# Integrating the 2-D Klein-Gordon Tangent Map

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The 2-D Klein-Gordon Hamiltonian is:

$$H = \sum_{x,y} \frac{p_{x,y}^2}{2} + \frac{\epsilon_{x,y} q_{x,y}^2}{2} + \frac{|q_{x,y}|^{\sigma+2}}{\sigma+2} - \frac{1}{2W}\left[(q_{x+1,y} - q_{x,y})^2 + (q_{x,y+1} - q_{x,y})^2\right] \tag{1}$$

which is separable into

$$\begin{aligned} H &= T(\vec{p}) + V(\vec{q}) \\ T(\vec{p}) &= \sum_{x,y} \frac{p_{x,y}^2}{2}, \\ V(\vec{q}) &= \sum_{x,y} \frac{\epsilon_{x,y} q_{x,y}^2}{2} + \frac{|q_{x,y}|^{\sigma+2}}{\sigma+2} - \frac{1}{2W}\left[(q_{x+1,y} - q_{x,y})^2 + (q_{x,y+1} - q_{x,y})^2\right] \end{aligned}$$

Since the Hamiltonian is nicely seperable, we can consider the variationals derived from the *Tangent Dynamic Hamiltonian (TDH)*, defined as

$$H_V(\vec{\delta q}, \vec{\delta p}; t) = \sum_{x,y} \frac{\delta p_{x,y}^2}{2} + \sum_{x,y} \sum_{u,v} \left[\mathbf{D}^2 V(\vec{q}(t))\right]_{x,y,u,v} \delta q_{x,y} \delta q_{u,v} \tag{2}$$

where

$$\left[\mathbf{D}^2 V(\vec{q}(t))\right]_{x,y,u,v} = \left.\frac{\partial^2 V}{\partial q_{x,y} \partial q_{u,v}}\right|_{\vec{q}=\vec{q}(t)}$$

Previously, the first derivative was found to be

$$\frac{\partial V}{\partial q_{x,y}} = \epsilon_{x,y} q_{x,y} + |q_{x,y}|^{\sigma} q_{x,y} - \frac{1}{W}\left[q_{x-1,y} + q_{x+1,y} + q_{x,y-1} + q_{x,y+1} - 4q_{x,y}\right]$$

And the second derivative yields yet again a Jacobi 5-stencil

$$\frac{\partial V}{\partial q_{u,v} \partial q_{x,y}} = \begin{cases} \epsilon_{x,y} + (\sigma+1)|q_{x,y}|^{\sigma} + \frac{4}{W}; & u = x,\ v = y \\ -\frac{1}{W}; & u = x \pm 1,\ v = y \\ -\frac{1}{W}; & u = x,\ v = y \pm 1 \end{cases}$$

Computationally, this is a fairly sparse tensor with only the diagonal depending on the trajectory $\vec{q}(t)$.

The former very easily integrates as

$$\partial_t u_{j,k} = \frac{\partial A}{\partial p_{j,k}} = p_{j,k} \quad \mapsto \quad u_{j,k}(t+\tau) = u_{j,k}(t) + \tau p_{j,k}(t)$$

For $B$, we'll need to expand to include the full $u_{j,k}$ stencil

$$\begin{aligned} B &= \ldots + \frac{\epsilon_{j,k} u_{j,k}^2}{2} + \frac{|u_{j,k}|^{\sigma+2}}{\sigma+2} + \ldots \\ &- \frac{1}{2W}\left[\ldots (u_{j,k} - u_{j-1,k})^2 + (u_{j+1,k} - u_{j,k})^2 + (u_{j,k} - u_{j,k-1})^2 + (u_{j,k+1} - u_{j,k})^2 + \ldots\right] \end{aligned}$$

In the differentiation, note that

$$\frac{\partial}{\partial u}\frac{|u|^{\sigma+2}}{\sigma+2} = |u|^{\sigma+1}\frac{\partial}{\partial u}|u| = |u|^{\sigma+1}\frac{u}{|u|} = |u|^{\sigma} u$$

Differentiating

$$\begin{aligned} \partial_t p_{j,k} &= -\frac{\partial B}{\partial u_{j,k}} \\ &= -\epsilon_{j,k} u_{j,k} - |u_{j,k}|^{\sigma} u_{j,k} + \frac{1}{W}\left(u_{j-1,k} + u_{j+1,k} + u_{j,k-1} + u_{j,k+1} - 4u_{j,k}\right) \end{aligned}$$

