



## An adaptive mesh solute transport model

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## An Adaptive Mesh Solute Transport Model,

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### Abstract

An adaptive mesh solute transport model is presented. The adaptive mesh scheme is implemented in a one-way multiply nested version of the hydrobiological model DIVAST (Depth Integrated Velocity and Solute Transport). The scheme allows the inner meshes of finer resolution to follow physical features such as solute plumes, thereby minimising the fine resolution coverage and thus the computational cost. If a physical feature moves during the course of a simulation, the fine resolution meshes move with it. Mesh movement can be either specified or automatic. The model was tested using a model of Galway Bay to simulate the discharge of a conservative tracer from a wastewater treatment plant. Results show that the model is capable of predicting solute transport to a high degree of accuracy and that adaptive meshing provides an efficient alternative to the classical zoom nesting techniques.

**Keywords:** adaptive mesh, one-way nested model, solute transport, DIVAST

## 1 Introduction

One of the main aims of the hydrobiological modeller is the optimisation of computational cost. This is particularly important as numerical models become increasingly complex, simulating an increasing number of physical, chemical and biological parameters, and thus requiring greater computational effort. Methods of reducing computational cost while maintaining model accuracy are therefore highly valued.

Horizontal resolution is one of the main determinants of the computational cost of a modelling project; higher resolution gives greater accuracy at a higher computational cost, lower resolution gives less accuracy but at a substantially lower computational cost. The trade-off between horizontal resolution, accuracy and computational effort is one of the great dilemmas of the numerical modeller.

Classical zoom nesting techniques (see Spall and Holland [1], Fox and Maskell [2], Barth, et al. [3]) can significantly reduce the computational effort required to model a specific phenomena. An inherent problem with static structured grids used in many hydrobiological models is that the computational cost is not optimal. Open boundary requirements usually mean that the area(s) of interest often comprise only a small percentage of the structured grid domain. In order to resolve detailed features within the fixed grid geometry it is necessary to increase the resolution across the whole domain, thereby significantly increasing computational effort. Nested grids provide high resolutions only in the areas of interest, thus significantly reducing the computational cost; however, the locations where high resolution is provided are dependent on the modeller's experience and perception. Further, like the regular grid, the grid structure remains unchanged during the simulation and it remains difficult to resolve features within the fixed grid geometry. In the current approach an adaptive mesh model has been developed allowing nested, fine-grid meshes to be generated throughout the parent coarse model domain. This type of model allows grid structure to change during the simulation making it easier to resolve features within the area of interest as the grid geometry is no longer fixed. This capability can lead to further significant reductions in computational cost compared to the classical zoom nested model.

The Authors have developed an adaptive mesh, multiply nested model capable of simulating hydrodynamics and solute transport. It is based on the hydrobiological model DIVAST (Depth Integrated Velocity and Solute Transport), a depth integrated, time-variant model capable of simulating two-dimensional distributions of currents, water surface elevations and water quality constituents (see Falconer, et al. [4]). The model is of the one-way nested variety and provides two methods of facilitating dynamically moving nests during the model simulation: user-specified and automatic. The paper gives details of the nesting procedure and the implementation of the adaptive mesh scheme. The performance of the model was tested using a model of Galway Bay, a large bay on the west coast of Ireland. The discharge of a conservative tracer from the wastewater treatment plant at Mutton Island was simulated and the results of the nested model were compared with those from coarse and fine resolution models of the Bay. The adaptive mesh model was found to accurately predict the solute transport and gave significant cost savings over the traditional static grid models. A selection of model results are presented and discussed.

## **2 Model Details**

### **2.1 Governing Equations**

The governing differential equations used by the model to determine the water surface elevation and depth-integrated velocity fields in a horizontal plane are based on integrating the three-dimensional Navier-Stokes equations over the water depth. This results in a two-dimensional model which resolves variables in two mutually

perpendicular horizontal directions ( $x$  and  $y$ ). The depth-integrated continuity and  $x$ -direction momentum equations can be shown to be given by equations (1) and (2) respectively [4]:

$$\frac{\partial \zeta}{\partial t} + \frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} = 0 \quad (1)$$

$$\frac{\partial q_x}{\partial t} + \beta \left[ \frac{\partial U q_x}{\partial x} + \frac{\partial V q_y}{\partial y} \right] = \quad (2)$$

