THE MOHID CONCEPT

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CHAPTER SYNOPSIS

Mathematical models transform conservation principles into quantification tools. They must satisfy the Gauss theorem when applied to a physical space delimited by open surfaces and must guarantee conservation when dealing with transformation processes that in environmental systems are mostly due to biological activity, involving energy fluxes in the form of mass transfer between consumers and producers.
MOHID is an environment modelling system dealing with transport and with biogeochemical transformation processes in complex geometries. It was developed to be used by researchers and by professionals and to be applicable to a large range of scales and physical conditions. Researchers require tools able to test hypotheses and compare options. Professionals require efficiency for quick results production. A wide range of scales requires the consideration of the corresponding transport processes and of interactions between scales.
This chapter describes the MOHID architecture and engineering developed to satisfy the requirements derived from the range of user profiles, physical scales and biogeochemical processes to be considered. The architecture designed permitted the integration of several models in the modelling system and the engineering adopted simplified the development of the information tools necessary to manage field data and model results in complex systems.

1 INTRODUCTION

The actual MOHID architecture was designed in the late nineties based on previous team experience and on the information technologies becoming available to the FORTRAN modelling community resulting from the publication of the new FORTRAN 90 language, but also from the development of standard data formats as HDF[1] and of more performing personal computers. Together with the HDF format personal computers permitted the use of small pieces of software not available in former mainframes that have strongly improved modellers productivity.

Scientific developments carried up to the nineties in the framework of a set of Ph.D theses concerned with hydrodynamics [1-4] and with eulerian ecological modelling [5] and M.Sc. theses mostly concerned with lagrangian transport [6] and ecological modelling [7,8] supported the design of the MOHID architecture. These developments included 2D and 3D developments, mesoscale and Boussinesq wave modelling and eulerian and lagrangian models. These developments generated different models of difficult maintenance in a quick scientific and technological evolving context. The need to combine them generating a modular system where differences were handled in specific parts of the code was high.

The new MOHID model should be able to deal with 2D and 3D simulations, to deal with Eulerian, Cartesian or Lagrangian vertical coordinates, to deal Eulerian or Lagrangian transport references and to use the same biogeochemical formulations independently of the number of spatial dimensions or space reference and should allow alternative formulations for every process in order to be flexible in terms of scientific developments.

[1] HDF was developed by the National Center for Supercomputing Applications and is now supported by The HDF Group: http://www.hdfgroup.org/)

The finite-volume method already used by Martins [4] was adopted to make the spatial description independent of the vertical coordinate and of the number of vertical dimensions and all the transformations processes occurring inside the volume were programed using a 0D formulation in order to make them independent of the spatial reference, being the code sharable by the eulerian and the lagrangian formulations.

A fractional time step was used in order to split the resolution of processes using the most adequate temporal discretization or calculation sequence in each of them. This approach was necessary to decouple the resolution of the transport and transformation processes, but also to decouple the resolution of biogeochemical processes creating the independence need to aggregate developments carried out by different people.

The resolution of evolution equations in their integral form simplified the design of the desired architecture. This form requires the explicit consideration of fluxes across the surfaces surrounding the integration volumes easing conservation during transport which is often violated in mathematical models when flux divergence is computed.

After accomplishment of the requirements described above a modular system to simulate free surface flows was achieved in the early years of 2000 decade. The Leitão [9] thesis was the first accomplished using this new concept that was described in [10]. The flexibility of the system simplified the subsequent development of a MOHID version to simulate catchments and all together these developments created a user's community that justified heavy investments on Information Technologies. *MohidStudio*[2] was developed to simplify the implementation of the model, assessment and processing of input data and the management of simulations, ncluding results visualizing and archiving. *AquaSafe*[3] was designed to automate procedures including the production of web services to integrate results of different models and field data in order to adequate the products to corporate user needs.

