Conceptual and computational challenges when coupling a groundwater model with ocean and river models

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Groundwater, river and ocean models are usually operated almost independently. If an interdisciplinary scientific contact exists, rough boundary conditions are found generally in the results of the other models. Indeed, many important coupled processes take place in the coastal zones involving all the ecohydrodynamical aspects. So that it is very important to introduce the interactions between the groundwater model on one hand and the ocean and river models on the other hand.

In the framework of the SALMON project (Sea Air Land Modelling Operational Network), the main concepts of these interactions have been studied and the computational challenges identified. In practice, the connection of the different models is planned through a specific interface, a Junction, designed to allow the data exchange between models based on different numerical methods. As each model has its own time and space discretizations, the Junction must organize the data exchanges including time and space interpolations schemes. The design of this Junction concept is made taking advantage of the clustered RS/6000 machines in the form of an IBM SP2 computer and by using the PVM software for the exchange of data between the different tasks running on the processors and the Data Explorer (DX) software for the visualization of the results.

The connection of the models through the Junction obliges to consider developments of each model. For the Groundwater Model, one of the main challenge will be probably to develop the parallel computing for multi-contaminant transport.

1 Introduction

Coastal or delta plains situated at the major river mouths are zones where an important fresh water demand is recorded. The human activities (urban, agricultural and industrial) in these regions lead to important degradations of the water quality. The purpose of the SALMON (Sea Air Land Modelling Operational Network) project is to develop from three existing models (ocean, river, and groundwater) developed at the University of Liège a joint model able to handle the description of water fluxes and quality in a whole system of regional scale including marine, river, groundwater and atmospheric inputs. In this complete three-fold model, fluxes of water, contaminants, nutrients,... must be computed in each model and transferred from one sub-model to another at the common boundaries. The clustered RS/6000 machines in the form of an SP2 computer provided by IBM (for the purpose of this research project) seem to be the appropriate platform to reach these goals taking advantage of a parallel computing environment.

Concerning the developments of the Groundwater Model (GM), year I of the project was dedicated to two main aspects: (1) tests and developments of the groundwater transport model to treat more accurately the density effect induced by salt water intrusion into an aquifer, (2) to develop the concepts of the main interactions to be taken into account when linking the Groundwater Model to River and Sea Models. About the validation tests of the coupled flow and transport Groundwater Model, one can find details in Dassargues [1] with comparisons with results published among others by Galeati et al. [2], and Hassanizadeh & Leijnse [3]. More tests are still in progress taking into account heterogeneities in the groundwater domain, inducing important variations of the Courant and Peclet numbers which can lead to strong constraints in terms of time and space discretization.

The main aspects treated hereafter concern the conceptual and computational developments which are needed to integrate the interactions linking the Groundwater Model (GM) to the River Model (RM) and the Ocean Model (OM). In this context, the purpose of this first step in the SALMON project was to define the most important interactions which are to be taken into account and to define conceptually how to take these interactions into account in a parallel computing environment.

2 Interactions between Groundwater and Ocean Models

On the boundary separating Ocean and Groundwater Models, two kinds of informations are to be exchanged: water pressures (or piezometric heads), and concentrations in different solute contaminants.

2.1 Exchange of water pressure and salt concentration values

For groundwater, the first contamination to be taken into account is produced by the salt water intrusion from the bottom of the ocean into the nearby geological formations. Assuming that groundwater fluxes into the ocean are not influencing water levels and salt concentration in the OM, the boundary condition for the groundwater flow is given by prescribed piezometric heads (h_0) corresponding to seawater pressure (p_0). For transport, as mentioned previously [1], the way of treating this sea-water boundary can influence strongly the results and usually, a prescribed concentration (C_0) is chosen when the flow is directed inward (for the groundwater model) and a zero dispersive flux when the flow is directed outward. The values of p_0 and C_0 coming unilaterally from the OM, should be actualized after each Δt of this model (figure 1).

2.2 Exchange of contaminated fluxes with prescribed solute concentrations

The bilateral exchanges, to be considered at each time step (Δt), are the convective contaminated fluxes. The GM provides, on parts of the common boundary, outwards computed fluxes (q) and the associated concentrations (C_i). If needed, inwards fluxes (for the GM) and associated concentrations can be considered from the OM on the other parts of the boundary (lower part of figure 1).

