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Integrating water quality models in the High Level Architecture (HLA) environment

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Abstract. HLA (High Level Architecture) is a computer architecture for constructing distributed simulations. It facilitates interoperability among different simulations and simulation types and promotes reuse of simulation software modules. The core of the HLA is the Run-Time Infrastructure (RTI) that provides services to start and stop a simulation execution, to transfer data between interoperating simulations, to control the amount and routing of data that is passed, and to co-ordinate the passage of simulated time among the simulations. The authors are not aware of any HLA applications in the field of water resources management. The development of such a system is underway at the UFZ –Centre for Environmental Research, Germany, in which the simulations of a hydrodynamic model (DYNHYD), eutrophication model (EUTRO) and sediment and micro-pollutant transport model (TOXI) are interlinked and co-ordinated by the HLA RTI environment. This configuration enables extensions such as (i) "cross-model" uncertainty analysis with Monte Carlo Analysis: time synchronisation allows EUTRO and TOXI simulations to be made after each successive simulation time step in DYNHYD, (ii) information transfer from EUTRO to TOXI to compute organic carbon fractions of particulate matter in TOXI, (iii) information transfer from TOXI to EUTRO to compute extinction coefficients in EUTRO and (iv) feedback from water quality simulations to the hydrodynamic modeling.

1 Introduction

This paper conceptualizes the integration of computer models used to simulate river water quality in the High Level Architecture (HLA) platform. There has been an impetus to configure models into modeling systems due to the integrative and more holistic approach science has taken to tackle environmental management problems. This is particularly the case for the management of large river basins (e.g. European Water Framework Directive [2000/60/EC]).

HLA is a program specifically developed for the coupling of models into one system (see Fig. 1). The models are represented as Federates (stand-alone computer programs) to and from which information is communicated by the Run Time Infrastructure (RTI), which is the core of the HLA. It provides services to start and stop a simulation execution, transfer data between interoperating simulations, control the amount and routing of data that is passed and co-ordinate the passage of simulated time among the simulations (Kuhl et al., 1999). One particular strength of the RTI is its ability of sequencing command inter-communication amongst the Federates in a very efficient manner. An additional advantage is its ease of communication of Federates on different computer systems via a network.

HLA has been used for a number of applications such as:

- communication and synchronisation media for modelling of hybrid systems (e.g. water level control in a two tank system) (Borshchev et al., 2002),
- modelling and simulation of processes associated with software system acquisition activities which concerns the funding, management, engineering, system integration, deployment and long-term support of large software systems (Choi and Scacchi, 2001),
- developing multi-agent systems for applications in mobile robotics (Das and Reyes, 2002),
- providing online/real-time location information of streetcars of the public transportation company in Magdeburg, Germany (Klein, 2000),
- traffic reduction schemes based on space-based quantization (Lee and Zeigler, 2002),
- designing simulation environments for human training (esp. military personnel) (Maamar, 2003).

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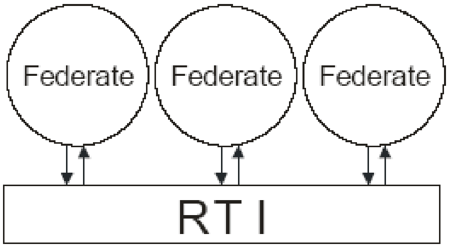

Fig. 1. The HLA environment (adapted from Petty, 2002).

The authors are unaware of any applications in water quality simulation. A project has been initiated in Germany to develop a flood forecasting system integrating a hydrological model, GIS (Geographical Information System) and up-to-date rainfall data (Schulze et al., 2002) but the project is still in its infancy.

In this paper the Water Quality Simulation Program version 5 (WASP5) is used to illustrate the capabilities gained in the simulation process by integrating its submodels into a HLA federation. The submodels include the hydrodynamics (DYNHYD), eutrophication (EUTRO) and sediment and micro-pollutant transport (TOXI) of surface waters. The HLA implementation induces better interactive transfer of information between the submodels to extend predictive ability and uncertainty analyses. The paper concludes with a comparison of the HLA method with conventional model coupling and object-oriented approaches.

