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Breaking water waves and geometric integration

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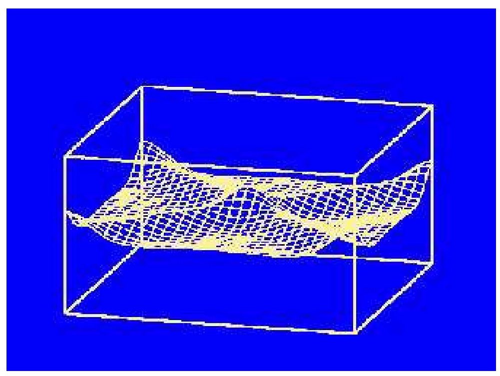


The widely used governing equations for modelling water waves are Hamiltonian, and therefore one would expect that symplectic integrators would be appropriate for time integration. In this lecture the use of symplectic or other geometric integrators for water waves is discussed. For a simple free surface (a graph) the Hamiltonian formulation is canonical, but still the use of symplectic integrators is not straightforward. For general surfaces, for example breaking waves, one needs a coordinate-free Hamiltonian formulation, and this was first proposed by BENJAMIN & OLVER (1982). For breaking waves the Hamiltonian structure is no longer canonical, and new ideas from geometric integration are needed.

Equations governing water wave dynamics

Assume that the free surface is a single-valued function of horizontal position (x, z),

$$y = \eta(x, z, t)$$

For inviscid irrotational flow, the velocity field is determined by a velocity potential

$$\mathbf{u}(x, y, z, t) = \nabla\phi(x, y, z, t)$$

Let

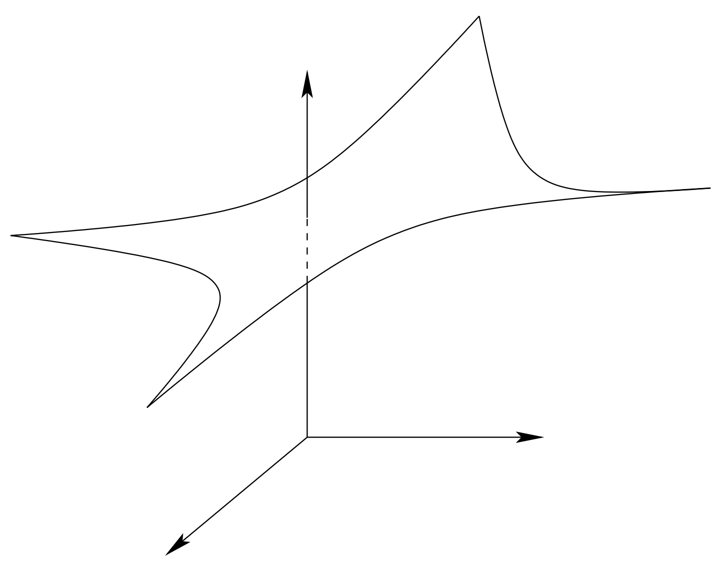
$$\Phi(x, z, t) = \phi(x, y, z, t)\Big|_{y=\eta(x,z,t)},$$

and suppose that $\phi(x, y, z, t)$ is a harmonic function in the fluid interior.

Then the governing equations take the form

$$\left.\begin{aligned} \Phi_t &= \frac{\delta H}{\delta \eta} \\ \eta_t &= -\frac{\delta H}{\delta \Phi} \end{aligned}\right\} \quad \text{Zakharov (1968) formulation}$$

where $H(\eta, \Phi)$ is the total energy.



Symplectic integrator ?

The total energy density takes the form

$$H(\eta, \Phi) = \tfrac{1}{2}\langle \Phi, G(\eta)\Phi\rangle + \tfrac{1}{2} g\eta^2 \,.$$

where $G(\eta)$ is the Dirichlet-Neumann operator, and g is the gravitational constant. As far as I'm aware, a symplectic integrator has never been implemented for this problem.

Typically, a boundary element method is used for spatial discretization, and then a standard time integration.

