# Fractional order convergence of time-discretizations for semilinear PDEs

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*Summary*. A discretization of an ODE is of order $p$ if the trajectory error is of magnitude $h^p$, where $h$ is the time step size. When we discretize a PDE in space first we obtain an ODE on a high dimensional space. Discretizing this ODE in time by an order $p$ numerical method does however in general NOT give an order $p$ accurate time discretization. Indeed when the spatial accuracy is very high the trajectory error of the full time-space discretization is $Ch^p$ where $C$ is very big. In this case convergence is lost UNLESS the continuous solution has some spatial regularity. In this talk we show how to obtain fractional order convergence in the case where the continuous solution has some regularity, but not enough to obtain full order convergence.

## Discretization error for ODEs

Let us first consider an ODE $\dot{y} = f(y)$ where $y : \mathbb{R}^n \to \mathbb{R}^n$ is smooth. Let $y(t)$ be its exact solution and $y(0) = y^0$. We discretize this ODE by an order $p$ method $y^1 = \Psi^h(y^0)$. This means that the local error $\|y(h) - y^1\|$ satisfies

$$\|y(h) - y^1\| = O(h^{p+1}). \tag{1}$$

For fixed $T > 0$ if $t = nh \leq T$, then the global trajectory error $E_n(h) = \|y(t) - y^n\|$ satisfies $E_n(h) = O(h^p)$ where $y^n = (\Psi^h)^n(y^0)$ is the $n$th iterate of $\Psi^h$. To obtain the error bound (1) we Taylor expand both $y^1 = \Psi^h(y^0)$ and $y(h)$ in $h$. If the first $p$ derivatives of $\Psi^h$ and $y(h)$ coincide then $\Psi^h$ is a method of order $p$. As an example we consider the implicit midpoint rule (IMPR) which has order $p = 2$ and is given by

$$y^1 = y^0 + hf(\frac{1}{2}(y^0 + y^1)), \tag{2}$$

see eg. [2].

## The semilinear wave equation

We now consider semilinear PDEs of the form

$$U_t = AU + B(U) = F(U) \tag{3}$$

on some Hilbert space $\mathcal{Y}$ where $A$ is a skew-self adjoint operator, i.e. $A^* = -A$ and $B : \mathcal{Y}^\ell \to \mathcal{Y}^\ell$ is smooth for any $\ell \geq 0$ where $\mathcal{Y}^\ell = D(A^\ell)$. An example is the semilinear wave equation with periodic boundary conditions

$$u_{tt} = u_{xx} - V'(u), \quad u(0) = u(2\pi), \tag{4}$$

where $V(\cdot) : \mathbb{R} \to \mathbb{R}$ is a smooth potential. This equation is Hamiltonian with energy

$$H(u, u_t) = \int_0^{2\pi} \left(\frac{1}{2}(u_x^2 + u_t^2) + V(u)\right) \mathrm{d}x.$$

We write (4) in the form (3) by setting $U = (u, v)$, where $v = u_t$, and

$$A = \mathbb{Q}_0 \tilde{A}, \quad \tilde{A} = \begin{pmatrix} 0 & 1 \\ \partial_x^2 & 0 \end{pmatrix}, \quad B(U) = \begin{pmatrix} 0 \\ -V'(u) \end{pmatrix} + \mathbb{P}_0 \tilde{A} U.$$

Here $\mathbb{P}_0$ is the spectral projector of $\tilde{A}$ to the eigenvalue 0 and $\mathbb{Q}_0 = 1 - \mathbb{P}_0$. Note that $\tilde{A}$ has spectrum $\operatorname{spec}(\tilde{A}) = \{\mathrm{i}m, m \in \mathbb{Z}\}$, with eigenvectors $(\frac{\mathrm{e}^{\mathrm{i}mx}}{\mathrm{i}m}, \mathrm{e}^{\mathrm{i}mx})$ for $m \neq 0$ and with eigenvector $(1, 0)$ and generalized eigenvector $(0, 1)$ when $m = 0$. Hence the solution operator of the linear system (3) (where $B \equiv 0$) given by $e^{tA}$ is an isometry ($\|e^{tA}\|_\mathcal{Y} = 1$) with finite energy solutions if we set $\mathcal{Y} = \mathcal{H}^1 \times \mathcal{L}_2$. Here we define the Sobolev space $\mathcal{H}^\ell$, $\ell \geq 0$, as the space of functions for which the inner product

$$\langle u, v \rangle_{\mathcal{H}^\ell} = \hat{u}_0 \overline{\hat{v}_0} + \sum_{m \in \mathbb{Z}} m^{2\ell} \hat{u}_m \overline{\hat{v}_m} \tag{5}$$

is finite. We denote by $\hat{u}_m$, $\hat{v}_m$ the Fourier coefficients of $u(x) = \frac{1}{\sqrt{2}} \sum_{m \in \mathbb{Z}} \hat{u}_m \mathrm{e}^{\mathrm{i}mx}$ and $v(x) = \frac{1}{\sqrt{2}} \sum_{m \in \mathbb{Z}} \hat{v}_m \mathrm{e}^{\mathrm{i}mx}$. Moreover $\mathcal{L}_2$, corresponding to $\ell = 0$ in (5), is the space of square integrable functions.
Using a variation of constant formula it can then be shown that there is a unique solution $U(t)$ of (3) in a mild sense [3]. For this solution to be a classical solution, i.e. a solution which satisfies equation (3), we need that $AU(t) \in \mathcal{Y}$, which means $U(t) \in D(A) = \mathcal{Y}_1$. In the case of the semilinear wave equation (4) the operator $A$ acts like $\mathrm{i}m$ on the $m$th Fourier mode, so, in view of (5), we need $U = (u, v) \in \mathcal{Y}_1 = \mathcal{H}^2 \times \mathcal{H}^1$. If the initial value $U(0) = U^0$ of the solution $U(t)$ of the evolution equation (3) lies in $\mathcal{Y}_\ell$, $\ell \in \mathbb{N}$, then $A^\ell U(t) \in \mathcal{Y}$ and $U(t)$ is $\ell$ times differentiable in $t$ in the $\mathcal{Y}$ norm.

