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Creating Planet Microbe Data Packages

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Marine microbial ecology requires the systematic comparison of biogeochemical and sequence data to analyze environmental influences on the distribution and variability of microbial communities. With ever-increasing quantities of metagenomic data, there is a growing need to make datasets Findable, Accessible, Interoperable, and Reusable (FAIR) across diverse ecosystems. FAIR data is essential to developing analytical frameworks that integrate microbiological, genomic, ecological, oceanographic, and computational methods. Although community standards defining the minimal metadata required to accompany sequence data exist, they haven't been consistently used across projects, precluding interoperability. Moreover, these data are not machine-actionable or discoverable by cyberinfrastructure systems. By making 'omic and physicochemical datasets FAIR to machine systems, we can enable sequence data discovery and reuse based on machine-readable descriptions of environments or physicochemical gradients.

In this work, we developed a novel technical specification for dataset encapsulation for the FAIR reuse of marine metagenomic and physicochemical datasets within cyberinfrastructure systems. This includes using Frictionless Data Packages enriched with terminology from environmental and life-science ontologies to annotate measured variables, their units, and the measurement devices used. This approach was implemented in Planet Microbe, a cyberinfrastructure platform and marine metagenomic web-portal. Here, we discuss the data properties built into the specification to make global ocean datasets FAIR within the Planet Microbe portal. We additionally discuss the selection of, and contributions to marine-science ontologies used within the specification. Finally, we use the system to discover data by which to answer various biological questions about environments, physicochemical gradients, and microbial communities in meta-analyses. This work represents a future direction in marine metagenomic research by proposing a specification for FAIR dataset encapsulation that, if adopted within cyberinfrastructure systems, would automate the discovery, exchange, and re-use of data needed to answer broader reaching questions than originally intended.

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https://www.planetmicrobe.org/

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Setup

1 Step one including downloading the relevant repositories. You'll want to download the relevant repositories to the same directory.

1.1 Open a terminal or shell program and navigate to a base working directory.

1.2 Clone the planet-microbe-datapackages repository:

```
git clone git@github.com:hurwitzlab/planet-microbe-datapackages.git
```

Note you could also use the https version

1.3 Clone the planet-microbe-scripts repository

```
git clone git@github.com:hurwitzlab/planet-microbe-scripts.git
```

Prepare datapackage.json

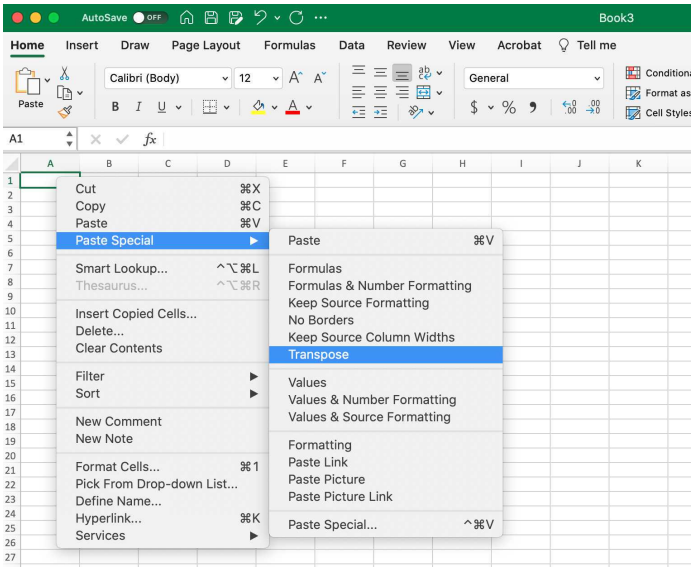
2 Prepare data for creation of Planet Microbe Frictionless Datapackage

How to create the datapackage.json wrapper for your tabular dataset(s).

2.1 Prepare ONTOLOGY_MAPPING.tsv file(s)

Make sure to do this for every individual TSV file that is part of one datapackage product

This can be done by transposing the column headers of your tabular dataset to be the items in the first row of a new csv file. Simply copy and paste the column headers of the original dataset using excel (or similar program) and in a new sheet past them (transposed).



