Adjoint-based optimization of a regional water elevation model

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Key Points:

\begin{itemize}
  \item Adjoint-based optimization is used to optimize bottom friction coefficient in 2D water elevation model for the North Sea and Baltic Sea
  \item The discrete adjoint model is automatically generated by leveraging a symbolic representation of the discrete forward model equations
  \item The optimization method is robust and results in significant improvement in the sea surface height performance at tide gauge locations
\end{itemize}

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Abstract

Calibration of unknown model parameters is a crucial task in most ocean model applications. We present an adjoint-based optimization of a bottom friction coefficient in North Sea-Baltic Sea simulation. The system is modeled with an unstructured mesh finite element shallow water model. The adjoint model provides a gradient of model misfit with respect to spatially-varying bottom friction field. A gradient-based quasi-Newton optimization method is applied to minimize the misfit. A key benefit of adjoint-based optimization is that the cost of does not depend on the number of unknown variables. Adjoint models are typically very laborious to implement manually. In this work, we leverage a domain specific language framework in which the discrete adjoint model can be obtained automatically. The adjoint model is both exactly compatible with the discrete forward model and computationally efficient. Optimizing spatially-variable parameter fields is typically an under-determined problem as there are more degrees of freedom compared to the amount of observational data which can lead to over-fitting. In this work, we employ Hessian-based regularization to penalize the curvature of the friction field to overcome this problem. We simulate the sea surface height (SSH) dynamics in the North Sea-Baltic Sea for a 3-month period in 2019. We show that the optimization process is robust and results in significant improvement of the model performance: SSH performance is comparable or better compared to existing state-of-the-art Baltic Sea models. The results are especially encouraging in the Danish Straits region, characterized by complex small-scale topography, highlighting the benefit of unstructured meshes.

Plain Language Summary

Ocean circulation models have several unknown parameters that must be tuned for each application in order to produce physically meaningful results. The tuning process can be a very laborious and time consuming task. In this paper, we investigate an automated way to tune the model’s friction at the sea bed to minimize the model’s error in predicted sea surface height. The method is based on a novel way of defining the model’s equations which enables solving such optimization problems automatically. The methodology is tested in the North Sea and Baltic Sea. The modeled sea surface height is compared against observations at several tide gauges. We show that by optimizing the bottom friction, the model’s capability to predict sea surface height improves significantly. Moreover, we show that the optimization process is robust and computationally efficient.

1 Introduction

Numerical modeling is an indispensable tool in oceanography and climate sciences. One of its major bottlenecks, however, is fitting the model state to observations. Model configuration must be carefully tuned and calibrated to replicate observational data. In addition to merely running simulations, one also needs to quantify the uncertainty of model predictions (Kalmikov & Heimbach, 2014; Loose & Heimbach, 2021), and estimate unknown parameters (Heemink et al., 2002; Zaron et al., 2011; Zhang et al., 2011; Almeida et al., 2018; Warder et al., 2022). The bottom friction coefficient, for example, is commonly regarded as an unknown free parameter in coastal applications (Zhang et al., 2011). In addition, as the amount of high-resolution observational data increases, sophisticated data assimilation methods are needed to synthesize the observation data and fill in the gaps with a physically meaningful ocean state. All of these use cases are examples of inverse modeling.

Adjoint models provide an efficient way to solve inverse modeling problems. In short, adjoint models allow evaluating the gradient of model outputs with respect to the model’s internal state, forcing fields, or parameters. The drawback is that implementing the adjoint model is technically challenging and labor intensive (Marotzke et al., 1999; Heemink et al., 2002; Vidard et al., 2015). The adjoints of the ROMS and NEMO ocean models,
for example, have been implemented manually, by differentiating each operator of the model (Moore et al., 2004; Vidard et al., 2015). Maintaining such a hard-coded adjoint, however, requires constant human intervention as the models evolve; both ROMS and NEMO adjoint models now lag behind the latest forward model versions. In the case of the MITgcm model, on the other hand, the adjoint has been derived via Automatic Differentiation (AD), i.e. by differentiating the Fortran source code automatically (Marotzke et al., 1999). Despite the automation, however, this procedure imposes constraints on the way the model code is written, requires significant expert intervention, and may result in an inefficient adjoint code (Vidard et al., 2015). For the majority of ocean models, adjoint capability is not available and inverse problems are difficult to solve, e.g. one has to rely on ensemble runs to obtain statistical estimates of the model’s sensitivity.

Adjoint models come in two flavors, continuous and discrete adjoints. In the former, the adjoint equations are derived directly from the continuous model equations and then discretized with a method of choice (e.g. finite volume (FV) or finite element (FE) method). In the discrete adjoint case, on the other hand, one differentiates the discrete (e.g. FV/FE) equations to derive an adjoint that is exactly compatible with the discrete forward model. Differentiating the model source code, as in the case of AD, also results in a discrete adjoint. There are advantages and disadvantages to both continuous and discrete adjoint approaches (Sirkes & Tziperman, 1997). For example, the continuous adjoint approach is flexible in the sense that the user is able to choose different discretization methods for the forward and adjoint equations, but comes with the burden of being tedious and error-prone to implement. The discrete adjoint approach, on the other hand, is less flexible, but involves little or no user effort and produces gradients that are exactly compatible with the discretized forward model. This is greatly beneficial in applications – such as the one considered in this paper – where gradient-based optimization methods are used, since the convergence of such methods is ensured.

In this work, we use an unstructured mesh FE ocean model, Thetis (Kärnä et al., 2018), for which the discrete adjoint model can be derived automatically. Thetis has been implemented in the generic Firedrake FE modeling framework (Rathgeber et al., 2016). Firedrake uses a domain specific language (Unified Form Language, (Alnæs et al., 2014)) to describe the FE weak forms. An automated code generator (Homolya et al., 2018) is then used to generate C code to evaluate the terms of the weak form. The equations are assembled as a linear system and solved in parallel with the PETSc solver library (Balay et al., 2021). Leveraging the symbolic representation, it is possible to derive the discrete adjoint model automatically by differentiating the symbolic FE equations (Farrell et al., 2013). The pyadjoint library handles the taping of the solve calls, solving the adjoint equation and evaluating the gradient of the cost function.

We use the discontinuous Galerkin FE 2D shallow water implementation of the Thetis model (Kärnä et al., 2018) to simulate tidal and atmospherically-driven water elevation dynamics in the North Sea and the Baltic Sea. Our primary focus is on the Baltic Sea and the Danish Straits, but as the North Sea is tightly coupled to the dynamics, the two seas must be simulated as a single dynamical system (Kärnä et al., 2021). We use the adjoint model to optimize the model’s bottom friction coefficient to improve the representation of water elevation dynamics with respect to tide gauge observations.

The two seas exhibit quite different water elevation dynamics. The North Sea is a tidal system with semi-diurnal tides. Tidal range varies from over 6 m in the English channel to roughly 0.4 m in Skagerrak. Tides are effectively filtered out in the Danish waters and only weak tides (<10 cm range) are observed in the Baltic Sea. The atmospherically-induced water elevation gradient across the Danish Straits controls the water volume exchange to and from the Baltic Sea in synoptic and longer time scales. Consequently, water elevation in the Baltic Sea is mainly governed by episodic filling and emptying of the basin, storm surges as well as atmospherically-generated seiche oscillations (coastal Kelvin waves).
Previously adjoint models have been used in several coastal ocean applications. Almeida et al. (2018) use the Delft3D-FLOW model to simulate a section of the Columbia River. A continuous adjoint was implemented for the model and used to optimize the model’s bathymetry based on surface velocity measurements. As the continuous adjoint model does not match exactly with the discrete forward model, a careful solution strategy was devised to avoid numerical instabilities.

