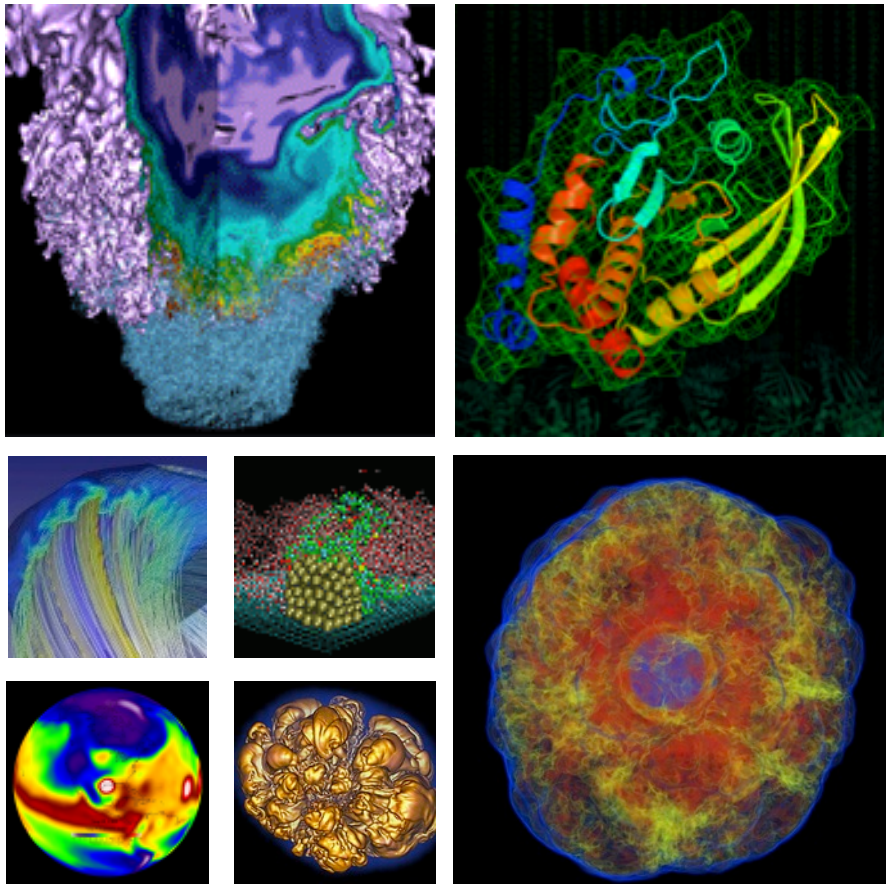
Databases and Data analytic frameworks at NERSC



Yushu Yao (yyao@lbl.gov)

NERSC Data Analytic Services

Big and Diverse Computing Facility
6000+ Users, 700+ Projects
3+ PetaFlops (20+pf more coming)
50+ PB Storage