For example in a recent state of the art paper, RK4 is used. To see the implications of this, consider the linear problem in 2D with periodic boundary conditions in the horizontal direction,

$$\eta(x,t) = \sum_{j=1}^{\infty} q_j(t)\cos jx + p_j(t)\sin jx$$

Then $(q_j(t), p_j(t))$ for $j = 1, 2, \ldots$ decouple into an infinite number of harmonic oscillators

$$\begin{aligned} \dot{q}_j &= \omega_j\, p_j \\ \dot{p}_j &= -\omega_j q_j \end{aligned}$$

with frequencies

$$\omega_j^2 = gj\tanh(jh)\,, \quad j = 1, 2, \ldots\,,$$

where h is the still water depth.

Coupled harmonic oscillators and RK4

Take N modes; then

$$\mathbf{u}_t = \mathbf{A}\mathbf{u}\,, \quad \mathbf{u} \in \mathbb{R}^{2N}$$

with

$$\mathbf{A} = \mathbf{A}_1 \oplus \cdots \oplus \mathbf{A}_j \oplus \cdots$$

and

$$\mathbf{A}_j = \omega_j \mathbf{J}\,, \quad \mathbf{J} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

The orbit of each mode is circular with the radius determined by initial data, since

$$\frac{d}{dt}\dot{I}_j = 0 \quad \text{where} \quad I_j(t) = \|\mathbf{u}_j(t)\|^2\,.$$

where $\mathbf{u}_j(t) = (q_j(t), p_j(t))$.

The standard RK-4 method for this linear system for one step $t \mapsto t+h$ reduces to

$$\mathbf{u}^{n+1} = [\mathbf{I} + h\mathbf{A} + \tfrac{1}{2}h^2\mathbf{A}^2 + \tfrac{1}{3!}h^3\mathbf{A}^3 + \tfrac{1}{4!}h^4\mathbf{A}^4]\mathbf{u}^n\,. \tag{1}$$

which decouples into

$$\begin{aligned}\mathbf{u}_j^{n+1} &= [\mathbf{I} + h\mathbf{A}_j + \tfrac{1}{2}h^2\mathbf{A}_j^2 + \tfrac{1}{3!}h^3\mathbf{A}_j^3 + \tfrac{1}{4!}h^4\mathbf{A}_j^4]\mathbf{u}_j^n \\ &= [(1 - \tfrac{1}{2}\alpha^2 + \tfrac{1}{4!}\alpha^4)\mathbf{I} + (\alpha - \tfrac{1}{3!}\alpha^3)\mathbf{J}]\mathbf{u}_j^n\,,\end{aligned}$$

where $\alpha = \omega_j h$.

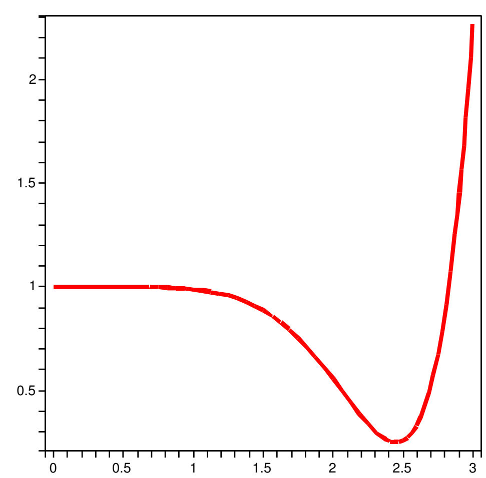
Harmonic oscillators and RK4

$$\mathbf{u}_j^{n+1} = [(1 - \tfrac{1}{2}\alpha^2 + \tfrac{1}{4!}\alpha^4)\mathbf{I} + (\alpha - \tfrac{1}{3!}\alpha^3)\mathbf{J}]\mathbf{u}_j^n \,,$$

where $\alpha = \omega_j h$. RK4 method distorts circles as follows

$$I(\mathbf{u}_j^{n+1}) = \left(1 - \frac{(h\omega_j)^6}{72} + \frac{(h\omega_j)^8}{576}\right) I_j(\mathbf{u}_j^n)$$

In the figure, $I(\mathbf{u}_j^{n+1})/I(\mathbf{u}_j^n)$ is shown plotted versus $h\omega_j$.



For the distortion to be less than unity requires $\omega_j h < \sqrt{8}$ for all j.

If $0 < \omega_j h < \sqrt{8}$ the amplitude of the oscillator is damped, and if $\omega_j h > \sqrt{8}$ the amplitude is growing.

