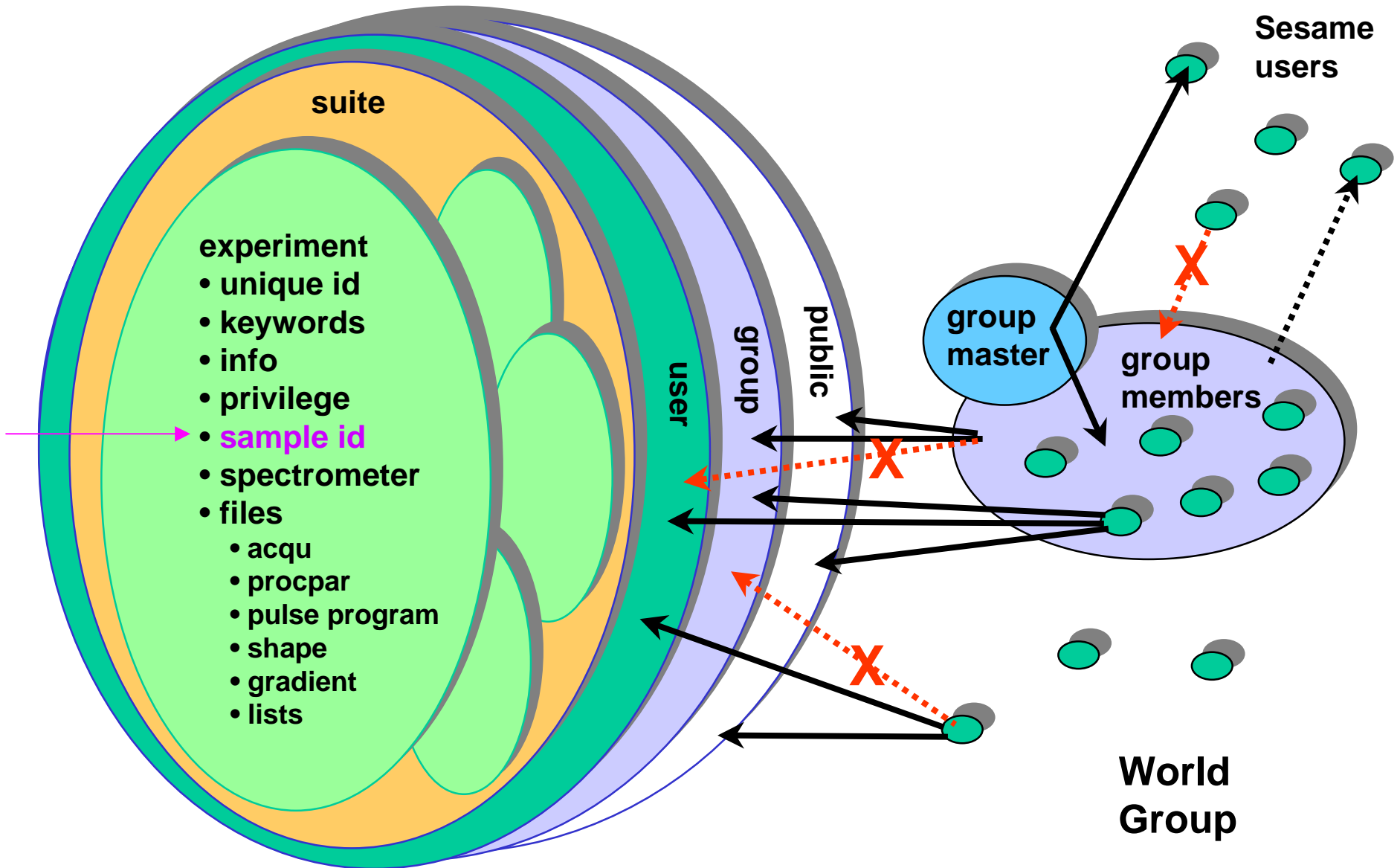


## Collaborative groups in Sesame

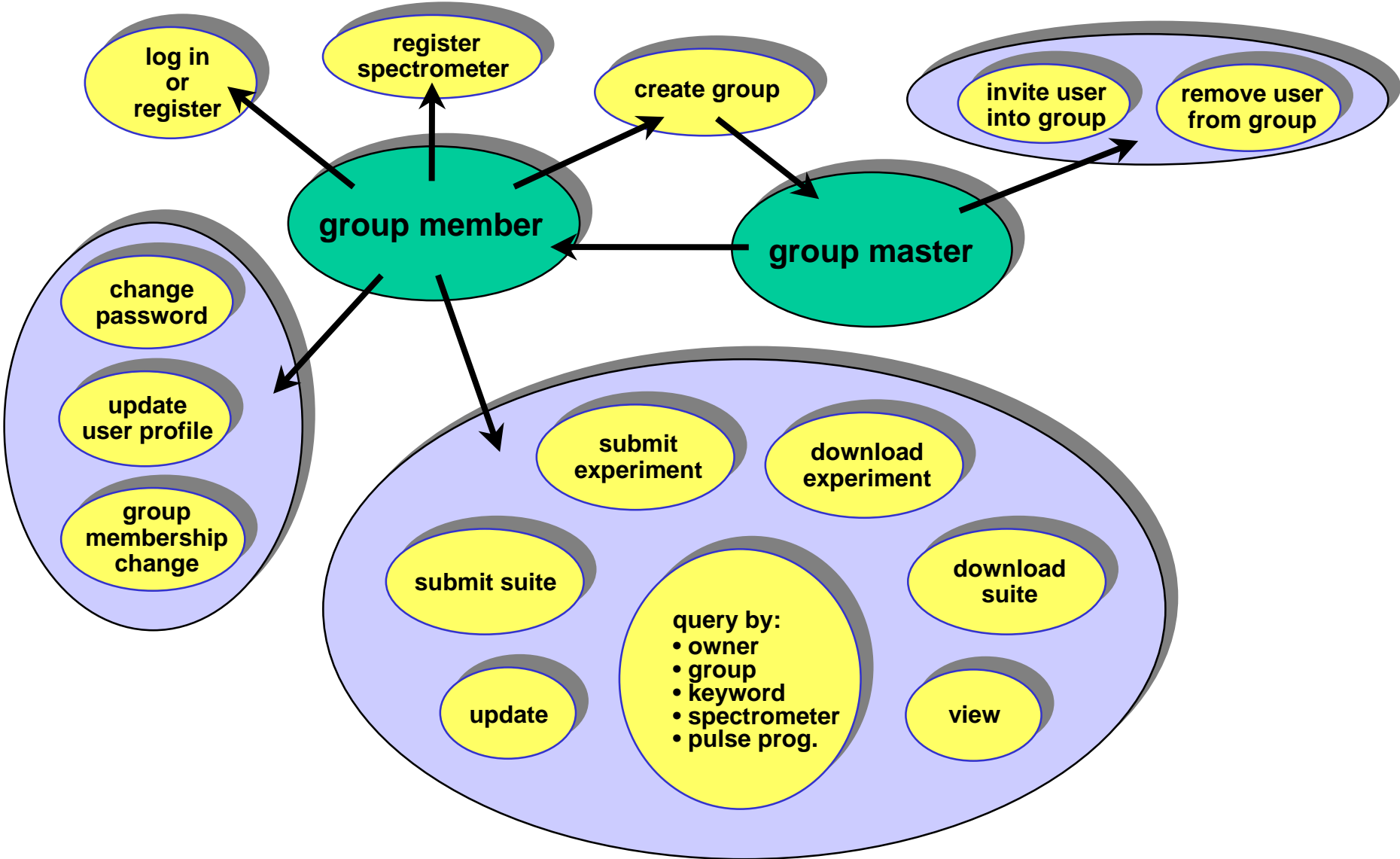
There are three privilege levels in the system: user, group and world. The privilege level controls access to information on the application modules in the system. Files marked by user privilege flags are visible to the owner, but invisible to other users who have no indication that the information is present. Users who have access to particular information (either by virtue of being a group member or world member) can upload it and become the owner of the copy. This copy can be stored by the user as is or modified prior to being stored. An owner can relax the current restriction on a data set, by setting the group or public flag. If a data set is public, it is downloadable by anyone, including a newly-registered user. The group flag helps to share data among virtual (e.g., far-flung collaborators on projects) or geographical (e.g., facility, department) groups. Every user can form a group, but can join one only if the owner of the group invites him. An invitation can be accepted, in which case the invited user becomes a member of a group, or it can be refused. Group members can resign from a group at any time. Also the owner of a group can remove any of the members. This way, the data sharing can be fully controlled at any level.

The **Camel** application module provides a solution to the problem of storing, recovering, and disseminating parameters used in NMR data acquisitions.

# Camel data objects



# Camel methods



# Screenshots

Ouroborus

Lamp

Jar

Sand

Camel