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RESEARCH ARTICLE

Supplementary Material

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1. Derivation of the adjoint model and gradients for surface waves

Define an inner product

$$\langle f, g \rangle = \int_t \int_y \int_x f(x,y,t) g^*(x,y,t) dxdydt, \tag{S1}$$

where g^* is the complex conjugate of function g. Similarly, the cost function can be written as

$$J = \frac{1}{2} \int_t \int_y \int_x (\eta - \eta_M)^2 dxdydt = \frac{1}{2} \langle \eta - \eta_M, \eta - \eta_M \rangle . \tag{S2}$$

Let $\boldsymbol{\mathcal{W}}(\boldsymbol{q}) = \boldsymbol{0}$ denote the wave model, i.e., equations (2.1) and (2.2) of the main paper, where $\boldsymbol{q} = [\eta, \Phi]^T$ with the superscript T denoting the transpose, and define a Lagrangian as

$$L = J - \langle \boldsymbol{\mathcal{W}}(\boldsymbol{q}), \boldsymbol{\lambda} \rangle , \tag{S3}$$

where $\boldsymbol{\lambda} = [\lambda_1, \lambda_2]^T$ are the Lagrangian variables. Because $\boldsymbol{\mathcal{W}}(\boldsymbol{q}) = 0$ at every time instant, L is equal to J. Given a small perturbation $\delta\eta_0$ to the initial surface elevation η_0 and perturbation $\delta\Phi_0$ to the initial velocity potential Φ_0, there is a perturbation δL to the Lagrangian. Then δL is expressed as

$$\delta L = \langle \delta\eta, \eta - \eta_M \rangle - \left\langle \boldsymbol{\mathcal{W}}'(\boldsymbol{\delta q}), \boldsymbol{\lambda} \right\rangle , \tag{S4}$$

where $\boldsymbol{\mathcal{W}}'(\boldsymbol{q}) = \boldsymbol{0}$ is the linearised wave model at $\boldsymbol{q_0} = [\eta_0, \Phi_0]^T$. The adjoint equations $\boldsymbol{\mathcal{W}}^*$, i.e., equations (2.3) and (2.4) of the main paper, satisfy

$$\left\langle \boldsymbol{\mathcal{W}}'(\boldsymbol{\delta q}), \boldsymbol{\lambda} \right\rangle = \left\langle \boldsymbol{\delta q}, \boldsymbol{\mathcal{W}}^*(\boldsymbol{\lambda}) \right\rangle + B.T., \tag{S5}$$

where B.T. denotes the boundary term

$$\begin{aligned} B.T. = & \int_y \int_x \left[\delta\eta(t_f)\lambda_1(t_f) + \delta\Phi(t_f)\lambda_2(t_f) \right] dxdy \\ & - \int_y \int_x \left[\delta\eta(t_0)\lambda_1(t_0) + \delta\Phi(t_0)\lambda_2(t_0) \right] dxdy. \end{aligned} \tag{S6}$$

Set $\lambda_1(t_f) = \lambda_2(t_f) = 0$ as the initial conditions for the adjoint model and $\boldsymbol{W}^*(\boldsymbol{\lambda}) = [\eta - \eta_M, 0]^T$, δL can be written as

$$\delta L = -B.T. = \int_y \int_x [\delta\eta(t_0)\lambda_1(t_0) + \delta\Phi(t_0)\lambda_2(t_0)]\, dxdy. \tag{S7}$$

Because

$$\delta J = \delta L = \int_y \int_x \left(\frac{\partial J}{\partial \eta_0}\delta\eta_0 + \frac{\partial J}{\partial \Phi_0}\delta\Phi_0 \right) dxdy, \tag{S8}$$

the gradients of the cost function to the initial wave field are

$$\begin{aligned} \frac{\partial J}{\partial \eta_0} &= \lambda_1(t_0), \\ \frac{\partial J}{\partial \Phi_0} &= \lambda_2(t_0). \end{aligned} \tag{S9}$$

