Starting MOHID Lagrangian

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Immediate concern: CleanAtlantic

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- Develop modelling methodologies and capabilities to tackle a domain such as the Atlantic ocean;
- Model **several types** of litter and their evolution in time (degradation, biofouling, aging, etc);
- Identify accumulation zones, account for main sources and predict trends.

Not so immediate concerns: MOHID development

- The Lagrangian Modules are **very large** (+40 KLOCs each);
- They have aged ungracefully:
  - considerable computational and coding overhead has been introduced by continuous add-ons;
  - memory usage is not optimized
  - **not internally modular** (like most of MOHID)
- As a standalone module, they are slow

- The Lagrangian Modules are **very comprehensive**;
- Do many things:
  - Plumes and jets;
  - Water quality;
  - Sediments;
  - Oil;
  - etc
- **Integrated** in the MOHID system

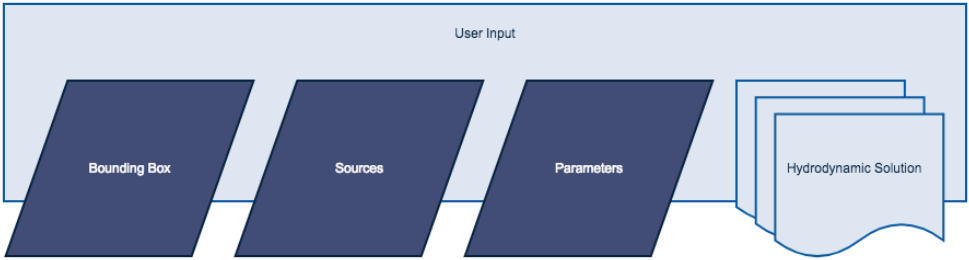
Functional Specifications

In order to be useful in the context of Maretec and the MOHID users, the new Lagrangian code should comply with:

- **Uni-directional** coupling to a hydrodynamic solution;
- Be **medium-independent**, i.e., should work across Water, Land and atmosphere;
- Present a **large collection of tracer types** and their respective methods;
- Be **efficient** ($O(10^7)$ tracers), **fast** (KISS and parallel), **extendible** (highly modular) and **readable** (it will never be finished, new coders should be kept in mind)

First looks

Our Lagrangian code should **expose** to the 'user' the following control structure



Defining a Source

Sources are complex objects:

- Geometry and location
- Lifespan
- Trajectory
- Properties to imprint on the Tracers
- Emitting rate of Tracers

Defining a useful Tracer

Our 'main' entity is probably opaque to the user. A **Pure Lagrangian Tracer** should consist of:

Parameters

- Id
- Id of the Source
- Maximum velocity
- ...

Statistics

- Average position
- Average velocity
- Average depth
- ...

State

- Active
- Age
- Position
- Velocity
- Acceleration
- Depth
- ...

Another Tracer!

A **Pure Lagrangian Tracer** is useful as a **template for other types of Tracers**. We can just make our 'plastic' tracer by adding some other properties to it:

Plastic parameters

- Density
- Degradation rate
- Size
- Particulate
- ...

Plastic statistics

- ...

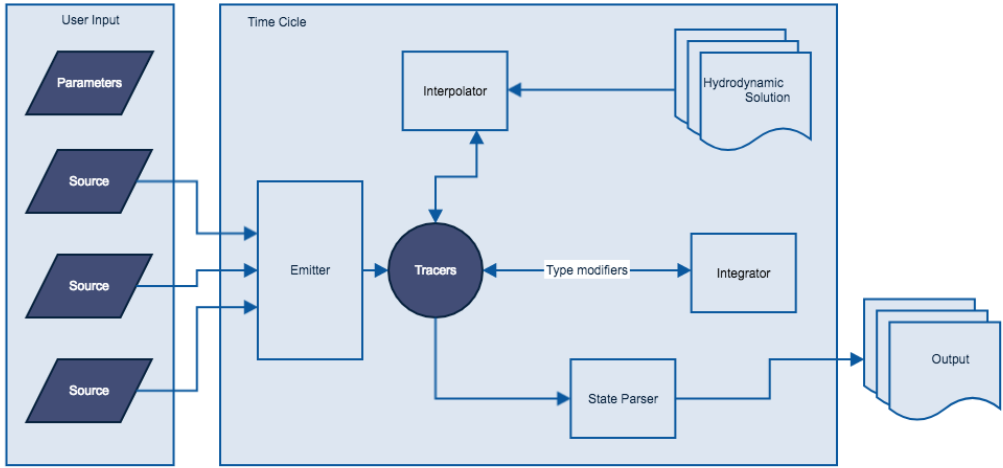
Plastic state

- Radius
- Condition
- Concentration
- ...

