

Term Project

(Mathematics, Computational Science & Engineering)

Discretization of Linear Dirac Equations in 1D

submitted by

Nisha Maria Kannookadan, M.Sc.

Supervisor: Prof. Dr. Ralf Hiptmair (SAM, D-MATH)

Assistant: Dr. Tomas Dohnal

ETH - Swiss Federal Institute of Technology Zurich

SAM - Seminar for Applied Mathematics

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Chapter 1

Definition of the Term Project

1.1 Basic Model Problem

Given a real valued function $f \in C^0([0, T], W^{1, \infty}(\Omega))$, $\Omega \subset \mathbb{R}^d$, we consider the initial boundary value problem: seek $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$. $v = v(\mathbf{x}, t)$ such that

$$\begin{aligned} \partial_t \mathbf{u} &= -if \mathbf{grad} v - \frac{i}{2} \mathbf{grad} f v && \text{in } [0, T] \times \Omega, \\ \partial_t v &= if \operatorname{div} \mathbf{u} + \frac{i}{2} \mathbf{grad} f \cdot \mathbf{u} && \text{in } [0, T] \times \Omega, \\ v &= 0 && \text{on } [0, T] \times \partial\Omega, \end{aligned} \tag{1.1}$$
$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) \quad , \quad v(\mathbf{x}, 0) = v_0(\mathbf{x}).$$

1.2 Weak Forms

- We may just test the two equations in (1.1) and integrate over Ω : seek $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$. $v = v(\mathbf{x}, t)$ such that

$$\begin{aligned} (\partial_t \mathbf{u}, \mathbf{q})_0 &= (-if \mathbf{grad} v - \frac{i}{2} \mathbf{grad} f v, \mathbf{q})_0 && \forall \mathbf{q} \in \mathbf{H}(\operatorname{div}, \Omega), \\ (\partial_t v, w)_0 &= (if \operatorname{div} \mathbf{u} + \frac{i}{2} \mathbf{grad} f \cdot \mathbf{u}, w)_0 && \forall w \in H_0^1(\Omega), \end{aligned} \tag{1.2}$$

where $(u, v)_0 := \int_{\Omega} u \bar{v} \, dx$.

- Another option is to aim integration by parts at the second equation: seek $\mathbf{u} \in (L^2(\Omega))^d$, $v \in H_0^1(\Omega)$, such that

$$\begin{aligned} (\partial_t \mathbf{u}, \mathbf{q})_0 &= (-if \mathbf{grad} v - \frac{i}{2} \mathbf{grad} f v, \mathbf{q})_0 && \forall \mathbf{q} \in (L^2(\Omega))^d, \\ (\partial_t v, w)_0 &= -\frac{i}{2} (\mathbf{u} \cdot \mathbf{grad} f, w)_0 - i \int_{\Omega} f \mathbf{u} \cdot \mathbf{grad} \bar{w} \, dx && \forall w \in H_0^1(\Omega). \end{aligned} \tag{1.3}$$

- A third option is to apply integration by parts to the first equation: seek $\mathbf{u} \in \mathbf{H}(\text{div}, \Omega)$, $v \in L^2(\Omega)$ such that

$$\begin{aligned} (\partial_t \mathbf{u}, \mathbf{q})_0 &= \int_{\Omega} \frac{i}{2} \mathbf{grad} f \cdot \bar{\mathbf{q}} v + i v f \text{div} \bar{\mathbf{q}} \, dx & \forall \mathbf{q} \in \mathbf{H}(\text{div}, \Omega), \\ (\partial_t v, w)_0 &= (i f \text{div} \mathbf{u} + \frac{i}{2} \mathbf{grad} f \cdot \mathbf{u}, w)_0 & \forall w \in L^2(\Omega). \end{aligned} \quad (1.4)$$

1.3 Conservation Property

The evolution respects conservation of total charge: $\frac{d}{dt} Q = 0$ for

$$Q(t) := \int_{\Omega} |\mathbf{u}|^2 + |v|^2 \, dx. \quad (1.5)$$

1.4 Galerkin Discretization

The variational formulations (1.2) – (1.4) allow a straightforward Galerkin discretization: We equip Ω with some mesh and choose \mathcal{V} and \mathcal{W} as finite element subspace of $L^2(\Omega)$, $\mathbf{H}(\text{div}, \Omega)$ and $H_0^1(\Omega)$, respectively. The simplest choice in 1D is piecewise linear / piecewise constant functions on some (non necessarily uniform) grid.

1.5 Timestepping

The timestepping scheme has to preserve the conservation of Q in the fully discrete setting. This suggests the choice of implicit Runge-Kutta-Gauss timestepping [1, Sect. 6.3.2], [1, Thm. 6.58].

For the ordinary differential equation $\dot{y} = f(t, y)$ the simplest representative of this class of Runge-Kutta methods is given by

$$y^{k+1} = y^k + \tau \delta y \quad , \quad \delta y = f\left(t^k + \frac{1}{2}\tau, y^k + \frac{1}{2}\tau \delta y\right).$$

Here, $\tau > 0$ is the size of the timestep. If the ODE is linear, that is, $\dot{y} = \mathbf{A}(t)y$ with a time-dependent linear operator $\mathbf{A} = \mathbf{A}(t)$, then the scheme reduces to

$$\frac{y^{k+1} - y^k}{\tau} = \mathbf{A}\left(t^k + \frac{1}{2}\tau\right) \left(\frac{y^{k+1} + y^k}{2}\right). \quad (1.6)$$

Let $\langle \cdot, \cdot \rangle$ be a (sesqui-linear) inner product on the phase space, for which $\mathbf{A}(t)$ is skew-symmetric for all times, that is,

$$\langle \mathbf{A}(t)y, z \rangle = -\langle y, \mathbf{A}(t)z \rangle \quad \forall y, z, t.$$

Writing $\|\cdot\|$ for the norm arising from $\langle \cdot, \cdot \rangle$, (1.6) involves

$$\begin{aligned} \|y^{k+1}\|^2 - \|y^k\|^2 &= \operatorname{Re} \langle y^{k+1} - y^k, y^{k+1} + y^k \rangle \\ &= \operatorname{Re} \frac{\tau}{2} \langle \mathbf{A}(t^k + \frac{1}{2}\tau)(y^{k+1} + y^k), y^{k+1} + y^k \rangle = 0. \end{aligned}$$

Let us assume that for the solution of any initial value problem form $\dot{y} = \mathbf{A}(t)y$ holds

$$\|y(t)\| = \|y(t^0)\| \quad \forall t. \quad (1.7)$$

Then

$$0 = \frac{d}{dt} \|y(t)\|^2 = 2 \operatorname{Re} \langle y(t), \mathbf{A}(t)y(t) \rangle \quad \forall t. \quad (1.8)$$

Since the trajectories of solutions cover the entire phase space, the operator $\mathbf{A}(t)$ has to be skew-symmetric.

Apply these considerations to (1.2) – (1.4) with $y = \begin{pmatrix} \mathbf{u} \\ v \end{pmatrix}$ and the inner product $(\cdot, \cdot)_0$.

We also observe that for constant f (1.1) boils down to a first order wave equation. For the wave equation explicit reversible timestepping schemes (known as Störmer-Verlet or leapfrog) display an excellent approximate conservation of charge, see [2, Sect. 1.7].

1.6 Task

1. Rederive the weak formulations and prove charge conservation.
2. Consider (1.1) for $d = 1$ and $\Omega =]0, 1[$ and examine the cases
 - (a) $f \equiv 1$ (constant function),
 - (b) $f(x) = x e^{-2x}$ (spatially varying function),
 - (c) $f(x, t) = x e^{-tx}$ (varying in space and time).

Discretize the initial value problem based on (1.2) – (1.4) on an equidistant spatial mesh and lowest order finite elements. Timestepping should be done using the implicit midpoint rule (see Sect. 1.5) or an explicit leapfrog-type scheme (optional).

3. Investigate the convergence of the methods in terms of spatial and temporal resolution (meshwidth and timestep).

Chapter 2

Weak Forms

2.1 Rederivation of the Weak Form (1.2)

$$\begin{aligned}(\partial_t \mathbf{u}, \mathbf{q})_0 &= \int_{\Omega} \partial_t \mathbf{u} \bar{\mathbf{q}} \, d\mathbf{x} \\ &= \int_{\Omega} (-if \operatorname{grad} v - \frac{i}{2} \operatorname{grad} f v,) \bar{\mathbf{q}} \, d\mathbf{x} \\ &= (-if \operatorname{grad} v - \frac{i}{2} \operatorname{grad} f v, \mathbf{q})_0\end{aligned}\quad \forall \mathbf{q} \in \mathbf{H}(\operatorname{div}, \Omega)$$

$$\begin{aligned}(\partial_t v, w)_0 &= \int_{\Omega} \partial_t v \bar{w} \, d\mathbf{x} \\ &= \int_{\Omega} (if \operatorname{div} \mathbf{u} + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u}) \bar{w} \, d\mathbf{x} \\ &= (if \operatorname{div} \mathbf{u} + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u}, w)_0\end{aligned}\quad \forall w \in H_0^1(\Omega)$$

2.2 Rederivation of the Weak Form (1.3)

$$\begin{aligned}
(\partial_t \mathbf{u}, \mathbf{q})_0 &= \int_{\Omega} \partial_t \mathbf{u} \bar{\mathbf{q}} \, dx \\
&= \int_{\Omega} (-if \, \mathbf{grad} v - \frac{i}{2} \, \mathbf{grad} f v,) \bar{\mathbf{q}} \, dx \\
&= (-if \, \mathbf{grad} v - \frac{i}{2} \, \mathbf{grad} f v, \mathbf{q})_0 \quad \forall \mathbf{q} \in (L^2(\Omega))^d
\end{aligned}$$

$$\begin{aligned}
(\partial_t v, w)_0 &= \int_{\Omega} \partial_t v \bar{w} \, dx \\
&= \int_{\Omega} (if \, \text{div} \mathbf{u} + \frac{i}{2} \, \mathbf{grad} f \cdot \mathbf{u}) \bar{w} \, dx \\
&= \int_{\Omega} if \, \text{div} \mathbf{u} \bar{w} + \frac{i}{2} \, \mathbf{grad} f \cdot \mathbf{u} \bar{w} \, dx \\
&= \int_{\Omega} \text{div} \mathbf{u} \cdot (if \bar{w}) + \frac{i}{2} \, \mathbf{grad} f \cdot \mathbf{u} \bar{w} \, dx \\
&\stackrel{\text{P.I.}}{=} - \int_{\Omega} \mathbf{u} \cdot \mathbf{grad} (if \bar{w}) \, dx + \int_{\partial \Omega} if \bar{w} (\mathbf{u} \cdot \mathbf{n}) \, dS \\
&\quad + \int_{\Omega} \frac{i}{2} \, \mathbf{grad} f \cdot \mathbf{u} \bar{w} \, dx \\
&\stackrel{\text{P.R.}}{=} - \int_{\Omega} \mathbf{u} \cdot (if \, \mathbf{grad} \bar{w} + i \, \mathbf{grad} f \bar{w}) \, dx \\
&\quad + \int_{\Omega} \frac{i}{2} \, \mathbf{grad} f \cdot \mathbf{u} \bar{w} \, dx \\
&= - \int_{\Omega} \mathbf{u} \cdot if \, \mathbf{grad} \bar{w} \, dx - \int_{\Omega} \mathbf{u} \cdot i \, \mathbf{grad} f \bar{w} \, dx \\
&\quad + \int_{\Omega} \frac{i}{2} \, \mathbf{grad} f \cdot \mathbf{u} \bar{w} \, dx \\
&= -i \int_{\Omega} f \mathbf{u} \cdot \mathbf{grad} \bar{w} \, dx + i \int_{\Omega} (-\mathbf{u} \cdot \mathbf{grad} f + \frac{1}{2} \, \mathbf{grad} f \cdot \mathbf{u}) \bar{w} \, dx \\
&= -i \int_{\Omega} f \mathbf{u} \cdot \mathbf{grad} \bar{w} \, dx - \frac{i}{2} \int_{\Omega} (\mathbf{u} \cdot \mathbf{grad} f) \bar{w} \, dx \\
&= -i \int_{\Omega} f \mathbf{u} \cdot \mathbf{grad} \bar{w} \, dx - \frac{i}{2} (\mathbf{u} \cdot \mathbf{grad} f, w)_0 \\
&= -\frac{i}{2} (\mathbf{u} \cdot \mathbf{grad} f, w)_0 - i \int_{\Omega} f \mathbf{u} \cdot \mathbf{grad} \bar{w} \, dx \quad \forall w \in H_0^1(\Omega)
\end{aligned}$$

P.I.: Partial integration

P.R.: Product rule

2.3 Rederivation of the Weak Form (1.4)

$$\begin{aligned}
(\partial_t \mathbf{u}, \mathbf{q})_0 &= \int_{\Omega} \partial_t \mathbf{u} \cdot \bar{\mathbf{q}} \, dx \\
&= \int_{\Omega} (-if \, \mathbf{grad} v - \frac{i}{2} \, \mathbf{grad} f v) \bar{\mathbf{q}} \, dx \\
&= \int_{\Omega} -if \, \mathbf{grad} v \bar{\mathbf{q}} - \frac{i}{2} \, \mathbf{grad} f \cdot (v \bar{\mathbf{q}}) \, dx \\
&\stackrel{\text{P.I.}}{=} \int_{\Omega} v \cdot \text{div} (if \bar{\mathbf{q}}) \, dx - \int_{\partial\Omega} v (if \bar{\mathbf{q}} \cdot \mathbf{n}) \, dS \\
&\quad - \int_{\Omega} \frac{i}{2} \, \mathbf{grad} f \cdot (v \bar{\mathbf{q}}) \, dx \\
&\stackrel{\text{P.R.}}{=} \int_{\Omega} v (\mathbf{grad} if \cdot \bar{\mathbf{q}} + if \, \text{div} \bar{\mathbf{q}}) - \frac{i}{2} \, \mathbf{grad} f \cdot (v \bar{\mathbf{q}}) \, dx \\
&= \int_{\Omega} i \, \mathbf{grad} f \cdot (v \bar{\mathbf{q}}) - \frac{i}{2} \, \mathbf{grad} f \cdot (v \bar{\mathbf{q}}) \, dx + \int_{\Omega} if v \, \text{div} \bar{\mathbf{q}} \, dx \\
&= \int_{\Omega} \frac{i}{2} \, \mathbf{grad} f \cdot \bar{\mathbf{q}} v + if v \, \text{div} \bar{\mathbf{q}} \, dx \quad \forall \mathbf{q} \in \mathbf{H}(\text{div}, \Omega)
\end{aligned}$$

$$\begin{aligned}
(\partial_t v, w)_0 &= \int_{\Omega} \partial_t v \cdot \bar{w} \, dx \\
&= \int_{\Omega} (if \, \text{div} \mathbf{u} + \frac{i}{2} \, \mathbf{grad} f \cdot \mathbf{u}) \bar{w} \, dx \\
&= (if \, \text{div} \mathbf{u} + \frac{i}{2} \, \mathbf{grad} f \cdot \mathbf{u}, w)_0 \quad \forall w \in L^2(\Omega)
\end{aligned}$$

P.I.: Partial integration

P.R.: Product rule

Chapter 3

Conservation Property

3.1 Proof of the Total Charge Conservation

To show: $\frac{d}{dt}Q = 0$ for Q in (1.5)