Giving

$$p_{j,k}(t+\tau) = p_{j,k}(t) - \tau\left[\epsilon_{j,k} u_{j,k} + |u_{j,k}|^{\sigma} u_{j,k} - \frac{1}{W}\left(u_{j-1,k} + u_{j+1,k} + u_{j,k-1} + u_{j,k+1} - 4u_{j,k}\right)\right]$$

**Corrector**

The corrector step is defined from $C = \{\{A,B\},B\}$. Expanding the brackets gives

$$\{A,B\} = \sum_{j,k} \frac{\partial A}{\partial u_{j,k}}\frac{\partial B}{\partial p_{j,k}} - \frac{\partial A}{\partial p_{j,k}}\frac{\partial B}{\partial u_{j,k}}$$

Since we have $A(p)$ and $B(u)$, the first term is zero

$$\{A,B\} = -\sum_{j,k} \frac{\partial A}{\partial p_{j,k}}\frac{\partial B}{\partial u_{j,k}}$$

The fact $\partial_p B = 0$ can be used again to simplify the next bracket

$$\begin{aligned} \{\{A,B\},B\} &= -\sum_{j,k} \frac{\partial}{\partial p_{j,k}}\left(\frac{\partial A}{\partial p_{j,k}}\frac{\partial B}{\partial u_{j,k}}\right)\frac{\partial B}{\partial u_{j,k}} \\ &= -\sum_{j,k}\left(\frac{\partial^2 A}{\partial p_{j,k}^2}\frac{\partial B}{\partial u_{j,k}} + \frac{\partial A}{\partial p_{j,k}}\frac{\partial^2 B}{\partial p_{j,k}\partial u_{j,k}}\right)\frac{\partial B}{\partial u_{j,k}} \end{aligned}$$

Previously, it was found

$$\frac{\partial A}{\partial p_{j,k}} = p_{j,k}, \qquad \frac{\partial B}{\partial u_{j,k}} = \epsilon_{j,k}u_{j,k} + |u_{j,k}|^{\sigma}\, u_{j,k} - \frac{1}{W}\left(u_{j-1,k} + u_{j+1,k} + u_{j,k-1} + u_{j,k+1} - 4u_{j,k}\right)$$

therefore the mixed derivative term goes to zero, giving

$$\{\{A,B\},B\} = -\sum_{j,k} \frac{\partial^2 A}{\partial p_{j,k}^2}\left(\frac{\partial B}{\partial u_{j,k}}\right)^2$$

Substituting the previously found values

$$C = \{\{A,B\},B\} = -\sum_{j,k}\left[\epsilon_{j,k}u_{j,k} + |u_{j,k}|^{\sigma}\, u_{j,k} - \frac{1}{W}\left(u_{j-1,k} + u_{j+1,k} + u_{j,k-1} + u_{j,k+1} - 4u_{j,k}\right)\right]^2$$

The corrector's momentum change is

$$\partial_t p_{j,k} = -\frac{\partial C}{\partial u_{j,k}}$$

which in order to do, we'll need to write out the full $u_{j,k}$ stencil. This is easily done by considering the variable

$$\zeta_{j,k} = \epsilon_{j,k}u_{j,k} + |u_{j,k}|^{\sigma}\, u_{j,k} - \frac{1}{W}\left(u_{j-1,k} + u_{j+1,k} + u_{j,k-1} + u_{j,k+1} - 4u_{j,k}\right)$$

Note that $\zeta_{j,k}$ contains the $u_{j,k}$ stencil. We can expand $C$ to a $\zeta_{j,k}$ stencil

$$C \;=\; \ldots - \zeta_{j-1,k}^2 - \zeta_{j+1,k}^2 - \zeta_{j,k-1}^2 - \zeta_{j,k+1}^2 - \zeta_{j,k}^2 - \ldots$$

