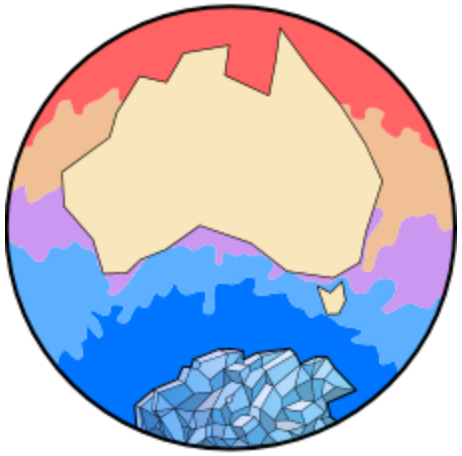


Building your own intake-esm datastore

Standardising analysis of climate model datasets

Anton Steketee, Charles Turner, Dougie Squire, Marc White, Romain Beucher

Australia's climate simulator

ACCESS National Research Infrastructure

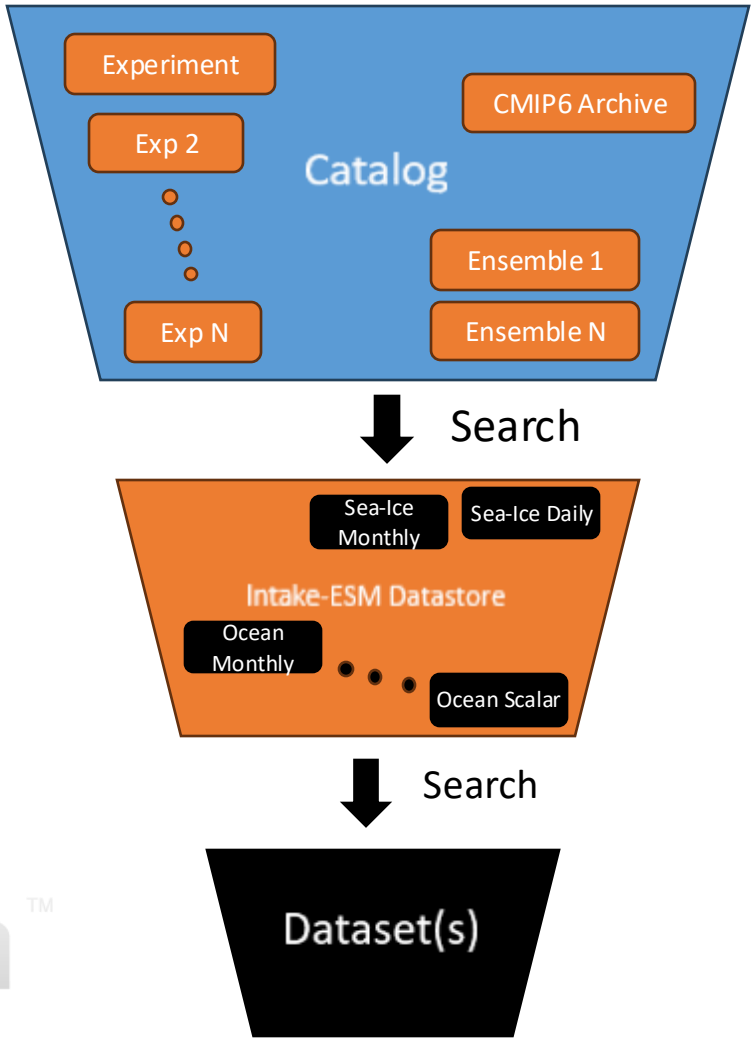
ACCESS-NRI Intake Catalog

A catalog provides functionality for searching, discovering and loading data.

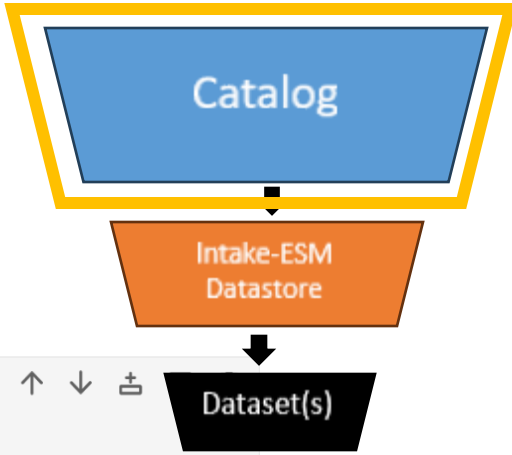
Data can be searched by many attributes, including:

- Experiment name
- Model
- Realm / Model Component
- Data Frequency
- Variable Name
- Variable Standard & Long Names

The ACCESS-NRI Intake Catalog is built upon Intake-ESM, and only shows data stored at the NCI.