2.2 Next add the following as the new column headers:

parameter	rdf type purl label	rdf type purl	pm:searchable	units label	units purl	measurement source purl label	measurement source purl	pm:measurement source protocol	pm:source url	frictionless type	frictionless format

2.3 ⚠

Populate the new ONTOLOGY_MAPPING.tsv one column at a time.

The "pm:searchable" column is a boolean flag (TRUE or FALSE) for columns that have a corresponding "rdf type purl" annotation columns. If the column from the dataset is about a physicochemical variable from the pmo_searchable_terms.tsv that you want to made searchable make sure to fill it out completely and set the "pm:searchable" to "TRUE". Otherwise the for a given column it can be set to false and everything else left blank.

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1. Fill in the "rdf type purl" column with IRIs from of terms from this **pmo_searchable_terms.tsv**.
2. Fill in the "units purl" column with IRIs from of terms from the UO (Units Ontology) which you can view and browser from here.
3. Fill in the "measurement source purl" columns with term from the OBI (Ontology for Biomedical Investigations) device hierarchy, which you can view and browser from here.
4. Fill in the "pm:source url" column with any link relevant to the dataset columns collection or source e.g., "https://www.ncbi.nlm.nih.gov/bioproject/213098"
5. Fill in the "frictionless type" column with one of: "string", "number", "date", or "datetime".
6. If necessary, fill in the "frictionless format" column for dates datetypes with custom formatting string patterns, e.g., "%Y-%m-%dT%H:%M" or default for ISO standard datetimes.
7. If uploading INSDC submited data (from EBI or NCBI) make sure to fill out one column with a "Biosample identifier assigned by the National Center for Biotechnology Information" aka "http://purl.obolibrary.org/obo/PMO_00000122"
8. If uploading MIxS compliant data make sure to annotated the appropriate columns for following ENVO MIxS triad:

```
biome http://purl.obolibrary.org/obo/ENVO_00000428
environmental feature http://purl.obolibrary.org/obo/ENVO_00002297
environmental material http://purl.obolibrary.org/obo/ENVO_00010483
```

Note that the columns "rdf type purl label', "units label" and "measurement source purl label" do not need to be filled in those are just for your convenience as you fill out the accompanying "purl" columns.

2.4 An example filled out ONTOLOGY_MAPPING.tsv file might look like the following:

parameter	rdf type purl label	rdf type purl	pm:searchable	units label	units purl	measuremen
SampleID_Tara	centrally registered identifier	http://purl.obolibrary.org/obo/IAO_0000578	FALSE			
BioSample	Biosample identifier assigned by the National Center for Biotechnology Information	http://purl.obolibrary.org/obo/PMO_00000122	FALSE			
Chlorophyll Sensor	concentration of chlorophyll in water	http://purl.obolibrary.org/obo/ENVO_3100036	TRUE	miligram per cubic meter	http://purl.obolibrary.org/obo/PMO_00000132	https://www
Depth	depth of water	http://purl.obolibrary.org/obo/ENVO_3100031	TRUE	meter	http://purl.obolibrary.org/obo/UO_0000008	https://www
Description	comment on investigation	http://purl.obolibrary.org/obo/OBI_0001898	FALSE			
Event Date/Time End	specimen collection time measurement datum stop	http://purl.obolibrary.org/obo/PMO_00000009	TRUE	time unit	http://purl.obolibrary.org/obo/UO_0000003	https://www
Event Date/Time Start	specimen collection time measurement datum start	http://purl.obolibrary.org/obo/PMO_00000008	TRUE	time unit	http://purl.obolibrary.org/obo/UO_0000003	https://www
Event Label	centrally registered specimen collection event identifier	http://purl.obolibrary.org/obo/PMO_00000056	FALSE			
Latitude End	latitude coordinate measurement datum stop	http://purl.obolibrary.org/obo/PMO_00000079	TRUE	degree	http://purl.obolibrary.org/obo/UO_0000185	https://www