In this expansion, ever instance of $u_{j,k}$ is present, so then

$$\begin{aligned}
\partial_t p_{j,k} &= -\frac{\partial C}{\partial u_{j,k}} \\
&= 2\zeta_{j-1,k}\frac{\partial \zeta_{j-1,k}}{\partial u_{j,k}} + 2\zeta_{j+1,k}\frac{\partial \zeta_{j+1,k}}{\partial u_{j,k}} + 2\zeta_{j,k-1}\frac{\partial \zeta_{j,k-1}}{\partial u_{j,k}} + 2\zeta_{j,k+1}\frac{\partial \zeta_{j,k+1}}{\partial u_{j,k}} + 2\zeta_{j,k}\frac{\partial \zeta_{j,k}}{\partial u_{j,k}}
\end{aligned}$$

Looking term by term

$$\begin{aligned}
\zeta_{j,k} &= \epsilon_{j,k}u_{j,k} + |u_{j,k}|^{\sigma}\, u_{j,k} - \frac{1}{W}\left(u_{j-1,k} + u_{j+1,k} + u_{j,k-1} + u_{j,k+1} - 4u_{j,k}\right) \\
\zeta_{j-1,k} &= \epsilon_{j-1,k}u_{j-1,k} + |u_{j-1,k}|^{\sigma}\, u_{j-1,k} - \frac{1}{W}\left(u_{j-2,k} + u_{j,k} + u_{j-1,k-1} + u_{j-1,k+1} - 4u_{j-1,k}\right) \\
\zeta_{j+1,k} &= \epsilon_{j+1,k}u_{j+1,k} + |u_{j+1,k}|^{\sigma}\, u_{j+1,k} - \frac{1}{W}\left(u_{j,k} + u_{j+2,k} + u_{j+1,k-1} + u_{j+1,k+1} - 4u_{j+1,k}\right) \\
\zeta_{j,k-1} &= \epsilon_{j,k-1}u_{j,k-1} + |u_{j,k-1}|^{\sigma}\, u_{j,k-1} - \frac{1}{W}\left(u_{j-1,k-1} + u_{j+1,k-1} + u_{j,k-2} + u_{j,k} - 4u_{j,k-1}\right) \\
\zeta_{j,k+1} &= \epsilon_{j,k+1}u_{j,k+1} + |u_{j,k+1}|^{\sigma}\, u_{j,k+1} - \frac{1}{W}\left(u_{j-1,k+1} + u_{j+1,k+1} + u_{j,k} + u_{j,k+2} - 4u_{j,k+1}\right)
\end{aligned}$$

And noting the derivative

$$\frac{\partial}{\partial u}\left|u\right|^{\sigma}u=\sigma\left|u\right|^{\sigma-1}\frac{\partial\left|u\right|}{\partial u}u+\left|u\right|^{\sigma}=\left(\sigma+1\right)\left|u\right|^{\sigma}$$

We then have

$$\begin{aligned}\frac{\partial\zeta_{j,k}}{\partial u_{j,k}} &= \epsilon_{j,k}+\left(\sigma+1\right)\left|u_{j,k}\right|^{\sigma}+\frac{4}{W}\\ \frac{\partial\zeta_{j\pm1,k}}{\partial u_{j,k}} &= \frac{\partial\zeta_{j,k\pm1}}{\partial u_{j,k}}=-\frac{1}{W}\end{aligned}$$

And finally

$$\partial_t p_{j,k}=-\frac{2}{W}\left(\zeta_{j-1,k}+\zeta_{j+1,k}+\zeta_{j,k-1}+\zeta_{j,k+1}\right)+2\zeta_{j,k}\left(\epsilon_{j,k}+\left(\sigma+1\right)\left|u_{j,k}\right|^{\sigma}+\frac{4}{W}\right)$$

which can be re-written as

$$\partial_t p_{j,k}=2\Big(\epsilon_{j,k}+\left(\sigma+1\right)\left|u_{j,k}\right|^{\sigma}\Big)\zeta_{j,k}-\frac{2}{W}\left(\zeta_{j-1,k}+\zeta_{j+1,k}+\zeta_{j,k-1}+\zeta_{j,k+1}-4\zeta_{j,k}\right)$$

which is then simply updated

$$p(t+\tau)=p(t)+2\tau\left[\Big(\epsilon_{j,k}+\left(\sigma+1\right)\left|u_{j,k}\right|^{\sigma}\Big)\zeta_{j,k}-\frac{1}{W}\left(\zeta_{j-1,k}+\zeta_{j+1,k}+\zeta_{j,k-1}+\zeta_{j,k+1}-4\zeta_{j,k}\right)\right]$$