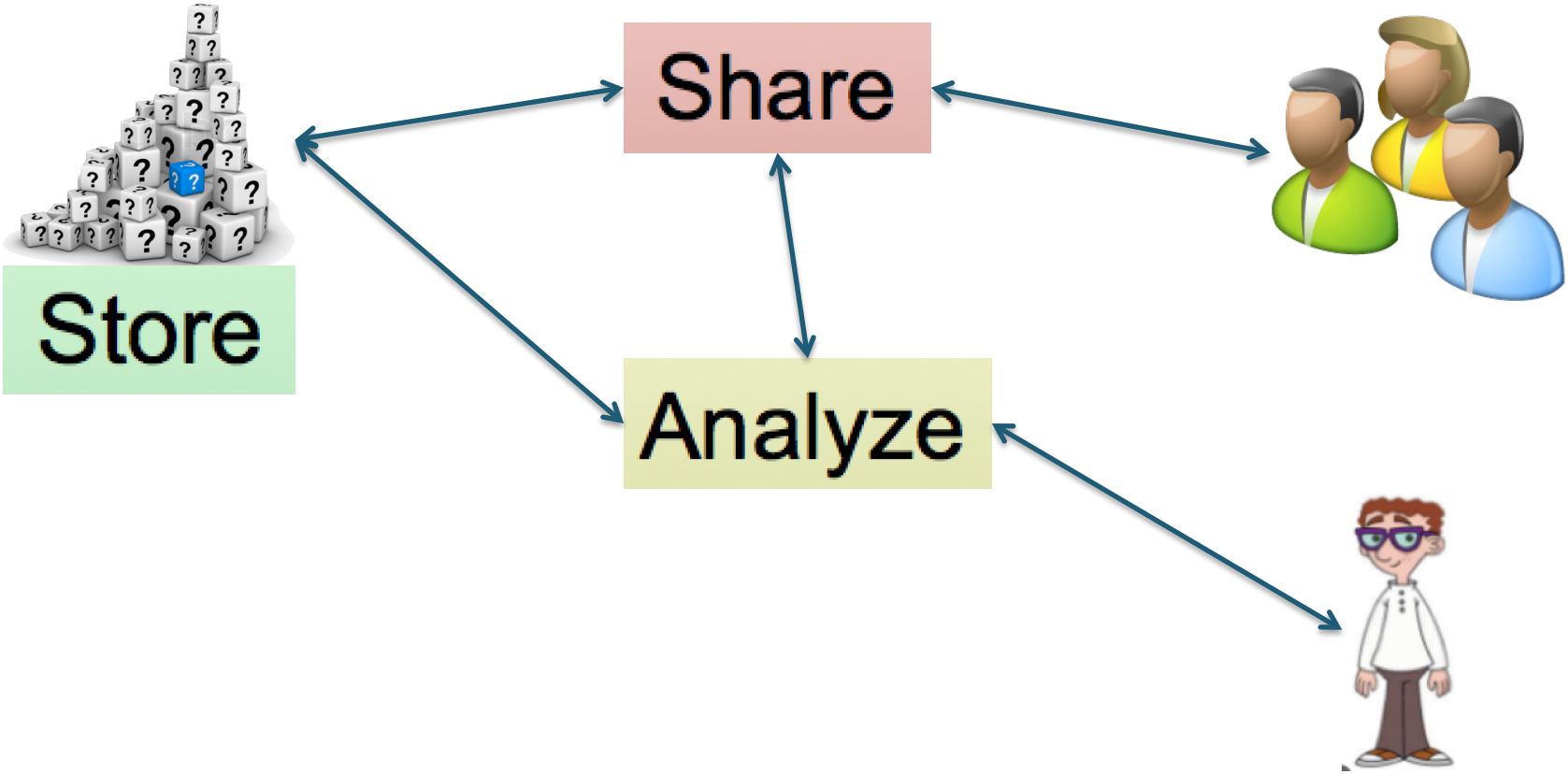
Production Data Services

Science Engagement

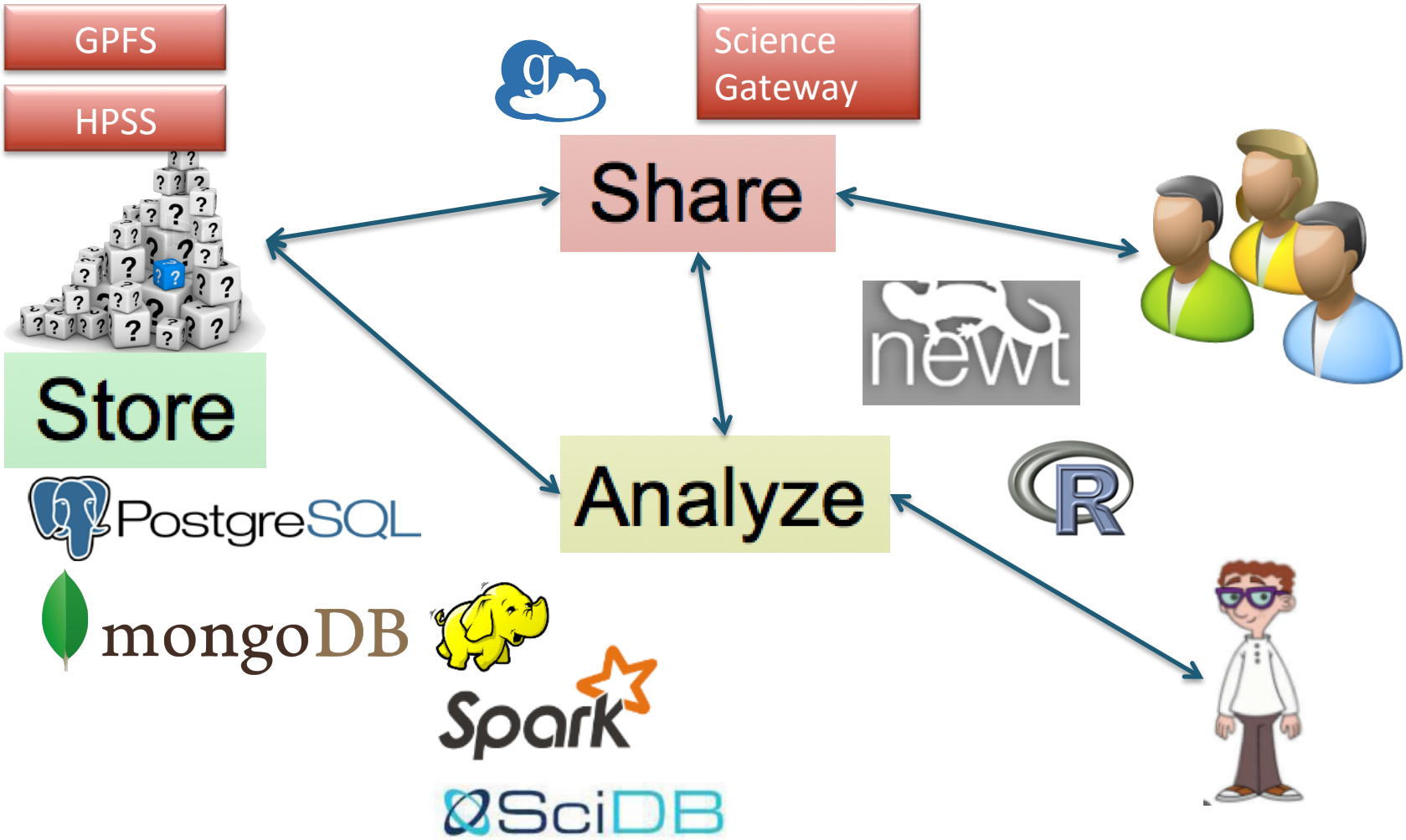
Usability Scale

Management Analysis Share

Store/Share/Analyze Data At NERSC



Store/Share/Analyze Data At NERSC



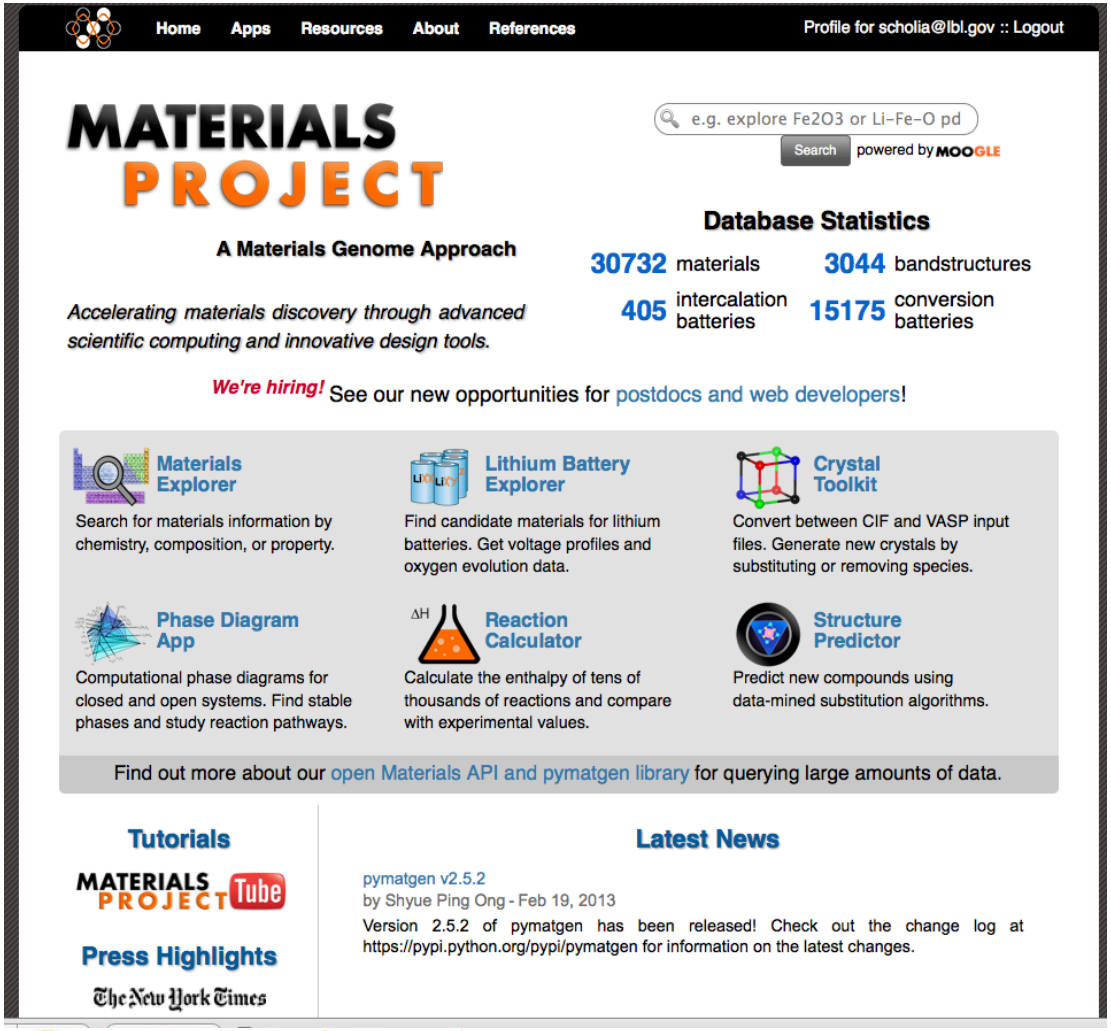
Science Gateway Services

- **Publish data on the web**
  - Create a www directory in your project space and put your data on the web
- **Build sophisticated web portals**
  - Build full stack web applications for your science at NERSC using Python/Django, PHP, Ruby on Rails
- **NEWT – the NERSC REST API**
  - Use the NEWT REST HTTP API to access NERSC HPC resources directly from your web apps.
  - Support for Authentication, Jobs, Commands, Files, Persistent Store, NIM, System Information at NERSC

Gateway examples - http://portal.nersc.gov
NEWT – https://newt.nersc.gov
Science Gateway information http://www.nersc.gov/users/science-gateways/

Example Gateway: Materials Project

http://www.materialsproject.org



- Web Server Hosted at NERSC
- Jobs Submitted to NERSC Systems as needed
- Data Stored in different DB and Storage Systems
- **You can do this too**

Traditional SQL Database Services

- **PostgreSQL and MySQL**

- **Good For:**
  - Structured, Relational Data
  - Mid-Size, <=several GB in total
  - Transactional Operations

