Numerical Diffusion
in ELM Advection Schemes for Water Quality Simulations with QSim-3D

Bundesanstalt für Gewässerkunde

What is the problem?

The basic ELM scheme, used in QSim-3D, exibits considerable numerical diffusion

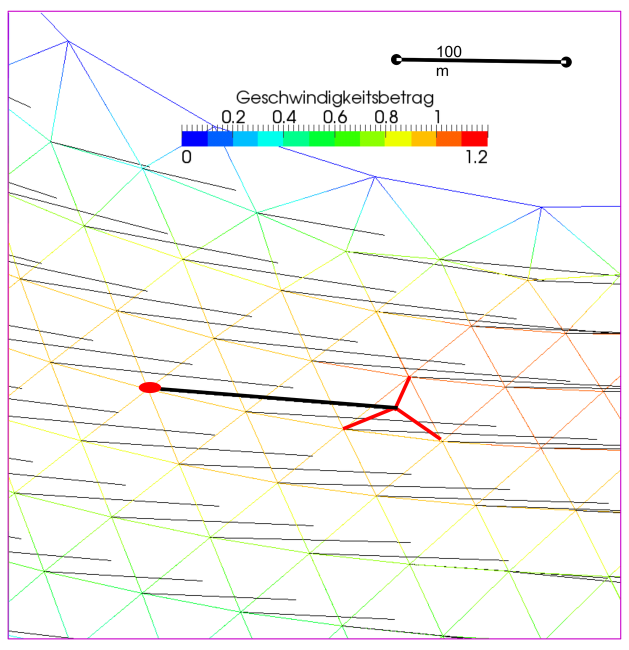


Figure 1 visualizes streamline backtracking. The mesh lines are colored with velocity magnitude. The black lines connect each node (red dot) with the origin of its streamline (black lines are no streamlines, which would be curved). The red star connects the streamline origin with the nodes, whose values are used to interpolate the concentration at the streamline origin.

In QSim-3D the advection part in a transport equation ist discretized with the ELM (Euler-Lagrange-Method), sometimes also called Method of Characteristics or Semi-Lagrangian Method.

The advected concentration difference in a timestep is taken as the difference between the actual value and the value at the origin of a backtracked streamline
.
The hydraulic drivers used for Qsim-3d (casu, SCHISM) do backtracking for momentum advection anyway. These streamline origins can be stored and reused in subsequent (offline coupled) water quality simulations with Qsim-3D.

In 2D-depth averaged computaions a linear Interpolation of the conservative variable (concentration times depth) is used to evaluate the value at the streamline origin.

$$D_{num} \le 0.25 \cdot \Delta x^2 / \Delta t$$

Equation 1 (same symbols as in eq. 2)

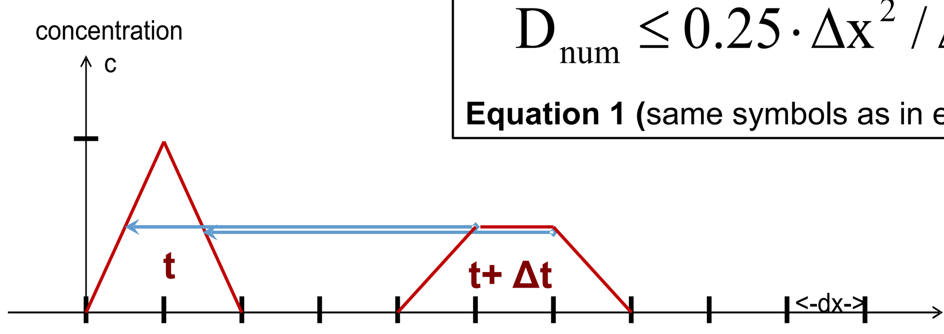


Figure 2 illustrates numerical diffusion in a 1D example in a constant velocity field. The red distributions show the concentration at the start and the end of the time step. The blue arrows symbolize the backtracked streamlines.

The local Courant number in this case is 3.5 The numerical diffusion is connected with the rest (0.5) behind the whole number (3). This example exibits the maximum of numerical diffusivity. Equation 1 quantifies this upper limit (for constant grid spacing). With the Courant number approaching a whole number, numerical diffusivity tends to zero.

Numerical diffusivity can be reduced by the use of finer grids and larger time steps.

How large is the problem?

