Deltares

Enabling Delta Life

DFMWAQ with Python

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Agenda

- D-Flow with processes use case

- Why might you want to use scripting?

- Arranging the input data

- Making the model

- Making a restart file

- Examining the balances

- Making coastal water quality boundaries (if there is time)

- Still beta!

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Use case

- In the past

Total time for simulation →

Parallelizability ↓

| Hydro model | | WQ model |

- Common now

| Hydro model | | WQ model |

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D-FLOW with processes – parallelizing water quality simulations

- **Pro**: no more big water balance files

- **Pro**: *no other coupling problems (e.g. changes in segment nrs)*

- **Pro**: no parallelized transport solver in D-WAQ needed

- **Con**: rerunning hydrodynamics is expensive (in CPU time)

- It is common that you might want to **compare the speed** of an **online** model with that of an **offline** model

- For this you need to be able to **create the same model twice** using quite different architectures

- It is best to do this in a structured way

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Typical workflow to consider

1. The user has a D-FLOW hydrodynamic model that they want to use as the foundation of a water quality model

2. Run the FLOW model, obtain coupling output files, and import into DeltaShell

3. Set up the water quality simulation and run D-WAQ

What if you want to see if D-FLOW with processes is a good choice for your application??

Option 1:

- Augment the D-FLOW model in Deltashell to include processes (shown in previous workshop)

Option 2:

- 'Grow' a new model using the old D-FLOW model and a sub file

- **This is what we will look at today**

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'Grow' a D-FLOW with processes model

- Model Prerequisites:

  - A D-FLOW model

  - A sub file

  - Deltashell-format boundary condition files (optional)

- These will be provided for this workshop

- Python Prerequisites

- Download the following repository: https://github.com/RSchueder/dflowutil

- Follow readme instructions

dflowutil

Utilities for Delft3D FLOW Flexible Mesh in python. It contains utilities useful for both hydrodynamic and integrated water quality simulations.
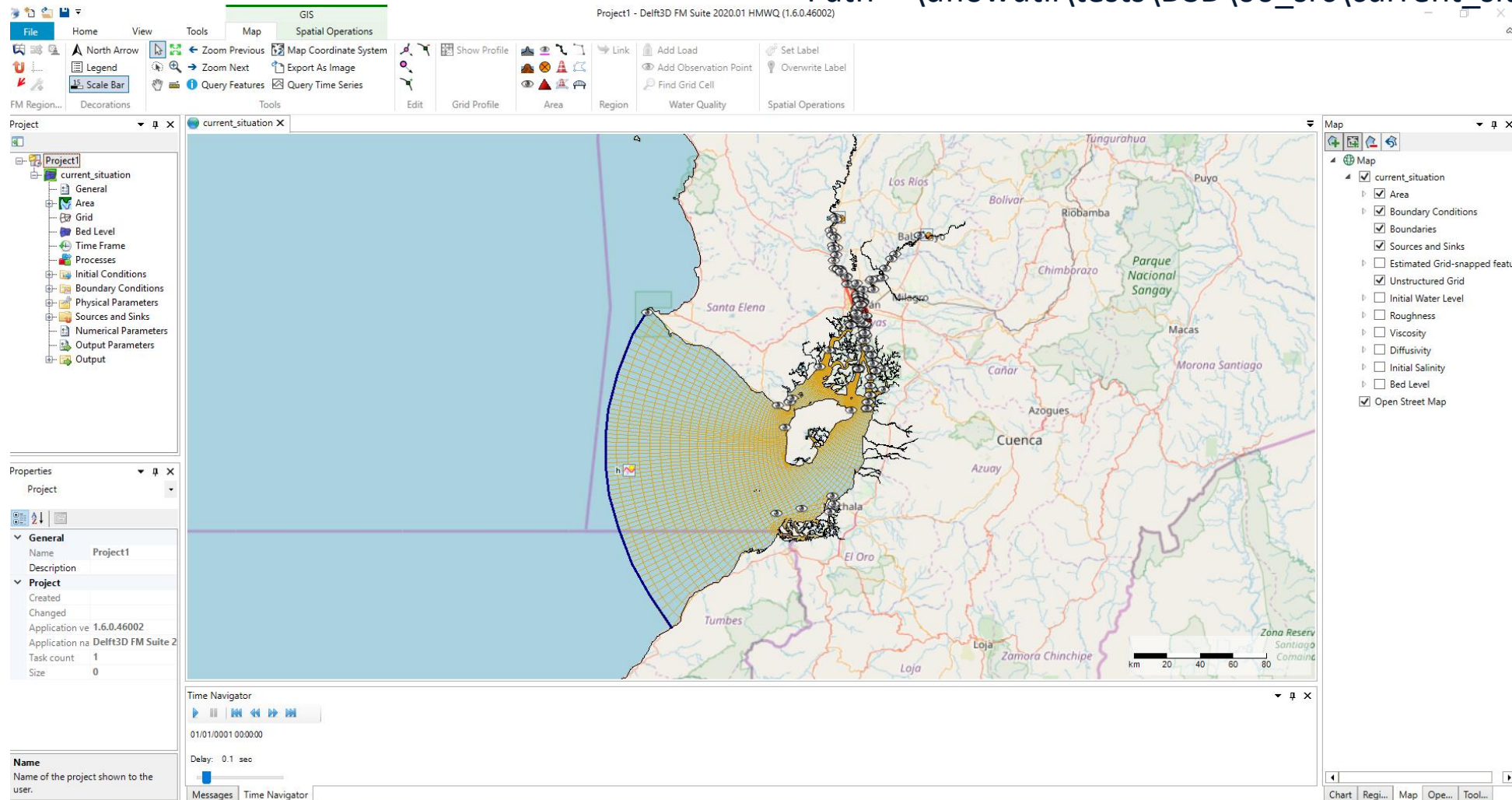
INSTALL