2 Modelling methods

The WASP5 modeling system (Ambrose et al., 1993) is used to simulate the hydrodynamics, water quality and transport of sediment and micro-pollutants in a river. It is a conglomeration of three models (see Fig. 2):

1. DYNHYD – uses the St. Venant equation (full dynamic wave) to calculate the flow of water through a water body. With the volume continuity equation and Mannings equation of flow through a channel, mean interfacial flows $\overline{Q}$, water volumes V, mean current velocity $\overline{v}$ and mean water depth $\overline{d}$ of each discretized unit can be simulated dynamically. These variables are transferred as input to the two models, EUTRO and TOXI, described next:

2. EUTRO – simulates the transport and transformation of variables important in describing the eutrophication processes (high productivity) in surface waters. Oxygen plays a central role in the system and is balanced between sources (production through photosynthesis by phytoplankton growth and re-aeration from the atmosphere via the water surface) and sinks (oxygen demand by organic matter and bottom sediments; respiration; nitrification). The dynamics of nutrients (phosphorus and nitrogen) complement the phytoplankton growth.

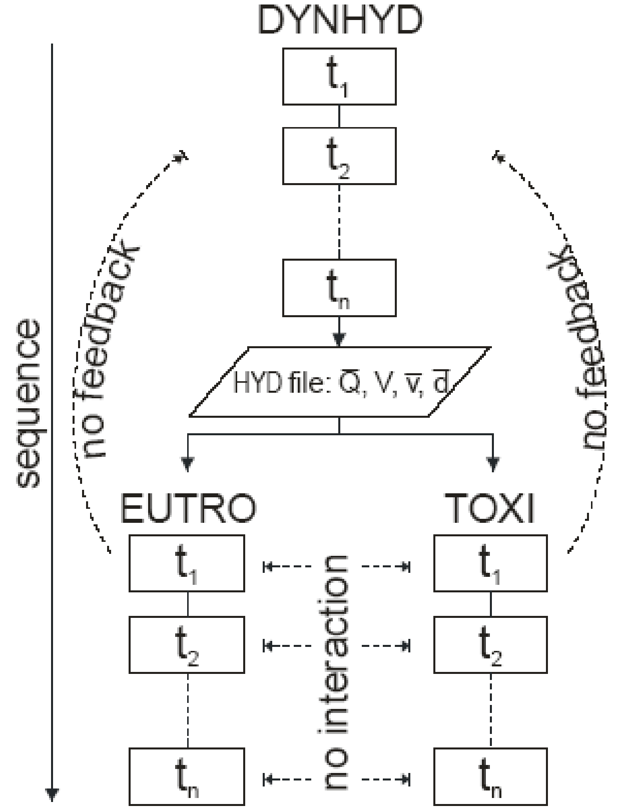

Fig. 2. Sequence of submodel simulations in the original WASP5.

3. TOXI – simulates the transport of sediments and micro-pollutants. Transport processes induce advection, dispersion and sedimentation and resuspension of particulate matter to and from the bottom sediments and diffusion of dissolved matter between the water body and bottom sediments. These substances may also undergo transformations such as equilibrium sorption, volatilization, ionization, photolysis, hydrolysis and biodegradation.

The sequence of simulation flow is illustrated in Fig. 2. The hydrodynamic simulation must be completed first to generate interfacial flows, water volumes, mean velocities and mean depths of each discretized unit. These variables are stored in a hydrodynamic file (*.hyd) for subsequent input to EUTRO and TOXI.

In its original version, no interaction occurs between EUTRO and TOXI and feedback from these two models to DYNHYD is also not possible. More flexibility is obtained when these models are coupled together in the HLA platform as shown in Fig. 3. Since the RTI is programmed in the C++ language and the three WASP5 models in Fortran, a wrapper needs to be integrated into each model to allow calls to be made to and from the models by the RTI.

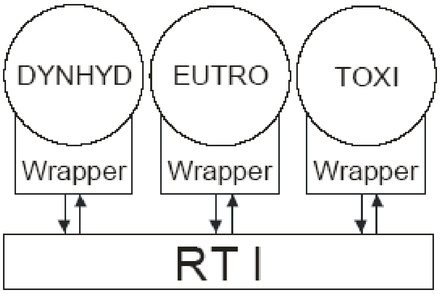

Fig. 3. Implementation of the WASP5 submodels DYNHYD, EUTRO and TOXI in HLA.