ACCESS-NRI Intake Catalog



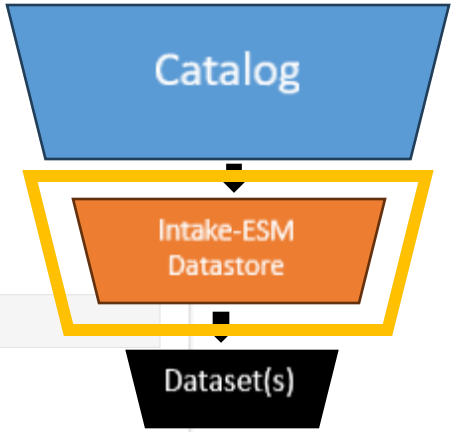
[1]:
```
import intake

catalog = intake.cat.access_nri
```

[2]:
```
catalog
```

access_nri catalog with 94 source(s) across 2268 rows:

name	model	description	realm	frequency	variab
01deg_jra55v13_ryf9091	{ACCESS-OM2}	{0.1 degree ACCESS-OM2 global model configuration with JRA55-do v1.3 RYF9091 repeat year forcing (May 1990 to Apr 1991)}	{ocean, sealce}	{3mon, 1mon, fx, 3hr, 1day}	{ANGLET, buoyfreq2_wt, dyu, fsalt_ai_m, tx_tran sss_m, frazil_r total_ocean_fprec, ke_tc total_ocean_lw_hea bih_fric_v, vocn_r frazil_3d_int_z, sig2_r tx_trans_rho, tau_ sfc_hflux_fr
01deg_jra55v140_iaf	{ACCESS-	{Cycle 1 of 0.1 degree ACCESS-OM2 global model	{ocean,	{1day,	{ANGLET, buoyfreq2_w bmf_u, u, dyu, fsalt_ai_r tx_trans, frazil_r total_ocean_fprec, ke_tc

Each experiment is an Intake-ESM Datastore




```
[12]: catalog['025deg_jra55_iaf_omip2_cycle6']
```

025deg_jra55_iaf_omip2_cycle6 catalog with 8 dataset(s) from 1830 asset(s):

	unique
path	1830
realm	2
variable	296
frequency	3
start_date	855
end_date	854
variable_long_name	271
variable_standard_name	57
variable_cell_methods	6
variable_units	63
filename	1470
file_id	8
derived_variable	0

```
[13]: catalog['025deg_jra55_iaf_omip2_cycle6'].keys()

[13]: ['iceh_XXXX_XX.1mon',
       'iceh_XXXX_XX_daily.1day',
       'ocean_budget.1mon',
       'ocean_daily.1day',
       'ocean_grid.fx',
       'ocean_month.1mon',
       'ocean_scalar.1mon',
       'ocean_scalar_snapshot.1day']
```

How do I make my own Intake ESM Datastore?

Example with build-esm-datastore in command line

Through the command line: `build-esm-datastore` :

```
user@gadi $ mkdir catalog_dir  # Change this to whatever you like/seems sensible to you
user@gadi $ module load conda/analysis3-25.02
user@gadi $ build-esm-datastore --builder Mom6Builder --expt-dir
 /g/data/ik11/outputs/mom6-panan/panant-01-zstar-ACCESSyr2/ --cat-dir catalog_dir
```

In a Jupyter Notebook: use_datastore:

```
from access_nri_intake.experiment import use_datastore
from access_nri_intake.source import builders

expt_datastore = use_datastore(
    experiment_dir = '/g/data/ik11/outputs/mom6-panan/panant-01-zstar-ACCESSyr2/',
    catalog_dir = 'catalog_dir',
    builder=builders.Mom6Builder
)
```

How do I make my own Intake ESM Datastore?

Further info: https://access-nri-intake-catalog.readthedocs.io/en/latest/datastores/quickstart.html

```
from access_nri_intake.experiment import use_datastore
from access_nri_intake.source.builders import Mom6Builder

ds = use_datastore(
    experiment_dir="/g/data/ik11/outputs/mom6-panan/panant-01-zstar-ACCESSyr2/",
    catalog_dir="/home/189/ct1163/catalog_dir/",
    builder=Mom6Builder,
    datastore_name="experiment_datastore",
    description="PanAnt experiment with ACCESS-OM2-01 forcing",
              )
ds
```

```
Datastore found in /home/189/ct1163/catalog_dir, verifying datastore integrity...
Parsing experiment dir...
Datastore integrity verified!
Datastore found in /home/189/ct1163/catalog_dir/experiment_datastore.json!
Please note that this has not added the datastore to the access-nri-intake catalog.
To add to catalog, please run 'scaffold_catalog_entry' for help on how to do so.
```

experiment_datastore catalog with 13 dataset(s) from 12325 asset(s):