- $ python setup.py sdist bdist_wheel
- $ (optional) conda env create -f dflowutil.yml
- $ (optional) conda activate dflowutil
- $ pip install dist/dflowutil-0.1.3-py3-none-any.whl

tests.py provides an overview of key functionality

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The FLOW model we will be working with

Path = \dflowutil\tests\DSD\00_src\current_situation.mdu

dflowutil.DFMWAQModel

- dflowutil is a python *package*

- DFMWAQModel is a *module* of the package

- It is a class that holds information and function needed to build a new D-FLOW with processes model from a D-FLOW model

```python
class DFMWAQModel():

    def __init__(self, mdu, ext, subfile, new_dir, tref, ini=None, run_sys='linux', v=None, cores=None,
                 loads_data=None, bounds_data=None,
                 process_path=None):
        """
        DFMWAQ model initialized from DFM model inputs

        call DFMWAQModel.build() to build an initialized model
        Arguments:
            mdu {str} -- path to mdu
            ext {list} -- [ext1, ext2], if only one, still must be a list
            subfile {dflowutil.SubFile} -- a dflowutil.SubFile object
            new_dir {path} -- path where model will be built
            tref {datetime.datetime}
            ini {dict} -- sub name value pair for initial conditions. May be empty.
            v {str} -- version - i.e. 1.2.56.xxx.
            cores {list} -- [nodes, threads]
        """
```

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What does dflowutil.DFMWAQModel do?

- It builds an entire model from a sub file. This way there is no room for mistake in the ordering of substances in the loads file!

- It scans the mdu for all model assets, excluding boundary conditions (specify these explicitly)

- It creates boundary conditions for all transportable substances. The data is either dummy or is taken from deltashell-formatted *.csv files (if available)

- It creates initial conditions for all substances, either uniform, or as 2D field

```
def build(self):
    '''
    builds model based solely on attributes from initialization
    '''
    self.soursin()
    self.open_bnd()
    self.administrate_ext_files()
    self.merge_ext_files()
    self.run_set_file()
```

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How can I use it: making the model

\dflowutil\make_model.py

```
################################################################################
'''
model with boundary data
'''


process_path= r'd:\projects\dflowutil\tests\DSD\01_substances\proc_def.dat'
system = 'windows'
mdu = r'd:\projects\dflowutil\tests\DSD\00_src\current_situation.mdu'
sub_file = r'd:\projects\dflowutil\tests\DSD\01_substances\guayas_V11.sub'

# boundaries for the mdu
ext = [r'd:\projects\dflowutil\tests\DSD\00_src\plant_loads_current_local.ext',
       r'd:\projects\dflowutil\tests\DSD\00_src\sea_riv_boundary_local_bc.ext']

# water quality data
loads_data  = [r'd:\projects\dflowutil\tests\DSD\03_loads\full_model_ds.csv']
bounds_data = [r'd:\projects\dflowutil\tests\DSD\02_boundaries\river_ds.csv',
               r'd:\projects\dflowutil\tests\DSD\02_boundaries\sea_ds.csv']

# location of new model
new_model_dir = 'd:\\projects\\dflowutil\\tests\\DSD\\R01\\'

# sub file to use
substances = SubFile(sub_file)

# initial conditions
ini = {'OXY' : 7}
tref = datetime.datetime(2000, 1, 1)
ecuador_model = DFMWAQModel(mdu, ext, substances, new_model_dir, tref,
                            bounds_data = bounds_data, loads_data = loads_data,
                            run_sys = system, process_path = process_path)
ecuador_model.build()

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

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Set up conda environment and running

\dflowutil\make_model.py

