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An integrated, multi-modelling approach for the assessment of water quality: lessons from the Pinios River case in Greece

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Abstract: Major factors influencing water quality along a river are land use practices, seasonal hydro-meteorological conditions, groundwater interactions and wastewater discharges. These complex water quantity and water quality aspects demand integrated solution approaches. The study links hydrologic, hydraulic and water quality models using the OpenMI standard to evaluate water quality in the Pinios River in Greece. OpenMI allows data to be exchanged at run time, between models from different providers, thus facilitating integrated modelling. The Pinios River was selected due to its high intensity of cultivation with water demanding crops. The objectives of the overall project, of which this study forms a part, were to assess water quality during extreme events and identify areas where any further pollution could be critical. A multi-modelling approach was utilized, where two separate integrated models were developed by two different research groups, each combining, using OpenMI, commercial and academic model components, thus creating a form of modelling ensemble. The assumptions and results are compared and critically discussed. The study's conclusions also address generic integrated modelling issues such as the benefit of bi-directional links and integrated model stability. They also identify challenges in model comparison, within a multi-modelling framework in view of differences in conceptualization, discretisation and solving schemes chosen by different researchers, which become apparent once the barriers for direct comparison are alleviated, with the use of approaches such as OpenMI.

Keywords: decision support; integrated modelling; multi-modelling; pollution; uncertainty; water quality

INTRODUCTION

The water environment in Europe (and overseas), faces increasing pressures from multiple facets of human activities, including water abstractions and wastewater generation from urban developments and agriculture. Current environmental legislation (of which the Water Framework Directive (2000/60/EC) is the more often quoted example), sets ever more stringent requirements for water quantity and quality objectives in water bodies, in the presence of natural variability and uncertainty. This trend necessitates the use of better tools (Gourbesville, 2008) able to capture the interactions between interventions, natural processes and environmental objectives. Such tools, modelling the environment (preferably) at the catchment scale, require data availability (due to the number of processes that need to be modelled), processing power (due to the complexity of individual models) and a way of seamless interaction between them (due to the requirement of interaction between models). This paradigm of focusing on process interactions through the coupling of multiple individual models, which has been known for some time as "integrated modelling" (Beven, 2007) is now moving even further away from large allencompassing models, towards a more model-component based approach (Argent, 2005) where each model is seen as a component of the integrative whole.

This approach also enables the exploration of the effect of changing model representations within the integrated model (or model ensemble) by swapping one model with another (Figure 1).

Such a capability presents multiple benefits:

- □ It facilitates the improvement of integrated models, whenever a better modelling component becomes available for some part of the system (something valuable to software developers (see Argent, 2005))
- □ It allows a direct comparison of the effect of different system conceptualisations on the uncertainty of the results (which is crucial in situations where the modelled system is highly complex e.g. in climate model ensembles (Fowler and Ekstrom, 2009) but also in complex water management problems (Makropoulos et al., 2008)). This approach is often termed multi-modelling (Stranger, 2000).
- □ It allows for a seamless switching between data sources, by changing modelling components that link the integrated model to specific databases (e.g. online data source, (Fotopoulos et al (in press)).
- □ It allows a harmonious, synergistic co-existence between model components from different developers (incl. for example commercial models and research prototypes)



Figure 1. A component-based multi-modelling approach

However, to allow for such a seamless (drag n drop) "swapping" of model components there is a need for modelling mechanisms (standards, frameworks etc (Argent, 2004)) that handle the (possibly bi-directional) data exchange between models, in runtime. In this work we used, one of the most promising technologies available for model linking: the OpenMI (Open Modelling Interface) Standard (Moore and Tindall, 2005). OpenMI is a software component interface definition for the computational core (the engine) of the hydrological and hydraulic models (Gregersen et al., 2007).

The OpenMI Standard dictates the way models can be linked to other models and exchange information in real (run) time (Gregersen et al., 2007) without using external files. In this way, integrated models can be created using OpenMI compliant models (or model components) from different providers, thus enabling the end-user to select those models that are best suited to a particular problem. OpenMI supports two-way links where the involved models mutually depend on results calculated by each other (Gregersen et al., 2007). Linked models may run asynchronously with respect to timesteps and data represented on different geometries (grids) can be exchanged seamlessly (Figure 2).