And then paper, tires, algae, radioactive isotopes, (...)

Once a simulation is launched

This part is mostly hidden from a 'user'



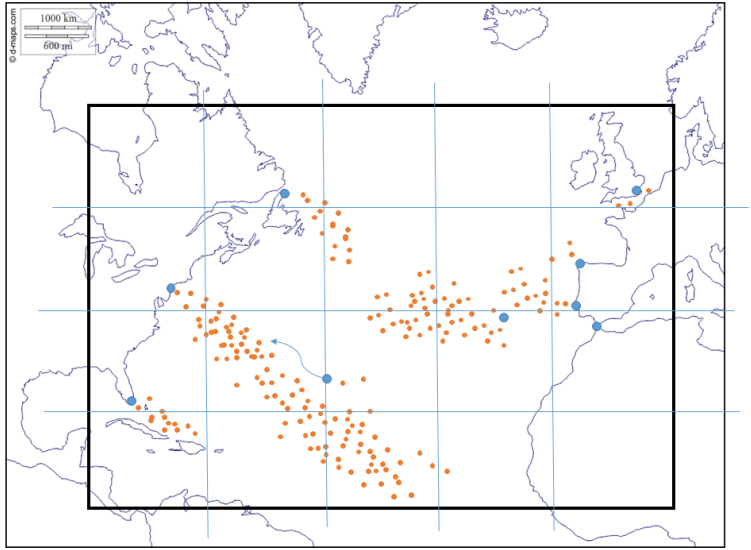
Organizing a Tracer library

A tracer type-properties library can be built over time, keeping information nice and clean:

```
<property name="bag_1">
    <particulate value="false" />
    <density value="0.7" />
    <radius value="0.2" />
    <condition value="0.95" />
    <degradation_rate value="1" />
</property>
```

A shared .xml file can be used as a library, were new entries can be added as need arises.

Ensuring scalability



Ensuring scalability - I

Employ domain decomposition even in a serial run

- Background hydrodynamic solution can be read in sub-domain blocks
- Different procedures can be done per block
- Allows higher-order optimizations on memory access patterns

Ensuring scalability - II

Finding your place in the domain takes time/memory in an arbitrary mesh:

Using memory (scales badly)

- use Ceiling()/dx and Floor()/dx on coordinates to find my grid cell
- need to store every dx in a variable resolution mesh
- what if someone gives us an unstructured mesh?

Using processor (scales at large)

- use a space filling curve and map to that
- very elegant way to decouple the problem from the mesh

Z-Order to the rescue!

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So what makes our problem 'hard'?

Sources and Tracers seem bo be simple enough, as entities. Integrating a tracer in time is essentially variations on the theme

$$\frac{D\boldsymbol{x}_i}{Dt} =< \boldsymbol{u} > (\boldsymbol{x}_i, t)$$

or

$$\frac{D\boldsymbol{V}_i}{Dt} = f(< \boldsymbol{u} > (\boldsymbol{x}_i, t))$$

Most processes rely on estimating an ambient quantity: velocity, temperature, salinity, colour...

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Interpolation - I

Assuming decent memory management, interpolation is our 'hard' problem in offline mode:

- file reading for every step
- find tracer positions on the mesh
- access mesh variables per interesting cell, per tracer
- implicit and/or higher-order schemes require several ambient time-steps...

Simple for a few Tracers, doesn't scale for large numbers. Fortunately it is open for optimizations and maps well to a parallel problem!

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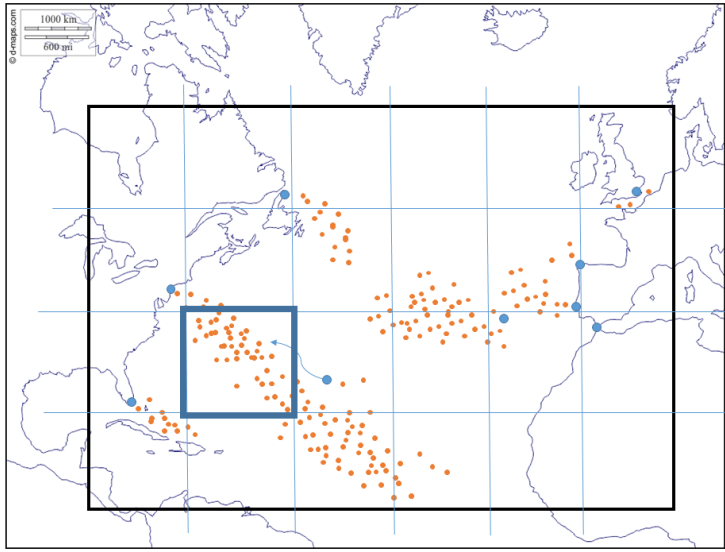
Interpolation - II