Method 1:
Assessment of numerical diffusivity (in use)

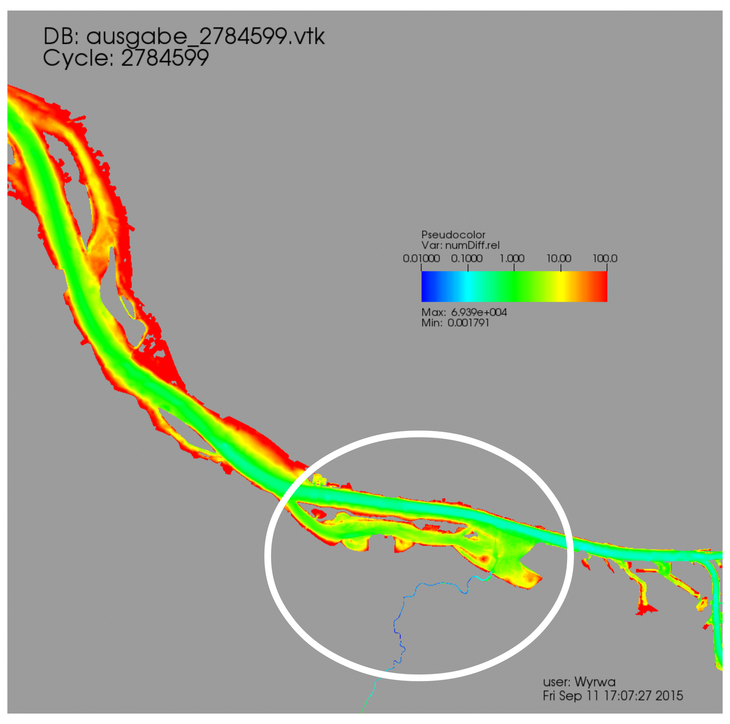


Figure 3 central part of Elbe estuary model. End of flood flow close to high water. Coloring shows relative numerical diffusivity from equation 2. White circle marks refined mesh

The significance of numerical diffusion for diffusive processes in the estuary gets clear when related to an estimate for the real diffusion. Here the Elder approach for longitudinal mixing in 2D depth averaged open channel flows is used.

Equation 2

$$\frac{D_{num}}{D_{Elder}} < \frac{0.25 \cdot \Delta x^2 / \Delta t}{5.93 \cdot v_\tau \cdot d}$$

D – diffusivity
Δx – grid spacing
Δt – time step
v_τ – friction velocity
d – water depth

Relating the upper limit for numerical diffusion to an established estimate for the real diffusion allows the following conclusions:

- In the deep fairway with its fast flows the numerical diffusion is less or equal the natural one.
- In the slow flows in shallow areas, the numerical diffusion might be significantly larger then natural.
- Mesh refinement can shrink numerical diffusion to a bearable ammount

Method 2:
Local measure for numerical diffusivity (under development)

Numerical diffusion is evaluated for a concentration peak at a single node. Concentration distributions can be seen as a linear combination of such concentration peaks.

Numerical diffusion is generated by concentration differences produced by the advection scheme along a streamline. Such a difference is visualized in fig. 4 and forms the right hand side of eq. 3.

A value for numerical diffusivity is now build by relating the afore mentioned difference to the divergence of the concentration gradient. The left hand side symbolizes this for 1D.

Equation 3

$$\frac{\Delta(\Delta c / \Delta x)}{\Delta x} \cdot D_{num} = \frac{c_j^{n+1} - c_{j,ur}^{n}}{\Delta t}$$

D – diffusivity
Δx – grid spacing
Δt – time step
c_j^{n+1} – concentration at node j in current time step
$c_{j,ori}^{n}$ – concentration at the origin of streamline leading to node j in previous time step

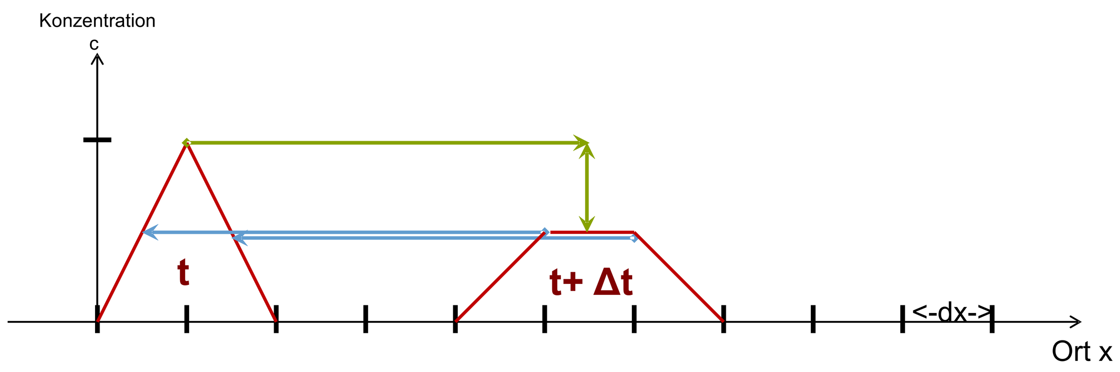


Figure 4 peak reduction can be measured in a 1D example assuming constant grid spacing and constand velocity. Colors like in Fig. 2; the green arrow symbolizes the forward streamline. At the location of the green arrow tip the concentration difference caused by the advection scheme can be measured (green double arrow).