Proof:

$$\begin{aligned} Q(t) &= \int_{\Omega} |\mathbf{u}|^2 + |v|^2 \, d\mathbf{x} \\ &= \int_{\Omega} \mathbf{u} \cdot \bar{\mathbf{u}} + v \cdot \bar{v} \, d\mathbf{x} \\ &= \int_{\Omega} \mathbf{u} \cdot \bar{\mathbf{u}} \, d\mathbf{x} + \int_{\Omega} v \cdot \bar{v} \, d\mathbf{x} \\ &= (\mathbf{u}, \mathbf{u})_0 + (v, v)_0 \end{aligned}$$

$$\begin{aligned} \frac{d}{dt}Q(t) &= \frac{d}{dt}((\mathbf{u}, \mathbf{u})_0 + (v, v)_0) \\ &= \frac{d}{dt}(\int_{\Omega} \mathbf{u} \cdot \bar{\mathbf{u}} \, d\mathbf{x} + \int_{\Omega} v \cdot \bar{v} \, d\mathbf{x}) \\ &= \frac{d}{dt} \int_{\Omega} \mathbf{u} \cdot \bar{\mathbf{u}} \, d\mathbf{x} + \frac{d}{dt} \int_{\Omega} v \cdot \bar{v} \, d\mathbf{x} \\ &\stackrel{\text{P.R.}}{=} \int_{\Omega} \partial_t \mathbf{u} \bar{\mathbf{u}} + \mathbf{u} \partial_t \bar{\mathbf{u}} \, d\mathbf{x} + \int_{\Omega} \partial_t v \bar{v} + v \partial_t \bar{v} \, d\mathbf{x} \\ &= \int_{\Omega} \partial_t \mathbf{u} \bar{\mathbf{u}} \, d\mathbf{x} + \int_{\Omega} \mathbf{u} \partial_t \bar{\mathbf{u}} \, d\mathbf{x} + \int_{\Omega} \partial_t v \bar{v} \, d\mathbf{x} + \int_{\Omega} v \partial_t \bar{v} \, d\mathbf{x} \\ &= (\partial_t \mathbf{u}, \mathbf{u})_0 + (\mathbf{u}, \partial_t \mathbf{u})_0 + (\partial_t v, v)_0 + (v, \partial_t v)_0 \\ &= (\partial_t \mathbf{u}, \mathbf{u})_0 + \overline{(\partial_t \mathbf{u}, \mathbf{u})_0} + (\partial_t v, v)_0 + \overline{(\partial_t v, v)_0} \\ &= 2 * \operatorname{Re}(\partial_t \mathbf{u}, \mathbf{u})_0 + 2 * \operatorname{Re}(\partial_t v, v)_0 \\ &= 2 * \operatorname{Re}((\partial_t \mathbf{u}, \mathbf{u})_0 + (\partial_t v, v)_0) \stackrel{?}{=} 0 \end{aligned}$$

P.R.: Product rule

3.1.1 Proof of Charge Conservation of Weak Form (1.2)

$$\begin{aligned}
\frac{d}{dt}Q(t) &= 2 * \operatorname{Re}((\partial_t \mathbf{u}, \mathbf{u})_0 + (\partial_t v, v)_0) \\
&= 2 * \operatorname{Re}((-if \operatorname{grad} v - \frac{i}{2} \operatorname{grad} f v, \mathbf{u})_0 + (if \operatorname{div} \mathbf{u} + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u}, v)_0) \\
&= 2 * \operatorname{Re}(\int_{\Omega} (-if \operatorname{grad} v - \frac{i}{2} \operatorname{grad} f v) \bar{\mathbf{u}} \, dx + \int_{\Omega} (if \operatorname{div} \mathbf{u} + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u}) \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} + if \operatorname{div} \mathbf{u} \bar{v} + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} + \operatorname{div} \mathbf{u} (if \bar{v}) + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v} \, dx) \\
&\stackrel{\text{P.I.}}{=} 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \mathbf{u} \cdot \operatorname{grad} (if \bar{v}) \, dx \\
&\quad + \int_{\partial \Omega} if \bar{v} (\mathbf{u} \cdot \mathbf{n}) \, dS + \int_{\Omega} \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v} \, dx) \\
&\stackrel{\text{P.R.}}{=} 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \mathbf{u} \cdot (if \operatorname{grad} \bar{v} + i \operatorname{grad} f \bar{v}) \\
&\quad + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \mathbf{u} \cdot if \operatorname{grad} \bar{v} - \mathbf{u} \cdot i \operatorname{grad} f \bar{v} \\
&\quad + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \mathbf{u} \cdot if \operatorname{grad} \bar{v} \\
&\quad + (-i \operatorname{grad} f \cdot \mathbf{u} \bar{v} + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v}) \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \mathbf{u} \cdot if \operatorname{grad} \bar{v} - \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \overline{if \operatorname{grad} \bar{v} \cdot \mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \frac{i}{2} \overline{\operatorname{grad} f \bar{v} \cdot \mathbf{u}} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \overline{if \operatorname{grad} \bar{v} \cdot \mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \frac{i}{2} \overline{\operatorname{grad} f \bar{v} \cdot \mathbf{u}} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} + \overline{if \operatorname{grad} v \cdot \bar{\mathbf{u}}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} + \frac{i}{2} \overline{\operatorname{grad} f v \cdot \bar{\mathbf{u}}} \, dx) \\
&= 2 * \operatorname{Re}(- \int_{\Omega} (if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \overline{if \operatorname{grad} v \cdot \bar{\mathbf{u}}}) + (\frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \frac{i}{2} \overline{\operatorname{grad} f v \cdot \bar{\mathbf{u}}}) \, dx) \\
&= 2 * \operatorname{Re}(- \int_{\Omega} 2 * \operatorname{Im}(if \operatorname{grad} v \cdot \bar{\mathbf{u}}) + 2 * \operatorname{Im}(\frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}}) \, dx) \\
&= 2 * 0 = 0
\end{aligned}$$

$$\begin{aligned}
\forall \mathbf{u} &\in \mathbf{H}(\operatorname{div}, \Omega), \\
\forall v &\in H_0^1(\Omega).
\end{aligned}$$

P.I.: Partial integration

P.R.: Product rule

3.1.2 Proof of Charge Conservation of Weak Form (1.3)

$$\begin{aligned}
\frac{d}{dt}Q(t) &= 2 * \operatorname{Re}((\partial_t \mathbf{u}, \mathbf{u})_0 + (\partial_t v, v)_0) \\
&= 2 * \operatorname{Re}((-if \operatorname{grad} v - \frac{i}{2} \operatorname{grad} f v, \mathbf{u})_0 - \frac{i}{2}(\mathbf{u} \cdot \operatorname{grad} f, v)_0 - i \int_{\Omega} f \mathbf{u} \cdot \operatorname{grad} \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} (-if \operatorname{grad} v - \frac{i}{2} \operatorname{grad} f v) \bar{\mathbf{u}} - \frac{i}{2} \mathbf{u} \cdot \operatorname{grad} f \bar{v} - if \mathbf{u} \cdot \operatorname{grad} \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \frac{i}{2} \mathbf{u} \cdot \operatorname{grad} f \bar{v} - if \mathbf{u} \cdot \operatorname{grad} \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - if \mathbf{u} \cdot \operatorname{grad} \bar{v} - \frac{i}{2} \operatorname{grad} f v \cdot \bar{\mathbf{u}} - \frac{i}{2} \mathbf{u} \cdot \operatorname{grad} f \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \overline{if \operatorname{grad} v \cdot \bar{\mathbf{u}}} - \frac{i}{2} \bar{\mathbf{u}} \cdot \operatorname{grad} f v - \frac{i}{2} \mathbf{u} \cdot \operatorname{grad} f \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} -if \operatorname{grad} v \cdot \bar{\mathbf{u}} + \overline{if \operatorname{grad} v \cdot \bar{\mathbf{u}}} - \frac{i}{2} \bar{\mathbf{u}} \cdot \operatorname{grad} f v + \frac{i}{2} \overline{\mathbf{u} \cdot \operatorname{grad} f \bar{v}} \, dx) \\
&= 2 * \operatorname{Re}(- \int_{\Omega} (if \operatorname{grad} v \cdot \bar{\mathbf{u}} - \overline{if \operatorname{grad} v \cdot \bar{\mathbf{u}}}) + (\frac{i}{2} \bar{\mathbf{u}} \cdot \operatorname{grad} f v - \frac{i}{2} \overline{\mathbf{u} \cdot \operatorname{grad} f \bar{v}}) \, dx) \\
&= 2 * \operatorname{Re}(- \int_{\Omega} 2 * \operatorname{Im}(if \operatorname{grad} v \cdot \bar{\mathbf{u}}) + 2 * \operatorname{Im}(\frac{i}{2} \bar{\mathbf{u}} \cdot \operatorname{grad} f v) \, dx) \\
&= 2 * 0 = 0
\end{aligned}$$

$$\begin{aligned}
\forall \mathbf{u} &\in (L^2(\Omega))^d, \\
\forall v &\in H_0^1(\Omega).
\end{aligned}$$

3.1.3 Proof of Charge Conservation of Weak Form (1.4)

$$\begin{aligned}
\frac{d}{dt}Q(t) &= 2 * \operatorname{Re}((\partial_t \mathbf{u}, \mathbf{u})_0 + (\partial_t v, v)_0) \\
&= 2 * \operatorname{Re}(\int_{\Omega} \frac{i}{2} \operatorname{grad} f \cdot \bar{\mathbf{u}} v + ivf \operatorname{div} \bar{\mathbf{u}} \, dx) + (if \operatorname{div} \mathbf{u} + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u}, v)_0 \\
&= 2 * \operatorname{Re}(\int_{\Omega} \frac{i}{2} \operatorname{grad} f \cdot \bar{\mathbf{u}} v + ivf \operatorname{div} \bar{\mathbf{u}} + if \operatorname{div} \mathbf{u} \bar{v} + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} \frac{i}{2} \operatorname{grad} f \cdot \bar{\mathbf{u}} v + \frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v} + ivf \operatorname{div} \bar{\mathbf{u}} + if \operatorname{div} \mathbf{u} \bar{v} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} \frac{i}{2} \operatorname{grad} f \cdot \bar{\mathbf{u}} v + \overline{\frac{i}{2} \operatorname{grad} f \cdot \mathbf{u} \bar{v}} + if \operatorname{div} \bar{\mathbf{u}} v + \overline{if \operatorname{div} \mathbf{u} \bar{v}} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} \frac{i}{2} \operatorname{grad} f \cdot \bar{\mathbf{u}} v - \frac{i}{2} \operatorname{grad} f \cdot \bar{\mathbf{u}} v + if \operatorname{div} \bar{\mathbf{u}} v - \overline{if \operatorname{div} \mathbf{u} \bar{v}} \, dx) \\
&= 2 * \operatorname{Re}(\int_{\Omega} 2 * \operatorname{Im}(\frac{i}{2} \operatorname{grad} f \cdot \bar{\mathbf{u}} v) + 2 * \operatorname{Im}(if \operatorname{div} \bar{\mathbf{u}} v) \, dx) \\
&= 2 * 0 = 0
\end{aligned}$$

$$\begin{aligned}
\forall \mathbf{u} &\in \mathbf{H}(\operatorname{div}, \Omega), \\
\forall v &\in L^2(\Omega).
\end{aligned}$$

Chapter 4

Discretization of the Initial Value Problem

4.1 Discretization in space

All three problems in weak formulations have the form:

Seek $\mathbf{u} \in U$. $v \in V$ such that

$$\begin{aligned} \frac{d}{dt} \mathbf{a}(\mathbf{u}, \mathbf{q}) &= \mathbf{ce}(v, \mathbf{q}) & \forall \mathbf{q} \in U, \\ \frac{d}{dt} \mathbf{b}(v, w) &= \mathbf{df}(\mathbf{u}, w) & \forall w \in V \end{aligned} \quad (4.1)$$

where \mathbf{a} , \mathbf{b} , \mathbf{ce} , \mathbf{df} are bilinear forms. \mathbf{q} and w are testfunctions.

Its **finite element discretization** has the following form:

Seek $\mathbf{u}_N \in U_N$. $v_N \in V_N$ such that

$$\begin{aligned} \frac{d}{dt} \mathbf{a}(\mathbf{u}_N, \mathbf{q}) &= \mathbf{ce}(v_N, \mathbf{q}) & \forall \mathbf{q} \in U_N, \\ \frac{d}{dt} \mathbf{b}(v_N, w) &= \mathbf{df}(\mathbf{u}_N, w) & \forall w \in V_N. \end{aligned} \quad (4.2)$$

This problem corresponds to a linear system of equations with $2N$ unknowns, since in terms of the basisfunctions $\vec{\mathbf{N}}$ and $\vec{\mathbf{S}}$

$$\begin{aligned} \mathbf{u}_N(x, t) &= \sum_{i=1}^N \mu_i \mathbf{N}_i(x), \\ v_N(x, t) &= \sum_{i=1}^N \nu_i \mathbf{S}_i(x), \\ \mathbf{q} &= \sum_{j=1}^N \mathbf{N}_j(x) \text{ and} \\ w &= \sum_{j=1}^N \mathbf{S}_j(x). \end{aligned}$$

Inserting this into (4.2), we obtain

$$\begin{aligned}
\frac{d}{dt} \mathbf{a}(\mathbf{u}_N, \mathbf{q}) &= \mathbf{ce}(v_N, \mathbf{q}) \\
\frac{d}{dt} \mathbf{a}(\sum_{i=1}^N \mu_i N_i(\mathbf{x}), \sum_{j=1}^N N_j(\mathbf{x})) &= \mathbf{ce}(\sum_{i=1}^N \nu_i S_i(\mathbf{x}), \sum_{j=1}^N N_j(\mathbf{x})) \\
\frac{d}{dt} \sum_{i=1}^N \mu_i \mathbf{a}(N_i(\mathbf{x}), \sum_{j=1}^N N_j(\mathbf{x})) &= \sum_{i=1}^N \nu_i \mathbf{ce}(S_i(\mathbf{x}), \sum_{j=1}^N N_j(\mathbf{x})) \\
\frac{d}{dt} \sum_{i=1}^N \mu_i \sum_{j=1}^N \mathbf{a}(N_i(\mathbf{x}), N_j(\mathbf{x})) &= \sum_{i=1}^N \nu_i \sum_{j=1}^N \mathbf{ce}(S_i(\mathbf{x}), N_j(\mathbf{x})) \\
\frac{d}{dt} \sum_{i=1}^N \mu_i \cancel{\sum_{j=1}^N} \mathbf{a}(N_i(\mathbf{x}), N_j(\mathbf{x})) &= \sum_{i=1}^N \nu_i \cancel{\sum_{j=1}^N} \mathbf{ce}(S_i(\mathbf{x}), N_j(\mathbf{x})) \\
\frac{d}{dt} \mathbf{A} \vec{\mu} &= \mathbf{CE} \vec{v} \\
\mathbf{A} \dot{\vec{\mu}} &= \mathbf{CE} \vec{v}
\end{aligned}$$

and

$$\begin{aligned}
\frac{d}{dt} \mathbf{b}(v_N, w) &= \mathbf{df}(\mathbf{u}_N, w) \\
\frac{d}{dt} \mathbf{b}(\sum_{i=1}^N \nu_i S_i(\mathbf{x}), \sum_{j=1}^N S_j(\mathbf{x})) &= \mathbf{df}(\sum_{i=1}^N \mu_i N_i(\mathbf{x}), \sum_{j=1}^N S_j(\mathbf{x})) \\
\frac{d}{dt} \sum_{i=1}^N \nu_i \mathbf{b}(S_i(\mathbf{x}), \sum_{j=1}^N S_j(\mathbf{x})) &= \sum_{i=1}^N \mu_i \mathbf{df}(N_i(\mathbf{x}), \sum_{j=1}^N S_j(\mathbf{x})) \\
\frac{d}{dt} \sum_{i=1}^N \nu_i \sum_{j=1}^N \mathbf{b}(S_i(\mathbf{x}), S_j(\mathbf{x})) &= \sum_{i=1}^N \mu_i \sum_{j=1}^N \mathbf{df}(N_i(\mathbf{x}), S_j(\mathbf{x})) \\
\frac{d}{dt} \sum_{i=1}^N \nu_i \cancel{\sum_{j=1}^N} \mathbf{b}(S_i(\mathbf{x}), S_j(\mathbf{x})) &= \sum_{i=1}^N \mu_i \cancel{\sum_{j=1}^N} \mathbf{df}(N_i(\mathbf{x}), S_j(\mathbf{x})) \\
\frac{d}{dt} \mathbf{B} \vec{v} &= \mathbf{DF} \vec{\mu} \\
\mathbf{B} \dot{\vec{v}} &= \mathbf{DF} \vec{\mu}.
\end{aligned}$$

