Symplecticity of the Störmer-Verlet algorithm for coupling between the shallow water equations and horizontal vehicle motion

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In this technical report it is proved that the Störmer-Verlet algorithm, applied to the dynamically coupled problem of shallow water sloshing in a horizontally moving vehicle reported in [2], is symplectic if the $\sigma-$integral is discretized using the trapezoidal rule.

The starting point is the governing equations for shallow water fluid motion in a vehicle constrained to move horizontally with position $q(t)$. The governing equations in the Lagrangian particle path formulation are [2]

$$x_{tt} + g\frac{\chi_a}{x_a^2} - g\frac{\chi}{x_a^3}\,x_{aa} + \ddot{q} = 0\,, \quad \ddot{q} + \nu q = \rho g \int_0^L h h_x \,\mathrm{d}x\,.$$

The first equation corresponds to equation (1.4) in [2] and the second equation corresponds to equation (1.2) in [2]. The Hamiltonian formulation of these equations, with coordinates $(q(t), x(a,t), p(t), w(a,t))$ is given in §4.2 of [2]. The symplectic form is

$$\Omega = \int_0^L \mathrm{d}w \wedge \mathrm{d}x \,\rho\chi\,\mathrm{d}a + \mathrm{d}p \wedge \mathrm{d}q\,. \tag{0.1}$$

1 Störmer-Verlet discretization

Consider the Störmer-Verlet discretization for the Hamiltonian formulation as presented in §6 in [2],

$$\begin{aligned}
p^{n+\frac{1}{2}} &= p^n - \tfrac{1}{2}\nu\Delta t\, q^n \\
w_i^{n+\frac{1}{2}} &= w_i^n + \frac{g\Delta t\Delta a}{4\chi_i}\left(\frac{\chi_{i-1}^2}{\left(x_i^n - x_{i-1}^n\right)^2} - \frac{\chi_i^2}{\left(x_{i+1}^n - x_i^n\right)^2}\right), \quad i = 2, ..., N\,, \\
x_i^{n+1} &= x_i^n + \Delta t\, w_i^{n+\frac{1}{2}} - \tfrac{\Delta t}{m_v}p^{n+\frac{1}{2}} + \tfrac{\Delta t}{m_v}\sigma^{n+\frac{1}{2}}\,, \quad i = 2, ..., N\,, \\
q^{n+1} &= q^n + \tfrac{\Delta t}{m_v}p^{n+\frac{1}{2}} - \tfrac{\Delta t}{m_v}\sigma^{n+\frac{1}{2}} \\
p^{n+1} &= p^{n+\frac{1}{2}} - \tfrac{1}{2}\nu\Delta t q^{n+1} \\
w_i^{n+1} &= w_i^{n+\frac{1}{2}} + \frac{g\Delta t\Delta a}{4\chi_i}\left(\frac{\chi_{i-1}^2}{\left(x_i^{n+1} - x_{i-1}^{n+1}\right)^2} - \frac{\chi_i^2}{\left(x_{i+1}^{n+1} - x_i^{n+1}\right)^2}\right), \quad i = 2, ..., N\,,
\end{aligned}$$

where

$$\sigma^n = \int_0^L w^n \, \rho\chi \, \mathrm{d}a \, .$$

The choice of quadrature formula for σ^n will affect symplecticity. At first we discretized using Simpson's rule, but this choice does not preserve symplecticity (this will be apparent in the proof below). We found that the trapezoidal rule does indeed preserve symplecticity.