$$f q_y - gH \frac{\partial \zeta}{\partial x} + \frac{\tau_{xw}}{\rho} + \frac{\tau_{xb}}{\rho} + 2 \frac{\partial}{\partial x} \left[ \varepsilon H \frac{\partial U}{\partial x} \right] + \frac{\partial}{\partial y} \left[ \varepsilon H \left[ \frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right] \right]$$

where,  $\zeta$  = water surface elevation above mean water level  
 $t$  = time  
 $q_x, q_y$  = depth-integrated velocity flux components in the  $x, y$  directions  
 $\beta$  = momentum correction factor  
 $U, V$  = depth-integrated velocity components in the  $x, y$  directions  
 $f$  = Coriolis parameter  
 $g$  = gravitational acceleration  
 $H$  = total depth of water column  
 $\tau_{xw}$  = surface wind shear stress components in the  $x$  direction  
 $\tau_{xb}$  = bed shear stress component in the  $x$  direction  
 $\rho$  = fluid density  
 $\varepsilon$  = depth averaged turbulent eddy viscosity

Solute transport processes are incorporated into the model using the 2D, depth-integrated advective-diffusion equation [4]:

$$\frac{\partial H\phi}{\partial t} + \left[ \frac{\partial HU\phi}{\partial x} + \frac{\partial HV\phi}{\partial y} \right] - \frac{\partial}{\partial x} \left[ HD_{xx} \frac{\partial \phi}{\partial x} + HD_{xy} \frac{\partial \phi}{\partial y} \right] \quad (3)$$

$$- \frac{\partial}{\partial y} \left[ HD_{yx} \frac{\partial \phi}{\partial x} + HD_{yy} \frac{\partial \phi}{\partial y} \right] - H[S_o + S_d + S_k] = 0$$

where,  $\phi$  = solute concentration  
 $[D_{xx}, D_{xy}, D_{yx}, D_{yy}]$  = depth-integrated dispersion-diffusion coefficients in the horizontal planes  
 $S_o$  = source or sink input  
 $S_d$  = first order decay rate or growth rate of the solute  
 $S_k$  = total kinetic transportation rate

The finite difference scheme used in the model is based upon the Alternating Direction Implicit (ADI) technique which involves the sub-division of each timestep

into two half-timesteps. A space-staggered orthogonal grid system is used where water elevation and solute concentration are specified at the centre of the grid cell and velocity components,  $U$  and  $V$ , specified at the centre of the cell sides. Water depths are also specified at the centre of the cell sides.

### 3 Adaptive Mesh Nested Model

The adaptive mesh model is a one-way nested model. In a one-way nest, the fine grid boundary conditions are interpolated from the coarser grid. This is the only information exchange (from coarse to fine) and interaction between grids is therefore only one-way. In a two-way nested model the fine grid solution replaces the coarse grid solution at each timestep giving two-way interaction. Two-way nested models are necessarily more complex and computationally expensive and a one-way nesting approach was deemed best for this research.

#### 3.1 The Nested Model

The nested model allows finer spatial resolution to be focused over a region of interest by introducing an additional grid (or grids) into the simulation. A simulation therefore involves one outer grid which contains one or more inner nested grids. Each nested region is entirely contained within a single coarser grid, referred to as the *parent* grid. The finer, nested grids are referred to as *child* grids. The nested grids are rectangular and are aligned with the parent grid within which they are nested. The open boundary conditions for each child grid are obtained from its parent. The nested grids allow any integer spatial ( $\Delta x_{coarse}/\Delta x_{fine}$ ) and temporal refinements of the parent grid (the spatial and temporal refinements are usually, but not necessarily the same).

The model allows multiple levels of nesting, in which case children are also parents. The fine grids may be telescoped to any depth (i.e., a parent grid may contain one or more child grids, each of which in turn may successively contain one or more child grids) and several fine grids may share the same parent at the same level of nesting. Figure 1 shows an example of the grid structure for a multiply nested model. The nested model is effectively a number of models running concurrently where each model operates on the set of grids at a particular level of nesting. The adaptive meshing scheme means that any valid fine grid may either be a static domain or a moving nest. Overlapping nested grids, where a coarse grid point is contained in more than a single child grid (i.e. both of which are at the same nest level as the parent), are not permitted for solute transport simulations; however, they *are* permitted when hydrodynamics alone are simulated. In addition, no grid can have more than a single parent, i.e. no child grid can cross its parent's open boundaries.

