medna-metadata

Release latest

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medna-metadata is a data management system for tracking environmental DNA samples from field data collection to bioinformatics analyses.

The Sequencing and Bioinformatics Metadata project is funded through the Maine-eDNA RII Track-1 EPSCoR grant supported by the National Science Foundation award #OIA-1849227. Maine-eDNA is a Maine coast-wide research effort to determine the efficacy of ecosystem monitoring through environmental DNA (eDNA). For more in-depth information related to Maine-eDNA, see the Maine-eDNA home page. The metadata project is directly related to the goals of Theme 3: Macrosystem eDNA Integration, but also involved in Theme 1: Sustainable Fisheries and Theme 2: Harmful and Shifting Species. Our efforts contribute to the Data Management and Data Analysis Pipeline work groups. The Sequencing and Bioinformatics Metadata project is a collaboration between the Coordinated Operating Research Entities (CORE) environmental DNA (eDNA) Laboratory and the Data Management Team to facilitate the development of a web application for the management and tracking of eDNA samples (medna-metadata; GitHub).

Kimble, M., Allers, S., Campbell, K., Chen, C., Jackson, L. M., King, B. L., Silverbrand, S., York, G., & Beard, K. (2022). medna-metadata: An open-source data management system for tracking environmental DNA samples and metadata. *Bioinformatics*, btac556. https://doi.org/10.1093/bioinformatics/btac556

Check out the *Installation* section for further information, including how to setup the project.

Note: This project is under active development.

CHAPTER

ONE

CONTENTS

1.1 Installation

Important: Ubuntu (20.04 LTS is recommended)

See also:

If you've never set up a server before, DigitalOcean provides an extensive variety of tutorials that we highly recommend. Several of the steps below were adapted from their tutorials.

- Initial Server Setup With Ubuntu 20.04
- Django, PostgreSQL, NGINX, Gunicorn, and Ubuntu 20.04

It's recommended to visit these tutorials to understand some of the rational behind the steps below.

The following instructions provide guidance on installing MeDNA-Metadata on Ubuntu 20.04.

Important: Instances of `youruser` need to be replaced with a relevant username. For example, references to `/home/youruser/` must be adjusted to the active Ubuntu username. The simplest solution would be to use the same username throughout the setup process, as long as it is **not** the root username. Never use root. For more information, see the aforementioned Initial Server Setup With Ubuntu 20.04.

1.2 Clone the Repository

To clone the most recent stable release as read-only:

```
git clone -b stable/1.0.1 https://github.com/Maine-eDNA/medna-metadata.git
```

To clone the development branch:

```
git clone -b main git@github.com:Maine-eDNA/medna-metadata.git
```

1.3 Docker Setup

1.3.1 Install Requirements

Ubuntu 20.04

Deploying with docker requires docker and docker-compose. Docker-compose must be able to run at least version 3.8. DigitalOcean provides tutorials on How to Install and Use Docker on Ubuntu 20.04 and How To Install and Use Docker Compose on Ubuntu 20.04.

After following DigitalOcean's tutorials, create a symbolic link of the installation to the `docker-compose` command

```
sudo ln -s ~/.docker/cli-plugins/docker-compose /usr/bin/docker-compose
```

Important: This allows you to call `docker-compose` from the command line, and is highly recommended to avoid future headaches.

The `docker/` directory has `medna.env.txt` and `medna.env.db.txt`, which contain all environmental variables for docker deployment. These files are necessary for docker. Other files that affect docker are:

- `entrypoint.sh`
- `.dockerignore`
- contents of `docker/` directory
- settings in `medna_metadata/settings.py`

Navigate to the `docker/` directory

```
cd medna-metadata/docker/
```

Make a copy of `medna.env.txt` and `medna.env.db.txt` in the same `docker/` directory with the `.txt` extension removed (e.g., `medna.env.db`, `medna.env`)

```
cp medna.env.txt medna.env
cp medna.env.db.txt medna.env.db
```

`medna.env`:

```
#####################################################################
# django general settings; loaded in settings.py
# The secret key must be a large random value and it must be kept secret.
# https://docs.djangoproject.com/en/4.0/ref/settings/#std:setting-SECRET_KEY
# https://docs.djangoproject.com/en/4.0/ref/settings/#std-setting-TIME_ZONE
# List of time zones: https://en.wikipedia.org/wiki/List_of_tz_database_time_zones
#####################################################################
DJANGO_SECRET_KEY=your_secret_key
DJANGO_ALLOWED_HOSTS=localhost 127.0.0.1 your_ip_address [::1]
DJANGO_SETTINGS_MODULE=medna_metadata.settings
DJANGO_DEBUG=False
DJANGO_LOG_LEVEL=info
TIME_ZONE=America/New_York
```

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```
#####################################################################
# Creates a superuser account (a user who has all permissions).
# https://docs.djangoproject.com/en/4.0/ref/django-admin/#createsuperuser
#####################################################################
DJANGO_SUPERUSER_PASSWORD=your_superuser_password
DJANGO_SUPERUSER_EMAIL=your_superuser_email@domain.com
DJANGO_SUPERUSER_USERNAME=your_superuser_email@domain.com

#####################################################################
# web_start.sh settings
# DJANGO_MANAGEPY_MIGRATE - build database tables; calls the migrate management cmd -␣
↪https://docs.djangoproject.com/en/4.0/topics/migrations/
# DJANGO_DATABASE_FLUSH - empty database of all data; calls the flush management cmd -␣
↪https://docs.djangoproject.com/en/4.0/ref/django-admin/#flush
# DJANGO_SUPERUSER_CREATE - create a superuser account; calls the createsuperuser␣
↪management cmd - https://docs.djangoproject.com/en/4.0/ref/django-admin/
↪#createsuperuser
# DJANGO_DEFAULT_GROUPS_CREATE - create default permissions groups; calls custom create_
↪default_groups management cmd (admin, gradstudent, intern)
# DJANGO_DEFAULT_USERS_CREATE - create default user; calls custom create_default_user␣
↪management cmd
# DJANGO_DATABASE_LOADDATA - load database with base data from fixtures; calls loaddata␣
↪management cmd - https://docs.djangoproject.com/en/4.0/ref/django-admin/#loaddata
# DJANGO_COLLECT_STATIC - calls the collectstatic management cmd - https://docs.
↪djangoproject.com/en/4.0/ref/contrib/staticfiles/
# entrypoint.sh settings
# ENTRYPOINT_DATABASE & ENTRYPOINT_MESSAGING - name of entrypoint to wait for; do not␣
↪change these values unless updating entrypoint.sh and the type of messaging server or␣
↪database
#####################################################################
DJANGO_MANAGEPY_MIGRATE=on
DJANGO_DATABASE_FLUSH=on
DJANGO_SUPERUSER_CREATE=on
DJANGO_DEFAULT_GROUPS_CREATE=on
DJANGO_DEFAULT_USERS_CREATE=on
DJANGO_DATABASE_LOADDATA=on
DJANGO_COLLECT_STATIC=on
ENTRYPOINT_DATABASE=postgres
ENTRYPOINT_MESSAGING=rabbitmq

#####################################################################
# django database settings; loaded in settings.py
# https://docs.djangoproject.com/en/4.0/ref/settings/#databases
#####################################################################
DJANGO_DATABASE_NAME=medna_metadata
DJANGO_DATABASE_TESTNAME=test_medna_metadata
DJANGO_DATABASE_USERNAME=your_db_user
DJANGO_DATABASE_PASSWORD=your_db_password
DJANGO_DATABASE_HOST=medna_metadata_pgdb
DJANGO_DATABASE_PORT=5432