This leads to the problem in matrix form

$$\begin{bmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{B} \end{bmatrix} \begin{pmatrix} \dot{\vec{\mu}} \\ \dot{\vec{v}} \end{pmatrix} = \begin{bmatrix} 0 & \mathbf{CE} \\ \mathbf{DF} & 0 \end{bmatrix} \begin{pmatrix} \vec{\mu} \\ \vec{v} \end{pmatrix} \quad (4.3)$$

with

$$\begin{aligned}
\mathbf{A}^{N,N} &: \mathbf{a}(N_i(\mathbf{x}), N_j(\mathbf{x})) & 1 \leq i \leq N, 1 \leq j \leq N, \\
\mathbf{B}^{N,N} &: \mathbf{b}(S_i(\mathbf{x}), S_j(\mathbf{x})) & 1 \leq i \leq N, 1 \leq j \leq N, \\
\mathbf{CE}^{N,N} &: \mathbf{ce}(S_i(\mathbf{x}), N_j(\mathbf{x})) & 1 \leq i \leq N, 1 \leq j \leq N, \\
\mathbf{DF}^{N,N} &: \mathbf{df}(N_i(\mathbf{x}), S_j(\mathbf{x})) & 1 \leq i \leq N, 1 \leq j \leq N, \\
\vec{\mu}^N &: \mu_i, & 1 \leq i \leq N, \\
\vec{v}^N &: \nu_i, & 1 \leq i \leq N.
\end{aligned}$$

The matrices \mathbf{A} , \mathbf{B} , \mathbf{CE} , \mathbf{DF} depend on the individual bilinear forms of the weak formulations. Each weak forms' basisfunctions are determined by the spaces of \mathbf{u} resp. \mathbf{q} and of v resp. w .

These matrices and basisfunctions are derived for each weak formulation in the next three subsections.

4.1.1 Weak Formulation (1.2)

Bilinear forms:

$$\begin{aligned}
a(\mathbf{u}, \mathbf{q}) &= (\mathbf{u}, \mathbf{q})_0 \\
b(v, w) &= (v, w)_0 \\
ce(v, \mathbf{q}) &= (-if \mathbf{grad}v - \frac{i}{2} \mathbf{grad}fv, \mathbf{q})_0 \\
df(\mathbf{u}, w) &= (if \operatorname{div}\mathbf{u} + \frac{i}{2} \mathbf{grad}f \cdot \mathbf{u}, w)_0
\end{aligned} \tag{4.4}$$

Spaces and the corresponding basisfunctions to it:

$$\begin{aligned}
\forall \mathbf{u} \text{ resp. } \mathbf{q} \in \mathbf{H}(\operatorname{div}, \Omega) &\implies \mathbf{N} \hat{=} \text{hatfunction} \\
\forall v \text{ resp. } w \in H_0^1(\Omega) &\implies \mathbf{S} \hat{=} \text{hatfunction} \\
&\implies \mathbf{N} = \mathbf{S} \hat{=} \text{hatfunction}
\end{aligned} \tag{4.5}$$

Substituting the adequate basisfunctions into the the combination of (4.3) and (4.4), leads to the entries of the matrices:

$$\mathbf{A}^{N,N} : a(N_i(x), N_j(x)) = (N_i(x), N_j(x))_0 = \int_{\Omega} N_i(x) \overline{N_j(x)} dx \quad 1 \leq i \leq N, 1 \leq j \leq N,$$

$$\mathbf{B}^{N,N} : b(S_i(x), S_j(x)) = (S_i(x), S_j(x))_0 = \int_{\Omega} S_i(x) \overline{S_j(x)} dx \quad 1 \leq i \leq N, 1 \leq j \leq N,$$

$$\begin{aligned}
\mathbf{CE}^{N,N} : ce(S_i(x), N_j(x)) &= (-if \mathbf{grad}S_i(x) - \frac{i}{2} \mathbf{grad}fS_i(x), N_j(x))_0 \\
&= \int_{\Omega} (-if \mathbf{grad}S_i(x) - \frac{i}{2} \mathbf{grad}fS_i(x)) \overline{N_j(x)} dx \\
&= \int_{\Omega} -if \mathbf{grad}S_i(x) \overline{N_j(x)} - \frac{i}{2} \mathbf{grad}fS_i(x) \overline{N_j(x)} dx \quad 1 \leq i \leq N, 1 \leq j \leq N,
\end{aligned}$$

$$\begin{aligned}
\mathbf{DF}^{N,N} : df(N_i(x), S_j(x)) &= (if \operatorname{div}N_i(x) + \frac{i}{2} \mathbf{grad}f \cdot N_i(x), S_j(x))_0 \\
&= \int_{\Omega} (if \operatorname{div}N_i(x) + \frac{i}{2} \mathbf{grad}f \cdot N_i(x)) \overline{S_j(x)} dx \\
&= \int_{\Omega} if \operatorname{div}N_i(x) \overline{S_j(x)} + \frac{i}{2} \mathbf{grad}f \cdot N_i(x) \overline{S_j(x)} dx \quad 1 \leq i \leq N, 1 \leq j \leq N.
\end{aligned}$$

4.1.2 Weak Formulation (1.3)

Bilinear forms:

$$\begin{aligned}
a(\mathbf{u}, \mathbf{q}) &= (\mathbf{u}, \mathbf{q})_0 \\
b(v, w) &= (v, w)_0 \\
ce(v, \mathbf{q}) &= (-if \mathbf{grad}v - \frac{i}{2} \mathbf{grad}fv, \mathbf{q})_0 \\
df(\mathbf{u}, w) &= -\frac{i}{2}(\mathbf{u} \cdot \mathbf{grad}f, w)_0 - i \int_{\Omega} f \mathbf{u} \cdot \mathbf{grad}\overline{w} dx
\end{aligned} \tag{4.6}$$

Spaces and the corresponding basisfunctions to it:

$$\begin{aligned}
\forall \mathbf{u} \text{ resp. } \mathbf{q} \in (L^2(\Omega))^d &\implies \mathbf{N} \hat{=} \text{constant linear function} \\
\forall v \text{ resp. } w \in H_0^1(\Omega) &\implies \mathbf{S} \hat{=} \text{hatfunction}
\end{aligned} \tag{4.7}$$

Substituting the basisfunctions into the combination of (4.3) and (4.7) as above, leads to:

$$\mathbf{A}^{N,N} : a(N_i(\mathbf{x}), N_j(\mathbf{x})) = (N_i(\mathbf{x}), N_i(\mathbf{x}))_0 = \int_{\Omega} N_i(\mathbf{x}) \overline{N_i(\mathbf{x})} d\mathbf{x} \quad 1 \leq i \leq N, 1 \leq j \leq N,$$

$$\mathbf{B}^{N,N} : b(S_i(\mathbf{x}), S_j(\mathbf{x})) = (S_i(\mathbf{x}), S_j(\mathbf{x}))_0 = \int_{\Omega} S_i(\mathbf{x}) \overline{S_j(\mathbf{x})} d\mathbf{x} \quad 1 \leq i \leq N, 1 \leq j \leq N,$$

$$\begin{aligned} \mathbf{CE}^{N,N} : ce(S_i(\mathbf{x}), N_j(\mathbf{x})) &= (-if \mathbf{grad} S_i(\mathbf{x}) - \frac{i}{2} \mathbf{grad} f S_i(\mathbf{x}), N_j(\mathbf{x}))_0 \\ &= \int_{\Omega} (-if \mathbf{grad} S_i(\mathbf{x}) - \frac{i}{2} \mathbf{grad} f S_i(\mathbf{x})) \overline{N_j(\mathbf{x})} d\mathbf{x} \\ &= \int_{\Omega} -if \mathbf{grad} S_i(\mathbf{x}) \overline{N_j(\mathbf{x})} - \frac{i}{2} \mathbf{grad} f S_i(\mathbf{x}) \overline{N_j(\mathbf{x})} d\mathbf{x} \quad 1 \leq i \leq N, 1 \leq j \leq N, \end{aligned}$$

$$\begin{aligned} \mathbf{DF}^{N,N} : df(N_i(\mathbf{x}), S_j(\mathbf{x})) &= -\frac{i}{2} (N_i(\mathbf{x}) \cdot \mathbf{grad} f, S_j(\mathbf{x}))_0 - i \int_{\Omega} f N_i(\mathbf{x}) \cdot \mathbf{grad} \overline{S_j(\mathbf{x})} d\mathbf{x} \\ &= -\frac{i}{2} \int_{\Omega} N_i(\mathbf{x}) \cdot \mathbf{grad} f \overline{S_j(\mathbf{x})} d\mathbf{x} - i \int_{\Omega} f N_i(\mathbf{x}) \cdot \mathbf{grad} \overline{S_j(\mathbf{x})} d\mathbf{x} \\ &= -\frac{i}{2} \int_{\Omega} N_i(\mathbf{x}) \cdot \mathbf{grad} f \overline{S_j(\mathbf{x})} - if N_i(\mathbf{x}) \cdot \mathbf{grad} \overline{S_j(\mathbf{x})} d\mathbf{x} \quad 1 \leq i \leq N, 1 \leq j \leq N. \end{aligned}$$

4.1.3 Weak Formulation (1.4)

Bilinear forms:

$$\begin{aligned} a(\mathbf{u}, \mathbf{q}) &= (\mathbf{u}, \mathbf{q})_0 \\ b(v, w) &= (v, w)_0 \\ ce(v, \mathbf{q}) &= \int_{\Omega} \frac{i}{2} \mathbf{grad} f \cdot \overline{\mathbf{q}} v + iv f \operatorname{div} \overline{\mathbf{q}} d\mathbf{x} \\ df(\mathbf{u}, w) &= (if \operatorname{div} \mathbf{u} + \frac{i}{2} \mathbf{grad} f \cdot \mathbf{u}, w)_0 \end{aligned} \quad (4.8)$$

Spaces and the corresponding basisfunctions to it:

$$\begin{aligned} \forall \mathbf{u} \text{ resp. } \mathbf{q} \in \mathbf{H}(\operatorname{div}, \Omega) &\implies \mathbf{N} \hat{=} \text{hatfunction} \\ \forall v \text{ resp. } w \in L^2(\Omega), \text{ but } v = 0 \text{ on } [0, T] \times \partial\Omega &\implies \mathbf{S} \hat{=} \text{hatfunction} \\ \implies \mathbf{N} = \mathbf{S} \hat{=} \text{hatfunction} & \end{aligned} \quad (4.9)$$

Substitution as before:

$$\mathbf{A}^{N,N} : a(N_i(\mathbf{x}), N_j(\mathbf{x})) = (N_i(\mathbf{x}), N_i(\mathbf{x}))_0 = \int_{\Omega} N_i(\mathbf{x}) \overline{N_i(\mathbf{x})} d\mathbf{x} \quad 1 \leq i \leq N, 1 \leq j \leq N,$$

$$\mathbf{B}^{N,N} : b(S_i(\mathbf{x}), S_j(\mathbf{x})) = (S_i(\mathbf{x}), S_j(\mathbf{x}))_0 = \int_{\Omega} S_i(\mathbf{x}) \overline{S_j(\mathbf{x})} d\mathbf{x} \quad 1 \leq i \leq N, 1 \leq j \leq N,$$

$$\begin{aligned} \mathbf{CE}^{N,N} : ce(S_i(\mathbf{x}), N_j(\mathbf{x})) &= \int_{\Omega} \frac{i}{2} \mathbf{grad} f \cdot \overline{S_i(\mathbf{x})} N_j(\mathbf{x}) + i N_j(\mathbf{x}) f \operatorname{div} \overline{S_i(\mathbf{x})} d\mathbf{x} \quad 1 \leq i \leq N, 1 \leq j \leq N, \end{aligned}$$

$$\begin{aligned} \mathbf{DF}^{N,N} : df(N_i(\mathbf{x}), S_j(\mathbf{x})) &= (if \operatorname{div} N_i(\mathbf{x}) + \frac{i}{2} \mathbf{grad} f \cdot N_i(\mathbf{x}), S_j(\mathbf{x}))_0 \\ &= \int_{\Omega} (if \operatorname{div} N_i(\mathbf{x}) + \frac{i}{2} \mathbf{grad} f \cdot N_i(\mathbf{x})) \overline{S_j(\mathbf{x})} d\mathbf{x} \\ &= \int_{\Omega} if \operatorname{div} N_i(\mathbf{x}) \overline{S_j(\mathbf{x})} + \frac{i}{2} \mathbf{grad} f \cdot N_i(\mathbf{x}) \overline{S_j(\mathbf{x})} d\mathbf{x} \quad 1 \leq i \leq N, 1 \leq j \leq N, \end{aligned}$$

4.2 Discretization in time

The discretization in time is independent of the concrete weak formulation. Its same for all three weak formulations, so it can be explained for the general form (4.3) which can be transformed to

$$\begin{aligned} \mathbf{M}_{\text{glo}} \dot{\vec{y}} &= \mathbf{A}_{\text{glo}} \vec{y} & \text{for } 0 \leq t \leq T \\ y(0) &= y_0 \end{aligned} \quad (4.10)$$

with

$$\mathbf{M}_{\text{glo}} = \begin{bmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{B} \end{bmatrix}, \quad \mathbf{A}_{\text{glo}} = \begin{bmatrix} 0 & \mathbf{CE} \\ \mathbf{DF} & 0 \end{bmatrix} \quad (4.11)$$

and

$$\vec{y} = \begin{pmatrix} \vec{\mu} \\ \vec{\nu} \end{pmatrix}, \quad \dot{\vec{y}} = \begin{pmatrix} \dot{\vec{\mu}} \\ \dot{\vec{\nu}} \end{pmatrix}. \quad (4.12)$$

We discretize (4.10) as follows: Set

$$\begin{aligned} \tau &:= \frac{T}{M} \text{ with } M > 0 \in \mathbb{N} \text{ is the timestep and} \\ t_k &= k * \tau \text{ for } k = 0, 1, 2, \dots, M. \end{aligned}$$

The aim is to calculate for $k = 0, 1, 2, \dots, M$ an approximation y_k for $y(t_k)$. There are a lot of methods to do this. In this work timestepping is done with two different schemes: the implicit Runge-Kutta-Gauss timestepping (midpoint rule) and the explicit leapfrog scheme. These schemes are presented in the next sections.

4.2.1 Implicit Runge-Kutta-Gauss Timestepping

This timestepping scheme is also known as the midpoint rule. The theory to this scheme was presented in section 1.5.

The problem (4.10) has to be replaced by the finite differences method, y_0 is given:

$$\mathbf{M}_{\text{glo}} \frac{y^{k+1} - y^k}{\tau} = \mathbf{A}_{\text{glo}}(t^k + \frac{1}{2}\tau) \left(\frac{y^{k+1} + y^k}{2} \right) \quad (4.13)$$

Solving for y^{k+1} , we get

$$y^{k+1} = y^k \left(\frac{2\mathbf{M}_{\text{glo}} + \mathbf{A}_{\text{glo}}(\mathbf{t}^k + \frac{1}{2}\tau)\tau}{2\mathbf{M}_{\text{glo}} - \mathbf{A}_{\text{glo}}(\mathbf{t}^k + \frac{1}{2}\tau)\tau} \right), \quad (4.14)$$

we need to compute this for $0 \leq k \leq M - 1$.