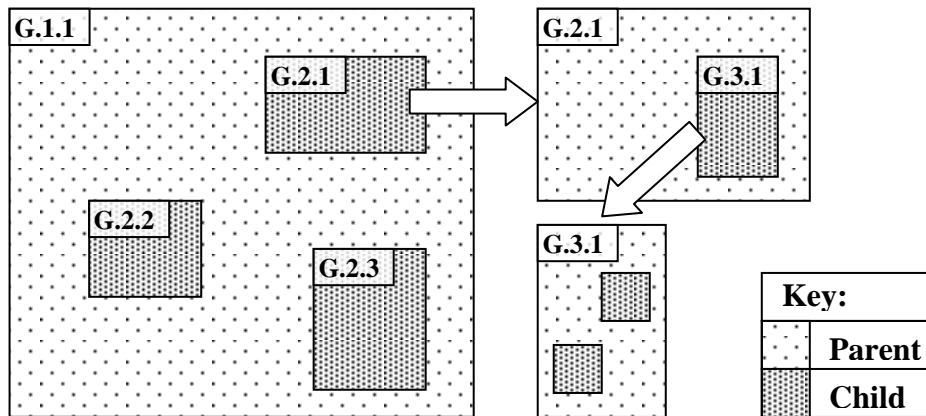


Figure 1: Nested model grid structure for multiple nesting.

### 3.2 Model Grids

DIVAST uses a space-staggered grid system as shown in Figure 2. Water surface elevation and solute concentration are discretised at the centre of each grid cell while water depth and normal velocity and flux components are specified at the centre of each cell interface.

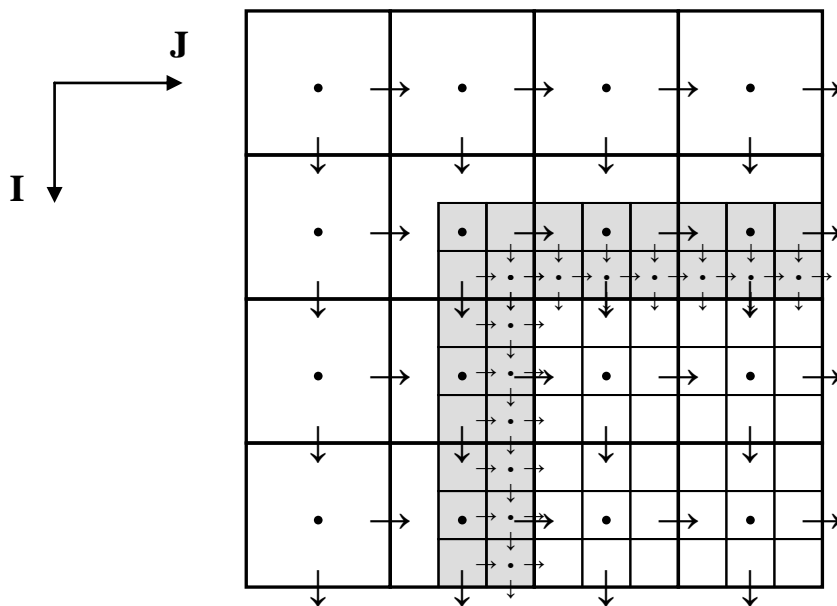


Figure 2: The relative position of the coarse (heavy lines) and fine grid (fine lines) and the halo layer (shaded). • show the position of elevations, → the J-direction velocity and flux components and depths and ↓ the I-direction velocity and flux components and depths. The large symbols are associated to the coarse grid and the small symbols to the fine grid. For clarity, only the positions of the variables imposed by boundary conditions are shown for the fine grid.

The implementation of the nesting procedure in the model allows the specification of any integer grid ratio ( $\Delta x_{coarse}/\Delta x_{fine}$ ). However, an odd grid ratio is preferable as it ensures that each grid value of the overlapping region of a parent grid coincides with a value from its child grid. A schematic of a nested grid using a 3:1 grid ratio is shown in Figure 2.

The interface between a parent and child grid consists of a halo layer, two fine grid cells in width; this constitutes the nested grid boundary. The nested open boundaries are driven by water elevations and current velocities obtained from interpolation of parent grid data. For the inner cells of the halo layer, elevations and velocities (both normal and tangential to the boundary) are required. For the outer cells, tangential velocities alone are required (see Figure 2).