The paper compares two OpenMI integrated models (with a number of common components) developed by different research groups which were applied to the same case: a part of the Pinios River basin in Greece.



Figure 2. OpenMI configuration editor: linking variables to be exchanged between models

Both integrated models explore water quality issues and specifically the influence of diffused pollution sources on the river quality. First a description of the problem is included to facilitate the understanding of the approach. Then the methodology is explained, by focusing on the model ensembles and some results are presented and discussed. The main discussion of the paper is in the presentation of insights from the comparison between these integrated models and the role of OpenMI in enabling this comparison.

2. STATING THE PROBLEM

The Pinios River catchment is the Greek pilot basin for the Water Framework Directive. The catchment drains an area of approximately 10,500 km² and the area of interest in this study is the upper part of the river (until the Ali Efenti bridge) where hydrologic, hydraulic, and water quality are modelled to investigate source and impact of pollution (Figure 3). Agriculture is the main source of income for the Thessaly Water District and the Pinios catchment is intensively cultivated with water demanding crops. Most of the pollution in the area arises from non-point sources (including for example livestock, which is the most important source of BOD pollution in the area).



Figure 3. Thessaly and the Pinios River

The increased irrigation of the basin has seriously decreased groundwater levels and river flow. Additionally, the fertilizers and pesticides used for the agricultural activities resulted to water quality degradation. Furthermore, untreated industrial waste and municipal wastewater discharged into Pinios have added to the local water pollution issues. Illegal damping areas are flushed in the river during storm events. The aim of the study was to create a model of the hydrology (rainfall-runoff) and couple it with a river hydraulics model and a river water quality model so that sources and fate of pollutants in the catchment could be modelled as a basis for prioritising interventions and assessing their performance.



Figure 4. Two alternative integrated model representations for the same case

3. METHODOLOGY

To achieve the case study objectives and to investigate the validity of the perceived benefits of multi-model component-based representations, identified in the introduction, two alternative integrated model representations (Figure 4) set up by different research groups were used. The model components (ie. the individual process models) in each case were migrated into OpenMI and linked using the OpenMI configuration editor. The schematizations of the models (reach lengths, inflow nodes, pollution nodes) are shown in Figure 5. It is interesting to notice that Integrated Model 1 was designed to evaluate water quality along the whole length of Pinios river. However, the comparison study between the two integrated models was conducted at selected locations along the first 75 km of the main Pinios channel.