Does one choose the time step so that the largest frequency is stable? Or choose a larger time step and then using smoothing to stabilize the high frequencies?

Contrast with an elementary symplectic method such as the implicit midpoint rule which preserves the circles of all the harmonic oscillators, regardless of frequency.

Irrotational waves and simple free surface

It is an open problem to implement a symplectic integrator in the case where the free surface is represented as a graph.

On the other hand ...

- Representation of the free surface with a graph is a special choice of parameterization.
- Can the free surface be represented in a coordinate free way?
- Can a coordinate free representation of the surface be incorporated into a Hamiltonian formulation?
- What is the appropriate geometric integrator for a coordinate-free representation of the free surface?
- These issues arise in a practical way when one is interested in simulating overhanging and breaking water waves

Coordinate-free representation of free surface

What changes when we represent the free surface as an abstract mapping from a reference space into $\mathbb{R}^3$? Of the form,

$$\mathbf{X}(a,b,t) = (X(a,b,t), Y(a,b,t), Z(a,b,t)), \quad (a,b) \in \mathscr{D} \subset \mathbb{R}^2 .$$

The kinematic condition is replaced by the more general condition

$$\mathbf{n} \cdot \mathbf{X}_t = \nabla\phi \cdot \mathbf{n}$$

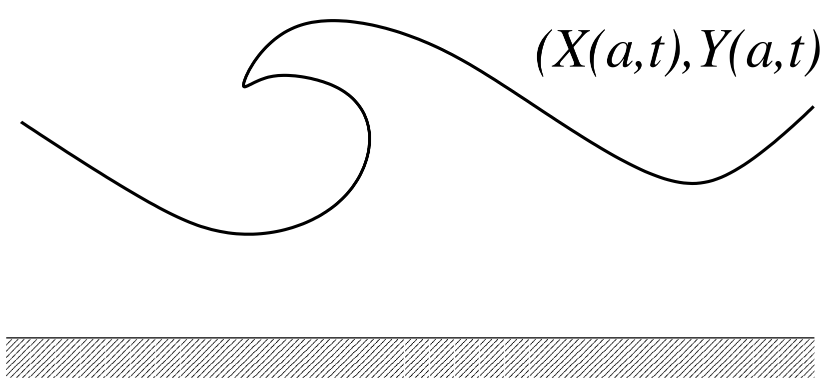
where $\mathbf{n}$ is the unit normal at the free surface. Note that there is some non-uniqueness in this condition since it is equivalent to

$$\mathbf{X}_t = \nabla\phi + \gamma_1(a,b,t)\mathbf{T}_1 + \gamma_2(a,b,t)\mathbf{T}_2 ,$$

where $\{\mathbf{T}_1, \mathbf{T}_2\}$ is an orthonormal basis for the tangent space of the surface, and γ_1 and γ_2 are arbitrary. The non-uniqueness is representative of the *reparameterization symmetry*.

What about a Hamiltonian formulation for this case?

It is not well known that BENJAMIN & OLVER (1982) (in a brief appendix of a long paper) showed that there is a Hamiltonian formulation for this case, which differs in important ways from the Zakharov formulation. They give the formulation in 3D, but we will discuss the 2D case, with $\mathbf{X}(a,t) = (X(a,t), Y(a,t))$.



Benjamin-Olver Hamiltonian formulation

The coordinates for the Hamiltonian formulation are $X(a,t)$, $Y(a,t)$ and $\Phi(a,t)$ where

$$\Phi(a,t) = \phi(x,y,t)\big|_{x=X(a,t),y=Y(a,t)} .$$

The equations are

$$\begin{bmatrix} 0 & -\Phi_a & Y_a \\ \Phi_a & 0 & -X_a \\ -Y_a & X_a & 0 \end{bmatrix} \begin{pmatrix} X \\ Y \\ \Phi \end{pmatrix}_t = \begin{pmatrix} \delta H/\delta X \\ \delta H/\delta Y \\ \delta H/\delta \Phi \end{pmatrix}$$

or

$$\mathbf{K}(\mathbf{U})\mathbf{U}_t = \nabla H(\mathbf{U}) ,$$

which can also be cast into the illuminating form

$$\mathbf{U}_a \times \mathbf{U}_t = \nabla H(\mathbf{U}) , \quad \mathbf{U} = (X, Y, \Phi) .$$

The Hamiltonian function is the total energy and the symplectic form is generated by

$$\Theta = \int_S \Phi \, \mathrm{d}\mathbf{X} \cdot \mathbf{n} \, \mathrm{d}S = \int_{a_1}^{a_2} \Phi(X_a \mathrm{d}Y - Y_a \mathrm{d}X) \, \mathrm{d}a ,$$

with $\omega = \mathrm{d}\Theta$.