4.2.2 Explicit Leapfrog Scheme

The leapfrog scheme is an explicit scheme, so we have to take the CLF-stability-condition into account.

Theory

The problem is of the following form

$$\begin{aligned} \mathbf{M}_u \dot{\vec{\mu}} &= \mathbf{G} \vec{\eta} \\ \mathbf{M}_v \dot{\vec{\eta}} &= -\mathbf{G}^H \vec{\mu}, \end{aligned} \quad (4.15)$$

this can be reduced to the scheme

$$\begin{aligned} \mathbf{M}_u \frac{\vec{\mu}^{k+1} - \vec{\mu}^k}{\tau} &= \mathbf{G} \vec{\eta}^{k+0.5} \\ \mathbf{M}_v \frac{\vec{\eta}^{k+1.5} - \vec{\eta}^{k+0.5}}{\tau} &= -\mathbf{G}^H \vec{\mu}^{k+1}. \end{aligned} \quad (4.16)$$

This is the leapfrog timestepping.

(4.16) can be transformed to

$$\begin{aligned} \vec{\mu}^{k+1} &= \frac{\mathbf{G} \vec{\eta}^{k+0.5} * \tau + \mathbf{M}_u \vec{\mu}^k}{\mathbf{M}_u}, \\ \vec{\eta}^{k+1.5} &= \frac{-\mathbf{G}^H \vec{\mu}^{k+1} * \tau + \mathbf{M}_v \vec{\eta}^{k+0.5}}{\mathbf{M}_v}. \end{aligned} \quad (4.17)$$

These formulas have a recursive scheme, the solution of one equation needs to be plugged into the other and this goes on recursively. To start, we need to compute $\vec{\eta}^{k+0.5}$ with $k=0$, which can be done with another explicit scheme, e.g. the theta scheme. $\vec{\mu}^0$ is given.

Applying this scheme to our problem, (4.10) can be written as

$$\begin{aligned} \mathbf{A} \dot{\vec{\mu}} &= \mathbf{C} \mathbf{E} \vec{\eta}, \\ \mathbf{B} \dot{\vec{\eta}} &= \mathbf{D} \mathbf{F} \vec{\mu}, \end{aligned} \quad (4.18)$$

which has the same structure as (4.15) with $\mathbf{D} \mathbf{F} = -\mathbf{C} \mathbf{E}^H$. This can be reduced similar to the theory to

$$\begin{aligned} \mathbf{A} \frac{\vec{\mu}^{k+1} - \vec{\mu}^k}{\tau} &= \mathbf{C} \mathbf{E} \vec{\eta}^{k+0.5} \\ \mathbf{B} \frac{\vec{\eta}^{k+1.5} - \vec{\eta}^{k+0.5}}{\tau} &= \mathbf{D} \mathbf{F} \vec{\mu}^{k+1}. \end{aligned} \quad (4.19)$$

and solved for $\vec{\mu}^{k+1}$ and $\vec{\eta}^{k+1.5}$

$$\begin{aligned} \vec{\mu}^{k+1} &= \frac{\mathbf{C} \mathbf{E} \vec{\eta}^{k+0.5} * \tau + \mathbf{A} \vec{\mu}^k}{\mathbf{A}}, \\ \vec{\eta}^{k+1.5} &= \frac{\mathbf{D} \mathbf{F} \vec{\mu}^{k+1} * \tau + \mathbf{B} \vec{\eta}^{k+0.5}}{\mathbf{B}}. \end{aligned} \quad (4.20)$$

$\bar{\mu}^0$ is given, $\bar{\eta}^{0.5}$ is computed with the explicit θ -scheme ($\theta = 0$): Replace (4.10) by finite differences, y^0 is given.

Compute

$$\mathbf{M}_{\text{glo}} \frac{\bar{y}^{m+1} - \bar{y}^m}{\tau_\theta} = \theta \mathbf{A}_{\text{glo}} \bar{y}^{m+1} + (1 - \theta) \mathbf{A}_{\text{glo}} \bar{y}^m \quad \text{for } 0 \leq m \leq M - 1. \quad (4.21)$$

with

$$\begin{aligned} \tau_\theta &:= \frac{T}{M_\theta} \text{ with } M_\theta = n * M, n \in \mathbb{N}, \\ t_m &:= m * \tau_\theta \text{ for } k = 0, 1, 2, \dots, M_\theta. \end{aligned}$$

For a given y^m , y^{m+1} can be computed. We need to compute $y(t_m)$ for $t_m = 0.5$ and from that we get $\eta^{0.5}$, which we need for the explicit leapfrog timestepping.

As mentioned before, we need to take the CLF-condition into account to assure stability.

CLF-condition

The θ -scheme is stable for (4.21)

1. for $0 \leq \theta < 0.5$, if

$$\frac{-2}{1-2\theta} \leq x \leq 0$$

or

$$0 \leq \tau_\theta \lambda_{i,N} \leq \frac{2}{1-2\theta} \quad \text{for } 1 \leq i \leq N \quad (4.22)$$

2. for $0.5 \leq \theta \leq 1$, it is stable for all combinations of $\tau_\theta \lambda_{i,N}$.

$\lambda_{i,N}$ are the eigenvalues of the space – operator.

Chapter 5

Results

5.1 Conservation of Charge

In this section, we show that the total charge is conserved over time and that it has the same value independent of the weak formulations.

5.1.1 Function a: $f \equiv 1$

This is the constant function. The results are presented for each weak formulation and both timestepping schemes.

Weak Formulations (1.2)

Midpoint Rule:

The figure 5.1 shows the charge in dependence of time. For the discretization in space and time, 1024 degrees of freedom were used.

Interpretation of the result:

The plot shows that the charge stays constant through time. The charge is $3.5 + 0i$.

Leapfrog Scheme:

The figure 5.2 shows the charge for the leapfrog scheme. The settings for the discretization are same as for the midpoint rule.

Interpretation of the result:

The charge is not really constant in the leapfrog scheme, but it fluctuates around the value we expect to be constant, here is the value $3.5+0i$.

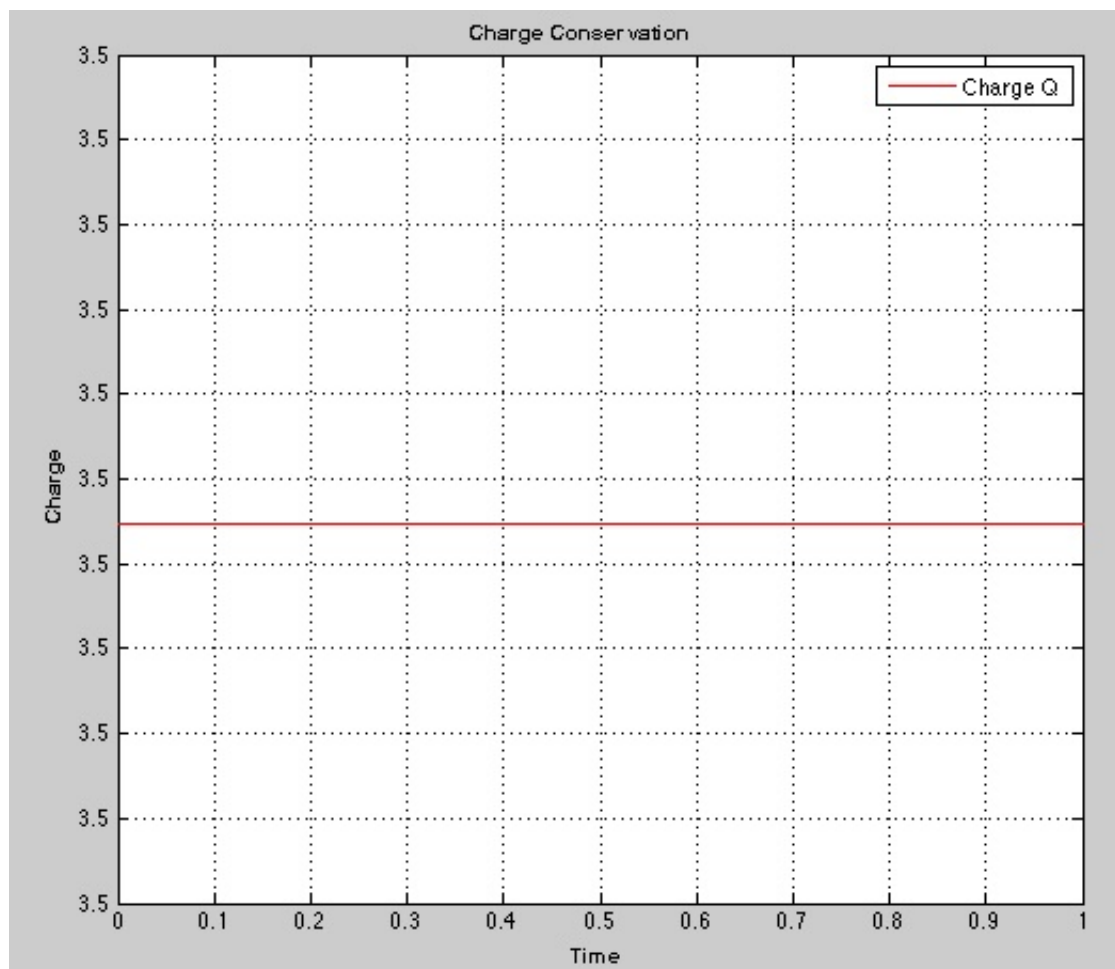


Figure 5.1: (1.2)-a - Conservation of charge: 1024 spatial and temporal dofs (midpoint rule)

The results are similar for the different weak formulations, functions and timestepping schemes. Just the number of spatial and temporal degrees of freedom need to be adapted in the leapfrog timestepping schemes to assure stability.

In the following the results are plotted for completeness.

Weak Formulations (1.3)

Midpoint Rule:

See figure 5.3.

Leapfrog Scheme:

The figure 5.4 shows the charge for the leapfrog scheme. Using only 512 spatial dofs and 1024 temporal dofs assures stability.

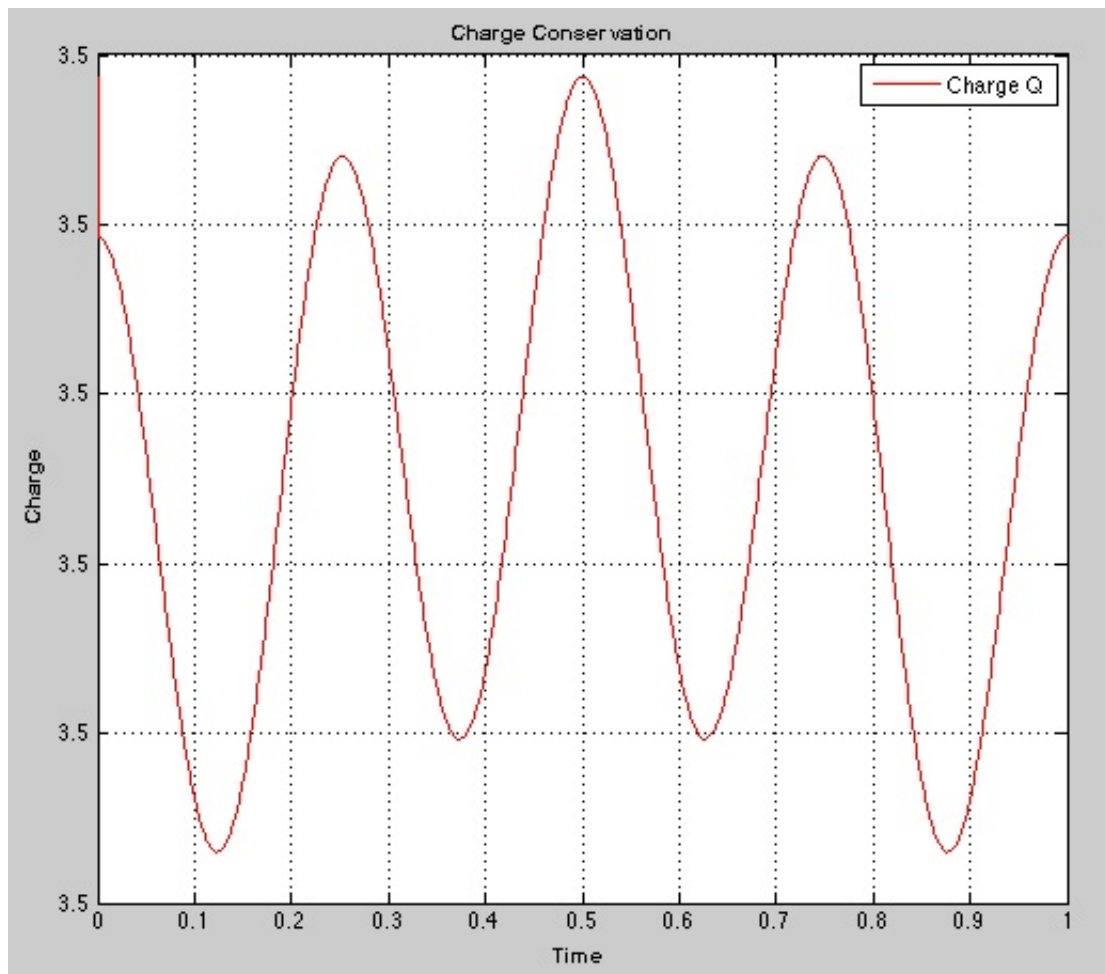


Figure 5.2: (1.2)-a - Conservation of charge: 1024 spatial and temporal dofs (leapfrog)

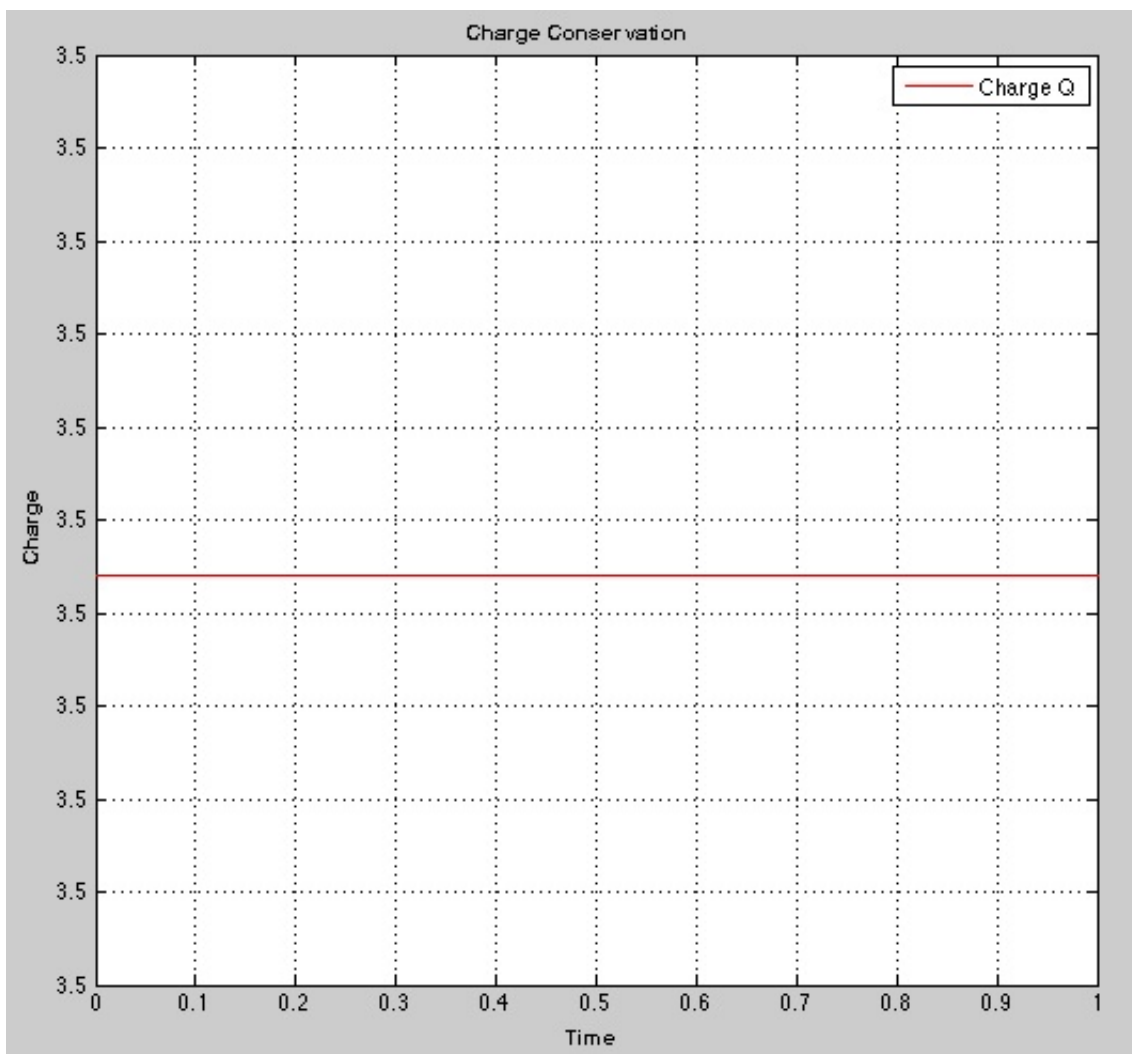


Figure 5.3: (1.3)-a - Conservation of charge: 1024 spatial and temporal dofs (midpoint rule)

Weak Formulations (1.4)

Midpoint Rule:

See figure 5.5.

