SUPPORTING MARINE ENVIRONMENT RESEARCH BY MODELING

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Abstract: The Centre of Informatics – Tri-City Academic Supercomputer and Network (CI TASK) was founded over twenty-five years ago, in 1994. It was a very important initiative undertaken as a result of rapid development of computer technology and one of its main goals was to integrate the computer resources of scientific communities in the Tri-City. CI TASK started to provide computing resources and the first steps in the world of high-performance computing must have been proved to be a significant challenge. The scientific community of the Institute of Oceanology has been cooperating with that computing centre since the very beginning.

Currently, CI TASK provides the widest set of tools and hardware that can be used for ocean modeling purposes. The main goal of this work is expression of appreciation and gratitude for the people who have contributed to the developing of this institution and helped in the work using their tools. CI TASK has been helpful in a great number of past and present tasks, however, in this paper we would like to present only three results of our work – a coupled ice-ocean model of the Baltic Sea, assessment of contamination for potential leakage from chemical munition dumped after the Second World War, and the currently operating SatBaltic system.

Keywords: Modeling-Baltic Sea, coupled models, regional models, hydrodynamic modeling, eBalticGrid system, SatBaltic system

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1. Introduction

The oceans and their marginal seas cover over 70 percent of Earth's surface. The volume of these waters is approximately 1370 million km3 and they play a crucial role for life on Earth. Nearly 94 percent of the life on Earth is aquatic.

Water is home for thousands of different species of marine plants and animals. They support various branches of economy and provide us with food.

These gigantic masses of oceanic waters absorb energy, their currents transfer heat, atmospheric gases and other substances, thus exerting a strong influence on the climate and living conditions on Earth. The world's ocean is the largest heat reservoir on the planet: it is the place where 93% of the energy surplus is stored within our climate system as a result of the increasing concentration of greenhouse gases.

Nowadays, observation of the sea environment conducted to obtain high-quality physical and chemical parameters along trans-oceanic sections is done with the help of research vessels, sections, mooring buoys and satellites. Typically, these observations are carried out in a short timescale (for example, observations performed from aboard a research vessel) or as long term *in situ* measurements based on moorings placed at specific locations. It is well known that direct measurements yield the most accurate results, but conducting surveys that would be representative for each point of the ocean/sea area would be very expensive, logistically difficult, sometimes dangerous and probably impossible. Satellite images provide a lot of data, but their streams of measurements could contain some gaps, for example, resulting from the cloud cover. Furthermore, such data is often limited to the surface or subsurface water column only.

One of the basic tools used in today's oceanography for the purpose of getting to know physical processes in the oceans are numerical models. These are basically ordinary computer programs using mathematical models to describe physical processes based on the Navier-Stokes primitive equations. Solving them directly is sometimes very difficult, therefore, approximate methods of solutions are used. Thanks to numerical models, it is possible to calculate different physical parameters characterizing the ocean/sea state with the user defined resolution.

During the last decades, the development of computer technology has resulted in an increased interest in large-scale modeling as well as in improving the models.

About two decades ago, the horizontal resolution of global scale models was of the order of one degree, which corresponds to a distance of about 120 km. Currently, a standard resolution on the global scale is 1/10 degrees and the resolution of models at a regional scale has increased up to one nautical mile.

Models are currently used for making hind cast scenarios and could cover a period of a century. Also, many simulations with different CO_2 emission scenarios are provided.

Since the time when TASK was founded, the Institute of Oceanology has been performing numerical calculations on a shared architecture. The first problem solved at IOPAN where numerical methods on TASK's system were applied was Monte Carlo tracing technique in different optical aspects of oceanography.

