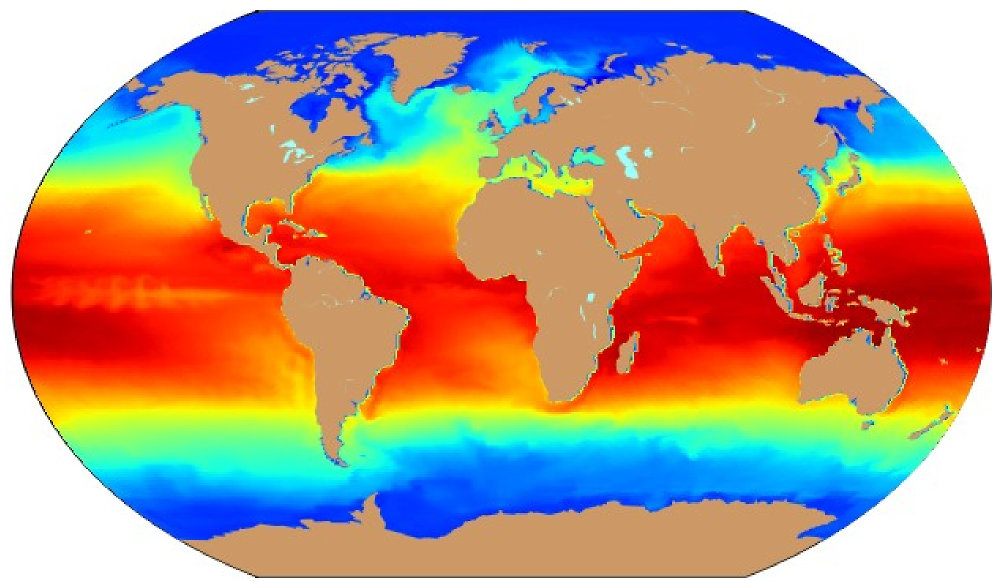
A gentle introduction to OMUSE: A Python framework for multiphysics simulations in Oceanography



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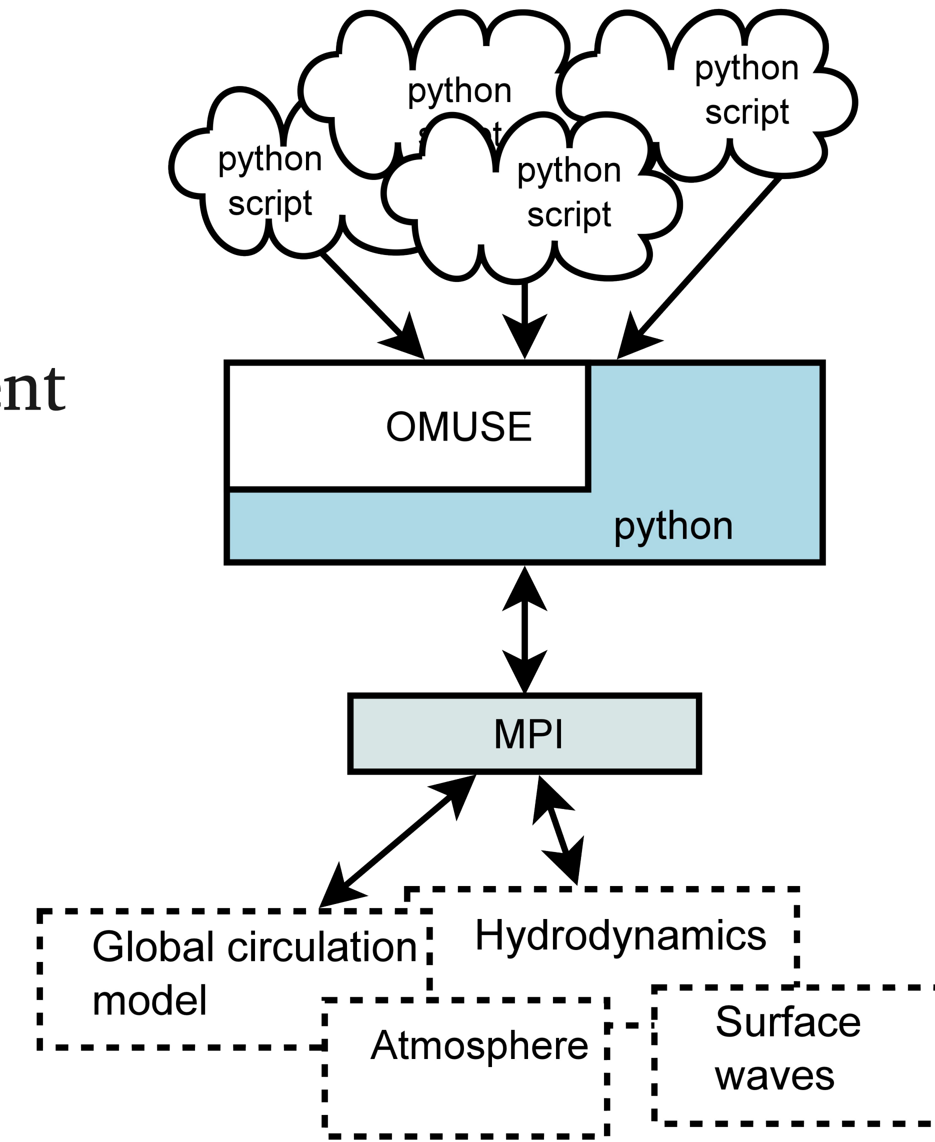
What is OMUSE?