Both file 'import' and the interpolation can be done on a block basis



Interpolation - III

Once the block is in memory, two general approaches can be considered

Tracer oriented

- typically bi-linear interpolation
- another z-order curve can be built to optimize mesh node access
- simple, easy and robust
- one interpolation/quantity/Tracer/time step
- limited optimizations available

Block oriented

- interpolate all the tile!
- splines, Lagrange interpolators, etc
- one interpolation/quantity/layer/time step
- further abstracts the Tracers from the ambient mesh
- may be useful for many Tracers
- available libraries

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Go Parallel

We described a very parallel problem

Distributed memory (MPI style)

- domain decomposition based
- blocks can be mapped to processes
- communication is minimized - just send tracers from one block to another
- load balancing is not trivial, but we might be limited to the domain decomposition of the hydrodynamic solution already stored, so we have limited responsibility...

Shared memory (OMP style)

- each process (block or block group) can be further subdivided into cells
- cells re-use all the block code
- load balancing is trivial and with plenty of options
- because memory becomes more coalesced, efficiency should increase
- directive based acceleration should be sufficient

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I/O formats

We should stay agnostic and portable - standard formats

Input files

- Demand NetCDF files (HDF5 is not a format...)
- Not sure about geometries, shapefiles

Output files

- again, NetCDF should be default
- There are people working exclusively on post-processors - use them.

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Mapping the problem to Fortran

Follow the golden rules of Fortran and use OOP (Fortran 2008+):

- Minimize global variables (parameters and nothing else if possible)
- Use external libraries to handle strings, vectors, file I/O and guarantee KIND portability across systems
- Be paranoid about compartmentalization and re-usability of code
- Avoid pointers
- Be pleasant to compilers and future coders
- ...

Fortran is very good with OOP nowadays

- 'Everything' is an object from a given class
- Take advantage of unlimited polymorphic classes to reduce code size and hence bug probability
- already have some library APIs ready to share

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Start with the basics - file structure

The code should be organized as both a **library** and an **application**, an implementation of the library using its API (Application Programming Interface). So:

Project tree

- Application
  - MOHIDLagrangian.exe
    - MOHIDLagrangian.f90
- Library
  - MOHIDLagrangian.lib
    - tracers.f90
    - interpolation.f90
    - sources.f90
    - ...

This is inherently **modular**, **clean** and generates a .lib that can be used inside MOHID for online solutions.

Start with the basics - code documentation

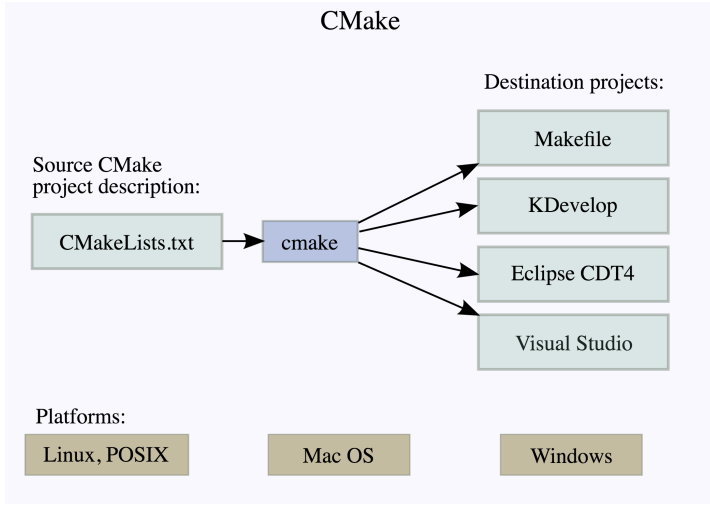
The code should be **self documented**:

```
type :: paper_state_class      !<Type - State variables of a
tracer object representing a paper material
real(prec) :: radius            !< Tracer radius (m)
real(prec) :: condition         !< Material condition (1-0)
real(prec) :: concentration     !< Particle concentration
end type
```

I've been using Doxygen, that interprets these comments and generates documentation. There are many options so we can structure the documentation to our liking. Right now I'm generating **html** and **latex** documentation.

Start with the basics - build solutions

I use Cmake to generate my solutions:



Start with the basics - Continuous Integration, tests, GIT use

- Use continuous integration (automatic builds)
- Use unit tests and grow you higher order tests
- Be paranoid about commits (my average is 8-10 a day) and branch (one per feature)

Next few months

- Continue implementation of basic framework tools
- Arrive at a barebones working model
- Test the interpolation ideas (compare bilinear to continuous in quality/performance)
- Search for turbulent diffusion models to include
- Search/implement closure models for different tracer types, starting with litter