The discretized boundary conditions for $x(a,t)$ and $w(a,t)$ are

$$\begin{aligned} x_1^{n+1} &= 0\,, \quad x_{N+1}^{n+1} = L\,, \\ w_1^{n+1/2} &= w_{N+1}^{n+1/2} = \tfrac{1}{m_v} p^{n+\frac{1}{2}} - \tfrac{1}{m_v}\sigma^{n+\frac{1}{2}}\,. \end{aligned}$$

2 The discretized symplectic form

Using the trapezoidal rule, and noting that $\delta x_1^n = \delta x_{N+1} = 0$, the discretization of the symplectic form (0.1) is

$$\boldsymbol{\Omega}^n = \boldsymbol{\omega}^n + \delta p^n \wedge \delta q^n \quad \text{with} \quad \boldsymbol{\omega}^n := \sum_{i=2}^{N} \delta w_i^n \wedge \delta x_i^n \, \rho\chi_i \Delta a \, . \tag{2.1}$$

We say that the numerical scheme is symplectic if

$$\boldsymbol{\Omega}^{n+1} = \boldsymbol{\Omega}^n \quad \text{for all} \quad n\,.$$

3 Variational equations

In order to test for symplecticity, the variational equations associated with the discretization are required. The most complicated ones are the equations for δw_i^n. The first one is

$$\delta w_i^{n+\frac{1}{2}} \;=\; \delta w_i^n + \tfrac{g\Delta t\Delta a}{4\chi_i}\left(-2\tfrac{\chi_{i-1}^2}{\left(x_i^n - x_{i-1}^n\right)^3}(\delta x_i^n - \delta x_{i-1}^n) + 2\tfrac{\chi_i^2}{\left(x_{i+1}^n - x_i^n\right)^3}(\delta x_{i+1}^n - \delta x_i^n)\right)\,,$$

for $i = 2, ..., N$. To simplify, define

$$A_i^n = \frac{1}{2} g\Delta t\Delta a \frac{\chi_i^2}{\left(x_{i+1}^n - x_i^n\right)^3}\,.$$

Then, for $i = 2, \ldots, N$,

$$\begin{aligned} \delta w_i^{n+\frac{1}{2}} &= \delta w_i^n + \frac{A_i^n}{\chi_i}\delta x_{i+1}^n - \frac{A_i^n}{\chi_i}\delta x_i^n - \frac{A_{i-1}^n}{\chi_i}\delta x_i^n + \frac{A_{i-1}^n}{\chi_i}\delta x_{i-1}^n\,, \\ \delta x_i^{n+1} &= \delta x_i^n + \Delta t\, \delta w_i^{n+\frac{1}{2}} - \tfrac{\Delta t}{m_v}\delta p^{n+\frac{1}{2}} + \tfrac{\Delta t}{m_v}\delta\sigma^{n+\frac{1}{2}}\,, \\ \delta w_i^{n+1} &= \delta w_i^{n+1/2} + \frac{A_i^{n+1}}{\chi_i}\delta x_{i+1}^{n+1} - \frac{A_i^{n+1}}{\chi_i}\delta x_i^{n+1} - \frac{A_{i-1}^{n+1}}{\chi_i}\delta x_i^{n+1} + \frac{A_{i-1}^{n+1}}{\chi_i}\delta x_{i-1}^{n+1}\,. \end{aligned}$$

The variational equations for (q,p) are

$$\begin{aligned} \delta p^{n+\frac{1}{2}} &= \delta p^n - \tfrac{1}{2}\nu\Delta t\,\delta q^n \\ \delta q^{n+1} &= \delta q^n + \tfrac{\Delta t}{m_v}\delta p^{n+\frac{1}{2}} - \tfrac{\Delta t}{m_v}\delta\sigma^{n+\frac{1}{2}} \\ \delta p^{n+1} &= \delta p^{n+\frac{1}{2}} - \tfrac{1}{2}\nu\Delta t\,\delta q^{n+1}\,. \end{aligned}$$

The boundary variations are

$$\begin{aligned} \delta w_1^{n+1/2} &= \delta w_{N+1}^{n+1/2} = \tfrac{1}{m_v}\delta p^{n+\frac{1}{2}} - \tfrac{1}{m_v}\delta\sigma^{n+\frac{1}{2}} \\ \delta x_1^{n+1} &= \delta x_{N+1}^{n+1} = 0\,. \end{aligned} \tag{3.1}$$