MongoDB

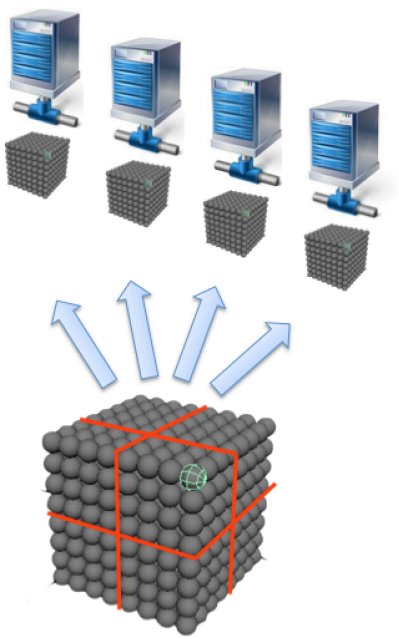
- **Key-value pair / Text database**

- **Good For:**
  - Un-Structured, Text Data
  - Mid-Size to Large, e.g. 10 GB of Text
  - E.g: for metadata that has ever changing schema

To request a MongoDB/PostgreSql/MySQL database:
https://www.nersc.gov/users/science-gateways/science-gateway-databases/

SciDB For High Usability Big Data Analytic

- **Why?** It's painful to manage and analyze terabytes of data. Need a unified solution that's easy to use.
- **What?** SciDB is a parallel database for array-structured data, great for **Terabytes** of:
  - **Time series, spectrums, imaging**, etc
- The greatest benefit of SciDB is:
  - **Usability**: Use HPC hardware without learning parallel programming and parallel I/O.



