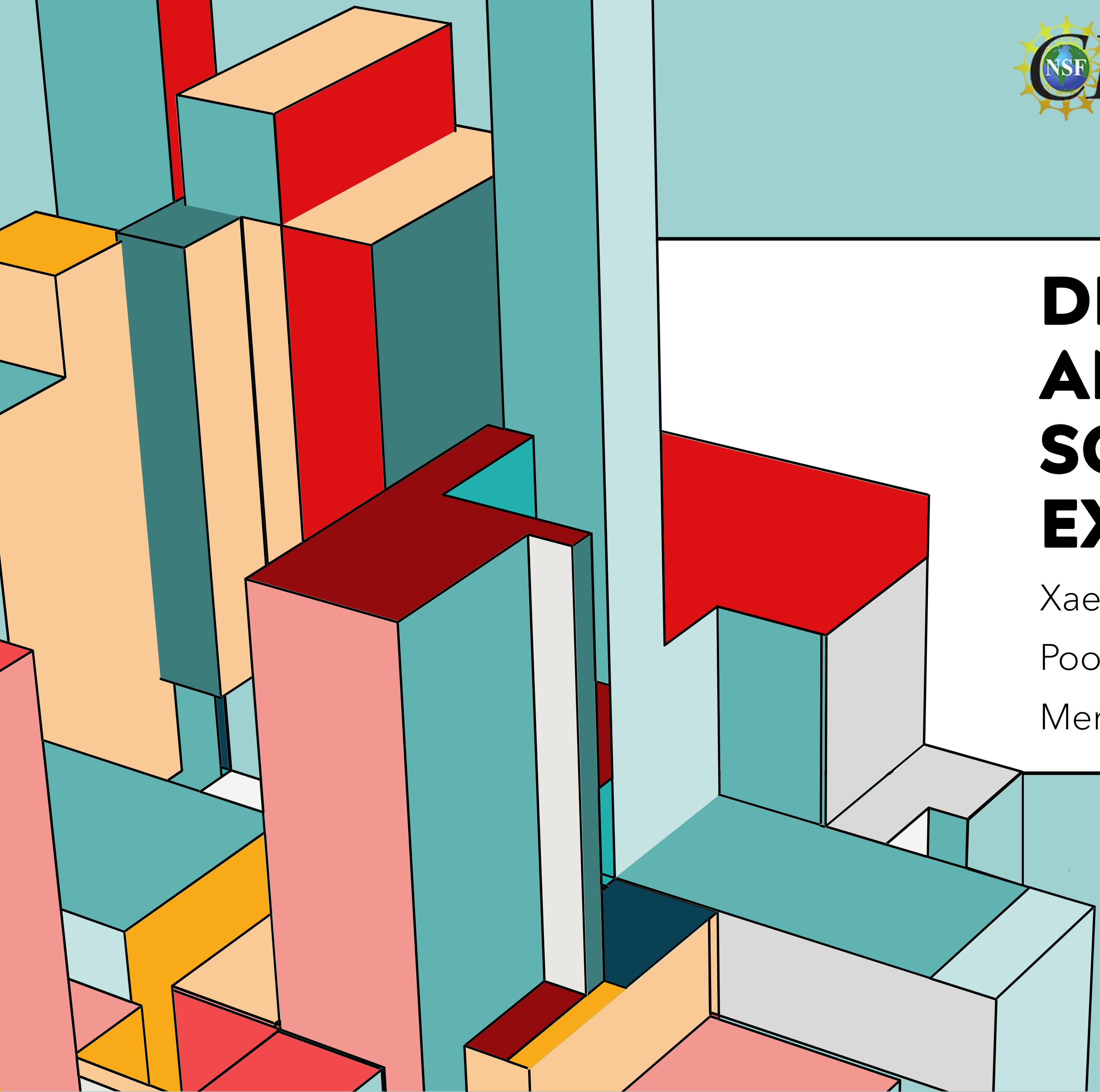


# DEVELOPING AN ANALYSIS SOFTWARE'S API EXTENSION

Xael Shan

Poolesville Highschool

Mentor - Jeff Krzywon, Elizabeth Kelley

# SASVIEW OVERVIEW

## What is SANS?

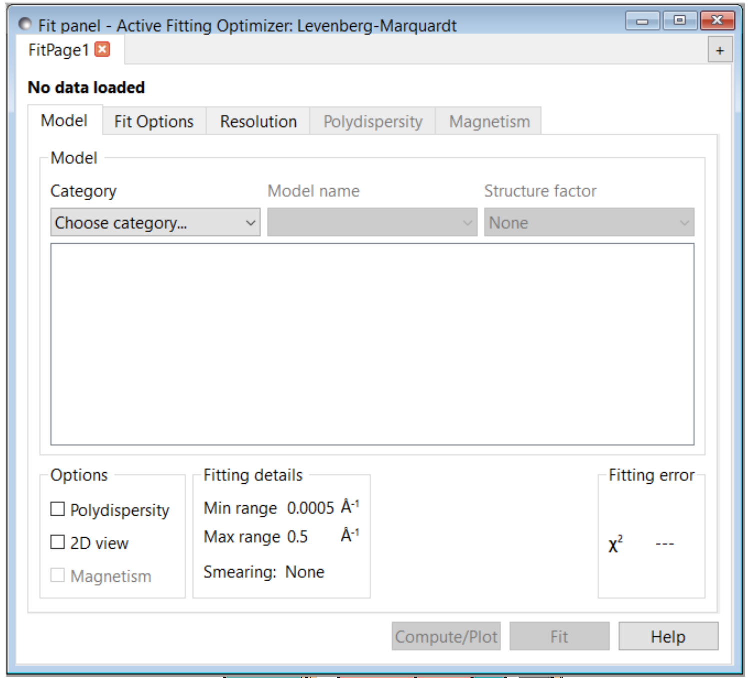
NCNR is a user facility that uses neutron scattering: Small Angle Neutron Scattering (SANS)

- Shoots neutron through a sample

## What is SasView?

SasView is an analysis software that takes the data from SANS:

- Analysis Tools
    - Fit
- SasCalc Tools



No data loaded

Category: Choose category...
Structure factor: None

☐ Polydispersity
☐ 2D view
☐ Magnetism

Min range 0.0005 $Å^{-1}$
Max range 0.5 $Å^{-1}$
Smearing: None

$\chi^2$ ---

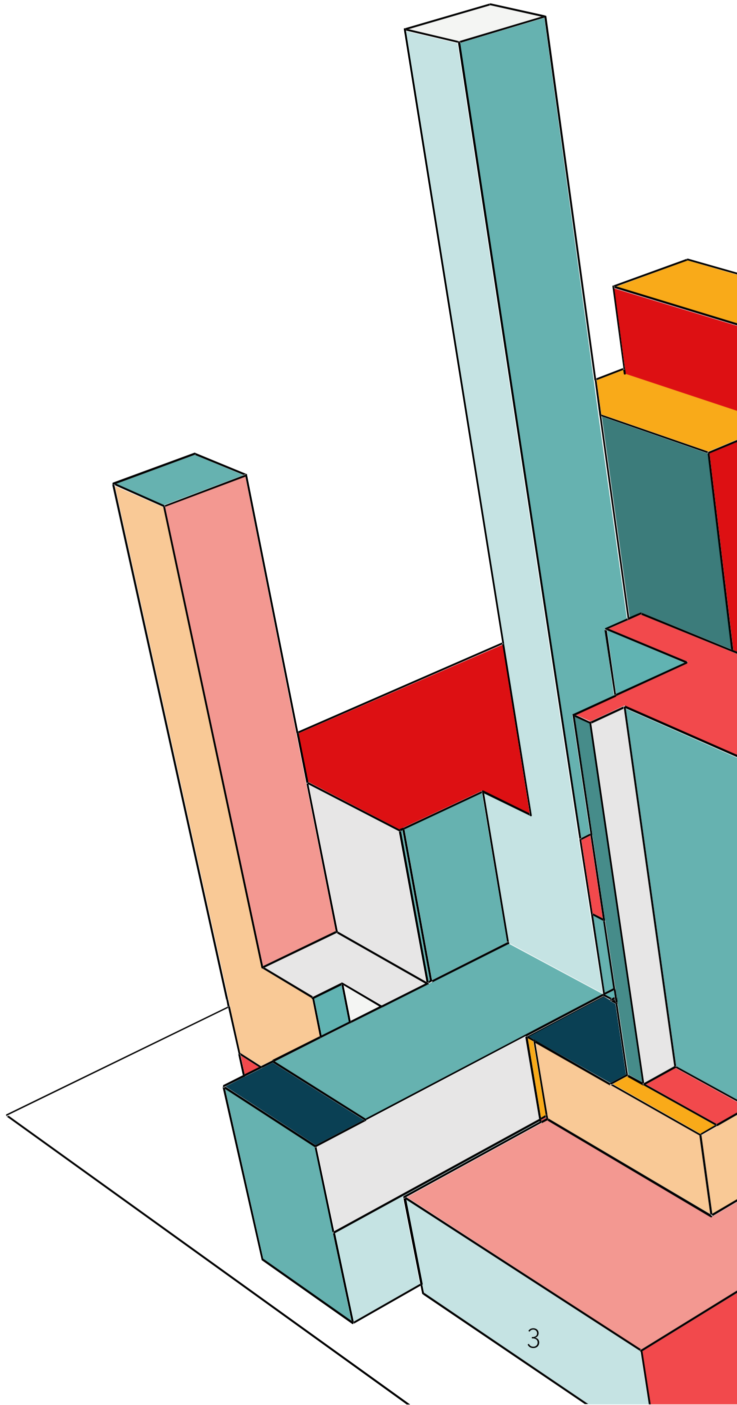
## PROJECT OVERVIEW

### The Project

Create a website-based application to give more control and flexibility to extend Sasview functions

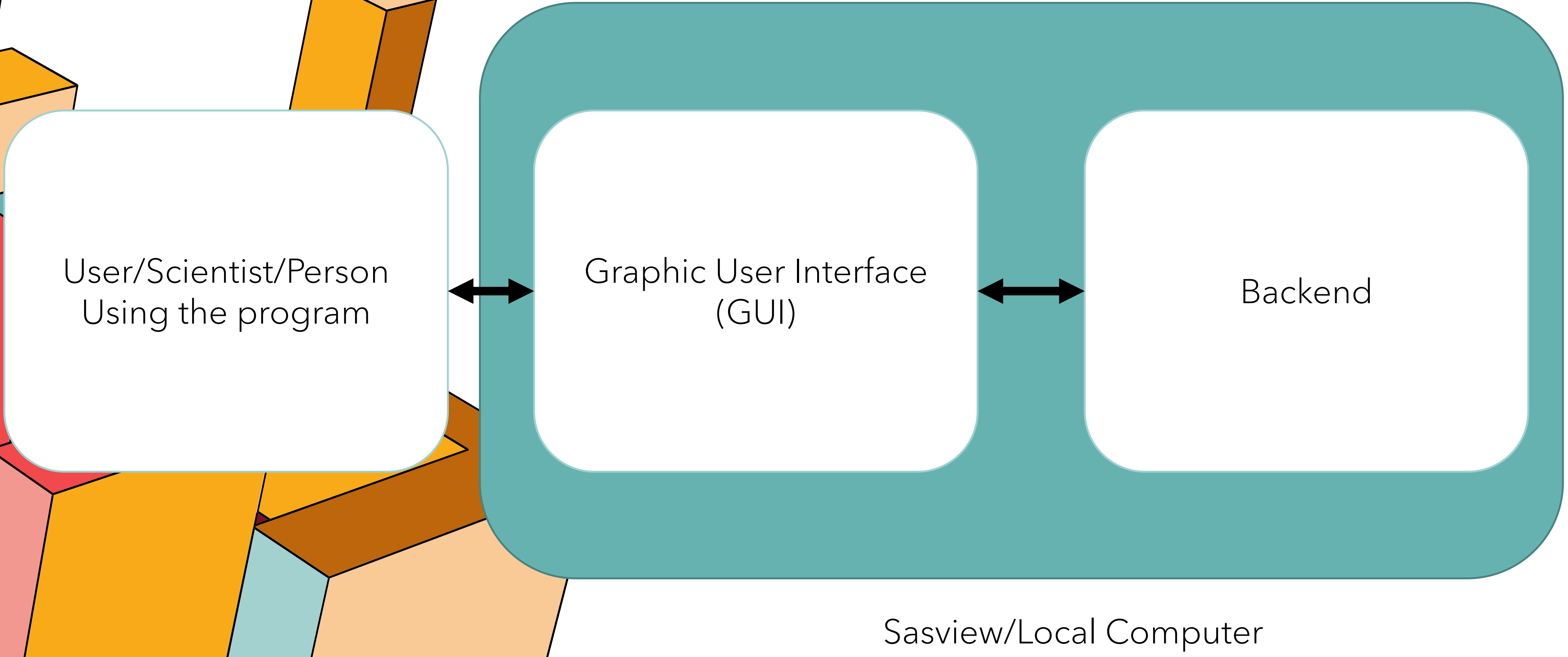
### Goals

- Create a working model of a website-based application
- Use application to analyze bicelle data
- Future Publish API