Kernel of $\mathbf{K}$ is $\{\mathbf{U}_a\}$. The kernel is due to the reparameterization symmetry.

Explicit equations for time integration

$$\mathbf{K}(\mathbf{U})\mathbf{U}_t = \nabla H(\mathbf{U})\,,$$

with

$$\mathbf{K} = \begin{bmatrix} 0 & -\Phi_a & Y_a \\ \Phi_a & 0 & -X_a \\ -Y_a & X_a & 0 \end{bmatrix} = \mathbf{U}_a \times$$

Now

$$\mathbf{K}^T\mathbf{K} = \|\mathbf{U}_a\|^2 \left[\mathbf{I} - \frac{\mathbf{U}_a\mathbf{U}_a^T}{\|\mathbf{U}_a\|^2}\right]\,,$$

and so

$$\mathbf{U}_t = \mathbf{J}(\mathbf{U})\nabla H(\mathbf{U}) + \mathrm{Ker}(\mathbf{K})\,, \quad \mathbf{J} = \frac{1}{\|\mathbf{U}_a\|^2}\mathbf{K}^T$$

or

$$\mathbf{U}_t = \mathbf{J}(\mathbf{U})\nabla H(\mathbf{U}) + \gamma(a,t)\mathbf{U}_a\,.$$

- $\gamma(a,t)$ is arbitrary.
- Can one choose γ to optimize the form of the equations?
- While $\mathbf{K}(\mathbf{U})$ is a linear function of $\mathbf{U}$, $\mathbf{J}(\mathbf{U})$ is a nonlinear function of $\mathbf{U}$.
- Can one choose γ to optimize the numerical scheme?
- Nonzero γ is equivalent to a time-dependent reparameterization.
- What are the implications of time-dependent reparameterization?

Special case: 2D equations with periodic B.C.

With periodic boundary conditions, the equations can be simplified by using time-dependent conformal mapping, and a Fourier series expansion on the reference space.

$$\begin{bmatrix} 0 & -\Phi_a & Y_a \\ \Phi_a & 0 & -X_a \\ -Y_a & X_a & 0 \end{bmatrix} \begin{pmatrix} X \\ Y \\ \Phi \end{pmatrix}_t = \begin{pmatrix} -gYY_a + \widehat{\mathcal{H}(A)} \\ gYX_a + A \\ -\widehat{\mathcal{H}}(\Phi_a) \end{pmatrix}$$

where $\widehat{\mathcal{H}}(\cdot)$ is the Hilbert transform, e.g. on Fourier space

$$\widehat{\mathcal{H}}(\mathrm{e}^{\mathtt{i}jx}) = \mathtt{i}\mathrm{sign}(j)\mathrm{e}^{ijx}$$

and A has a simple expression in terms of Y and Φ.

By expanding X, Y and Φ in a Fourier series, the system can be reduced to a large system of ODEs of the form

$$\mathbf{K}^N(\mathbf{U}^N)\mathbf{U}_t^N = \nabla H(\mathbf{U}^N)\,, \quad \mathbf{U}^N \in \mathbb{R}^{3N}\,,$$

with $\mathbf{K}_N(\mathbf{U}^N)$ a linear function of $\mathbf{U}^N$,

$$\mathbf{K}_N(\mathbf{U}^N) = \mathbf{K}_1 \oplus \cdots \mathbf{K}_j \oplus \cdots\,, \quad \mathbf{K}_j = c_j \mathbf{U}^j \times\ .$$

Reminiscent of the structure of coupled rigid bodies, but with this structure in the symplectic operator rather than the Poisson operator.

What is the appropriate choice of geometric integrator?

Curvature driven free surface flow

A model problem which is useful for studying the reparameterization question in isolation is the normal motion of a closed plane curve driven by its local curvature.

This "curve-shortening" problem is a model for a number of phase transition and front dynamics.