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Latitude Start	latitude coordinate measurement datum start	http://purl.obolibrary.org/obo/PMO_00000076	TRUE	degree	http://purl.obolibrary.org/obo/UO_0000185	https://www
Longitude End	longitude coordinate measurement datum stop	http://purl.obolibrary.org/obo/PMO_00000078	TRUE	degree	http://purl.obolibrary.org/obo/UO_0000185	https://www
Longitude Start	longitude coordinate measurement datum start	http://purl.obolibrary.org/obo/PMO_00000077	TRUE	degree	http://purl.obolibrary.org/obo/UO_0000185	https://www
Nitrate Sensor	concentration of nitrate in water	http://purl.obolibrary.org/obo/ENVO_3100022	TRUE	micromole per litre	http://purl.obolibrary.org/obo/UO_0010003	https://www
Oxygen Sensor	concentration of oxygen in water	http://purl.obolibrary.org/obo/ENVO_09200021	TRUE	micromole per kilogram	http://purl.obolibrary.org/obo/UO_0010004	https://www
Salinity Sensor	liquid water salinity	http://purl.obolibrary.org/obo/PMO_00000014	TRUE	practical salinity unit	http://purl.obolibrary.org/obo/PMO_00000037	https://www
Size Fraction Lower Threshold	aquatic sample minimum filter fractionation size threshold	http://purl.obolibrary.org/obo/PMO_00000022	TRUE	micrometer	http://purl.obolibrary.org/obo/UO_0000017	https://www
Size Fraction Upper Threshold	aquatic sample maximum filter fractionation size threshold	http://purl.obolibrary.org/obo/PMO_00000023	TRUE	micrometer	http://purl.obolibrary.org/obo/UO_0000017	https://www
Temperature	temperature of water	http://purl.obolibrary.org/obo/ENVO_09200014	TRUE	degree Celsius	http://purl.obolibrary.org/obo/UO_0000027	https://www
purl_biome	biome	http://purl.obolibrary.org/obo/ENVO_00000428	TRUE			
purl_feature	environmental feature	http://purl.obolibrary.org/obo/ENVO_00002297	TRUE			
purl_material	environmental material	http://purl.obolibrary.org/obo/ENVO_00010483	TRUE			

2.5 Creating Data Package Templates

This example command is how one can generate a tabular data package JSON template for the OSD data set:

```
cd planet-microbe-scripts

cat example_ontology_mappings/OSD.tsv | ./scripts/schema_tsv_to_json.py
> example_data_packages/osd/datapackage.json
```

The JSON was then hand-edited to add missing information and correct names, types, and units.

For more information on FD Table Schemas see http://frictionlessdata.io/specs/table-schema/

This can be replicate for a new dataset by running the similar command with the newly created ONTOLOGY_MAPPING.tsv file(s). Recreate this command in the new directory with the new project files in the planet-microbe-datapackages repository. E.g.,

```
cd planet-microbe-datapackages/NEW_DATASET/

cat ONTOLOGY_MAPPING.tsv | #PATH_TO_planet-microbe-
scripts_REPO#./scripts/schema_tsv_to_json.py >
datapackage_component1.json
```

2.6 Finalize the **datapackage_component.json** file

Open the file in a text editor such as atom or sublime text and modify the following information specific to the resource in question.