2 THE CONSERVATION EQUATION

MOHID is formulated using the integral approach stated in Equation 1, which describes the conservation principle – "The rate of accumulation inside a control volume balances the input and output fluxes plus sources minus sinks":

$$\frac{\partial}{\partial t}\left(\iiint_{CV} \beta dV\right) = -\iint_{surface}\left[\left(\beta \vec{u}.\vec{n}\right) + \left(-\vartheta\vec{\nabla}c.\vec{n}\right)\right]dA + \iiint_{CV}(S_0 - S_i)dV \tag{1}$$

where CV is the Control Volume, u is the fluid velocity relative to the volume surface ϑ is the diffusivity and (S_0–S_i) are the property β rate of production per unit of volume. Using the Gauss theorem, Equation 1 is transformed into the differential conservation equation:

$$\frac{\partial \beta}{\partial t} = -\frac{\partial}{\partial x_j}\left(u_j\beta - \vartheta\frac{\partial \beta}{\partial x_j}\right) + (S_o - S_i) \tag{2}$$

[2] *MohidStudio* is a trademark of Action Modulers (http://www.actionmodulers.com) and software aims to simplify the implementation of MOHID and facilitate the interaction between modelling and field data.

[3] *Aquasafe* is a trademark of Hidromod (http://www.hidromod.com). It was designed to automate procedures including the production of web services to integrate results of different models and data.

Equation 2 states that the rate of change of a property in a point balances the divergence of the advection plus diffusion fluxes at that point plus the production minus the consumption rate per unit of volume. Manipulating Equation 2 one can write the conservation equation in a lagrangian reference where the time derivative states that the rate of change in an elementary volume of fluid balances diffusion across its boundaries plus sources minus sinks:

$$\frac{d\beta}{dt} = \frac{\partial}{\partial x_j}\left(\vartheta \frac{\partial \beta}{\partial x_j}\right) + (S_o - S_i) \tag{3}$$

If the surface of the control volume used into Equation 1 is moving at the fluid velocity Equation 3 is obtained. In this case the surface could be deformed, but the total volume inside the surface would remain constant. If instead the surface of the controle volume could also move in order to build an envelope of the molecules initially inside the volume[4] the space occupied by the control volume would increase in time, but the total flux of β across the surface would be zero. The volume increase is a result of the entrainment of surrounding fluid and consequently the concentration β inside the control volume will change according to the difference between the concentration inside the volume and the concentration of the entrained fluid. The MOHID lagrangian module computes dilution through a volume increasing rate.

3 MOHID ASSESSMENT OF ENVIRONMENTAL SYSTEMS

Equation 1 requires volume integration to compute rates of accumulation and rates of transformation and surface integration to compute rates of exchange due to advection and to diffusion. The calculation of these fluxes requires the knowledge of the velocity and diffusivity along the Control-Volume (*CV*) surface, which value depends on the scales resolved by the model.

3.1 Aquatic environments

Figure 1 shows the MOHID vertical layout for aquatic systems. On the top of the water column is separated from the atmosphere by the air-water interface and the benthic layer separates the water column from the sediment at the bottom. MOHID includes modules for the processes in the water column, in the sediments and in the interfaces and uses atmospheric information provided by meteorological models or data from meteorological stations to describe the atmosphere.

Air-water fluxes are the only variables owned by the air-water interface. They can be specified by the meteorological model or computed using air temperature, moisture, wind speed, cloud cover and solar radiation and coefficients provided by the user. Precipitation has to be specified by the user. On the contrary the benthic interface layer lying between the water column and the sediment computes fluxes but is also owner of state variables having negligible mobility (filter feeders, microphytobenthos, decomposers, etc.).