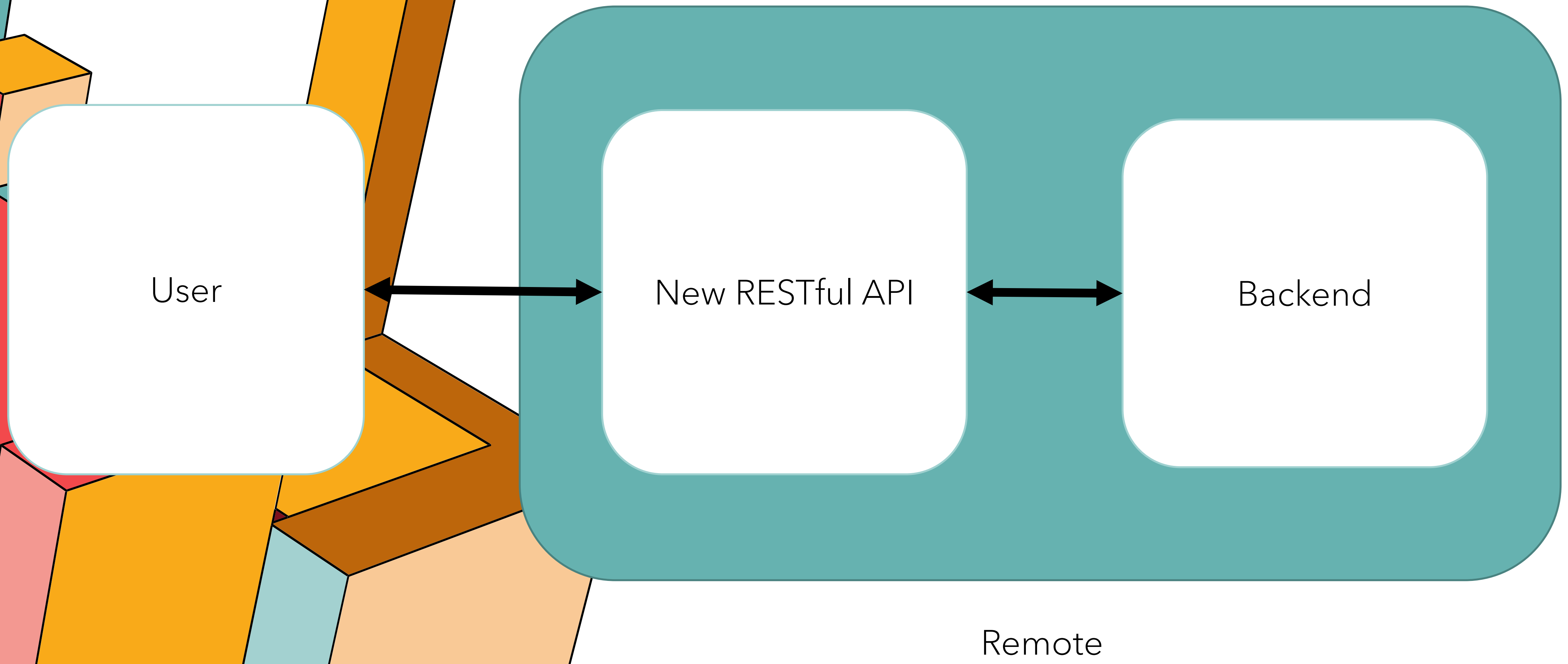


CHRNS CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING NIST

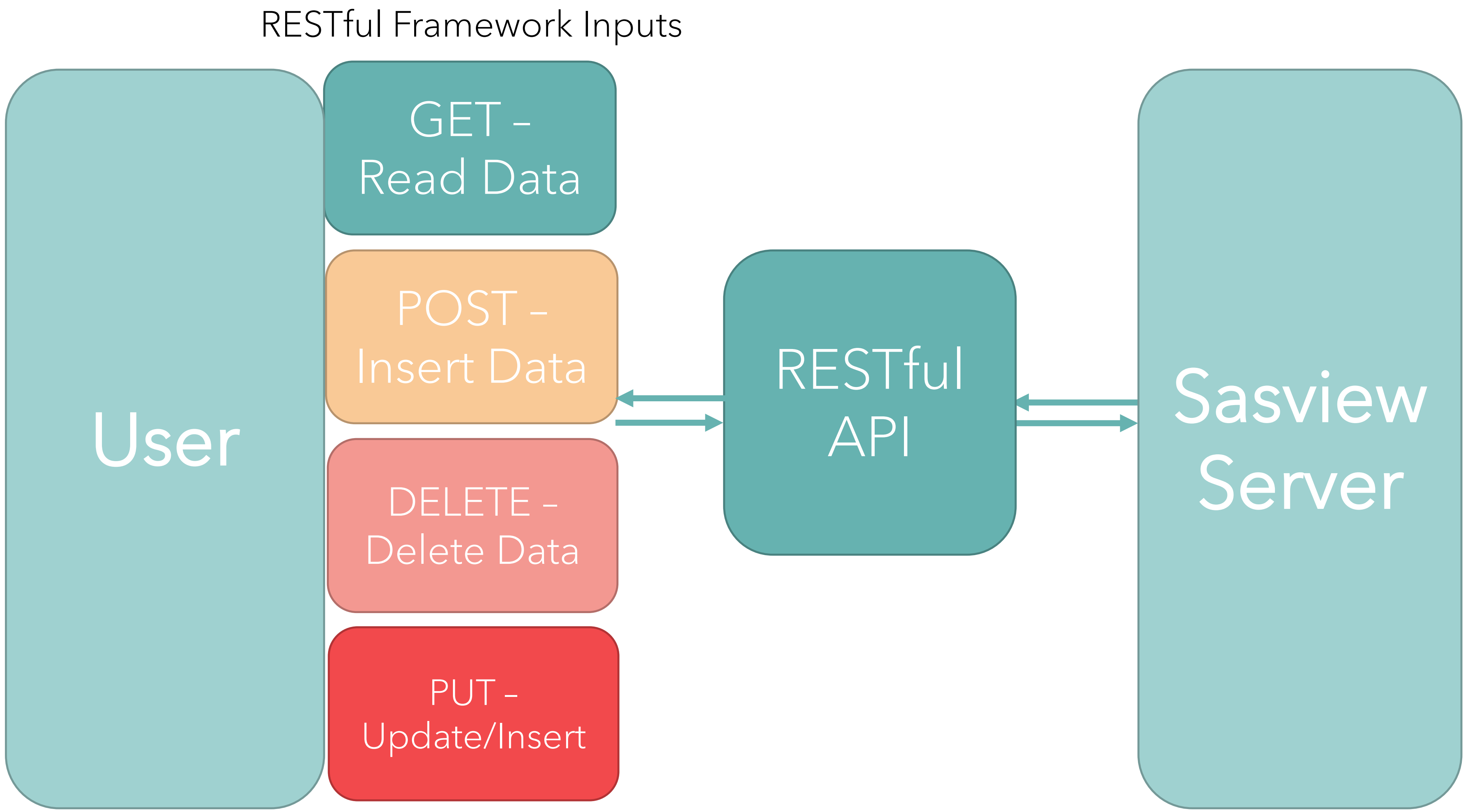
## Current Layout


User/Scientist/Person Using the program
Graphic User Interface (GUI)
Backend
Sasview/Local Computer

# Proposed Layout



# WHAT IS AN API



## WHY DO MORE?

Why create "another" Sasview

**Accessible**

**Experimental benefits**

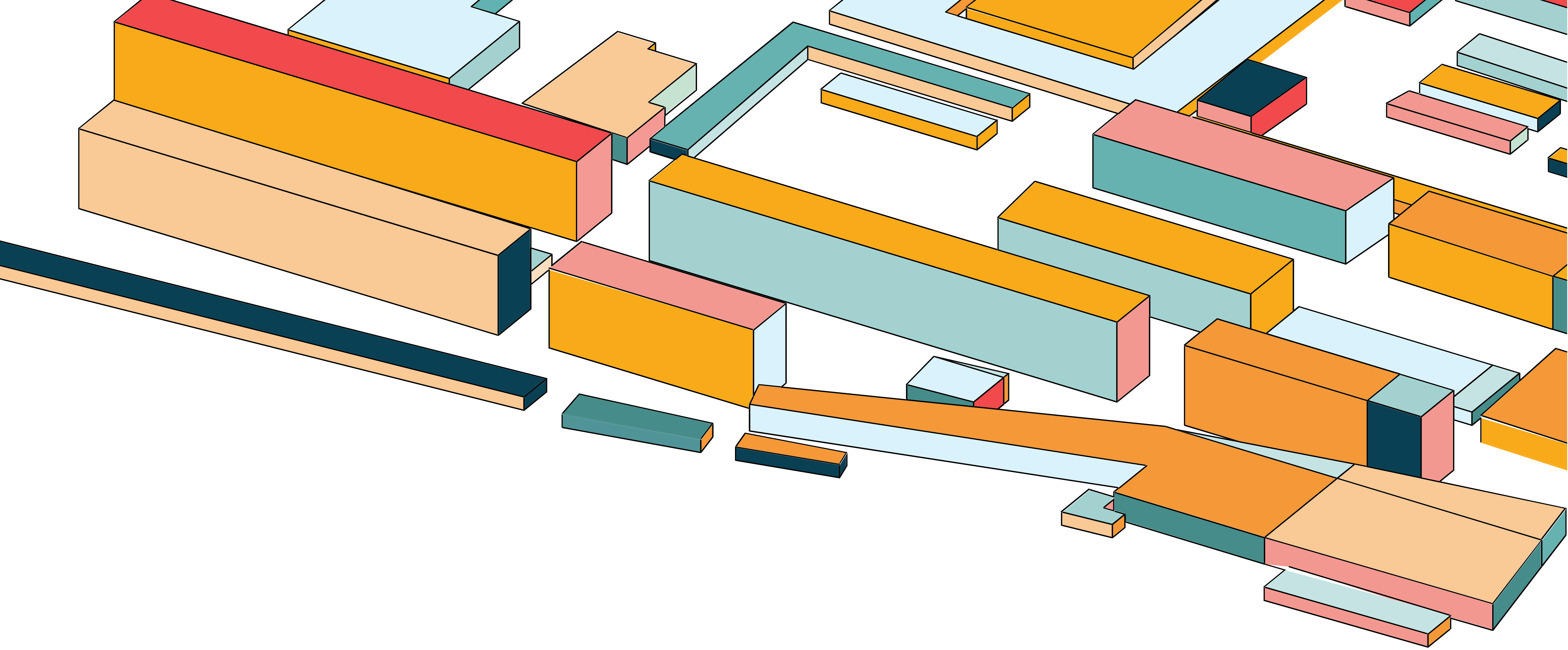
**Operating System Deployment**

Alleviate Resources

Non-Equilibrium (Structure of Materials) Initiative

Overcomes Window, Linux, Mac Requirements

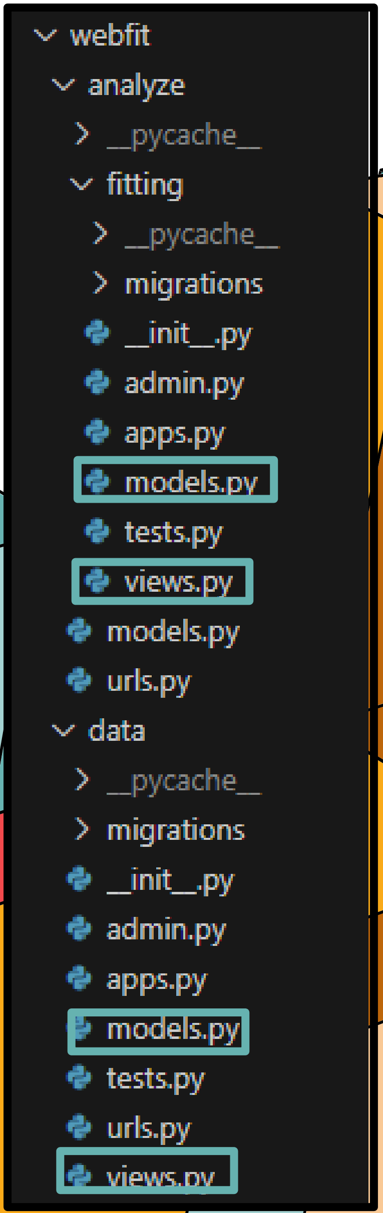
Automation!



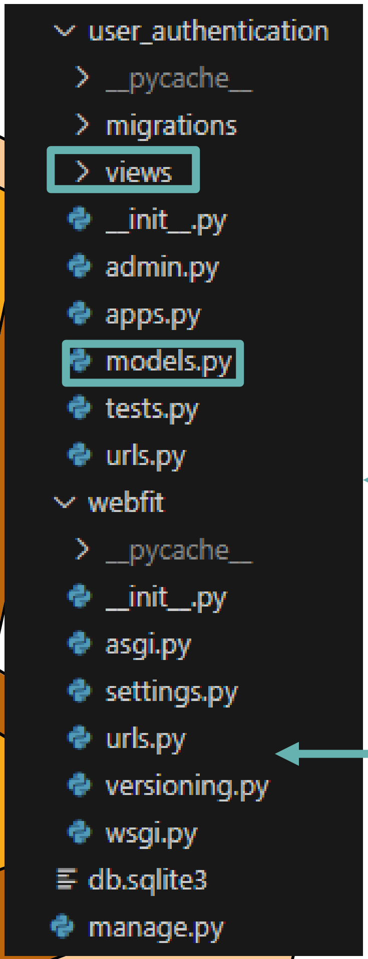
## MAKING THE API

# DJANGO

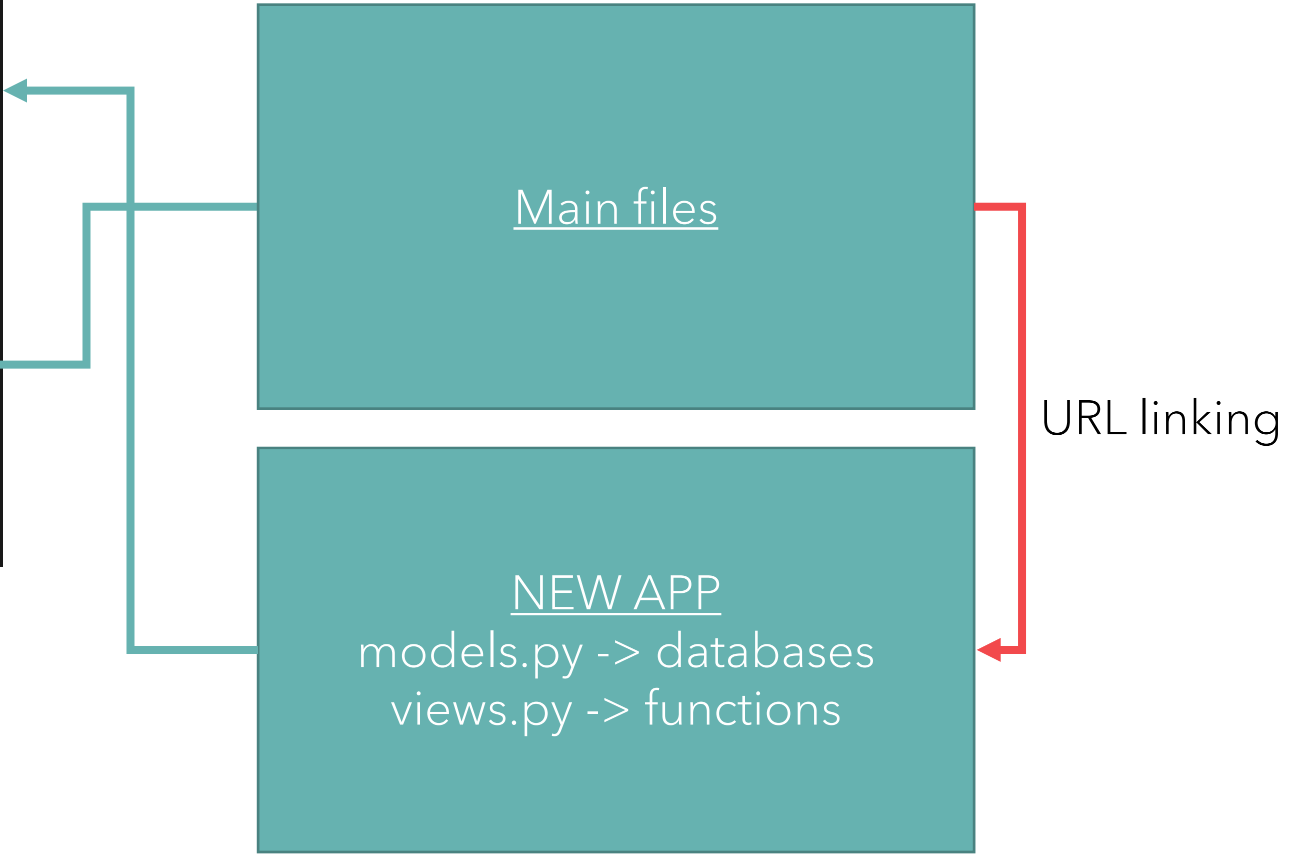
Modularity!



```
webfit
  analyze
    __pycache__
    fitting
      __pycache__
      migrations
      __init__.py
      admin.py
      apps.py
      models.py
      tests.py
      views.py
    models.py
    urls.py
  data
    __pycache__
    migrations
    __init__.py
    admin.py
    apps.py
    models.py
    tests.py
    urls.py
    views.py
```

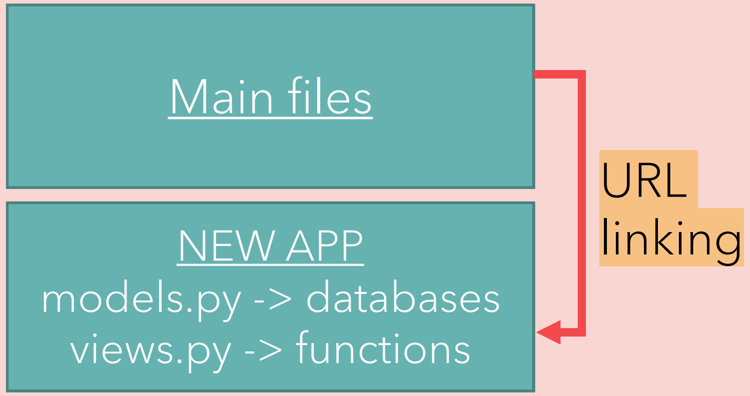


```
user_authentication
  __pycache__
  migrations
  views
  __init__.py
  admin.py
  apps.py
  models.py
  tests.py
  urls.py
webfit
  __pycache__
  __init__.py
  asgi.py
  settings.py
  urls.py
  versioning.py
  wsgi.py
db.sqlite3
manage.py
```



# WHAT I IMPLEMENTED

How this was made from scratch



## Urls

- Links everything together!
- Allows the user to get to function

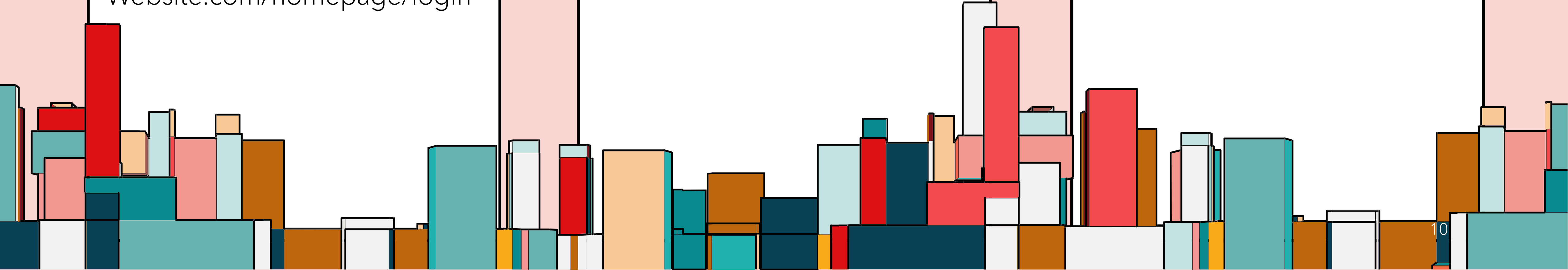
Website.com/homepage/
Website.com/homepage/login