Leapfrog Scheme:

See figure 5.6.

5.1.2 Function b: $f(x) = xe^{-2x}$

Weak Formulations (1.2)

Midpoint Rule:

See figure 5.7.

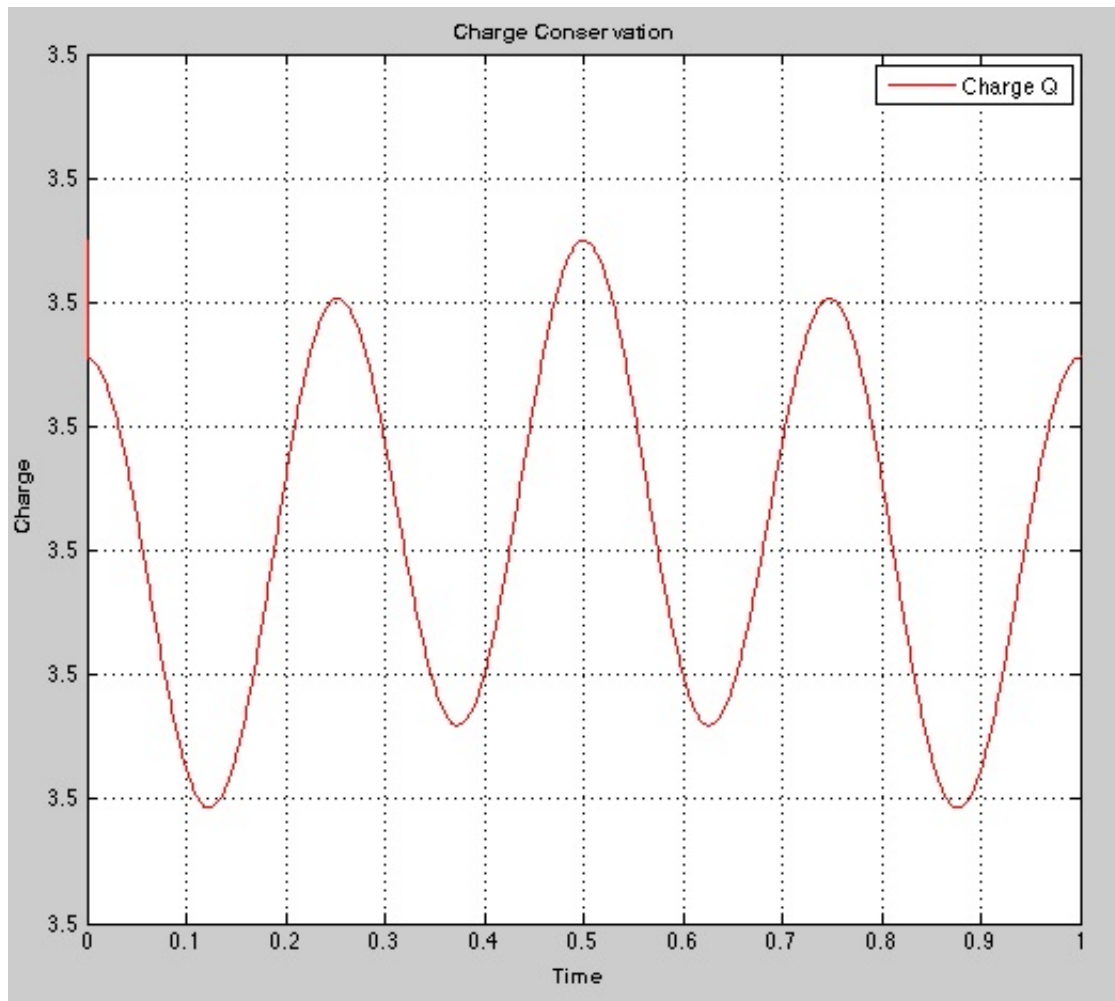


Figure 5.4: (1.3)-a - Conservation of charge: 512 spatial and 1024 temporal dofs (leapfrog)

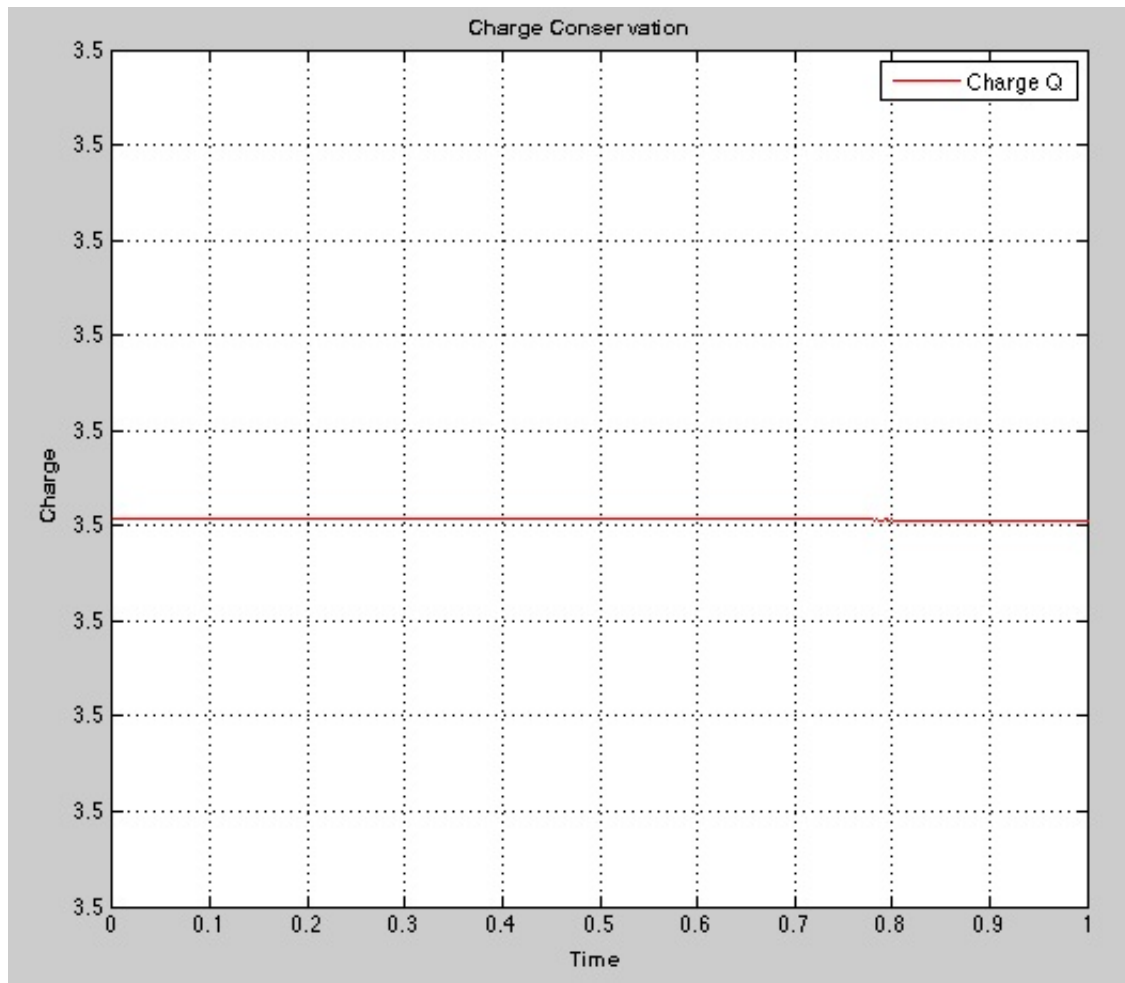


Figure 5.5: (1.4)-a - Conservation of charge: 1024 spatial and temporal dofs (midpoint rule)

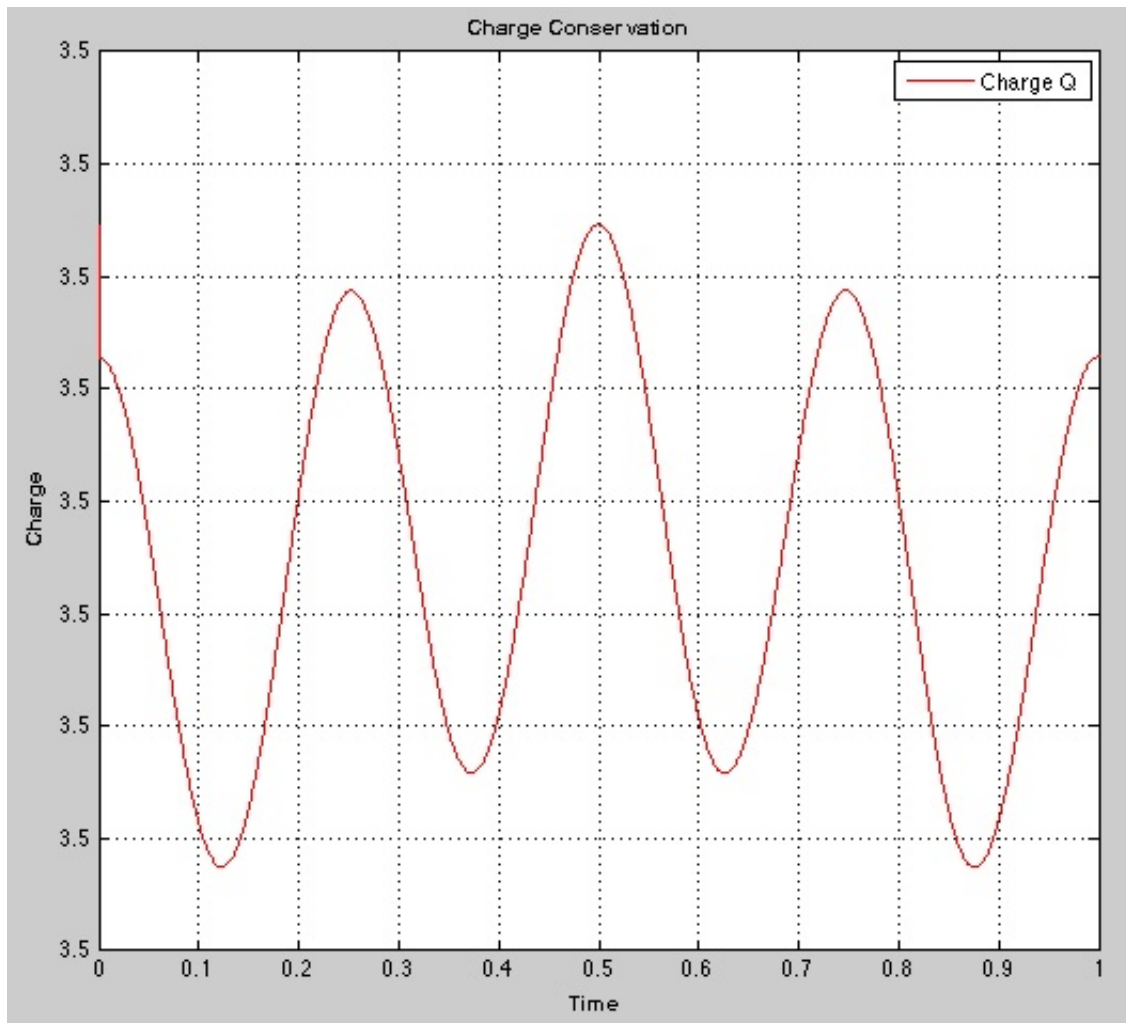


Figure 5.6: (1.4)-a - Conservation of charge: 1024 spatial and 2048 temporal dofs (leapfrog)

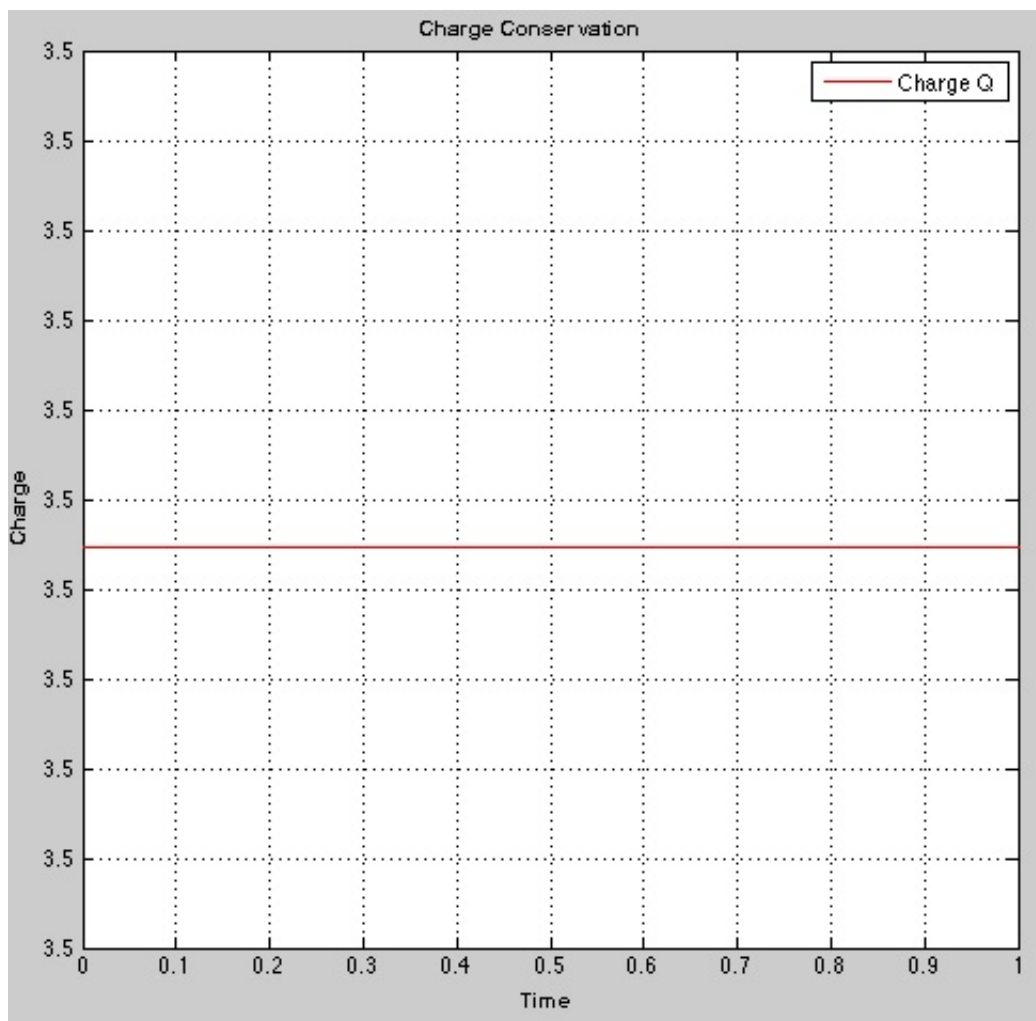


Figure 5.7: (1.2)-b - Conservation of charge: 1024 spatial and temporal dofs (midpoint rule)

Leapfrog Scheme:

See figure 5.8.