Let $\mathbf{X}(a,t) = (X(a,t), Y(a,t))$ where a parameterizes the curve. Then the governing equation for the curve $X(a,t)$ is

$$\mathbf{n} \cdot \mathbf{X}_t = \kappa \,,$$

where $\mathbf{n}$ is the unit normal

$$\mathbf{n} = \frac{1}{\ell} \begin{pmatrix} -Y_a \\ X_a \end{pmatrix} , \quad \ell = \sqrt{X_a^2 + Y_a^2} \,,$$

and κ is the surface curvature

$$\kappa(a,t) = \frac{X_a Y_{aa} - Y_a X_{aa}}{\ell^3} \,.$$

The dynamics of $\mathbf{X}(a,t)$ is not unique since only the normal velocity is prescribed. This becomes apparent when the governing equation is expressed in the form

$$\mathbf{X}_t = \kappa \mathbf{n} + \gamma(a,t) \mathbf{t} \,, \quad \mathbf{t} = \frac{1}{\ell} \begin{pmatrix} X_a \\ Y_a \end{pmatrix} ,$$

with $\gamma(a,t)$ arbitrary.

- T.Y. HOU, J.S. LOWENGRUB & M.J. SHELLEY. *Removing the stiffness from interfacial flows with surface tension*, J. Comput. Phys. **114** 312–338 (1994).

Curvature driven free surface flow

$$\mathbf{X}_t = \kappa \mathbf{n} + \gamma(a,t)\mathbf{t}\,,$$

Can choose $\gamma(a,t)$ to optimize the numerical scheme.

Choosing γ is equivalent to a time-dependent reparameterization. To see this, first suppose γ is zero,

$$\mathbf{X}_t = \kappa \mathbf{n}\,,$$

Introduce a time-dependent reparameterization

$$a = h(b,t) \quad \text{for some } h(b,t) \text{ satisfying } h_b \neq 0 \text{ for all } (b,t)$$

Then with

$$\widehat{\mathbf{X}}(b,t) = \mathbf{X}(h(b,t))$$

it follows that $\widehat{\mathbf{n}} = \mathbf{n}$, $\widehat{\mathbf{t}} = \mathbf{t}$ and $\widehat{\kappa} = \kappa$ and so

$$\begin{aligned} \tfrac{\partial}{\partial t}\widehat{\mathbf{X}}(b,t) &= \mathbf{X}_t + \mathbf{X}_a h_t \\ &= \kappa\mathbf{n} + h_t \ell \mathbf{t} \\ &= \widehat{\kappa}\widehat{\mathbf{n}} + \ell h_t \widehat{\mathbf{t}} \end{aligned}$$

that is,

$$\widehat{\mathbf{X}}_t = \widehat{\kappa}\widehat{\mathbf{n}} + \gamma\widehat{\mathbf{t}} \quad \text{with} \quad \gamma = \frac{h_t}{h_b}\,\widehat{\ell}\,.$$

The water-wave problem has the same structure but with the normal velocity determined by a third equation for Φ.

Summary and comments

- Appropriate geometric integrator for time evolution of water waves is still largely unsolved.
- When the surface is a graph, the symplectic structure associated with the Zakharov Hamiltonian formulation is canonical (albeit infinite-dimensional), but the kinetic energy depends on the "position variables".
- Of interest to combine symplectic integration with BEM methods.
- The Hamiltonian structure changes substantially when using the coordinate free Hamiltonian formulation of Benjamin and Olver.
- Symplectic form in the BO formulation is non-constant – a Lie-Poisson type structure on the "left". Can Lie-Poisson type integrators be adapted to this setting?
- The coordinate-free Hamiltonian formulation generalizes easily to interfacial waves and problems like the nonlinear Kelvin-Helmholtz instability. Φ is simply replaced by

$$\zeta(a,b,t) = \rho\Phi(a,b,t) - \rho'\Phi'(a,b,t)\,.$$

- There is a potential to take advantage of reparameterization symmetry in designing numerical schemes.
- Analogy with curvature-driven curve-shortening flow.

• T.B. BENJAMIN & TJB. *Reappraisal of the Kelvin-Helmholtz problem. Part I: Hamiltonian formulation*, J. Fluid Mech. **333**, 301–325 (1997).