## Models.py

- Database structure
- Define what the user inputs
- Make sure user can't put in malicious data

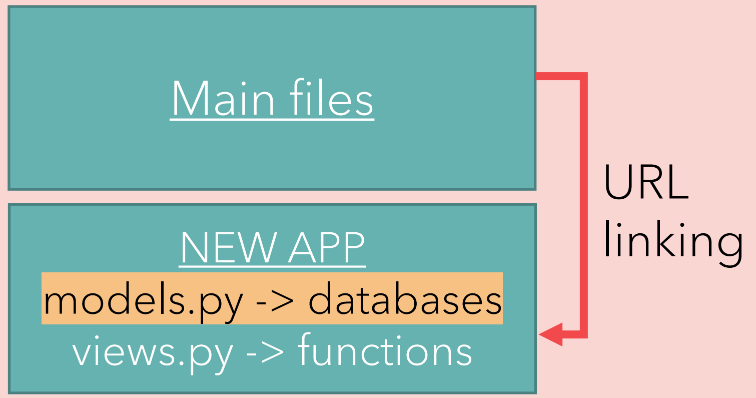
## Views.py

- Translator
- Puts into databases
- Defines how user's data looks



# WHAT I IMPLEMENTED

How this was made from scratch



## Urls

- Links everything together!
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Website.com/homepage/
Website.com/homepage/login

## Models.py

- Database structure
- Define what the user inputs
- Make sure user can't put in malicious data

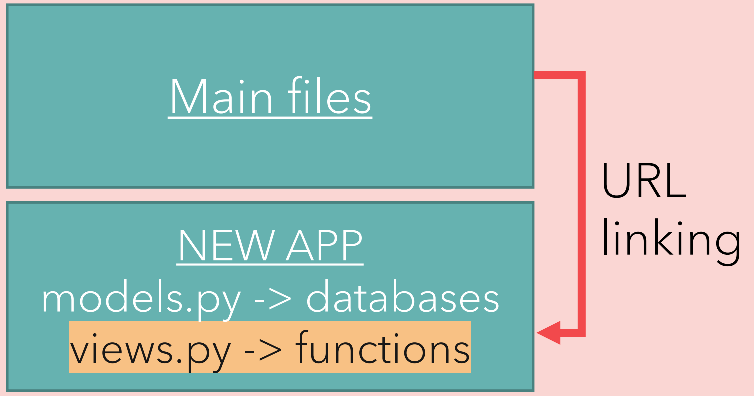
## Views.py

- Translator
- Puts into databases
- Defines how user's data looks

| Data id | user | file | file_name | is_public |
|---|---|---|---|---|
| 1 | None | <File_obj> | Data.txt | True |
| 2 | None | | | |
| 3… | None | | | |

# WHAT I IMPLEMENTED

How this was made from scratch



## Urls

- Links everything together!
- Allows the user to get to function

Website.com/homepage/
Website.com/homepage/login

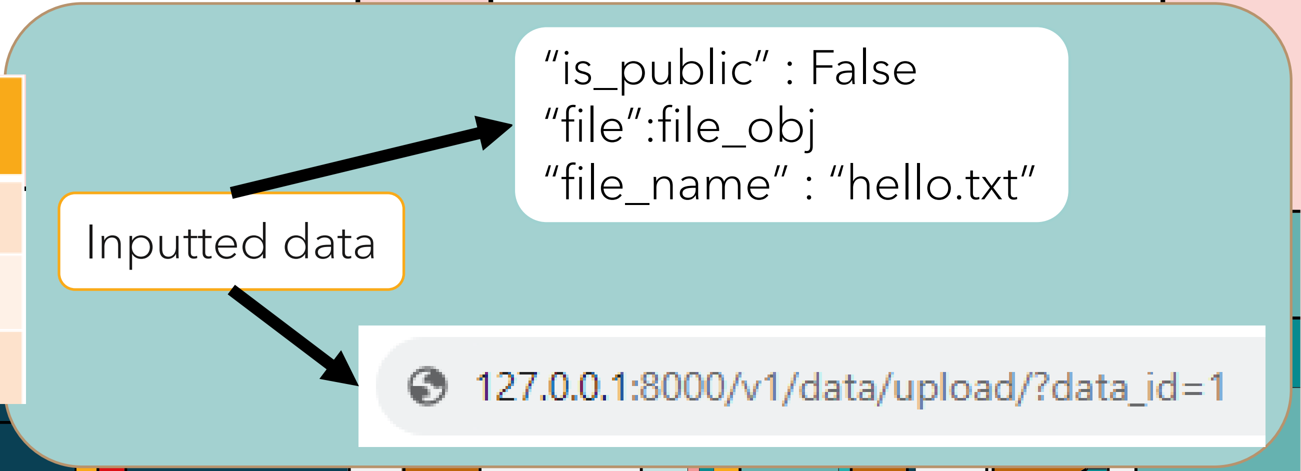
## Models.py

- Database structure
- Define what the user inputs
- Make sure user can't put in malicious data

## Views.py

- Translator
- Puts into databases
- Defines how user's data looks

| Data id | user | file | file_name | is_public |
|---|---|---|---|---|
| 1 | None | <File_obj> | Data.txt | True |
| 2 | None | <File_obj> | Hello.txt | False |
| 3… | None | | | |



"is_public" : False
"file":file_obj
"file_name" : "hello.txt"

127.0.0.1:8000/v1/data/upload/?data_id=1

# WHERE ARE WE NOW!

**1**

Database

Created!

**2**

Views

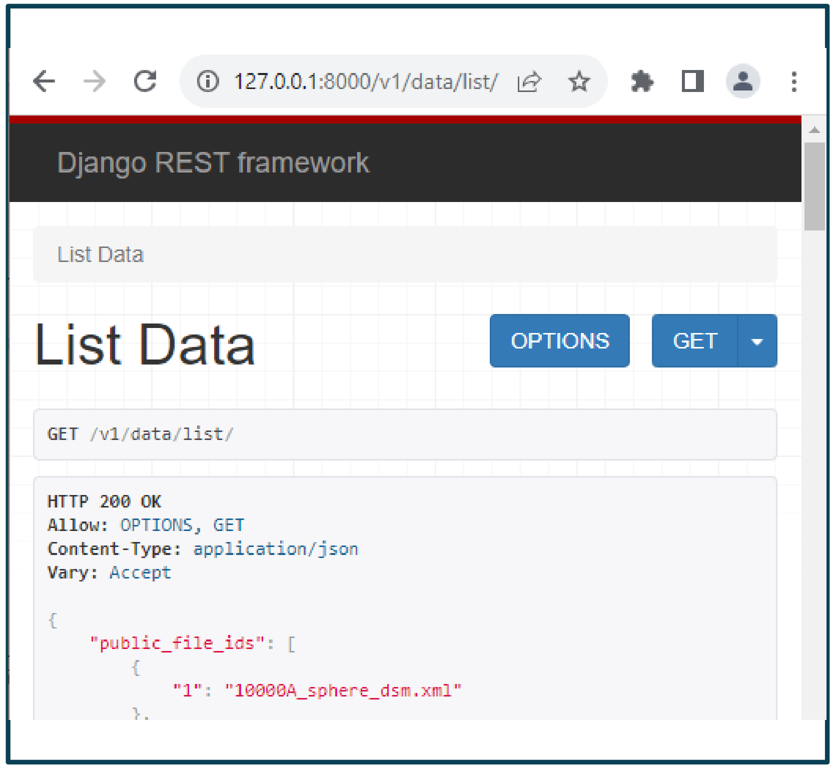
Written!

**3**

Let's show it working!

The working model

# MULTIPLE WAYS TO BE A USER

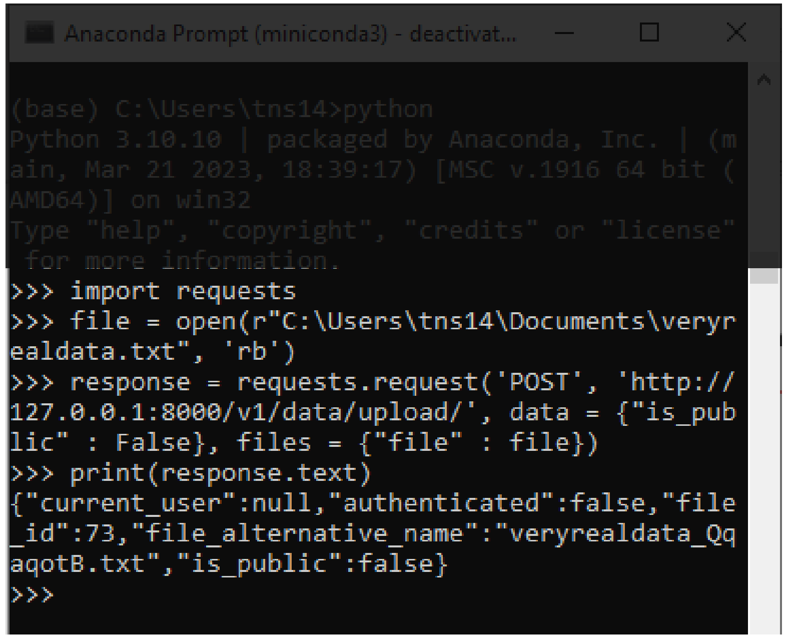


# List Data

```
GET /v1/data/list/
```

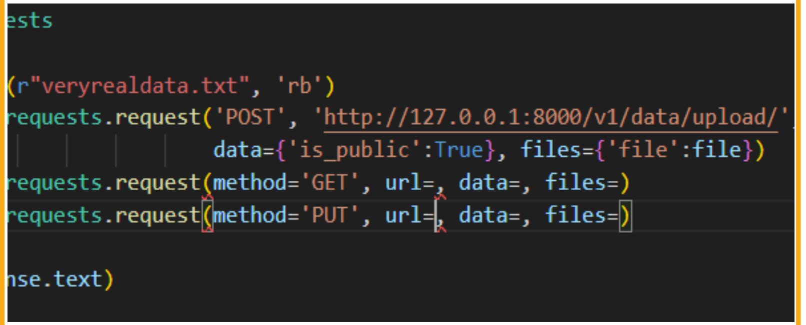
```
HTTP 200 OK
Allow: OPTIONS, GET
Content-Type: application/json
Vary: Accept

{
    "public_file_ids": [
        {
            "1": "10000A_sphere_dsm.xml"
        },
```

Development Server: API view



```
(base) C:\Users\tns14>python
Python 3.10.10 | packaged by Anaconda, Inc. | (m
ain, Mar 21 2023, 18:39:17) [MSC v.1916 64 bit (
AMD64)] on win32
Type "help", "copyright", "credits" or "license"
 for more information.
>>> import requests
>>> file = open(r"C:\Users\tns14\Documents\veryr
ealdata.txt", 'rb')
>>> response = requests.request('POST', 'http://
127.0.0.1:8000/v1/data/upload/', data = {"is_pub
lic" : False}, files = {"file" : file})
>>> print(response.text)
{"current_user":null,"authenticated":false,"file
_id":73,"file_alternative_name":"veryrealdata_Qq
aqotB.txt","is_public":false}
>>>
```