Weak Formulations (1.3)

Midpoint Rule:

See figure 5.9.

Leapfrog Scheme:

See figure 5.10.

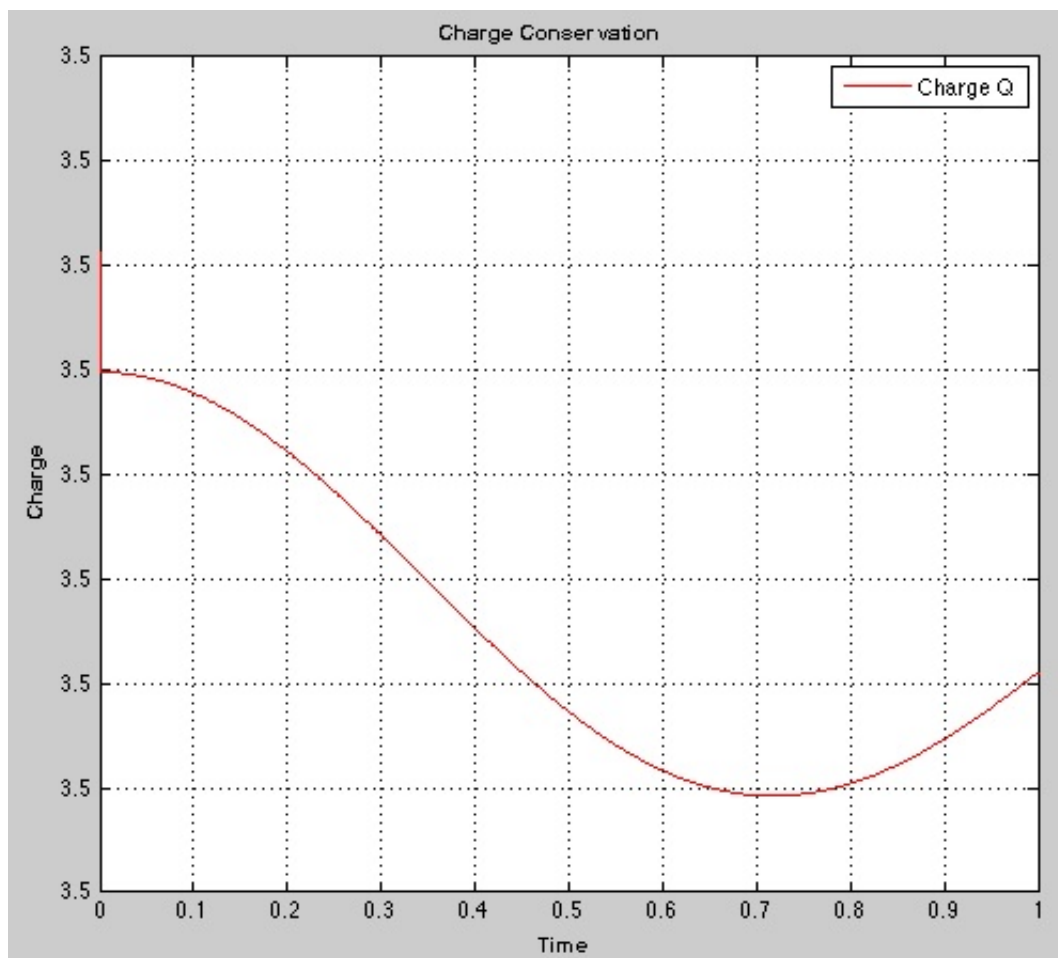


Figure 5.8: (1.2)-b - Conservation of charge: 1024 spatial and temporal dofs (leapfrog)

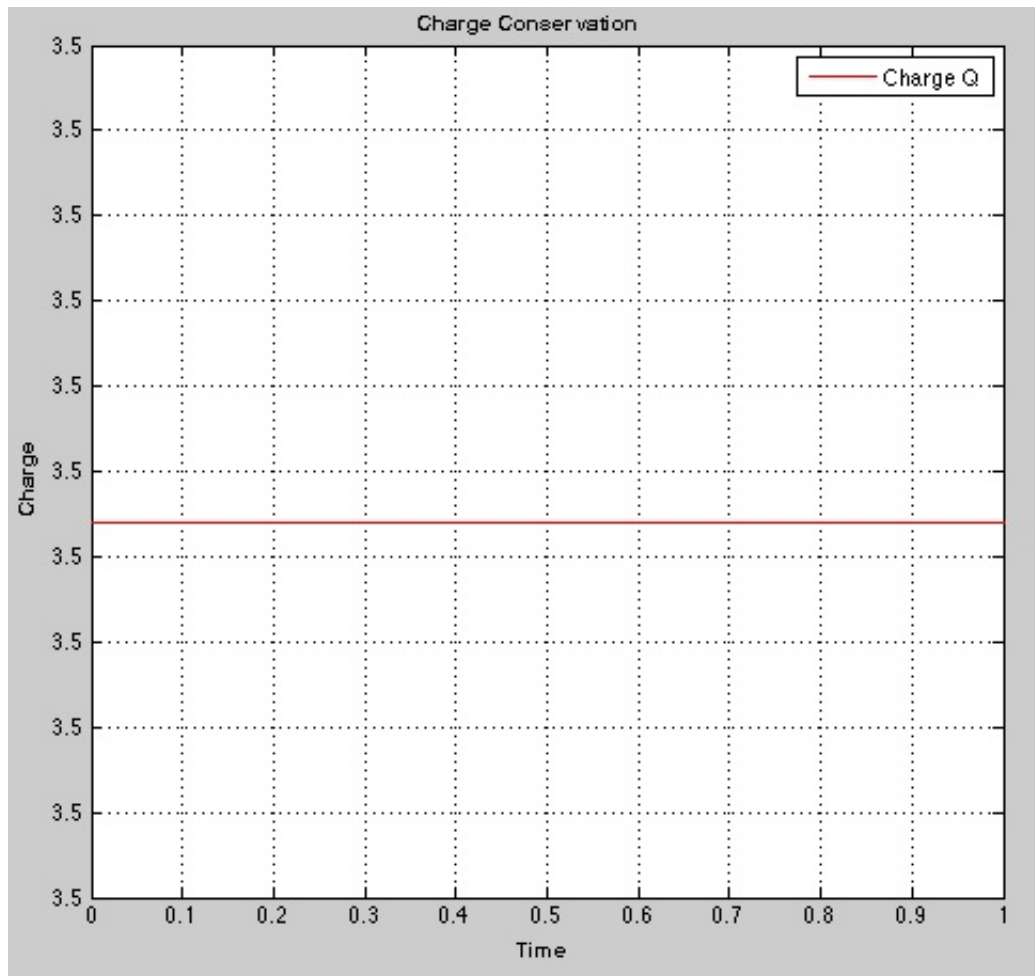


Figure 5.9: (1.3)-b - Conservation of charge: 1024 spatial and temporal dofs (midpoint rule)

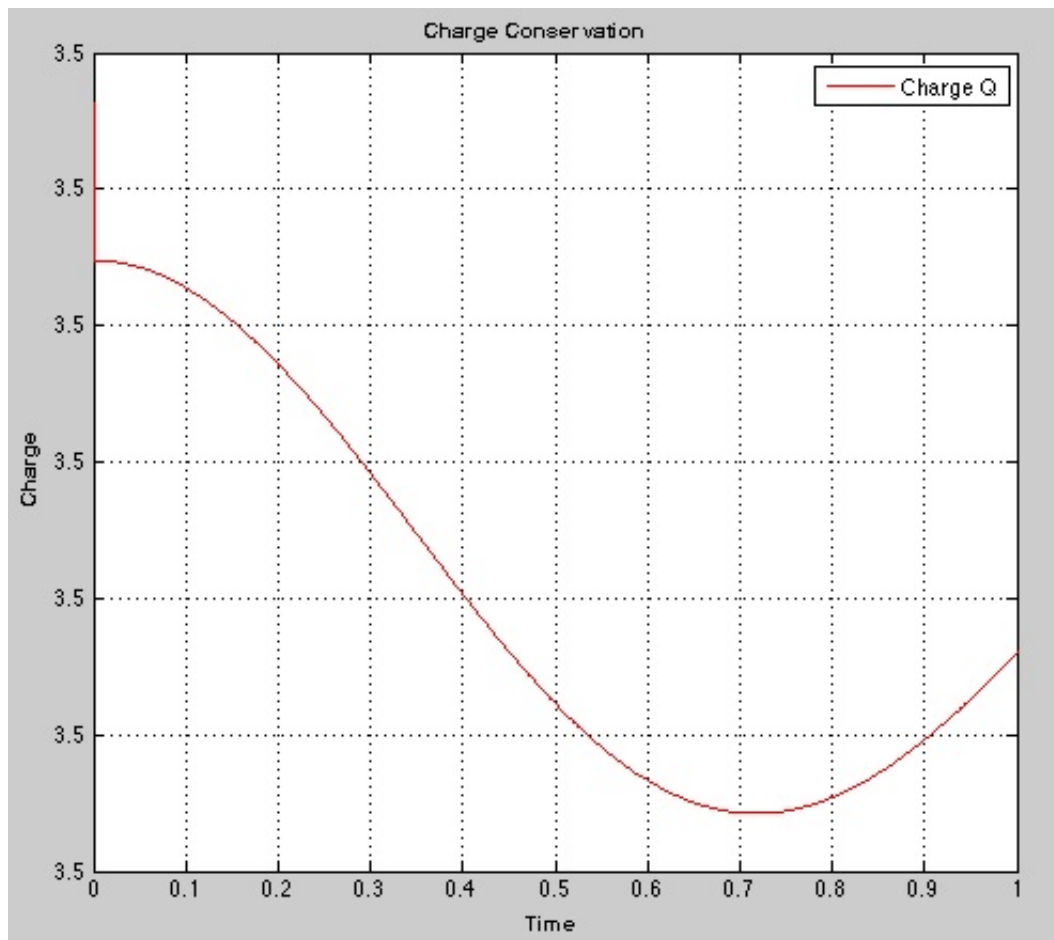


Figure 5.10: (1.3)-b - Conservation of charge: 1024 spatial and 1024 temporal dofs (leapfrog)

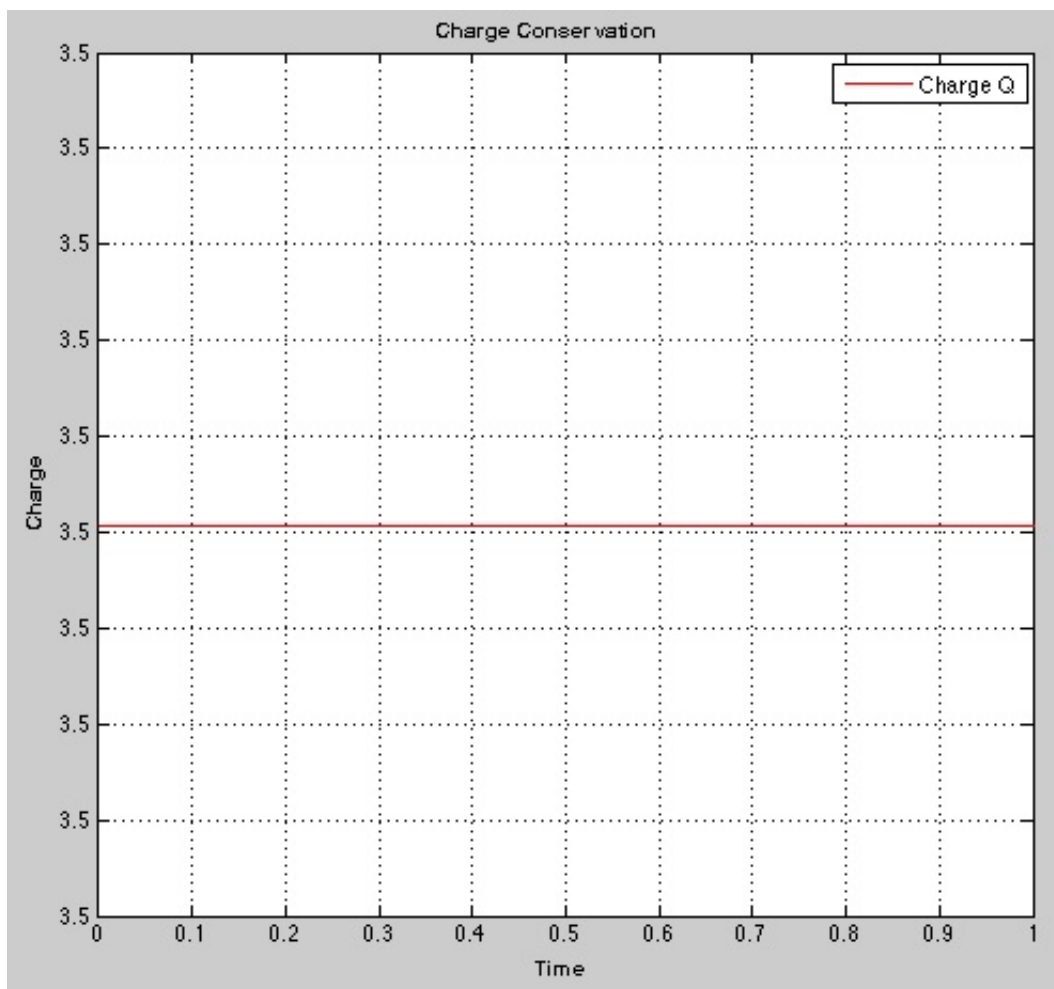


Figure 5.11: (1.4)-b - Conservation of charge: 1024 spatial and temporal dofs (midpoint rule)

Weak Formulations (1.4)

Midpoint Rule:

See figure 5.11.

Leapfrog Scheme:

See figure 5.12.

5.1.3 Function c: $f(x, t) = xe^{-tx}$

Weak Formulations (1.2)

Midpoint Rule:

See figure 5.13.