3.1 The (q,p) component of the symplectic form

$$\begin{aligned} \delta p^{n+1}\wedge\delta q^{n+1} &= (\delta p^{n+\frac{1}{2}} - \tfrac{1}{2}\nu\Delta t\delta q^{n+1})\wedge\delta q^{n+1} \\ &= \delta p^{n+\frac{1}{2}}\wedge\delta q^{n+1} \\ &= \delta p^{n+\frac{1}{2}}\wedge(\delta q^n - \tfrac{\Delta t}{m_v}\delta\sigma^{n+\frac{1}{2}}) \\ &= (\delta p^n - \tfrac{1}{2}\nu\Delta t\,\delta q^n)\wedge(\delta q^n - \tfrac{\Delta t}{m_v}\delta\sigma^{n+\frac{1}{2}})\,, \end{aligned}$$

and so

$$\delta p^{n+1}\wedge\delta q^{n+1} = \delta p^n\wedge\delta q^n - \frac{\Delta t}{m_v}\delta p^n\wedge\delta\sigma^{n+\frac{1}{2}} + \tfrac{1}{2}\nu\frac{\Delta t^2}{m_v}\delta q^n\wedge\delta\sigma^{n+\frac{1}{2}}\,.$$

3.2 The (x,w) component of the symplectic form

From the definitions; for $i=2,\ldots,N$,

$$\begin{aligned} \delta w_i^{n+1}\wedge\delta x_i^{n+1} &= \delta w_i^{n+1/2}\wedge\delta x_i^{n+1} \\ &\quad + \frac{A_i^{n+1}}{\chi_i}\delta x_{i+1}^{n+1}\wedge\delta x_i^{n+1} + \frac{A_{i-1}^{n+1}}{\chi_i}\delta x_{i-1}^{n+1}\wedge\delta x_i^{n+1}\,. \end{aligned}$$

But

$$\begin{aligned} \delta w_i^{n+1/2}\wedge\delta x_i^{n+1} &= \delta w_i^{n+1/2}\wedge\left(\delta x_i^n - \tfrac{\Delta t}{m_v}\delta p^{n+\frac{1}{2}} + \tfrac{\Delta t}{m_v}\delta\sigma^{n+\frac{1}{2}}\right) \\ &= \delta w_i^n\wedge\delta x_i^n \\ &\quad + \frac{A_i^n}{\chi_i}\delta x_{i+1}^n\wedge\delta x_i^n + \frac{A_{i-1}^n}{\chi_i}\delta x_{i-1}^n\wedge\delta x_i^n \\ &\quad - \frac{\Delta t}{m_v}\delta w_i^{n+1/2}\wedge\delta p^{n+1/2} + \frac{\Delta t}{m_v}\delta w_i^{n+1/2}\wedge\delta\sigma^{n+1/2}\,. \end{aligned}$$

Hence

$$
\begin{aligned}
\delta w_i^{n+1} \wedge \delta x_i^{n+1} \;=\;& \delta w_i^n \wedge \delta x_i^n \\
&+\frac{A_i^n}{\chi_i}\delta x_{i+1}^n \wedge \delta x_i^n + \frac{A_{i-1}^n}{\chi_i}\delta x_{i-1}^n \wedge \delta x_i^n \\
&+\frac{A_i^{n+1}}{\chi_i}\delta x_{i+1}^{n+1} \wedge \delta x_i^{n+1} + \frac{A_{i-1}^{n+1}}{\chi_i}\delta x_{i-1}^{n+1} \wedge \delta x_i^{n+1} \\
&-\frac{\Delta t}{m_v}\delta w_i^{n+1/2} \wedge \delta p^{n+1/2} + \frac{\Delta t}{m_v}\delta w_i^{n+1/2} \wedge \delta\sigma^{n+1/2} .
\end{aligned}
$$