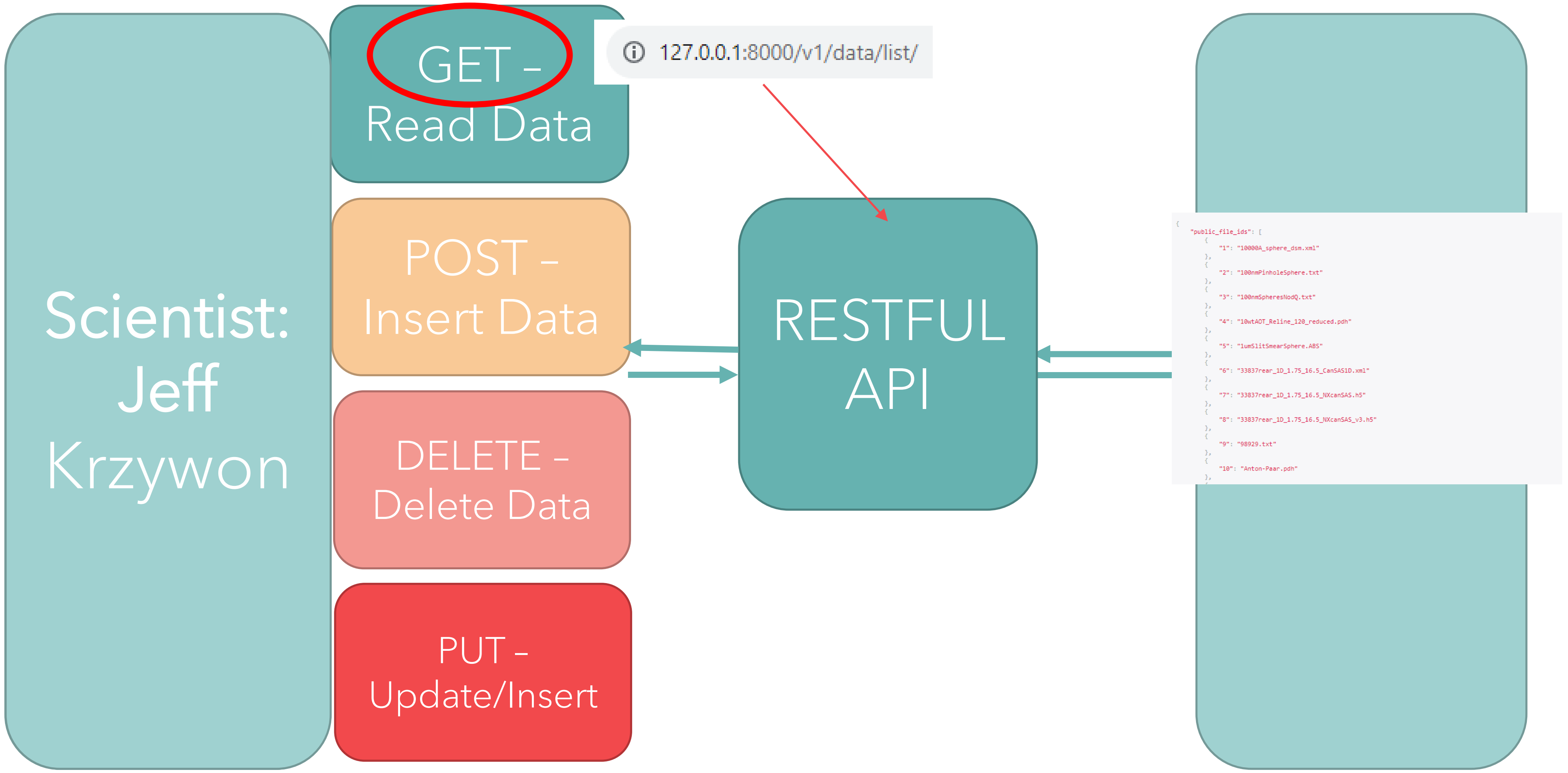
Terminal/Command pallet



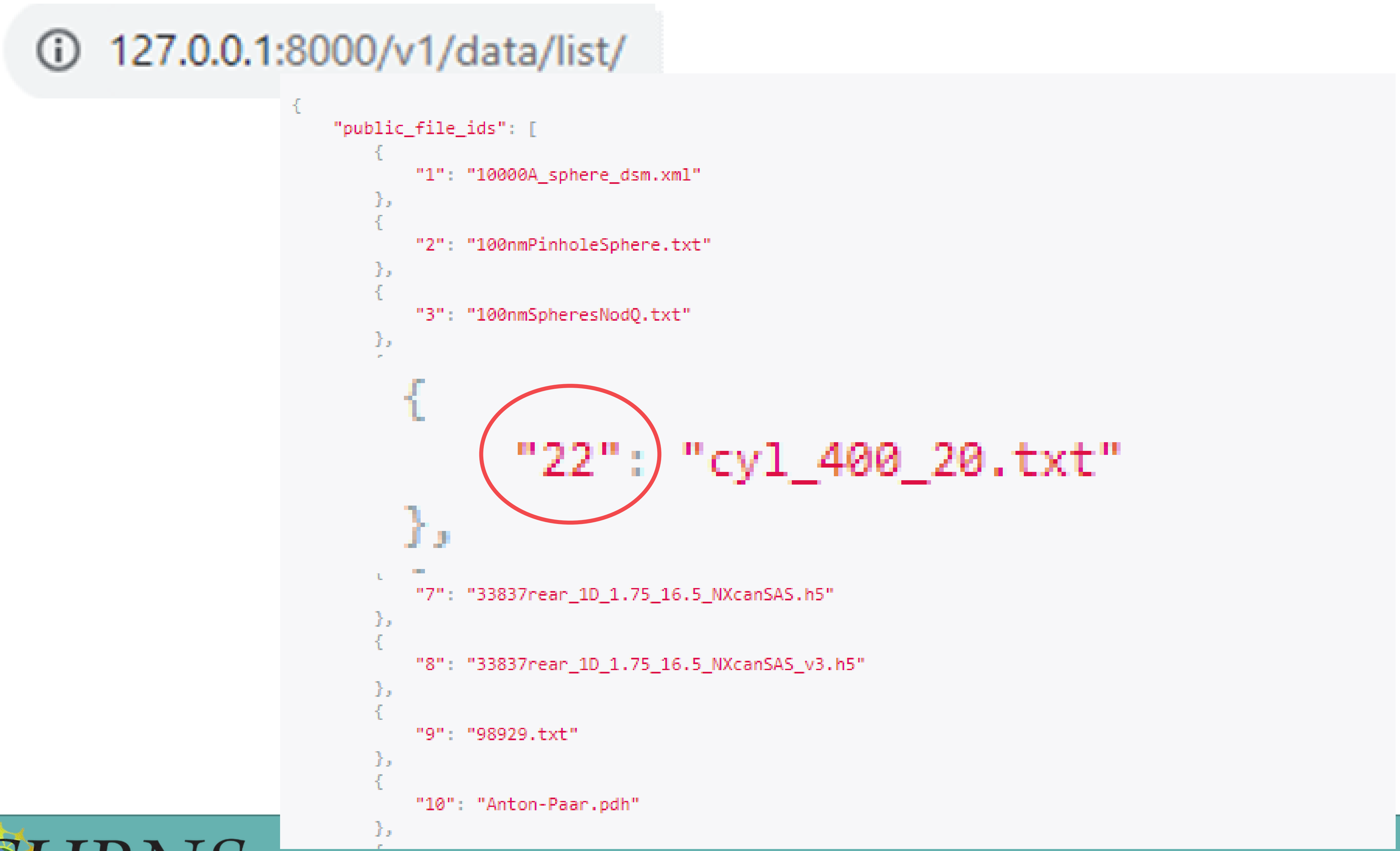
```
ests

(r"veryrealdata.txt", 'rb')
requests.request('POST', 'http://127.0.0.1:8000/v1/data/upload/'
                data={'is_public':True}, files={'file':file})
requests.request(method='GET', url=, data=, files=)
requests.request(method='PUT', url=, data=, files=)

nse.text)
```

Script

## RESTful Framework Inputs

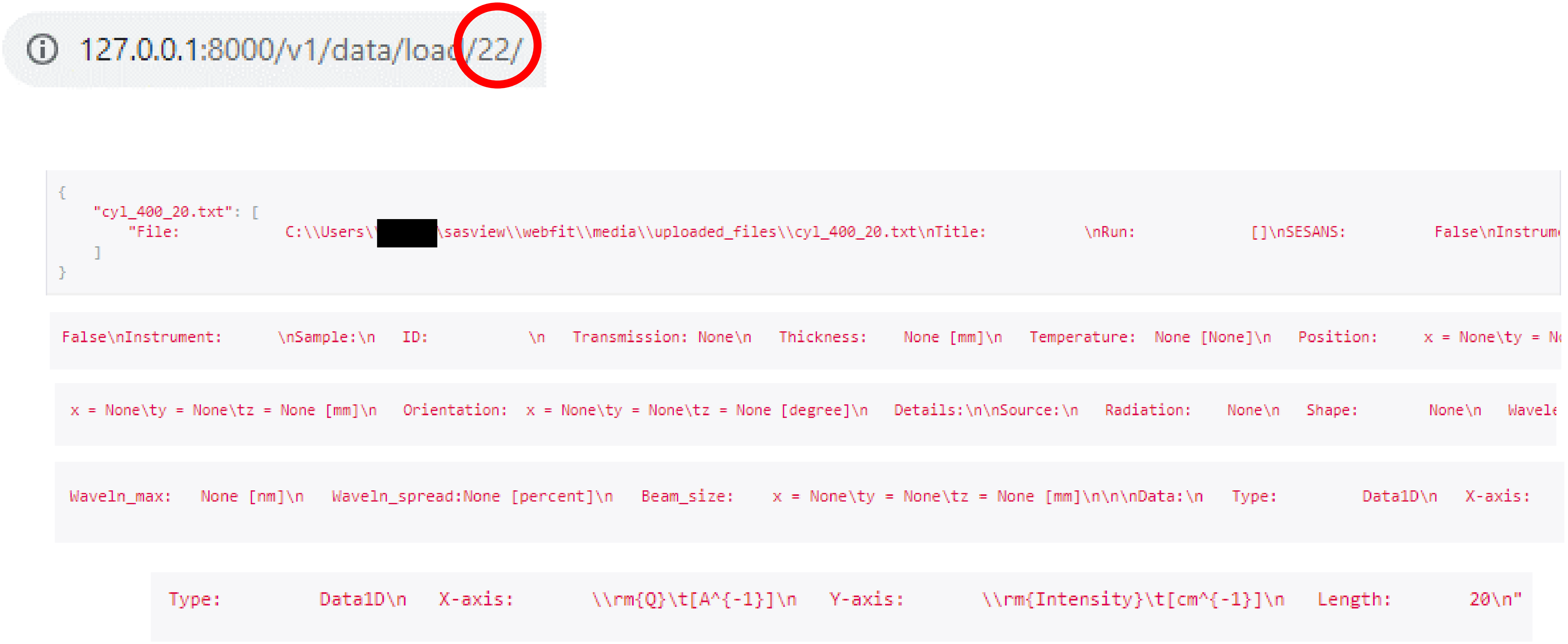


```
{
    "public_file_ids": [
        {
            "1": "10000A_sphere_dsm.xml"
        },
        {
            "2": "100nmPinholeSphere.txt"
        },
        {
            "3": "100nmSpheresNodQ.txt"
        },
        {
            "4": "10wtAOT_Reline_120_reduced.pdh"
        },
        {
            "5": "1umSlitSmearSphere.ABS"
        },
        {
            "6": "33837rear_1D_1.75_16.5_CanSAS1D.xml"
        },
        {
            "7": "33837rear_1D_1.75_16.5_NXcanSAS.h5"
        },
        {
            "8": "33837rear_1D_1.75_16.5_NXcanSAS_v3.h5"
        },
        {
            "9": "98929.txt"
        },
        {
            "10": "Anton-Paar.pdh"
        },
```



127.0.0.1:8000/v1/data/list/

```
{
    "public_file_ids": [
        {
            "1": "10000A_sphere_dsm.xml"
        },
        {
            "2": "100nmPinholeSphere.txt"
        },
        {
            "3": "100nmSpheresNodQ.txt"
        },
          {
              "22": "cyl_400_20.txt"
          },
            "7": "33837rear_1D_1.75_16.5_NXcanSAS.h5"
        },
        {
            "8": "33837rear_1D_1.75_16.5_NXcanSAS_v3.h5"
        },
        {
            "9": "98929.txt"
        },
        {
            "10": "Anton-Paar.pdh"
        },
```



127.0.0.1:8000/v1/data/load/22/

```
{
    "cyl_400_20.txt": [
        "File:            C:\\Users\\[redacted]\sasview\\webfit\\media\\uploaded_files\\cyl_400_20.txt\nTitle:          \nRun:           []\nSESANS:          False\nInstrum
    ]
}
```

```
False\nInstrument:      \nSample:\n    ID:            \n    Transmission: None\n    Thickness:     None [mm]\n    Temperature:  None [None]\n    Position:      x = None\ty = N
```

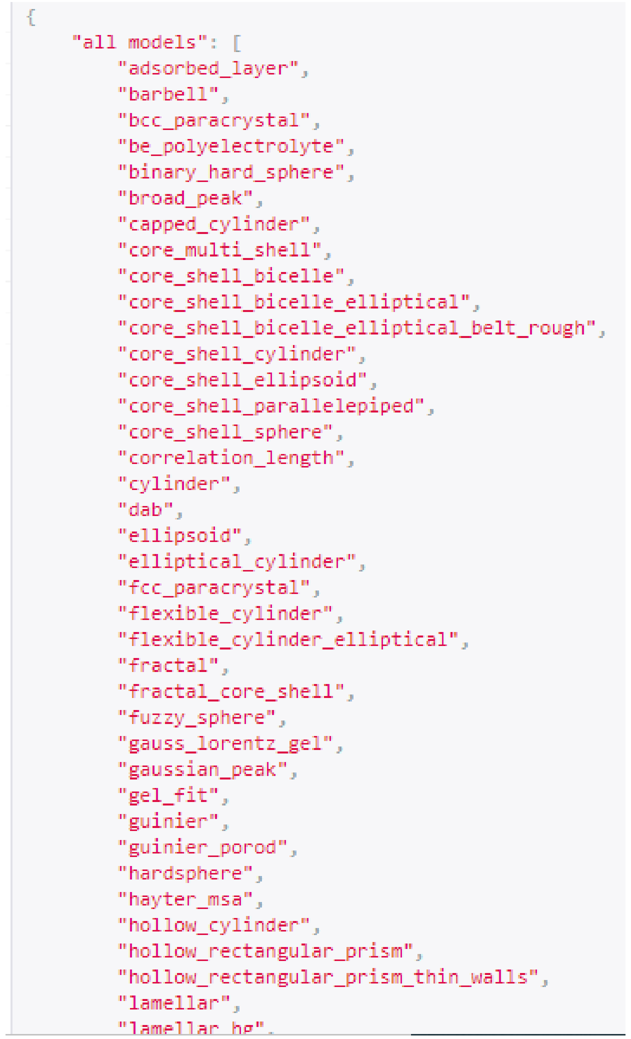
```
x = None\ty = None\tz = None [mm]\n    Orientation:  x = None\ty = None\tz = None [degree]\n    Details:\n\nSource:\n    Radiation:     None\n    Shape:          None\n    Wavele
```

```
Waveln_max:    None [nm]\n    Waveln_spread:None [percent]\n    Beam_size:     x = None\ty = None\tz = None [mm]\n\n\nData:\n    Type:          Data1D\n    X-axis:
```

```
Type:          Data1D\n    X-axis:        \\rm{Q}\t[A^{-1}]\n    Y-axis:        \\rm{Intensity}\t[cm^{-1}]\n    Length:        20\n"
```

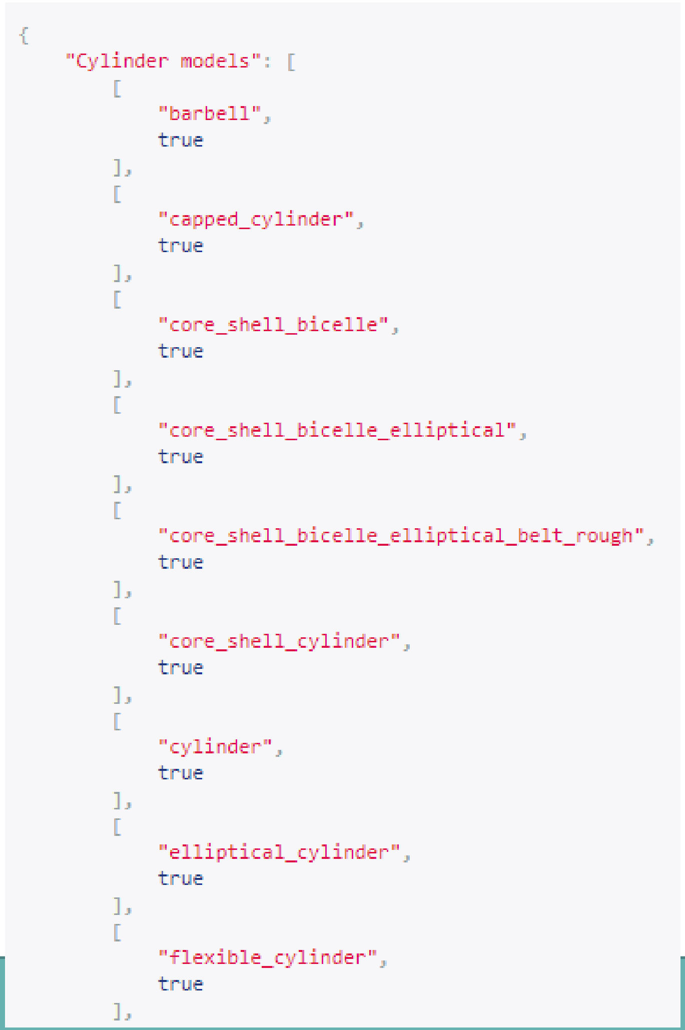
CHRNS CENTER FOR HIGH RESOLUTION NEUTRON SCATTERING NSF NIST

127.0.0.1:8000/v1/analyze/fit/models/



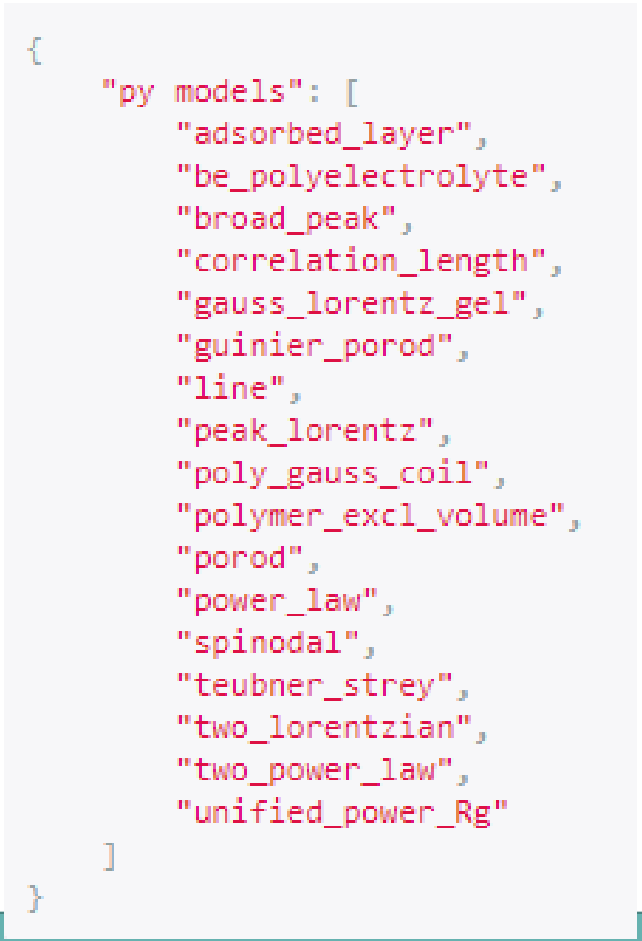
```
{
    "all models": [
        "adsorbed_layer",
        "barbell",
        "bcc_paracrystal",
        "be_polyelectrolyte",
        "binary_hard_sphere",
        "broad_peak",
        "capped_cylinder",
        "core_multi_shell",
        "core_shell_bicelle",
        "core_shell_bicelle_elliptical",
        "core_shell_bicelle_elliptical_belt_rough",
        "core_shell_cylinder",
        "core_shell_ellipsoid",
        "core_shell_parallelepiped",
        "core_shell_sphere",
        "correlation_length",
        "cylinder",
        "dab",
        "ellipsoid",
        "elliptical_cylinder",
        "fcc_paracrystal",
        "flexible_cylinder",
        "flexible_cylinder_elliptical",
        "fractal",
        "fractal_core_shell",
        "fuzzy_sphere",
        "gauss_lorentz_gel",
        "gaussian_peak",
        "gel_fit",
        "guinier",
        "guinier_porod",
        "hardsphere",
        "hayter_msa",
        "hollow_cylinder",
        "hollow_rectangular_prism",
        "hollow_rectangular_prism_thin_walls",
        "lamellar",
        "lamellar_hg",
```

```
{
"category" : "cylinder"
}
```