### 3.3 Adaptive Mesh Scheme

The adaptive mesh scheme allows for any nested domain to move anywhere within the boundaries of its parent domain. All of the specifics described for the fine grid domains in the previous sections apply also to moving nests. In general, all nests are eligible to be moving nests and the user must specify whether a nested grid is to be static or dynamic. The model provides two methods of facilitating dynamically moving nests during the model simulation: specified and automatic. For a specified move, the timing of a nest move and the extent of the lateral move is defined entirely by the user. For the automatically moving nest, the fine grid is initialized to cover a particular feature, such as a solute plume, and the nest then intelligently moves to maintain the plume within its boundaries according to some predetermined rule. Enabling a nested grid to follow the movement of a feature of interest in such an intelligent manner ensures that the total area of domain where high resolution is required is kept to a minimum, thus optimising the computational cost.

Adaptive meshing is facilitated in the following manner. At the end of a parent grid timestep the model must check if any dynamic child grids require a move. If so the grid is moved to the new location depending on user specifications or a predetermined rule. After a nested domain has moved, the majority of the data in the domain is still valid. The data that is valid is shifted with the domain; the invalid data is discarded. As a result of the move, some of the grid cells in the moving child domain will have no data; these data are obtained from interpolation of the parent grid data. The model then proceeds as normal.

### 3.4 Nesting Procedure

Although the model allows multiple levels of nesting, the nesting procedure is explained for clarity in the case of a single moving nest. For multiple nesting, the procedure described holds for every pair of parent and child grids. The procedure is presented in graphical form in Figure 3; it can be summarised as follows:

1. integrate parent grid one timestep ( $t+\Delta t_c$ )
2. interpolate (time-wise) required parent grid data to current timestep of child grid ( $t$ )
3. spatially interpolate child grid open boundary data from parent grid data at current timestep of child grid ( $t$ )
4. integrate child grid one timestep ( $t+\Delta t_f$ )
5. repeat Steps 2  $\rightarrow$  4 to current timestep of parent grid ( $t+\Delta t_c$ )
6. check if child grid must be moved
  - if yes: move grid and interpolate from parent to child for missing data
  - if no: proceed to Step 7
7. return to Step 1 and continue

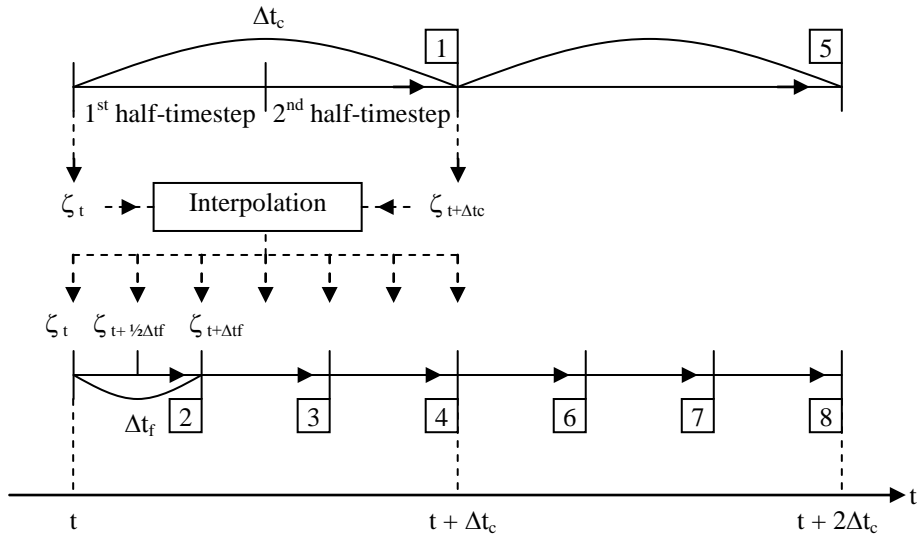


Figure 3: The nesting procedure. The subscripts  $c$  and  $f$  signify coarse and fine grids. For clarity, the only variable shown is water surface elevation,  $\zeta$ .

The order of time integration within the model can be seen in Figure 3. Time integration proceeds from the outermost parent grid to the innermost child. The integration of a certain parent grid can only proceed when all child grids have been integrated up to the time-level of that grid. It should be noted that DIVAST uses the Alternating Direction Implicit (ADI) solution technique to solve the governing finite difference equations; this requires that each timestep is split into two. This does not affect the order of time integration as each parent grid is integrated by one full timestep before the model proceeds to the child. However, it does affect the temporal interpolation process as each child grid requires boundary data at each half-timestep. In relation to the interpolation of nested open boundary data, a linear technique is used for temporal interpolation while an inverse distance weighted technique is used for spatial interpolation. Both techniques have been found to give accurate results.