Heemink et al. (2002) presented an adjoint-based inverse model of a 3D shallow water model and used it to optimize bottom friction, vertical viscosity coefficient and bathymetry in an application to the European Continental Shelf. The adjoint model was implemented manually. A common problem in parameter estimation is that the problem is typically underdetermined: in the case of a spatially-varying parameter field, there are far too many degrees of freedom compared to the amount of observation data. Heemink et al. (2002) reduced the dimensionality of the problem by allowing the parameter fields to vary only in predefined subdomains of the model grid. The choice of subdomains was informed by inspecting the gradient of the cost function, calculated with the adjoint, and also expert knowledge of the system dynamics (e.g., amphidromic points).

Zhang et al. (2011) used a shallow water adjoint model to optimize constant and spatially-variable bottom friction coefficient for the Bohai Sea and Yellow Sea. Also here, the dimensionality of the problem was reduced by optimizing the friction values only in a sparse subset of the model grid points and using linear interpolation in between.

Besides inversion and optimization of uncertain model parameters, the availability of adjoint-based gradient information of specified outputs of interest in an ocean model, has a large number of other potentially powerful applications. The gradient can be used in sensitivity analyses to provide invaluable insight in the sensitivity of the model with respect to various inputs, and estimate uncertainties in the outcomes. Warder et al. (2021) studied the spatial and temporal sensitivities of a storm surge model of the North Sea with respect to bottom friction, bathymetry and wind forcing using Thetis and its automated adjoint. In coastal engineering applications the adjoint can be used to drive the design optimization of engineering structures and their interaction with the coastal environment. As an example, the automated adjoint derived through the same pyadjoint approach has been used to study the optimal placement of a large number of tidal turbines in (Funke et al., 2014, 2016; Goss et al., 2021). The flexibility of this symbolic language approach allows for easy extension of the adjoint calculations to coupled models implemented in the same framework – as demonstrated in (Clare et al., 2022) where inversion and sensitivity analyses where performed with Thetis coupled to a morphodynamic model. Finally, adjoint sensitivity information can be used for goal-oriented error estimation in mesh adaptation approaches where the mesh is adapted to optimize the model accuracy for a specified quantity of interest, as demonstrated within the Thetis model in (Wallwork et al., 2020).

The novelty of the present work can be summarized as follows. First, we leverage a domain specific language modeling framework in which the discrete adjoint model and the evaluation of the gradient of the cost function can be obtained automatically. Therefore the user only needs to implement the forward model and the cost function. Second, we use regularization to constrain the underdetermined bottom friction optimization problem, i.e. we optimize a spatially-varying friction field but include an additional term in the cost function to penalize the second derivatives of the field to control its smoothness. We show that the optimization procedure works well in a large and complex North Sea-Baltic Sea domain that exhibits water elevation variability across several time scales. The present work is therefore a step toward automated model calibration methodology that does not require manual implementation of the adjoint model, running expensive ensemble simulations, or extensive expert knowledge of the system dynamics.
The 2D shallow water model and its discretization is presented in Section 2. The variational inverse problem and its application to bottom friction optimization is presented in Section 3. Section 4 outlines the model configuration for the North Sea-Baltic Sea, followed by results, discussion, and conclusions in Sections 5, 6, 7, respectively. Further details on the forward and inverse modelling techniques are provided in Appendix A and Appendix B.

2 Shallow-water model

Denoting the free surface elevation and depth averaged velocity by \( \eta \) and \( \mathbf{u} = (u, v) \), respectively, the shallow water equations in non-conservative form read

\[
\frac{\partial \eta}{\partial t} + \nabla \cdot (H \mathbf{u}) = 0
\]

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + f \mathbf{e}_z \wedge \mathbf{u} + g \nabla \eta + \frac{1}{\rho_0} \nabla p_a = D \mathbf{u} + \tau_w + \tau_b
\]

where \( H = \eta + h \) is the total water column depth, \( h \) is the bathymetry, \( f \) is the Coriolis parameter, \( \mathbf{e}_z \) an upward vertical unit vector, \( g \) the gravitational acceleration, \( \rho_0 \) the constant reference water density, \( p_a \) the atmospheric pressure, \( D \mathbf{u} = \nabla \cdot (\nu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \) is the viscosity operator and \( \nu \) is the horizontal eddy viscosity, \( \tau_w \) and \( \tau_b \) denote the surface (wind) and bottom stresses, respectively.

In this work, we use the wind stress formula by Large and Yeager (2008):

\[
\tau_w = C_{DW} |\mathbf{u}_w| \mathbf{u}_w
\]

\[
C_{DW} = \begin{cases} a_1 \frac{|\mathbf{u}_w|}{|\mathbf{u}_w|} + a_2 + a_3 |\mathbf{u}_w| + a_8 |\mathbf{u}_w|^6, & |\mathbf{u}_w| < 33 \text{ m/s}, \\ 0.00234, & \text{otherwise} \end{cases}
\]

where \( \mathbf{u}_w \) stands for the wind velocity at 10 m height; the \( a_i \) coefficients are defined in Large and Yeager (2008).

The bottom friction is parametrized by the Manning formula,

\[
\tau_b = C_D |\mathbf{u}| \mathbf{u}
\]

\[
C_D = \frac{g \mu^2}{H^{1/3}}
\]

where \( \mu \) is the Manning friction coefficient. Generally \( \mu \) can be regarded as an unknown, spatially-variable, model and mesh-dependent parameter.

2.1 Finite element discretization

We use the Thetis model implementation of the shallow water equations (Kärnä et al., 2018). The 2D model domain and its boundary are denoted by \( \Omega \) and \( \Gamma \), respectively. The boundary consists of open ocean (\( \Gamma_o \)) and closed land (\( \Gamma_c \)) parts, i.e. \( \Gamma = \Gamma_o \cup \Gamma_c \).

Thetis supports several finite element families. In this work, the equations are discretized with linear discontinuous (DG\(_1\)) finite elements (see Fig. 1). The same element is used for both of the prognostic fields, \( \eta \) and \( \mathbf{u} \). Let \( \phi \) and \( \phi \) denote the scalar and vector valued test functions in the DG\(_1\) function space. The weak form of the shallow water problem is obtained by multiplying the governing equations (1-2) by the test functions \( \phi \) and \( \phi \), respectively and integrating over the domain \( \Omega \):

\[
\int_{\Omega} \frac{\partial \eta}{\partial t} \phi \, dx + S_{\text{div}} = 0, \quad \forall \phi
\]

\[
\int_{\Omega} \frac{\partial \mathbf{u}}{\partial t} \cdot \phi \, dx + S_{\text{adv}} + S_{\text{cor}} + S_{\text{pg}} + S_{\text{pa}} = S_{\text{visc}} + S_{\tau}, \quad \forall \phi.
\]
Figure 1. Finite elements: a) linear continuous; b) linear discontinuous; and c) quadratic continuous scalar element. The dots denote scalar degrees of freedom. For vector-valued fields, each component is stored as a scalar.

The bilinear forms of each term, $S_\cdot$, are defined below.