→ Oceanographic Multi-PUrpose Software Environment

→ OMUSE is a Python environment for oceanographic numerical experiments



Goals:

- provide a homogeneous enviroment to run *community* codes
- enable new code couplings and interactions between components
- facilitate multi-physics and multi-scale simulations

Why OMUSE?

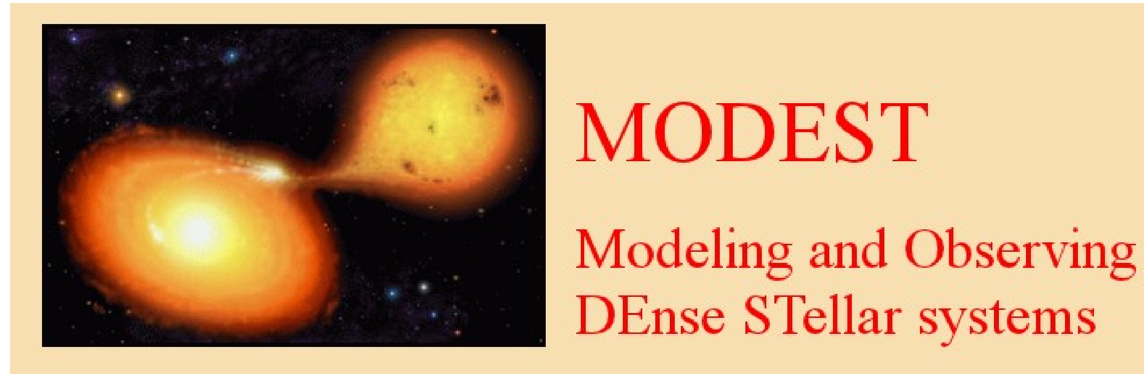
many excellent oceanographic codes have been written,
so why OMUSE?

traditional monolithic codes present challenges:
- difficult to learn&use,
- difficult to maintain and adapt,
- difficult to couple with other models,
- difficult to extend with new physics

so why not build on the legacy of the oceanographic community
and build a toolbox using existing codes?

History of OMUSE

- OMUSE build on AMUSE, started in the MODEST community



- development of predecessor and prototype around 2006: MUSE
- MUSE features retained in AMUSE: python based, 4 domains
- around 2009: more formal development started with funding from NOVA and later NWO,
- main development team in Leiden
- actively being used by 15+ groups worldwide
- 30+ publications, 8+ theses

History of OMUSE

- 2012 – 2013: discussions on wider applicability, call from the NLeSc for interdisciplinary projects, interest from Henk Dijkstra

- 2014: start of development @IMAU of OMUSE with funding from NLeSc, OMUSE main developers: Pelupessy (IMAU) & van Werkhoven (NLeSc)

- 2015 – 2016: current development of prototype & initial capability

'Hello Ocean'

“imports”

```
from omuse.units import units
from omuse.community.qgmodel.interface import QGmodel
from amuse.io import read_set_from_file
```

“initial cond.”

```
input=read_set_from_file('initial_condition')
```

“instantiate community code”

```
code=QGmodel()
```

“initialize model”

```
code.parameters.dt=0.5 | units.hour
code.grid.psi=input.psi
```

