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Ongoing developments in TELEMAC and TOMAWAC at IMDC

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***Abstract*—In this paper, various ongoing developments in TELEMAC and TOMAWAC are presented. The presented developments are:**

1. **Two-way coupling between TELEMAC-2D and TELEMAC-3D.**

2. **Implementation of surface rollers in TOMAWAC.**

3. **The implementation of a functionality to export history files (data on a limited number of locations in the computational domain, such that typically a much higher output frequency can be used) in TELEMAC, TOMAWAC and GAIA**

4. **Implementations to switch off horizontal diffusion in TELEMAC-3D, which lead to large speed-up of calculations with advected tracers.**

I. Coupling between TELEMAC-2D and TELEMAC-3D

A. Background and motivation

In many engineering applications, one has to deal with problems that involve three-dimensional flow effects in large areas. However, the three-dimensional flow effects are often important in only a part of the model domain. An example is the Scheldt estuary in Belgium (Fig.1). In this estuary, the effect of density currents due to the variation in salinity is important, especially in the area around Antwerp, for which the use of three-dimensional calculations is necessary. In these areas, an estuarine turbidity maximum (ETM) occurs, and also for the correct simulation of such an ETM, three-dimensional calculations are necessary. However, in the upstream parts of the estuary, which still have a large tidal variation, three-dimensional effects are less important. Instead, the tributaries are narrower, leading to the need of smaller mesh sizes and smaller time steps, such that the upstream part has a large impact on the calculation time of the model. Because of this, a large speed-up could in principle be obtained by performing simulations using a two-way coupled TELEMAC-2D and TELEMAC-3D model, where the TELEMAC-2D model is used in the upstream part of the estuary, and TELEMAC-3D in the downstream part.

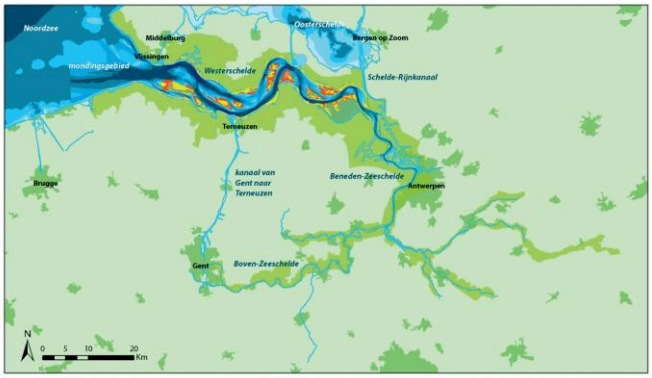

Fig.1 Overview of the Scheldt Estuary (from VNSC communications).

B. Objective and limitations

The objective is to develop a two-way coupling between TELEMAC-2D and TELEMAC-3D. This coupling has the following requirements:

- The coupling must work in parallel.
- Each sub-model can use different parameters. Especially, each model must have its own time step, which must be a multiple of each other.
- The coupling should be able to handle meshes with different extends (i.e. some overlap between the meshes must be possible).
- The changes to the existing TELEMAC-2D and TELEMAC-3D code should be as limited as possible.

C. Implementation

The coupling between TELEMAC-2D and TELEMAC-3D is implement in the Fortran version of the TELEMAC-API (the file homere_api.F). Many of the ideas for the coupling are inspired by the previous work coupling TELEMAC-2D to MASCARET [1]. Based on the finding in that work, it was opted for a method, in which both models are run consecutively (i.e. a multiplicative Schwartz method). Hence first TELEMAC-2D is run for one or more sub-steps, followed by TELEMAC-3D. The number of sub-steps for each of the models depends on the ratio of time steps in TELEMAC-2D and TELEMAC-3D. At the last sub-step, water levels and velocities at the location of the open boundaries are collected and communicated to the other model using the TEL2TOM functionality [2]. TEL2TOM is a parallel coupling facility, developed originally to couple TELEMAC and TOMAWAC on different meshes. It provides parallel communication, as well as spatial interpolation using weighting coefficients that have to be determined during the pre-processing stage. Time interpolation or extrapolation is performed on the communicated water levels and velocities. The information that is applied on the boundaries are water levels (η) and flow rates *(q=Hu)*, with *H* the water depth and *u* the flow velocity. Here, the flow rate is applied at an inflow boundary and the water level at an outflow boundary. These two variables were chosen, because some experiments showed that using these two variables, substantially more stable results were obtained than using water levels and velocities on the boundaries.

