

# Introduction to Scientific Computing

## Discrete Energy

### Explicit time stepping and numerical energy

To obtain a numerical solution of the 1D heat equation, we have derived the following explicit scheme

$$v_j^{(m+1)} = v_j^{(m)} + \frac{\tau}{h^2} \left( v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)} \right). \quad (1)$$

For the resulting numerical solutions  $v^{(m)}$  we introduce the discrete energy

$$E^{(m)} := h \sum_{j=1}^{n-1} \left( v_j^{(m)} \right)^2$$

for each time step  $m$ .

We would like to show that the discrete energy also decreases in time, i.e.:

$$E^{(m+1)} \leq E^{(m)} \quad \text{for } m \geq 0.$$

Thus, we compute the difference of the energy in two subsequent time steps:

$$\begin{aligned} E^{(m+1)} - E^{(m)} &= h \sum_{j=1}^{n-1} \left( \left( v_j^{(m+1)} \right)^2 - \left( v_j^{(m)} \right)^2 \right) \\ &= h \sum_{j=1}^{n-1} \left( v_j^{(m+1)} + v_j^{(m)} \right) \left( v_j^{(m+1)} - v_j^{(m)} \right). \end{aligned}$$

Remembering our explicit time-stepping scheme,

$$v_j^{(m+1)} = v_j^{(m)} + \frac{\tau}{h^2} \left( v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)} \right), \quad (2)$$

$$\text{or } v_j^{(m+1)} - v_j^{(m)} = \frac{\tau}{h^2} \left( v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)} \right), \quad (3)$$

we get

$$\begin{aligned}
E^{(m+1)} - E^{(m)} &= \frac{\tau}{h} \sum_{j=1}^{n-1} \left( v_j^{(m+1)} + v_j^{(m)} \right) \left( v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)} \right) \\
&= \frac{\tau}{h} \left\{ \underbrace{\sum_{j=1}^{n-1} v_j^{(m)} \left( v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)} \right)}_{=: S^{(m)}} \right. \\
&\quad \left. - 2 \sum_{j=1}^{n-1} v_j^{(m+1)} v_j^{(m)} + \sum_{j=1}^{n-1} v_j^{(m+1)} \left( v_{j-1}^{(m)} + v_{j+1}^{(m)} \right) \right\} \\
&= \frac{\tau}{h} \left\{ S^{(m)} - 2 \sum_{j=1}^{n-1} v_j^{(m+1)} v_j^{(m)} + \sum_{j=1}^{n-1} v_j^{(m+1)} \left( v_{j-1}^{(m)} + v_{j+1}^{(m)} \right) \right\}
\end{aligned}$$

### Estimates for Discrete Energy

The three sums can be examined separately.

- For the term  $S^{(m)}$ , we can use *summation by parts* (see separate worksheet, eq. 8) to get

$$S^{(m)} = \sum_{j=1}^{n-1} v_j^{(m)} \left( v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)} \right) = -(v_1^{(m)})^2 - \sum_{j=1}^{n-1} \left( v_{j+1}^{(m)} - v_j^{(m)} \right)^2 \leq 0.$$

Thus, this term is always negative.

- In the second sum, we can apply the time stepping scheme (1), and obtain

$$\begin{aligned}
-2 \sum_{j=1}^{n-1} v_j^{(m+1)} v_j^{(m)} &= -2 \sum_{j=1}^{n-1} \left( v_j^{(m)} + \frac{\tau}{h^2} \left( v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)} \right) \right) v_j^{(m)} \\
&= -2 \underbrace{\sum_{j=1}^{n-1} (v_j^{(m)})^2}_{= \frac{1}{h} E^{(m)}} - 2 \frac{\tau}{h^2} \underbrace{\sum_{j=1}^{n-1} v_j^{(m)} \left( v_{j-1}^{(m)} - 2v_j^{(m)} + v_{j+1}^{(m)} \right)}_{= S^{(m)}} \\
&= -\frac{2}{h} E^{(m)} - 2 \frac{\tau}{h^2} S^{(m)}
\end{aligned}$$

- and finally, using the inequality  $ab \leq \frac{1}{2} (a^2 + b^2)$ ,

$$\begin{aligned}
\sum_{j=1}^{n-1} v_j^{(m+1)} \left( v_{j-1}^{(m)} + v_{j+1}^{(m)} \right) &= \sum_{j=1}^{n-1} v_j^{(m+1)} v_{j-1}^{(m)} + \sum_{j=1}^{n-1} v_j^{(m+1)} v_{j+1}^{(m)} \\
&\leq \frac{1}{2} \sum_{j=1}^{n-1} \left[ (v_j^{(m+1)})^2 + (v_{j-1}^{(m)})^2 \right] + \frac{1}{2} \sum_{j=1}^{n-1} \left[ (v_j^{(m+1)})^2 + (v_{j+1}^{(m)})^2 \right]
\end{aligned}$$

$$\begin{aligned}
&= \underbrace{\sum_{j=1}^{n-1} \left(v_j^{(m+1)}\right)^2}_{=\frac{1}{h}E^{(m+1)}} + \frac{1}{2} \underbrace{\sum_{j=1}^{n-1} \left(v_{j-1}^{(m)}\right)^2}_{\leq \frac{1}{h}E^{(m)}} + \frac{1}{2} \underbrace{\sum_{j=1}^{n-1} \left(v_{j+1}^{(m)}\right)^2}_{\leq \frac{1}{h}E^{(m)}} \\
&\leq \frac{1}{h} \left(E^{(m+1)} + E^{(m)}\right)
\end{aligned}$$

Putting these three results together, we get that

$$\begin{aligned}
E^{(m+1)} - E^{(m)} &\leq \frac{\tau}{h} \left( S^{(m)} - \frac{2}{h}E^{(m)} - 2\frac{\tau}{h^2}S^{(m)} + \frac{1}{h} \left(E^{(m+1)} + E^{(m)}\right) \right) \\
&= \frac{\tau}{h} \left( 1 - 2\frac{\tau}{h^2} \right) S^{(m)} + \frac{\tau}{h^2} \left( E^{(m+1)} - E^{(m)} \right),
\end{aligned}$$

which is equivalent to

$$\left(1 - \frac{\tau}{h^2}\right) \left(E^{(m+1)} - E^{(m)}\right) \leq \frac{\tau}{h} \left(1 - 2\frac{\tau}{h^2}\right) S^{(m)}.$$

We already know that  $S^{(m)} \leq 0$ . As  $\tau$  and  $h$  are positive, the right hand side will be negative if (and only if)

$$-1 + 2\frac{\tau}{h^2} \leq 0 \quad \Leftrightarrow \quad \frac{\tau}{h^2} \leq \frac{1}{2}.$$

As a consequence, the left hand side has got to be negative, too:

$$\left(1 - \frac{\tau}{h^2}\right) \left(E^{(m+1)} - E^{(m)}\right) \leq 0.$$

However, if  $\frac{\tau}{h^2} \leq \frac{1}{2}$ , then  $1 - \frac{\tau}{h^2} > 0$ , which means that

$$E^{(m+1)} - E^{(m)} \leq 0.$$

### Conclusion:

As the final result, we may state that the energy function  $E^{(m)}$  is decreasing, if a certain restriction of the size of the time step is enforced:

$$E^{(m+1)} - E^{(m)} \leq 0 \quad \text{if} \quad \frac{\tau}{h^2} \leq \frac{1}{2}.$$

For larger time steps, energy conservation is not guaranteed, and the numerical scheme might diverge.