Multiply by $\rho\chi_i\Delta a$

$$
\begin{aligned}
\rho\chi_i\Delta a\,\delta w_i^{n+1} \wedge \delta x_i^{n+1} \;=\;& \rho\chi_i\Delta a\,\delta w_i^n \wedge \delta x_i^n \\
&+\rho\Delta a A_i^n\delta x_{i+1}^n \wedge \delta x_i^n + \rho\Delta a A_{i-1}^n\delta x_{i-1}^n \wedge \delta x_i^n \\
&+\rho\Delta a A_i^{n+1}\delta x_{i+1}^{n+1} \wedge \delta x_i^{n+1} + \rho\Delta a A_{i-1}^{n+1}\delta x_{i-1}^{n+1} \wedge \delta x_i^{n+1} \\
&-\frac{\Delta t\Delta a}{m_v}\rho\chi_i\delta w_i^{n+1/2} \wedge \delta p^{n+1/2} + \frac{\Delta t\Delta a}{m_v}\rho\chi_i\delta w_i^{n+1/2} \wedge \delta\sigma^{n+1/2} .
\end{aligned}
\tag{3.2}
$$

3.3 Proof that the sum of the A_i^n terms vanish

Before summing to obtain the symplectic form, first it is shown that the A_i^n terms vanish when summed. From the definition,

$$
\sum_{i=2}^{N} A_i^n\delta x_{i+1}^n \wedge \delta x_i^n = \sum_{i=2}^{N-1} A_i^n\delta x_{i+1}^n \wedge \delta x_i^n = \sum_{i=3}^{N} A_{i-1}^n\delta x_i^n \wedge \delta x_{i-1}^n
$$

using the fact that $\delta x_{N+1}^n = 0$, and shifting the index by one in the second equality. Similarly,

$$
\sum_{i=2}^{N} A_{i-1}^n\delta x_{i-1}^n \wedge \delta x_i^n = \sum_{i=3}^{N} A_{i-1}^n\delta x_{i-1}^n \wedge \delta x_i^n = -\sum_{i=3}^{N} A_{i-1}^n\delta x_i^n \wedge \delta x_{i-1}^n ,
$$

using the fact that $\delta x_1^n = 0$ and skew-symmetry of wedge. Hence

$$
\sum_{i=2}^{N} A_i^n\delta x_{i+1}^n \wedge \delta x_i^n + \sum_{i=2}^{N} A_{i-1}^n\delta x_{i-1}^n \wedge \delta x_i^n = 0 . \tag{3.3}
$$

A similar argument proves that

$$
\sum_{i=2}^{N} A_i^{n+1}\delta x_{i+1}^{n+1} \wedge \delta x_i^{n+1} + \sum_{i=2}^{N} A_{i-1}^{n+1}\delta x_{i-1}^{n+1} \wedge \delta x_i^{n+1} = 0 . \tag{3.4}
$$

4 Summing to obtain the discrete symplectic form

Since $\delta x_1^n = 0$ and $\delta x_{N+1}^n = 0$ for all n, we need only sum the terms in (3.2) from $i = 2$ to $i = N$. Summing and using (3.3) and (3.4) results in

$$\boldsymbol{\omega}^{n+1} = \boldsymbol{\omega}^n - \frac{\Delta t}{m_v}\left(\sum_{i=2}^{N} \rho\chi_i \Delta a \delta w_i^{n+1/2}\right) \wedge \delta p^{n+1/2} + \frac{\Delta t}{m_v}\left(\sum_{i=2}^{N} \rho\chi_i \Delta a \delta w_i^{n+1/2}\right) \wedge \delta\sigma^{n+1/2}. \quad (4.1)$$

This equation needs to be combined with the (q, p) equation

$$\delta p^{n+1} \wedge \delta q^{n+1} = \delta p^n \wedge \delta q^n - \frac{\Delta t}{m_v}\delta p^n \wedge \delta\sigma^{n+\frac{1}{2}} + \tfrac{1}{2}\nu\frac{\Delta t^2}{m_v}\delta q^n \wedge \delta\sigma^{n+\frac{1}{2}}. \quad (4.2)$$