D. Limitations of the implementation.

The use of the TELEMAC-API leads to the limitations, that only one TELEMAC-2D model can be coupled with only one TELEMAC-3D model. Such a model can however consist of many different, unconnected domains. These domains must have the same physical and numerical parameters (such as the time step). Further, the coupling of additional TELEMAC modules (such as GAIA or WAQTEL) seems only possible with one of the two models (either TELEMAC-2D or TELEMAC-3D), but not to both of them. In the current implementation, coupling of tracers (e.g. temperature or salinity) is not implemented, but this could be done with relatively limited effort. Finally, in the existing TELEMAC code, there are a couple of functionalities, where the code of TELEMAC-2D and TELEMAC-3D are interlinked. The most important of these functionalities are the use of tidal boundary conditions (TPXO) and the use of meteorological data (wind and atmospheric pressure). Therefore, in the current implementation of the 2D-3D coupling, these features can only be used in TELEMAC-2D. Note that this limitations could be solved with relatively limited efforts by some cleaning of the code for these specific functionalities.

E. Preliminary results

A first test is performed to verify the correct implementation of the coupling. In this test, a TELEMAC-2D model, with two disconnected sections (an inflow section and an outflow section) is coupled to a TELEMAC-3D model with 20 vertical nodes in between (Fig. 2). The model represents a river (with flow from left to right), with some connected branch in the middle of the domain. The total length of the domain is 100 km, with a mesh size of 50 m, leading to 24169 nodes in the 2D domain and 3865 nodes in the 3D domain. The overlap between the two domains is 1 km at each side. The mesh in the overlap is the same in both meshes (although this is not strictly necessary for the coupling), except from a few small changes, to prevent overconstrained triangles at the boundaries of the subdomain. At the transitions between the domains, a water level boundary condition is used downstream, and a velocity boundary condition upstream. A slowly varying discharge boundary condition was applied at the upstream boundary of the 2D domain.

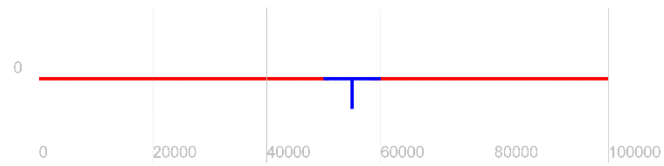

Fig. 2 Overview of the model domain. The TELEMAC-2D model is red, the TELEMAC-3D domain is blue.

The preliminary results of the water levels of the two models are shown in Fig. 3. It can be seen in this figure that the water levels coincide at the location where of the downstream boundary of the subdomains, thus showing that the implementation is correct. The water level in the 3D domain is however rather noisy. This becomes much worse when the time step is increased (in this test a rather small time step of 1 s was used). The cause of thee instabilities is currently being investigated.

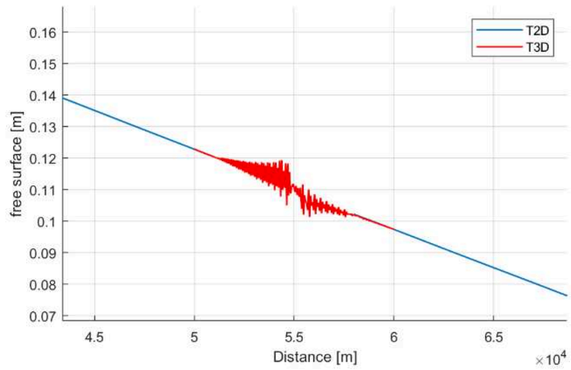

Fig. 3 Preliminary results of the water level in the two models after three hours of simulations.

F. Future work

The current implementation is limited to unidirectional flow, because the type of the boundary conditions (water level or velocity boundary) at the connections between the TELEMAC-2D domain and the TELEMAC-3D domain is currently set in the .cli files. The first step that will be performed is a functionality to change the type of the boundary condition depending on the flow conditions (flow direction and Froude number), such that also problems with changing flow directions (such as tides) can be simulated.

Further, in the current implementation, each model performs one iteration (i.e. there is no real Schwarz loop) per time step. While this is beneficial for calculation times (especially multiple iterations with TELEMAC 3D do not seem desirable), performing multiple iterations when needed, may make the model more stable. This will be investigated.