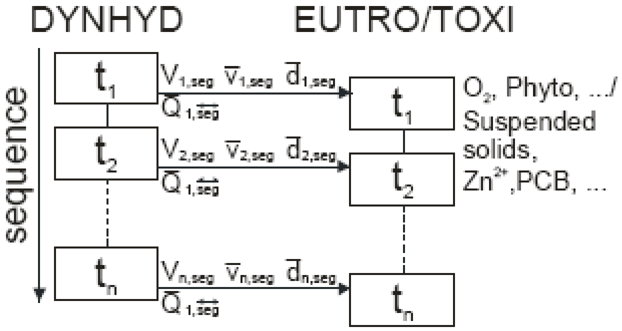

Fig. 4. WASP5 submodel simulation sequence in HLA.

3 HLA implementation

An initial configuration of the simulation sequencing in the HLA environment is shown in Fig. 4. Storage of the hydrodynamic variables is avoided and can be passed after each time step directly to EUTRO and TOXI. All three models can now be run simultaneously and the simulation time steps are synchronized by the RTI. Hence, for example, the simulation of EUTRO and TOXI at time step 2 (t_2) occurs as soon as the t_2 simulation of DYNHYD is completed. DYNHYD than immediately begins simulation of its time step 3 (t_3) while EUTRO and TOXI are computing their t_2. There is a saving in computation time when the three models are networked together and run in parallel on three different processors or on a multi processor computer. Also, Intels® Hyperthreading expedites the simulations.

3.1 Monte-Carlo uncertainty analysis

An important advantage of such a configuration is the extensive capabilities it provides for Monte-Carlo uncertainty analysis. The effect of certain variations of change in the parameter values (e.g. Fig. 5a and b) in DYNHYD on the variables in EUTRO and TOXI can now be explored. Up to 10 000 runs of the same simulation are carried out, in which a different parameter setting is chosen for each run. The DYNHYD parameters are randomly selected from a probability distribution of its values. This evokes a distribution of the EUTRO and TOXI variables (e.g. oxygen O_2 and suspended sediments *SS*), from which the contribution of uncertainty of each parameter on the water quality description can be made. In the conventional simulation sequence (Fig. 2) only an uncertainty analysis of the parameters on the variables of the same model could be made (see for example Lindenschmidt et al., 2003; Lindenschmidt et al., 2004a). With the HLA implementation, "cross-model" uncertainty analyses were made possible (Lindenschmidt et al., 2004b and 2004c).

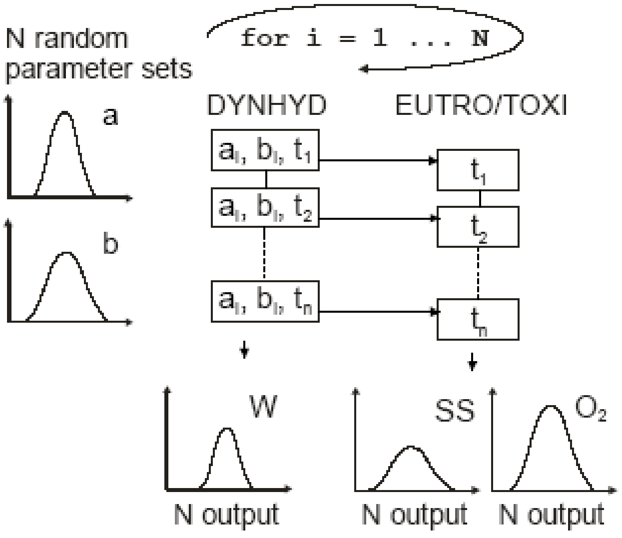

Fig. 5. Monte-Carlo analysis of the WASP5 federation.

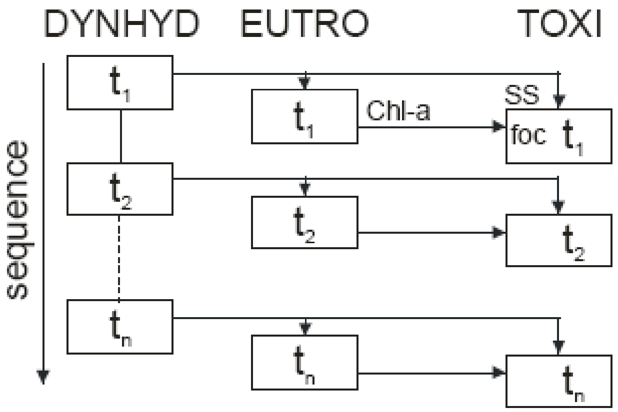

Fig. 6. Flow of information from EUTRO to TOXI to calculate *foc*.