#####################################################################
```

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```
# django database backup custom setting; loaded in settings.py
# setting DB_BACKUPS to True will automatically backup the full database
# daily at 4:30AM local time - this can be changed in medna_metadata/settings.py
# under CELERYBEAT_SCHEDULE
# https://django-dbbackup.readthedocs.io/en/master/index.html
######################################################################
DB_BACKUPS=False

######################################################################
# django smtp (email) settings; loaded in settings.py
# https://docs.djangoproject.com/en/4.0/topics/email/
######################################################################
DJANGO_EMAIL_HOST_USER=your_email@domain.com
DJANGO_EMAIL_HOST_PASSWORD=your_email_password

######################################################################
# django-storages settings; loaded in settings.py
# https://django-storages.readthedocs.io/en/latest/backends/amazon-S3.html#amazon-s3
######################################################################
AWS_ACCESS_KEY_ID=your_access_key_id
AWS_SECRET_ACCESS_KEY=your_access_key
AWS_REGION=your_aws_region
AWS_STORAGE_BUCKET_NAME=your_storage_bucket_name
AWS_STORAGE_BUCKET_SUBFOLDER_NAME=your_storage_bucket_subfolder_name

######################################################################
# RabbitMQ docker settings
# https://www.rabbitmq.com/configure.html
# https://hub.docker.com/_/rabbitmq
######################################################################
RABBITMQ_DEFAULT_USER=your_rabbitmq_user
RABBITMQ_DEFAULT_PASS=your_rabbitmq_password
RABBITMQ_DEFAULT_VHOST=your_rabbitmq_vhost
RABBITMQ_HOST=medna_metadata_rabbitmq
RABBITMQ_PORT=5672

######################################################################
# Celery settings
# https://docs.celeryq.dev/en/stable/userguide/configuration.html
######################################################################
CELERY_RESULT_BACKEND=rpc
CELERY_BROKER_URL=pyamqp://your_rabbitmq_user:your_rabbitmq_password@medna_metadata_
↪rabbitmq:5672/your_rabbitmq_vhost
CELERYD_NODES=worker
CELERYD_NUM_NODES=1
CELERY_BIN=/home/django/.virtualenvs/mednaenv/bin/celery
CELERY_APP=medna_metadata.celery.app
CELERYD_MULTI=multi
CELERYD_OPTS=''
CELERYD_PID_FILE=/var/run/celery/%n.pid
CELERYD_LOG_FILE=/var/log/celery/%n%I.log
CELERYD_LOG_LEVEL=INFO
```

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```
CELERYBEAT_PID_FILE=/var/run/celery/beat.pid
CELERYBEAT_LOG_FILE=/var/log/celery/beat.log

######################################################################
# Gunicorn settings
# https://docs.gunicorn.org/en/stable/settings.html
# https://docs.gunicorn.org/en/stable/settings.html#logging
# https://github.com/benoitc/gunicorn/blob/master/examples/logging.conf
# https://stackoverflow.com/questions/36424335/how-to-perform-log-rotation-with-gunicorn
######################################################################
GUNICORN_CONFIG_FILE=/your/path/to/medna-metadata/docker/gunicorn-logging.conf
```

`medna.env.db`:

```
######################################################################
# PostGIS docker settings; loaded in settings.py
# https://registry.hub.docker.com/r/postgis/postgis/
######################################################################
POSTGRES_USER=your_db_user
POSTGRES_PASSWORD=your_db_password
POSTGRES_DB=medna_metadata
```

Open and update the environmental variables with desired settings in a text editor such as VIM

```
sudo vim medna.env
```

Write and exit the VIM text editor:

```
:wq!
```

Repeat these steps with `medna.env.db`.

Once settings are verified, run `sudo docker-compose -f docker-compose.yml up -d --build` from the `docker/` directory to build and deploy medna-metadata from the Dockerfiles in `docker/web/` and `docker/nginx/`, PostgreSQL with PostGIS, RabbitMQ, Celery, Gunicorn, and NGINX.:

```
cd medna-metadata/docker/
sudo docker-compose -f docker-compose.yml up -d --build
```

After the containers are up, it will take a moment for the application to set itself up. Once it is done, it will be accessible at *http://localhost:8000*

1.4 Manual Setup

1.4.1 Install Requirements

Ubuntu 20.04

Install Ubuntu Requirements:

```
cd medna-metadata
sudo bash requirements/ubuntu-requirements.sh
```

It will run the following installation commands:

```
# Ubuntu 20.04
# sudo bash ubuntu-requirements.sh
apt-get update && apt-get install -y --no-install-recommends apt-utils
# Django with Postgres, Nginx, and Gunicorn on Ubuntu 20.04
apt update && apt -y install \
 libpq-dev postgresql postgresql-contrib nginx curl vim netcat
# GDAL, GEOS, PROJ.4, python deps
apt-get -y install \
 binutils libproj-dev gdal-bin \
 python3-dev python3-pip python3-venv python3-wheel \
 rabbitmq-server
# PostGIS
apt -y install \
 postgis postgresql-12-postgis-3
# Certbot and Nginx plugin
apt -y install \
 certbot python3-certbot-nginx
```

Create a Virtual Environment and Set Environmental Variables

Create a virtual environment with venv:

```
sudo -H pip install --upgrade pip
sudo -H pip install virtualenvwrapper
sudo -H pip install virtualenv
```

Dotenv is a python library for reading in environmental variables from a file:

```
pip install django-dotenv
```

Add environmental variables to the bottom of bashrc, which reloads environmental variables anytime the server reboots.

The environmental variables required to run this application are listed in `docker/bashrc.txt`:

```
######################################################################
# django general settings; loaded in settings.py
# The secret key must be a large random value and it must be kept secret.
# https://docs.djangoproject.com/en/4.0/ref/settings/#std:setting-SECRET_KEY
# https://docs.djangoproject.com/en/4.0/ref/settings/#std-setting-TIME_ZONE
# List of time zones: https://en.wikipedia.org/wiki/List_of_tz_database_time_zones
######################################################################
export DJANGO_SECRET_KEY='your_secret_key'
export DJANGO_ALLOWED_HOSTS='localhost www.yourdomain.com [::1]'
export DJANGO_SETTINGS_MODULE=medna_metadata.settings
export DJANGO_DEBUG=False
export DJANGO_LOG_LEVEL='info'
export TIME_ZONE='America/New_York'

######################################################################
# django database settings; loaded in settings.py
# https://docs.djangoproject.com/en/4.0/ref/settings/#databases
```

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```
########################################################################
export DJANGO_DATABASE_NAME='medna_metadata'
export DJANGO_DATABASE_TESTNAME='test_medna_metadata'
export DJANGO_DATABASE_USERNAME='your_db_user'
export DJANGO_DATABASE_PASSWORD='your_db_password'
export DJANGO_DATABASE_HOST='localhost'
export DJANGO_DATABASE_PORT=''

########################################################################
# django database backup custom setting; loaded in settings.py
# setting DB_BACKUPS to True will automatically backup the full database
# daily at 4:30AM local time - this can be changed in medna_metadata/settings.py
# under CELERYBEAT_SCHEDULE
# https://django-dbbackup.readthedocs.io/en/master/index.html
########################################################################
export DB_BACKUPS=False

########################################################################
# django smtp (email) settings; loaded in settings.py
# https://docs.djangoproject.com/en/4.0/topics/email/
########################################################################
export DJANGO_EMAIL_HOST_USER='your_email@domain.com'
export DJANGO_EMAIL_HOST_PASSWORD='your_email_password'

########################################################################
# django-storages settings; loaded in settings.py
# https://django-storages.readthedocs.io/en/latest/backends/amazon-S3.html
########################################################################
export AWS_ACCESS_KEY_ID='your_access_key_id'
export AWS_SECRET_ACCESS_KEY='your_secret_access_key'
export AWS_REGION='your_aws_region'
export AWS_STORAGE_BUCKET_NAME='your_bucket'
export AWS_STORAGE_BUCKET_SUBFOLDER_NAME='your_bucket_subfolder'

########################################################################
# Celery settings
# https://docs.celeryq.dev/en/stable/userguide/configuration.html
########################################################################
export CELERY_RESULT_BACKEND='rpc'
export CELERY_BROKER_URL='pyamqp://your_rabbitmq_user:your_rabbitmq_
↪password@localhost:5672/your_rabbitmq_vhost'

########################################################################
# virtualenv settings
# https://virtualenvwrapper.readthedocs.io/en/latest/install.html#python-interpreter-
↪virtualenv-and-path
########################################################################
export WORKON_HOME=$HOME/.virtualenvs
export PROJECT_HOME=$HOME/medna-metadata
export VIRTUALENVWRAPPER_PYTHON=/usr/bin/python3
source /usr/local/bin/virtualenvwrapper.sh
```

These environmental variables must be updated with values specific to your deployment.