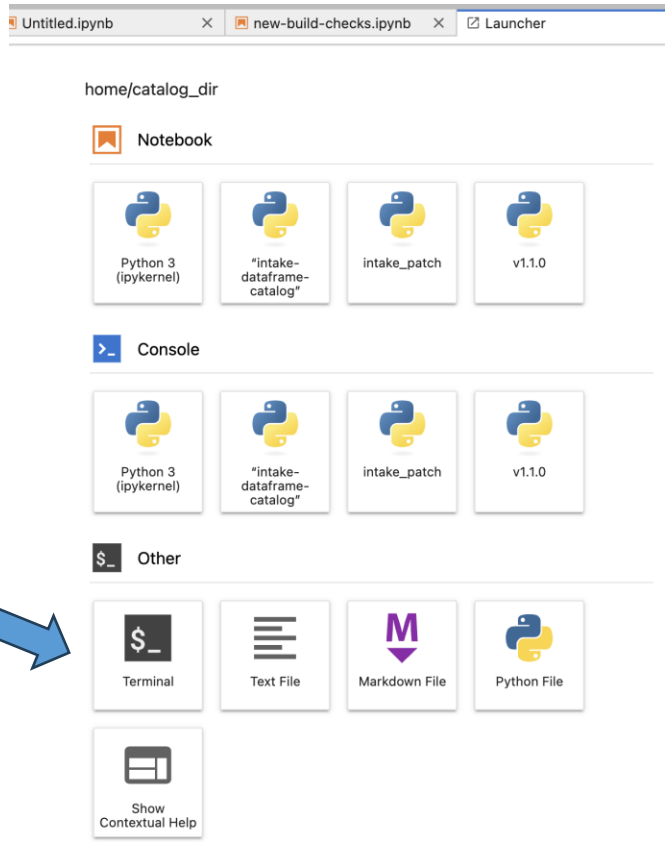
	unique
filename	12325
file_id	13

```
$ build-esm-datastore --builder Mom6Builder --expt-dir  /g/data/ik11/outputs/mom6-panan/panant-01-zstar-ACCESSyr2/ --cat-dir .
Datastore found in current directory, verifying datastore integrity...
Parsing experiment dir...
Experiment directory and datastore do not match (missing files from datastore). Datastore regeneration required...
Building esm-datastore...
...
Sucessfully built esm-datastore!
Saving esm-datastore to /home/189/ct1163/catalog_dir
/home/189/ct1163/catalog_dir/venv/lib/python3.11/site-packages/intake_esm/cat.py:186: PydanticDeprecatedSince20: The `dict` method is deprecated; use `model_dump` instead.
  data = self.dict().copy()
Successfully wrote ESM catalog json file to: file:///home/189/ct1163/catalog_dir/experiment_datastore.json
Hashing catalog to prevent unnecessary rebuilds.
This may take some time...
Catalog sucessfully hashed!
Datastore sucessfully written to /home/189/ct1163/catalog_dir/experiment_datastore.json!
Please note that this has not added the datastore to the access-nri-intake catalog.
To add to catalog, please run 'scaffold-catalog-entry' for help on how to do so.
To open the datastore, run `intake.open_esm_datastore('/home/189/ct1163/catalog_dir/experiment_datastore.json', columns_with_iterables=['variable'])` in a Python session.
```

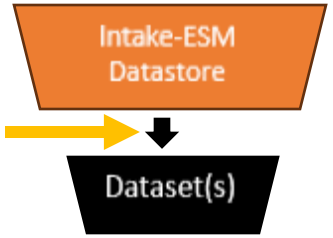
How do I make my own Intake ESM Datastore?

Further info: https://access-nri-intake-catalog.readthedocs.io/en/latest/datastores/quickstart.html

If building a catalog from the terminal, we recommend you do so from an ARE instance terminal, not by SSH'ing into a Gadi login node



Datastore keys define different datasets



[36]:
```
datastore
```

intake_esm_ds catalog with 95 dataset(s) from 95 asset(s):

	unique
path	95
realm	2
variable	235
frequency	3
start_date	1
end_date	2
variable_long_name	216
variable_standard_name	51
variable_cell_methods	20
variable_units	25
filename	95
file_id	95
derived_variable	0