Currently, TASK's Tryton cluster provides over 38 000 cores with peak performance close to 1.5 PFLOPS. Using shared supercomputers it is possible

to make a lot more numerical calculations. Currently, our Institute utilizes that potential in many ways:

(a) three operational systems have been implemented:

– Coupled Ecosystem Model of the Baltic Sea,
– eBalticGrid system (a coupled ice-ocean model of the Baltic Sea),
– Satellite Environment Control of the Baltic Sea (part of SatBaltic System);

(b) models are used to predict contamination by potential leakage from dumped chemical munition;

(c) data analysis from many sources;

(d) using and testing atmosphere, ocean and ice models:

– Parallel Ocean Program (POP) – a large scale ocean model,
– Community Earth System Model (a large scale coupled global system model),
– Princeton Ocean Model (a regional ocean model),
– Regional Arctic System Model (a global scale coupled system model for the Pan-Arctic domain),
– MIKE by DHI (a small scale system model).

In the section below we present only three selected issues listed above – the coupled ice-ocean model of the Baltic Sea, estimation of contamination caused by potential leakage of dumped chemical munition in the Baltic Sea and the SatBaltic System.

2. Coupled ice-ocean model of the Baltic Sea

The coupled ice-ocean model is a regional adaptation of the Community Earth System Model (CESM, [1, 2]) for the Baltic Sea. Our regional adaptation consists of two active components: the ocean model and the ice model. Although we can assume that the ice cover does not have any direct influence on the bottom currents, it is an important part of the heat and momentum budget, therefore, it should not be ignored. The main part – the ocean model – is based on the Los Alamos National Laboratory (LANL) Parallel Ocean Program (POP, [3, 4]), which evolved from the global ocean model with the added free surface formulation [5]. It is a z-level coordinate, general circulation ocean model (GCM) that solves 3-dimensional primitive equations for stratified fluid, using the hydrostatic and Boussinesq approximations. Numerically, the model computes spatial derivatives in the spherical coordinates using the finite difference technique. The arrangement of the model variables in the horizontal direction is according to the Arakawa B-grid [6].

The setup of the adapted model is presented in Figure 1.

The model was modified to ensure proper representation of the Baltic Sea [7, 8]. The main modifications and settings in the model included:

(a) biharmonic mixing was selected to represent horizontal mixing;
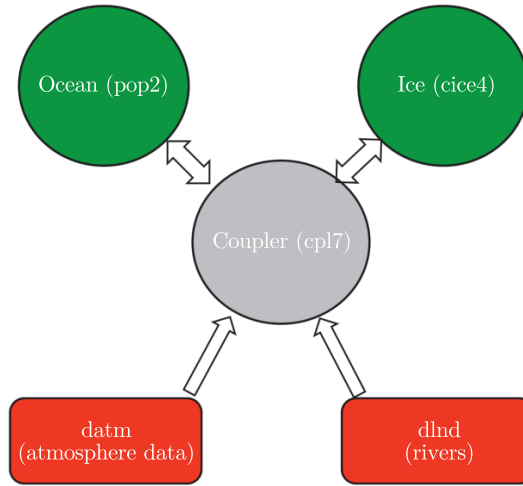
Figure 1. Set up of the Community Earth System Model adapted for the Baltic Sea (active components – green circles)

(b) vertical mixing was used as k-profile parameterization [9], but the turbulent viscosity vertical profile was modified for better fitting of local turbulences;

(c) the barotropic equation was modified to implement lateral boundaries;

(d) the roughness dependence on the cell thickness was also added;

(e) the horizontal resolution was set to 1/48 degrees;

(f) the vertical resolution for most of the Baltic Sea was 5 meters.

The model was validated against the satellite and experimental data. The hydraulic flow through Øresund is presented in Figure 2 as an example. The vertical axis presents the volume flux through the section presented and the horizontal axis was calculated as the sea level difference between the two ends of the strait. The solid line represents experimental data, the red points are derived from the model results.

It is clearly visible that the model adequately represents the hydraulic flow through Øresund. This results from the implemented quadratic drag formula – the bottom friction is proportional to the square of velocity. The sea level differences in our model are lower than the measured values. This is a consequence of free surface representation in the model. The model consists of linear approximation of the barotropic equation that requires a small free surface variability. This approach provides lower than actual sea level variation and, as a consequence, a little smaller barotropic velocity.