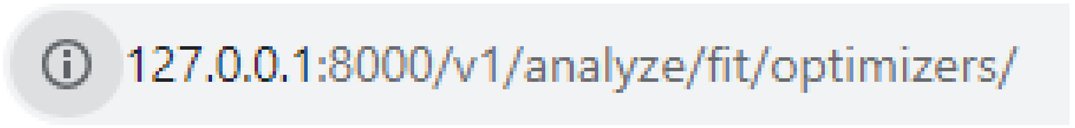


```
{
    "Cylinder models": [
        [
            "barbell",
            true
        ],
        [
            "capped_cylinder",
            true
        ],
        [
            "core_shell_bicelle",
            true
        ],
        [
            "core_shell_bicelle_elliptical",
            true
        ],
        [
            "core_shell_bicelle_elliptical_belt_rough",
            true
        ],
        [
            "core_shell_cylinder",
            true
        ],
        [
            "cylinder",
            true
        ],
        [
            "elliptical_cylinder",
            true
        ],
        [
            "flexible_cylinder",
            true
        ],
```

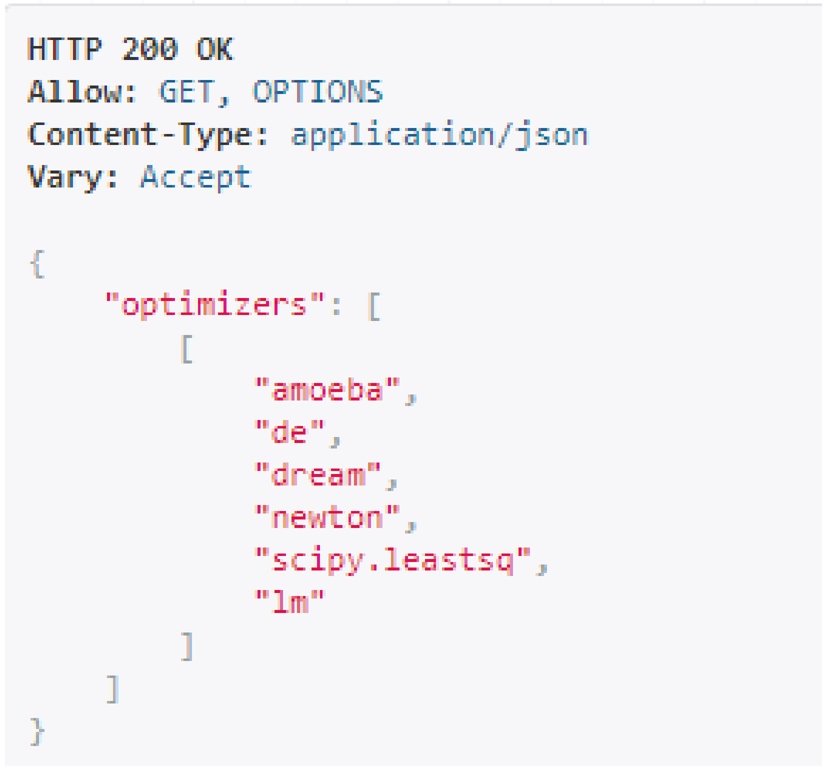
```
{
"kind" : "py"
}
```



```
{
    "py models": [
        "adsorbed_layer",
        "be_polyelectrolyte",
        "broad_peak",
        "correlation_length",
        "gauss_lorentz_gel",
        "guinier_porod",
        "line",
        "peak_lorentz",
        "poly_gauss_coil",
        "polymer_excl_volume",
        "porod",
        "power_law",
        "spinodal",
        "teubner_strey",
        "two_lorentzian",
        "two_power_law",
        "unified_power_Rg"
    ]
}
```

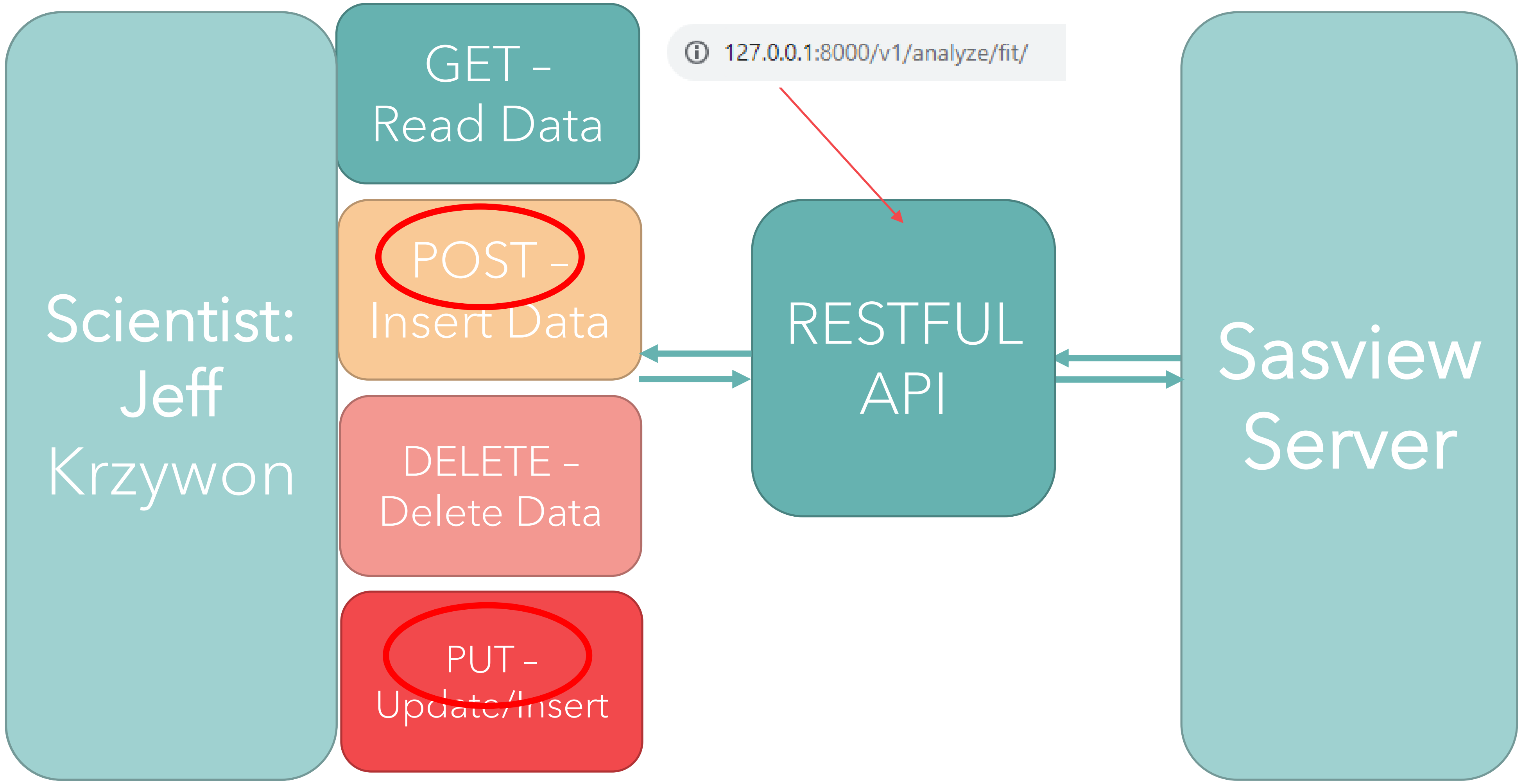


127.0.0.1:8000/v1/analyze/fit/optimizers/

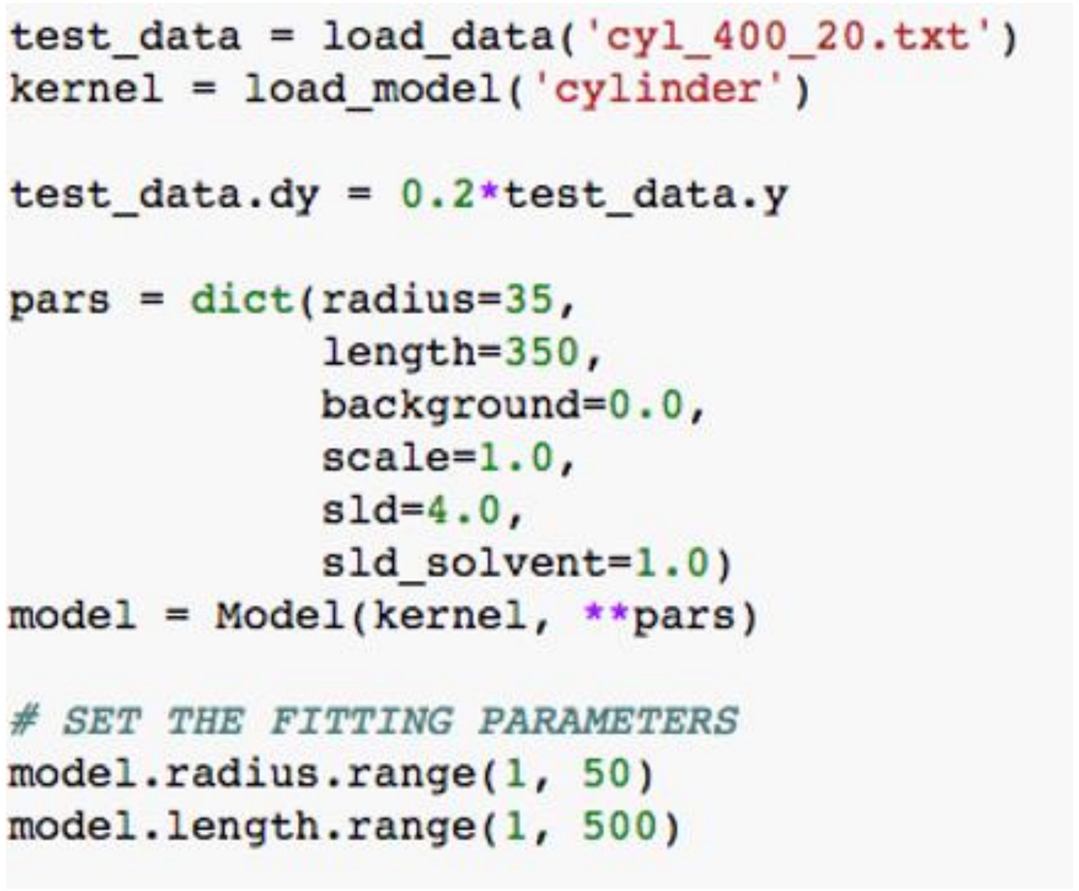


```
HTTP 200 OK
Allow: GET, OPTIONS
Content-Type: application/json
Vary: Accept

{
    "optimizers": [
        [
            "amoeba",
            "de",
            "dream",
            "newton",
            "scipy.leastsq",
            "lm"
        ]
    ]
}
```

## RESTful Framework Inputs



127.0.0.1:8000/v1/analyze/fit/

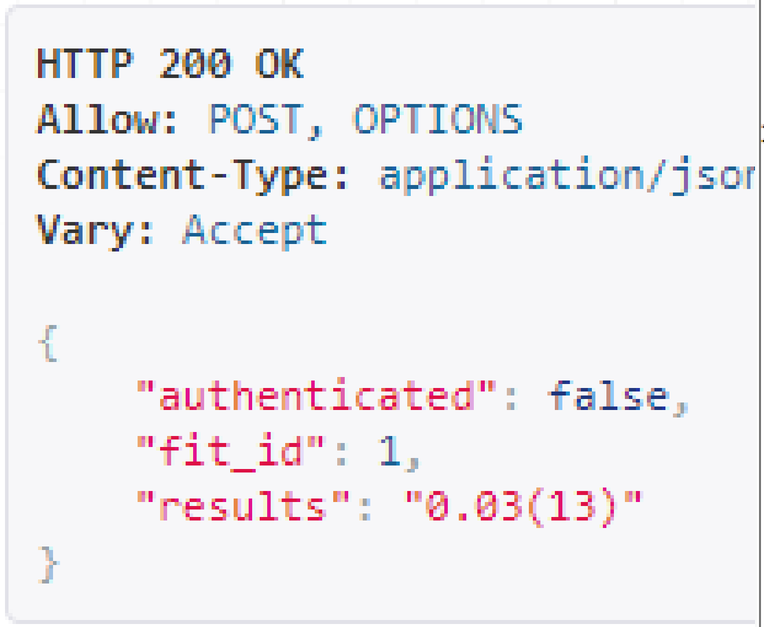


```
test_data = load_data('cyl_400_20.txt')
kernel = load_model('cylinder')

test_data.dy = 0.2*test_data.y

pars = dict(radius=35,
            length=350,
            background=0.0,
            scale=1.0,
            sld=4.0,
            sld_solvent=1.0)
model = Model(kernel, **pars)

# SET THE FITTING PARAMETERS
model.radius.range(1, 50)
model.length.range(1, 500)
```

127.0.0.1:8000/v1/analyze/fit/

```json
{
      "model":"cylinder",
      "data_id":22,
      "optimizer":"amoeba",
      "parameters" :
      [
          {
              "name":"radius",
              "value":35,
              "data_type":"int",
              "lower_limit":1,
              "upper_limit":50
          },
          {
              "name":"length",
              "value":350,
              "data_type":"int",
              "lower_limit":1,
              "upper_limit":500
          },
          {
              "name":"background",
              "value":0.0,
              "data_type":"float"
          },
          {
              "name":"scale",
              "value":1.0,
              "data_type":"float"
          },
          {
              "name":"sld",
              "value":4.0,
              "data_type":"float"
          },
          {
              "name":"sld_solvent",
              "value":1.0,
              "data_type":"float"
          }
      ]
}
```

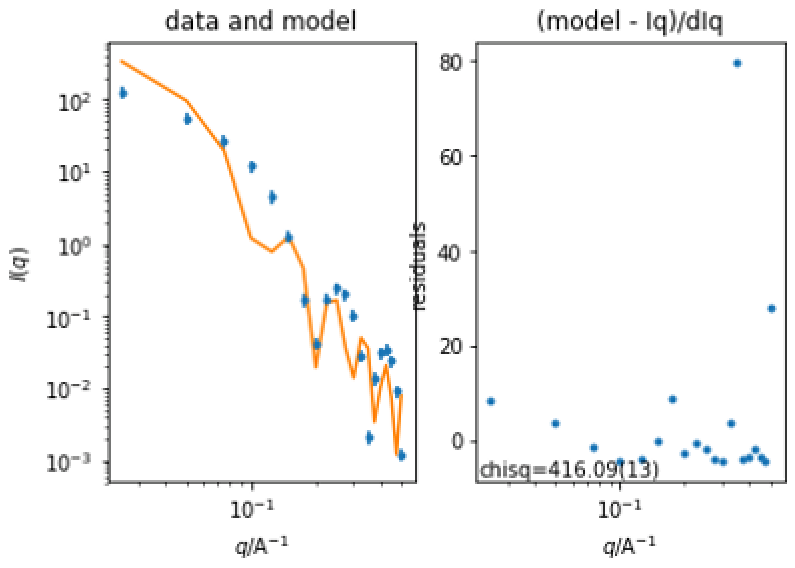
127.0.0.1:8000/v1/analyze/fit/



```
HTTP 200 OK
Allow: POST, OPTIONS
Content-Type: application/jsor
Vary: Accept

{
    "authenticated": false,
    "fit_id": 1,
    "results": "0.03(13)"
}
```

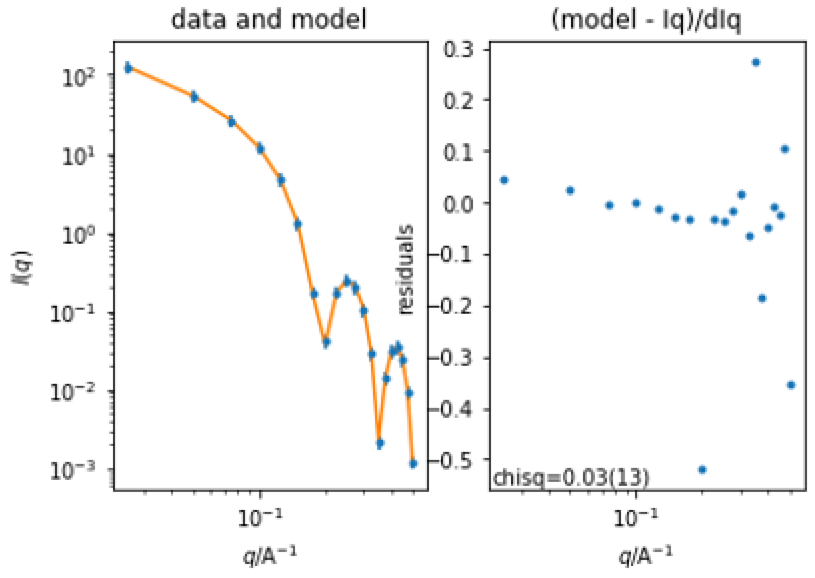
## Before fit

```
Initial chisq 416.09(13)
```