### Implicit midpoint time discretization of semlinear wave equation

Applying the implicit midpoint rule (2) to the evolution equation (3) and rearranging gives

$$U^1 = \Psi^h(U^0) = (1 - \frac{h}{2}A)(1 - \frac{h}{2}A)^{-1}U^0 + h(1 - \frac{h}{2}A)^{-1}B(\frac{1}{2}(U^0 + U^1))$$

which can be solved by the contraction mapping theorem. If $U^0 \in \mathcal{Y}_\ell$ with $\ell \geq 3$ then the derivatives $\partial_t^j U(t) \in \mathcal{Y}$ of the solution $U(t)$ of (3) exist for $j = 1, 2, 3$, and similarly $\partial_h^j \Psi^h(U^0) \in \mathcal{Y}$ exists for $j = 0, 1, 2, 3$. In this case the local error $\|U(h) - U^1\|_\mathcal{Y}$ is well defined and of order $O(h^3)$ and the global error is of order $O(h^2)$ as in the case of ODEs.

### Main result

Here we investigate the case when the initial value $U(0) = U^0$ lies in $\mathcal{Y}_\ell$ with $\ell < p + 1$, i.e. $\ell < 3$ for our example, the implicit midpoint rule (2) . We show that for such initial data $U^0$ the global error $\|U(t) - U^n\|_\mathcal{Y}$ where $t = nh$ and $U^n = (\Psi^h)^n(U^0)$, satisfies

$$E_n(h) = \|U(t_n) - U^n\|_\mathcal{Y} = ch^{\frac{\ell p}{p+1}}, \quad \text{where} \quad t_n = nh \leq T, \tag{6}$$

with the constant $c$ depending on $T > 0$. For linear evolution equations such a result was proved in [1]. For the IMPR (2) we get an order of convergence $q(\ell) = 2\ell/3$. Let us discretize (4) in space as well, say by finite differences, using that

$$u_{xx}(x) = \frac{u(x + k) - 2u(x) + u(x - k)}{k^2} + O(k^3).$$

The global space time discretization error then in general satisfies

$$\|U(t_n) - U_k^n\| = O(\|A_k\|^3)h^3, \quad \text{where } x_m = mk \in [0, 2\pi].$$

Here $U_k^n = \{U_k^n(x_m)\}$, with $U_k^n(x_m)$ the space time discretization of $U(t)$ at $(t, x) = (t_n, x_m)$. Moreover $A_k$, the space discretization of $A$, satisfies $\|A_k\| = O(1/k)$ (in the norm descending from $\mathcal{Y}$). Hence when spatial and temporal stepsizes $k$ and $h$ are of the same order then in general the discretization error is $O(1)$, so there is no convergence. This corresponds to the case $\ell = 0$ in (6). But if $U^0 \in \mathcal{Y}_\ell$, $\ell > 0$, then we numerically observe an order of convergence $q(\ell)$ as shown in Figure 1 (solid line), which is in good agreement with the theoretical result $q(\ell) = p\ell/(p + 1)$ (dashed line). To produce the figure we have chosen $V'(u) = u - 4u^2$ for $\ell = j/2$, $j = 0, \ldots, 6$, on the interval $t \in [0, 0.5]$, and use a fine spatial mesh (with $N = 1000$ grid points on $[0, 2\pi]$). As initial values we choose $U^0 = (u^0, v^0) \in \mathcal{Y}_\ell$ where

$$u^0(x) = \sum_{k=0}^{N=1} \frac{c_u}{k^{\ell+1/2+\epsilon}}(\cos kx + \sin kx), \quad v^0(x) = \sum_{k=0}^{N=1} \frac{c_v}{k^{\ell+1/2+\epsilon}}(\cos kx + \sin kx).$$

Here $c_u$ and $c_v$ are such that $\|U^0\|_{\mathcal{Y}_\ell} = 1$, with $U^0 = (u^0, v^0)$, and $\epsilon = 10^{-8}$. We integrate the semilinear wave equation with the above initial data for the time steps $h = 0.1, 0.095, 0.09, \ldots, 0.05$, when $\ell > 0$. To estimate the trajectory error, we compare the numerical solution to a solution calculated using a smaller time step, $\tilde{h} = 10^{-3}$ for $\ell > 0$ and $\tilde{h} = 10^{-4}$ for $\ell = 0$. From the assumption $E_n(h) = ch^q$ we get $\log E_n(h) = \log c + q \log h$. Fitting a line to those data, we take the gradient of the line as our estimated order of convergence $q(\ell)$ of the trajectory error.

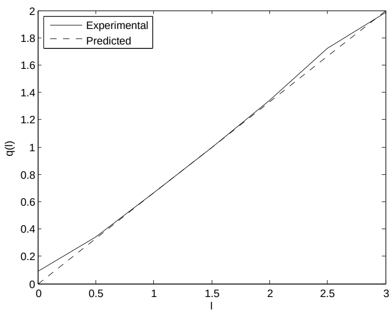


Figure 1: Plot of a numerical estimate of $q(\ell)$ against $\ell$ for the implicit midpoint rule applied to the semilinear wave equation, with the prediction of (6) for comparison. Courtesy of [4].

## References

[1] P. Brenner and V. Thomée, *On rational approximations of semigroups*, SIAM J. Numer. Anal., 16(4): 683âĂŞ-694, 1979.

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