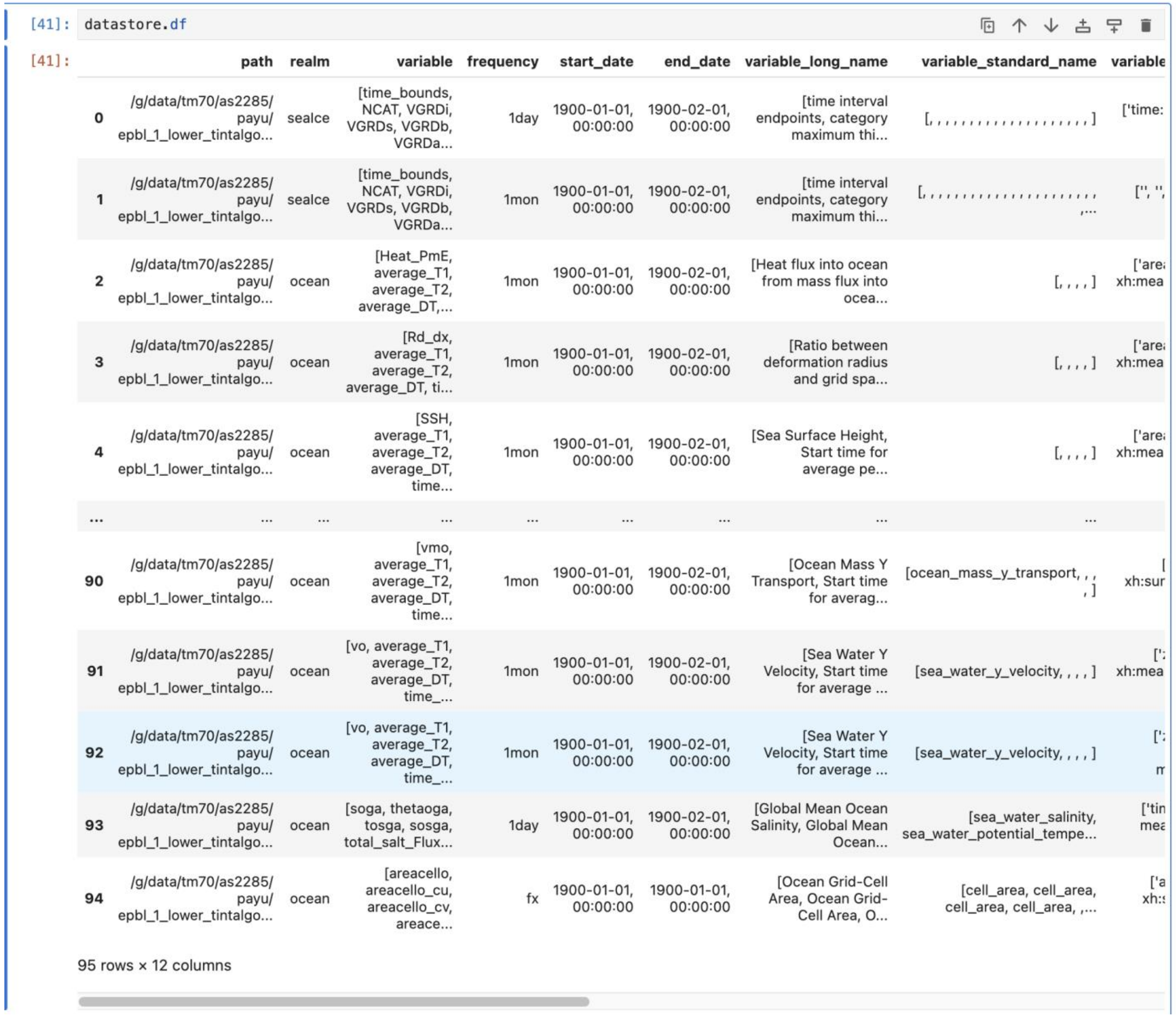
[28]:
```
datastore.keys_info()
```

[28]:

key	file_id	frequency
access_om3_cice_XXXX_XX.1day	access_om3_cice_XXXX_XX	1day
access_om3_cicem_1900_01.1mon	access_om3_cicem_1900_01	1mon
access_om3_mom6_2d_Heat_PmE_1mon_mean_XXXX_XX.1mon	access_om3_mom6_2d_Heat_PmE_1mon_mean_XXXX_XX	1mon
access_om3_mom6_2d_Rd_dx_1mon_mean_XXXX_XX.1mon	access_om3_mom6_2d_Rd_dx_1mon_mean_XXXX_XX	1mon
access_om3_mom6_2d_SSH_1mon_mean_XXXX_XX.1mon	access_om3_mom6_2d_SSH_1mon_mean_XXXX_XX	1mon
...	...	...
access_om3_mom6_3d_vmo_1mon_mean_XXXX_XX.1mon	access_om3_mom6_3d_vmo_1mon_mean_XXXX_XX	1mon
access_om3_mom6_3d_vo_1mon_mean_XXXX_XX.1mon	access_om3_mom6_3d_vo_1mon_mean_XXXX_XX	1mon
access_om3_mom6_3d_vo_1mon_pow02_XXXX_XX.1mon	access_om3_mom6_3d_vo_1mon_pow02_XXXX_XX	1mon
access_om3_mom6_scalar_1day_XXXX_XX.1day	access_om3_mom6_scalar_1day_XXXX_XX	1day
access_om3_mom6_static.fx	access_om3_mom6_static	fx

95 rows × 2 columns

Dataframe view shows assets



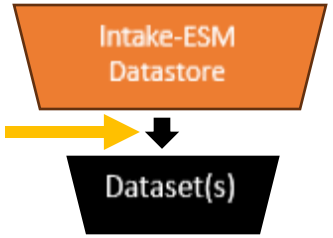
```
[41]: datastore.df
```

[41]:

	path	realm	variable	frequency	start_date	end_date	variable_long_name	variable_standard_name	variable
0	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	sealce	[time_bounds, NCAT, VGRDi, VGRDs, VGRDb, VGRDa...	1day	1900-01-01, 00:00:00	1900-02-01, 00:00:00	[time interval endpoints, category maximum thi...	[, , , , , , , , , , , , , , , , , , , ,]	['time:
1	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	sealce	[time_bounds, NCAT, VGRDi, VGRDs, VGRDb, VGRDa...	1mon	1900-01-01, 00:00:00	1900-02-01, 00:00:00	[time interval endpoints, category maximum thi...	[, ,...	['', '',
2	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	ocean	[Heat_PmE, average_T1, average_T2, average_DT,...	1mon	1900-01-01, 00:00:00	1900-02-01, 00:00:00	[Heat flux into ocean from mass flux into ocea...	[, , , ,]	['are: xh:mea
3	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	ocean	[Rd_dx, average_T1, average_T2, average_DT, ti...	1mon	1900-01-01, 00:00:00	1900-02-01, 00:00:00	[Ratio between deformation radius and grid spa...	[, , , ,]	['are: xh:mea
4	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	ocean	[SSH, average_T1, average_T2, average_DT, time...	1mon	1900-01-01, 00:00:00	1900-02-01, 00:00:00	[Sea Surface Height, Start time for average pe...	[, , , ,]	['are: xh:mea
...	...	...	...	...	...	...	...	...	
90	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	ocean	[vmo, average_T1, average_T2, average_DT, time...	1mon	1900-01-01, 00:00:00	1900-02-01, 00:00:00	[Ocean Mass Y Transport, Start time for averag...	[ocean_mass_y_transport, , , ,]	[xh:sur
91	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	ocean	[vo, average_T1, average_T2, average_DT, time_...	1mon	1900-01-01, 00:00:00	1900-02-01, 00:00:00	[Sea Water Y Velocity, Start time for average ...	[sea_water_y_velocity, , , ,]	[': xh:mea
92	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	ocean	[vo, average_T1, average_T2, average_DT, time_...	1mon	1900-01-01, 00:00:00	1900-02-01, 00:00:00	[Sea Water Y Velocity, Start time for average ...	[sea_water_y_velocity, , , ,]	[': m
93	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	ocean	[soga, thetaoga, tosga, sosga, total_salt_Flux...	1day	1900-01-01, 00:00:00	1900-02-01, 00:00:00	[Global Mean Ocean Salinity, Global Mean Ocean...	[sea_water_salinity, sea_water_potential_tempe...	['tin mea
94	/g/data/tm70/as2285/ payu/ epbl_1_lower_tintalgo...	ocean	[areacello, areacello_cu, areacello_cv, areace...	fx	1900-01-01, 00:00:00	1900-01-01, 00:00:00	[Ocean Grid-Cell Area, Ocean Grid-Cell Area, O...	[cell_area, cell_area, cell_area, cell_area, ,...	['a xh:

95 rows × 12 columns

Finding a variable by name



[46]:
```
datastore.search(variable='sos')
```

intake_esm_ds catalog with 1 dataset(s) from 1 asset(s):

	unique
path	1
realm	1
variable	5
frequency	1
start_date	1
end_date	1
variable_long_name	5
variable_standard_name	2
variable_cell_methods	1
variable_units	1
filename	1
file_id	1
derived_variable	0

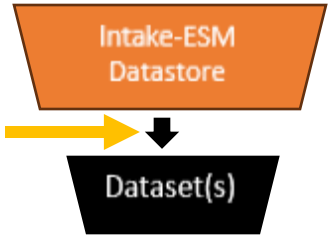
[51]:
```
datastore.search(variable='sos').keys()
```

[51]:
```
['access_om3_mom6_2d_sos_1mon_mean_XXXX_XX.1mon']
```

[52]:
```
datastore.search(variable_standard_name='sea_surface_salinity').keys()
```

[52]:
```
['access_om3_mom6_2d_sos_1mon_mean_XXXX_XX.1mon',
 'access_om3_mom6_scalar_1day_XXXX_XX.1day']
```

Finding a dataset by attribute

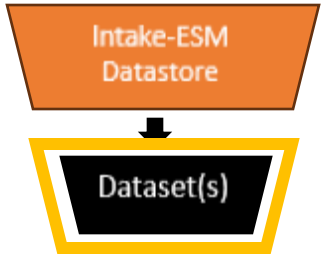



```
[53]: datastore.search(realm='seaIce', frequency='1mon')
```

intake_esm_ds catalog with 1 dataset(s) from 1 asset(s):

	unique
path	1
realm	1
variable	81
frequency	1
start_date	1
end_date	1
variable_long_name	81
variable_standard_name	1
variable_cell_methods	1
variable_units	1
filename	1
file_id	1
derived_variable	0

Opening a dataset with multiple variables




```
[21]: from dask.distributed import Client

[22]: client = Client(threads_per_worker=1)

[23]: client
```

[23]:

Client

Client-83b75012-df7b-11ef-8ebc-00000188fe80

Connection method: Cluster object **Cluster type:** distributed.LocalCluster

Dashboard: /proxy/8787/status

Launch dashboard in JupyterLab

▸ Cluster Info

```
[24]: seaice_ds = datastore.search(realm='seaIce', frequency='1mon').to_dask()

      seaice_ds
```