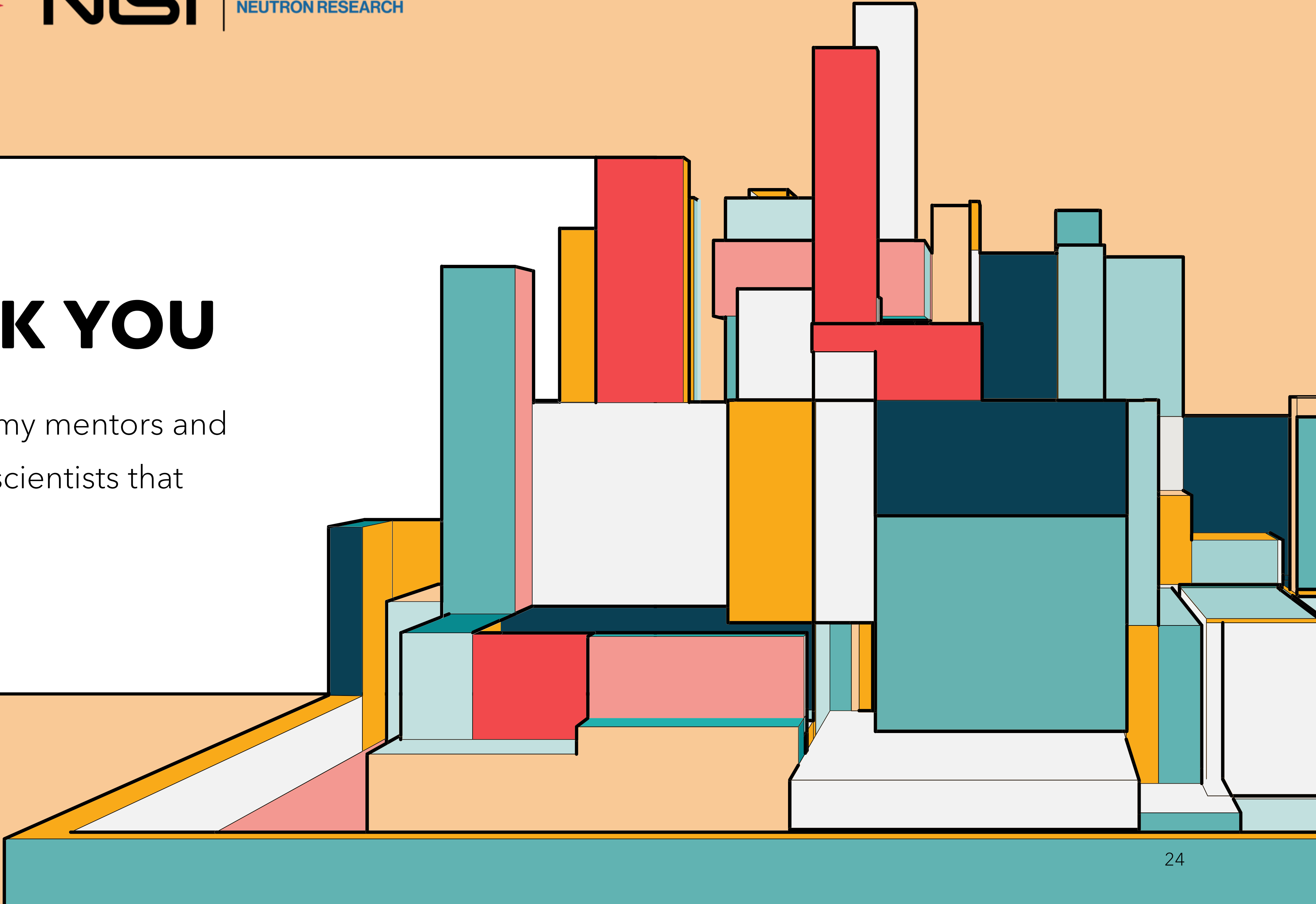
## After fit

```
Final chisq 0.03(13)
length : 464.9(55)
radius : 19.977(64)
```



## THANK YOU

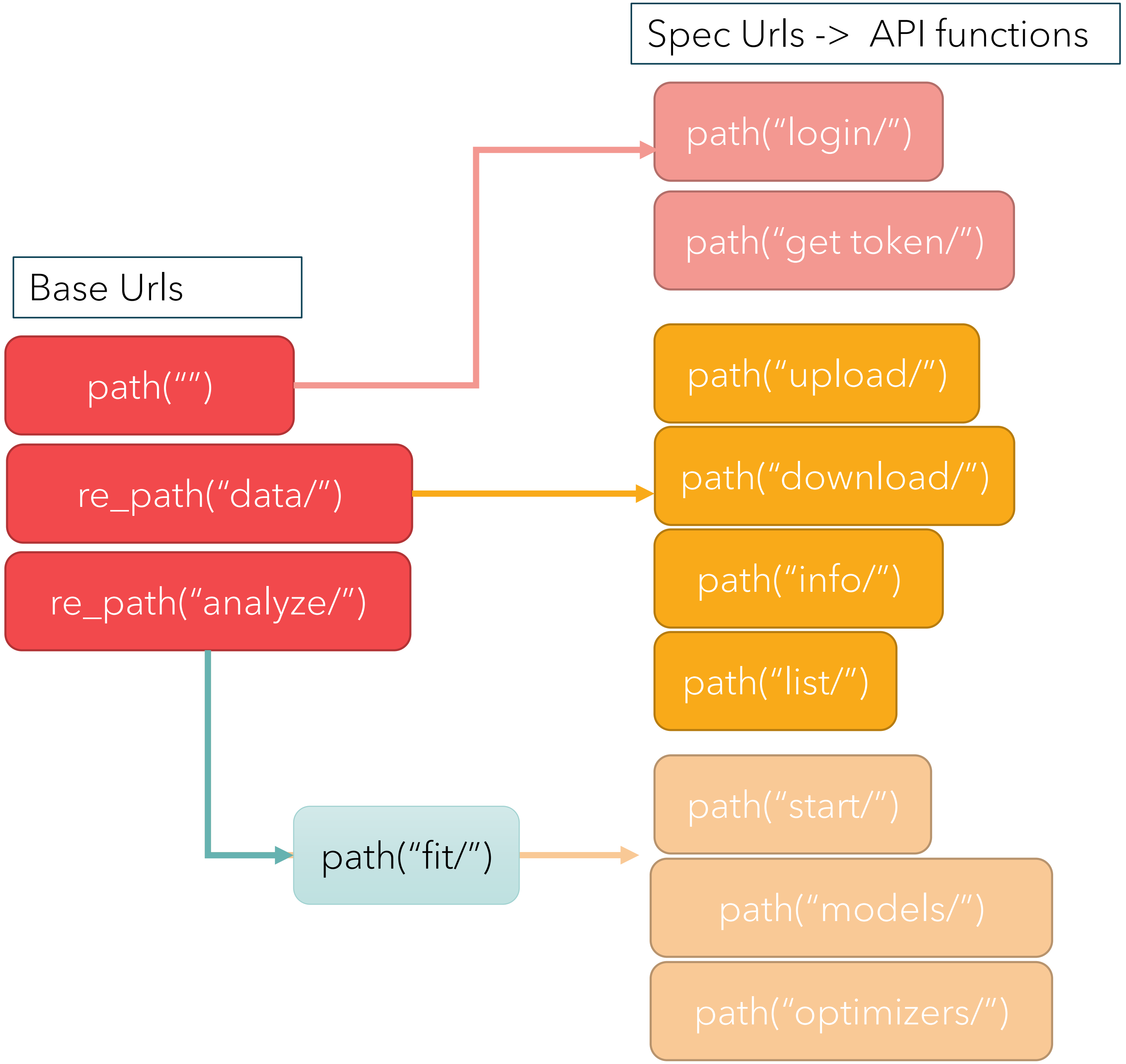
Especially to my mentors and other NCNR scientists that helped me!



# URL PATHING

- Links everything together!
- Allows the user to get to function
- Modular
  - Add in new paths easy

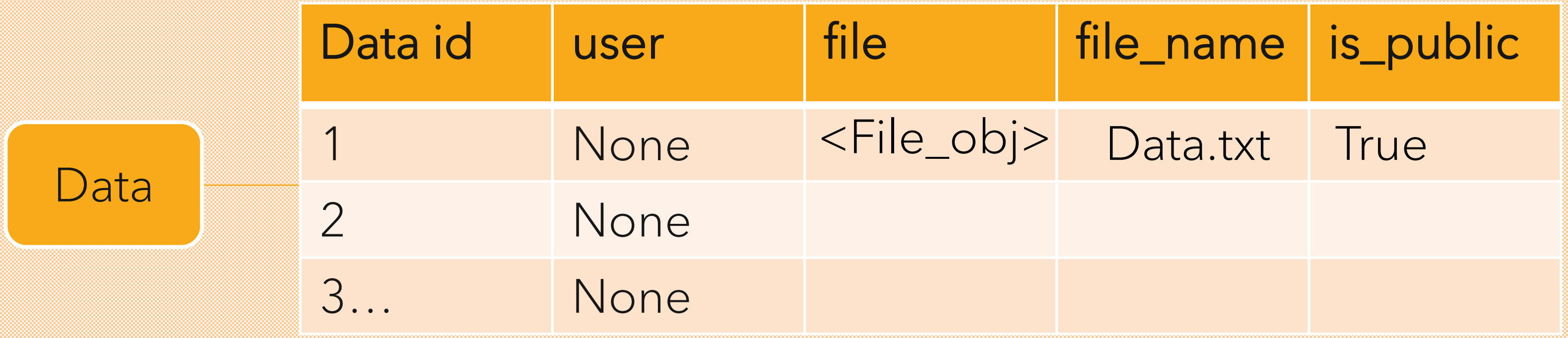
Ref: Django Rest Framework Versioning



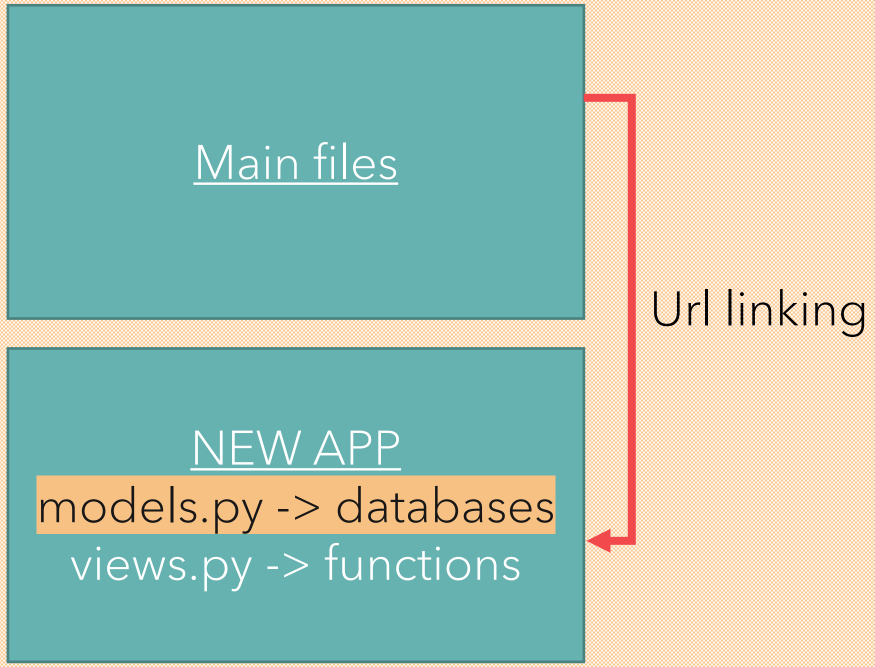
## SETTING UP DATABASES

Models for Django

- Define what the user inputs
- Make sure user can't put in malicious data



| Data id | user | file | file_name | is_public |
|---|---|---|---|---|
| 1 | None | <File_obj> | Data.txt | True |
| 2 | None | | | |
| 3… | None | | | |

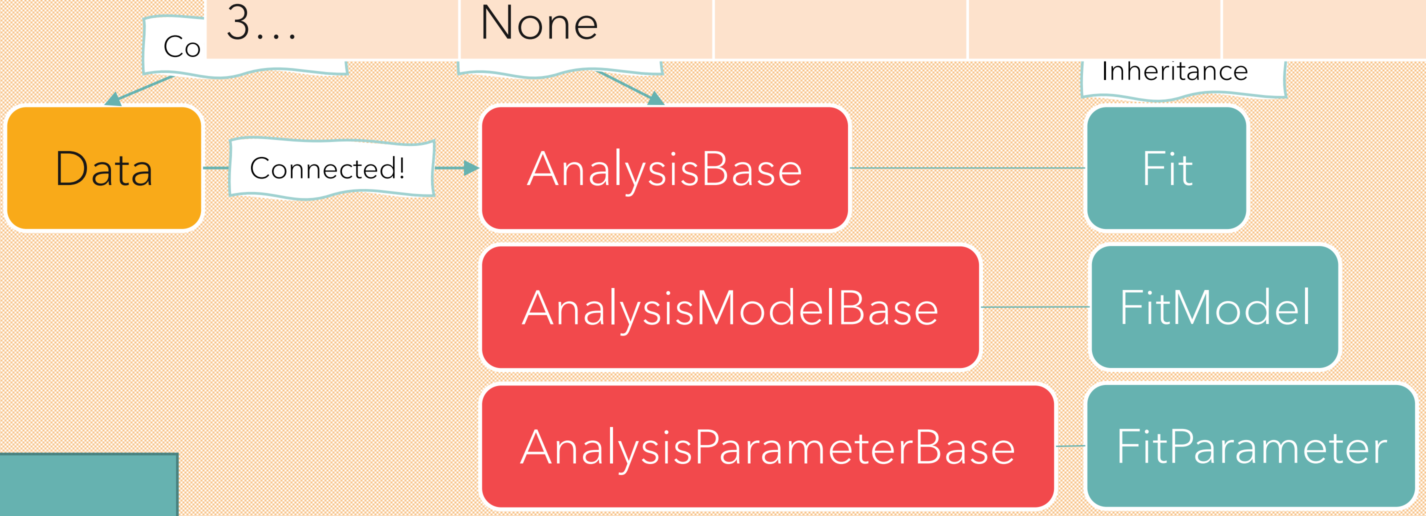


# SETTING UP DATABASES

## Models for Django

- Data – holds imported data for users
- Analysis – holds data for analysis
- Fit – extends analysis, specific data for fit

| Data id | user | file | file_name | is_public |
|---|---|---|---|---|
| 1 | None | <File_obj> | Data.txt | True |
| 2 | None | | | |
| 3… | None | | | |