| 11 | NTEGRATE | MODEL | 1 | | | | INTEG | RATED | MODEL 2 |
|------------|--------------|-------------|-------|-------------|--|---|-----------------|----------------------|--------------------------------------|
| | 1 | 1 | . 1 | Tributarie | es & Pollution loads | | OTIS Node ID | Distance d/s (km) | Description / Node type |
| | 2 | | 1 | | Malakasiotiko | _ | ▶ 1 | 0 | Upstream node |
| | <u>_</u> | Ionas (Ga | vros) | | | | 2 | 6 | Auxiliary node |
| | /- | | | | lonas (Gavros) | _ | ► 3 | 6 | Major tributary node |
| | | | | | Mantania | | ♦ 4 | 8 | Tributary node |
| WWTPTRI03 | → 16 | | | | Mpatsa | | ► 5 | 12 | Tributary node |
| | | | 2 | | | | 6 | 15 | Auxiliary node |
| INDTRI008 | → 42 43 ◆ | Potraikos | | ww | (FPTRI03 (Kalampaka) | | 7 | 15 | Pollution node (WWTP) |
| DIDTDI006 | > 11 | | | | | | 8 | 19 | Node (Sarakina) |
| INDIRI006 | - 44 | | | | Bitoumitis | | ▶ 9 | 21 | Tributary node |
| | | | | | | | 10 | 24 | Node |
| INDTRI005 | → 48 | | | | | | 11 | 30 | Node |
| | | | 3 | | Palaiopotamos | | ▶ 12 | 34 | Tributary node |
| WWTPTRI01 | ▶ 51 | | | | | | 13 | 37 | Node |
| | 51.4 | Pamissos | | | | | 14 | 39 | Water Quality node (Fotada) |
| | 34 🔫 | | | | | | 15 | 41 | Auxiliary node |
| | | | | | Portaikos | _ | 16 | 41 | Major tributary nod |
| INDTRI004 | ► 56 | | 4 | | INDTRI008 (Dairy) | | | | Pollution node |
| | | Litheos | | | INDTRI006 (Tannery) | | 17 | 41 | (Industries) |
| | 73 🗲 | | | | | | 18 | 44 | Node |
| | | | 1 | | | | 19 | 47 | Auxiliary node |
| WWTPTRI02 | → 81 | | 5 | | Litheos1 | _ | ▶ 20 | 47 | Major tributary node |
| | 85 🗲 | Enippeas | | Untreated s | INDTRI005 (Dairy) ewage City of Trikala | | 21 | 47 | Pollution node (Industries & Sewa |
| | | Amygdalea | 6 1 | | | | | | Water Quality node |
| | 104 | _ | , | | | | 22 | 49 | (Karavoporo) |
| | | | 1 | | | | 23 | 52 | Node |
| INDLAR015 | → 141 | Almyros | 7 | | | | 24 | 53 | Auxiliary node |
| INDLAR008 | ▶ 142◀ | 1 | | | Pamissos | | 25 | 53 | Wates Quality and |
| WWTPLAR01 | → 143 | | | | | | 26 | 56 | (Gef Menala Kalva |
| | | 1 | | | Moistiria | | 20 ► 27 | 50 | Tributany node |
| DIDI AD021 | N 145 | | | | | | - 21 | 00 | Water Quality node |
| INDLAR021 | 145 | 1 | | | | | 28 | 63 | (Agnantero Piniou) |
| INDLAR018 | 140 | | | Me | egarema+Litheos2 - | | | | |
| | | | 8 | | WWTPTRI01 | | 29 | 71 | Tributary node |
| INDLAR020 | ▶ 151 | | | | | | 30 | 73 | Node |
| | | | | | | | 31 | 75 | Node |
| INDLAR019 | → 158 | | | | | | 32 | 77 | Ali Efenti bridge |
| | 1 | Titarissios | | | | | | | |
| | 169 | | | | | | | | |
| | | | 9 | | | | | | |
| | 212 | 1 | 2 | | | | | | |
| | 213 | | | | | | | | |

Figure 5. The two integrated model schematizations

3.1 Integrated Model #1

An integrated 1-D linked scheme was developed using the OpenMI standard to simulate hydrodynamics and water quality in rivers and streams. The integrated scheme consisted of the rainfall runoff NAM module of MIKE 11, the hydrodynamic model RISH-1D and the water quality model RISQ-1D (Figure 7a); the latter two models were developed in NTUA (Stamou and Douka, 2010). The MIKE 11 NAM module is a deterministic, conceptual and lumped rainfall-runoff model. The main inputs for the NAM module include precipitation and potential evaporation for each sub-catchment, as well as measured discharge for the calibration procedure (DHI, 2009). RISH-1D is based on Saint-Venant equations, which are discretized using the implicit weighted four-point Priessmann scheme and solved by the iterative method of Newton -Raphson. RISQ-1D consists of mass balance equations for the water quality variables of interest that are descritized using the second order accurate implicit Crank-Nicolson method and solved via the Thomas algorithm. RISH-1D and RISQ-1D were calibrated and validated for the total length of the Pinios River. The available field measurements, used in the computations, had a high level of uncertainty; moreover, there was also significant uncertainty in the estimation of pollution loads. Despite these limitations, the separate and linked model run successfully, simulating flow and water quality at selected locations during low (June 1998) and high (December 1998) flow conditions (Figure 6).



Figure 6. Calibration and validation of integrated model 1(June and December 1998)



Figure 7a. OpenMI Configuration for representation #1

Figure 7b. BOD values determined by separate and OpenMI-linked runs at two locations (nodes 101 and 146) along the Pinios River.