## 4 Models

Three models of Galway Bay were developed: a coarse model, a fine model and a nested model. The extent of the model domain was the same for each model and is shown in Figure 4. For simplicity the nested model had only one level of nesting with a 3:1 grid ratio. The spatial and temporal resolutions were as follows:

1. Coarse Model:  $\Delta x = 300\text{m}$ ,  $\Delta t = 60\text{s}$
2. Fine Model:  $\Delta x = 100\text{m}$ ,  $\Delta t = 20\text{s}$
3. Nested Model: Parent Grid -  $\Delta x = 300\text{m}$ ,  $\Delta t = 60\text{s}$   
Child Grid -  $\Delta x = 100\text{m}$ ,  $\Delta t = 20\text{s}$

The parent grid in the nested model was a copy of the coarse grid model with the same resolutions and hydrodynamic parameters while the child grid was a copy of the fine grid model.

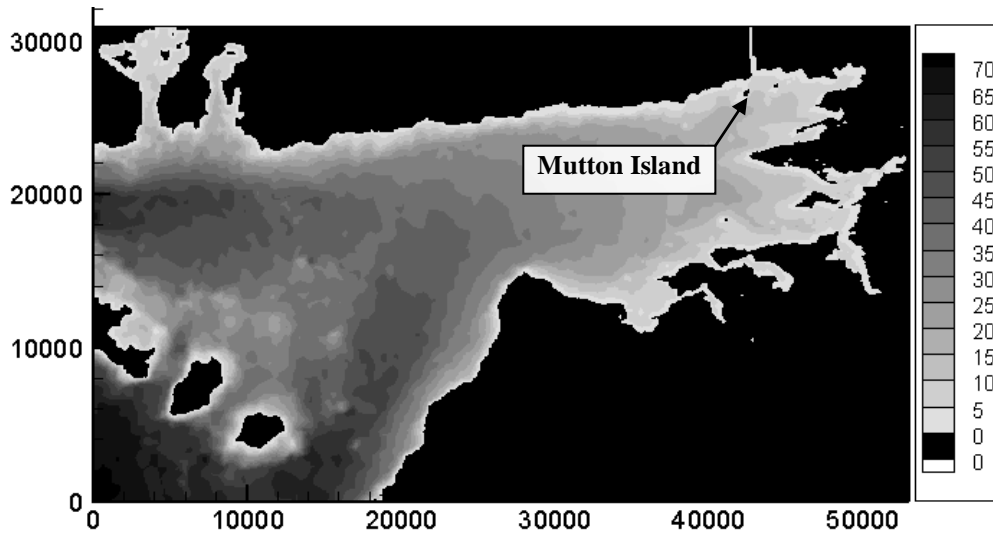


Figure 4: Galway Bay model domain [all units in metres].

All three models simulated the same discharge scenario where a conservative tracer was discharged from the wastewater treatment plant at Mutton Island (see Figure 4). The discharge began at 12.5hrs (the time of high water) and finished at 12.6hrs. The discharge was specified with a flow rate of  $10\text{m}^3/\text{s}$  and a concentration of  $50,000\text{mg/l}$ . The model simulation time was 50 hours. Model data was output in two formats, firstly as instantaneous snapshots of the model domain at particular instances in time and secondly as time series at the locations shown in Figure 5.

In the nested model the adaptive mesh moves were user-specified at the beginning of the simulation. The times and extents of the moves were determined from the solute transport results of the fine model so that the nested domain would always enclose the solute plume. The nest was moved twice during the simulation at 18.75hrs and 31.25hrs. The locations of the nested domain during the course of the

simulation are shown in Figure 5. At 18.75hrs the extents of the nest moved from Nest 1 to Nest 2 and at 31.25hrs the extents again moved from Nest 2 to Nest 3.