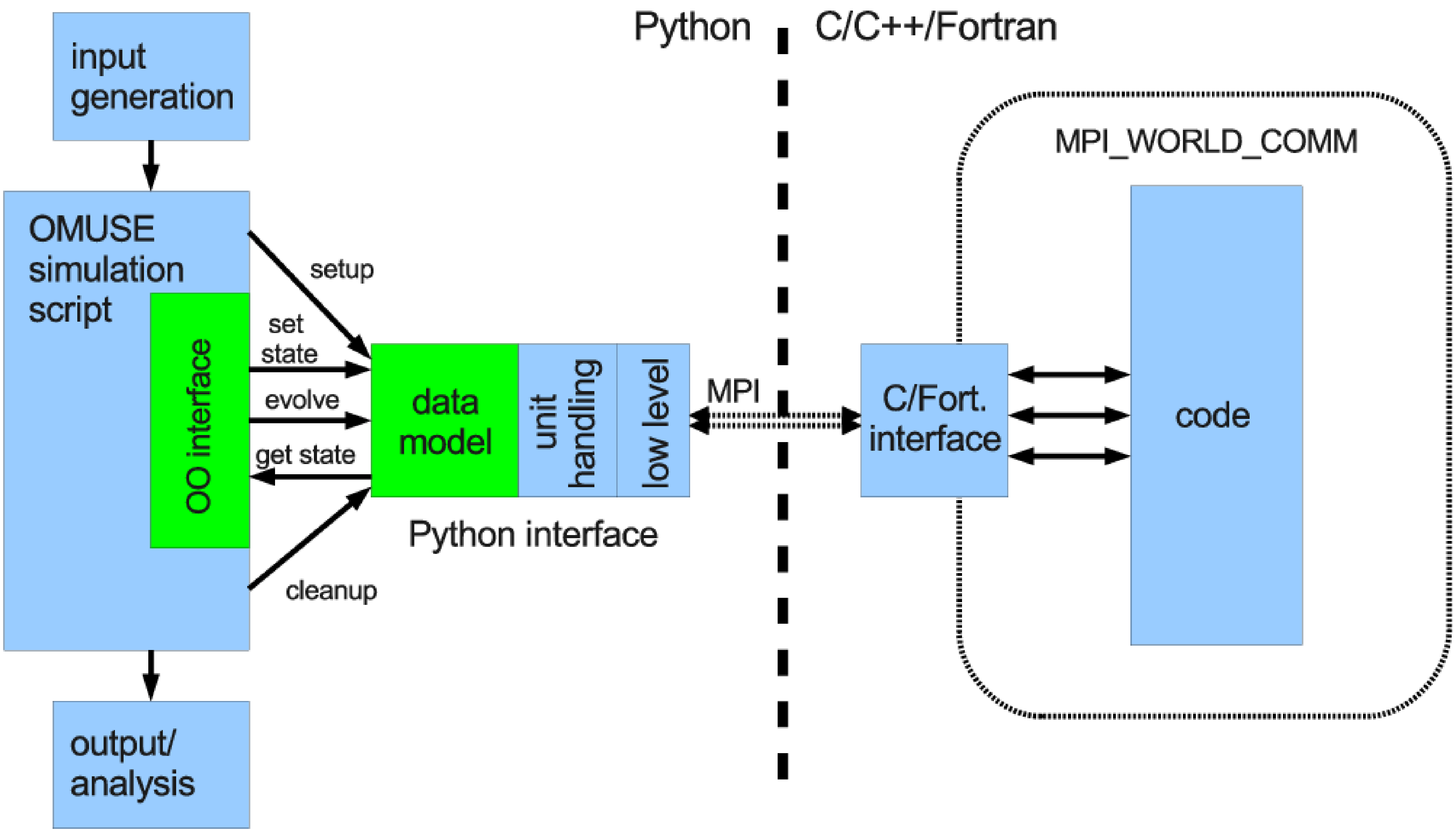
“evolve”

```
code.evolve_model(1.| units.day)
```

“analysis”

```
print code.grid.psi.max().in_(units.Sv/units.km)
```

OMUSE interface design



AMUSE & OMUSE design highlights

- python based:
  algorithmic flexibility and ease of programming
- remote function interfaces:
  built-in parallelism & separation of memory space, thread safety
- unit algebra module: units imposed
- automatic state handling
- object oriented interfaces
- error handling & stopping conditions
- testing integral part of AMUSE development:
  2000+ tests covering the base framework, support libraries
  and the community interfaces (>80% code coverage),
- test suite run daily on different (virtual) machines

Current status of OMUSE

initial set of codes currently in OMUSE:

- QGmodel: solves barotropic vorticity equation on rectangular cartesian grid
- ADCIRC: shallow water coastal model, solves 2D or 3D momentum equations
- SWAN: wave propagation model, implicit, solves spectral action balance equation
- POP: solves three-dimensional primitive equations for ocean dynamics
- QGCM: multi-layer QG solver, atmosphere + ocean
- under consideration: XBEACH, SELFE, Delft3D, ...