2.3 Organization of the information exchanges

All the information exchanges will be managed by the Junction (see paragraph 4) at each time step of the GM. The values to be exchanged have to be known at each node of the finite element grid which is lying on the 2D border as the groundwater model is 3D. Since the discretizing concepts of both models are quite different, the Junction will also have to interpolate the values from one model in order to prepare information to be provided to the other.

If more than one solute is concerned in the exchanges with the OM, multiple GM's must run in parallel, each of them dealing with another solute contaminant concentration. It implies the use of the same code in a parallel environment (single task on multi-processors). In a first step, this technique can be applied assuming that there is no physico-chemical reactions between the different species, and that no density effect influences the flow. This last statement is untrue for the salt and consequently the simulations relative to all the other solute contaminants have to wait informations at each time step from the coupled flow-transport simulation of the seawater intrusion (lower part of figure 1).

3 Interactions between Groundwater and River Models

When studying groundwater, river is often considered as forming a 1D or 2D boundary where one of the following flow conditions is chosen [4]: (1) piezometric heads are imposed at the boundary in contact with the river (Dirichlet conditions), the values being set equal to the elevation of the free surface of the river, (2) inwards or outwards fluxes are computed at nodes of the boundary depending of the difference between water head in the aquifer and in the river (Fourier condition). This last type of condition is more general and the computed flux can be written:

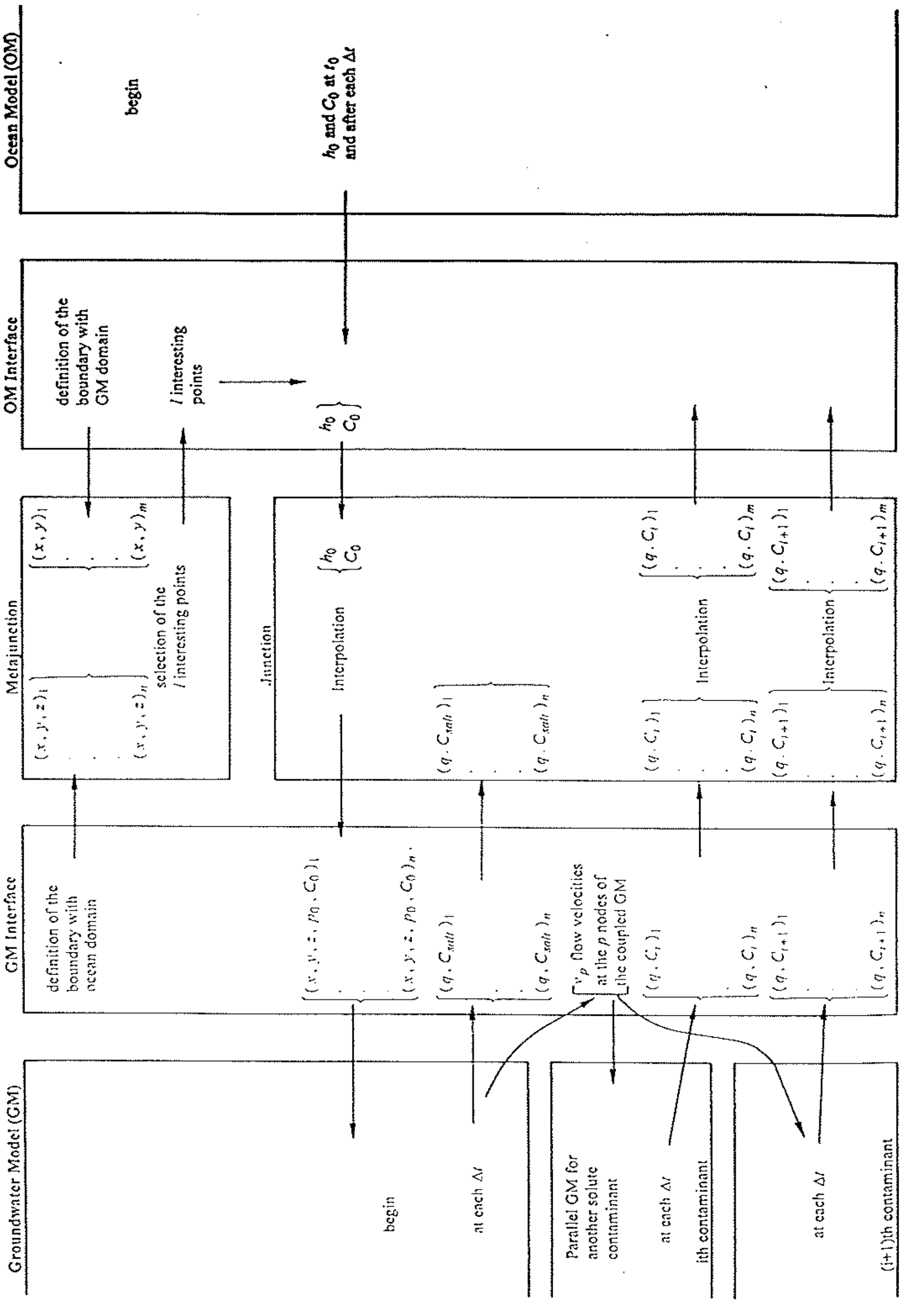

Figure 1: Conceptual schema of the information exchanges to be managed by the Junction (see §4) between Groundwater Model and Ocean Model.

$$q = \frac{K_r}{e_r} \cdot (h_g - h_r) \qquad (1)$$

with K_r and e_r respectively the hydraulic conductivity and the thickness of the bottom of the river, h_g being the groundwater piezometric head and h_r is the water level in the river. A conceptual schema of the exchanges is given at the figure 2. At each time step, computation of the flux can be done by the Junction (see paragraph 4) and the information is returned to each model, one receiving a certain amount of water corresponding to the volume lost by the other and the exchanged value is considered as a constant for the next time step.

For the solute transport aspect, the bilateral exchanges are considered as only depending of the advective and dispersive contaminated fluxes so that solute concentrations are associated to the advective and dispersive fluxes computed by the junction at each time step. As for the interactions between the GM and the OM, if more than one solute is concerned in the exchanges with RM [6], multiple GM's must work in parallel, each of them dealing with a different solute contaminant. If the advective flux is directed into the GM, the associated concentrations are provided by the RM (C_{r_i}), and they have to be dispatched by the Junction to each concerned GM. On the contrary, when and where the advective flux is directed from the GM's to the RM the associated concentrations (C_{g_i}) are provided by the GM's (in parallel) and they have to be transferred for input in the RM.

4 Concepts of Junction and Meta-junction

The distributed-memory parallel systems and the Parallel Virtual Machine (PVM) software allow us to run meta-models comprising several different models applied to several connected domains. Initially, as defined by Beckers & Schmitz [5], the Junction was an entity which was managing the connections between models of the same type (OM's) applied on adjacent subdomains in a parallel computing environment. The role of the Junction is extended to the connection of domains with different time steps, with different grid size, with different state variables and with different models. The Junction must be able to perform the necessary interpolations and treatments of the data from one model before passing them to the other adjacent model: (1) interpolation in space and time (time steps or mesh sizes are not identical), (2) aggregation and desaggregation of data (e.g. when a model handles nitrogen concentration as state variable and the others various derived forms as nitrate, ammoniac,...). The generalization introduced by the Junction compared to a generalized domain decomposition method is the fact that it must be able to connect (1) the Ocean, River and GM's, (2) each of these models at regional scale with sub-models at local scale and (3) two of more GM's each of them running with different contaminants. Figure 3 shows the situation when 2 different models are connected. We distinguish "Servers" as special subroutines dedicated to specific tasks as for example, I/O or integral functions (for balance studies). Each model has its own servers, so that each model performs the I/O operations as if it were alone. The exchange of informations is organised only in the region where they