The results of the preliminary tests showed that the results can be influenced substantially by reflections at the (downstream) boundaries. Test using Thompson boundary conditions did not show any improvements. For the good functioning of the coupling, it seems necessary to develop non-reflective boundary conditions. Different options exist for this. One option, is to perform nudging (e.g. [5]). With this option, the momentum equations are changed, such that the flow velocities are nudged toward the externally prescribed boundary conditions. Another option is to use Flather boundary conditions (e.g. [5]), which use a radiation condition on outflow boundaries to prevent reflections. It is to be investigated, which of these is the most appropriate option. It is noted that the development of non-reflective boundary conditions would be beneficial for many other applications as well.

Finally, further testing of the functionality needs to be performed.

II. Surface rollers in TOMAWAC

A. Background and motivation

When waves break, a part of the wave energy is transferred to surface rollers. These propagate shoreward, thus causing a delay between the point, where the waves begin to break and the point, where wave setup and longshore currents develop. In additional the surface rollers transfer mass towards the coast, thus influencing the return current that occurs. Finally, they can influence the stirring up of sediment

B. Objective and limitations

The objective is to implement a model for the evolution of the energy of the surface rollers, and its influence on the long-shore currents. The effect of surface rollers on the stirring up of sediment and on the Stokes drift are currently neglected.

C. Implementation

In the implementation, we follow the work by Zenner [8]. More information can also be found in for example [6]. According to these references, the surface roller energy E_r per unit of mass is given by:

$$E_r = \frac{1}{2} A \frac{\overline{U_{roller}^2 + W_{roller}^2}}{L}$$

Here, L is the wave length, A is cross-sectional area of the surface roller, and U_{roller} and W_{roller} the velocity components in the horizontal and vertical direction respectively. The overbar denotes averaging over a roller. The evolution of the surface roller energy is given by the following differential equation:

$$\frac{\partial E_r}{\partial t} + \frac{\partial c_x E_r}{\partial x} + \frac{\partial c_y E_r}{\partial y} = D_w - D_r$$

Here c_x and c_y are the x and y components of the phase velocity of the waves. D_w is the is the energy dissipation due to breaking of the waves (which is calculated in TOMAWAC using the depth induced breaking routines, e.g. using the formulation of Battjes and Jansen), and D_r is the energy dissipation of the surface rollers, which is parametrized as:

$$D_r = 2 \frac{\beta_s}{\beta_2} \frac{g}{c} E_r$$

Here, β_s and β_2 are calibration parameters, and g is the gravitational acceleration.

The effect of the surface rollers of the current comes from its effect on the radiation stresses, which are given by:

$$S_{xx} = S_{xx,waves} + \cos^2\theta E_r$$

$$S_{xy} = S_{xy,waves} + \cos\theta \sin\theta \, E_r$$

$$S_{yy} = S_{yy,waves} + \sin^2\theta E_r$$

Here, S_{xx} S_{xy} and S_{yy} are the different components of the radiation stress tensor, $S_{xx,wave,}$ $S_{xy,waves.}$ $S_{yy,waves}$ the radiation stress components from the surface waves (as calculated in TOMAWAC), and θ the mean wave direction.

This differential equation is implemented in TOMAWAC using a fractional step method. The advection step is solved first using the method of characteristics. The velocity field is determined every time step from the peak period, water depth and mean wave direction calculated by TOMAWAC (for the moment ignoring the effect of wave-current interaction). After the advection step, the source and sink terms are applied. Here, D_r is calculated using an implicit numerical discretisation while D_w uses an explicit discretisation. D_w is exported directly from the calculation of the depth induced breaking term of Battjes-Janssen in TOMAWAC. Currently, this is only implemented in a new version of the breaking source term (which can be switched on by setting the keyword DEPTH-INDUCED BREAKING DISSIPATION=10). This new implementation of the source term speeds up the calculation of the depth-induced breaking significantly by the following modifications:

- The use of an implicit numerical scheme with Newton-Raphson iteration. This additionally has the advantage that it makes the computation more robust and that the user does not need to specify the number of time steps for the breaking iterations; the number of iterations is determined automatically using a convergence criterion.
- The use of threshold to make sure the depth-induced breaking is only calculated on the mesh points, where depth induced breaking is important (i.e. shallow points).
- The calculation of the energy dissipation for the mean action density only, because the source term of Battjes-Janssen leads to an energy dissipation that is constant for each component in the spectrum. Only after all the iterations for breaking are performed, the energy dissipation is applied over the spectrum.