5 Quadrature rule for σ^n

The terms in parentheses in (4.1) are partial approximations of σ^n. It is pretty clear that if we use Simpson's rule for σ^n, then the discretization will not be symplectic since the sum terms in (4.1) will not cancel. However, if we use the trapezoidal rule then the relevant terms will cancel. Therefore approximate σ^n as

$$\sigma^n = \frac{1}{2}\rho\Delta a\left(\chi_1 + \chi_{N+1}\right) w_1^n + \sum_{i=2}^{N} \rho\chi_i w_i^n \,\Delta a\,,$$

using the fact that $w_1^n = w_{N+1}^n$. The sum in (4.1) is then

$$\left(\sum_{i=2}^{N} \rho\chi_i \Delta a \delta w_i^{n+1/2}\right) = \delta\sigma^{n+\frac{1}{2}} - \frac{1}{2}\rho\Delta a\left(\chi_1 + \chi_{N+1}\right)\delta w_1^{n+\frac{1}{2}}.$$

6 Checking symplecticity

Adding the two terms in (4.1) and (4.2)

$$\begin{aligned}\boldsymbol{\Omega}^{n+1} &= \boldsymbol{\Omega}^n \\ &\quad - \tfrac{\Delta t}{m_v}\left(\delta\sigma^{n+\frac{1}{2}} - \tfrac{1}{2}\rho\Delta a\left(\chi_1 + \chi_{N+1}\right)\delta w_1^{n+\frac{1}{2}}\right) \wedge \delta p^{n+1/2} \\ &\quad + \tfrac{\Delta t}{m_v}\left(\delta\sigma^{n+\frac{1}{2}} - \tfrac{1}{2}\rho\Delta a\left(\chi_1 + \chi_{N+1}\right)\delta w_1^{n+\frac{1}{2}}\right) \wedge \delta\sigma^{n+1/2} \\ &\quad - \tfrac{\Delta t}{m_v}\delta p^n \wedge \delta\sigma^{n+\frac{1}{2}} + \tfrac{1}{2}\nu\tfrac{\Delta t^2}{m_v}\delta q^n \wedge \delta\sigma^{n+\frac{1}{2}}.\end{aligned}$$

Noting that $\delta\sigma^{n+\frac{1}{2}} \wedge \delta\sigma^{n+\frac{1}{2}} = 0$, $\delta p^{n+\frac{1}{2}} = \delta p^n - \frac{1}{2}\nu\Delta t\delta q^n$, and that

$$\delta w_1^{n+\frac{1}{2}} = m_v^{-1}\left(\delta p^{n+1/2} - \delta\sigma^{n+1/2}\right),$$

this expression simplifies to

$$\boldsymbol{\Omega}^{n+1} = \boldsymbol{\Omega}^n\,,$$

proving symplecticity of the scheme.

7 Remarks

Suppose we start in (2.1) with a different quadrature rule

$$\boldsymbol{\omega}^n := \sum_{i=2}^{N} e_i \, \delta w_i^n \wedge \delta x_i^n \, \rho \chi_i \Delta a \,,$$

where e_i are weightings associated with the chosen quadrature formula. Then this choice will filter through and σ^n can be evaluated with the same quadrature formula. However, the scheme will not be symplectic. In this case the proof breaks down in the proof that the A-terms vanish in §3.3.

Unless, the potential term,

$$\frac{g}{x_a} \frac{\partial}{\partial a} \left(\frac{\chi}{x_a} \right) ,$$

is discretized differently, the symplectic form should be discretized using the trapezoidal rule. Although, since δx_1^n and δx_{N+1}^n both vanish, one could equally well use a left or right Riemann sum.

Since $w_1^n = w_{N+1}^n$ for all n, the integrand in σ^n will be periodic when $\chi_1 = \chi_{N+1}$. This is the case for example when the initial condition is the flat state, $h = h_0$. Hence the integrand can be extended to all a as a periodic function. The trapezoidal rule is known to have excellent properties for periodic functions [3]. However, although the integrand is a continuous periodic function, it may not be a smooth periodic function.

References

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