Open ~/.bashrc with a text editor such as VIM:

```
sudo vim ~/.bashrc
```

Scroll to the bottom of bashrc and type i to insert into the file. Write and exit the VIM text editor:

```
:wq!
```

Tip: To write and quit within the VIM text editor, [esc], :wq!, and [enter]

Load the environmental variables:

```
source ~/.bashrc
```

Make a copy of gunicorn.env.txt in the same docker/ directory with the .txt extension removed (e.g., gunicorn.env)

```
cp docker/gunicorn.env.txt docker/gunicorn.env
```

gunicorn.env:

```
######################################################################
# django general settings; loaded in settings.py
# The secret key must be a large random value and it must be kept secret.
# https://docs.djangoproject.com/en/4.0/ref/settings/#std:setting-SECRET_KEY
# https://docs.djangoproject.com/en/4.0/ref/settings/#std-setting-TIME_ZONE
# List of time zones: https://en.wikipedia.org/wiki/List_of_tz_database_time_zones
######################################################################
DJANGO_SECRET_KEY=your_secret_key
DJANGO_ALLOWED_HOSTS=localhost [::1]
DJANGO_DEBUG=True
DJANGO_LOG_LEVEL=info
TIME_ZONE=America/New_York

######################################################################
# django database settings; loaded in settings.py
# https://docs.djangoproject.com/en/4.0/ref/settings/#databases
######################################################################
DJANGO_DATABASE_NAME=medna_metadata
DJANGO_DATABASE_TESTNAME=test_medna_metadata
DJANGO_DATABASE_USERNAME=your_db_user
DJANGO_DATABASE_PASSWORD=your_db_password
DJANGO_DATABASE_HOST=localhost
DJANGO_DATABASE_PORT=''

######################################################################
# django database backup custom setting; loaded in settings.py
# setting DB_BACKUPS to True will automatically backup the full database
# daily at 4:30AM local time - this can be changed in medna_metadata/settings.py
# under CELERYBEAT_SCHEDULE
# https://django-dbbackup.readthedocs.io/en/master/index.html
######################################################################
DB_BACKUPS=False
```

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```
######################################################################
# django smtp (email) settings; loaded in settings.py
# https://docs.djangoproject.com/en/4.0/topics/email/
######################################################################
DJANGO_EMAIL_HOST_USER=your_email@domain.com
DJANGO_EMAIL_HOST_PASSWORD=your_email_password

######################################################################
# django-storages settings; loaded in settings.py
# https://django-storages.readthedocs.io/en/latest/backends/amazon-S3.html
######################################################################
AWS_ACCESS_KEY_ID=your_access_key_id
AWS_SECRET_ACCESS_KEY=your_access_key
AWS_REGION=your_aws_region
AWS_STORAGE_BUCKET_NAME=your_storage_bucket_name
AWS_STORAGE_BUCKET_SUBFOLDER_NAME=your_storage_bucket_subfolder_name

######################################################################
# Celery settings
# https://docs.celeryq.dev/en/stable/userguide/configuration.html
######################################################################
CELERY_RESULT_BACKEND=rpc
CELERY_BROKER_URL=pyamqp://your_rabbitmq_user:your_rabbitmq_password@localhost:5672/your_
↪rabbitmq_vhost
CELERYD_NODES=worker
CELERYD_NUM_NODES=1
CELERY_BIN=/your/path/to/bin/celery
CELERY_APP=medna_metadata.celery.app
CELERYD_MULTI=multi
CELERYD_OPTS=''
CELERYD_PID_FILE=/var/run/celery/%n.pid
CELERYD_LOG_FILE=/var/log/celery/%n%I.log
CELERYD_LOG_LEVEL=INFO
CELERYBEAT_PID_FILE=/var/run/celery/beat.pid
CELERYBEAT_LOG_FILE=/var/log/celery/beat.log

######################################################################
# Gunicorn settings
# https://docs.gunicorn.org/en/stable/settings.html
# https://docs.gunicorn.org/en/stable/settings.html#logging
# https://github.com/benoitc/gunicorn/blob/master/examples/logging.conf
# https://stackoverflow.com/questions/36424335/how-to-perform-log-rotation-with-gunicorn
######################################################################
GUNICORN_CONFIG_FILE=/your/path/to/medna-metadata/docker/gunicorn-logging.conf
```

Update the environmental variables with values specific to your deployment in a text editor such as VIM

```
sudo vim docker/gunicorn.env
```

Type `i` to insert into the file. Write and exit the VIM text editor:

```
:wq!
```

Warning: MeDNA-Metadata **will not** successfully deploy without setting these environmental variables.

Create and activate virtualenvwrapper:

```
mkvirtualenv --python /usr/bin/python3.8 mednaenv
```

Important:

The version of python varies and you will have to check or install it.

- Python with Virtualenvwrapper
- Change Ubuntu's Default Python Version

Activate the virtual environment:

```
workon mednaenv
```

Install python requirements to the virtualenv:

```
pip install -U -r requirements/prod.txt
```

The following python libraries will install: .. literalinclude:: ../../requirements/base.txt

language
env

```
-r base.txt

gunicorn==20.1.0
```

1.4.2 Create PostgreSQL database with PostGIS Extension

Create the database for your project:

```
sudo -u postgres psql -c "CREATE DATABASE medna_metadata;"
```

Create a database user and add them to the project with a secure password:

```
sudo -u postgres psql -c "CREATE USER youruser WITH PASSWORD 'yourdbpassword';"
```

Recommended settings from the Django project:

```
sudo -u postgres psql -c "ALTER ROLE youruser SET client_encoding TO 'utf8';"
sudo -u postgres psql -c "ALTER ROLE youruser SET default_transaction_isolation TO 'read␣
↪committed';"
sudo -u postgres psql -c "ALTER ROLE youruser SET timezone TO 'UTC';"
```

Set `youruser` as the administrator for the medna_metadata database:

```
sudo -u postgres psql -c "GRANT ALL PRIVILEGES ON DATABASE medna_metadata TO youruser;"
```

Grant privileges to the `youruser` database user to create databases for Django tests:

```
sudo -u postgres psql -c "ALTER USER youruser CREATEDB NOSUPERUSER NOCREATEROLE;"
```

Add the PostGIS extension to medna_metadata:

```
sudo -i -u postgres psql -d medna_metadata -c "CREATE EXTENSION postgis;"
```

Tip: It would be advantageous here to use the same username as your selected Ubuntu username.

Migrate the Database Tables

Migrate the database schema to PostgreSQL from within the same directory as `manage.py` Within each app there is a migration directory which contains files which tell the database how to create the database tables. These have been pre-generated and added to this repository to simplify the process of deplying the medna-metadata application:

```
python manage.py migrate users
python manage.py migrate utility
python manage.py migrate field_site
python manage.py migrate sample_label
python manage.py migrate field_survey
python manage.py migrate wet_lab
python manage.py migrate freezer_inventory
python manage.py migrate bioinformatics
```

Now, if everything looked good (e.g., no error messages), complete the remaining migrations:

```
python manage.py migrate
```

1.4.3 Create Superuser

Creating a `superuser` adds an administrative user with full privileges to the MeDNA-Metadata project.

Create a superuser:

```
python manage.py createsuperuser
```

When prompted, enter in your preferred credentials (`youremail`, `yourpassword`).

1.4.4 Collect Static

Collecting static files will copy all static content into the directory specified in `settings.py`.

Collect static files:

```
python manage.py collectstatic
```

1.4.5 Test The Deployment

Temporarily create an exception for port 8000:

```
sudo ufw allow 8000
```

Test the project deployment:

```
python manage.py runserver 0.0.0.0:8000
```

In your web browser, visit the server's IP address followed by :8000

`http://youripaddress:8000`

If you're able to see a live project, then enter `[CTRL-C]` in to shut down the test deployment.

Test Gunicorn

Now test to see if the project can be deployed with Gunicorn:

```
gunicorn --bind 0.0.0.0:8000 medna_metadata.wsgi
```

See also:

If you were able to visit the same page while deployed with Gunicorn, continue onward. If not, some helpful troubleshooting steps can be found in the DigitalOcean tutorial on setting up Django with PostgreSQL, Gunicorn, and Nginx.

- Django with PostgreSQL, Gunicorn, and Nginx on Ubuntu 20.04

1.4.6 Create Gunicorn Socket and Service files (e.g., daemonizing!)

Leave the virtualenv:

```
deactivate
```

Create a systemd Socket file:

```
sudo vim /etc/systemd/system/gunicorn.socket
```

Write the following to the file:

```
[Unit]
Description=gunicorn socket

[Socket]
```

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```
ListenStream=/run/gunicorn.sock

[Install]
WantedBy=sockets.target
```

Write and exit the VIM text editor:

```
:wq!
```

Create a systemd service file:

```
sudo vim /etc/systemd/system/gunicorn.service
```

Modify then write the following to the file:

```
[Unit]
Description=gunicorn daemon
Requires=gunicorn.socket
After=network.target

[Service]
User=youruser
Group=youruser
WorkingDirectory=/path/to/medna-metadata
EnvironmentFile=/path/to/medna-metadata/docker/gunicorn.env
ExecStart=/path/to/.virtualenvs/mednaenv/bin/gunicorn \
          --log-config ${GUNICORN_CONFIG_FILE} \
          --workers 3 \
          --timeout 300 \
          --bind unix:/run/gunicorn.sock \
          medna_metadata.wsgi:application

[Install]
WantedBy=multi-user.target
```

Warning: You will need to replace the `User` and `Group` to the correct Ubuntu username and group and modify the `WorkingDirectory`, `EnvironmentFile`, and `ExecStart` to the actual directory MeDNA-Metadata is in.

Write and exit the VIM text editor:

```
:wq!
```

Enable the socket and service:

```
sudo systemctl start gunicorn.socket
sudo systemctl enable gunicorn.socket
```

Check for the socket file's status (it should be green):

```
sudo systemctl status gunicorn.socket
```

Check for the existence of the sock file:

```
file /run/gunicorn.sock
```

If there is no file, check the socket's logs and troubleshoot:

```
sudo journalctl -u gunicorn.socket
```

Test the socket activation (should be grey & inactive):

```
sudo systemctl status gunicorn
```

Test the socket activation mechanism through curl:

```
curl --unix-socket /run/gunicorn.sock localhost
```

Now see if Gunicorn is "running":

```
sudo systemctl status gunicorn
```

If you need to troubleshoot, check `journalctl` and `daemon-reload` and `restart gunicorn` when the service, socket, settings, or env files are edited:

```
sudo journalctl -u gunicorn
sudo systemctl daemon-reload
sudo systemctl restart gunicorn
```

1.4.7 Setup Celery and RabbitMQ

Celery task management and the RabbitMQ messaging server are used for task queues within the backend application. This allows for things such as queues of data transformations and workers that will spawn as resources are available.

See also:

- Celery First Steps
- Celery, RabbitMQ, and Ubuntu
- Celery and Django

Note: Celery and RabbitMQ should have already been installed with the requirements.txt and ubuntu-requirements.sh, but the commands are also provided here.

Install RabbitMQ messaging server:

```
sudo apt-get update
sudo apt-get install rabbitmq-server
```

Important: If you named your venv something other than `mednaenv`, use that here instead.

Activate the virtualenv:

```
workon mednaenv
```

Install Celery:

```
pip install -U "celery>=5.2.3"
```

Setup RabbitMQ

Add a user and a virtual host:

```
sudo rabbitmqctl add_user youruser yourpassword
sudo rabbitmqctl add_vhost yourvhost
sudo rabbitmqctl set_user_tags youruser yourtag
sudo rabbitmqctl set_permissions -p yourvhost youruser ".*" ".*" ".*"
```

Warning: You will need to replace `youruser`, `yourpassword`, `yourvhost`, `yourtag`, to the password, username, tag and hostname of your choosing. These are specific to RabbitMQ and not dependent on other applications. What is chosen is used to construct your CELERY_BROKER_URL.

Stop RabbitMQ:

```
sudo systemctl stop rabbitmq-server
```

Check to verify it is actually stopped:

```
sudo rabbitmqctl cluster_status
```

Start it up again:

```
sudo systemctl start rabbitmq-server
sudo systemctl restart rabbitmq-server
sudo systemctl status rabbitmq-server
```

Warning: For Celery and RabbitMQ to function, the CELERY_RESULT_BACKEND and CELERY_BROKER_URL variables must be set in `~/.bashrc` and `docker/gunicorn.env`. These variables should resemble the following:

- CELERY_RESULT_BACKEND='rpc'
- CELERY_BROKER_URL='pyamqp://youruser:yourpassword@localhost:port/yourvhost`

Create Celery Worker and Beat files (e.g., daemonizing!)

Like Gunicorn, celery should be run as a Systemd service. –

First, open your environment file:

```
sudo vim docker/gunicorn.env
```

Update or add the following Celery config settings to your environment file:

```
CELERY_RESULT_BACKEND='your_result_backend'
CELERY_BROKER_URL='transport://your_rabbitmq_user:your_rabbitmq_password@hostname:port/
↪your_rabbitmq_vhost'
```

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```
CELERYD_NODES='worker'
CELERY_BIN='/path/to/.virtualenvs/mednaenv/bin/celery'
CELERY_APP='medna_metadata.celery.app'
CELERYD_MULTI='multi'
CELERYD_OPTS=''
CELERYD_PID_FILE='/var/run/celery/%n.pid'
CELERYD_LOG_FILE='/var/log/celery/%n%I.log'
CELERYD_LOG_LEVEL='INFO'
CELERYBEAT_PID_FILE='/var/run/celery/beat.pid'
CELERYBEAT_LOG_FILE='/var/log/celery/beat.log'
```

Write and exit the VIM text editor:

```
:wq!
```

Now we need to create the Celery log and run directories and update their permissions:

```
sudo mkdir /var/run/celery/
sudo mkdir /var/log/celery/

sudo chgrp yourgroup /var/run/celery/
sudo chgrp yourgroup /var/log/celery/

sudo chmod g+rwx /var/run/celery/
sudo chmod g+rwx /var/log/celery/
```

Create a Celery service file:

```
sudo vim /etc/systemd/system/celery.service
```

Modify then write the following to the file:

```
[Unit]
Description=Celery Service
After=network.target rabbitmq-server.service
Requires=rabbitmq-server.service

[Service]
Type=forking
User=youruser
Group=yourgroup
EnvironmentFile=/path/to/medna-metadata/docker/gunicorn.env
WorkingDirectory=/path/to/medna-metadata
Environment=DJANGO_SETTINGS_MODULE=medna_metadata.settings
ExecStart=/bin/sh -c '${CELERY_BIN} -A ${CELERY_APP} multi start ${CELERYD_NODES} \
    --pidfile=${CELERYD_PID_FILE} --logfile=${CELERYD_LOG_FILE} \
    --loglevel="${CELERYD_LOG_LEVEL}" ${CELERYD_OPTS}'
ExecStop=/bin/sh -c '${CELERY_BIN} multi stopwait ${CELERYD_NODES} \
    --pidfile=${CELERYD_PID_FILE} --logfile=${CELERYD_LOG_FILE} \
    --loglevel="${CELERYD_LOG_LEVEL}"'
ExecReload=/bin/sh -c '${CELERY_BIN} -A ${CELERY_APP} multi restart ${CELERYD_NODES} \
    --pidfile=${CELERYD_PID_FILE} --logfile=${CELERYD_LOG_FILE} \
    --loglevel="${CELERYD_LOG_LEVEL}" ${CELERYD_OPTS}'
```

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```
Restart=always

[Install]
WantedBy=multi-user.target
```

Write and exit the VIM text editor:

```
:wq!
```

Warning: You will need to replace the `User` and `Group` to the correct Ubuntu username and group and modify the `WorkingDirectory` and `EnvironmentFile` to the actual directory MeDNA-Metadata is in.