D. Preliminary results

A first test was performed in the littoral test case. In this test case, waves, with an offshore significant wave height of 1.0 m propagate toward the coast under an angle. While propagating, towards the shore, they refract and start breaking thus generating a longshore current. The results of two test calculations, one without surface roller and one with surface rollers are shown in Fig. 4. This figure shows clearly that the surface rollers cause the wave-driven current to be moved closer to the shore. This is as expected from theory, and this is one of the main motivations for including the effect of surface rollers. Further, it causes the maximum longshore to increase. Interestingly, a current in the opposite direction is generated at the start of the breaking zone. The reason for this is not yet clear.

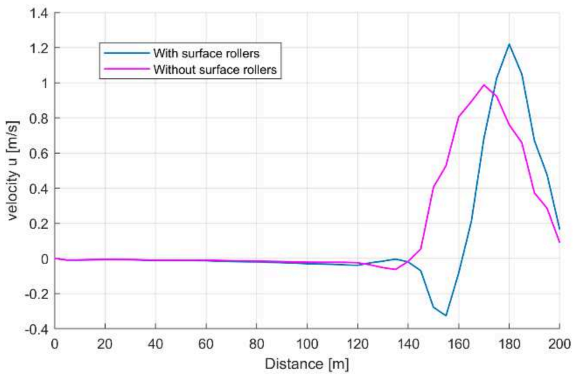

Fig. 4 The wave-generated longshore current in the littoral test case with and without surface rollers. The beach is on the right side of the figure

E. Future work

In the next phase, more extensive testing of this functionality is needed, in both schematic test cases and real applications, as well as using parallel computations. It seems especially needed to compare the results in a schematic test case, with some reference solution. Also, the implications of ignoring the effect of wave-current interaction need to be studied. Further, the effects of surface rollers on return currents and the stirring up of sediment may be implemented to improve the cross-shore modelling facilities in TELEMAC-TOMAWAC-GAIA. Finally, some work need be done on the IO with respect to this routine, such as adding keywords to the .CAS file and adding the possibility to export the surface roller energy to the TOMAWAC result files (this is currently done using a private array).

III. Improvements in input/output

A. Background and motivation

When working with TELEMAC, input and output are important to provide correct data to the model as well as to export the results of the simulations for postprocessing. Different computational environments provide different limitations in this respect. On HPC clusters, the storage space may be limited for the individual users, and hence the need arises to limit the amount of storage space taken by the input and output data in the model. Other advantages of limiting these data consist of shorter pre-processing and post-processing times, and shorter times needed to download data. Especially on older infrastructure, the time spend on IO may be a bottleneck for the duration of the computation.

B. Objective and limitations

The objective is to provide more flexibility in the TELEMAC-IO. More specific, the aim is to develop the functionality to make so called "history files", which are files which export time series of point-data or 1-d vertical profiles (for example at the location of a measurement station), but with a much higher time resolution than is typically used in the normal TELEMAC output files. Further, it is the objective to improve the *find_variable* subroutine, to limit the amount of IO in this routine.

C. Implementation

The functionality for exporting history files is implemented. This functionality reads coordinates of the required output points from a text file, performs linear interpolation on the data (using weight factors computed during the initialization of the model in order to have a fast performance; these weights are calculated such that they correspond to the P1 discretisation used in TELEMAC; the weight factors are saved for the entire calculation in order to save calculation time) and then stores the data using the existing HERMES IO-module. Finally, some adaptations to GRETEL were done, in order to be able to merge the generated output files of a parallel computation to a single output file.

In order to generate the history files, the following keyword were added to TELEMAC-3D (and similar in TOMAWAC, GAIA and TELEMAC-2D)

HISTORY COORDINATES FILE : the name of the file with the required output coordinates

2D HISTORY FILE: 2D results file with time series of depth-averaged point data

3D HISTORY FILE: 3D results file with time series of 1DV profile data

The format of the HISTORY COORDINATE FILE is as follows:

- On the first line, there are two numbers indicating:
  - The number of time periods for which data is written to the HISTORY FILE
  - The number of coordinates for which output is generated
- On the next lines, for each output period, three numbers indicating:
  - Start of the output period (in seconds since the start of the model)
  - End of the output period (in seconds since the start of the model)
  - Output time interval (in seconds)
- For each coordinate, three numbers and a string:
  - X-coordinate of the output point
  - Y-coordinate of the output point
  - Unique ID of each station (in order to easily encounter the output data in the output files). This ID will be written to the IKLE-array in the output file, which has a size [NPOINTSx1]. Note that the history files have different points. There is no mesh information, thus explaining that the length of the IKLE array is the same as the number of points in the history file.