3.2 EUTRO to TOXI interactions

Coupling EUTRO and TOXI together in the HLA environment allows ease of communication between the two models. Figure 6 shows an example of data transfer from EUTRO to TOXI.

The concentration of chlorophyll-a (*Chl-a*) is a variable in EUTRO which, in many cases, correlates well with the particulate organic carbon (*POC*) content in the water. By dividing *POC* with the concentration of suspended sediment

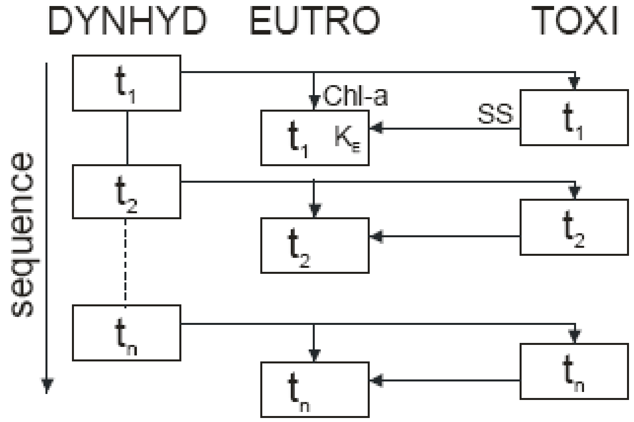

Fig. 7. Flow of information from TOXI to EUTRO to calculate K_E.

(SS) simulated in TOXI, the weight fraction of organic carbon in suspended matter (foc) is obtained (Ambrose et al., 1993; Chapra, 1997):

$$foc = \frac{POS}{SS} \tag{1}$$

The partitioning of heavy metals M in the water can now occur between the dissolved phase M_{DIS} and the organic carbon of the particulate phase M_{OC} using the partition coefficient K_{OC}

$$K_{oc} = \frac{K_D}{foc} \tag{2}$$

This is an extension of the simplified partitioning of heavy metals between the dissolved and total particulate fractions of heavy metals (M_{DIS} and M_{PART}) using the partition coefficient K_D:

$$M_{DIS} = \frac{1}{1 + K_D \cdot SS} \tag{3}$$

$$M_{PART} = \frac{K_D \cdot SS}{1 + K_D \cdot SS} \tag{4}$$

where SS is the concentration of suspended solids.

3.3 TOXI to EUTRO interactions

The transfer of information from TOXI to EUTRO is shown conceptually in Fig. 7. In the original WASP5 version, the extinction coefficient K_E of light passing through the water column is a constant parameter implemented for each discretized unit of the modelled river. With the communication between TOXI and EUTRO, K_E can now vary depending on the chlorophyll-a concentrations *Chl-a* (μg/l) and phytoplankton biomass *Phyto* (mg/l) computed in EUTRO and the suspended solids *SS* (mg/l) calculated in TOXI (equation modified from Schöl et al., 2002):

$$K_E = 0.052 \cdot (SS - Phyto) + 0.013 \cdot Chla + 1.06 \tag{5}$$

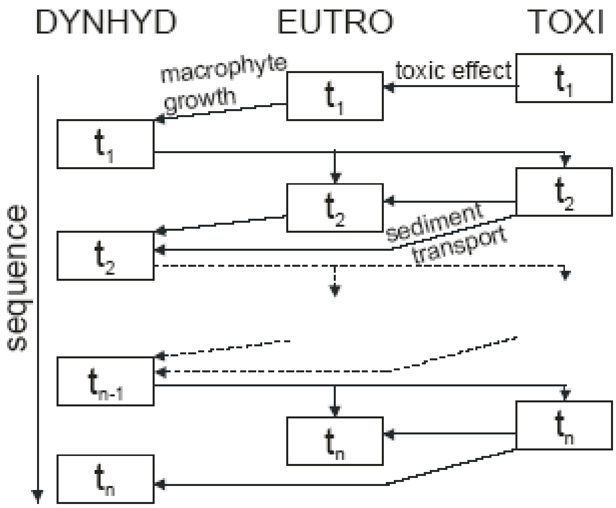

Fig. 8. Feedback from EUTRO and TOXI to DYNHYD.