We also need a celerybeat Systemd service for scheduling tasks.

Create a celerybeat file:

```
sudo vim /etc/systemd/system/celerybeat.service
```

Modify then write the following to the file:

```
[Unit]
Description=Celery Beat Service
After=network.target rabbitmq-server.service
Requires=rabbitmq-server.service

[Service]
Type=simple
User=youruser
Group=yourgroup
EnvironmentFile=/path/to/medna-metadata/docker/gunicorn.env
WorkingDirectory=/path/to/medna-metadata
Environment=DJANGO_SETTINGS_MODULE=medna_metadata.settings
ExecStart=/bin/sh -c '${CELERY_BIN} -A ${CELERY_APP} beat  \
    --pidfile=${CELERYBEAT_PID_FILE} \
    --logfile=${CELERYBEAT_LOG_FILE} --loglevel=${CELERYD_LOG_LEVEL}'
Restart=always

[Install]
WantedBy=multi-user.target
```

Write and exit the VIM text editor:

```
:wq!
```

Warning: You **must** replace the `User` and `Group` to the correct Ubuntu username and group and modify the `WorkingDirectory` and `EnvironmentFile` to the actual directory MeDNA-Metadata is in.

We can now start the celery and celerybeat services:

```
sudo systemctl daemon-reload
sudo systemctl start celery.service
sudo systemctl status celery.service

sudo systemctl start celerybeat.service
sudo systemctl status celerybeat.service
```

If any modifications are made to any `tasks.py` or `medna_metadata/celery.py`, restart `celerybeat` and `celeryworker`:

```
sudo systemctl restart celery.service && sudo systemctl restart celerybeat.service &&␣
↪sudo systemctl daemon-reload && sudo systemctl restart gunicorn
```

If you want these services to start automatically on boot, you can enable them as follows:

```
sudo systemctl enable celery.service
sudo systemctl enable celerybeat.service
```

Troubleshooting Celery

If you are trying to troubleshoot celery or celerybeat, be sure to check system logs for error messages:

```
sudo cat /var/log/syslog
sudo tail /var/log/syslog -n 40
```

You can also check RabbitMQ logs:

```
sudo tail /var/log/rabbitmq/rabbit@medna-metadata.log -n 50
```

To view Celery tasks as they are sent by RabbitMQ:

```
celery -A medna_metadata worker --pool=solo -l info
```

`[CTRL-C]` to exit.

1.4.8 Collect Static Files

Any time there is a change made to the python code, run the following to reload changes:

```
git pull && python manage.py collectstatic --noinput --clear && sudo systemctl daemon-
↪reload && sudo systemctl restart gunicorn.socket gunicorn.service
```

1.4.9 Configure Nginx

Create a nginx config file:

```
sudo vim /etc/nginx/sites-available/medna-metadata
```

Modify and write the following:

```
server {
    listen 80;
    server_name youripaddress yourdomain.com;

    location = /favicon.ico { access_log off; log_not_found off; }
    location /static/ {
        root /path/to/medna-metadata;
    }

    location / {
        include proxy_params;
        proxy_pass http://unix:/run/gunicorn.sock;
        proxy_set_header X-Forwarded-For $proxy_add_x_forwarded_for;
        proxy_connect_timeout 300s;
        proxy_read_timeout 300s;
    }
}
```

Warning: You **must** edit the `server_name` and `location` to the actual IP address or domain name and to the actual directory MeDNA-Metadata is in.

Write and exit the VIM text editor:

```
:wq!
```

Enable the file by linking it to sites-enabled:

```
sudo ln -s /etc/nginx/sites-available/medna-metadata /etc/nginx/sites-enabled
```

Test the Nginx configuration for syntaix errors:

```
sudo nginx -t
```

If there are no errors, restart Nginx:

```
sudo systemctl restart nginx
```

Delete port 8000 and allow Nginx in the firewall:

```
sudo ufw delete allow 8000
sudo ufw allow 'Nginx Full'
```

Troubleshooting Nginx and Gunicorn

See also:

For more information on troubleshooting Nginx and Gunicorn, please see the following:

- Django with PostgreSQL, NGINX, and Gunicorn on Ubuntu 20.04

1.4.10 SSL Certificates with Certbot

Run certbot:

```
sudo certbot --nginx -d yourdomain.com
```

Follow the prompt by enter in your `email address`, `[A]`, `[n]`, and `[2]`.

Verify Certbot auto-renewal:

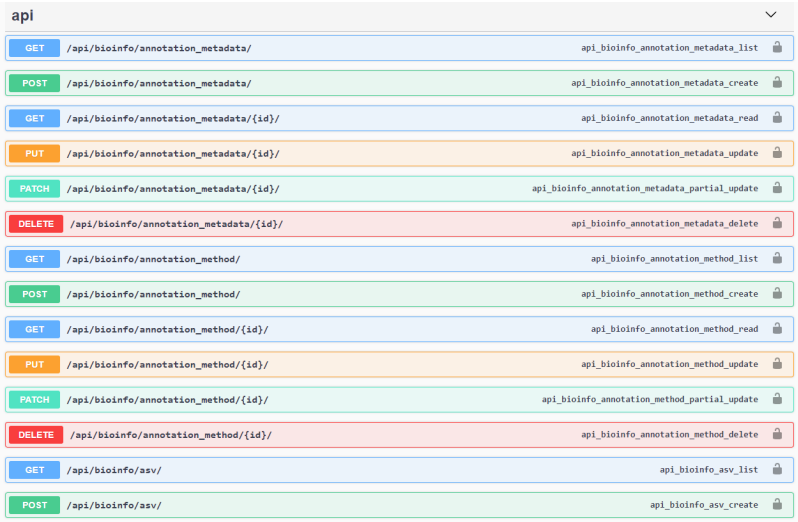
```
sudo certbot renew --dry-run
```

You should now be good to go and running with your desired server and domain.