Properties in the water column exchange material among them using the water as a transport agent. The planktonic properties move at the water speed, but particulate material can

[4] Random velocity associated to the Brownian movement (generating molecular diffusion) or to turbulent movement mix the initial fluid with surrounding fluid the surface has to have additional movement to surround the initial molecules, i.e., the volume increases as a result of diffusion.

have their own velocity too. It is the case of sediments that have its own settling velocity or oil that moves vertically in the water column to reach its stability depth (usually the surface) or fish larvae and dinoflagellates that can have alternated upward and downward movements in the water column. Macroalgae and suspended filter feeders are also water column properties – although they do not move with the water – because they can exchange material with several layers in the water column (macroalgae length can be long compared with water column height and thus with model vertical layer thickness).

The module Water-Properties manages the simulation in the water column. It uses the geometry, velocity, water fluxes, and diffusivity whose computation is managed by the Hydrodynamic module and invokes modules in charge of solving the equation terms associated to the property's activity (e.g., sources/sinks, settling, swimming, adsorption/desorption). The module water properties also manages the calculation of state variables derived from others, as is the case of water density or light intensity.

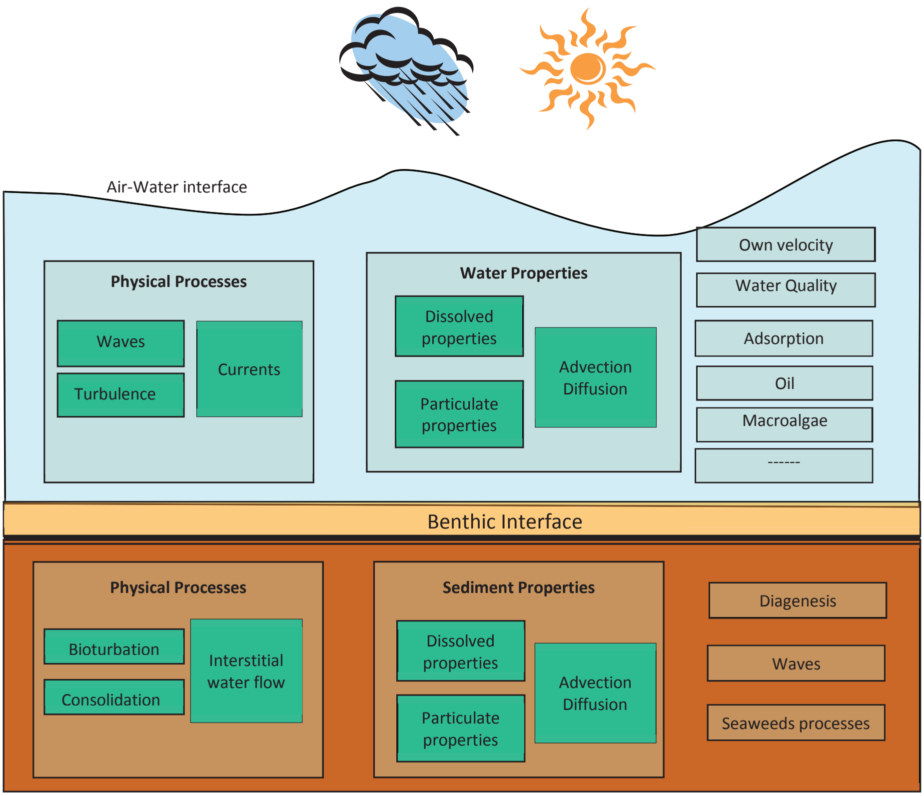

Figure 1. *Layout of MOHID vertical description of the aquatic environment. The water column is separated from the atmosphere by the Air-Water interface and from the consolidated sediment by the Benthic interface.*

Processes in the sediment have the same origin and structure as the processes occurring in the water column, but are much slower due to lower mobility of the dissolved material. There is advection due to interstitial water movement generated by sediment consolidation and/or by groundwater exfiltration. Diffusion is molecular in the lower layers and is induced by animals' activity – bioturbation – in the upper 10 cm layer. Like in the water column properties can be dissolved and unlike in the water column most material is particulate. Because of the low water content and mobility exchanges between deposited sediment and water column are slow and sediment is mostly anoxic.