However, a linear approximation of the free surface formulation does not have any strong influence on the modeled results. The model quality can be obtained when comparing the snapshot. For more than twenty years our Institute has been conducting standard transect surveys from the Gulf of Gdańsk to the Arkona Basin (this section is marked on the model bathymetry shown in Figure 3).
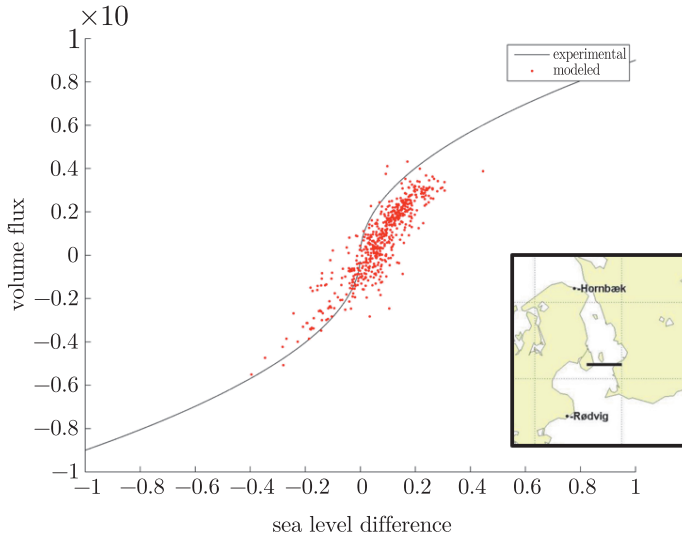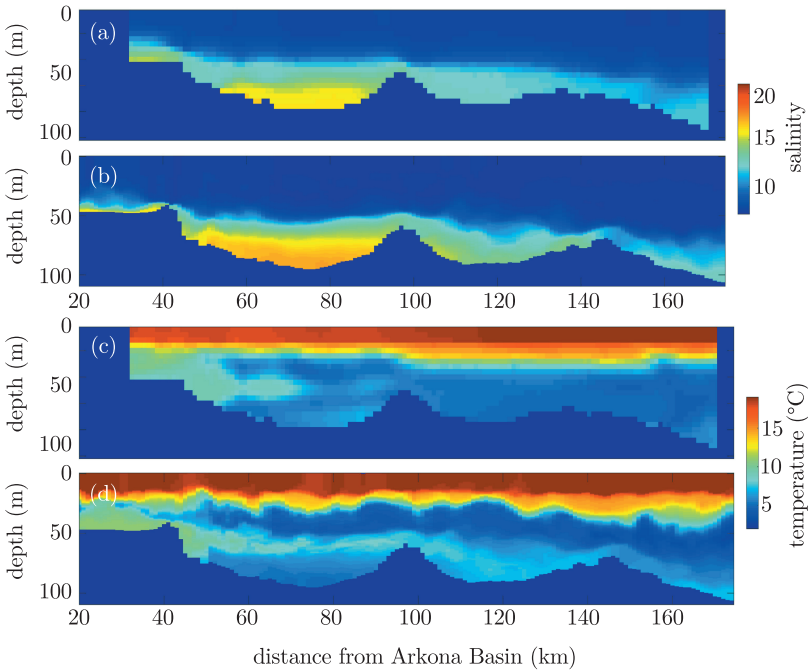
Figure 2. Hydraulic flow through Øresund (the section is shown as the insert)
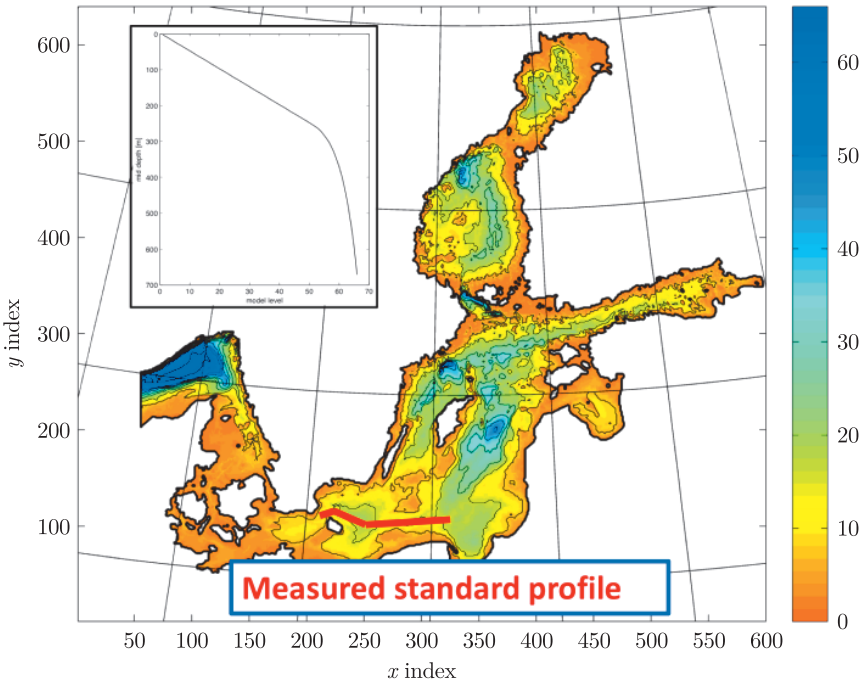
Figure 3. Model bathymetry with vertical levels (insert) and standard profile performed from R/V Oceania (red line)