[24]: xarray.Dataset

▸ Dimensions: (**time**: 1, nbnd: 2, nc: 5, nkice: 4, nksnow: 1, nkbio: 3, nkaer: 5, nj: 1142, ni: 1440)

▾ Coordinates:

time	(time)	object	1900-01-16 12:00:00
NCAT	(nc)	float64	dask.array<chunksize=(5,), meta=np.ndarray>

▸ Data variables: (80)

▸ Indexes: (1)

▸ Attributes: (26)

Datasets can have more than one variable

[58]:
```
search = datastore.search(variable=['sosga','tosga'])
search
```

intake_esm_ds catalog with 1 dataset(s) from 1 asset(s):

	unique
path	1
realm	1
variable	25
frequency	1
start_date	1
end_date	1
variable_long_name	25
variable_standard_name	12
variable_cell_methods	1
variable_units	1
filename	1
file_id	1
derived_variable	0

[59]:
```
mom_scalar_ds = search.to_dask()
mom_scalar_ds
```

[59]: xarray.Dataset

▸ Dimensions: (**time**: 31, **scalar_axis**: 1)

▾ Coordinates:

scalar_axis	(scalar_axis)	float64	0.0
time	(time)	object	1900-01-01 12:00:00 ... 1900-01-...

▾ Data variables:

sosga	(time, scalar_axis)	float64	dask.array<chunksize=(1, 1), meta=np.ndarray>
tosga	(time, scalar_axis)	float64	dask.array<chunksize=(1, 1), meta=np.ndarray>

▸ Indexes: (2)

▸ Attributes: (18)

Related variables are often in different datasets

[60]:
```
search = datastore.search(variable=['sos','tos'])
search
```

intake_esm_ds catalog with 2 dataset(s) from 2 asset(s):

	unique
path	2
realm	1
variable	6
frequency	1
start_date	1
end_date	1
variable_long_name	6
variable_standard_name	3
variable_cell_methods	1
variable_units	2
filename	2
file_id	2
derived_variable	0

[61]:
```
search.keys()
```

[61]:
```
['access_om3_mom6_2d_sos_1mon_mean_XXXX_XX.1mon',
 'access_om3_mom6_2d_tos_1mon_mean_XXXX_XX.1mon']
```

Related variables on the same grid can be merged

```
[74]: search = datastore.search(variable=['sos','tos'])

[75]: mom_dict = search.to_dataset_dict()

--> The keys in the returned dictionary of datasets are constructed as follows:
        'file_id.frequency'
100.00% [2/2 00:00<00:00]

[76]: import xarray as xr

[77]: mom_ds = xr.merge(mom_dict.values())

[78]: mom_ds
```

[78]: xarray.Dataset

▸ Dimensions: (**time**: 1, **yh**: 1142, **xh**: 1440)

▾ Coordinates:

xh	(xh)	float64	-279.9 -279.6 ... 79.62 79.88
yh	(yh)	float64	-80.94 -80.87 ... 89.84 89.95
time	(time)	object	1900-01-16 12:00:00

▾ Data variables:

tos	(time, yh, xh)	float32	dask.array<chunksize=(1, 1142, 1440), meta=np.nda...
sos	(time, yh, xh)	float32	dask.array<chunksize=(1, 1142, 1440), meta=np.nda...

▸ Indexes: (3)

▸ Attributes: (20)

Why do I need to know the models name for a variable?

[79]:
```
search = datastore.search(
    variable_standard_name=['sea_surface_salinity','sea_surface_temperature'],
)
```

[80]:
```
search.keys()
```

[80]:
```
['access_om3_mom6_2d_sos_1mon_mean_XXXX_XX.1mon',
 'access_om3_mom6_2d_tos_1mon_mean_XXXX_XX.1mon',
 'access_om3_mom6_2d_tos_1mon_min_XXXX_XX.1mon',
 'access_om3_mom6_scalar_1day_XXXX_XX.1day']
```

[81]:
```
search = datastore.search(
    variable_standard_name=['sea_surface_salinity','sea_surface_temperature'],
    file_id='access_om3_mom6_scalar_1day_XXXX_XX'
)
search
```

intake_esm_ds catalog with 1 dataset(s) from 1 asset(s):

	unique
path	1
realm	1
variable	25
frequency	1
start_date	1
end_date	1
variable_long_name	25
variable_standard_name	12
variable_cell_methods	1
variable_units	1
filename	1
file_id	1
derived_variable	0

See **Model Agnostic Analysis** at COSIMA-Recipes

https://cosima-recipes.readthedocs.io/en/latest/Tutorials/Model_Agnostic_Analysis.html

Why do I need to know the models name for a variable?

```
[45]: mom_scalar_ds = search.to_dask()
      mom_scalar_ds
```

[45]: xarray.Dataset

▸ Dimensions: (**scalar_axis**: 1, **time**: 31, **nv**: 2)

▾ Coordinates:

scalar_axis	(scalar_axis)	float64	0.0
time	(time)	object	1900-01-01 12:00:00 ... 1900-01-...
nv	(nv)	float64	1.0 2.0