3.4 EUTRO/TOXI feedback to DYNHYD

An extension of the WASP5 model by Shanahan (2001) includes the variable macrophytes. This allows interacting feedback constructs from EUTRO and TOXI to DYNHYD, shown in Fig. 8. Water bodies laden with many submerged plants may alter the hydrodynamics of the water course. High concentrations of particular micro-pollutants may inhibit the growth of phytoplankton and macrophytes. Alternatively, areas of greater or less sediment deposition may also influence the water flows and velocities, especially for shallow water bodies.

4 Discussion: model couplin

Figure 9 shows a comparative exercise between three different model coupling variants:

1. conventional – models are loosely coupled, in that information is transferred from one model to another by file storage and retrieval. Additional programming in the model source codes is not necessary. Sequence control is managed by batch files or an external program.

2. object oriented – in the open source project Object Modeling System (OMS) (David, 1997; http://oms.ars.usda.gov/; Hesser and Kralisch, 2003) models are refracted to single processes and only called when required for simulating a particular modeling exercise. The processes act on single represented objects called entities. A central kernel controls iteration in time and space and the data exchange is realised by global variables without the aid of buffer storage files. The time required for integrating new components is low but is extensive for the development of the entire system. Flexibility in the configuration of the modeling exercise is high.

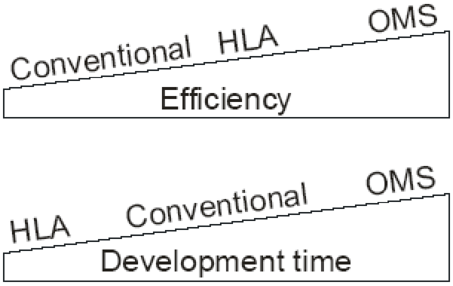

Fig. 9. Pros and cons of three model coupling approaches: conventional, HLA and OMS.

3. coupling platform (HLA) – entire models are easily and rapidly integrated into the simulation environment, but efficiency may be compromised since the execution of service and support routines that are similar in several coupled models need to be repeated. Programming in the source code is required to include RTI functionality, which eliminates the need for buffer storage of data for model interaction.

In order to obtain all the advantages of both OMS and HLA environments, a HLA component may be integrated into OMS to allow communication between the RTI and OMS (see Fig. 10). This HLA component would provide the necessary docking station for quick and easy testing of the models performance and capabilities. It also provides a means of coupling modelling systems that are being developed in parallel.

5 Software

The HLA software runs on a PC under Windows 95/98/NT/2000/XP and versions have been compiled for UNIX and LINUX environments. More information can be obtained from https://www.dmso.mil/public/transition/hlaandhttp://www.pitch.se/.

6 Conclusions

- The HLA platform provides a simple and fast way of coupling models together in a simple modeling system.
- Additional capabilities are extracted from modeling systems with several submodels, such as “cross-model” uncertainty analysis and submodel interaction and feedbacks.
- The RTI of a modeling system may serve as a docking mechanism to other modeling systems (such as OMS).

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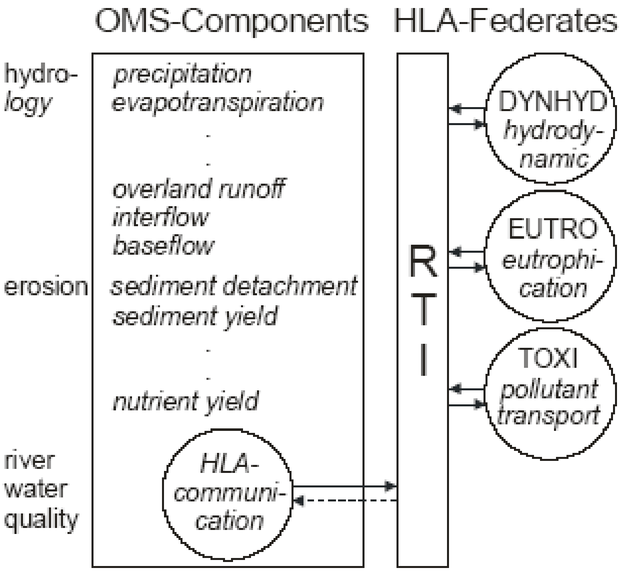

Fig. 10. HLA docking port in OMS.

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