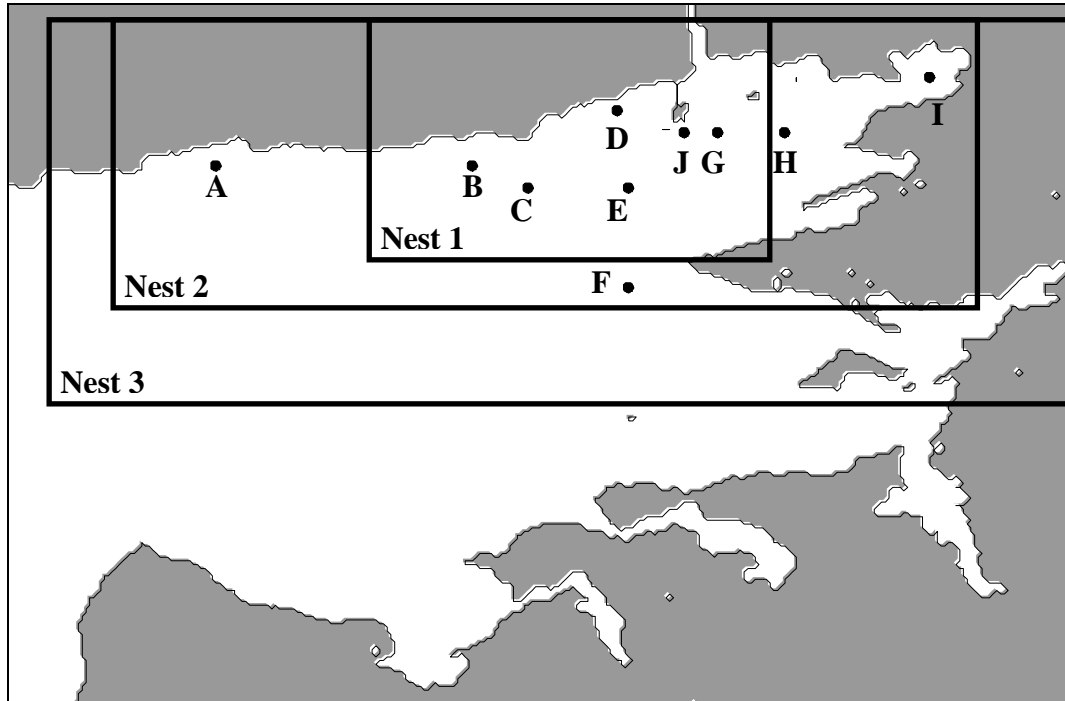


Figure 5: Inner Galway Bay showing locations of time series and nested domain.

## 5 Model Results

The fine model was assumed the ‘correct solution’ against which the other model results were compared. Coarse model results were first compared to the fine model to demonstrate the improvement in accuracy achieved as a result of improved resolution. The nested model results were then compared to the fine model results to determine the accuracy of the adaptive mesh model.

Figure 6 and Figure 7 compare the solute plume computed by the coarse model with that predicted by the fine model at times  $t=43.75\text{hrs}$  (low water) and  $t=50\text{hrs}$  (high water). It can be seen that the extents of the plumes are quite different with the spread of the tracer in the coarse model much larger on the western side at low water and on the eastern side at high water. Concentrations in the waters surrounding Mutton Island are also higher (by as much as 25%) in the coarse model than in the fine model. The differences observed in the plumes are due to differences in advection between the models as a result of the more accurate calculation of hydrodynamic activity by the fine model (see Nash and Hartnett [5]). The differences may be observed more readily by comparing solute concentration time series from the coarse and fine models. Figure 8 shows comparisons at Points E and

H. The coarse model concentrations are substantially different to the fine model concentrations at both locations.

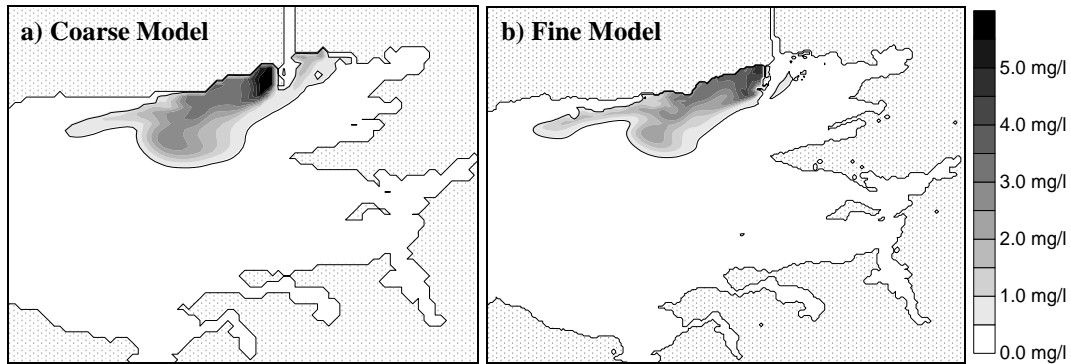


Figure 6: Solute plumes at time  $t = 43.75$ hrs, low water.