In shallow zones with low sediments deposition rate seaweeds can develop injecting organic matter inside the sediment through roots' growth and extracting mineral nutrients regenerated by organic matter mineralisation. In regions with high settling rate accretion of sediments is usually the main mechanism to maintain organic matter content in the sediment. The Sediment-Properties module manages the transport of properties inside the sediments computing advection using the water movement associated to the consolidation process (in absence of groundwater exfiltration) and diffusion using bioturbation diffusivity and invokes modules in charge of computing reactions and exchange between dissolved and particulate phases. Fluxes at the interface sediment-water are managed by the benthic layer which can accumulate particulate matter "fluff layer" and computes fluxes of dissolved properties.

Particulate material deposited in the fluff layer maintains its ordinary critical shear stress for erosion and is transferred into sediment at a low rate (or the order of mm/month). Material transferred into the sediment acquires its critical stress for erosion and generates a flux of properties as a function of the concentration in the benthic layer. Fluxes of dissolved material are computed using the concentration difference between water and sediment and an exchange coefficient function of the flow next to the bottom (in the first layer).

Salt marshes and tidal flats are a limit case of the representation shown in Figure 1. In these areas the sickness of the water column is zero at low water periods, allowing these zones to exchange directly with the atmosphere.

3.2 Land environments

Vertical structure of land environments is identical to vertical structure of aquatic environments, although the relative importance of the compartments is very much different. In fact, on land a water column is an exception, although it can occur during flood events or in ponds and in the sediment (i.e., in the soil) water flow is usually much more intense than in the aquatic sediment, being soil usually not saturated with water. As a consequence, in normal conditions, on land surface runoff occurs only in rivers and generalised surface runoff occurring only during storm events.

Figure 2 represents schematically the elements composing a catchment. The soil is the sediment equivalent in the aquatic environment. The river network (or ponds) is the water column equivalent in aquatic environment and soil surface is similar to salt marches, the major difference being the inundation frequency and the fact that the sediment below land surface is usually unsaturated.

The correspondence between compartments in land and aquatic environments permits the use of the same data structure to describe them and consequently both models can share the software architecture.

4 MOHID GEOMETRY

Evolution processes in a three dimensional environment are described by conservation Equations 1 to 3, which can describe balances to finite volumes or at one point. Mathematical models have to describe nature using discrete values computed in a grid. The consideration of the grid as a finite number of adjacent volumes to which the conservation Equation 1 is applied simplifies the respect of the mass conservation principle and permits the use of irregular grids as that shown in Figure 3.

MOHID has adopted the integral form of the equations, fluxes being computed over the faces of the finite volumes (cells). Inside the volumes source and sink terms are computed based on the local values. Diffusive fluxes are computed at each cell face using concentration values on each side of the face and advection is computed using the water discharge across the cell face and a concentration estimated using a spatial interpolation in order to generate upstream, central differences, QUICK or TVD methods.

Diffusivity and water fluxes are computed by the hydrodynamic module over the face using a staggered grid approach where velocities are computed on the faces of the cells described on Figure 3. In the hydrodynamic module (as in the hydrological module) a conservative approach is also considered for advection and diffusion, meaning that velocities are also computed using finite volumes obtained by interpolation of the control volumes used for scalars.