These measurements provide a vertical section of temperature and salinity along the measured profile. The example of the result is shown in Figure 4.

Figure 4. Modeled ((a) and (c)) and measured ((b) and (d)) horizontal profile (shown in Figure 3) of salinity ((a) and (b)) and temperature ((c) and (d)). The section was surveyed on 15 August 2004 and the modeled data is exactly for the same date

First of all, there is a very good comparison of results from *in situ* measurements with the model. The mixed layer depth is comparable to the clean visible three layer vertical structure of the Baltic Sea. Also, there is another distinct feature visible on the profile – warm water intrusion from the Arkona Basin into the Bornholm Basin. The incoming water is of lower density than the bottom layers and moves on the halocline. Thus, the intrusion is visible in the experimental data (d) as well as in the modeled result (c). Also, the thermocline in Figure 4 (d) is oscillating along the section. This is the effect of internal waves and it is not visible or is hardly visible in the model result. As mentioned above, the model has a linear free surface representation and an additional effect of this approximation is damping the fast waves.

The second active component in our system is the ice model. It is based on the Hibler model [10] and it is called CICE (**C**ommunity **I**ce **C**od**E**). The model uses elastic-viscous-plastic ice rheology [11, 12]. The Los Alamos CICE model is the result of an effort to develop a computationally efficient sea ice component for a fully coupled global atmosphere-ice-ocean-land climate model. It was designed to be compatible with the POP for the use on massively parallel computers. CICE has several interacting components: a thermodynamic model [13] that computes local growth rates of snow and ice due to vertical conductive, radiative and turbulent fluxes, along with snowfall; a model of ice dynamics which predicts the velocity

field of the ice pack based on a model of the ice material strength; a transport model that describes advection of the ice area concentration, ice volumes and other variables of the state; and a ridging parameterization that transfers ice among thickness categories based on energetic balances and rates of strain [14]. The CICE also has multiple thickness categories and ice thickness distribution evolves over time. The sea ice model provides ice distribution in space and time. The main physical parameters are concentration, thickness, drift and internal stress. It also provides deformation and ridging rates. A comparison between the modeled and measured sea ice concentration is shown in Figure 5 as an example of the result.
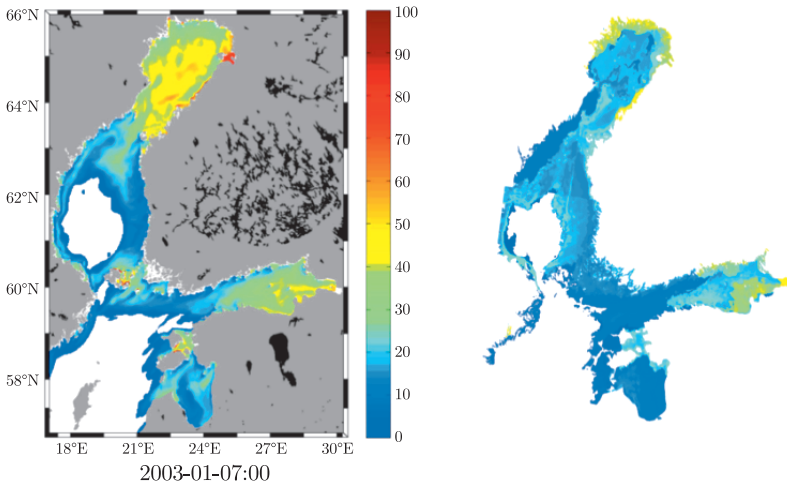
Figure 5. Modeled (left) and measured (right) sea ice concentration (2003-01-07)

