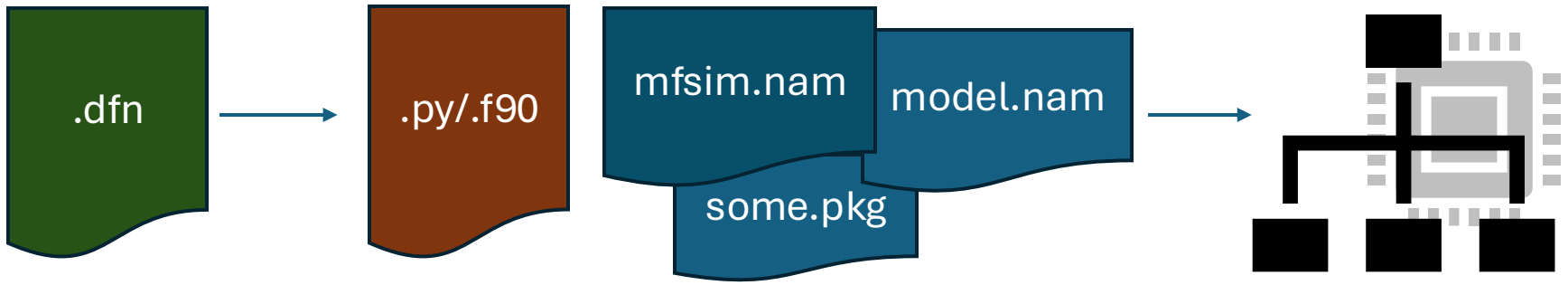
FloPy 4

Prototyping 7/26/24

#Goals

- Existing functionality maintained
- Easy to read/debug/contribute
- Easy to understand and use
- Pythonic – standard Python types and idioms

DFNs specify MF6 source and input files, input files specify simulations



Program roles

	read	write
dfn2f90.py	DFN	Fortran source
flopy	DFN, input files	Python source, Input files
mf6	Input files	Output files

Inspiration: ORMs

- Map relational database to user-facing API, usually OO
- Examples: SQLAlchemy, Django
- Principle: hide data source details

```python
from django.db import models


class Question(models.Model):
    question_text = models.CharField(max_length=200)
    pub_date = models.DateTimeField("date published")
```

Philosophy

A model is the single, definitive source of information about your data. It contains the essential fields and behaviors of the data you're storing. Django follows the DRY Principle. The goal is to define your data model in one place and automatically derive things from it. https://docs.djangoproject.com/en/5.0/intro/tutorial02/#creating-models

FloPy: OFM?

- Object-file mapping: map definition/input files to Python API
- Metaprogramming to discover constituent parameters/blocks
- Parameters and blocks provide access to spec as well as loaded values

```
mjreno, 9 hours ago | 1 author (mjreno)
class TestGwfIc(MFPackage):
    __test__ = False  # tell pytest not to collect

    export_array_ascii = MFKeyword(
        block="options",
        longname="export array variables to layered ascii files.",
        description="keyword that specifies input griddata arrays should be"
        "written to layered ascii output files.",
        optional=True,
        default_value=False,
    )
    export_array_netcdf = MFKeyword(
        block="options",
        longname="export array variables to netcdf output files.",
        description="keyword that specifies input griddata arrays should be"
        "written to the model output netcdf file.",
        optional=True,
        default_value=False,
    )
    strt = MFArray(
        block="griddata",
        longname="starting head",
        description="is the initial (starting) head---that is, head at the"
        "beginning of the GWF Model simulation.  STRT must be specified for"
        "all simulations, including steady-state simulations. One value is"
        "read for every model cell. For simulations in which the first stress"
        "period is steady state, the values used for STRT generally do not"
        "affect the simulation (exceptions may occur if cells go dry and (or)"
```

1 object model, 2 APIs

- Class attributes: block/parameter specifications

```
> GwfDis.top
MFArray(block='griddata', name='top', type=None, longname='
cell top elevation', description='is the top elevation for each cel
l in the top modellayer.', deprecated=False, in_record=False, lay
ered=False, optional=False, numeric_index=False, preserve_cas
e=False, repeating=False, tagged=False, reader=<MFReader.ur
word: 'urword'>, shape=(‘ncol’, ‘nrow’), default_value=None)
```

```
> help(GwfDis.nlay)
Help on MFInteger in module flopy4.scalar:

MFInteger(block=‘dimensions’, name=‘nlay’, type=…rw
ord: ‘urword’>, shape=None, default_value=None)
        is the number of the layers in the model grid
```

- Instance attributes: block/parameter values

```
> dis.top
array([[[4., 4., 4., 4., 4.],
        [4., 4., 4., 4., 4.],
        [4., 4., 4., 4., 4.],
        [4., 4., 4., 4., 4.],
        [4., 4., 4., 4., 4.]])
```

```
> dis.dimensions
{‘nlay’: 3, ‘nrow’: 5, ‘ncol’: 5}

> dis.nlay
3
```

```
> dis.options
{‘export_array_ascii’: True}
```

Resources

- https://docs.djangoproject.com/en/5.0/intro/tutorial02/#creating-models
- https://code.djangoproject.com/wiki/DevModelCreation
- https://code.djangoproject.com/wiki/DynamicModels
- https://docs.sqlalchemy.org/en/20/orm/extensions/hybrid.html#sqlalchemy.ext.hybrid.hybrid_property
- https://stackoverflow.com/questions/15247075/how-can-i-dynamically-create-derived-classes-from-a-base-class
- https://stackoverflow.com/questions/17929543/how-can-i-dynamically-create-class-methods-for-a-class-in-python
- https://docs.python.org/3/reference/datamodel.html?emulating-container-types=#emulating-container-types
- https://stackoverflow.com/questions/3387691/how-to-perfectly-override-a-dict
- https://numpy.org/doc/stable/user/basics.dispatch.html#basics-dispatch
- https://numpy.org/doc/stable/user/basics.interoperability.html#basics-interoperability
- https://stackoverflow.com/questions/55386602/how-to-overide-numpy-ufunc-with-array-ufunc