Let $T$ stand for the triangulation of the domain $\Omega$. The set of element interfaces is denoted by $\mathcal{I} = \{ k \cap k' \mid k, k' \in T \}$, and $\mathbf{n} = (n_x, n_y)$ denotes the outward unit normal vector of an interface $e \in \mathcal{I}$. On the interfaces, the $DG_1$ functions are discontinuous and do not have a unique value. We define the average and jump operators,

\[ \{a\} = \frac{1}{2}(a^+ + a^-), \]
\[ [a \mathbf{n}] = a^+ \mathbf{n}^+ + a^- \mathbf{n}^-, \]
\[ [u \cdot \mathbf{n}] = u^+ \mathbf{n}^+ + u^- \mathbf{n}^-, \]
\[ [u \mathbf{n}] = u^+ \mathbf{n}^+ + u^- \mathbf{n}^-, \]

where the superscripts ‘+’ and ‘−’ arbitrarily label the values on either side of the interface, and $\mathbf{n}^- = -\mathbf{n}^+$. 

The $Hu$ divergence term is integrated by parts:

\[ S_{div} = -\int_\Omega H(u \cdot \nabla \phi) \, dx + \int_\mathcal{I} (H'u^*) \cdot [\phi \mathbf{n}] \, dS + \int_{\Gamma_o} (Hu) \cdot \phi \mathbf{n} \, dS \]  

where $H'$ and $u^*$ denote the interface terms obtained from an approximate Riemann solver defined below. Note that the $Hu$ flux vanishes on the closed boundary $\Gamma_c$.

The advection term is also integrated by parts (also here the flux across $\Gamma_c$ vanishes):

\[ S_{adv} = -\int_\Omega \nabla_h \cdot (u \phi) \cdot u \, dx + \int_\mathcal{I} \{u\} \cdot [\phi(u \cdot \mathbf{n})] \, dS + \int_{\Gamma_o} u \cdot \phi(u \cdot \mathbf{n}) \, dS. \]

The Coriolis and atmospheric pressure gradient terms read

\[ S_{cor} = \int_\Omega f e_z \wedge u \cdot \phi \, dx, \]
\[ S_{pa} = \int_\Omega \frac{1}{\rho_0} \nabla p_a \cdot \phi \, dx. \]

The pressure gradient term is integrated by parts
\[
S_{pg} = -\int_{\Omega} g\eta \nabla \cdot \phi \, dx + \int_{\mathcal{I}} g\eta^* [\phi \cdot n] \, dS + \int_{\Gamma} g\eta \phi \cdot n \, dS.
\] (17)

The viscosity operator is discretized with the interior penalty method (Riviè re, 2008; Hillewaert, 2013):

\[
S_{\text{visc}} = \int_{\Omega} (\nabla \psi) : \tau_v \, dx - \int_{\mathcal{I}} [\psi n] \cdot [\tau_v] \, dS - \int_{\Gamma} \nu \nabla (H) \cdot (\nabla u + (\nabla u)^T) \cdot \phi \, dx.
\] (18)

\[
- \int_{\mathcal{I}} \nu [\psi n] \cdot [\nabla \psi] \, dS + \int_{\mathcal{I}} \sigma [\psi n] \cdot [\psi n] \, dS
\] (19)

\[
- \int_{\Omega} \nu \nabla (H) \cdot (\nabla u + (\nabla u)^T) \cdot \phi \, dx
\] (20)

where \( \tau_v = \nu \nabla u \) denotes the viscous flux. The last term is an additional source term that accounts for the bathymetry gradient. The viscous flux is zero on \( \Gamma_c \) and on \( \Gamma_o \).

Finally, the surface and bottom stress terms are given by

\[
S_T = \int_{\Omega} \frac{\tau_w + \tau_b}{H \rho_0} \cdot \phi \, dx.
\] (21)

In this work, we use the Roe fluxes to stabilize the \( S_{div} \) and \( S_{pg} \) terms:

\[
\eta^* = \{\eta\} + \sqrt{\frac{g}{H}} [u \cdot n]
\] (22)

\[
u^* = \{u\} + \sqrt{\frac{H}{g}} [\eta n]
\] (23)

\[
H^* = \eta^* + h.
\] (24)

The spatial integrals are evaluated with a standard Gauss quadrature rule of degree 3. Denoting the individual DG1 basis functions by \( \phi_i \) and \( \phi_i \), the discrete FE representation of \( \eta \) and \( u \) fields are \( \eta^h = \sum \eta_i \phi_i \) and \( u^h = \sum u_i \phi_i \), where \( \eta_i \) and \( u_i \) are the nodal values. The model state (dual) vectors are \( \eta^h = (\eta_1, \eta_2, \ldots) \), \( u^h = (u_1, u_2, \ldots, v_1, v_2, \ldots) \); the concatenated state vector is denoted by \( q_i = (u_i, \eta_i) \). Replacing the test functions in (7-8) by \( \phi_i \) and \( \phi_i \), respectively, the equations can be written in a vector form:

\[
\mathbf{M} \frac{\partial q_i^h}{\partial t} = \mathbf{S}(q^h),
\] (25)

where \( \mathbf{M} \) denotes the 3-block DG1 mass matrix, i.e. \( \mathbf{M} = \text{diag}(\mathbf{M}_\phi, \mathbf{M}_{\phi}, \mathbf{M}_{\phi}) \) and \( [\mathbf{M}_{\phi}]_{i,j} = \int_\Omega \phi_i \phi_j \, dx \), and \( \mathbf{S} \) denotes the remaining bilinear forms. Hereafter we omit the \( h \) superscript for brevity.

### 2.2 Time integration

The solution is marched in time with a fully implicit Runge-Kutta scheme. In this work, we use the two-stage, 2nd order accurate Diagonally Implicit Runge Kutta method DIRK(2,2), defined by the Butcher tableau (Ascher et al., 1997),
\begin{equation}
\begin{pmatrix}
c_1 \\
c_2 \\
\end{pmatrix}
\begin{pmatrix}
a_{1,1} & 0 & \gamma \\
a_{2,1} & a_{2,2} & 1 - \gamma \\
\end{pmatrix}
\begin{pmatrix}
g \\
p \\
\end{pmatrix}
\begin{pmatrix}
\gamma \\
0 \\
\end{pmatrix}
\begin{pmatrix}
1 \\
1 - \gamma \\
\end{pmatrix}
\end{equation}

with $\gamma = (2 - \sqrt{2})/2$.

Denoting the solution at time $t^n$ by $q^n$, and intermediate solutions by $q^{(i)}$, the $m$-stage DIRK iteration reads

\begin{align}
q^{(0)} &= q^n, \\
M q^{(i)} &= M q^{(i-1)} + \Delta t \sum_{j=1}^{i} a_{i,j} S(q^{(j)}), \quad \forall i = 1, \ldots, m, \\
q^{n+1} &= q^{(m)},
\end{align}

For brevity, we denote the entire nonlinear forward model update operator by $F$, i.e.

\begin{equation}
F(q^{n+1}, q^n) = 0.
\end{equation}

Agglomerating the model state over all $N$ time steps into a single vector $Q = (q^0, \ldots, q^N)$, we can re-write the entire forward operator as

\begin{equation}
F(Q) = 0.
\end{equation}

Note that the $F$ operator is only introduced to simplify notation, it is never assembled. Indeed, $F$ consists of nonlinear solves and it can only be evaluated by iterating over the time steps. As seen in (30), the forward update depends on past values of the model state. Let $\tilde{F}$ denote a linearized forward operator. Due to the time dependency, $\tilde{F}$ could be assembled into a lower-diagonal matrix operator. In what follows, we’ll see that the adjoint model requires a transpose of $\tilde{F}$, therefore reversing the time dependency.