Citation: Kai Blumberg, Alise J J. Ponsero, Bonnie Hurwitz Creating Planet Microbe Data Packages https://dx.doi.org/10.17504/protocols.io.bzsdp6a6

```
{
      "name": "#ADD NAME e.g., sample",
      "title": "#ADD tile",
      "profile": "#tabular-data-resource",
      "pm:resourceType": "#ADD TYPE",
      "path": "#ADD FILEPATH e.g., FILEPATH.tsv",
      "dialect": {
        "delimiter": "#Add delimiter e.g., \t",
        "header": true,
        "caseSensitiveHeader": true
      },
      "format": "csv",
      "mediatype": "text/tab-separated-values",
      "encoding": "UTF-8",
      "hash": "OPTIONALLY ADD file e.g.,
hasheac36d6747691e1061718509828598b1",
      "schema": {
        "fields": [ ...
}
```

Note the following "pm:resourceTypes" are accepted:

```
"pm:resourceType": "niskin",

"pm:resourceType": "campaign",

"pm:resourceType": "sample",

"pm:resourceType": "sampling_event",

"pm:resourceType": "ctd",
```

3 The following is an skeleton of the Planet Microbe Datapackage main json file for a new project

```
{
  "@context": {
    "pm": "http://purl.obolibrary.org/obo/PMO_00000000"
  },
  "profile": "tabular-data-package",
  "name": "#ADD NAME",
  "title": "#ADD TITLE",
  "description": "#ADD DESCRIPTION",
  "pm:selfUrl": "https://github.com/hurwitzlab/planet-microbe-
datapackages/tree/master/#ADD_DIR_NAME",
  "homepage": "#ADD HOMEPAGE",
  "keywords": [
    "#ADD KEYWORDS",
    "#ADD MORE KEYWORDS"
  ],
  "sources": [
    {
      "title": "#ADD SOURCE(s)",
      "path": "ADD URL FOR SOURCE"
    }
  ],
  "licenses": [
    {
      "name": "CC-BY-3.0",
      "title": "Creative Commons Attribution 3.0 Unported",
      "path": "https://creativecommons.org/licenses/by/3.0/"
    }
  ],
  "resources": [
    {#ADD datapackage_component1.json CODE HERE},
    {... #Add more datapackage components if needed}
  ]
}
```

Save this as a new (main) **datapackage.json** file for the project.

For each tabular dataset file that was prepared in the above steps open up the "datapackage_componentX.json" files one at a time and paste the entirety of the json file into the {}'s inside the "resources" block. This way each file will be annotated in a FAIR way that can be uploaded into the Planet Microbe Database.

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Make sure to also fill in the other information about the datapackage for example the "name" "description" "keywords" etc.

3.1 Optional Step, add constraints for select fields

Optionally for fields which should follow a numeric constraint such as such as Latitude and Longitude, add and or modify the json file for each column header for each resource to change them from something like the following:

```
{
    "name": "Latitude",
    "type": "number",
    "format": "default",
    "rdfType": "http://purl.obolibrary.org/obo/OBI_0001620",
},
```

into something like this with a constraint block specified with numerical values e.g., -90 and 90 for Latitude.

```
{
    "name": "Latitude",
     "type": "number",
     "format": "default",
     "rdfType": "http://purl.obolibrary.org/obo/OBI_0001620",
     "constraints": {
     "required": false,
     "minimum": -90,
     "maximum": 90
},
```

Validate datapackage.json

4 Validating Data Packages

First, make sure you have a Python 3 virtual environment setup:

```
virtualenv -p $(which python3) python3
source python3/bin/activate
pip install datapackage
```

Alternatively create a conda environment:

```
conda create --name planet_microbe
conda activate planet_microbe
conda install -c conda-forge datapackage
```

Run the validation script:

```
scripts/validate_datapackage.py [-r resource]
```

4.1 Example command to validate a Datapackage:

```
scripts/validate_datapackage.py ../planet-microbe-
datapackages/OSD/datapackage.json
```

5 Optional Step, run GoodTables validation for constraints

This is based on the original goodtables script avaiable from: https://goodtables.readthedocs.io/en/latest/

First install the goodtables library using pip:

```
pip install goodtables
```

Example call using the script

Citation: Kai Blumberg, Alise J J. Ponsero, Bonnie Hurwitz Creating Planet Microbe Data Packages https://dx.doi.org/10.17504/protocols.io.bzsdp6a6

```
goodtables OSD/datapackage.json
```


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