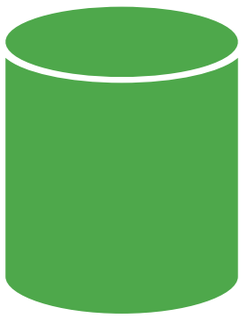
Wrap-up session

- Short tutorial & demo of MongoDB for those interested

- Hands-on help for installing Materials Project codes or mongoDB on your own systems

  - or any other questions you may have!

- `MPRester()` and `atomate` both use mongoDB
  - If you just want to use workflows, you only need:
    - a running mongoDB database
      - a basic understanding of query syntax
- But you can use mongoDB to store *any* kind of data
  - This session to be a short demo on how to do this
  - and how you can access your database in a general way *outside* `MPRester()` and `atomate`



A mongoDB database …

… contains collections …

of documents

A document: is not a file like a Word or Excel document

is more like a Python dict (or JSON file)

Setting up MongoDB

- **You don’t need to do this today, but in future…**

- For testing and development, you can run mongoDB locally: installation instructions on mongodb.com

  - very easy installation on macOS via homebrew: `brew install mongodb`

- For production, several options:

  - mongoDB as a service, both mlab.com and mongodb.com offer 500 MB mongoDB databases free to get started

  - many paid services exist, e.g. you can run your own mongoDB server with one-click setup on DigitalOcean (5$/mo. for 20 GB)

  - your local HPC facility may be able to help

pymongo

- `pymongo` is the standard way to interact with mongoDB via Python

- For now, we already have a mongoDB instance already running on the Jupyter Hub

  - Go to `mongo-primer/mongo-primer.ipynb`

Our Nobel example annotated

{} curly braces show we have a dict

our dictionary values are either strings

prizes is a list, because each laureate can have more than one prize

each individual prize is a dictionary containing information on that individual prize

dictionary keys are highlighted

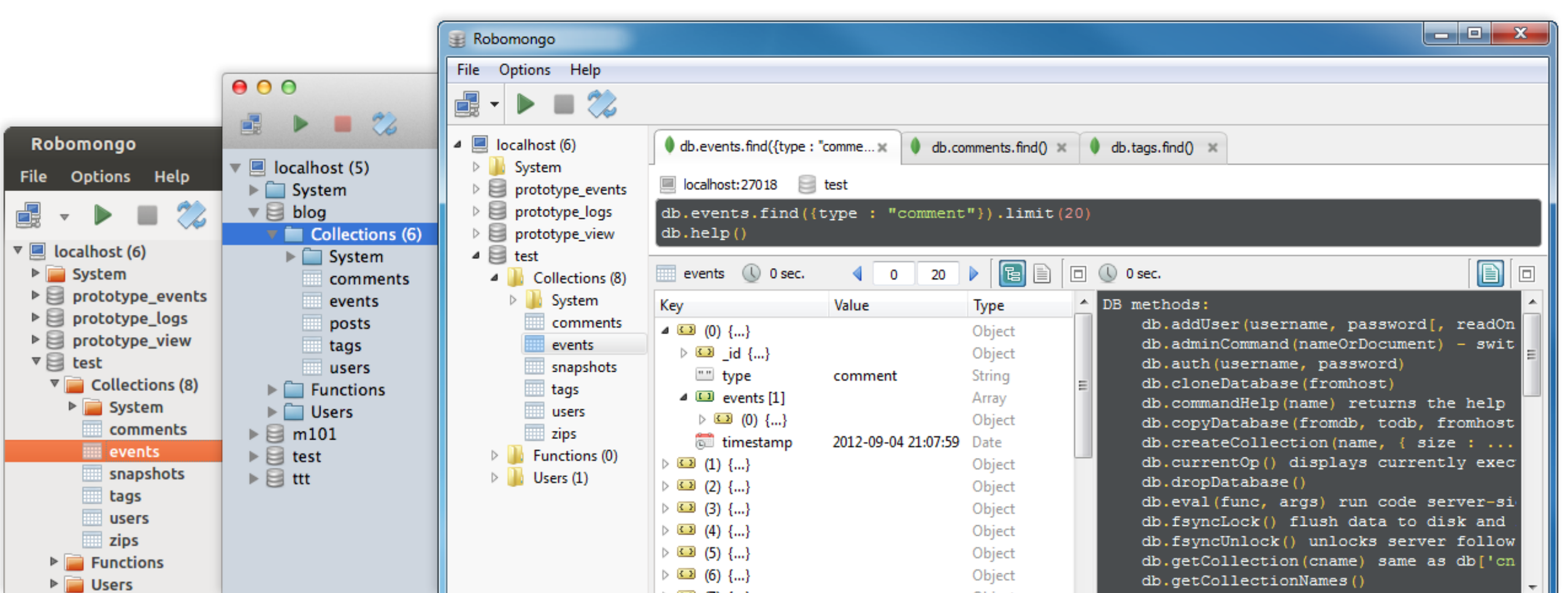
or our dictionary values can be lists (of more dictionaries)

similarily, affiliations is a list, because a laureate can have more than one affiliation

```
{'born': '1845-03-27',
 'bornCity': 'Lennep (now Remscheid)',
 'bornCountry': 'Prussia (now Germany)',
 'bornCountryCode': 'DE',
 'died': '1923-02-10',
 'diedCity': 'Munich',
 'diedCountry': 'Germany',
 'diedCountryCode': 'DE',
 'firstname': 'Wilhelm Conrad',
 'gender': 'male',
 'id': '1',
 'prizes': [
     {'affiliations':
         [{'city': 'Munich',
           'country': 'Germany',
           'name': 'Munich University'}],
      'category': 'physics',
      'motivation': '"in recognition of the extraordinary services he has
rendered by the discovery of the remarkable rays subsequently named after
him"',
      'share': '1',
      'year': '1901'}],
 'surname': 'Röntgen'}
```

Graphical Interface

- Several graphical interfaces available to browse data:
  - Our demo is using Robo 3T (formerly Robomongo), robomongo.org



Questions? 🤔