\section{Variational inverse problem}

The forward model depends on some unknown parameters, $\theta$, that need to be estimated, i.e. $F = F(Q, \theta)$. Let $J$ denote the user-defined, scalar-valued cost function we aim to minimize. The inverse optimization problem then reads

\begin{equation}
\min_{Q, \theta} J(Q, \theta), \quad \text{subject to } F(Q, \theta) = 0.
\end{equation}

The minimization problem can be solved with standard gradient-based optimization methods provided that one can compute the gradient of $J$:

\begin{equation}
\frac{dJ}{d\theta} = \frac{\partial J}{\partial Q} \frac{dQ}{d\theta} + \frac{\partial J}{\partial \theta}.
\end{equation}
Figure 2. Automated generation of the discrete adjoint model. The forward model updates the model state, \( q \), forward in time while the adjoint model iterates the adjoint variable, \( \lambda \), backward in time.

The latter term on the right hand side can be obtained by differentiating \( J \) symbolically. The first term is unknown and can be computed from the discrete adjoint equation,

\[
\frac{\partial \tilde{F}^T}{\partial L} = \frac{\partial J^T}{\partial Q},
\]

(34)

where \( L = (\lambda^0, \lambda^1, \ldots, \lambda^N) \) is the time-agglomerated adjoint variable and \( \tilde{F}^T \) is the transpose of the linearized forward model. The adjoint variables, \( \lambda^n \), have the same dimension as the model state, \( q^n \). That is, for the model state variables, \( \eta^n \) and \( u^n \), we have corresponding spatially and temporally varying adjoint fields. Note that due to the transpose, the adjoint equation must be solved backward in time (see Fig. 2).

Once \( L \) is known, the gradient of \( J \) can be computed:

\[
\frac{dJ}{d\theta} = -L^T \frac{\partial \tilde{F}}{\partial \theta} + \frac{\partial J}{\partial \theta}.
\]

(35)

The adjoint method is attractive as the cost of solving the adjoint equation, and hence evaluation of the gradient, does not depend on the number of unknown parameters, \( \theta \). This is in contrast to many other inverse modeling techniques such as finite difference approximation, the tangent linear model, or ensemble methods, where computational cost increases with the number of control variables.

With the pyadjoint library, the adjoint equation can be derived automatically (Farrell et al., 2013). Leveraging symbolic representation of the finite element discretization, (31), the adjoint equation is formed by differentiating the forward equations (Fig.2); a similar procedure is used to compute \( \partial \tilde{F}/\partial \theta \) and \( \partial J/\partial \theta \).

The time-dependent forward problem is solved first, and pyadjoint is used to record the sequence of forward solve operations on tape. The adjoint equation (34) is solved backward in time by rewinding the tape and applying the linearized adjoint operators (Fig.2). Once the adjoint variables, \( \lambda^n \), are known, \( dJ/d\theta \) can be evaluated.

Automated generation of the discrete adjoint model circumvents two major bottlenecks in adjoint modeling: First, implementing the adjoint model by hand is tedious,
often comparable to the cost of implementing the forward model itself. Thus most ocean models do not have adjoint capability, or the adjoint model tends to be poorly maintained as new features are added to the forward model. Second, we utilize the same code generator as with the forward model to obtain optimized low-level implementation for the adjoint model. Thus the adjoint is computationally efficient, in contrast to traditional automatic differentiation methods, for example, where one transposes every low-level code operation and the resulting adjoint implementation is often far from optimal (Vidard et al., 2015).

The presented inverse modeling procedure resembles the so-called four-dimensional variational assimilation (4D-Var) method (Le Dimet & Talagrand, 1986) widely used in geophysical applications. Compared to simpler methods (e.g. 3D-Var), the time dependency is consistently treated with the forward-backward solution procedure. In addition, the constraint (31) ensures that the solution always satisfies the model equations which is not the case in some (e.g. nudging) methods. One notable difference is that many existing 4D-Var implementations use the tangent linear model or ensemble methods to estimate the gradient which is generally more expensive compared to solving the adjoint equation.

Utilizing the gradient \( \frac{dJ}{d\theta} \), the optimization problem (32) is solved with a quasi-Newton method where the Hessian of \( J \) is estimated during the iteration. The convergence of the quasi-Newton method depends on several factors, e.g. nonlinearity of the problem and smoothness of the cost function. In this work, we employ additional regularization to ensure smoothness of the spatially-variable parameter field, \( \theta \).

### 3.1 Water elevation optimization

In this work, we minimize the model misfit with respect to water elevation observations by varying the Manning bottom friction coefficient field.

Let \( \eta_{o,i}^n, i = 1, \ldots, B, n = 1, \ldots, N \) denote the observation time series at \( B \) tide gauges. The model elevation field is interpolated in space at the tide gauge locations, resulting in corresponding modeled time series \( \eta_{m,i}^n \). If a tide gauge lies outside the model domain, a nearest element center is used. Time-averaged time series are denoted by \( \tilde{\eta}_{o,i} = \sum_n \eta_{o,i}^n / N \) and the bias-removed (centered) time series by \( \hat{\eta}_{o,i}^n = \eta_{o,i}^n - \tilde{\eta}_{o,i} \). The standard deviation of observations is given by \( (\sigma_{o,i})^2 = \sum_n (\hat{\eta}_{o,i}^n)^2 / N \). The Centered Root Mean Square Deviation (CRMSD) is

\[
(\text{CRMSD}_i)^2 = \frac{1}{N} \sum_{n=1}^{N} (\hat{\eta}_{m,i}^n - \hat{\eta}_{o,i}^n)^2. \tag{36}
\]

The cost function is then defined as

\[
J_o(Q, \theta) = \frac{1}{B} \sum_{i=1}^{B} \frac{1}{(\sigma_{o,i})^2} (\text{CRMSD}_i)^2, \tag{37}
\]

where \( T \) denotes the duration of the simulation in seconds.

Note that the misfit \( J_o \) is computed with the centered time series \( \hat{\eta}_{j,i}^n, j \in \{o, m\} \). This is necessary because the model exhibits an SSH offset with respect to the observations that is not known a-priori. The model bias \( \tilde{\eta}_{m,i} - \tilde{\eta}_{o,i} \) is affected by the bathymetry (defined approximately with respect to the mean sea level), river discharge, the SSH bias at the open boundary, simulated water transport between basins, and the reference level of the observations. Furthermore, the cost function is scaled by the inverse variance of the observations to ensure similar weight across the tidal and non-tidal tide gauges, for example. Indeed, the SSH variability (standard deviation) exceeds 3 m in the English
channel while only being a few centimeters in the Baltic Sea. Consequently, $J_o$ is equivalent to the variance of the model error normalized by the observation variance.