Current status of OMUSE

Development of support code:

- AMUSE framework support for different grid types
- grid transformations (e.g. dipolar, tripolar)
- remapping schemes
- triangulate package (building unstructered meshes)
- importers for netcdf data etc
- integrion of plotting libraries
- ext (utility functions, ..)
- unit support for 'oceanographic' specific units

OMUSE interface design

The interface to a code defines the way you talk to a code from python:

- interfaces are based on *physics* rather than *numerics*
- codes from the same domain use the *same interface*
- communicate *objects* rather than arrays
- *impose* the use of units
- model calling sequence in *state model*
- function calls are *remote*
- *stopping conditions* to detect events and guard integrity of the simulation results

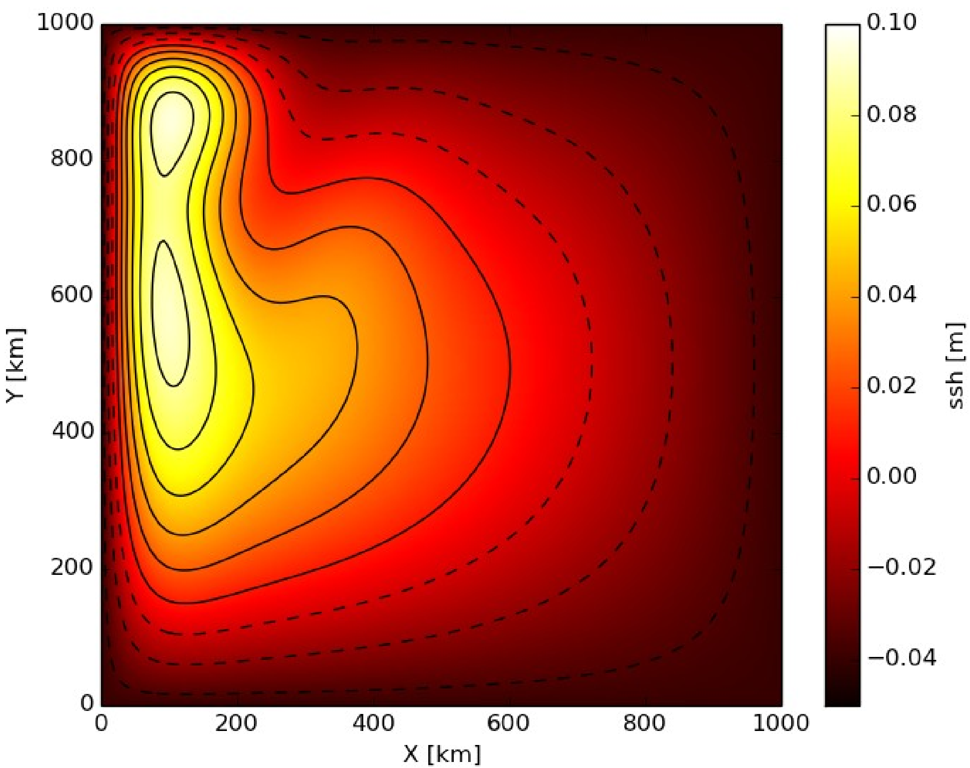
example: Quasi-geostrophic model

- `qgmodel` code (Viebahn 2014) , solves barotropic vorticity equation:

$$\frac{\partial}{\partial t}\nabla^2\psi + J(\psi, \nabla^2\psi) + \beta_0\frac{\partial\psi}{\partial x} = \frac{1}{\rho_0 H}\left(\frac{\partial\tau^y}{\partial x} - \frac{\partial\tau^x}{\partial y}\right) - R_H\nabla^2\psi + A_H\nabla^4\psi$$

easy example, because:

- small number of variables and parameters
- simple, fast solver
- regular cartesian grid



Quasi-geostrophic model

brief steps of implementation of the `QGModel` interface:

→ make code library

→ define interface: parameters, model setters and getters, units

→ rewrite main into `evolve_model`

→ define state model & grid variables

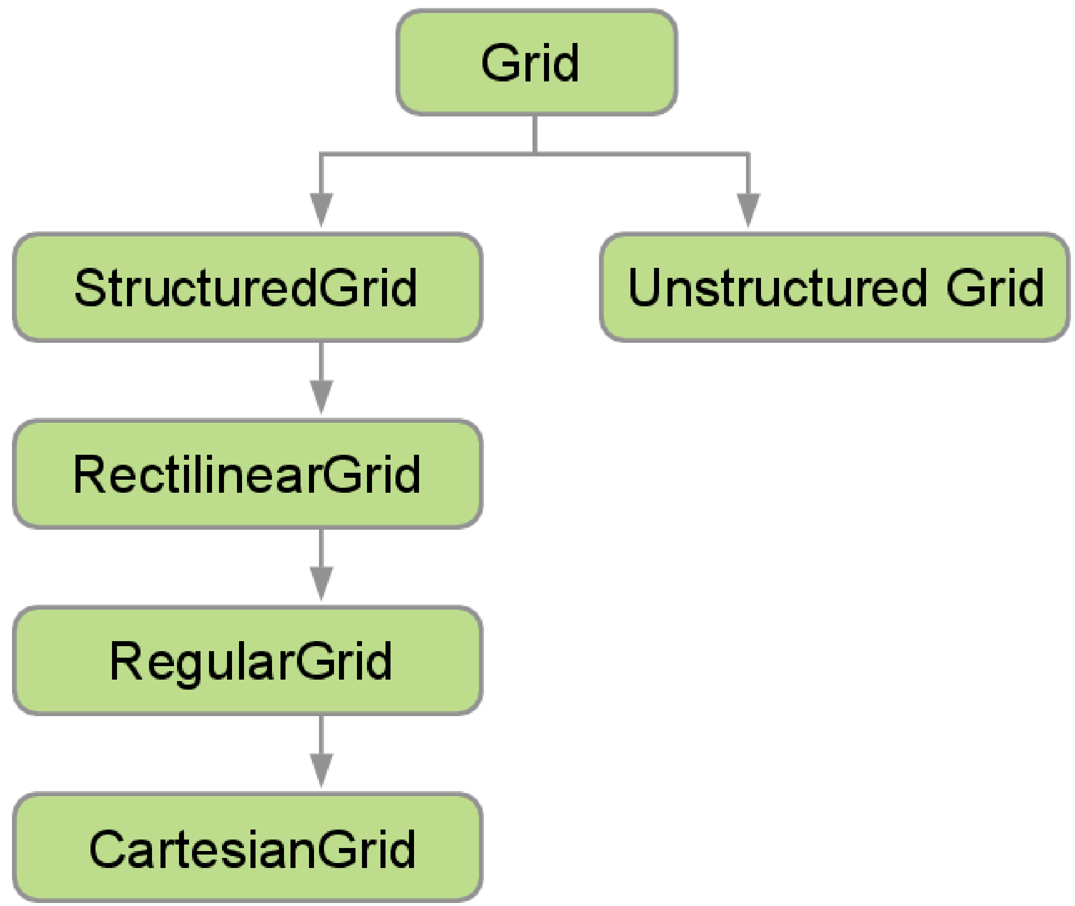
→ write tests!

extra steps:

- change hardcoded wind model → interface wind
- add interface boundary conditions
- add *fishpack* Poisson solver (for portability)

Datamodel: Grid support

- OMUSE uses high level objects to describe state of a system: grids and particles sets
- these can reference memory storage, disk storage or the state of a community code