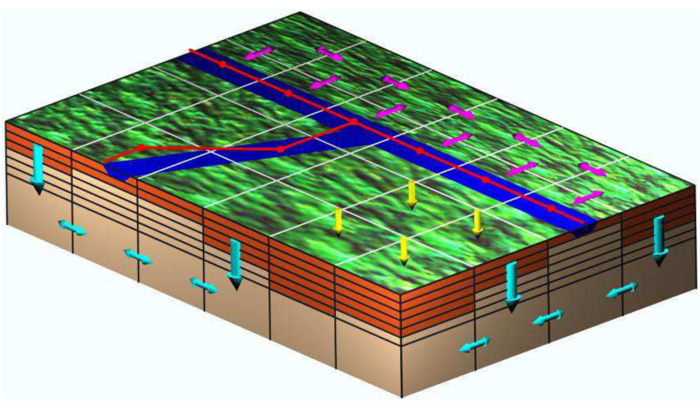

Figure 2. *Vertical description of a catchment. The surface gets rain and at surface we can have a river network in normal conditions and generalised surface runoff during rain events. It is also at surface that vegetation grows and in the soil one can have a non-saturated zone (vadose zone) on the top of a saturated zone. All these compartments can exchange water in two senses.*

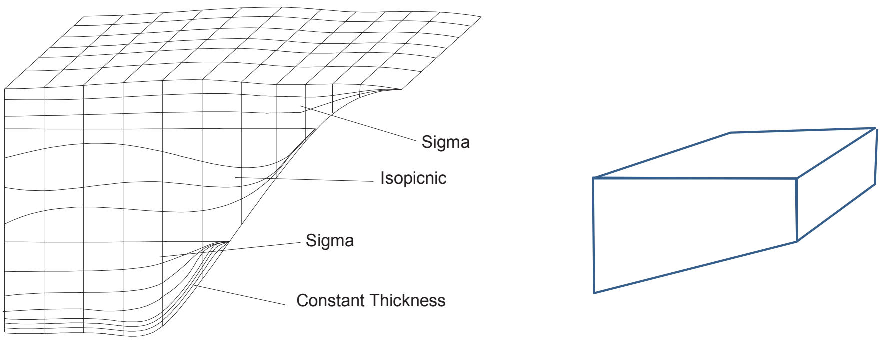

Figure 3. *Example of spatial descretization combining domains with different types of coordinates (left) and an example of a finite-volume (right).*

Most MOHID applications use parallelepiped control volumes with orthogonal horizontal axes simplifying the calculation of the internal products necessary to compute fluxes. However MOHID can also use curvilinear grids as that shown on Figure 4. The curvilinear grid is adequate to compute flows in horizontal anisotropic systems (e.g., rivers). It saves memory and increases the transversal resolution, but it requires simplifications for momentum fluxes calculation, to be computationally efficient.

On vertical direction the internal product involved on the calculation of fluxes is simple because the area of cell surfaces projected on a horizontal plane is constant and uniform for every vertical column. Vertical water fluxes are computed considering the rate of change of the cell volume and incompressibility.

5 VERTICAL COORDINATE

The integral form of the conservation equation adopted by MOHID permits a very versatile definition of vertical coordinates. The most suitable coordinate is the one that minimises advective fluxes between adjacent cells. In fact advective fluxes in presence of Courant numbers very much different from unit are a major source of numerical diffusion. Vertical velocities are usually much smaller than horizontal velocities and consequently the corresponding Courant number can be much smaller than one. The consideration of a lagrangian grid where cell boundaries have some vertical movement minimises the vertical diffusion.

Rigid rectangular coordinates are the simplest because, apart from the surface layer, they do not move in time. They are adequate to simulate horizontal flows where topography plays a minor role. This is the case of the deep oceans. On the contrary the sigma coordinate varies between zero at the bottom and 1 at the surface and consequently the layer thickness varies according to water column depth which depends on the bathymetry and on the movement of the free surface. Sigma coordinates are the most adequate to simulate the flow in coastal shallow areas. Both coordinates can be combined with the lagrangian coordinate option to minimize numerical diffusion associated to high frequency waves.