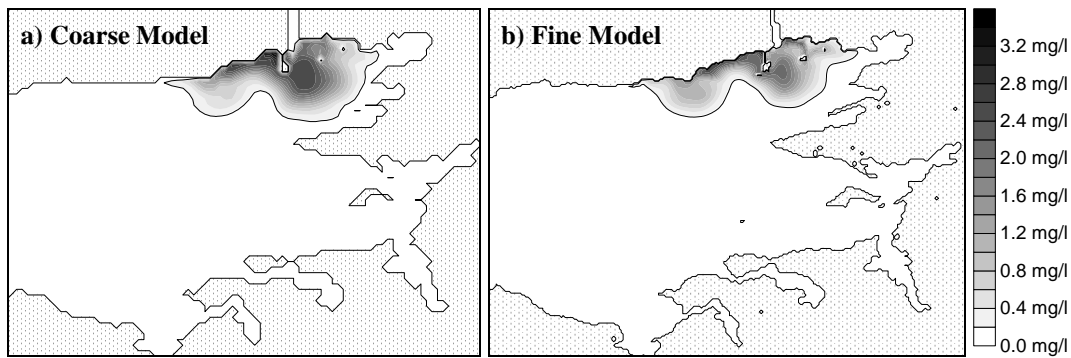


Figure 7: Solute plumes at time  $t = 50$ hrs, high water.

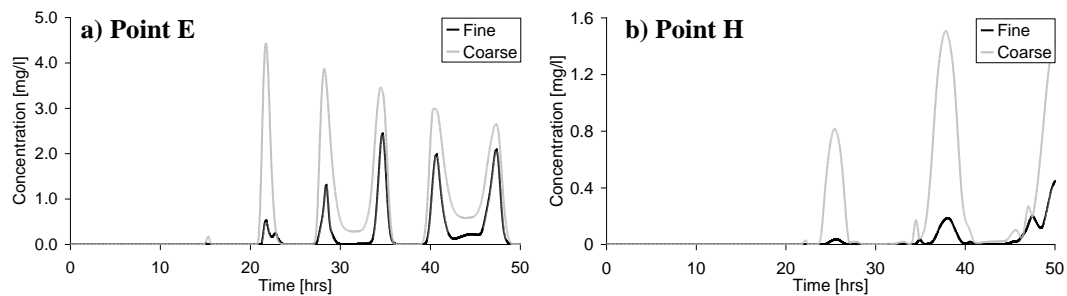


Figure 8: Comparison of tracer concentrations between coarse and fine models.

The accuracy of the adaptive mesh model was determined by comparing its results with those from the fine model; an accurate nested model should yield similar results to the fine resolution model. Figure 9 and Figure 10 compare the solute plume computed by the nested model with that predicted by the fine model at times  $t=43.75$ hrs (low water) and  $t=50$ hrs (high water). The plumes computed by the nested model can be seen to be almost identical to those of the fine model. Figure 11

compares the tracer concentrations predicted by both models at Points E and H. The nested model time series are for the most part coincidental with their fine model counterparts. Similar levels of accuracy were found at all of the other time series locations. The results indicate that the solute transport predictions of the adaptive mesh model are much improved on the coarse model and are almost as accurate as the fine model. The nested model is therefore well-behaved and accurate.

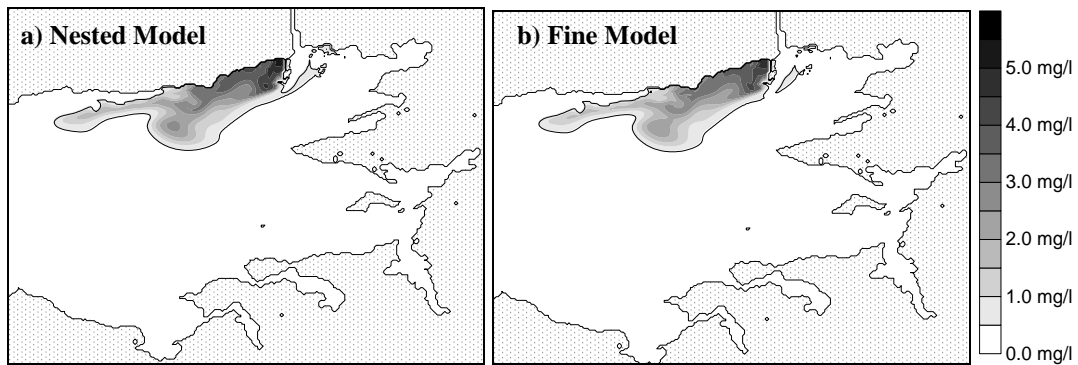


Figure 9: Solute plumes at time  $t = 43.75$ hrs, low water.