- The name of the station (for better readability of the coordinate file)

  An example is shown in Fig. 5.

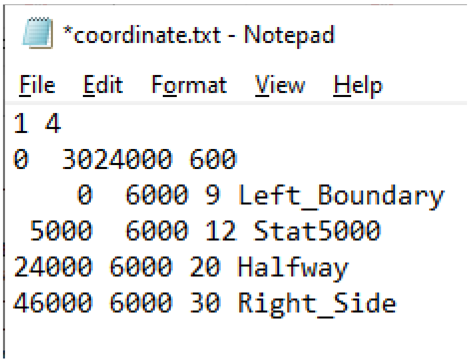

Fig. 5 Example of a HISTORY COORDINATE FILE

Finally, an updated version of *find_variable* was made. This function is used to read data from input files (e.g. for meteo data), including the time interpolation of the data. However, this function reads data from the previous and future moments in the input file, at each time step. This leads to a large amount of IO, in case the time step in the input file is much larger than the time step in the model. In the updated version, data from the previous and future time steps in the input files are stored in memory, thus limiting the amount of IO considerably.

IV. Improvements in 3D Scalar Transport and Stratified Flow

A. *Background and motivation*

In many practical problems, the transport of scalars is important. For example, these tracers can be different sediment fractions when using GAIA, or different water quality parameters when using WAQTEL maybe in combination with AED2. In many situations, these scalars vary strongly over the vertical, meaning that it is important to perform 3D simulations using TELEMAC-3D Using these modules can lead to problems with large number of advected tracers (in AED2, this can be up to at least 24). However, using many scalar variables can lead to large calculation times. Some of these tracers (like sediment salinity or temperature) are so called active tracers. This means that their concentration influences the density, and hence can change the flow due to the generation of baroclinic pressure gradients or stable vertical stratifications, which damp turbulence.

B. *Objective and limitations*

The objective is to improve the transport of scalars in TELEMAC-3D, in particular with the objective to decrease the calculation time of the simulation, and to diminish the artificial vertical mixing present in TELEMAC-3D.

C. *Implementation*

Profiling was done, in order to determine the bottlenecks with respect to the transport of tracers. From this is was found that diffusion formed a bottleneck, which is apparently because a large matrix needs to be solved to calculate the diffusion. This matrix is substantially larger than the matrix in the flow calculations, which contains only the 2D points, whereas the tracer diffusion is calculated using a matrix containing all 3D points. It was then realized that for many (but certainly not all) typical problems (e.g. dispersion of sediment plumes), the horizontal diffusion is not very important physically (in contrast to vertical diffusion, which is very important). This is particularly so, because the advection schemes that are typically used in TELEMAC (like NERDS) lead to a substantial amount of numerical diffusion, which seems to be of a similar magnitude as the horizontal diffusion calculated by the advection-diffusion solver. Also note that horizontal diffusion in large scale flows (such as in coasts or oceans) is a process that is physically not very well understood, making the values for the coefficients that need to be specified by the user rather uncertain.

It was then realized that for sediment, it is possible to switch off the horizontal diffusion and apply the vertical diffusion (with a fully implicit scheme), using the subroutine *set_diff* by setting these two settings in the .cas file:

SCHEME FOR DIFFUSION OF TRACERS = 0

ADVECTION-DIFFUSION SCHEME WITH SETTLING VELOCITY : 1

These settings only work in combination with residual distribution schemes (such NERD or LIPS). This is not a big disadvantage, as these are the most suited advection schemes for the transport of tracers in practical applications anyway.

In order to speed up calculation of tracers, the code was adapted (by specifying settling velocities and erosion/depositions terms with a default value of zero), such that horizontal diffusion can be switched off, and vertical diffusion is calculated for any tracer (not just sediment), by setting the previously shown keywords. In order to have all important physical processes, the surface boundary conditions and the explicit and implicit source terms were added to the *set_dif* subroutine, such they can also be taken into account for those tracers that need it.

Note that in those cases where horizontal diffusion is important, one could set IMPLICITATION FOR DIFFUSION = 0.0 in order to have the horizontal diffusion explicit. This is different from using SCHEME FOR DIFFUSION OF TRACERS = 2, because when using *set_dif*, an implicit scheme is still used vertically. In this way, the horizontal diffusion is taken into account for a fraction of the computation cost. There is a time step criterion involved:

$$\Delta T < \frac{\Delta X^2}{D_H}$$

Here, ΔX is a measure of the mesh spacing (e.g. the square root of the area of the triangle) ΔT is the time step and D_H is the horizontal diffusivity. For typical, engineering applications, this criterion allows rather large time steps, which are typically larger than the time step actually used in the model. Note that the use of *set_diff* ensures that the vertical diffusion is solved implicitly, which is important, because the time restriction for vertical diffusion is much more stringent due to the fact that in typical applications, the vertical mesh spacing is much finer than the horizontal one.