The ocean model in the described system is connected to the ice model via a central coupler (cpl7). This central component controls synchronization of all the models as well as the exchange of data between the models, it reads and interpolates data, and controls domain decompositions.

The coupled ice-ocean system is forced by atmospheric data from the Weather Research and Forecasting Model (WRF). All integrations have been operating on the Tryton cluster since 2015. Access to all the data is granted by the website ebaltic.plgrid.pl developed by TASK and the Institute of Oceanology, PAS.

The system can be used to make sections, enlarge selected areas and show variability in any given points. Furthermore, it provides data to the Multi Model Ensemble project directed by the German Federal Maritime and Hydrographic Agency (BSH) and to the SatBaltic system (described below). Also, it helps to assess the contamination area from potential leakage of dumped chemical munition. Currently, we are working on adding waves from another model. It is also planned to keep the system working.

3. Estimation of the contamination caused by potential leakage from chemical munition dumped in the Baltic Sea

It is a well-known fact that after the Second World War (WWII) the Allies decided to dump residual chemical munition into the sea. The main part was dropped into selected areas of the Baltic Sea and into Skagerrak (the precise dumping sites are not known, yet based on the past investigations and available information, it is possible to indicate some main regions of dumping: Skagerrak, the Bornholm Deep, the Gdansk Bay and the Gotland Basin – Figure 6). The exact total quantity of the dumped munitions is not known. The estimation varies between 60 000 and 200 000 tons. Currently, over 70 years after WWII there is no disposition from the decision makers what to do if somebody finds residues of chemical munition. There are no directives from the Helcom Commission or from the governments of the Baltic Sea countries in case of potential leakage. However, Swedish fishermen are still obligated to have the necessary special equipment in case of trawling lumps of viscous mustard gas from the sea floor with their nets in the Gotland Deep dumpsite area.

In our study we have implemented a passive tracer into a hydrodynamic model that is a part of the coupled ice-ocean model of the Baltic Sea (with the ca. 2.3 km horizontal and 5 m vertical resolution). This model is presented here as a part of the "Coupled ice-ocean model of the Baltic Sea" [7, 8].

**Figure 6.** Chemical munition dumping areas together with ship routes

Since there are no rules or laws that would define the procedure applicable in case of finding such dangerous munition, we were trying to estimate an area of potential contamination. Thus, for us it is important how to treat leakage of dangerous material. For this purpose we have assumed that there is a threshold

that defines a dangerous situation – if the concentration exceeds the assumed threshold, it is dangerous, and lower levels are safe. Based on that, we can say that:

(a) it is important how big the area where the concentration exceeds the assumed threshold is – it will be represented by the maximum distance from the source to the place where the concentration exceeds the assumed threshold;

(b) time dependence of the maximum concentration will provide information about the time scale of this process;

(c) the trajectory of the maximum concentration provides the balance between advection and diffusion;

(d) for better understanding, the distance to the place of the maximum concentration will be also shown.