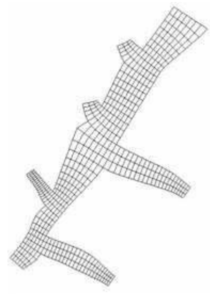

Figure 4. *Example of a curvilinear grid used in MOHID.*

Different coordinates can be combined in a simulation using the concept of a vertical dominium as shown on Figure 3. The simulation of ocean flows (or flows in deep artificial reservoirs) is dominated by baroclinic effects in the deeper zones and by topography in the shelf zone. The use of a Cartesian coordinate between the bottom and the shelf break and a sigma coordinate between the shelf break and the free surface is usually the most convenient combination. A 2D vertically integrated simulation is a particular case of a 3D sigma model. It is a 3D sigma model with just one layer.

MOHID includes procedures to combine Cartesian and sigma coordinates (lagrangian or not) using simple data specification. The user must specify the number of vertical domains to be used, the type of coordinate to use in each of them and the spatial step.

6 TEMPORAL DISCRETIZATION

Stability and accuracy but also computational software structure are determined by temporal discretization options. Explicit models generate the simplest codes but have to verify the CFL condition. The Crank-Nicolson (semi-implicit) codes have computation complexity identical to implicit codes and have better accuracy.

MOHID uses semi-implicit algorithms to compute the processes with higher stability restrictions and explicit algorithms for others. Gravity waves, vertical advection and diffusion and particulate matter settling are among the most restrictive processes and are computed using implicit algorithms.

Numerical instabilities are usually generated by excessive transport or consumption. Advection and diffusion generate instabilities when the material removed from one cell in a time step exceeds the existing material at the beginning of the time step and the sink terms generate instabilities when the consumption calculated by the model in one time step exceeds the existing material. The sequential calculation of processes in explicit algorithms minimises the probability of introducing instabilities and can simplify the algorithm itself (e.g., computing sequentially the transport in different directions) of computing sequentially the biogeochemical processes (e.g., respiration, natural mortality, predation, etc.). Equation 4 describes the procedure using the addition associative property:

$$\frac{\partial \beta}{\partial t} \approx \frac{\beta^{t+\Delta t} - \beta^{t}}{\Delta t} = \frac{\beta^{t+\Delta t} - \beta^{*}}{\Delta t} + \frac{\beta^{*} - \beta^{**}}{\Delta t} + ... + \frac{\beta^{***} - \beta^{t}}{\Delta t} \tag{4}$$

Applying this approach to Equation 5 one gets a set of algebraic equations as described in Equation 6.

$$\frac{\partial\beta}{\partial t} + u_j\frac{\partial\beta}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\vartheta\frac{\partial\beta}{\partial x_j}\right) + f_1 + f_2 \tag{5}$$

$$\begin{aligned}
\frac{\beta^{***}-\beta^{t}}{\Delta t} &= \left(-u_1\frac{\partial\beta}{\partial x_1}\right)^t + \left(-u_2\frac{\partial\beta}{\partial x_2}\right)^t + \frac{\partial}{\partial x_1}\left(\vartheta\frac{\partial\beta}{\partial x_1}\right)^t + \frac{\partial}{\partial x_2}\left(\vartheta\frac{\partial\beta}{\partial x_2}\right)^t \\
\frac{\beta^{**}-\beta^{***}}{\Delta t} &= \left(-u_3\frac{\partial\beta}{\partial x_3}\right)^{**} + \frac{\partial}{\partial x_3}\left(\vartheta\frac{\partial\beta}{\partial x_3}\right)^{**} \\
\frac{\beta^{*}-\beta^{**}}{\Delta t} &= (f_1)^{**} \\
\frac{\beta^{t+\Delta t}-\beta^{*}}{\Delta t} &= (f_2)^{*}
\end{aligned} \tag{6}$$

In the algorithms described in (6) the second step would be implicit and the others would be explicit. This procedure permits the optimization of the numerical algorithm and the subdivision of the model into modules that modify the state variables independently. The procedure is useful within a research group, but is especially useful to combine developments by several research groups. This is the case of biochemical models where sometimes higher trophic levels are computed using Energy Budget concepts instead of mass budgets as is the case for planktonic primary producers.