▾ Data variables:

soga	(time, scalar_axis)	float64	dask.array<chunksize=(1, 1), meta=np...
thetaoga	(time, scalar_axis)	float64	dask.array<chunksize=(1, 1), meta=np...
tosga	(time, scalar_axis)	float64	dask.array<chunksize=(1, 1), meta=np...
sosga	(time, scalar_axis)	float64	dask.array<chunksize=(1, 1), meta=np...

```
[46]: import cf_xarray

[50]: mom_scalar_ds.cf["sea_surface_salinity"]
```

[50]: xarray.DataArray 'sosga' (**time**: 31, **scalar_axis**: 1)

	Array	Chunk
Bytes	248 B	8 B
Shape	(31, 1)	(1, 1)
Dask graph	31 chunks in 2 graph layers	
Data type	float64 numpy.ndarray	

▾ Coordinates:

scalar_axis	(scalar_axis)	float64	0.0
time	(time)	object	1900-01-01 12:00:00 ... 1900-01-...

▾ Indexes:

scalar_axis	PandasIndex
time	PandasIndex

▾ Attributes:

units :	psu
long_name :	Sea Surface Salinity
cell_methods :	time: mean
time_avg_info :	average_T1,average_T2,average_DT
standard_name :	sea_surface_salinity

Ongoing Work

Panantarctic (GFDL-OM4) results are in xp65 environments, available for testing

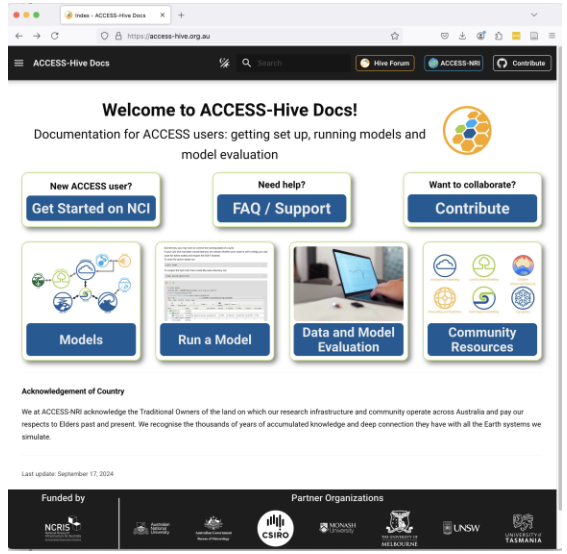
Request additional datasets into the main catalog at
- https://github.com/ACCESS-NRI/access-nri-intake-catalog

List of cosima recipes converted to intake and open pull-requests:
- https://github.com/COSIMA/cosima-recipes/issues/313

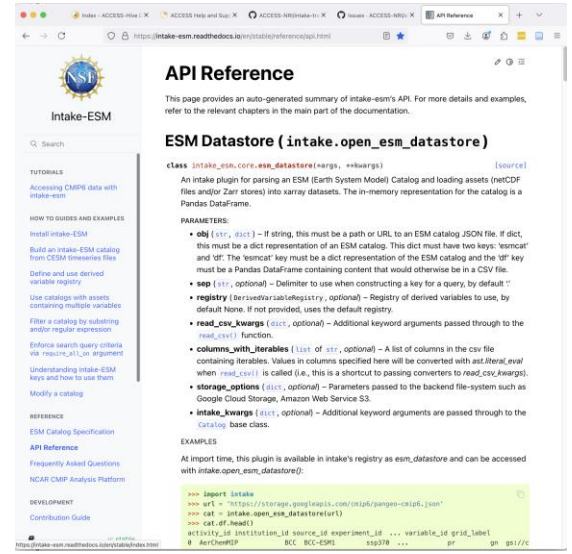
Updates & change since hh5 (xp65, conda/analysis3-25.02):
- Catalog now indexes grid variables
- `use_datastore/build-esm-datastore`
- More experiments and datasets indexed

NCI also have and add intake catalogs (e.g. ERA5, BARRA/BARPA, CMIP6)

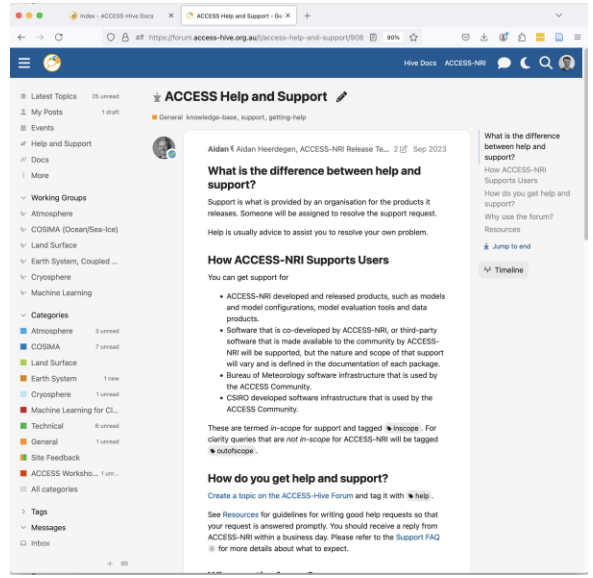
For ACCESS documentation – see ACCESS-HIVE