The control variable, $\theta$, is the spatially varying Manning bottom friction coefficient field. The Manning field is discretized in space with continuous linear elements (Fig. 1a). It is known that the optimization problem is ill-posed, i.e. there exist infinitely many Manning coefficient fields that minimize the cost function, $J_o$ (Zhang et al., 2011). In addition, $J_o$ typically exhibits multiple local minima that prevent convergence to the global optimum. To this end, we use spatial regularization to penalize local variability of the $\theta$ field, i.e. we augment the cost function with a regularization term $J_r(\theta)$,

$$
J(Q, \theta) = J_o(Q, \theta) + J_r(\theta) \tag{38}
$$

$$
J_r(\theta) = \alpha\|\mathcal{H}(\theta)(\Delta x)^4\|_2^2, \tag{39}
$$

where $\mathcal{H}(\theta)$ denotes the Hessian of the control field, $\|\cdot\|_2$ is the $L_2$ norm, $\Delta x$ is the local mesh element size, and $\alpha$ is an unknown regularization parameter. The scaling by $\Delta x$ means that we effectively penalize the $\theta$ variability within each element: $\partial \theta/\partial x \Delta x \approx \Delta \theta$. This regularization term ensures that the Manning coefficient field remains smooth while higher variability is allowed in regions with high mesh resolution. The finite element implementation for computing $\mathcal{H}(\theta)$ is presented in Appendix B. In addition to $J_r$, our tests indicated that it is necessary to use a sufficiently long optimization period $T$ to avoid over-fitting.

The optimization problem (32) is solved with the L-BFGS-B quasi-Newton method with bound constraints (Byrd et al., 1995) from the SciPy package (Virtanen et al., 2020). During the iteration, we impose bounds $10^{-3}$ s m$^{-1/3} \leq \mu \leq 5^{-1}$ s m$^{-1/3}$ for the Manning coefficient field; in practice the upper bound is never reached.

4 North Sea – Baltic Sea simulation

We apply the 2D shallow water model to the North Sea and Baltic Sea to simulate tidal and atmospherically-driven water elevation dynamics. The two seas are tightly coupled via the narrow and shallow Danish Straits (Fig. 3; Kärnä et al. (2021)).

4.1 Model configuration

The model domain covers the North Sea and Baltic Sea (Fig. 3). The open boundary is placed beyond the continental shelf to allow reliable imposition of the tides due to greater water depth and weaker currents (Heemink et al., 2002; de Brye et al., 2010). In addition, the domain is sufficiently large so that most atmospherically-driven events, such as storm surges, can be generated within the model.

Fig. 4 presents the triangular unstructured mesh, generated with GMSH (Geuzaine & Remacle, 2009). We first defined a scalar field indicating the desired mesh resolution across the domain. The coastal boundary line was extracted from the bathymetry raster at the 0.5 m contour. In order to generate a smooth coastline, the bathymetry was first smoothed with a Gaussian filter; stronger smoothing was applied in regions with coarser desired mesh resolution. This procedure ensures that the coastline is compatible with the bathymetric data and also appropriate for the intended mesh resolution. Higher mesh resolution is used along the coasts and especially in the Danish waters to better capture the complex geometry; resolution progressively decreases towards the open boundary.

Bathymetric data originates from the 1/16 arc minute EMODnet 2020 dataset (EMODnet Bathymetry Consortium, 2020). A second order $P_2$ discretization (Fig. 1c) is used for the bathymetry field, $h$, in order to improve the representation of small-scale features,
Figure 3. Model domain and bathymetry; (a) entire domain, (b) the Baltic Sea, and the (c) Danish Straits region. Red dots indicate tide gauge locations.

Figure 4. Triangular mesh of the model domain. The mesh consists of 53,558 elements whose size ranges from roughly 500 m to 23 km.
such as narrow channels in the Danish Straits. During our initial tests we noted that the geometry and bathymetry of the channels play an important role in both the volume flux between the North Sea and Baltic Sea, as well as the reflection and refraction of tides in the region. The procedure of generating the $P_2$ bathymetry field is described in Appendix A.

At the open boundary, the model is forced with the TPXO 9 (v1) global tidal model (Egbert & Erofeeva, 2002) using all 15 constituents. We impose only tidal water elevation; water velocity is relaxed towards zero using the Roe fluxes. Subtidal SSH variation is not imposed. This configuration was found to be sufficient to represent both the mean SSH and atmospherically-driven SSH variability in the region of interest (i.e. the Danish Straits and the Baltic Sea).

A constant-in-time river discharge is imposed at 428 major rivers across the domain. The mean river discharge was computed from the EHYPE watershed model (Donnelly et al., 2015) hindcast data.

Atmospheric wind stress and mean sea level pressure are imposed from the 2.5 km MetCoOp Ensemble Prediction System (MEPS) data obtained from the Norwegian Meteorological institute. The MEPS data set does not cover the western and southwestern parts of the model domain where the European Centre for Medium-range Weather Forecasts (ECMWF) HRES forecast data is used instead. The datasets are blended together in a 50 km overlapping region using a linear blending mask. Wind stress is computed with the (Large & Yeager, 2008) formulation from 10 m winds. The atmospheric pressure and wind stress fields are discretized with linear continuous $P_1$ elements (Fig. 1 a). Viscosity was set to a constant $5 \text{ m}^2/\text{s}$ throughout the domain.

The model time step was set to 1 h. The time step was chosen to minimize computational cost: A fully implicit solver allows longer time steps and can therefore reduce computational cost significantly (Kärnä et al., 2011). However, using a $\Delta t > 1$ h resulted in slower convergence of the solver and thus higher overall cost. Using 1 h time step for modeling tidal dynamics is appropriate as we are using a second-order implicit Runge-Kutta solver which can represent nonlinear processes accurately. In addition, during the Runge-Kutta sub-iteration, all forcing fields are evaluated twice in each time step which, again, increases the accuracy. Our preliminary tests did not show any significant deterioration of the SSH performance with 1 h time step (not shown). We did notice, however, that the commonly-used, asymptotically unstable Crank-Nicolson time integrator did exhibit numerical instability manifested in a noisier velocity field.

The modeled SSH is compared against tide gauge observations at 56 tide gauges across the model domain (Fig. 3). The observational data was obtained from the Copernicus Marine Service (CMEMS) catalog (E.U. Copernicus Marine Service, 2015b, 2015a). Only tide gauges that had nearly complete data coverage over the modeled period were included. The tide gauge time series were manually quality-checked to remove spurious SSH values (e.g., spikes).

### 4.2 Simulation period and initial condition

The Manning coefficient is optimized for a 16.5 day period, spanning from June 1 00:00 UTC to June 17 12:00 UTC, 2019. To exclude initial adjustment effects from the optimization, the cost function is not evaluated during the first 2.5 days, i.e. the model misfit is calculated over a 14-day period. This period is henceforth called the optimization period.

On June 1, 2019, the model is initialized from a spun-up initial state. Using a realistic initial condition is important for the optimization process. According to our sensitivity runs, the mean SSH in the Baltic Sea reaches an equilibrium in roughly 1 month
(not shown) and this transient adjustment must be excluded from the optimization process as it would skew the results. Moreover, a relatively good guess for the Manning field is needed for the spin-up as bottom friction affects the volume flux to/from the Baltic Sea and therefore the mean SSH. The initial condition was generated as follows: First, 10 iterations of the optimization process are carried out starting the model from rest (zero initial water elevation and velocity; the Manning coefficient was set to 0.03 s m\(^{-1/3}\) initially). As a result, a first guess of a suitable Manning coefficient field, \(\mu_0\), is obtained. Using the \(\mu_0\) field, a 1-month spin-up run (May 1, 2019 to June 1, 2019) is then carried out to generate an initial condition for June 1. The spin-up run used the ERA5 atmospheric reanalysis data as forcing (Hersbach et al., 2018).