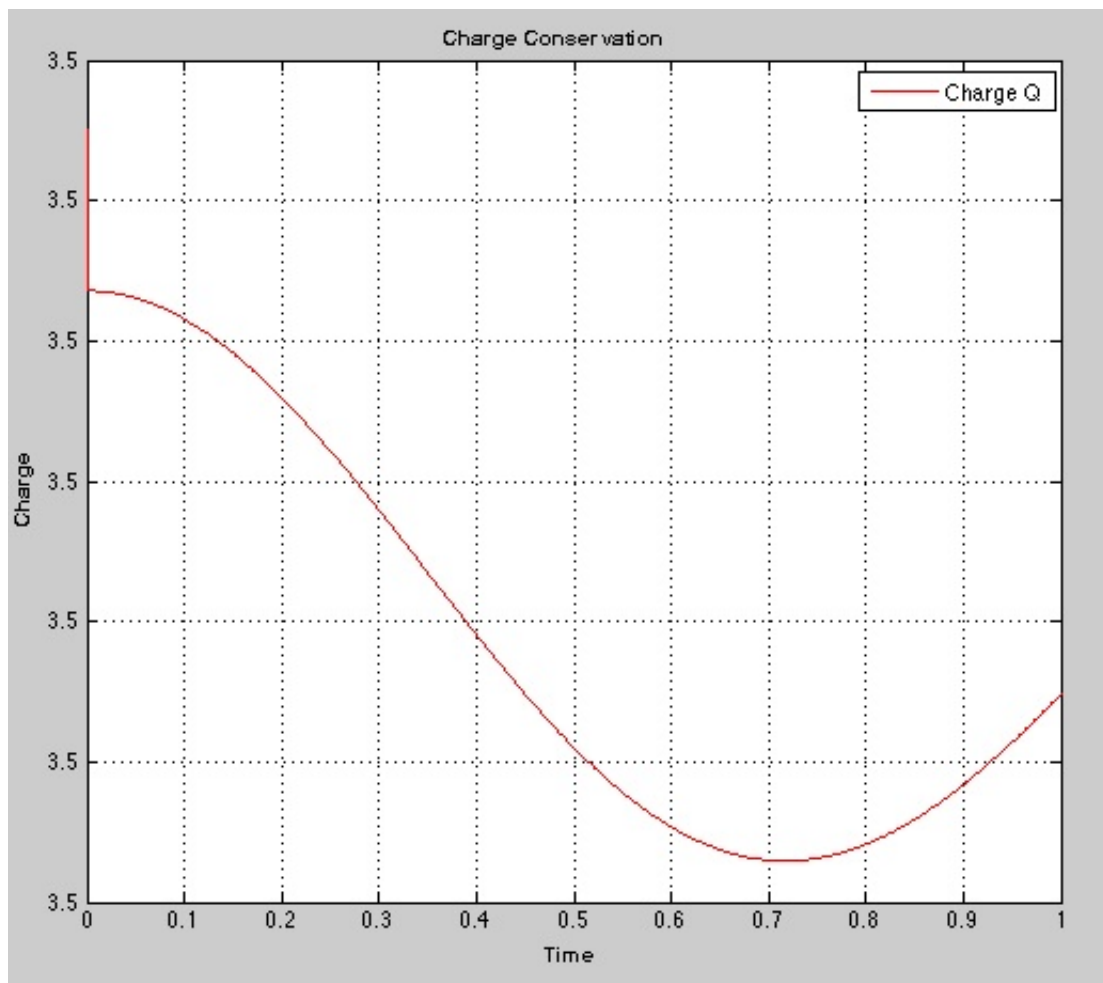


Figure 5.12: (1.4)-b - Conservation of charge: 1024 spatial and temporal dofs (leapfrog)

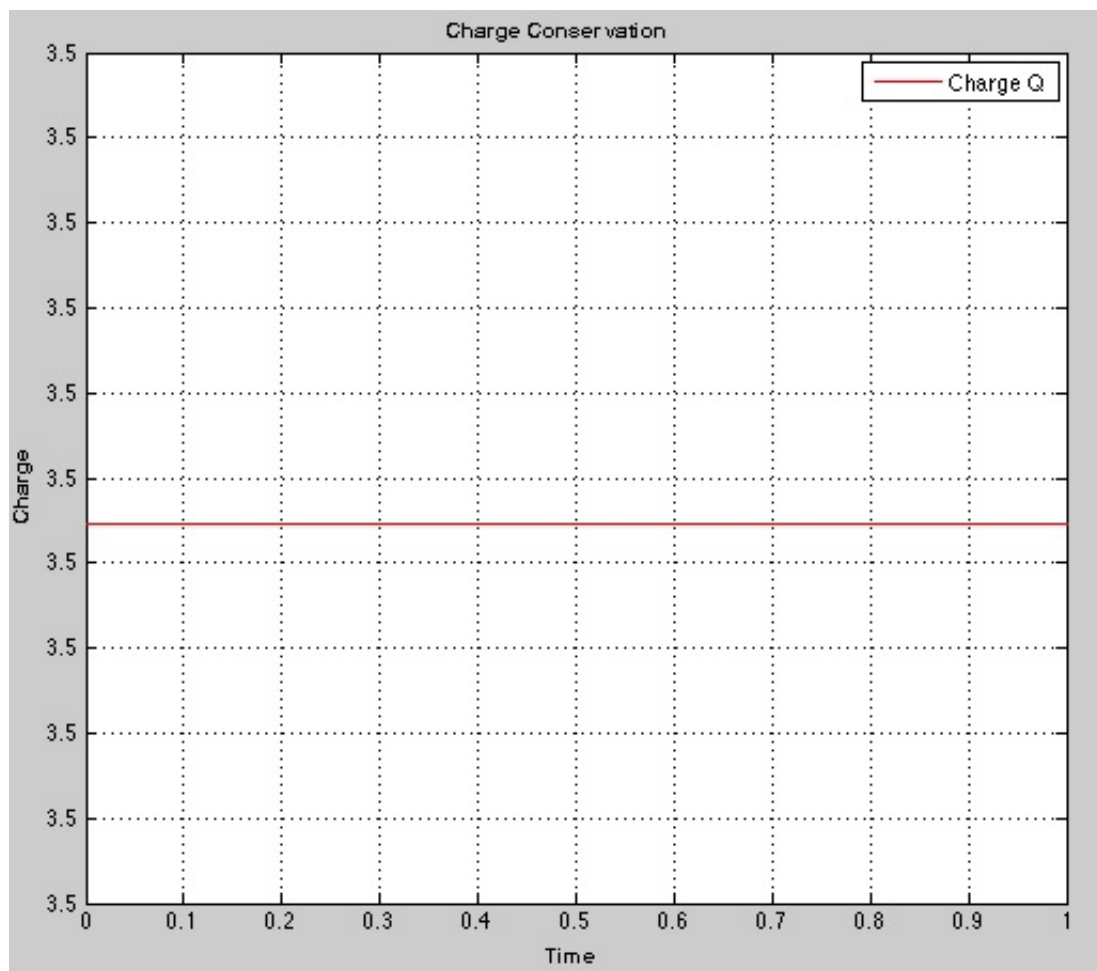


Figure 5.13: (1.2)-c - Conservation of charge: 1024 spatial and temporal dofs (midpoint rule)

Leapfrog Scheme:

See figure 5.14.

Weak Formulations (1.3)

Midpoint Rule:

See figure 5.15.

Leapfrog Scheme:

See figure 5.16.

Weak Formulations (1.4)

Midpoint Rule:

See figure 5.17.

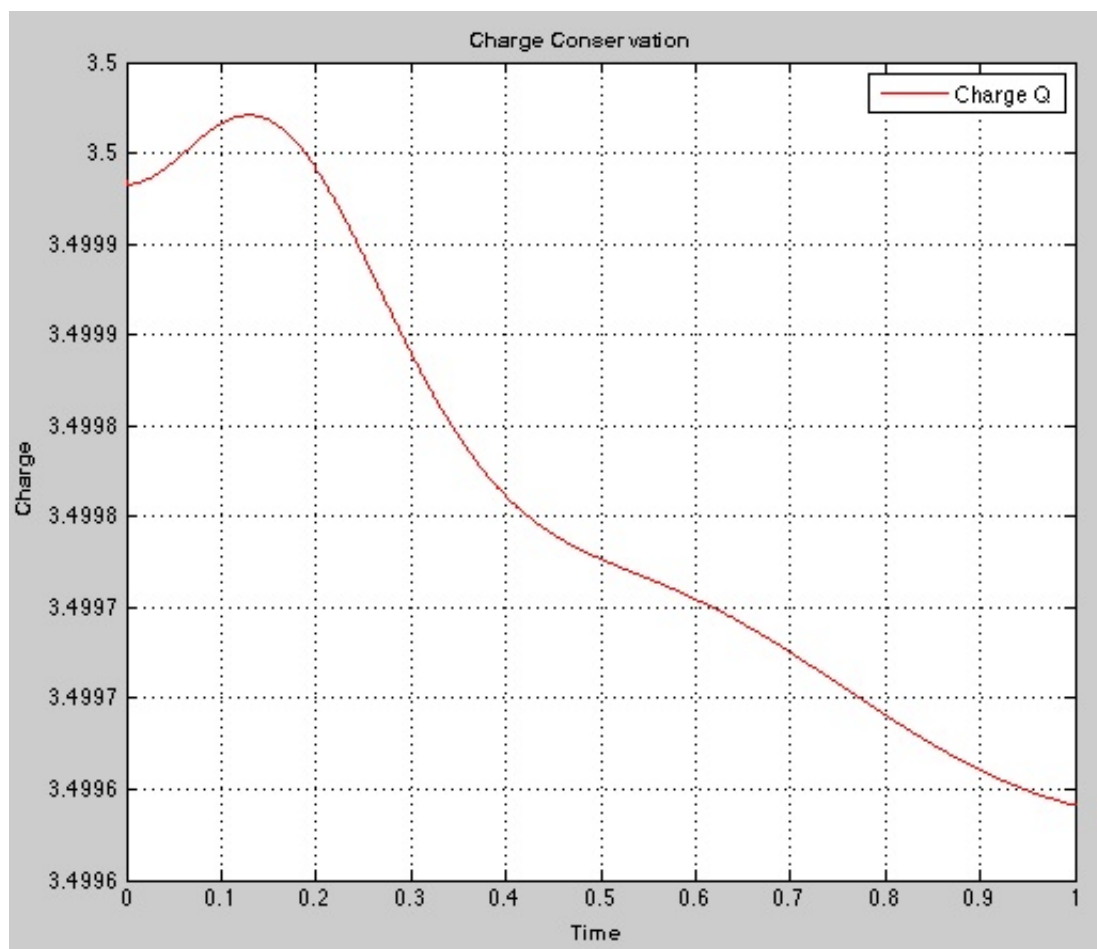


Figure 5.14: (1.2)-c - Conservation of charge: 1024 spatial and temporal dofs (leapfrog)

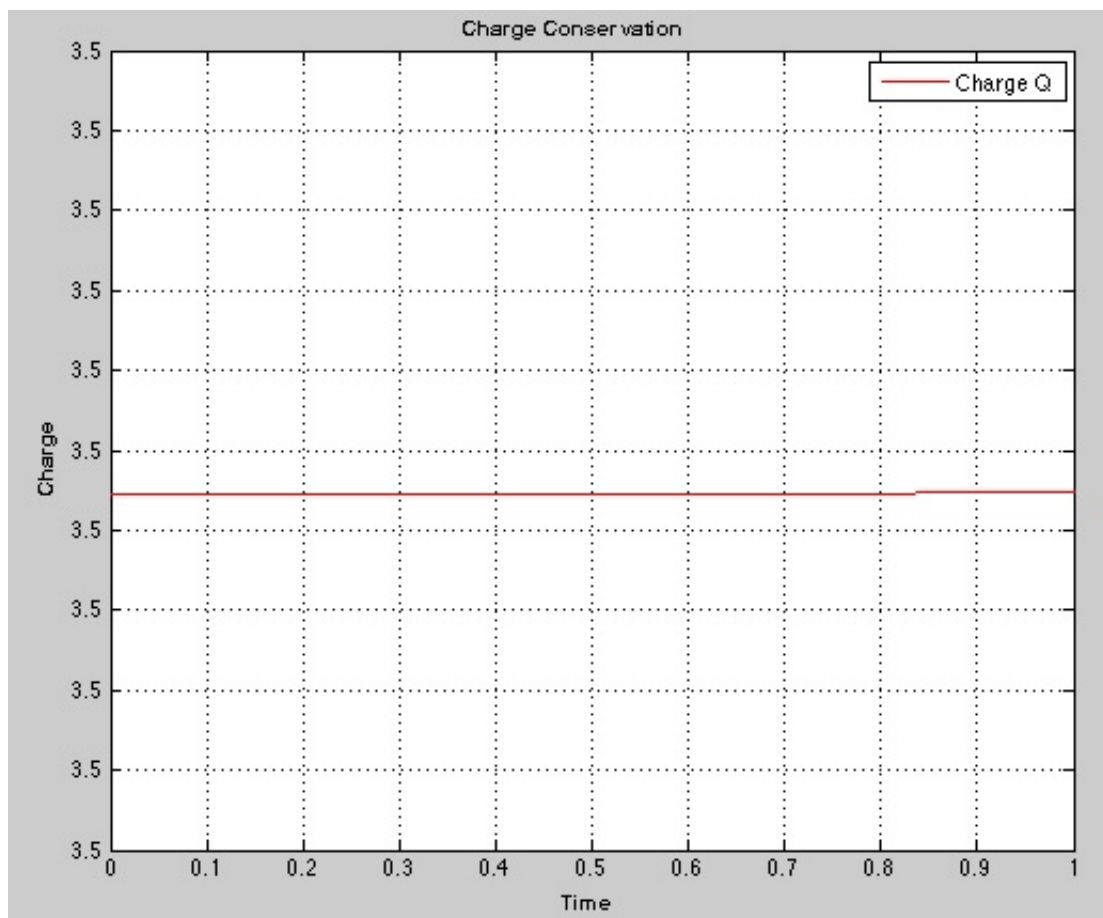


Figure 5.15: (1.3)-c - Conservation of charge: 1024 spatial and temporal dofs (midpoint rule)

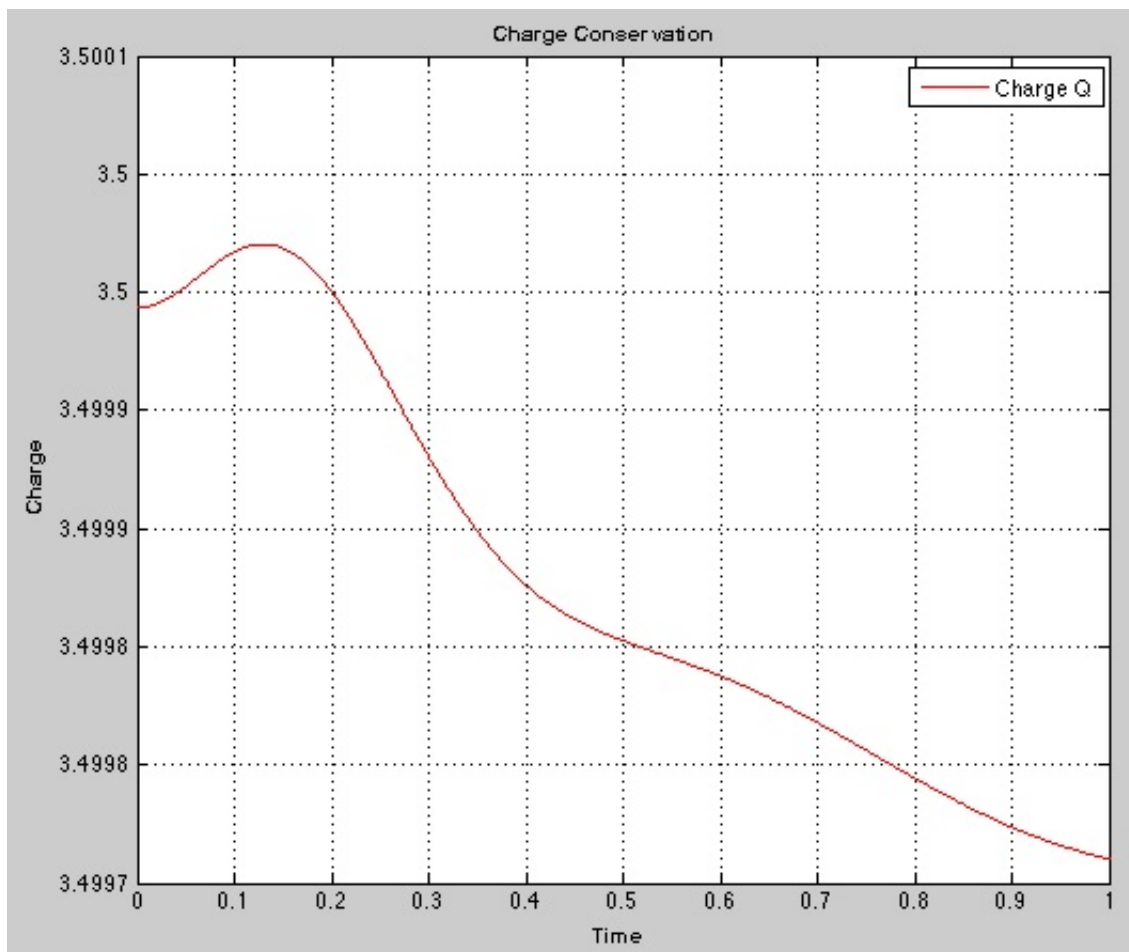


Figure 5.16: (1.3)-c - Conservation of charge: 750 spatial and 1500 temporal dofs (leapfrog)