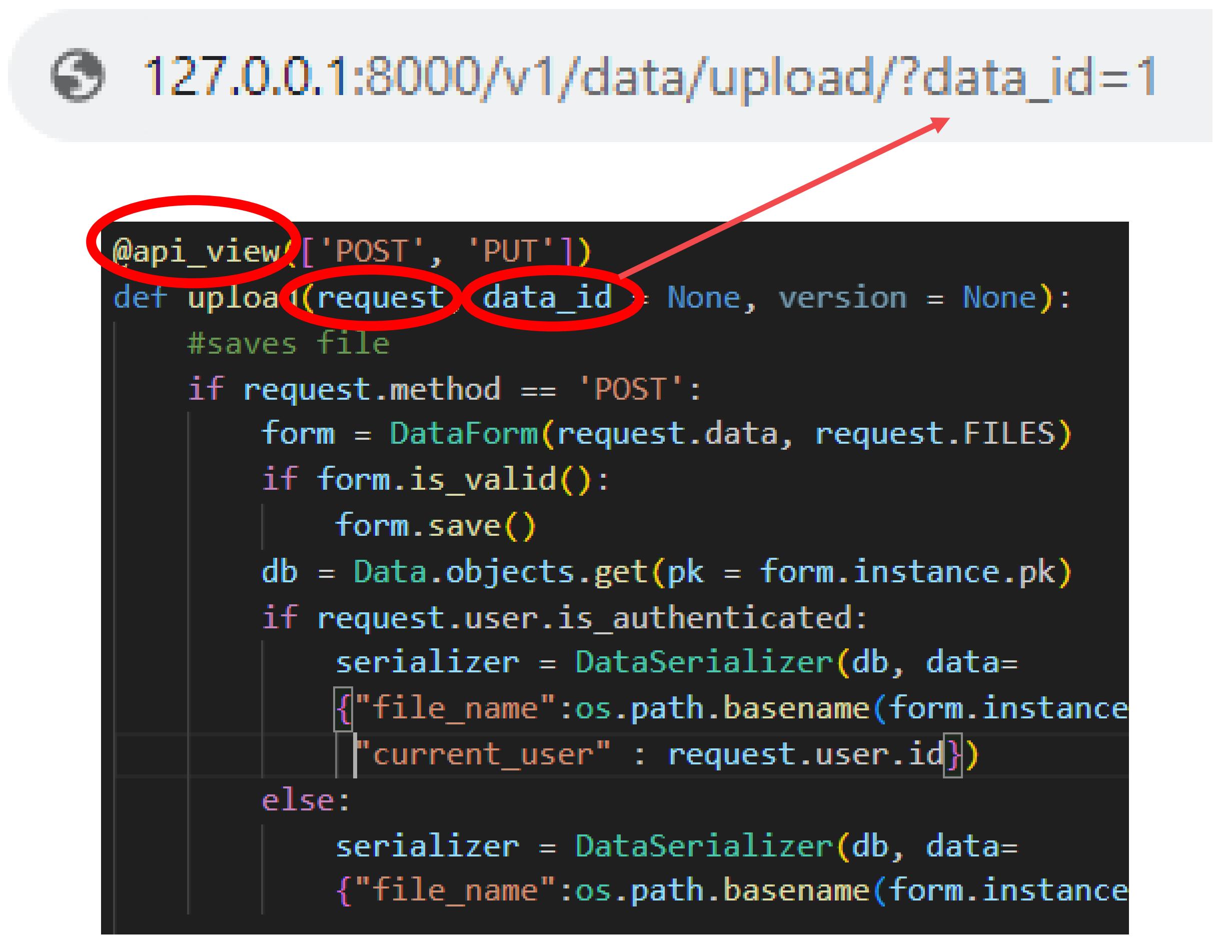


NEW APP
models.py -> databases
views.py -> functions

## VIEWS

- Views hold the meat of the code:
- Takes user request <- holds data
- Returns response <- specified by function

NEW APP
models.py -> databases
views.py -> functions

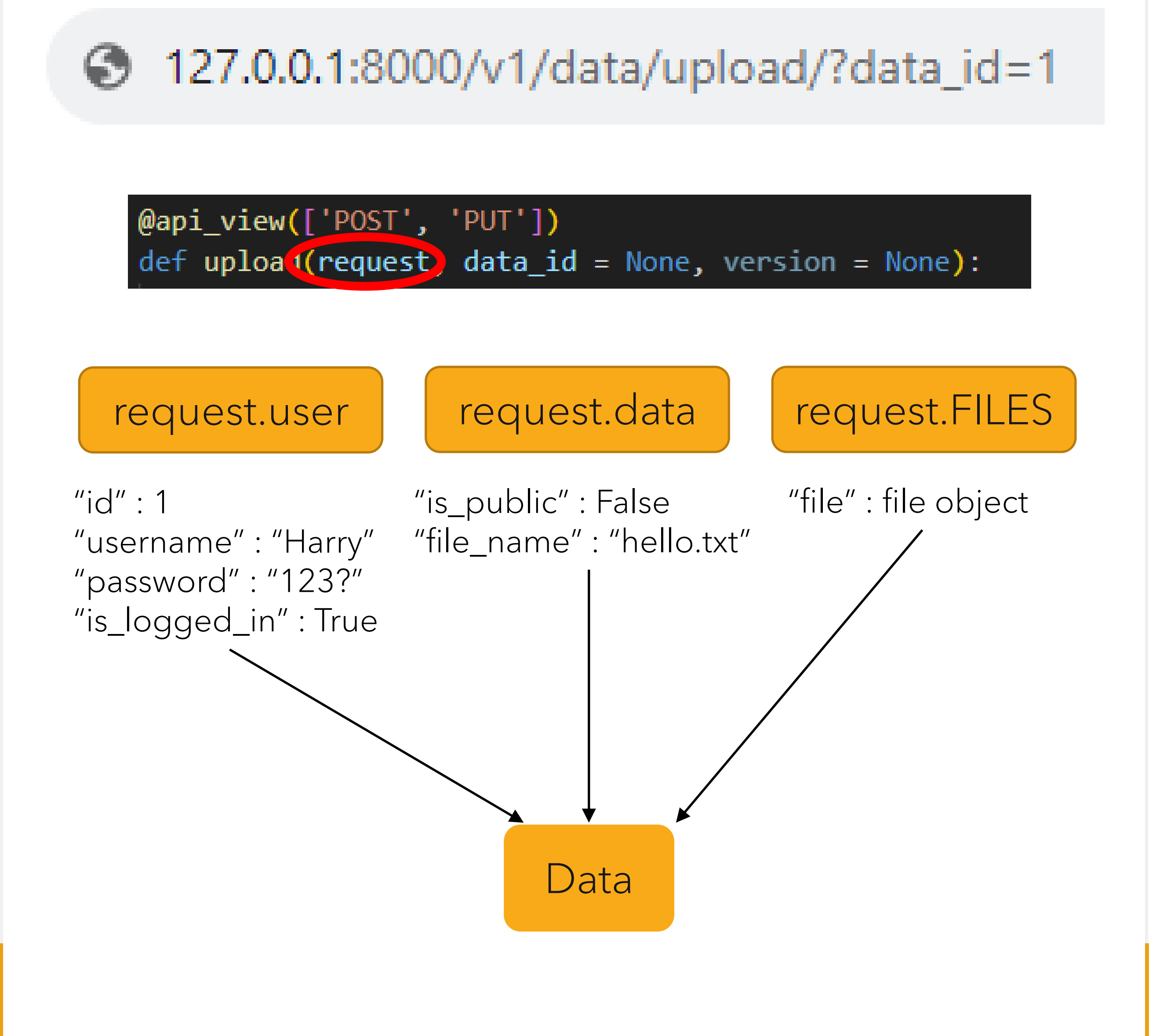

127.0.0.1:8000/v1/data/upload/?data_id=1

```
@api_view(['POST', 'PUT'])
def upload(request, data_id = None, version = None):
    #saves file
    if request.method == 'POST':
        form = DataForm(request.data, request.FILES)
        if form.is_valid():
            form.save()
        db = Data.objects.get(pk = form.instance.pk)
        if request.user.is_authenticated:
            serializer = DataSerializer(db, data=
            {"file_name":os.path.basename(form.instance
             "current_user" : request.user.id})
        else:
            serializer = DataSerializer(db, data=
            {"file_name":os.path.basename(form.instance
```

## VIEWS

- Views hold the meat of the code:
- Takes user request <- holds data
- Returns response <- specified by function

NEW APP
models.py -> databases
views.py -> functions

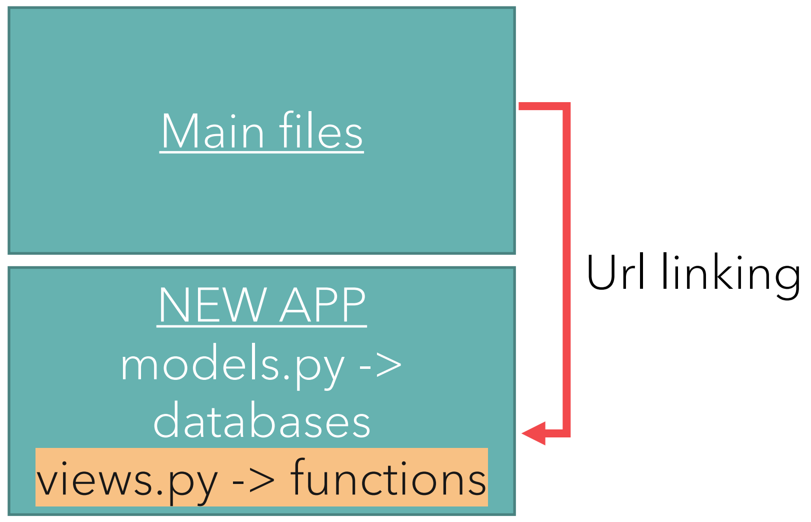


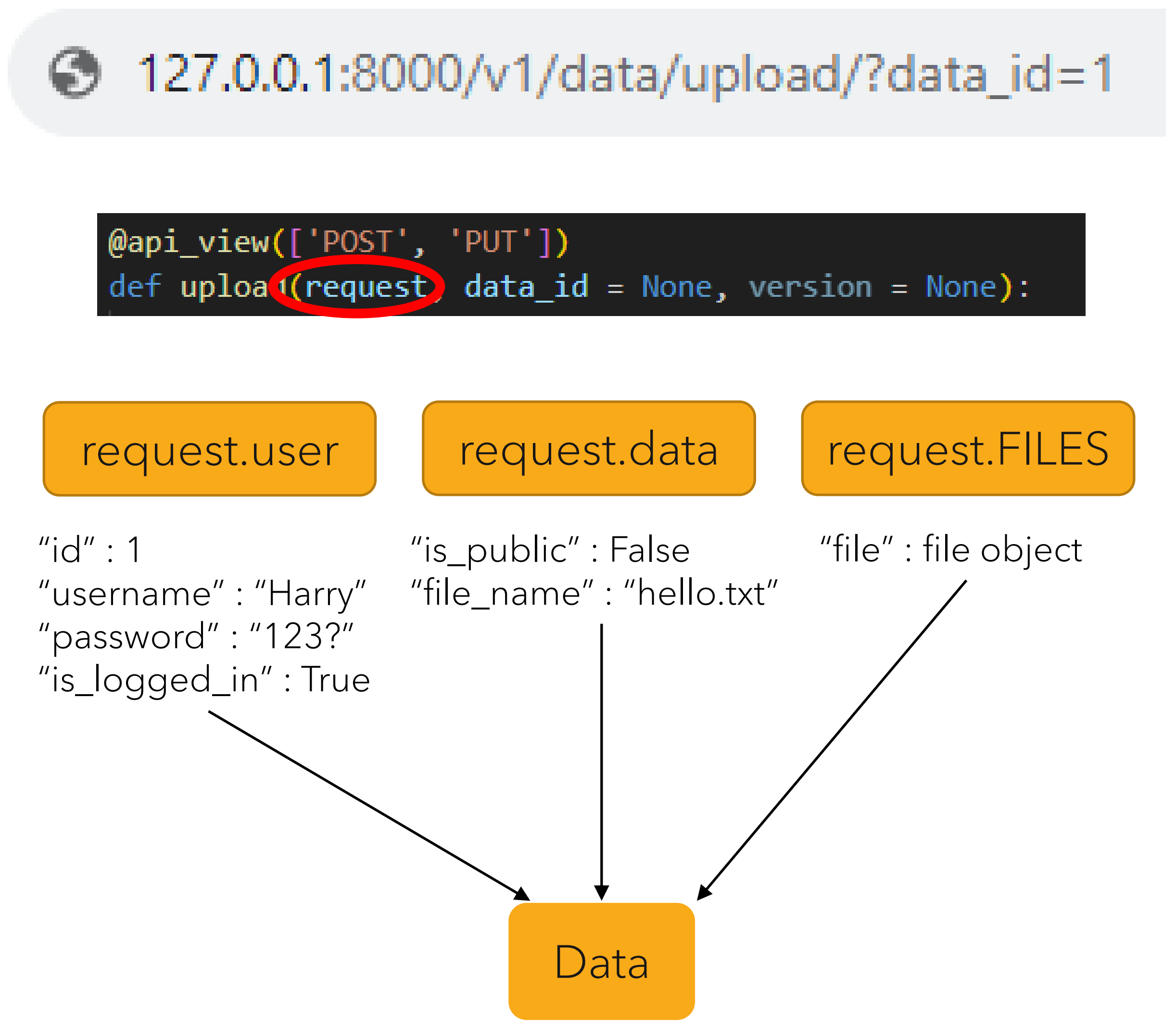
```
127.0.0.1:8000/v1/data/upload/?data_id=1
```

```
@api_view(['POST', 'PUT'])
def upload(request, data_id = None, version = None):
```

## VIEWS

- Translator
- Puts into databases
- Defines how user's data looks

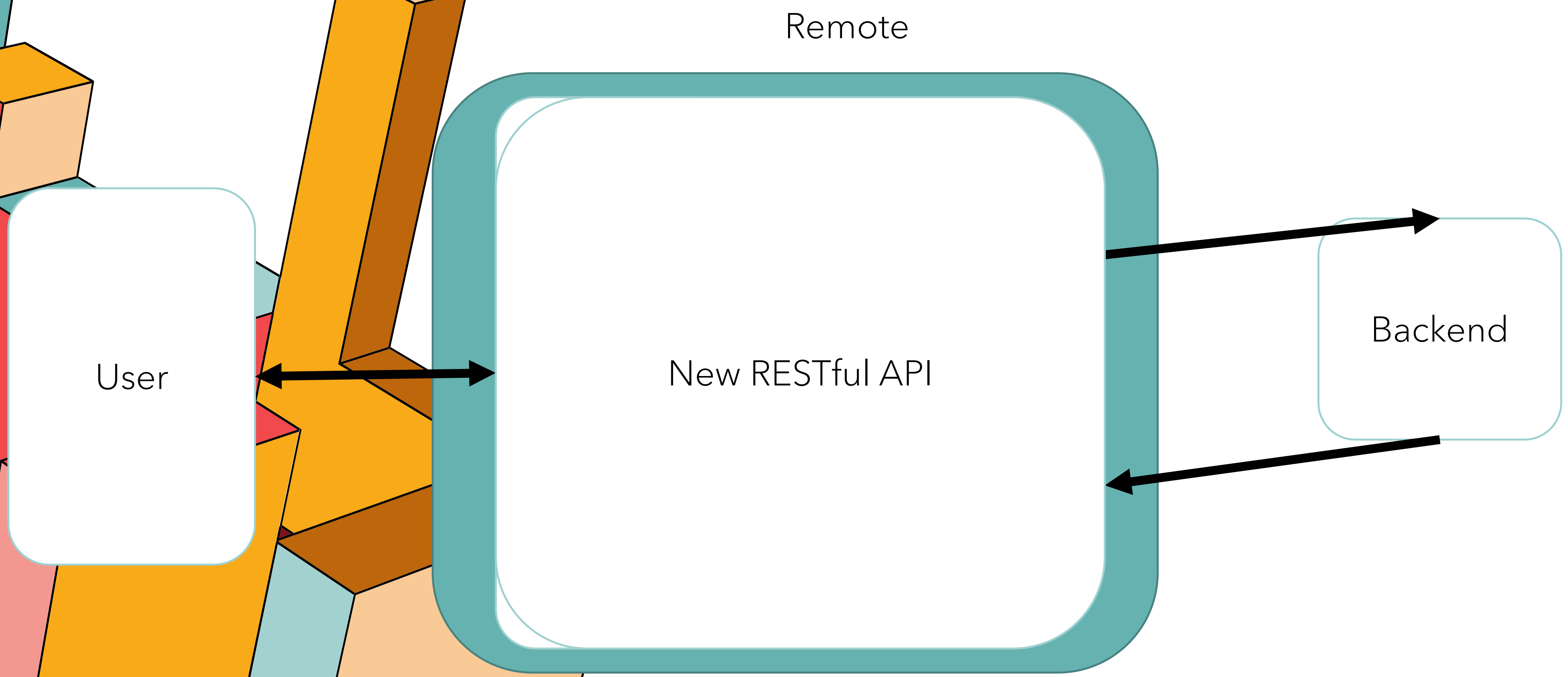




```
127.0.0.1:8000/v1/data/upload/?data_id=1
```

```
@api_view(['POST', 'PUT'])
def upload(request, data_id = None, version = None):
```