An example of the above listed parameters for a point located in the Slupsk Furrow is shown in Figure 7. Twelve simulations are shown – each one started on the first day of each month. It is important to add that a strong velocity causes a strong advection, thus, in the case of the Slupsk Furrow, the distance between the source and the location where the threshold values exceed the assumed level is not short.
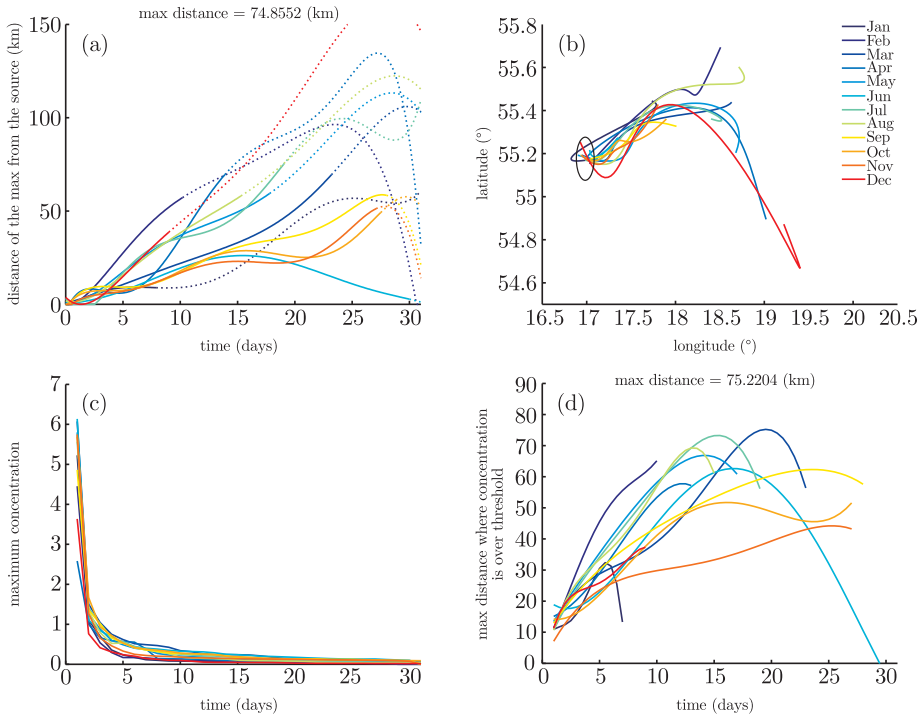
Figure 7. (a) Distance from the source to maximum tracer concentration, (b) Maximum concentration trajectories, (c) Maximum concentration vs. time, (d) Maximal range to the place where concentration is higher than the assumed threshold

This approach can be useful in the case of leakage and when operational data is available. However, when operational data is not available, it is possible to calculate the probability of contamination.

It is shown in Figure 8 (for the same location – the Slupsk Furrow). Multiplying this probability by the initial concentration provides an estimated contamination [15]. It is very important to have such distribution calculated for a selected, dangerous location – it facilitates greatly the contamination assessment, with no need to perform any calculations based on the operational system.
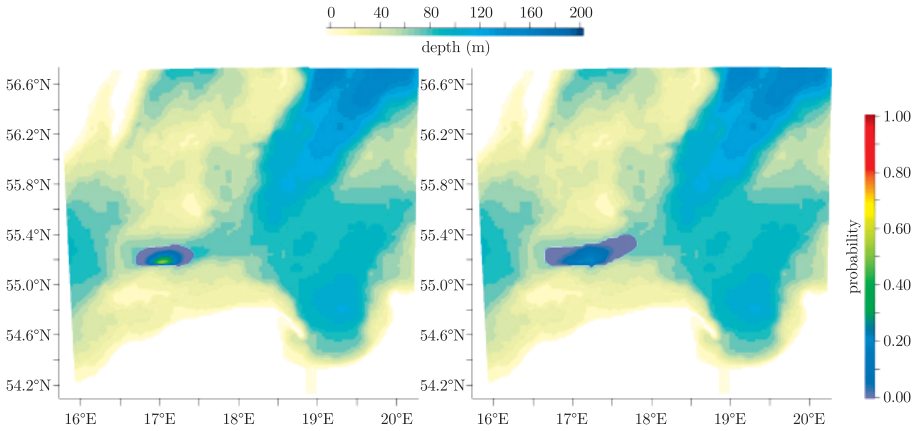
Figure 8. Probability of contamination based on the coupled ice-ocean model (left – two days after releasing, right – four days after releasing, instantaneous release)