D. Preliminary results

The settings prescribed in the previous section have been applied in many different model simulations. Indeed , a large speed up is obtained. Switching off horizontal diffusion appeared to have the following additional advantages:

- Simulations appear to be more stable (especially on tidal flats).
- The mass balance seem to be more correct (even when decreasing the accuracy of the solver to 10^{-12}).
- In case of stratified flow, horizontal diffusion can lead to some extra vertical mixing (especially when the vertical layers are not completely horizontal, e.g. when using sigma or double-sigma layers. This diminishes the stratification, leading to incorrect results (such as errors in the penetration of a salt wedge.

Two examples are presented here. First a schematic case was run using AED-2 with phytoplankton in a square basin with 133 nodes, with a time step of 60 s. This test case has 22-advected tracers. The calculation time with the traditional TELEMAC settings was 49 s for a simulation period of one day. Switching the horizontal diffusion off, the calculation time reduced to 20 s, giving a speed-up of a factor 2.5, while the results remained the same. In this case, the speed-up is still rather modest, which is due to the fact that the case is homogeneous, and hence the number of iterations of the matrix solver when solving horizontal diffusion of the tracers appears to be very low (either 0 or 1).

As a second example, a test case is run, in which the Rouse profile is calculated for a single sediment fraction using 10 vertical nodes. In this test case, the standard TELEMAC settings (with the default solver for the diffusion of tracers, which is conjugate gradient on a normal equation) resulted in a calculation time of 25 s, which reduced to 12 s in case the horizontal diffusion was switched off. In this case, the speed up is much larger. The reason is that in this case, the flow field and the concentration profile were not homogeneous, hence leading to a larger number of iterations to solve the implicit horizontal diffusion (the typical number of iterations for the matrix solver was around 10). Also in this case, the results were very similar for the cases with and without horizontal diffusion.

E. Future work

In the next phase, it is intended to change the first-order advection scheme in the *set_dif* subroutine to a second order scheme, in order to limit the numerical diffusion. Further, more attention will be paid to the stratified flow. Specifically, two issues are addressed. Hodges and Rueda [4] study the inclusion of density driven flows in a numerical algorithm rather similar to the wave-equation approach used in TELEMAC-3D [3]. They show that adding the baroclinic pressure gradient directly (such as done in TELEMAC-3D) leads to a system of equations that is unstable without any further dissipation. This means, that artificial currents can be created, when active tracers are present. Although these artificial currents are typically weak (a few cm/s), this may be a serious problem, particularly in situations where the flow is weak, such as in lakes or in the deep ocean. As a solution, they propose a prediction-corrector scheme, which is stable.

Further, it is important to calculate the baroclinic pressure gradient accurately. This can be very difficult, particularly in case the elevation of vertical layers vary in space such as when using sigma-coordinates or close to the bottom using z-double-sigma coordinates. Wang et al [7] proposed to use cubic-spline interpolation to perform accurate vertical interpolation to equal levels, in order to calculate the baroclinic pressure gradient more accurately.

It is intention to implement these two techniques in TELEMAC-3D and study whether these prevent artificial mixing of stratification in an idealized case.

V. SUMMARY AND CONCLUSIONS

In this paper, various ongoing developments in TELEMAC and TOMAWAC are presented. The presented developments are:

1.) Two-way coupling between TELEMAC-2D and TELEMAC-3D. In this task, TELEMAC-2D and TELEMAC-3D are coupled with the objective to decrease the calculation time substantially, by only applying TELEMAC-3D in the areas where three-dimensional processes are physically important. At the moment, a first test case is set up, which still shows instabilities that need to be addressed.

2.) Implementations of surface rollers in TOMAWAC. Here, an extra physical process is implemented in TOMAWAC. A first test in the littoral test case shows that the implementation changes the longshore current in a way as expected from theory.

3.) The functionality to export history files (data on a limited number of locations in the computational domain, such that typically a much higher output frequency can be used) in TELEMAC, TOMAWAC and GAIA

4.) the possibility to switch off horizontal diffusion in TELEMAC-3D, which lead to large speed-up of calculations with advected tracers.

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