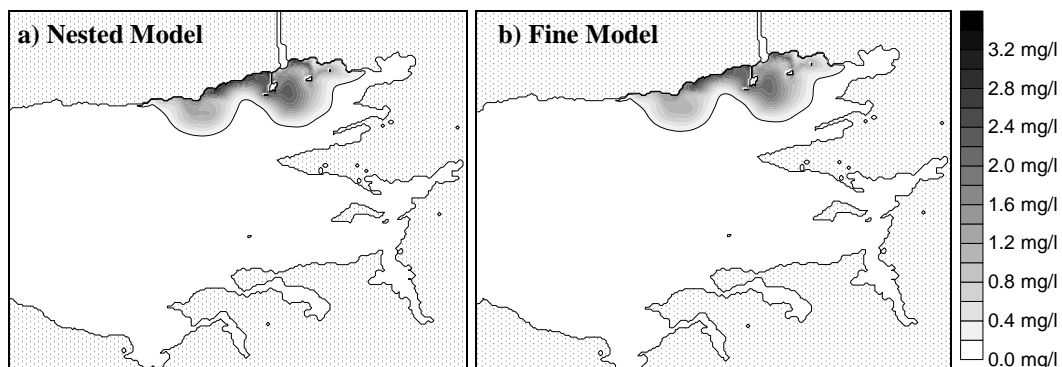


Figure 10: Solute plumes at time  $t = 50$ hrs, high water.

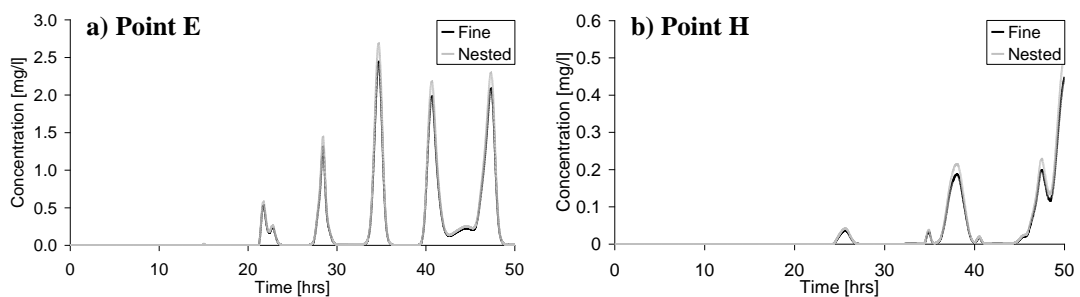


Figure 11: Comparison of tracer concentrations between nested and fine models.

## 5 Summary and Conclusions

The Author's have developed an adaptive mesh solute transport model. The model is a one-way nested version of the hydrobiological model DIVAST and allows multiple nesting, i.e. each parent grid can have one or more child grids, each of which in turn can successively have one or more children. The adaptive meshing scheme means that any valid nested child grid may either be a static domain or a moving domain. Extensive testing has shown that the model is stable and is capable of computing solute transport to a high degree of accuracy.

The adaptive mesh model provides two methods of facilitating dynamically moving nests during the course of a simulation: specified and automatic. For a specified move, the timing of a nest move and the extent of the lateral move is defined entirely by the user. For the automatically moving nest, the nest moves to maintain a feature within its boundaries according to some predetermined rule. The implementation of the adaptive mesh scheme ensures that the area over which high resolution is required (and therefore the computational effort) is kept to a minimum during the simulation. The adaptive mesh scheme therefore not only gives significant computational savings over non-nested models but also gives further savings over the classical zoom nested models. The computation time for a 50hr simulation using the nested model with user-specified dynamic nesting was 32mins. This compares with a time of 142mins for the fine model giving a computational saving of 77%. The computation time for the same simulation using a static nested grid model was 40mins giving a saving of 20% for the adaptive mesh model over the classical zoom nested model; this is a significant saving in its own right.

The Author's are currently developing a parallelised version of the nested model where each parent and child grid is assigned to a different processor. This will lead to further reductions of the computational cost of hydrobiological modelling.

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