Considering the dependence of the initial velocity potential on the initial surface elevation as shown by equation (2.8) of the main paper, δL can be further written as

$$\begin{aligned} \delta L &= -B.T. \\ &= \int_y \int_x \left\{ \delta\eta(t_0)\lambda_1(t_0) + \mathcal{F}^{-1}\left[\frac{-i\omega}{|\boldsymbol{k}|} \operatorname{sgn}(k_x)\mathcal{F}(\delta\eta(t_0)) \right] \lambda_2(t_0) \right\} dxdy \\ &= \int_y \int_x \delta\eta(t_0) \left\{ \lambda_1(t_0) - \mathcal{F}^{-1}\left[\frac{-i\omega}{|\boldsymbol{k}|} \operatorname{sgn}(k_x)\mathcal{F}\left(\lambda_2\left(t_0\right)\right) \right] \right\} dxdy. \end{aligned} \tag{S10}$$

The gradient in this case is then

$$\frac{\partial J}{\partial \eta_0} = \lambda_1(t_0) - \mathcal{F}^{-1}\left[\frac{-i\omega}{|\boldsymbol{k}|} \operatorname{sgn}(k_x)\mathcal{F}(\lambda_2(t_0)) \right]. \tag{S11}$$

Then Φ_0 is updated using equation (2.8) of the main paper to initialise the wave model.

2. Validation of the adjoint gradients

To verify the gradients calculated by the integration of the adjoint equations, we compare the results with those calculated directly from the finite difference method. The benchmark solution of the gradient information is obtained using a finite difference scheme, in which the gradient of the cost function with respect to η_0 at any point (i, j) is calculated as

$$\left.\frac{\partial J}{\partial \eta_0(i,j)}\right|_{Benchmark} = \frac{J_{\eta_0+\delta} - J_{\eta_0}}{\delta}, \tag{S12}$$

where J_{η_0} is calculated by equation (2.5) of the main paper with η_0, and $J_{\eta_0+\delta}$ is calculated by adding a small perturbation δ to $\eta_0(i, j)$. We set the magnitude of δ to be 1.0×10^{-6} m, sufficiently small to reduce the error caused by the finite difference approximation. The gradient of the cost function with respect to Φ_0 is calculated in a similar way. Figure S1 shows the comparison of the gradients at 20 different grid points in the first optimization iteration for case KA09-N00 in the main paper with the initial guess $(\eta_0, \Phi_0) = (0, 0)$. As shown in figure S1, the adjoint gradients agree with the gradients calculated by the finite difference method.

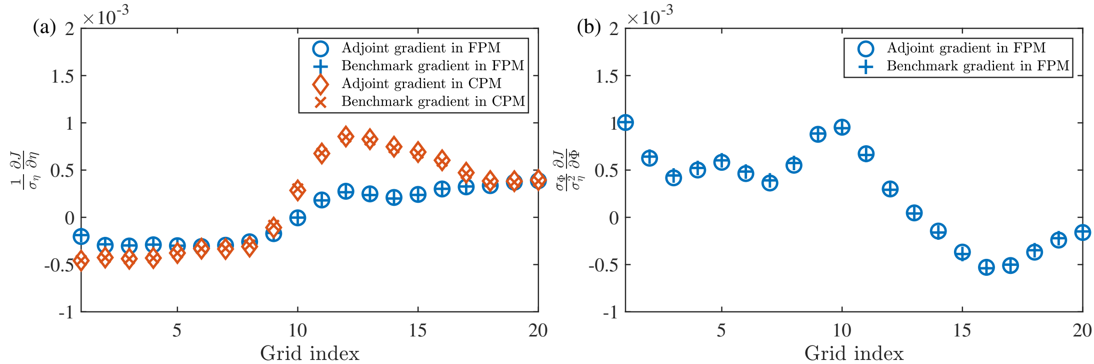

Figure S1. *Comparison between the adjoint gradient by the adjoint model in table 1 of the main paper and the benchmark gradient calculated using the finite difference method in Eq. (S12) at 20 grid points for case KA09-N00 of the main paper: (**a**) the values of normalised $\partial J/\partial \eta_0$ in FPM and CPM; (**b**) the values of normalised $\partial J/\partial \Phi_0$ in FPM (note that $\partial J/\partial \Phi_0$ are computed only in FPM). The gradients are normalised by $\sigma_\eta = 0.18$ m and $\sigma_\Phi = 1.04$ m^2/s, the root mean square of the initial true surface elevations and surface velocity potential, respectively.*