The Manning coefficient is initially set to 0.03 s m\(^{-1/3}\) everywhere in the model domain. We run the final optimization for 40 iterations, after which the changes in the friction field were small.

Once the optimal Manning coefficient field has been found, the results are validated with a 3-month simulation ranging from June 1 to August 31, 2019. The start date is the same as with the optimization period and the same model initial condition is used. The longer validation run allows to verify that the Manning coefficient has not been tuned to fit particular events during the optimization period (over-fitting), i.e., the optimized model is able to represent SSH dynamics accurately in general.

4.3 Performance metrics

The model skill is quantified with standard statistical metrics. Recall that \(\eta_{o,i}^n\) and \(\eta_{m,i}^n\), \(n = 1, \ldots, N\) denote the observed and modeled water elevation time series at station \(i\), respectively. The time-averaged and time-centered series are denoted by \(\bar{\eta}_o\) and \(\hat{\eta}_o\), respectively. The standard deviation and Centered Root Mean Square Deviation are denoted by \(\sigma_{o,i}\) and \(\text{CRMSD}_i\) (Sect. 3.1). In the following, we drop the station index \(i\) for brevity. The bias and correlation coefficient (\(R\)) are defined as:

\[
\text{BIAS} = \bar{\eta}_m - \bar{\eta}_o, \quad (40)
\]

\[
R = \frac{1}{\sigma_o \sigma_m} \frac{1}{N} \sum_{n=1}^{N} \hat{\eta}_m^n \hat{\eta}_o^n. \quad (41)
\]

CRMSD is related to \(\sigma_m\) and \(R\) through the equation,

\[
\text{CRMSD}^2 = \sigma_o^2 + \sigma_m^2 - \sigma_o \sigma_m R, \quad (42)
\]

which can be visualized in a Taylor diagram (Taylor, 2001). In this work, we are normalizing the Taylor diagram by scaling the variables with \(\sigma_o\):

\[
\text{NCRMSD}^2 = 1 + \sigma_m^2 - \sigma_m' R, \quad (43)
\]

\[
\text{NCRMSD} = \frac{1}{\sigma_o} \text{CRMSD}, \quad (44)
\]

\[
\sigma_m' = \frac{\sigma_m}{\sigma_o}, \quad (45)
\]

where NCRMSD and \(\sigma_m'\) are the normalized CRMSD and standard deviation of the model, respectively. Normalization leads to dimensionless metrics and permits the comparison of different data sets in a single figure.

5 Results

5.1 Optimization

Starting from a spatially uniform Manning coefficient field, we ran the optimization for 40 iterations. The evolution of the cost function is shown in Fig. 5. During the
first 5 iterations the cost function decreases rapidly and begins to stagnate between iterations 20 and 40. The regularization parameter, $\alpha$, was set to 400 as it appeared to result in a smooth Manning coefficient field without constraining the optimization too much.

The final optimized Manning coefficient field is shown in Fig. 6. The Manning field shows significant spatial variability throughout the model domain, i.e. not only in the vicinity of the tide gauge locations. This suggests that the optimization process alters the propagation of long surface waves instead of finding artificial local minima at the observation locations. In the North Sea and around the British Isles, the friction coefficient is altered to improve the propagation and reflection of the tides; In the Danish waters (panel b), friction is lowered in the Great Belt and across the Darss Sill. This is the dominant route for water transport between the Baltic Sea and the North Sea (Mohrholz et al., 2015; Gräwe et al., 2015; Mohrholz, 2018) and the friction coefficient has a great impact on the barotropic volume flux, driven by water elevation difference across the Danish Straits. In the Baltic Sea, the friction coefficient is altered at certain shallow regions, such as the Quark, Archipelago Sea and the Irbe Strait. These locations control the volume transport to the Bothnian Bay, Bothian Sea, and Gulf of Riga, respectively. With the used mesh, the Archipelago Sea is largely under-resolved which plausibly explains.
the need for higher friction. Overall, the optimized Manning coefficient field is complex and would be difficult to find through manual manipulation or brute force methods.

Example time series of the optimization process are shown in Fig. 7. In the Baltic Sea (panels a and b), the optimization mainly affects the slowly varying mean water elevation. This is related to the volumetric transport into the Baltic Sea. The Degerby station lies close to a nodal point of the basin’s seiche oscillations and thus it is often regarded as a metric of the total water volume in the basin. Panel (b) thus suggests that the emptying of the basin is initially underestimated; after 5 iterations, the model already tracks the observations fairly closely.

Panels (c) and (d) show examples of tidal stations in the Great Belt and Skager-rak, respectively. In both cases, the tidal range is initially overestimated but the model recovers a reasonable tidal range as the iteration progresses. The optimization also affects the phase of the tides to some extent. This is plausibly achieved by altering the relative strength of the tidal waves that propagate though the various parallel straits, for example. Based on our experience, these kinds of effects are difficult to achieve through manual manipulation of the Manning coefficient field. It should be noted that in the Danish Straits the solution converges slower compared to the Baltic stations (a and b) and the tidal waves are not fully replicated even after 40 iterations.

5.2 Validation

Model performance metrics for the validation period are presented in Fig. 8. The blue and red markers indicate the initial and optimized model, respectively. The optimization improves the model performance at all tide gauges. In the Baltic Sea, the CRMSD improves from 5 to 8 cm range to 2 to 6 cm range; In many locations in the Gotland Basin and the Bothian Sea, the optimized model reaches CRMSD of 3 cm or less. Slightly higher CRMSD is observed in the Bothian Bay and Gulf of Finland. In the Danish Straits, the deviation is higher, the optimized model’s CRMSD ranging between 4 and 8 cm. In this case, the improvement is substantial: At certain locations (e.g. Aarhus, Fredericia, Frederikshavn) the CRMSD is reduced by nearly a factor of 3. This is due to the complex reflection and interaction of tidal waves in this region which is difficult to replicate without careful tuning. For example, the tides propagate through the straits with different phase speeds, resulting in a complex superpositioning of tidal waves in the Great Belt; our initial tests indicate that a sufficiently good representation of the geometry is essential for capturing these processes.

The second panel in Fig. 8 shows the standard deviation of the observed and modeled time series; The black markers indicate the observations. Also here, the optimization clearly improves the performance. The model has a slight tendency to underestimate variability at certain stations in the Gulf of Bothnia and Danish Straits.

Fig. 9 presents a Taylor diagram for the validation data. Also here the improvement in model skill is clear. In the Baltic Sea (round markers) the optimized model performs very well; at most stations the correlation coefficient is above 0.95 and standard deviation is close to the observations. In the Danish waters (star markers), the correlation coefficient is lower but still above 0.83 in all cases.

Two time series examples are shown in Fig. 10. Panel (a) shows water elevation at Degerby station for the entire validation period. Similarly to Fig. 7, the uncalibrated model tends to underestimate the slowly-varying SSH changes, suggesting that the transport through the Danish Straits is underestimated. The optimized model, on the other hand, tracks the volumetric changes quite accurately. Panel (b) shows tidal SSH signal at Korsor station in the Great Belt for a 7-day period outside the optimization window. Also in this case, the optimized model produces both a realistic tidal range as well as sub-tidal variability.
Figure 7. Example time series during the optimization. The black line stands for the observation; colored lines indicate model results at different stages of the optimization progress; iteration 0 indicates the initial guess. The data sets have been bias corrected for visual comparison.
Figure 8. Performance metrics for each tide gauge for the validation period (June 1 to August 31, 2019). Sub-basins are indicated by the abbreviations: GoB, Gulf of Bothnia; AS, Archipelago Sea; GoF, Gulf of Finland; GB, Gotland Basin; BB, Bornholm Basin; AB, Arkona Basin; DS, Danish Straits; Kat, Kattegat.
Figure 9. Taylor diagram for tide gauge comparison for the validation period. The round and star symbols indicate stations in the Baltic Sea and Danish waters (Danish Straits and Kattegat), respectively.