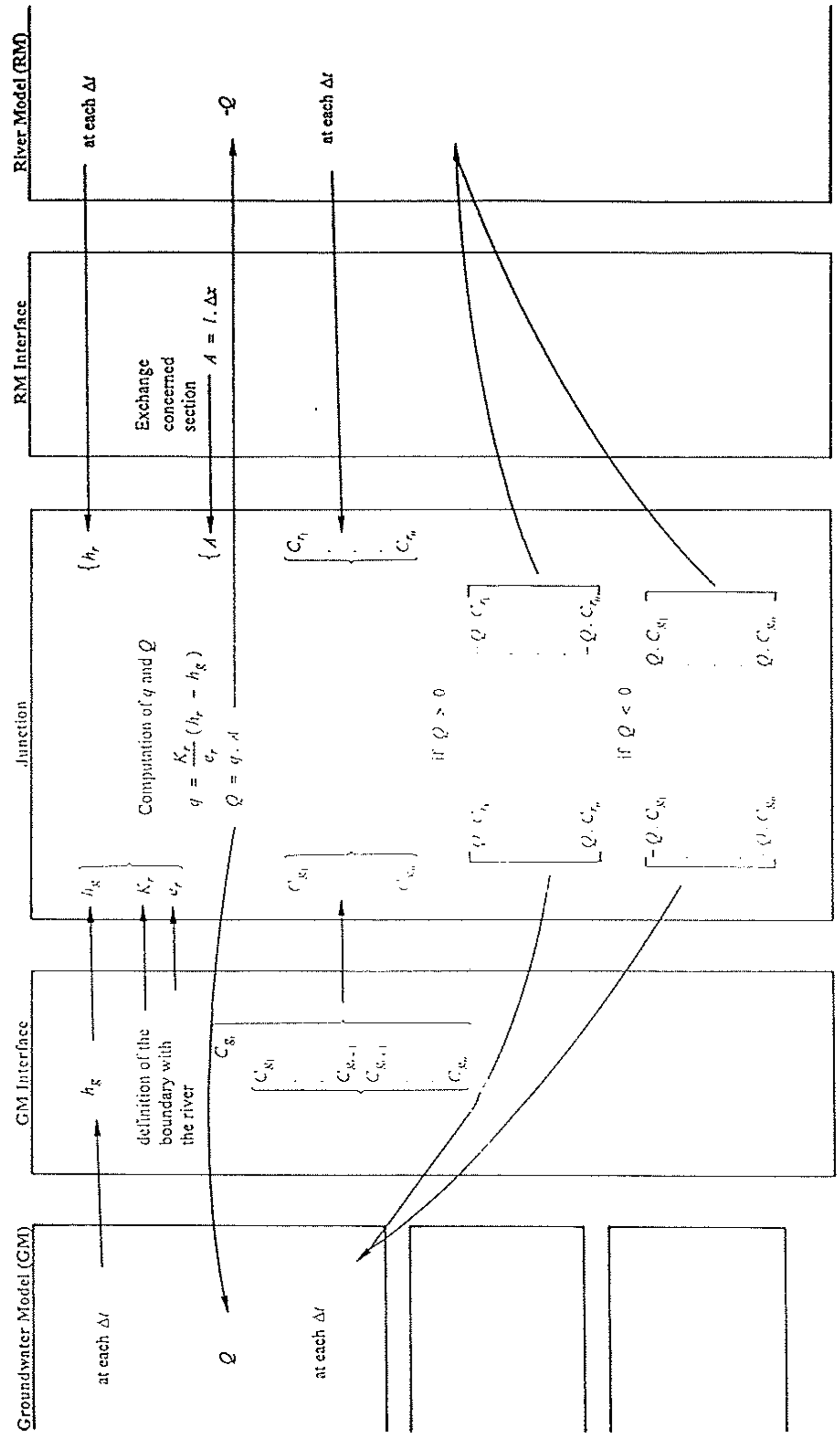

Figure 2: Conceptual schema of the information exchanges to be managed by the Junction between the Groundwater Model and the River Model.

are connected and only when it is required.The Junction is a task activated by the Meta-junction (figure 3) which is defined as a switch activating the tasks and sending the informations to allow the exchange of data with other tasks.