How to cope with the problem?

Option 1:
Careful design of discretisation

Advective transports in estuaries with a large tidal amplitude are much bigger than diffusive fluxes anyhow. But some tranport processes are of duffusive nature on the scale under consideration here, e.g. harbor basin mixing.

Discretisation can be designed in a way, so that numerical duffusion can aproximately cover diffusive processes.

Differences, detected in validation, can be checked with the methods described above. Enabeling the experinced modeller to distiguish possible origins.

Option 2:
Reduce numerical diffusion

This demands for the implementation of a higher order advection algorithm combined with a fine discretisation.

Higher order schemes are less diffusive but need to implement limiters to make the solution total variation diminishing (TVD). This slows down computation. Especially in water quality simulation where the limiter needs to be applied to each of the large number of concentrations individually.

A fine discretisation slows down computation even further.

Then full use of a diffusion model can be made.

Option 3:
Measure numerical diffusion

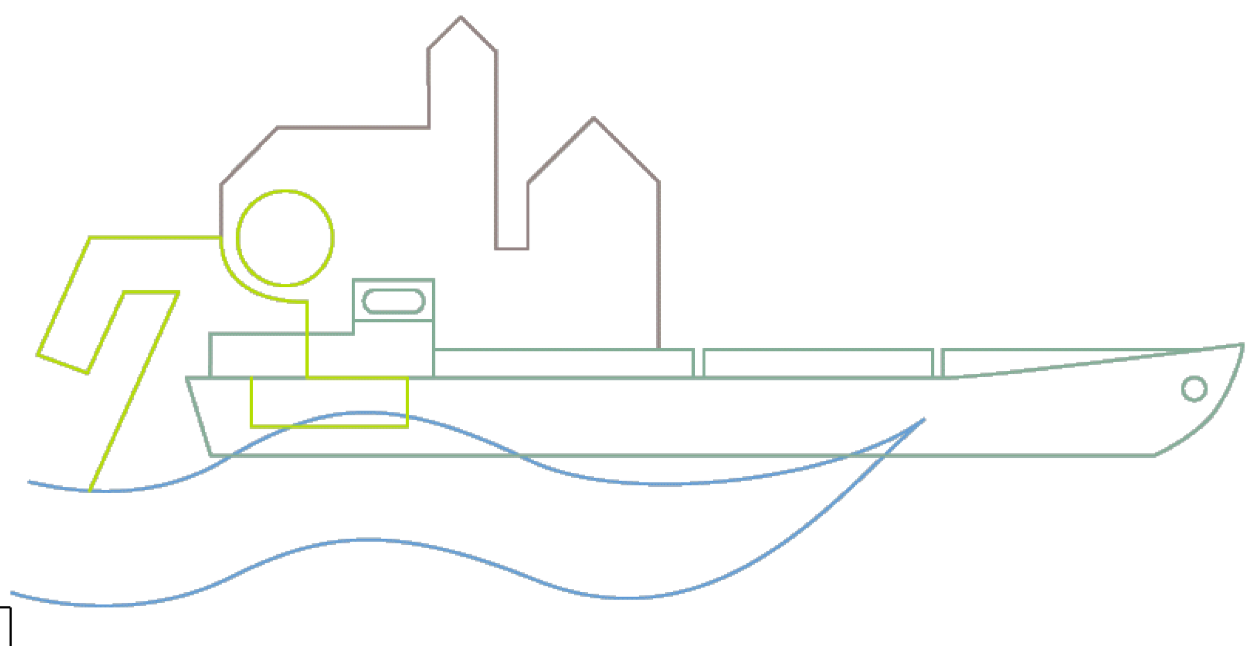
Schemes to measure numerical diffusivity locally at each node are under development.

First possibility: compute forward (green) streamline and detect peak reduction as depicted in the figure 4.

Second possibility: evaluate local courant number for each backtracked (blue in fig. 2 and 4) streamline, knowing the value of numerical diffusivity as a function of local Courant number. Appropriate concepts for specifying Courant number in 2D and 3D are needed.

If the locally varying numerical diffusivity is known, it can be augmented to the full value determined by a diffusion model. A warning can be issued if numerical diffusivity is too large.

Then there would be no need to reduce numerical diffusion in highly diffusive estuarine flows.



QSim

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Dr.-Ing. Jens Wyrwa

Federal Institute of Hydrology
(Part of German waterways)
Division U, Ecology
Am Mainzer Tor 1; 56068 Koblenz
Tel.: (0049) 261 / 1306 - 5254
wyrwa@bafg.de ; www.bafg.de

www.wyrwa.de