Datamodel: Grid remapping

→ abstraction for data transport: `channels`

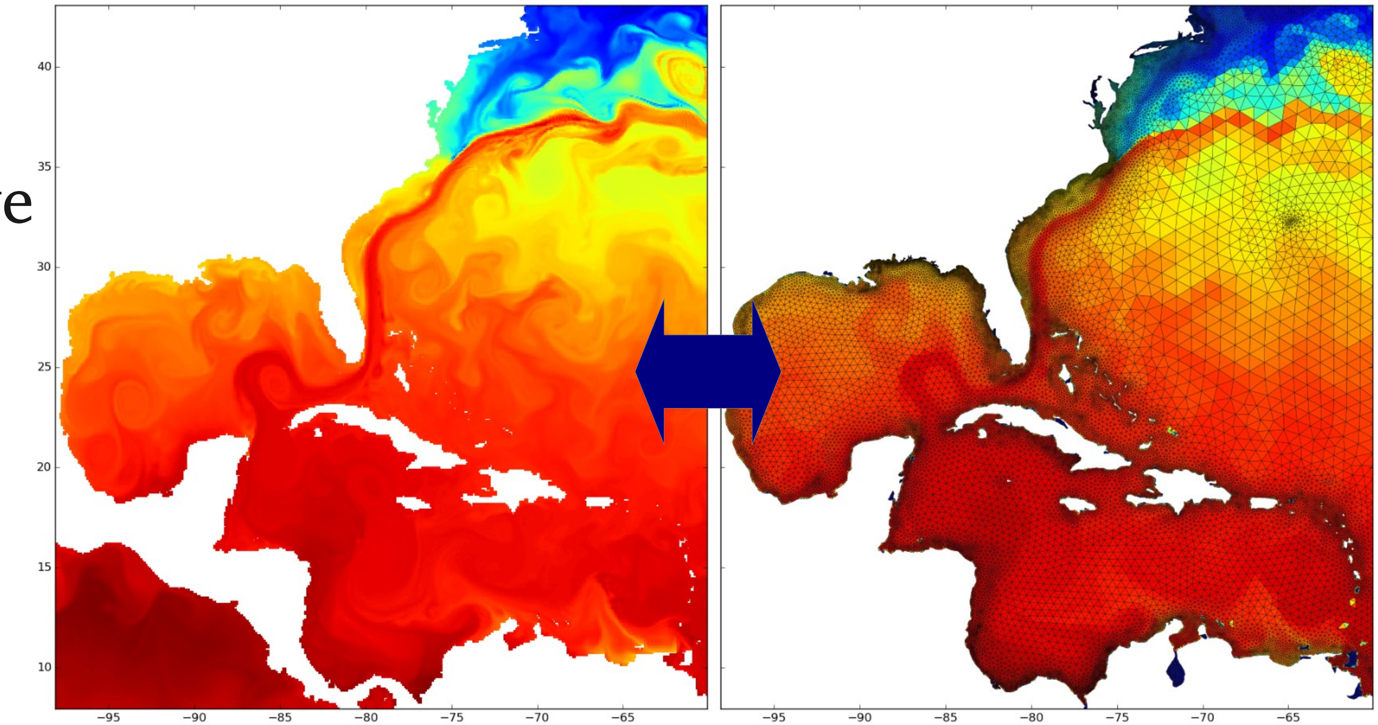
normal (copy): `channel.copy_attribute("density")`

functional transforms: `channel.transform( target, function, src)`

takes input attributes and transforms to (different) target attributes

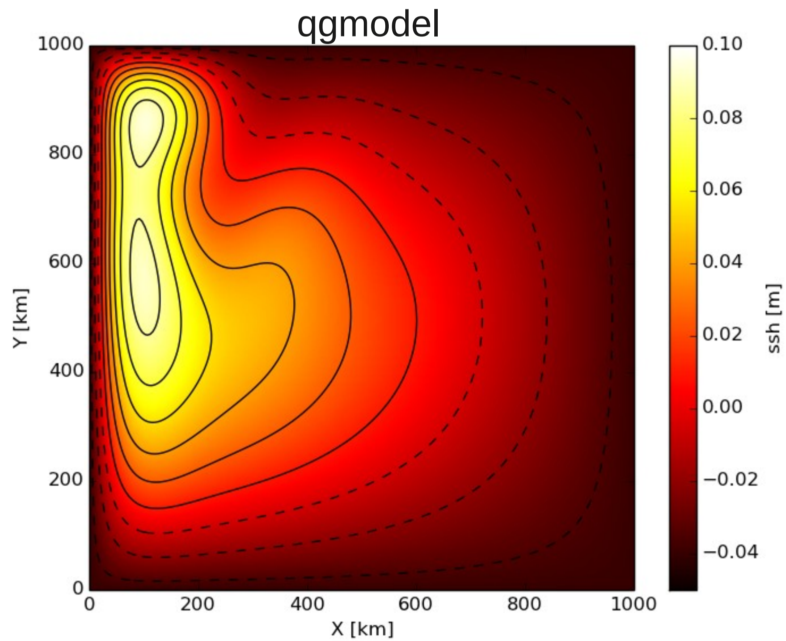
remapping channels:

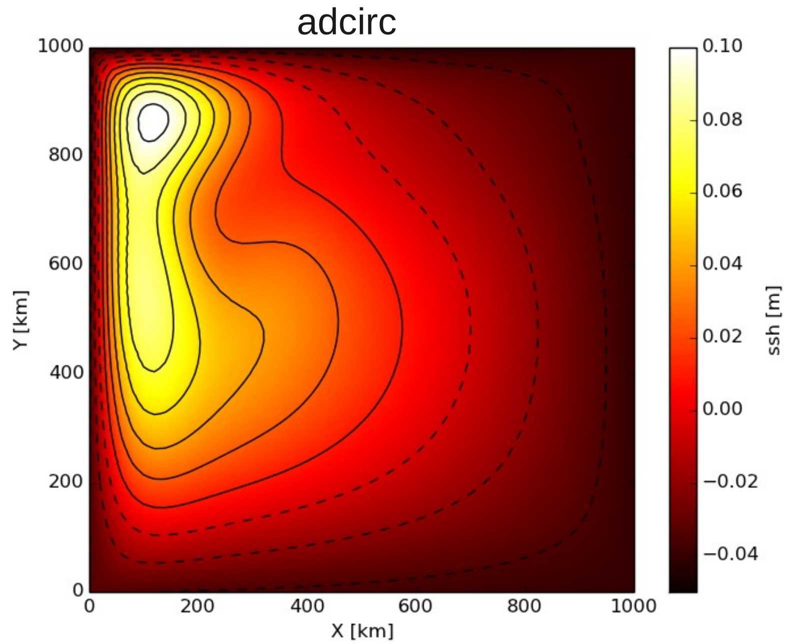
- remaps values between grids using a `remapper` object
- various remappers available: interpolate, conservative
- same semantics for usage.