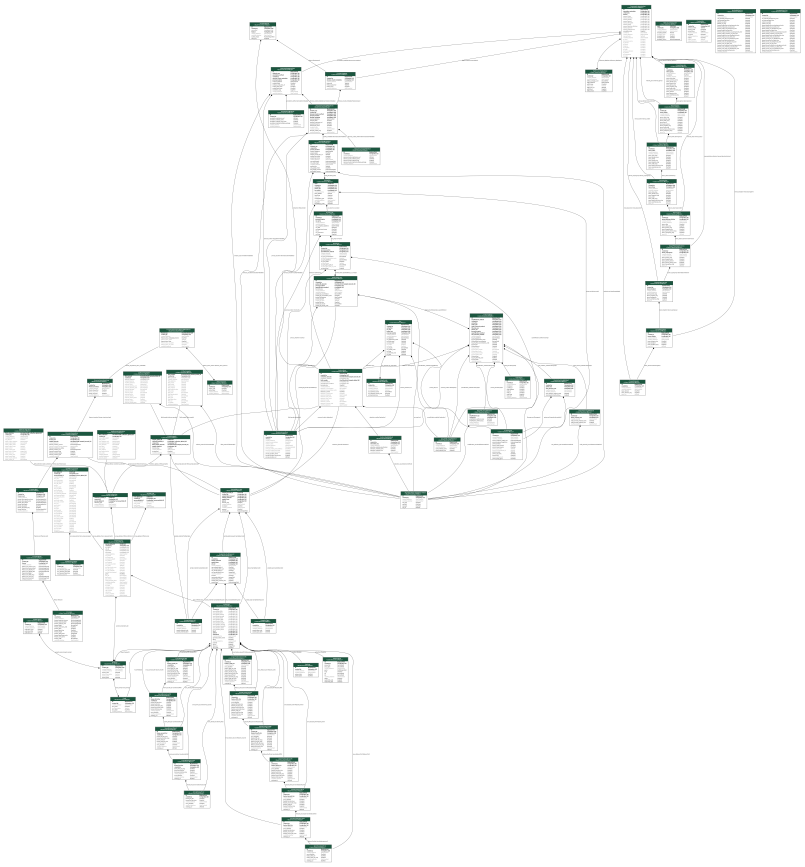
1.5 Application Programming Interface (API)

1.5.1 API Documentation

medna-metadata's API was written in the Django REST Framework and all API documentation are automatically generated with drf-yasg library. With an active deployment, simply navigate to `https://yourdomain.com/swagger/` to view details on all Create, Read, Update, and Delete (CRUD) operations.



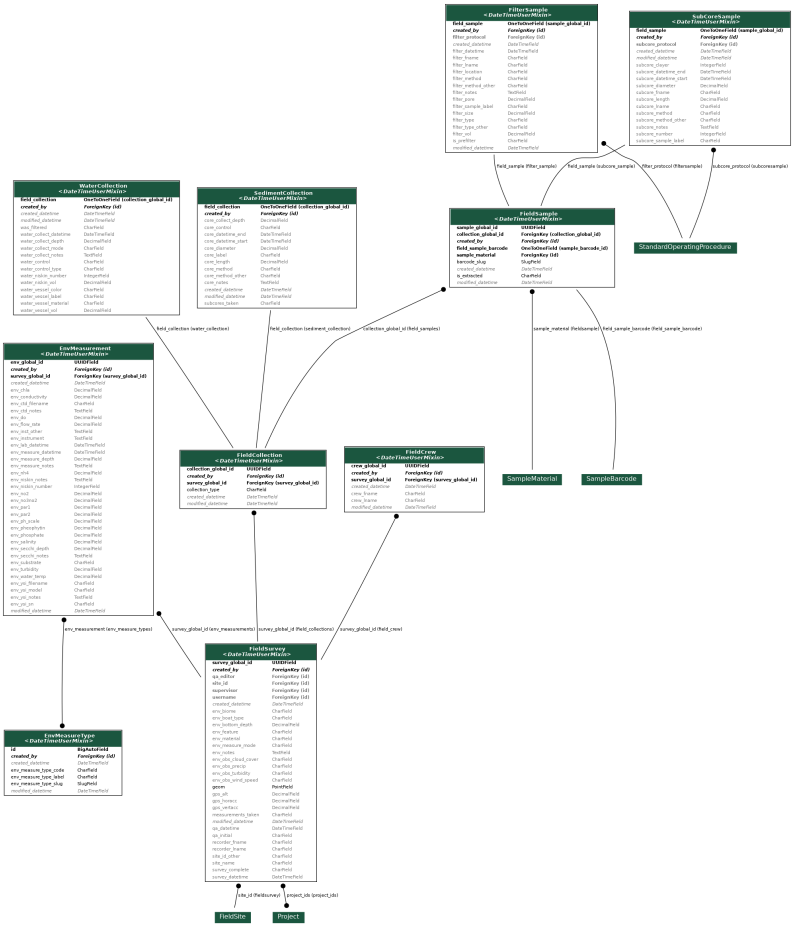
1.5.2 Database Design



Field Data Collection

Field data collection is project wide, and pertains to environmental and collection information related to sediment or water samples. These samples are barcoded and that barcode is used as a unique identifier. Barcodes are placed on filters for water samples, and on sub-cores for sediment samples. Each water collection is filtered using multiple filter types (Nitex, Glass Fiber Filter, Supor, or Cellulose Nitrate) and each filter represents one sample. If sediment is collected, it is initially collected as a core. After a core of sediment is collected, it is subdivided into sub-cores, and each sub-core represents one sample.

Filters, cores, and sub-cores are stored within -80°C lab freezers until extraction.



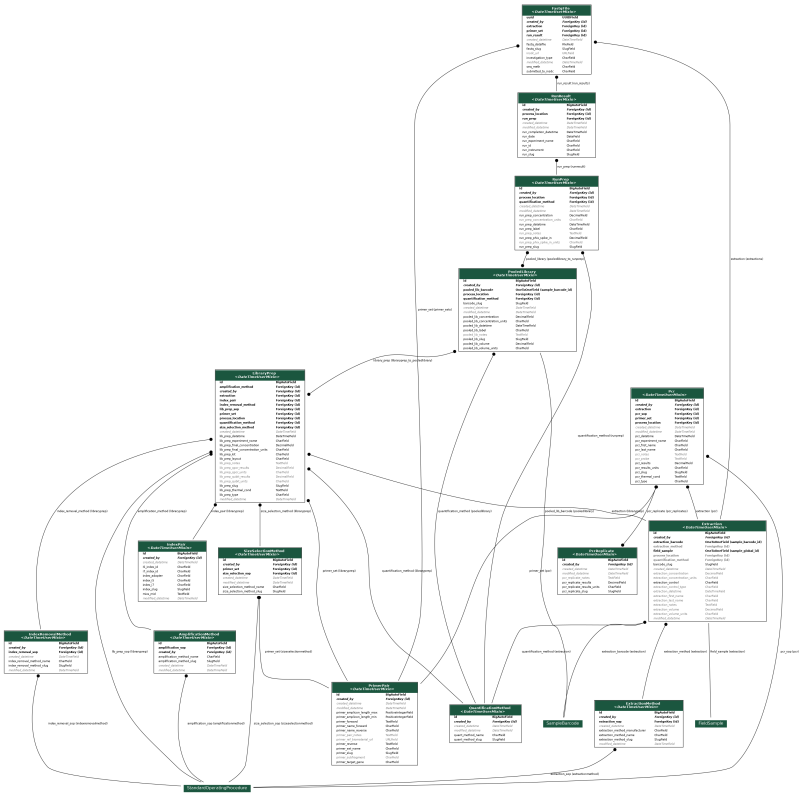
Wet Lab Processing

Wet lab processing is conducted by the Wet Laboratory. Wet lab processing pertains to all processing from extraction, Digital Droplet PCR (ddPCR), quantitative PCR (qPCR), and Next Generation Sequencing (NGS). After filtration or sub-coring, the samples are extracted. Extraction converts field samples into solutions of eDNA. Extractions share the same unique barcode identifier as samples.

The tables for LibraryPrep, PooledLibrary, RunPrep, RunResults, and FastqFile are all directly related to Next Generation Sequencing (NGS) and the generation of FastQ files. FastQ files contain the resulting sequences from NGS, and sequencing is typically performed by hardware equivalent to an Illumina MiSeq. These NGS tables also relate to information in the IndexPair and PrimerPair tables. The PCR and PCRReplicate tables pertain to additional analyses that can amplify or quantify eDNA samples and are also related to the PrimerPair table.

The PrimerPair table contains information related to the target gene, or DNA region of interest. Primers allow for the amplification of a specific region of DNA, which is important for the positive identification of a particular taxon or taxonomic group. The IndexPair table contains information related to a unique sequence that is used to identify each sample. During NGS, the samples are pooled together. Adding a unique index adapter to the sample sequences enables the separation of pooled samples after sequencing is complete. Separation of pooled samples occurs during a process called demutiplexing, which converts raw BCL files into two FastQ files for each sample.