Figure 10. Example time series from the validation run at the (a) Degerby and (b) Korsor stations. Panel (a) covers the entire validation period; gray shading indicates the 14-day optimization period. Panel (b) shows tidal variability in the Great Belt region. The black, blue and red lines stand for the observations, uncalibrated, and optimized model, respectively. The data sets have been bias corrected for visual comparison.
5.3 Computational cost

The simulations were carried out on AMD Rome 7H12 CPUs on the CSC Mahti cluster using 8 MPI processes. The forward model runs roughly 1800 times faster than real time: a 1-day and a 1-month simulation take roughly 48 s and 24 min, respectively. Evaluating the gradient of $J$ in the 16.5 day optimization period takes roughly 45 min, i.e. about 3.4 times longer than running the forward model. In each L-BFGS-B iteration typically only one, and at most two, gradient evaluations are needed. Running the entire optimization for 40 iterations took 36 h.

6 Discussion

We have presented an adjoint-based optimization of a 2D water elevation model. One of our main findings is that for the optimization process to work, the model misfit must be dominated by the control variable, i.e. bottom friction in this case. Otherwise, the optimization process may end up compensating errors due to other sources, e.g., by generating artificial friction patterns near the boundary in the case of poor boundary forcings. Consequently, one needs a sufficiently good mesh, bathymetry, boundary conditions and atmospheric forcing. The open boundaries should be located sufficiently far away from the domain of interest. In addition, a realistic initial condition is crucial for robust optimization. Our test runs showed that the model SSH bias in the Baltic Sea reaches an equilibrium in approximately 1 month, and this adjustment period must be excluded from the optimization period.

The present work is based on a 2D shallow water model. As such, our model does not include water density effects, baroclinic processes or wind waves, for example. Water density difference between the North Sea and the northern Baltic Sea introduces a steady elevation gradient across the Baltic basin. Baroclinic processes can be important especially in the Danish Straits where density gradients are strong and fluctuate with in- and outflow events. The freshwater outflow in Kattegat/Skagerrak can exhibit baroclinic eddies, which affect local water elevation. Wind wave effects are most pronounced under storm conditions and can enhance storm surges via Stokes drift or wave build-up near the coast (Kanarik et al., 2021). At the open boundary, we are not imposing subtidal SSH variability which can also affect SSH in the North Sea to some extent. However, our test runs suggest that including subtidal SSH forcing does not have a significant impact, possibly because the open boundaries are located beyond the shelf break. In the deep water, subtidal SSH variability remains relatively small and, on the other hand, our model domain is sufficiently large to permit the generation of storm surges.

Although water elevation in the Baltic Sea is mainly driven by atmospheric forcing and exchange through the Danish straits, river discharge can also affect local SSH and affect the long-term SSH gradient across the basin. In this work, we have used a time-averaged, constant-in-time river discharge from the largest rivers. This appears to be sufficient to replicate SSH variability with good accuracy.

One common pitfall in gradient-based optimization is over-fitting. The optimization process is underdetermined, i.e. there are much more degrees of freedom in the control field compared to the amount of observational data. In addition, the cost function typically exhibits many local minima. As such, the model can adjust to specific events or observation noise and lead to a friction field that is not generally applicable. To this end, some regularization is needed. Heemink et al. (2002) and Zhang et al. (2011), for example, reduced the dimensionality of the friction field considering only a small subset of the grid’s nodal values. In this work, we firstly noted that by far the best way to avoid over-fitting is to use a sufficiently long optimization period. Indeed, the Baltic Sea SSH variability happens on weekly time scales (Fig. 10 a). In addition, in the Danish Straits the tides are modulated by atmospheric forcing over several days (e.g., Fig. 7 c).
Initial tests with a 2-day optimization window resulted in rapid convergence and very low cost function values, but the model performed very poorly outside the optimization window. We chose the 16.5-day window as it is sufficiently long to yield generalizable results with a reasonable computational cost.

To control spatial over-fitting, we included an additional regularization term to penalize the second derivative of the control variable. The second derivatives were scaled with the local element size to allow larger changes in high-resolution regions (cf. 3.1). This procedure is sufficient to avoid strong “bipolar” friction adjustment at the tide gauge locations and results in a smooth Manning coefficient field (Fig. 6). The final Manning coefficient field is complex and highly variable across the domain. Most notably, friction is altered around the British Isles and the Irish Sea where no tide gauge data is used. It is worth noting, however, that shallow-water surface waves are typically relatively long and smooth which also reduces the risk of spatial over-fitting.

Based on our experiments, the presented friction optimization process appears to be robust: most tests resulted in a similar friction field with only small spatial differences. We did observe some dependency on the mesh, however. As such, the optimized friction field should be regarded as a model and mesh dependent parameter with limited physical interpretability (e.g. with respect to sea bed roughness). Indeed, capturing SSH dynamics requires suitable dissipation at the right locations and the model’s dissipation characteristics are governed by the discretization and mesh resolution.

We also experimented with a simultaneous optimization of bathymetry and friction but it did not have a significant impact on the model performance; typically most of the changes occurred in the friction field while bathymetry correction was minimal. This suggests that given a reasonable initial bathymetry field, the friction dominates the misfit. Moreover, to certain extent, small errors in bathymetry can be compensated by a suitable friction field.

The fact that the model skill is lower in the Danish waters compared to the Baltic Sea stations is consistent with other modeling results (Kärnä et al., 2021). Compared to the 1 nautical mile Nemo-Nordic 2.0 3D baroclinic model (Kärnä et al., 2021), the presented results are comparable or better. Although the simulation period, model configuration, and forcings are different, Kärnä et al. (2021) state that Nemo-Nordic yields CRMSD below 7 cm and 10 cm in the Baltic Sea and Danish waters, respectively, similar to our results. However, at certain locations, e.g. Fredericia, Nemo-Nordic 2.0 accuracy is lower, CRMSD being above 12 cm. This is most likely due to the fact that the complex geometry of the Danish Straits cannot be properly represented with a 1 nautical mile (1.8 km) regular grid.

The presented optimization method is a promising step towards automated calibration of ocean models. Bottom friction tuning is necessary in almost all coastal applications and manual tuning of spatially variable friction coefficient can be a very time consuming task. In the case of traditional ocean models with no adjoint model implementation, the options for automated tuning are limited: one would have to rely on ensemble-based estimates of the cost function gradient, for example. As the size of the ensemble is proportional to the number of control variable degrees of freedom, the computational cost in practice is significant. In our case, one iteration is 3.4 times more expensive compared to the forward model, i.e. the cost is roughly equivalent to running a 3-member ensemble. The accuracy, however, is much better as the gradient $\frac{dJ}{d\theta}$ is computed exactly.