What can you do with OMUSE?

- simplify setup and model runs,
- scripting simulations:
    - parameters searches
    - optimizations (e.g. MCMC)
    - event detection,
    - stoppage conditions
- 'online' data analysis
- cross verification: running problems with different codes and method
- coupling different codes to construct new solvers





Coupling codes in OMUSE

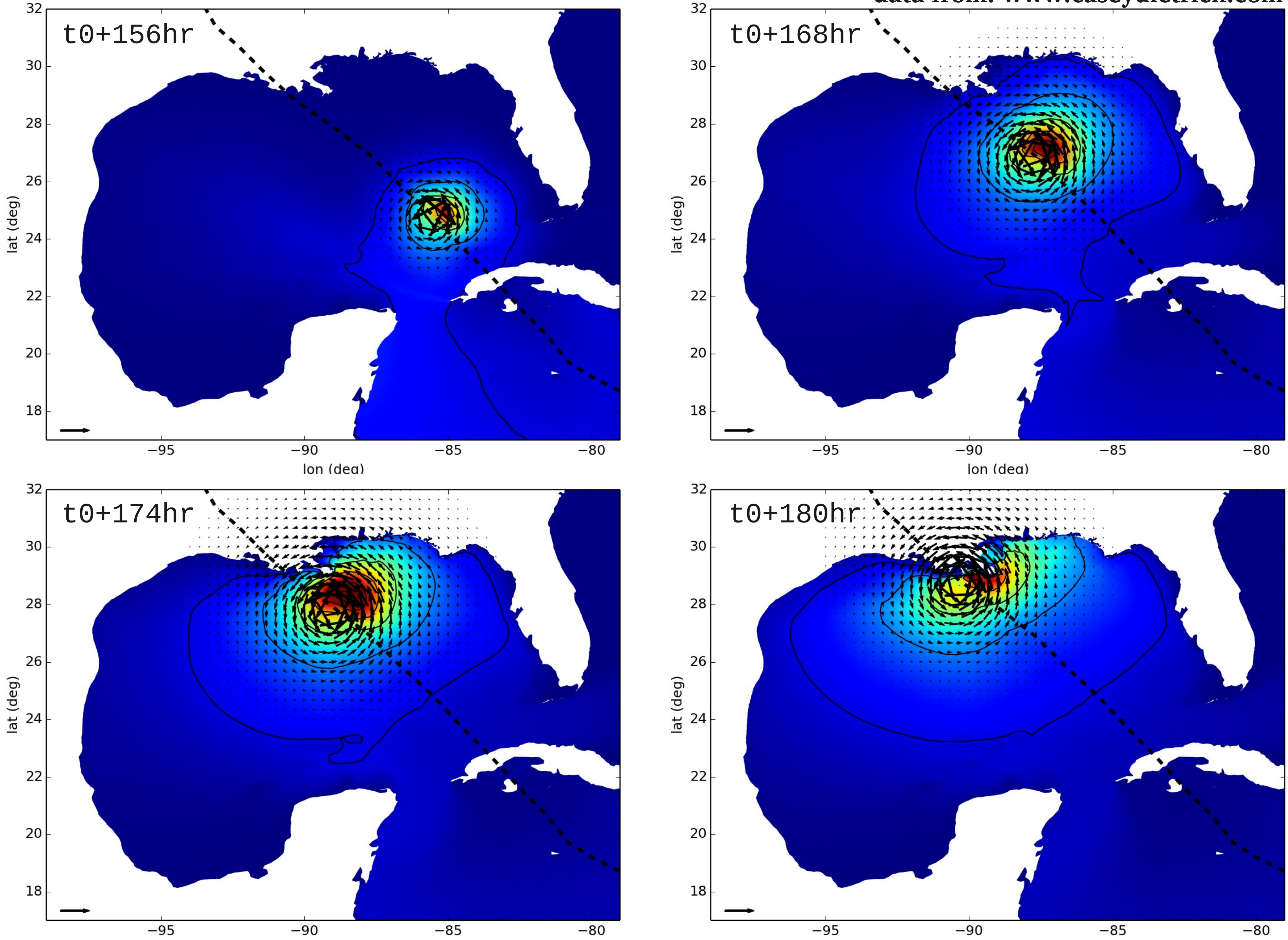
- the community code interfaces define a simple and homogeneous way of running codes,
- the interface provides read + write access to the state, forcings, boundary conditions etc. of a running code with very little overhead,
- code state is kept consistent by the interface,

→ the interface can be used to implement (explicit) couplings between different codes.