Extractions and pooled libraries are stored within the -80°C lab freezers until they are depleted.



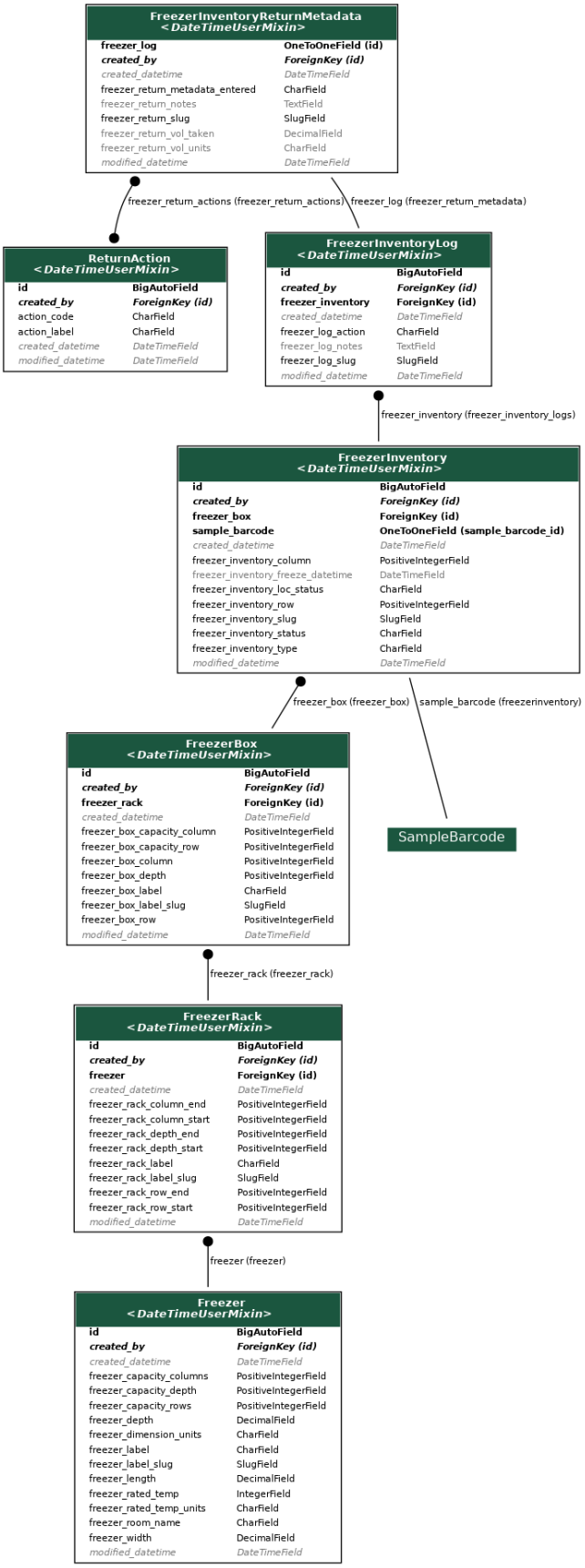
Freezer Inventory Tracking

Freezer inventory tracking is conducted by the Wet Laboratory, and pertains to the tracking of all filters, subcores, extractions, or pooled libraries that may be stored in -80°C lab freezers.

Occasionally a sediment core is not sub-cored within the same day it was collected, so it will be stored in -80°C lab freezers until it is sub-cored. Water collections will not be stored in -80°C lab freezers, but the filters that are taken from water are typically stored in freezers until they are extracted.

Extractions are stored within -80°C lab freezers, where they are temporarily removed from the freezer when further processing is performed. Only small portions are taken from an extraction each time they are removed from the freezer. After small portions are taken, extractions are placed back in the -80°C lab freezers until there is no more extraction remaining. The Wet Laboratory will track the amount taken from extractions, who has the extraction, and whether it was returned to the same freezer location.

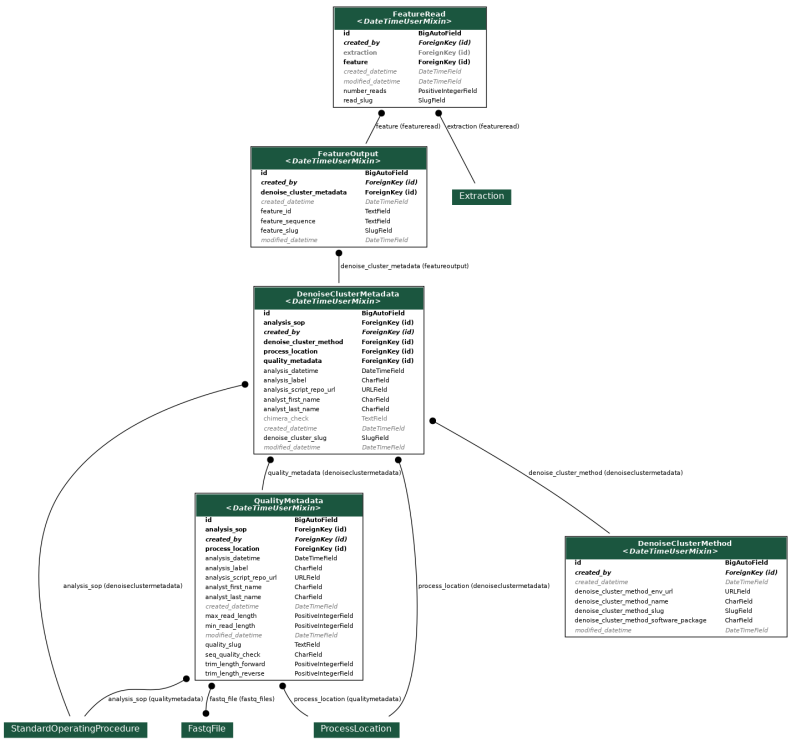
A pooled library may also function in a similar way to an extraction, in that it is a solution of eDNA that may be stored in the -80°C lab freezers. The Wet laboratory will also track the amount taken from a pooled library, who has the pooled library, and whether it was returned to the same freezer location.


FreezerInventoryReturnMetadata
<DateTimeUserMixin>
freezer_log OneToOneField (id)
created_by ForeignKey (id)
created_datetime DateTimeField
freezer_return_metadata_entered CharField
freezer_return_notes TextField
freezer_return_slug SlugField
freezer_return_vol_taken DecimalField
freezer_return_vol_units CharField
modified_datetime DateTimeField
freezer_return_actions (freezer_return_actions)
freezer_log (freezer_return_metadata)
ReturnAction
<DateTimeUserMixin>
id BigAutoField
created_by ForeignKey (id)
action_code CharField
action_label CharField
created_datetime DateTimeField
modified_datetime DateTimeField
FreezerInventoryLog
<DateTimeUserMixin>
id BigAutoField
created_by ForeignKey (id)
freezer_inventory ForeignKey (id)
created_datetime DateTimeField
freezer_log_action CharField
freezer_log_notes TextField
freezer_log_slug SlugField
modified_datetime DateTimeField
freezer_inventory (freezer_inventory_logs)
FreezerInventory
<DateTimeUserMixin>
id BigAutoField
created_by ForeignKey (id)
freezer_box ForeignKey (id)
sample_barcode OneToOneField (sample_barcode_id)
created_datetime DateTimeField
freezer_inventory_column PositiveIntegerField
freezer_inventory_freeze_datetime DateTimeField
freezer_inventory_loc_status CharField
freezer_inventory_row PositiveIntegerField
freezer_inventory_slug SlugField
freezer_inventory_status CharField
freezer_inventory_type CharField
modified_datetime DateTimeField
freezer_box (freezer_box)
sample_barcode (freezerinventory)
FreezerBox
<DateTimeUserMixin>
id BigAutoField
created_by ForeignKey (id)
freezer_rack ForeignKey (id)
created_datetime DateTimeField
freezer_box_capacity_column PositiveIntegerField
freezer_box_capacity_row PositiveIntegerField
freezer_box_column PositiveIntegerField
freezer_box_depth PositiveIntegerField
freezer_box_label CharField
freezer_box_label_slug SlugField
freezer_box_row PositiveIntegerField
modified_datetime DateTimeField
SampleBarcode
freezer_rack (freezer_rack)
FreezerRack
<DateTimeUserMixin>
id BigAutoField
created_by ForeignKey (id)
freezer ForeignKey (id)
created_datetime DateTimeField
freezer_rack_column_end PositiveIntegerField
freezer_rack_column_start PositiveIntegerField
freezer_rack_depth_end PositiveIntegerField
freezer_rack_depth_start PositiveIntegerField
freezer_rack_label CharField
freezer_rack_label_slug SlugField
freezer_rack_row_end PositiveIntegerField
freezer_rack_row_start PositiveIntegerField
modified_datetime DateTimeField
freezer (freezer)
Freezer
<DateTimeUserMixin>
id BigAutoField
created_by ForeignKey (id)
created_datetime DateTimeField
freezer_capacity_columns PositiveIntegerField
freezer_capacity_depth PositiveIntegerField
freezer_capacity_rows PositiveIntegerField
freezer_depth DecimalField
freezer_dimension_units CharField
freezer_label CharField
freezer_label_slug SlugField
freezer_length DecimalField
freezer_rated_temp IntegerField
freezer_rated_temp_units CharField
freezer_room_name CharField
freezer_width DecimalField
modified_datetime DateTimeField