```
Anaconda Prompt (Anaconda3)

(base) C:\Users\schueder>d:

(base) D:\>cd projects\dflowutil

(base) D:\projects\dflowutil>conda env create -f dflowutil.yml

CondaValueError: prefix already exists: D:\Anaconda3\envs\dflowutil


(base) D:\projects\dflowutil>conda activate dflowutil

(dflowutil) D:\projects\dflowutil> python make_model.py
```

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Examine the new model

- d:\projects\dflowutil\tests\DSD\R01\

⬆ [..]			<DIR>	11-11-2019 16:40	----
📁 [DFM_OUTPUT_current_situation]			<DIR>	11-11-2019 16:48	----
📄 run_model		bat	189	07-11-2019 12:17	-a--
📄 current_situation_dry		xyz	4,400	11-11-2019 16:40	-a--
📄 stage4_spot_ortho_DFM_reint_net		nc	6,367,500	11-11-2019 16:40	-a--
📄 guayas		ldb	3,844,515	11-11-2019 16:40	-a--
📄 bridgepiers_3_thd		pli	1,170	11-11-2019 16:40	-a--
📄 guayas_locations_obs		xyn	10,340	11-11-2019 16:40	-a--
📄 proc_def		dat	2,508,780	11-11-2019 16:40	-a--
📄 proc_def		def	42,652	11-11-2019 16:40	-a--
📄 bloom		spe	53,593	11-11-2019 16:40	-a--
📄 bloominp		d09	1,208	11-11-2019 16:40	-a--
📄 current_situation		mdu	16,595	11-11-2019 16:40	-a--
📄 L_Orquideas		pli	125	11-11-2019 16:40	-a--
📄 L_Orquideas		tim	65,234	11-11-2019 16:40	-a--

```
[processes]
SubstanceFile = d:\projects\dflowutil\tests\DSD\01_substances\guayas_V11.sub
AdditionalHistoryOutputFile      =
ProcesDataBaseFile               = proc_def.dat
DtProcesses                      = 600.                  # waq processes time step
DtMassBalance                    = 86400.  # waq mass balance output time step
ProcessFluxIntegration           = 1       # integration option (1: WAQ, 2: D-Flow FM)
```

Running the model

- We need to edit a batch file to allow for running in this exercise

- C:\Program Files (x86)\Deltares\Delft3D FM Suite 2020.01 HMWQ (1.6.0.46002)\plugins\DeltaShell.Dimr\kernels\x64\dflowfm\scripts\run_dflowfm_processes.bat

```
@ echo off
title %cd%
    rem
    rem This script is an example for running DFlowFM on Windows
    rem Adapt and use it for your own purpose
    rem

    rem
    rem Set the directories
    rem
set scriptdir=%~dp0
set dflowfmexedir=%scriptdir%\..\bin
set libdir=%scriptdir%\..\..\share\bin
set procdefbloomspedir=%scriptdir%\..\default
set path=%dflowfmexedir%;%libdir%;%path%