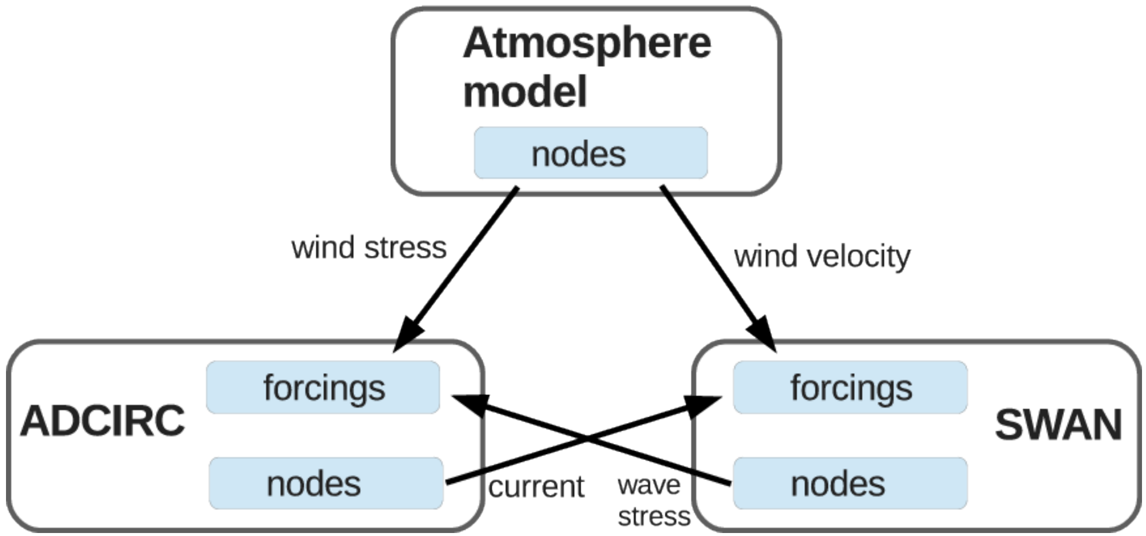
  + couplings can be formulated efficiently
  + couplings can be defined in a code agnostic way
  + coupling between codes running on different machines
  + easy to set up such that coupled code conform to interface spec.
  - overhead of framework calls

ADCIRC/ SWAN: Hurricane Gustave example

data from: www.caseydietrich.com



OMUSE coupled solver: ADCIRC/ SWAN




```
(1) channel1=hurricane.grid.new_channel_to( swan.forcings )
( ) channel2=hurricane.grid.new_channel_to( adcirc.forcings )
( ) channel3=adcirc.nodes.new_channel_to( swan.forcings )
( ) channel4=swan.nodes.new_channel_to( adcirc.forcings )
(2) while time<tend:
(3)     hurricane.evolve_model(time+dt/2)
(4)     channel1.copy_attributes(["tau_x","tau_y"])
( )     channel2.copy_attributes(["vx","vy"])
(5)     adcirc.evolve_model(time+dt/2)
( )     swan.evolve_model(time+dt/2)
(6)     channel3.copy_attributes(["current_vx","current_vy"])
( )     channel4.copy_attributes(["wave_tau_x","wave_tau_y"])
```

in short, OMUSE...

easy to use:

- effortless using of different codes
- automation of unit conversions, state handling
- no learning different I/O formats, parameter files, etc

encourages reproducability:

- open source policies
- easy cross verification across different codes and numerical methods
- low barrier for communication of experiments: portable scripts

OMUSE distribution:

- source repository, soon also binary release:

bitbucket.org/omuse/omuse

repository contains OMUSE specific code and open source community codes (all except ADCIRC)

- example script repository:

bitbucket.org/omuse/omuse-examples

- AMUSE frame work:

www.amusecode.org

Code papers: Pelupessy et al. 2016, under GMD discussion

(http://www.geosci-model-dev-discuss.net/gmd-2016-178/)

Pelupessy et al. 2013, A&A 557, 84