7 MODULAR STRUCTURE

A modular structure combined with object oriented programing is essential to develop complex models dealing with very much different processes and groups of state variables. This is essential for managing memory and especially to restrict the effects of software bugs to a single module. The temporal discretisation described above simplifies the implementation of the modular approach.

MOHID modules are combined in terms of geometrical requirements and in terms of groups of state variables. There is a central module (Module Model) in charge controlling the whole system and key modules as WaterProperties, Hydrodynamics, Geometry, AdvectionDiffusion, Atmosphere and Benthos that are always used to simulate free surface flows and the modules PorousMedia and SurfaceRunOff that are used in MOHID Land instead of the module Hydrodynamics.

The module WaterProperties defines the variables that will be simulated in each run. In this module are specified the modules and the state variables necessary to simulate a particular state variable. The Atmosphere Module specifies how the interaction with the atmosphere will be done. If fluxes are available (e.g., generated by an atmospheric model) MOHID will use those fluxes. Otherwise the module InterfaceAirWater will compute the fluxes using atmospheric state variables specified as boundary conditions.

8 SOFTWARE ENGINEERING

MOHID evolved from a sequential FORTRAN 77 model to an object oriented model programed in FORTRAN 95 and its subsequent evolutions. The whole structure of the system is divided into FORTRAN modules, each of them having the functionality of an object class. The design of MOHID uses several object oriented features like encapsulation, polymorphism, function overloading and inheritance. Objects have four standard methods: (i) constructor, (ii) selector, (iii) modifier and (iv) destructor.

The EnterData is a critical MOHID module. It parses ASCII data files written in format similar to XML and extracts information required by each module using a ”direct access” approach. This module permits a variable form of input data files, allowing input data files with unread data. This structure allows a user to develop alternative process formulations requiring different data sets without interfering with users requiring different inputs.

A detailed description of the software engineering approach is described in [11]. Each of the more than 50 classes that form the MOHID Framework is designed to fill out standard requirements, regarding programming rules and definition concepts, in order to establish a straightforward connection of the whole code. This standardization is reflected in memory organization, public methods systematization, possible object states, client/server relationship and errors management. Each class is responsible for managing a specific kind of information. The design of a class, in FORTRAN 95, can be accomplished by the MODULE statement allowing encapsulation (using the PRIVATE statement) assuring that all the information associated to an object is only changed by the object itself, reducing errors due to careless information handling in other classes.

A MOHID class is defined as a derived type, which has, in addition to its specific information, two required variables InstanceID and Next. InstanceID relates to the identification number of the class instance, that is the object’s ID, which is attributed when the object is created. Each time a new object is created, it is added to a collection of objects, stored in a linked list. Next relates to the object stored after the current in the list. Global class variables are designed to be one-way and can only be scanned in one direction.

Each class has only two global variables, defined as derived type pointers. They are the first object in the linked list (FirstObject), which works as an anchor or starting point to scan the list of instances of the module, and a pointer to the current active object (Me). The procedure to access an object is to, starting on the first object, scan the list and find the corresponding one through its ID number.

9 CONCLUDING REMARKS

An integrated modelling system must build on a wide scientific experience, on an integrator concept and must be supported by performing information technologies. MOHID development evolved along those lines. After a set of individual developments experience necessary to support an integrating concept was acquired. The integral form of the evolution equation showed to be the umbrella required for the numerical assessment of environmental systems. The integral approach associated to a flexible morphological and temporal description of the modelling object created the conditions to develop an integrated modelling architecture. The association of the modelling architecture to an adequate software engineering permitted the development of the MOHID system which is satisfying the needs of consultancy bodies and of researchers, being used in tenths of applied and research projects.

The MOHID code is open permitting the continuous inclusion of new developments. On aquatic ecosystems new developments are being carried on the benthic system, including on processes in the sediments and on terrestrial systems the interaction between the vadose and saturated zones and between these and surface water and their implications on vegetation development and soil pollution processes are being object of several projects.

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