4. Satellite Environment Control of the Baltic Sea (SatBaltic System)

The significant progress of satellite techniques made in recent years together with advances in our knowledge in various aspects of oceanography, also those related to satellite remote sensing, have made it possible for us to apply the satellite observations with much improved efficiency not only to the open oceans but also, with no less success, to other, more complex marine environments, such as the coastal waters and semi-enclosed basins. Satellite remote sensing provides relatively easy to access and cost efficient information used mainly in the climate related research, but also in many other fields, such as the marine management and industry.

However, there are still some critical environmental restrictions which limit the amount of available satellite data recorded in visible and infra-red spectral domains. The most significant, especially in European waters, is the occurrence of the cloud cover over the investigated area. Due to the cloudiness that blocks the useful signal applied in optical and infrared satellite remote sensing, the temporal coverage of the acquired data may decrease to 30% of the potentially

available information or even less in some subregions. That is a serious limitation of any operational system which is expected to provide data on a regular basis, regardless of the weather conditions. A solution can come with the support from eco-hydrodynamic models, which, if properly calibrated by satellite and *in situ* data, can fill gaps in the satellite imagery when clouds cover the investigated area.

The SatBaltic system, developed in recent years, has proposed such a solution. Merging satellite data with properly adopted models increases the accuracy of both satellite and modeled data and can provide a data stream at regular intervals, regardless of the weather conditions. The system provides a spatial distribution of a wide range of current biological, physical and chemical characteristics of the Baltic sea, together with all the historical data and short term forecast, on a daily basis. Some characteristics are provided for the very first time and has not been produced in any similar operational system. One of the greatest achievements developed and applied within the system is the advanced methodology applied for merging the satellite and modeled data in order to assure delivering operational products independently from the cloud cover over the Baltic Sea [16] (see Figure 9).
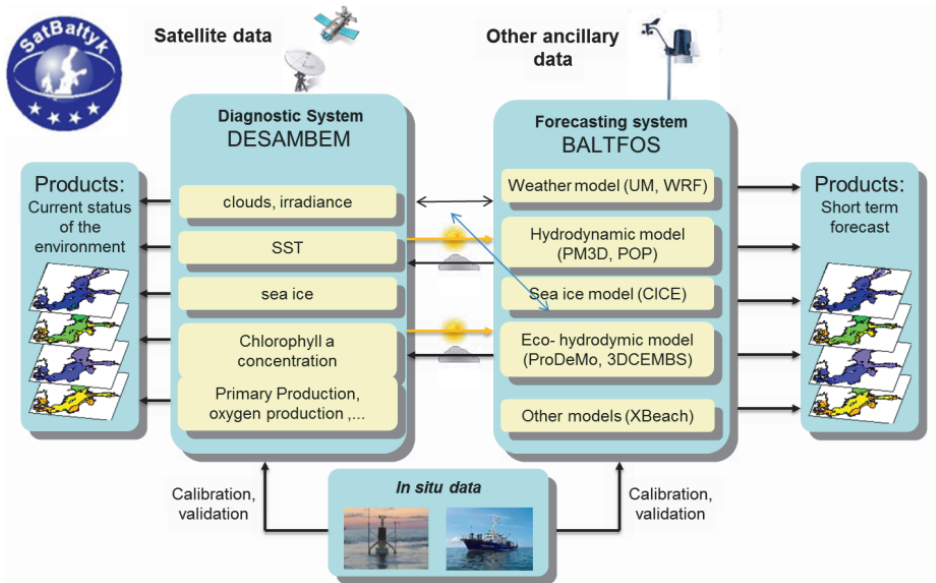

Figure 9. Schematic diagram of the SatBaltic System [17]

The system outcome consists of maps presenting the spatial distribution of more than 70 parameters (available through the SatBaltic website: `http://www.satbaltyk.pl/`, Figure 10). The parameters have been divided into the following eight groups:

(a) atmosphere, meteorology;
(b) hydrology;
(c) marine optics;

(d) energy balance;

(e) sea water components;

(f) phytoplankton, photosynthesis;

(g) coastal zone;

(h) threats.