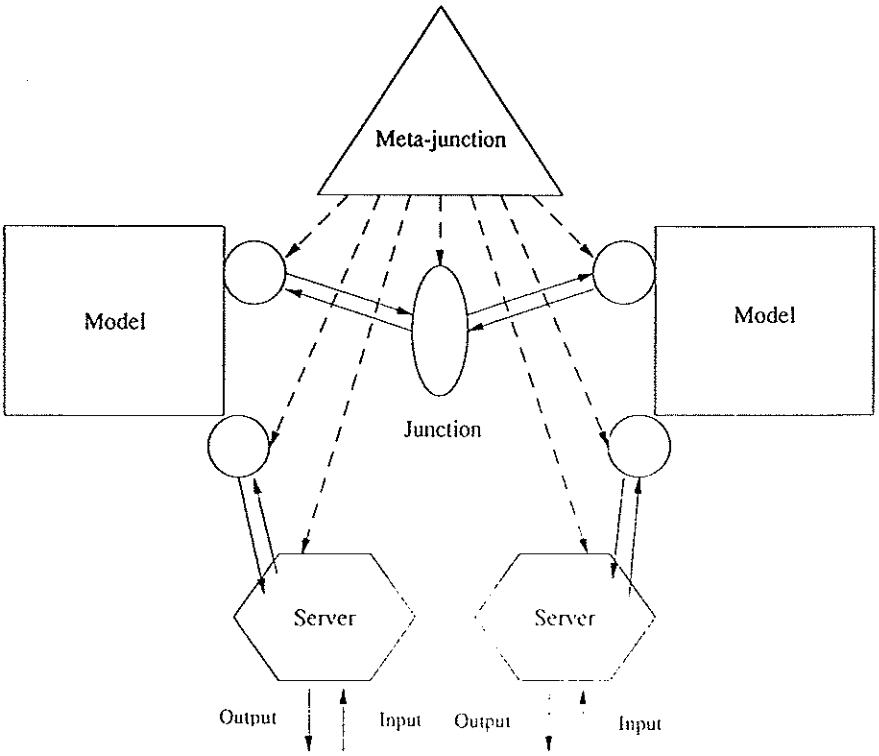

Figure 3: Running two connected models on a parallel machine. Each model has its own server. The Meta-junction creates and activates the Junction.

5 Time and space scale problems

At each time step, each model must send and receive the required information, but each model has its own time discretization. Strong differences are awaited in the chosen time steps from a model to another. The Junction must exchange informations with the different models at their own different time steps. It means time interpolations and organization of exchanges.

When a case study will be studied, problems will arise also with the choice of the spatial domain discretizations in each of the three models. For the OM, the usual scale of study makes possible that the model has a coastal boundary of few hundreds of kilometres. For the RM, it can represent also hundreds of kilometres in the inland direction. Consequently, the GM should cover a very large area including the whole river basin and the concerned coastal zones (i.e. more than 10000 km2)! At this scale, none of the groundwater simulation could be consistent due to spatial heterogeneity of the geological layers and the large number of required elements to solve numerically the transport equation in good conditions. If the parameters of the GM have to be taken at this scale, the study should be considered as only a theoretical exercise (for the groundwater aspect) and the results should be interpreted as so.

6 Conclusions: challenges for the future

At the end of Year I of the SALMON project, many difficulties and challenges have been identified and conceptually expressed in order to select the priorities for the good achievement of the project. Concerning the Groundwater Model exchanges with the River and Ocean Models the following priorities are selected: (1) testing the ability of the code to support large grids when treating the transport problem (using hybrid Eulerian-Lagrangian methods), (2) development of subdomains and Local Grid Refinement techniques with parallel processing, (3) develop the GM in the way to allow multi-component computations in parallel. During our future researches, other interactions between the Groundwater Models involving different solute contaminants could be studied and managed at the Junction level, taking into account the eventual chemical reactions between the different species.

Key-words: groundwater, ocean, river, interactions, parallel processing.

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References

1. Dassargues, A., 1994, Validation of a Finite Element code to simulate the coupled problem of salt transport in groundwater, Computer Techniques in Environmental Studies V, Proc. of ENVIROSOFT'94 San Francisco, vol.1, pp173-180, CMP.
2. Galeati, G., Gambolati, G. and Neuman, S.P., 1992, Coupled and partially coupled Eulerian-Lagrangian model of freshwater-seawater mixing, *Water Resources Research*, 28, 149-165.
3. Hassanizadeh, S.N. & Leijnse, T., 1988, On the modeling of brine transport in porous media, *Water Resources Research*, 24, 321-330.
4. Nawalany, M., 1994, Combining the analytical and finite element models of the river-groundwater interaction, Computational Methods in Water Resources X, vol. 1, pp. 83-90, Water Science and Technology Library, Kluwer Academic Publishers.
5. Beckers J.M. & Schmitz F., 1994, The Junction: a tool to parallelize ocean models by a domain decomposition, to connect different kind of models and to impose open boundary conditions, 7th SIAM Conference on Parallel Processing for Scientific Computing.
6. Vanderborght J.P., Smitz J., Everbecq E., Descy J.P., 1994, Pegase: un modèle de planification et de gestion de l'assainissement des eaux, Revue des Sciences de l'Eau, France.