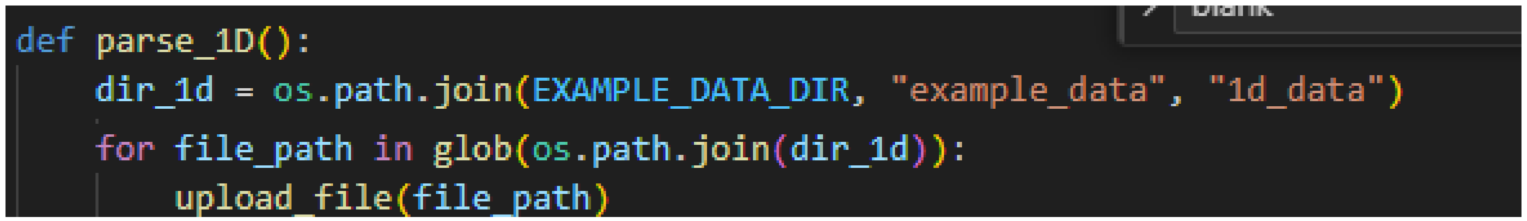
## Proposed Layout



# UPLOADING DATA

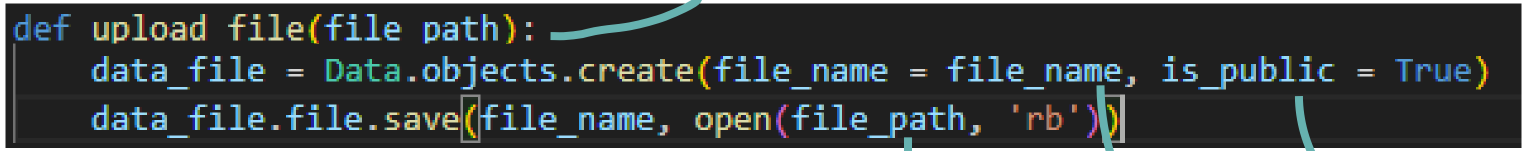
**Example Data**

->



```python
def parse_1D():
    dir_1d = os.path.join(EXAMPLE_DATA_DIR, "example_data", "1d_data")
    for file_path in glob(os.path.join(dir_1d)):
        upload_file(file_path)
```

```
example_data
        L  1d_data
                L    file1
                L    file2
```



```python
def upload_file(file_path):
    data_file = Data.objects.create(file_name = file_name, is_public = True)
    data_file.file.save(file_name, open(file_path, 'rb'))
```

Data =

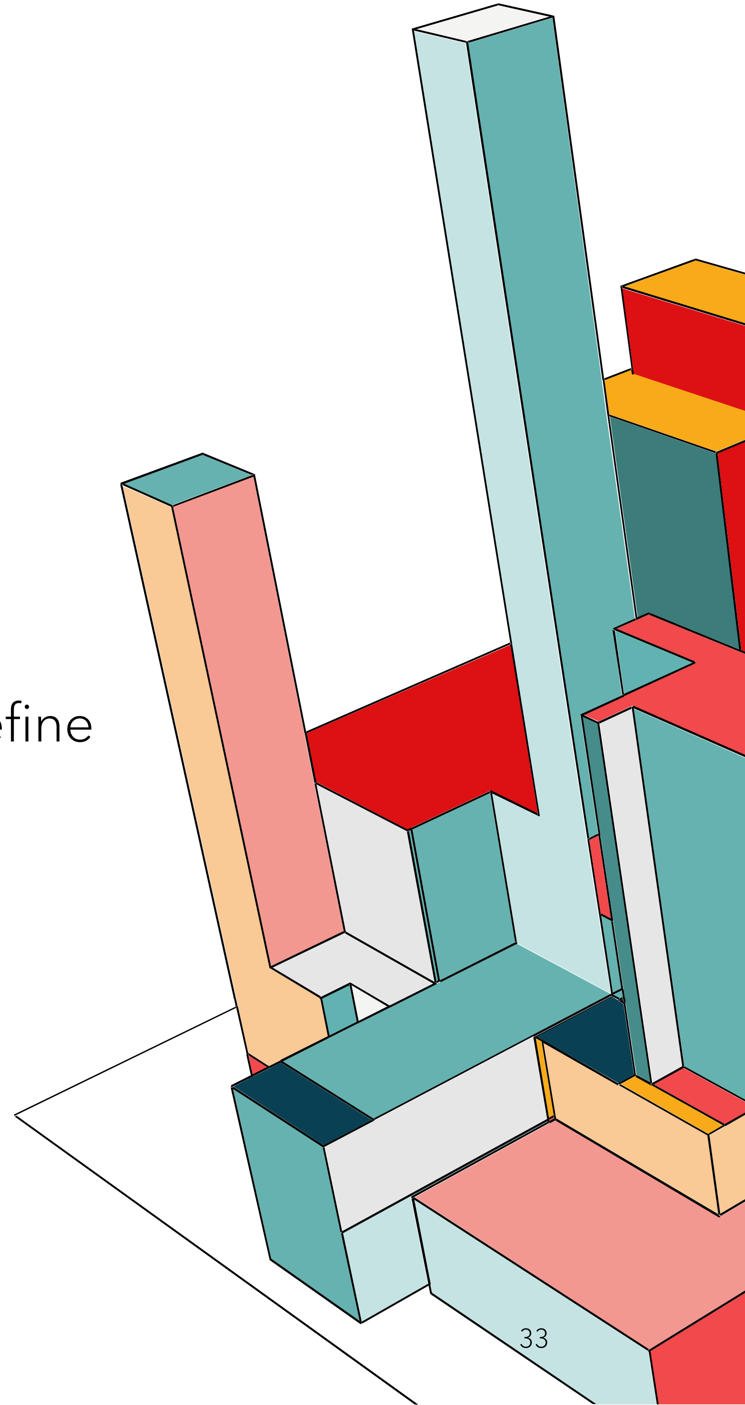
## OTHER FACTORS

### Why Django?

- Web framework
- Batteries Included
- DRY (Don't Repeat Yourself)
- Database backend
- Future View integration

### International

- Users all over the world!
- Different wants
    - Need something to define "public"
- Save Data and Fits



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## OTHER FACTORS

### What web framework?

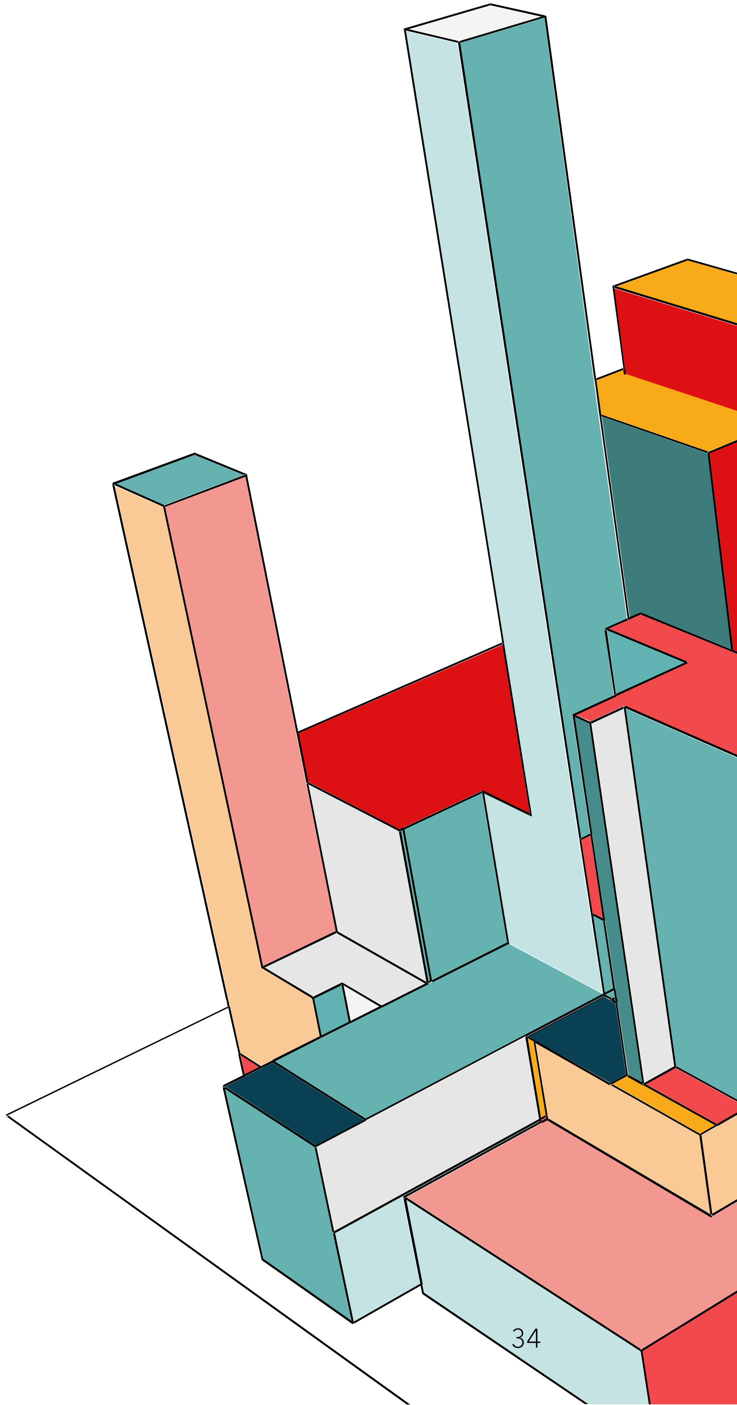
- Django
- Flask
- What's the best?

### International

- Users all over the world!
- Different wants
    - Need something to define "public"

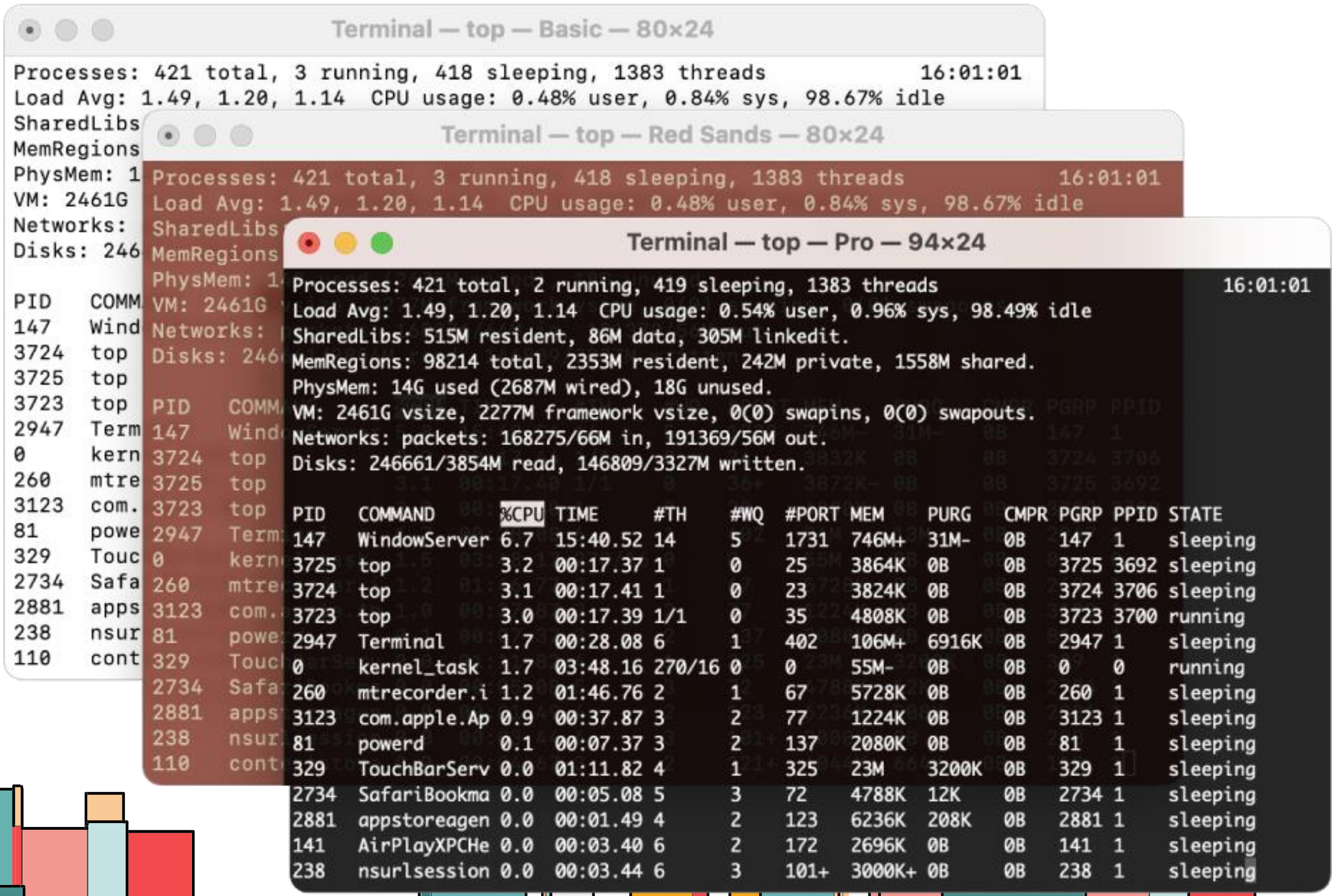
### Why Django?

- Defined database backend
- Allows for the future development of web application rather than just interface



# BACKEND?

terminal


Terminal — top — Basic — 80×24

```
Processes: 421 total, 3 running, 418 sleeping, 1383 threads           16:01:01
Load Avg: 1.49, 1.20, 1.14  CPU usage: 0.48% user, 0.84% sys, 98.67% idle
SharedLibs
MemRegions
PhysMem: 1
VM: 2461G
Networks:
Disks: 246

PID    COMM
147    Wind
3724   top
3725   top
3723   top
2947   Term
0      kern
260    mtre
3123   com.
81     powe
329    Touc
2734   Safa
2881   apps
238    nsur
110    cont
```

Terminal — top — Red Sands — 80×24

```
Processes: 421 total, 3 running, 418 sleeping, 1383 threads           16:01:01
Load Avg: 1.49, 1.20, 1.14  CPU usage: 0.48% user, 0.84% sys, 98.67% idle
SharedLibs
MemRegions
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3123   com.
81     powe
329    Touc
2734   Safa
2881   apps
238    nsur
110    cont
```

```
Processes: 421 total, 2 running, 419 sleeping, 1383 threads                          16:01:01
Load Avg: 1.49, 1.20, 1.14  CPU usage: 0.54% user, 0.96% sys, 98.49% idle
SharedLibs: 515M resident, 86M data, 305M linkedit.
MemRegions: 98214 total, 2353M resident, 242M private, 1558M shared.
PhysMem: 14G used (2687M wired), 18G unused.
VM: 2461G vsize, 2277M framework vsize, 0(0) swapins, 0(0) swapouts.
Networks: packets: 168275/66M in, 191369/56M out.
Disks: 246661/3854M read, 146809/3327M written.

PID  COMMAND      %CPU TIME     #TH    #WQ  #PORT MEM    PURG   CMPR PGRP PPID STATE
147  WindowServer 6.7  15:40.52 14     5    1731  746M+  31M-   0B   147  1    sleeping
3725 top          3.2  00:17.37 1      0    25    3864K  0B     0B   3725 3692 sleeping
3724 top          3.1  00:17.41 1      0    23    3824K  0B     0B   3724 3706 sleeping
3723 top          3.0  00:17.39 1/1    0    35    4808K  0B     0B   3723 3700 running
2947 Terminal     1.7  00:28.08 6      1    402   106M+  6916K  0B   2947 1    sleeping
0    kernel_task  1.7  03:48.16 270/16 0    0     55M-   0B     0B   0    0    running
260  mtrecorder.i 1.2  01:46.76 2      1    67    5728K  0B     0B   260  1    sleeping
3123 com.apple.Ap 0.9  00:37.87 3      2    77    1224K  0B     0B   3123 1    sleeping
81   powerd       0.1  00:07.37 3      2    137   2080K  0B     0B   81   1    sleeping
329  TouchBarServ 0.0  01:11.82 4      1    325   23M    3200K  0B   329  1    sleeping
2734 SafariBookma 0.0  00:05.08 5      3    72    4788K  12K    0B   2734 1    sleeping
2881 appstoreagen 0.0  00:01.49 4      2    123   6236K  208K   0B   2881 1    sleeping
141  AirPlayXPCHe 0.0  00:03.40 6      2    172   2696K  0B     0B   141  1    sleeping
238  nsurlsession 0.0  00:03.44 6      3    101+  3000K+ 0B     0B   238  1    sleeping
```