Figure 7b shows a comparison between BOD values, calculated by separate runs of each model component in configuration #1 and an OpenMI-integrated model of configuration #1. As an indication of a successful migration and physically meaningful model linking, in both nodes the values of the separate and linked configurations match well.

3.2 Integrated Model #2

In this model the hydraulic and water quality component were substituted with MIKE-11's hydraulic model and OTIS respectively. This configuration retains the NAM model (which

is part of MIKE11) as the rainfall runoff component (Figure 8). The MIKE11 hydrodynamic module (HD), which represents the core of MIKE11, uses an implicit, finite difference scheme for the computation of unsteady flows in rivers and estuaries. The computational method is based on the numerical solution of the St. Venant equations on the conservation of continuity and momentum. Main inputs for the HD model include cross-sectional information at various locations along the main river network, measured stage or discharge for model calibration, stage-discharge relationship, etc.

MIKE11 includes an advanced graphical user interface in order to facilitate data input and editing. Besides, generating stage and discharge for the points of the computational grid that represent the main model output, MIKE11 calculates additional outputs, including velocity and cross-sectional area. Discharge and cross-sectional area at selected locations are important inputs for the water quality model OTIS that utilised them for the calculation of BOD levels along the main river. The solute transport model OTIS (One-Dimensional Transport with Inflows and Storage) started being developed in the beginning of the 1990's by USGS (Runkel, 1998). OTIS simulates the fate and transport of water-borne solutes in streams and rivers. Specifically, OTIS calculates the solute concentrations that result from hydrologic transport and chemical transformation when providing the catchment loading. It is a one-dimensional model using the main assumption that pollutant concentration varies only in the longitudinal direction and not with width or depth. The model simulates various hydrologic and chemical processes including advection, dispersion, lateral inflow, transient storage, first-order decay and sorption using the advection-dispersion equation with additional terms to account for all the processes. All equations used within the model are solved numerically using a Crack-Nicolson finite-difference solution for each segment of the river. The model has the ability to simulate the fate and transport of both conservative and non-conservative pollutants (Runkel, 1998). Pollution loads from both point and nonpoint sources, flows and cross sectional area in the main river represent the main inputs for OTIS. Water quality measurements along the river are necessary for model calibration (Figure 9). At the end of the simulation OTIS generates the solute concentration at various selected locations along the modelled river and in the case of the particular application the concentration of BOD (Figure 10).



Figure 8. OpenMI Configuration for representation #2



Figure 9. Calibration and validation of integrated model #2 (October and December 1993)



Figure 10. BOD values determined from separate and OpenMI-linked simulation for a specific location.

It can be seen that the results of the individual models (run in sequence) match well with the results of the integrated model, exchanging data though OpenMI. As before this is an indicator of a successful migration and linking.

It should be noted however, that this is because the links established within this and the previous configuration, are one-directional. In the presence of bi-directional links, where data supplied by the "upstream" model are influenced by data provided by the "downstream" model, it is expected that differences would be observed between individual models (run in sequence) and the integrated model, without this being an implication of faulty migration and linking. On the contrary: provided that sufficiently detailed data sets are available to support model set up and calibration to capture (in some detail) interactions between different processes, the results of the integrated model would be expected to be more realistic, as this is exactly the type of problem that OpenMI enables to tackle.

4. RESULTS AND COMPARISON

The two integrated modelling configurations were developed by separate research teams to answer different water resources management questions and were therefore based on different assumptions and originally run for different time periods. To allow for a meaningful comparison, a common time period was selected (February 1998) to run both configurations. The same pollution loads were assumed for both configurations (for both diffused and point source) and the same BOD decay coefficient and dispersion coefficient were used in both RISQ-1D and OTIS. However, some assumptions remained different:

- □ The river schematisation used by OTIS does not match exactly the one used by RISH/RISQ. This results in a difference between the exact locations of the point sources which in turn affects BOD distribution along the river.
- □ Due to a simplifying assumption in OTIS, diffuse pollution loads enter only from the major four tributaries of Pinios with pollution loads from the smaller tributaries required to be added to these. This assumption however has an effect on the distribution of the BOD concentration along the river.
- □ The cross sections in the two configurations slightly varied in width along the main channel, with an average cross section width of 30 meters for all models. These (+/-3 meters) cross section variations along Pinios river improved the individual model calibrations and the stability of the linked runs. However, flow and stage changes fed in the water quality models (RISQ-1D and OTIS) inevitably varied in space and time.