    rem
    rem Run
    rem
"%dflowfmexedir%\dflowfm-cli.exe" --nodisplay --autostartstop %1 %2 %3 %4 %5 %6 %7 %8  --processlibrary "%procdefbloomspedir%\proc_def.dat" --bloomspecies "%procdefbloomspedir%\bloom.spe"
```

Ensure there are quotes here

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Run and take a break

d:\projects\dflowutil\tests\DSD*.*					
Name	Ext	Size	↑Date	Attr
[..]		<DIR>	11-11-2019 17:12	----
[00_src]		<DIR>	11-11-2019 16:36	----
[01_substances]		<DIR>	07-11-2019 16:15	----
[02_boundaries]		<DIR>	01-11-2019 09:55	----
[03_loads]		<DIR>	04-11-2019 13:45	----
[04_obs]		<DIR>	11-11-2019 17:13	----
[R01]		<DIR>	11-11-2019 16:40	----
[R02]		<DIR>	11-11-2019 16:54	----
run_model	bat	189	07-11-2019 12:17	-a--

Copy the bat file to the run directory

d:\projects\dflowutil\tests\DSD\R01*.*					
Name	Ext	Size	↑Date	Attr
[..]		<DIR>	11-11-2019 16:40	----
[DFM_OUTPUT_current_situation]		<DIR>	11-11-2019 16:48	----
run_model	bat	189	07-11-2019 12:17	-a--
current_situation_dry	xyz	4,400	11-11-2019 16:40	-a--
stage4_spot_ortho_DFM_reint_net	nc	6,367,500	11-11-2019 16:40	-a--

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Take a look at the results

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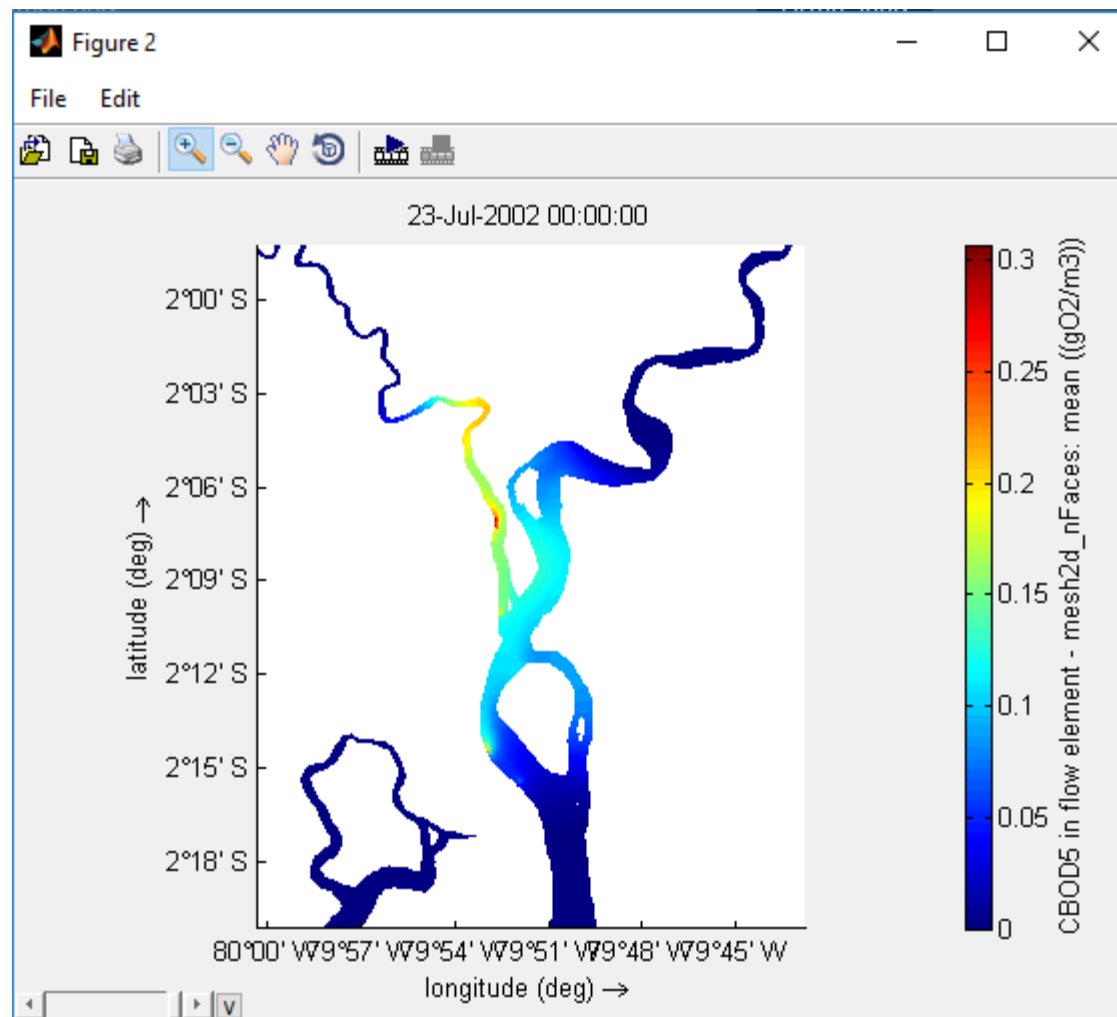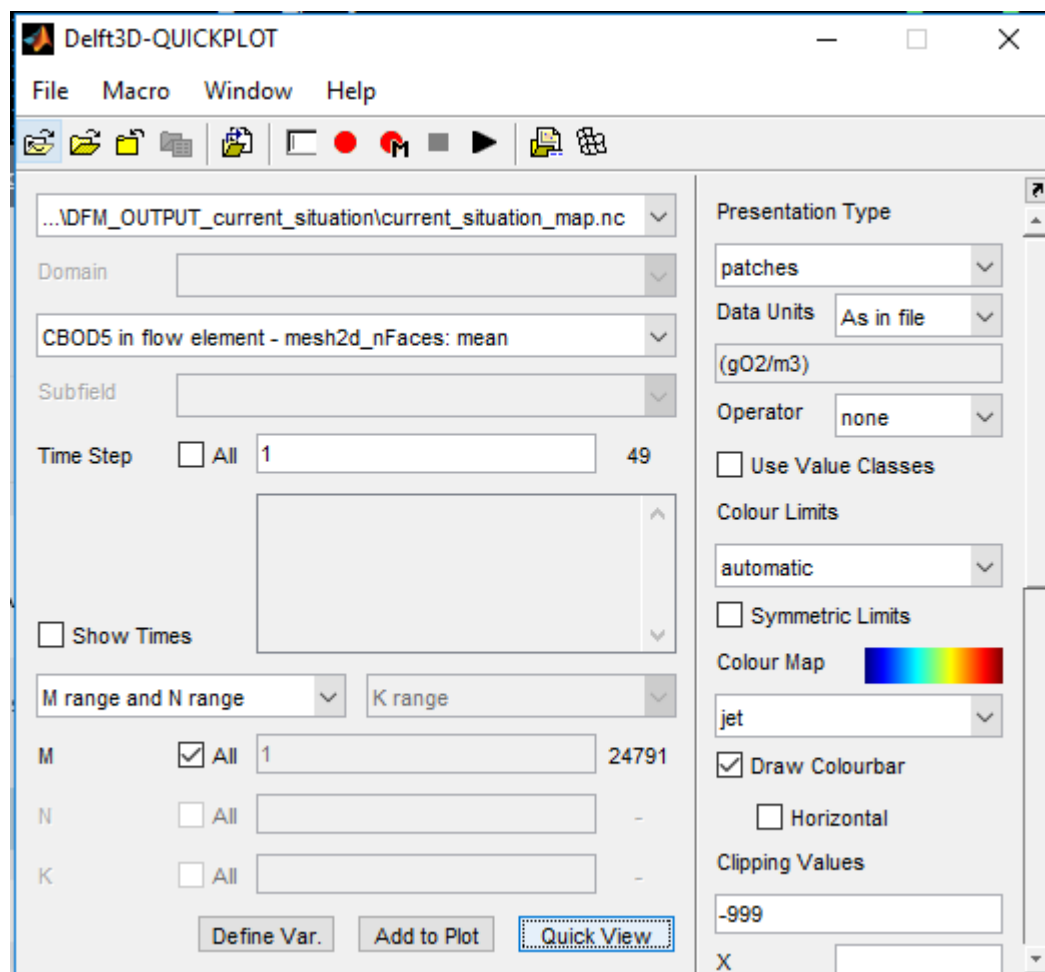
Making a restart