SciDB Distribute a big array on many nodes

Spark for In-Memory Map-Reduce

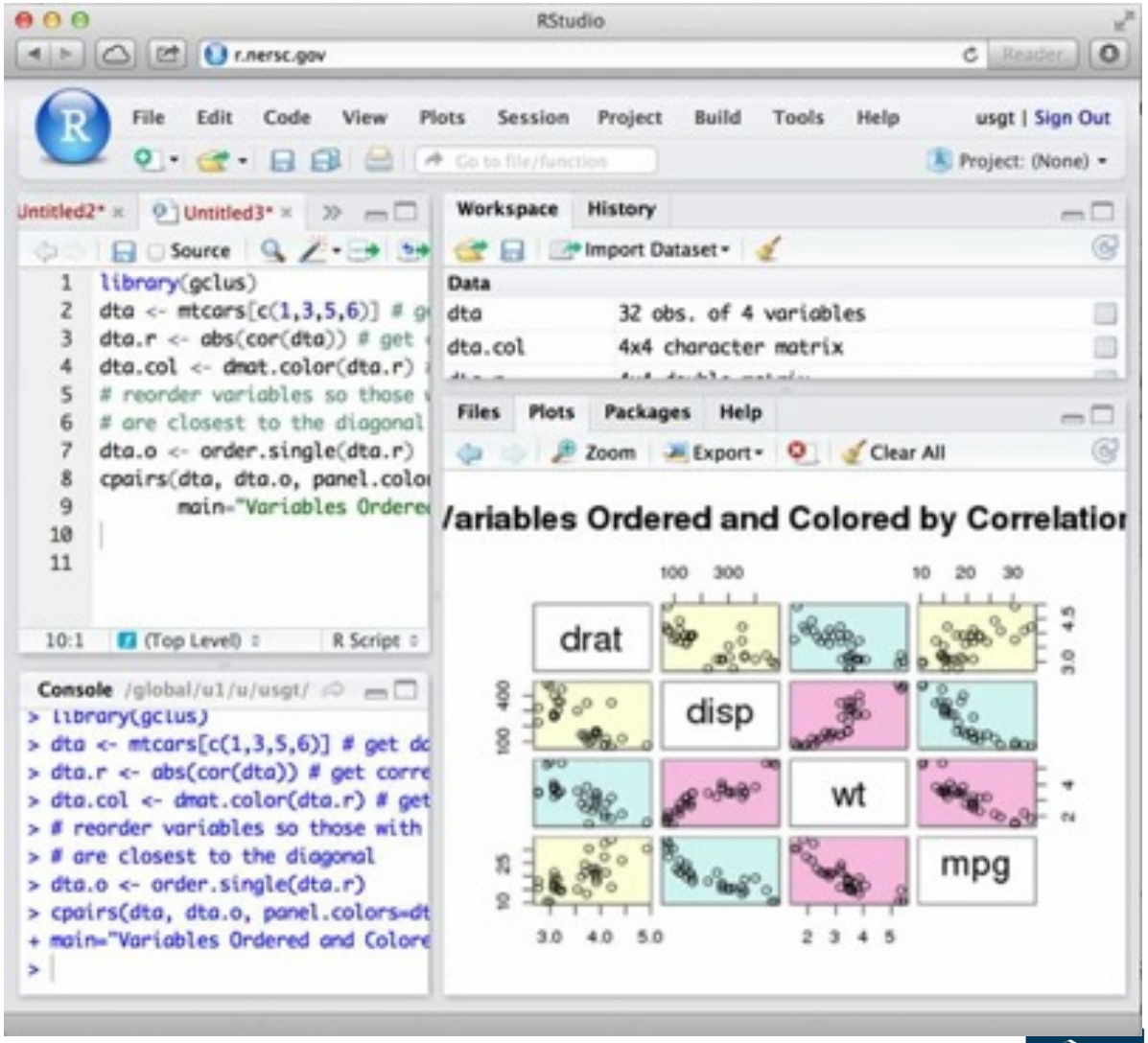
Lightning-Fast Cluster Computing

https://www.nersc.gov/users/software/data-visualization-and-analytics/spark-distributed-analytic-framework

- **Very efficient in-memory map-reduce data analytic framework.**

RStudio Service(Beta) – r.nersc.gov

Any NERSC user can go to r.nersc.gov and login with NIM Username/Password



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iPythonNotebook Service (Coming Soon)

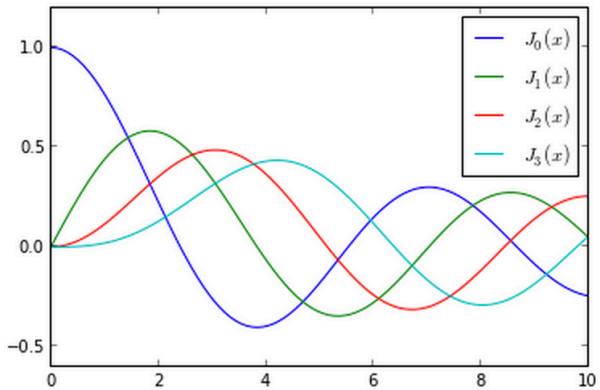
IP[y]: Notebook Lecture_3_Scipy (autosaved) Logout

File Edit View Insert Cell Kernel Help

Markdown Cell Toolbar: None Env: np18py27-1.9

In [6]:
```
x = linspace(0, 10, 100)

fig, ax = subplots()
for n in range(4):
    ax.plot(x, jn(n, x), label=r"$J_%d(x)$" % n)
ax.legend();
```



In [7]:
```
# zeros of Bessel functions
n = 0 # order
m = 4 # number of roots to compute
jn_zeros(n, m)
```

Out[7]:
```
array([  2.40482556,   5.52007811,   8.65372791,  11.79153444])
```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Links

- **Science Gateways:**
  - http://www.nersc.gov/users/science-gateways/
- **Database Request Form**
  - https://www.nersc.gov/users/science-gateways/science-database-request-form/
- **SciDB**
  - http://www.nersc.gov/users/computational-systems/testbeds/scidb/
- **Rstudio**
  - http://r.nersc.gov
- **Spark**
  - https://www.nersc.gov/users/software/data-visualization-and-analytics/spark-distributed-analytic-framework/