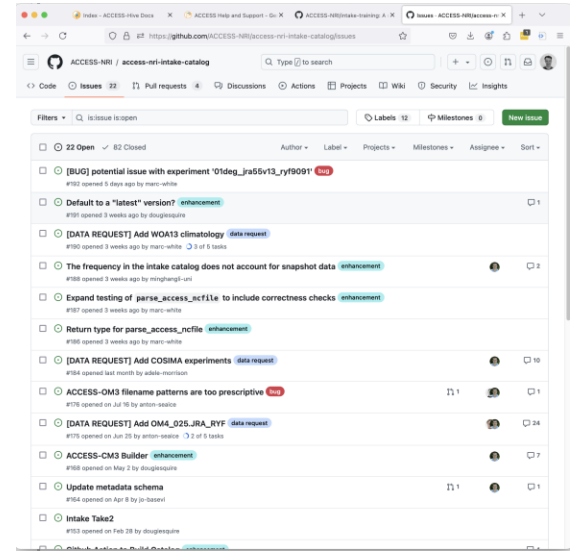
For intake documentation – see intake-esm website



For general support – use ACCESS-HIVE FORUM



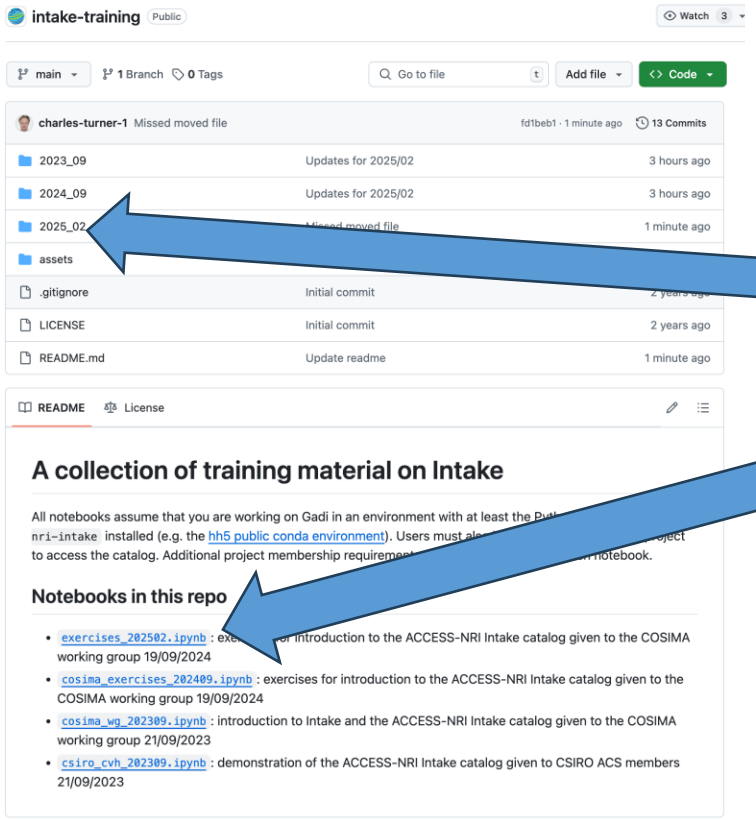
For bugs–use access-nri-intake-catalog github



Some other resources

https://cosima-recipes.readthedocs.io/en/latest/Tutorials/ACCESS-NRI_Intake_Catalog.html

https://github.com/ACCESS-NRI/intake-training/



Todays exercises can be found here

`use_datastore()` is not in hh5

Test set-up (very similar to a normal session for COSIMA Recipes):

Module directories

`/g/data/xp65/public/modules`

Modules

`conda/analysis3-25.02`

Projects:

gdata/xp65+gdata/$PROJECT
(+gdata/hh5+gdata/ik11+gdata/cj50
+gdata/oi10+gdata/ol01+gdata/fs38+gdata/p73)

Compute Size of `large` or greater.

Raise issues: https://github.com/ACCESS-NRI/ACCESS-Analysis-Conda

Exercises:

To follow the exercises:

```
$ git clone https://github.com/ACCESS-NRI/intake-training/
$ cd intake-training/2025_02
```

1. Make a datastore:

   datastore = use_datastore(…)

2. Find a single dataset:

```
search = datastore.search(…)
```

Start a dask cluster

Open the dataset:

```
search.to_dask()
```

3. Try another search which returns two variables.

```
search = datastore.search(variable=[…,…])
search.to_dataset_dict()
```

4. Try search with CF:

```
datastore.search(variable_standard_name='')
```

5. (Bonus) Run COSIMA recipe with your datastore, e.g:

https://github.com/COSIMA/cosima-recipes/blob/main/Recipes/Compare_SSH_model_obs.ipynb