```
new_model_dir = 'd:\\projects\\dflowutil\\tests\\DSD\\R02\\'
```
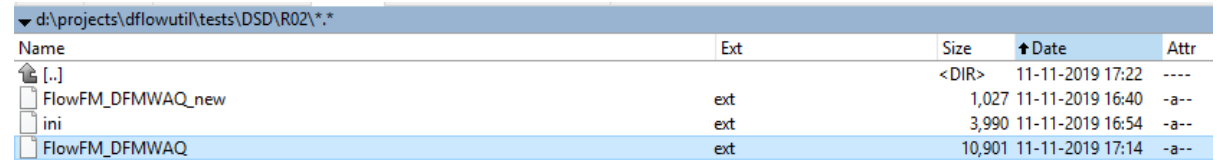
\dflowutil\make_model.py (already run)

```
'''
turn the last model into a restart
'''

sub_file = r'd:\projects\dflowutil\tests\DSD\01_substances\guayas_V11.sub'
map_dir = 'd:\\projects\\dflowutil\\tests\\DSD\\R01\\DFM_OUTPUT_current_situation\\'
new_model_dir = 'd:\\projects\\dflowutil\\tests\\DSD\\R02\\'
rst_to_xyz(map_dir, sub_file, -1, new_model_dir)
```

\dflowutil\make_restart.py

```
Anaconda Prompt (Anaconda3)

(base) C:\Users\schueder>d:

(base) D:\>cd projects\dflowutil

(base) D:\projects\dflowutil>conda env create -f dflowutil.yml

CondaValueError: prefix already exists: D:\Anaconda3\envs\dflowutil

(base) D:\projects\dflowutil>conda activate dflowutil

(dflowutil) D:\projects\dflowutil> python make_restart.py
```

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Adding the restart to the model

d:\projects\dflowutil\tests\DSD\R02*.*

Name	Ext	Size	Date	Attr
[..]		<DIR>	11-11-2019 17:22	----
FlowFM_DFMWAQ_new	ext	1,027	11-11-2019 16:40	-a--
ini	ext	3,990	11-11-2019 16:54	-a--
FlowFM_DFMWAQ	ext	10,901	11-11-2019 17:14	-a--

- Open R02/FlowFM_DFMWAQ.ext

- Open R02/ini.ext

- Copy contents from ini.ext -> FlowFM_DFMWAQ.ext

- In FlowFM_DFMWAQ.ext , rename:

  - initialtracers1 -> initialwaterlevel

  - initialtracersa1 -> initialsalinity

- Delete from top of FlowFM_DFMWAQ.ext :