Adjoint-based optimization has many similarities with machine learning methods (Sonnewald et al., 2021). Indeed, the backward-in-time adjoint iteration resembles the backpropagation training methods. In addition, regularization is a key ingredient to avoid over-fitting and a separate validation set is used to inform the final model selection.
this application, the cost function is defined as the centralized root mean square deviation, scaled by the observation variance. This is in fact equivalent to whitening the target signal (i.e. removing the bias and scaling to unit variance), commonly used as a preprocessing step in machine learning. In contrast to data-driven modeling, the benefit of adjoint-based physical modeling is that the results are guaranteed to be physically sound (i.e. satisfy the physical principles encoded in the forward equations; see eq. (32)).

7 Conclusions

We have presented adjoint-based bottom friction optimization in a 2D water elevation model for the Baltic Sea. The discrete adjoint model is automatically generated from the symbolic representation of the discrete forward model equations. The Manning coefficient optimization procedure is robust and yields good, generalizable results. Achieving similar performance via manual tuning would be challenging. The model performs well, especially in the complex Danish Straits region that is difficult to model with structured grid models (e.g., Kärnä et al. (2021)), highlighting the benefit of variable-resolution unstructured meshes.

Appendix A Quadratic bathymetry field

As the coastal topography exerts a leading-order control on water circulation, it is crucial to obtaining an accurate numerical representation of the bathymetry. Typically the accuracy of the bathymetric field is restricted by the mesh resolution. In this work, we discretize the bathymetry field with a second order $P_2$ element (Fig. 1 c) to increase the intrinsic resolution.

A common bottleneck with order $p > 1$ polynomials is the fact that it becomes difficult to ensure the monotonicity of the field near sharp gradients. Indeed, the polynomial representation typically leads to large oscillations that exceed the bounds of the original data. In the case of bathymetric data, the water depth may become negative in the vicinity of steep slopes, for example.

We generate a smooth $P_2$ bathymetry field as follows: First, we generate a refined triangular mesh by splitting each triangle uniformly into four (i.e. joining the $P_2$ element nodes). On the refined mesh, we define a preliminary $P_1$ bathymetry field and interpolate the raw raster bathymetry data on it. This field does not exhibit any spurious overshoots due to the linear basis functions. The preliminary bathymetry field is then smoothed with Laplacian diffusion. Given an preliminary bathymetry field $h^{(1)}$ and a test function $\phi$ in the $P_1$ space, the smoothing operator is

$$r = \frac{(|\nabla h^{(n)}| \Delta x)^\gamma}{2(h^{(n)})^\beta}$$  \hspace{1cm} (A1)

$$\int_{\Omega} (h^{(n+1)} - h^{(n)}) \phi dx = - \int_{\Omega} \alpha r \nabla h^{(n)} \cdot \nabla \phi dx, \quad \forall \phi$$  \hspace{1cm} (A2)

with $\alpha = 20$, $\gamma = 5/2$, and $\beta = 1/2$. On the right hand side, the Laplacian diffusion operator has been integrated by parts, omitting the interface terms. The diffusion coefficient, $r$, depends on the local bathymetry change in each element. It resembles the dimensionless bathymetry slope metric commonly used in sigma coordinate models (recovered by setting $\gamma = \beta = 1$; Haney (1991); Mellor et al. (1998)).

The smoother is applied 30 times. We then use $L^2$ projection to cast the smoothed preliminary bathymetry on a $P_2$ field on the original mesh. Although the procedure is not guaranteed to be monotonic, the smoothing step essentially ensures that the projection does not generate severe overshoots. A comparison of the final $P_2$ bathymetry and
Figure A1. Comparison of bathymetry fields in the Danish Straits region, a) the raster bathymetry data interpolated onto the P₁ elements; b) the final P₂ bathymetry field.

interpolated P₁ bathymetry are shown in Fig. A1. The P₂ discretization allows more realistic representation of the narrow channels in the Danish Straits. In the P₁ case, the channels are not entirely continuous which affects volume transport.

Appendix B Hessian recovery procedure

The cost function described in Subsection 3.1 involves a regularization term that depends on the Hessian of the control field. In practice, the control field is discretized using linear finite elements, which are not twice continuously differentiable. In order to approximate the second derivatives of the (continuous) control field, we apply an L² projection recovery procedure. The gradient of the discrete field is projected into L² space. A second application then obtains the Hessian approximation. We opt to perform the Hessian recovery in P₁ spaces and apply the two recovery steps simultaneously using a mixed finite element method.

Let θₜ denote the finite element approximation of the control field and gₜ and Hₜ denote the corresponding approximations of its gradient and Hessian, the latter of which we seek to obtain. Let φ and φ̄ denote test functions in vector and tensor P₁ spaces, respectively. The mixed formulation may then be written as

\[ \int_Ω gₜ \cdot φ \, dx = - \int_Ω θₜ(∇ \cdot φ) \, dx + \int_Γ θₜ(φ \cdot n) \, ds + \int_Γ \{θₜ\} \cdot [φ \cdot n] \, dS \quad ∀φ \quad (B1) \]

\[ \int_Ω Hₜ : φ \, dx = - \int_Ω gₜ \cdot (∇ \cdot φ) \, dx + \int_Γ gₜ \cdot (φ \cdot n) \, ds + \int_Γ \{gₜ\} \cdot [φ \cdot n] \, dS \quad ∀φ \quad (B2) \]

where \( \int_Ω A : B \, dx \) denotes the standard L² inner product on Ω for two tensors A and B. An advantage of the formulation in (B1)–(B2) is that it does not require the control field to have any derivatives at all, meaning it can be applied to both continuous and discontinuous fields.

Taken together, (B1) and (B2) give rise to a 2x2 block matrix system. We solve this system using Schur complement preconditioners and GMRES as the linear solver.
A major advantage of our approach is that, in addition to solving the adjoint shallow water equations, the automated adjoint model takes this solver step into account, as well as any other “post-processing” required to calculate the objective functional.

Data Availability Statement

The model source code used to perform the presented experiments is publicly available. Firedrake, and its components, may be obtained from https://www.firedrakeproject.org (last access: 21 April 2022); Thetis may be obtained from https://thetisproject.org (last access: 21 April 2022). The exact software versions used to produce the results in this paper have been archived on Zenodo (zenodo/Firedrake, 2022; zenodo/Thetis, 2022). The model configuration as well as the model and observation time series used to produce the presented results are preserved on Zenodo (zenodo/Data, 2022). Data analysis and visualization were carried out with Matplotlib (Hunter, 2007) and Iris (Met Office, 2010 - 2022) Python packages.

The MEPS atmospheric forecast data can be obtained from the Norwegian Meteorological Institute, https://github.com/metno/NWPdocs/wiki/Data-access (last access: 21 April 2022). The ECMWF (European Centre for Medium-Range Weather Forecasts) HRES atmospheric forecast data can be accessed from the ECMWF services, subject to license restrictions, https://www.ecmwf.int/en/forecasts/accessing-forecasts (last access: 21 April 2022). The ERA5 reanalysis atmospheric data can be downloaded from the Copernicus Climate Change Service (C3S) Climate Data Store (CDS) (Hersbach et al., 2018). The EHYYPE river runoff data can be obtained from the Swedish Meteorological and Hydrological Institute, subject to license restrictions. The TPXO global tidal atlas (TPXO9-atlas-v1; Egbert and Erofeeva (2002)) can be obtained from https://www.tpxo.net (last access: 21 April 2022). Bathymetric data is provided by the EModnet Bathymetry Consortium (2020). The observational data can be obtained from the Copernicus Marine Service (E.U. Copernicus Marine Service, 2015b, 2015a).

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