They include the current values of the solar radiation flux into the sea at various spectral intervals, the short- and long-wave radiation budget at the sea surface and in the upper layers of the atmosphere, the sea surface temperature, dynamic states of the water surface, concentrations of chlorophyll and other phytoplankton pigments, distribution of algal blooms, the occurrence of upwelling events, the characteristics of primary organic matter production and photosynthetically released oxygen in the water, and many, many others. Additionally, historical data is available, together with a short term forecast of some of the modeled parameters.

In order to ensure the highest quality of the results obtained from the system, a network of various instruments and platforms for *in situ* measurements of a number of physical, biological and chemical parameters of the sea, have been included in the system, allowing continuous validation and calibration of the system products.
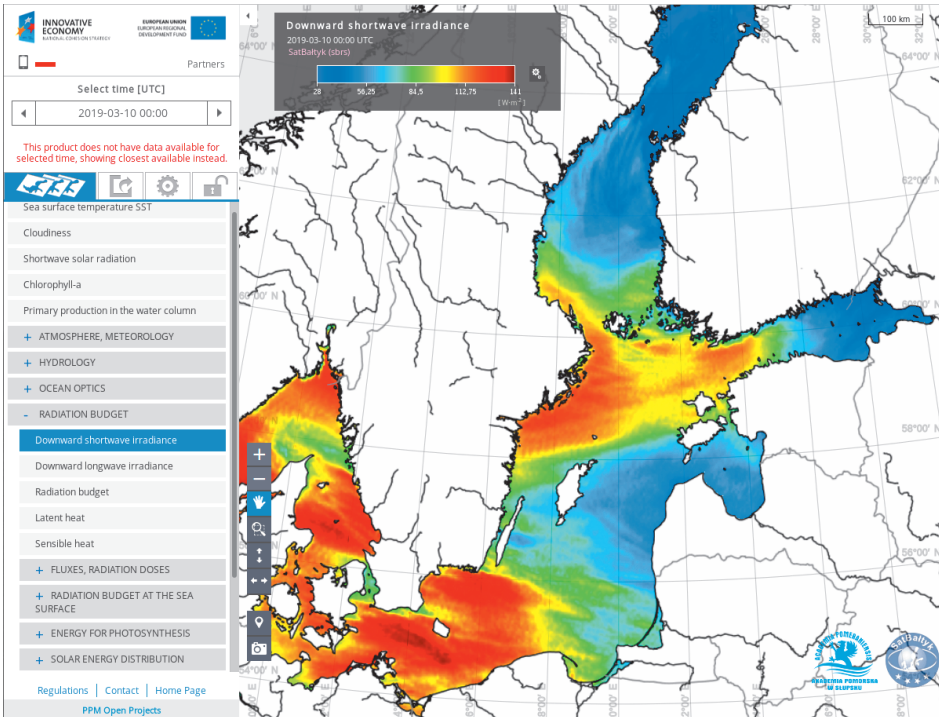

Figure 10. The SatBaltic website (`http://www.satbaltyk.pl/`)

5. Summary

The paper describes examples of different possibilities of implementing numerical modeling in physical oceanography using the CI TASK computer resources. Two of them work in the operational regime. The third one is an adaption of a passive tracer, one of the most important tools included in the ocean models for estimation of potential leakage from chemical munition dumped in the sea. The provided examples show the potential of numerical modeling in physical oceanography. The main limitations are computer resources which limit the domain size and resolution (vertical and horizontal). In spite of these limitations, the results are very promising and any improvements in the hardware performance will be consequently included in the next adaptation of modeling.

Acknowledgements

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