```
QUANTITY=initialwaterlevel
FILENAME=ini_waterlevel_20020722.xyz
FILETYPE=7
METHOD=5
OPERAND=O

QUANTITY=initialsalinity
FILENAME=ini_salinity_20020722.xyz
FILETYPE=7
METHOD=5
OPERAND=O
```

- Delete old initial conditions from bottom of file

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Adding a balance area to the model

- Good idea to include balances so you can examine the relative contribution of different loads

```
QUANTITY=waqmassbalanceareaDomain
FILENAME=domain.pol
FILETYPE=10
METHOD=4
OPERAND=O
VALUE=1.0
```

Add to -> \dflowutil\tests\DSD\R02\FlowFM_DFMWAQ.ext

- The domain.pol file was created when the model was created

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Run and take a break

Name	Ext	Size	↑Date	Attr
⬆ [..]		<DIR>	11-11-2019 17:12	----
[00_src]		<DIR>	11-11-2019 16:36	----
[01_substances]		<DIR>	07-11-2019 16:15	----
[02_boundaries]		<DIR>	01-11-2019 09:55	----
[03_loads]		<DIR>	04-11-2019 13:45	----
[04_obs]		<DIR>	11-11-2019 17:13	----
[R01]		<DIR>	11-11-2019 16:40	----
[R02]		<DIR>	11-11-2019 16:54	----
run_model	bat	189	07-11-2019 12:17	-a--

d:\projects\dflowutil\tests\DSD*.*

Copy the bat file to the run directory

d:\projects\dflowutil\tests\DSD\R02*.*

Name	Ext	Size	↑Date	Attr
⬆ [..]		<DIR>	11-11-2019 17:22	----
[DFM_OUTPUT_current_situation]		<DIR>	11-11-2019 17:22	----
run_model	bat	189	07-11-2019 12:17	-a--
stage4_spot_ortho_DFM_reint_net	nc	6,367,500	11-11-2019 16:40	-a--

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Take a look at the results

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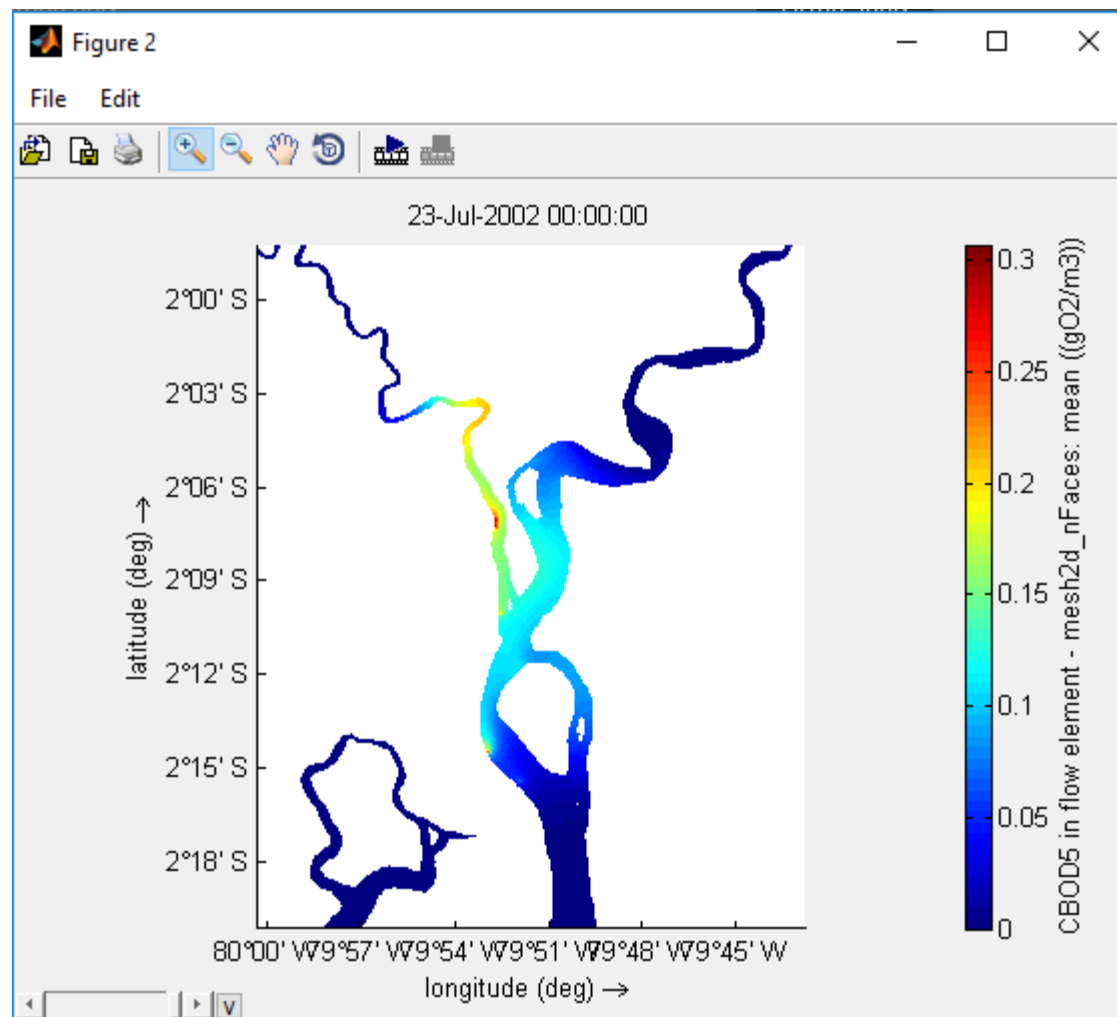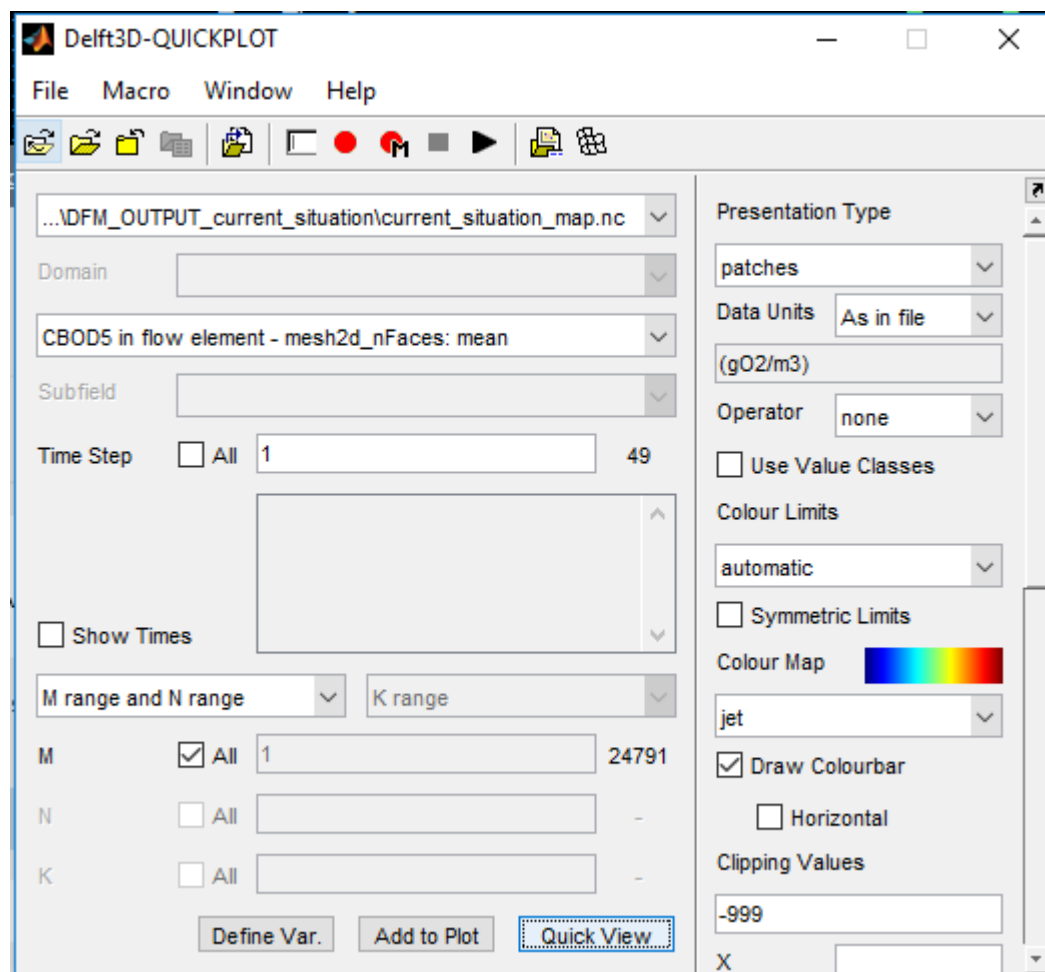
Create balances