Bioinformatics: Denoising or Clustering

The bioinformatic process of denoising (converting sequences within FastQ files to Amplicon Sequence Variants) or clustering (converting sequences within FastQ files to Operational Taxonomic Units), are represented by the DenoiseClusterMetadata, FeatureReads, and FeatureOutputs tables.

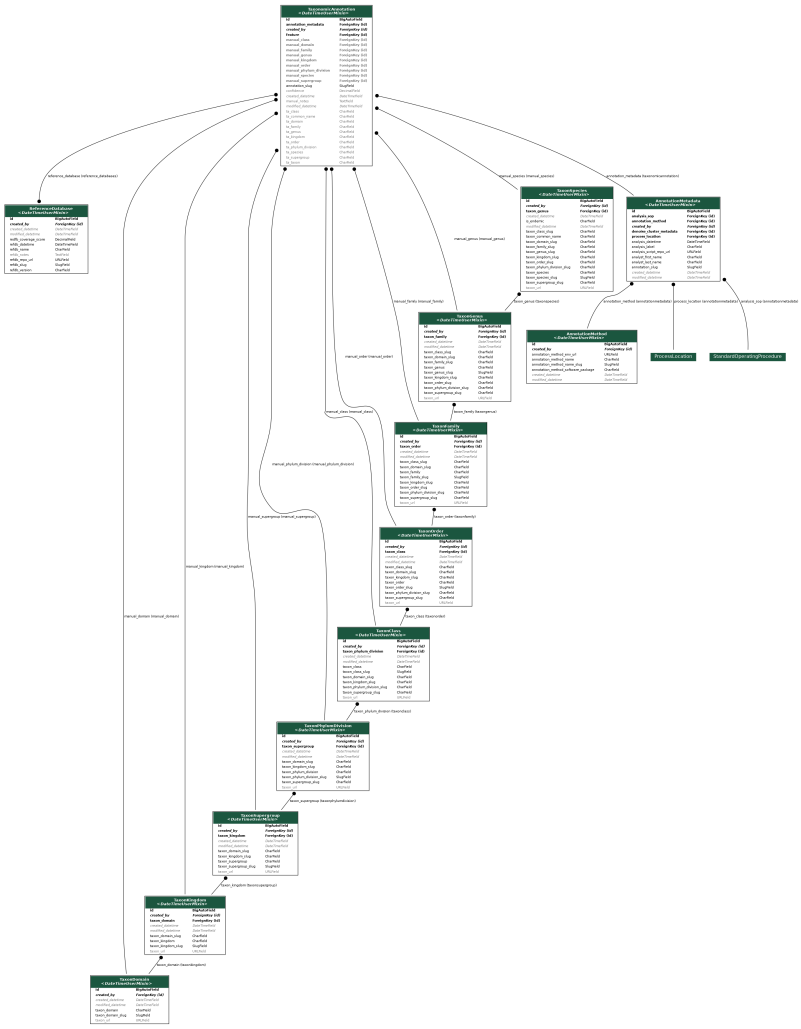
The DenoiseClusterMetadata table covers information related to the specifics of the bioinformatics analysis pipeline. This table enables users to track the process through which ASVs or OTUs were generated. The resulting sequences are listed in the FeatureOutput table. The number of reads, or count of each sequence in each sequencing run, is represented in the FeatureRead table.



Bioinformatics: Taxonomic Annotation

The bioinformatic process of taxonomic annotation is represented by the AnnotationMetadata, TaxonomicAnnotation, ReferenceDatabase, TaxonDomain, TaxonKingdom, TaxonClass, TaxonOrder, TaxonFamily, TaxonGenus, and TaxonSpecies tables.

The AnnotationMetadata table covers information related to the specifics of the bioinformatics analysis pipeline. This table enables us to track the process through which taxonomies are annotated to feature outputs from denoising or clustering. It is possible that taxonomic annotation may be performed multiple times on the same set of feature outputs. The TaxonomicAnnotation table retains the results of either BLAST or a trained classifier and also enables the annotation of manually verified taxonomy. The TaxonDomain, TaxonKingdom, TaxonClass, TaxonOrder, TaxonFamily, TaxonGenus, and TaxonSpecies tables represent curated regional species lists that can be referenced to manually associate verified taxonomy to a sequence through the TaxonomicAnnotation table.



1.6 Troubleshooting

When determining the source of an issue, there are a handful of avenues one can take while troubleshooting. The following are the most common and accessible options in Django.

1.6.1 DEBUG Mode

Django provides a DEBUG mode, where errors are displayed directly in the frontend (user facing web content) while browsing. This is helpful in that a developer is provided with the source of an error rather than a generic failure page. However, DEBUG mode consumes a significant amount of resources and the outputs publicly display secure information. It is not advised to use DEBUG mode on a production (live) server.

Within medna-metadata, Django's `DEBUG` mode can be toggled on (True) or off (False) through the `DJANGO_DEBUG` environmental setting. For manual installations of medna-metadata, this setting will be set in `bashrc` and `docker/gunicorn.env`. For a docker-compose installation, this setting will be set in `docker/medna.env`.

1.6.2 Logging

Another common method to find the source of an issue that is separate from `DEBUG` mode, is through log files. medna-metadata stores logs in a few locations:

- Django logs - `/tmp/`
- Gunicorn access and error logs - `/tmp/`
- Celery beat and worker logs - `/var/log/celery/`
- PostgreSQL logs - `/var/log/postgresql/`
- NGINX logs - `/var/log/nginx/`
- RabbitMQ logs - `/var/log/rabbitmq/`

Manual Installation Logs

If services were daemonized during a manual installation, additional information may be available through system status and logs

```
# show daemonization status - this shows if a service is running
sudo systemctl status gunicorn
sudo systemctl status nginx
sudo systemctl status celery.service
sudo systemctl status celerybeat.service

# show journal entries for each service
sudo journalctl -u gunicorn
sudo journalctl -u nginx
sudo journalctl -u celery.service
sudo journalctl -u celerybeat.service

# print system logs
sudo cat /var/log/syslog
sudo tail /var/log/syslog -n 40
```

Docker-Compose Installation Logs

For a docker-compose installation, log file directories are accessible after entering a docker container. To enter the medna-metadata docker container, use the following command:

```
sudo docker exec -it medna_metadata_web /bin/bash
```

To exit the docker container:

```
exit
```