Figure 11, below shows the results of both configurations at selected locations.



Figure 11. Comparative results of the two integrated model configurations at two locations

The two configurations were built with slightly different topographic characteristics, observed points, initial conditions and assumptions. Many of these differences were a direct result of individual model characteristics, strengths and limitations and the availability of segmented data sets. Furthermore, the input data discrepancies were enhanced by the different modelling techniques followed by different research groups. These variations are clearly depicted in the comparative modelling results presented for two river nodes (14 and 26) in Figure 11. At both locations, there is a significant lag between the BOD concentration peaks as well as between the BOD concentration valleys. It also appears that configuration #1 overestimates, while configuration #2 underestimates BOD concentrations at every location. This difference increases as we move downstream.

It is suggested that this variation is in effect a measure of the uncertainty related to this multi-model simulation. The visualisation of this (significant) uncertainty may be very important for decision making, including, but not restricted to, the identification of the required level of water treatment for local communities. If water at node 26, for example, was used for recreational purposes, that would necessitate a BOD<4 mg/l. This threshold, however, is in the middle of the uncertainty band produced by the multi-modelling approach – while each integrated model on its own would produce a more definitive (and perhaps misleadingly authoritative) answer.

5. CONCLUSIONS

The OpenMI standard was successfully used to link rainfall-runoff, hydraulic and water quality models, as components of an integrated model for the Pinios River catchment. Two alternative configurations of an integrated model were developed, by two different research groups, by substituting modelling components (ie. in this case whole domain models). Three models (RISH-1D, RISQ-1D, OTIS) developed by different providers (two separate research teams at NTUA and the OTIS developers in the USGS) were successfully migrated to OpenMI. An additional, commercial model (MIKE-11) which was already OpenMI compatible was used, albeit in different roles, in both configurations. The individual models were set up, calibrated and validated in the study area. The individual and OpenMI linked model runs matched well in both configurations, proving that linking models in OpenMI does not compromise the accuracy of model runs.

The comparative analysis of the two configurations illustrated the significant differences between model components and (consequently) modelling results, even when OpenMI is used as the integrating medium and model schemes are set up for the same study area by collaborating modelling teams. The comparison also introduces a series of questions regarding the extent to which alternative modelling configurations (or members of a multi-modelling ensemble) can be "objectively" compared to each other.

Comparisons between models are nothing new, and have been traditionally based on such criteria as computational speed (e.g. Ji et al., 1996), ease of model use (Saloranta et al., 2003), accurate forecasting of analytical solutions (Rossman and Boulos, 1996) or observed values (Habets et al., 2010) to name a few. However, all these metrics, with the possible exception of the last two, are significantly biased by the expertise of the modeller,

who more often than not is the developer of one of the models and the (reluctant) user of the other. The last two comparisons are unfortunately often difficult to perform, in exactly these situations where it is most needed: either in complex problems where analytical solutions are not possible or where field observations are scarce and modelling results are required exactly to substitute them. The ease with which alternative configurations of integrated models can be build using OpenMI however, change this picture, by often putting real end-users (as opposed to model developers) in the position to setup, run and ultimately assess these configurations.

We suggest that although by carefully selecting parameter values and identifying equivalent schematisations, models do become more comparable, this may not be a very productive exercise, as significant difference will inevitably remain. Perhaps a more productive way of working, would be to exploit these different assumptions, schematisations and parameterisations (assuming of course they are all well developed and supported by the evidence (Beck, 2002)) and use the ensemble of results to analyse, assess and visualise the underlying uncertainty (Potempski and Galmarini, 2009).

It could be argued that such an approach is becoming increasingly feasible through the use of OpenMI and coupled with techniques such as Evidence Theory (Bicik et al., 2009) could open new avenues of investigation on issues of epistemic uncertainty that have been lying "under the surface" of much of the modelling endeavour.

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