```
'''
examine balances
'''

sub_file = r'd:\projects\dflowutil\tests\DSD\01_substances\guayas_V11.sub'
bal_file = r'd:\projects\dflowutil\tests\DSD\R02\DFM_OUTPUT_current_situation\current_situation_wq_proc_bal.txt'
subs = SubFile(sub_file)
prn = BalanceFile(bal_file)
area = ['Domain']
period = ['933-934']
prn.extract_balances(area, period)
```

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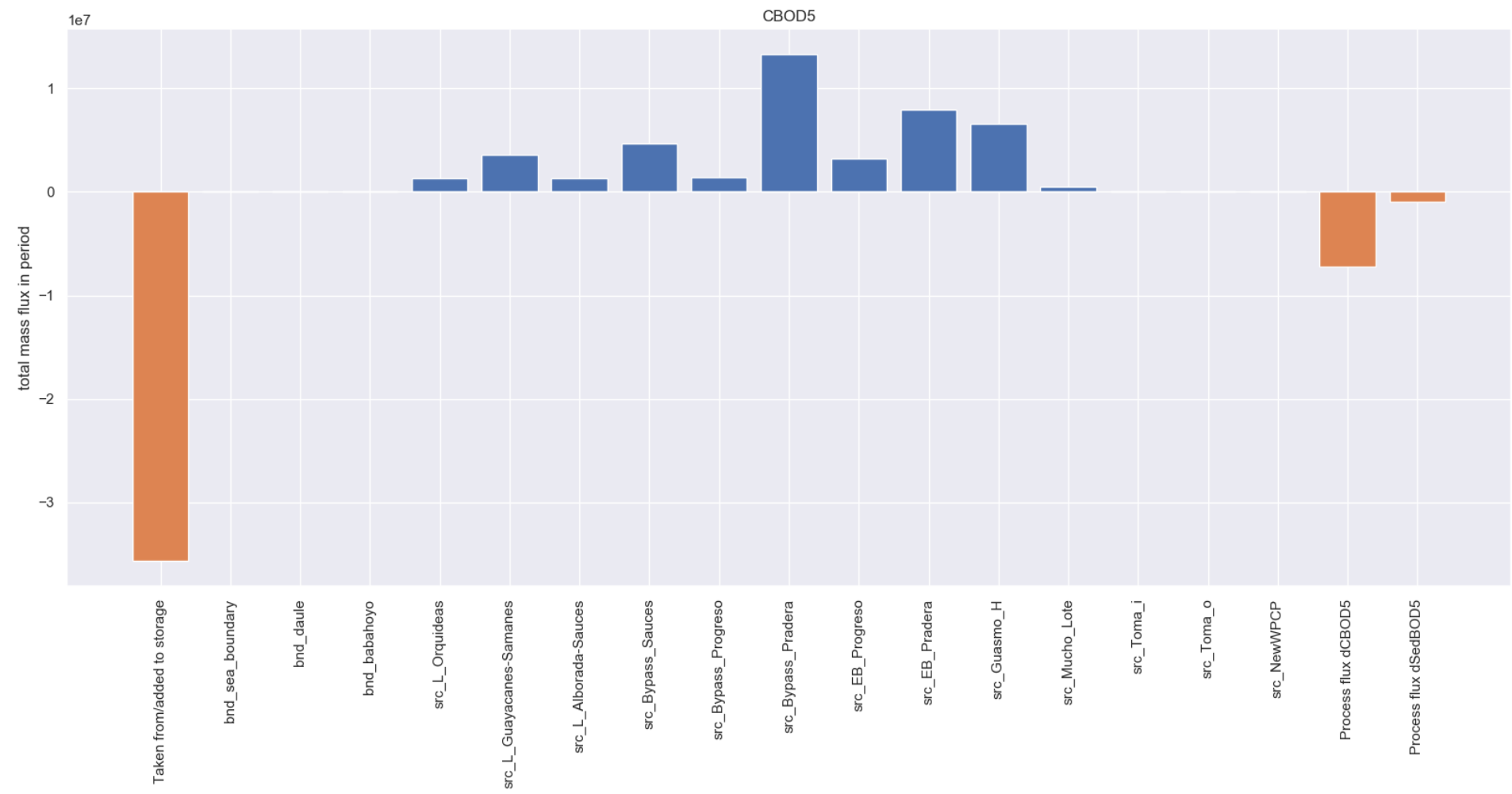# Create balances

```
'''
now do some plotting
'''


df = prn.areas
subs = SubFile(sub_file)
for domain in area:
    plt.close('all')
    for sub in subs.substances:
        if subs.transportable[sub] == 'active':
            fig = plt.figure()
            ax = fig.add_axes([0.1,0.3,0.8,0.6])
            print(sub)
            dfi = prn.areas[domain][sub]['Inflows']
            dfo = prn.areas[domain][sub]['Outflows']

            x = np.arange(0, len(dfi.columns))
            ax.bar(x, dfi.iloc[0])
            ax.bar(x, -dfo.iloc[0])
            ax.set_ylabel('total mass flux in period')
            plt.title(sub)
            plt.xticks(x, dfi.columns,rotation=90)
```

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Examine balances

Any questions?

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