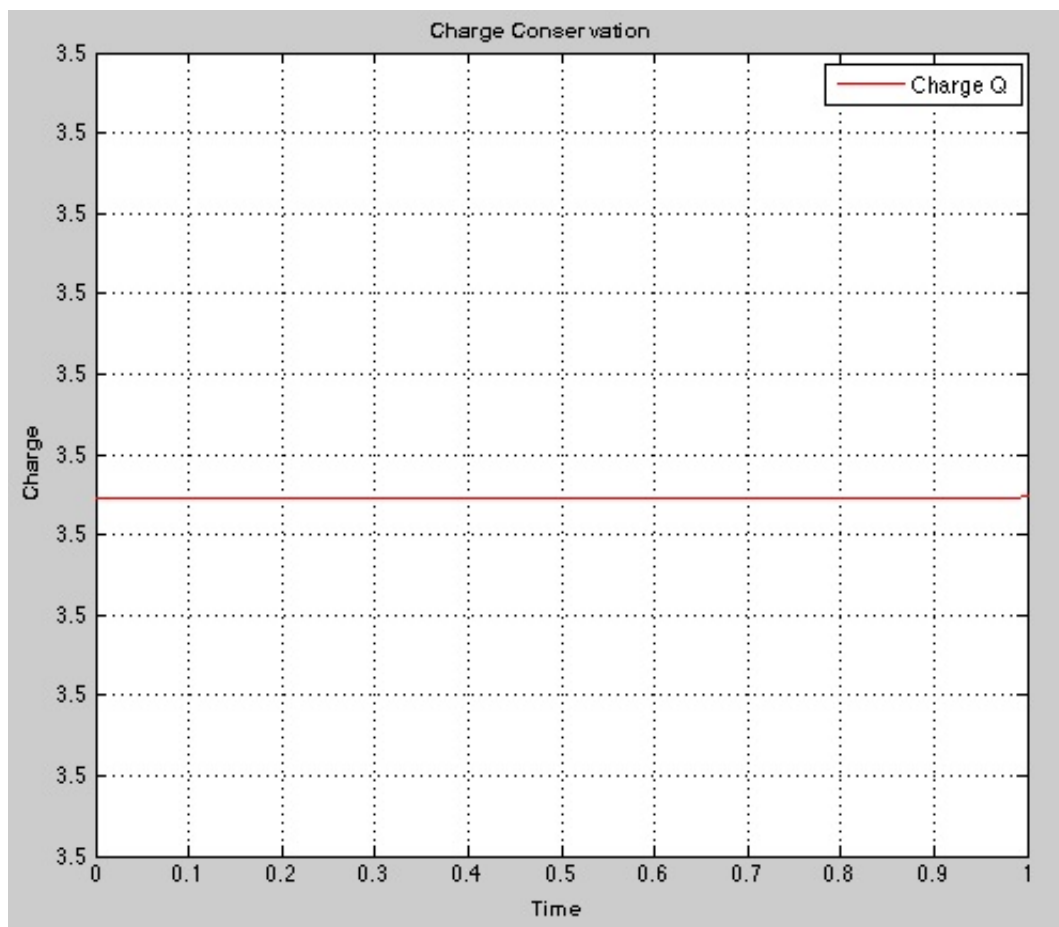


Figure 5.17: (1.4)-c - Conservation of charge: 1024 spatial and temporal dofs (midpoint rule)

Leapfrog Scheme:

See figure 5.18.

5.1.4 Conclusions

Midpoint rule

For the implicit Runge-Kutta-Gauss timestepping the total charge is conserved over time. The charge has the value $3.5+0i$ at all times.

Leapfrog scheme

For the explicit leapfrog-type scheme the total charge varies around the value $3.5+0i$. It is important to choose adequate number of degrees of freedom in terms space and time. The solutions are independent of the weak formulations.

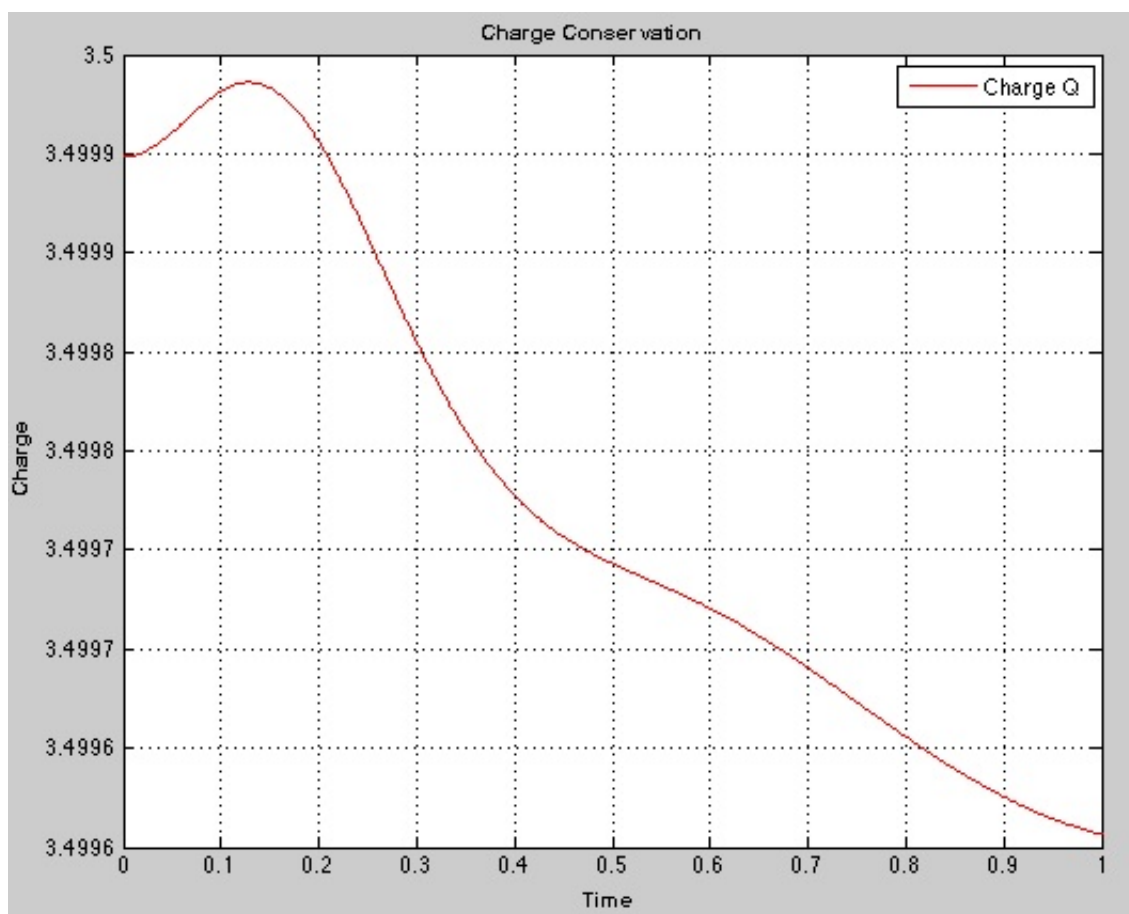


Figure 5.18: (1.4)-c - Conservation of charge: 512 spatial and 1024 temporal dofs (leapfrog)

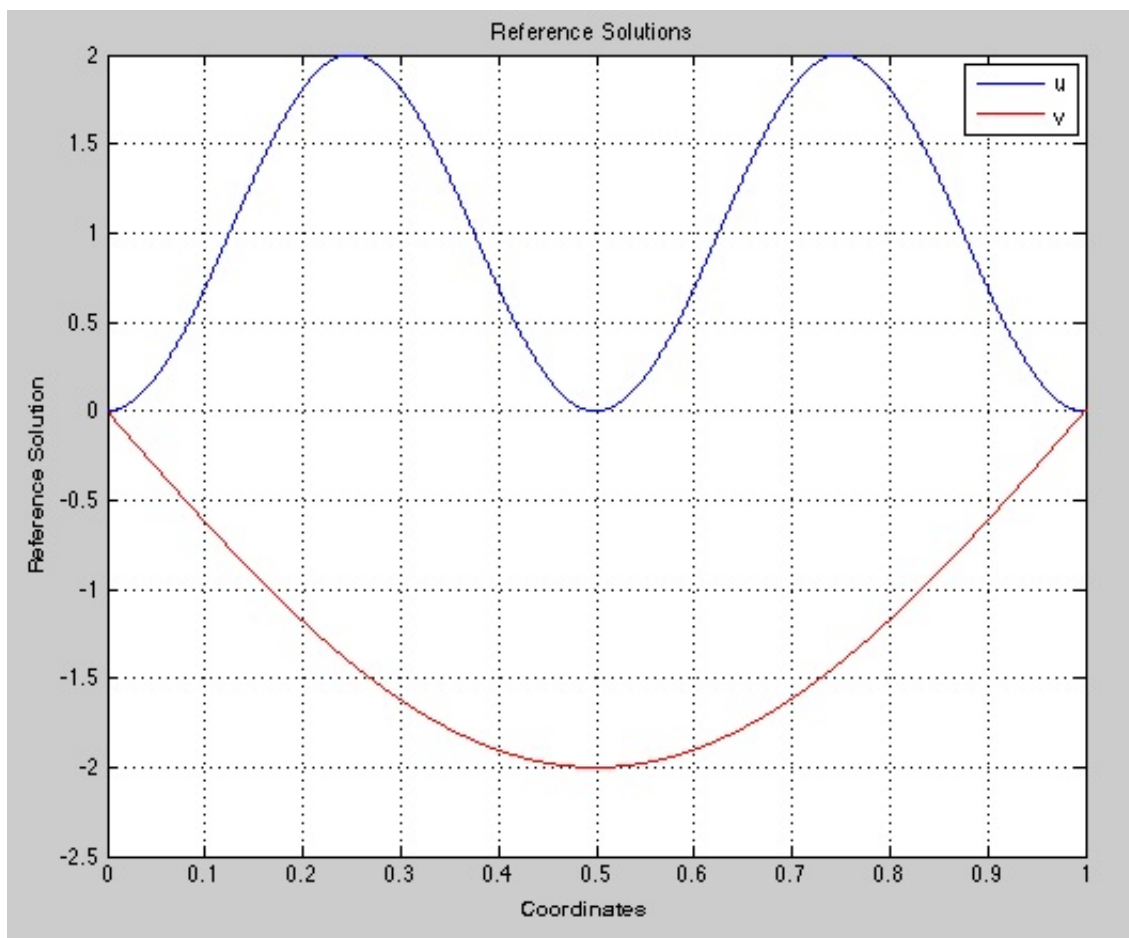


Figure 5.19: Reference solution $f \equiv 1$

5.2 Convergence Of The Methods

Now we look at the solutions of the investigations of the convergence of the methods in terms of spatial and temporal resolution (meshwidth and timestep). There is no exact solution known for this problem, so we need to compute reference solutions with 10000 spatial and temporal degrees of freedom for each of the given functions.

5.2.1 Reference Solutions

The reference solutions are plotted for each weak formulation.

Function a: $f \equiv 1$

see figure 5.19

Function b: $f(x) = xe^{-2x}$

see figure 5.20

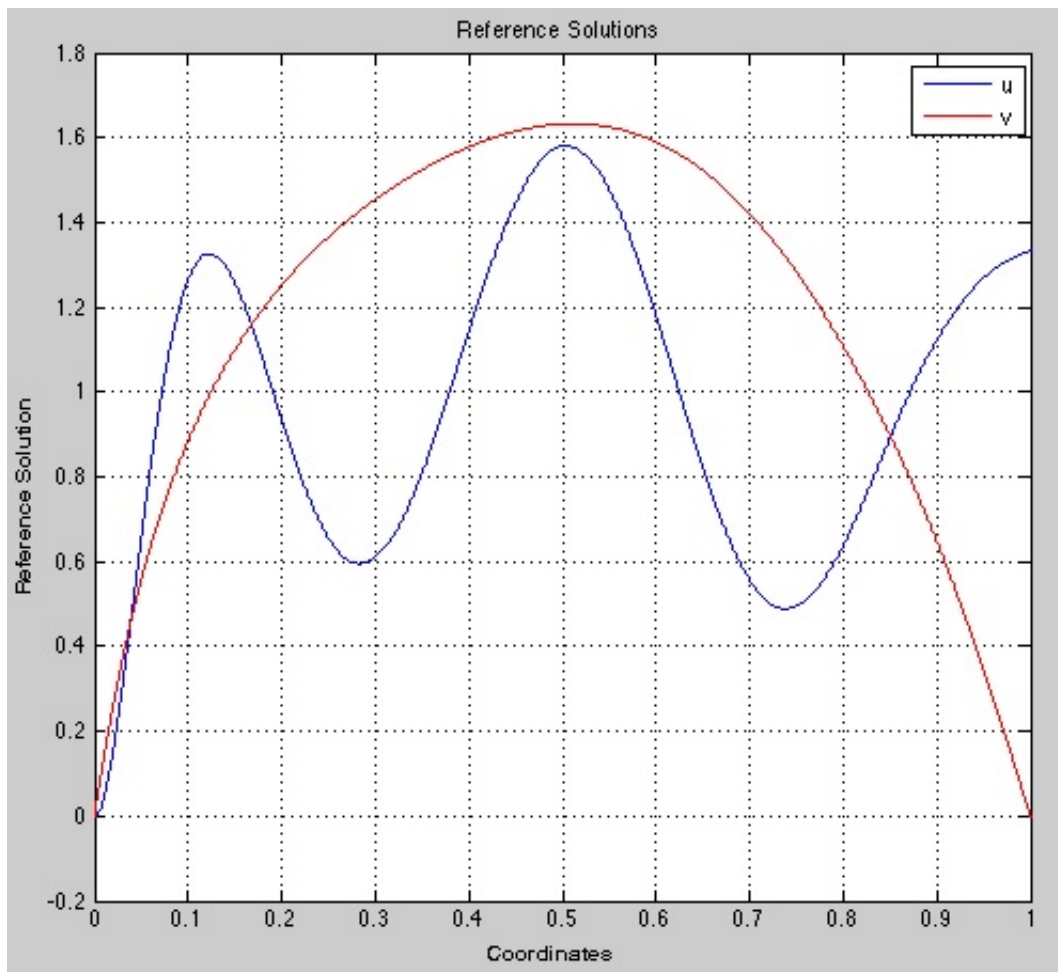


Figure 5.20: Reference solution $f(x) = xe^{-2x}$

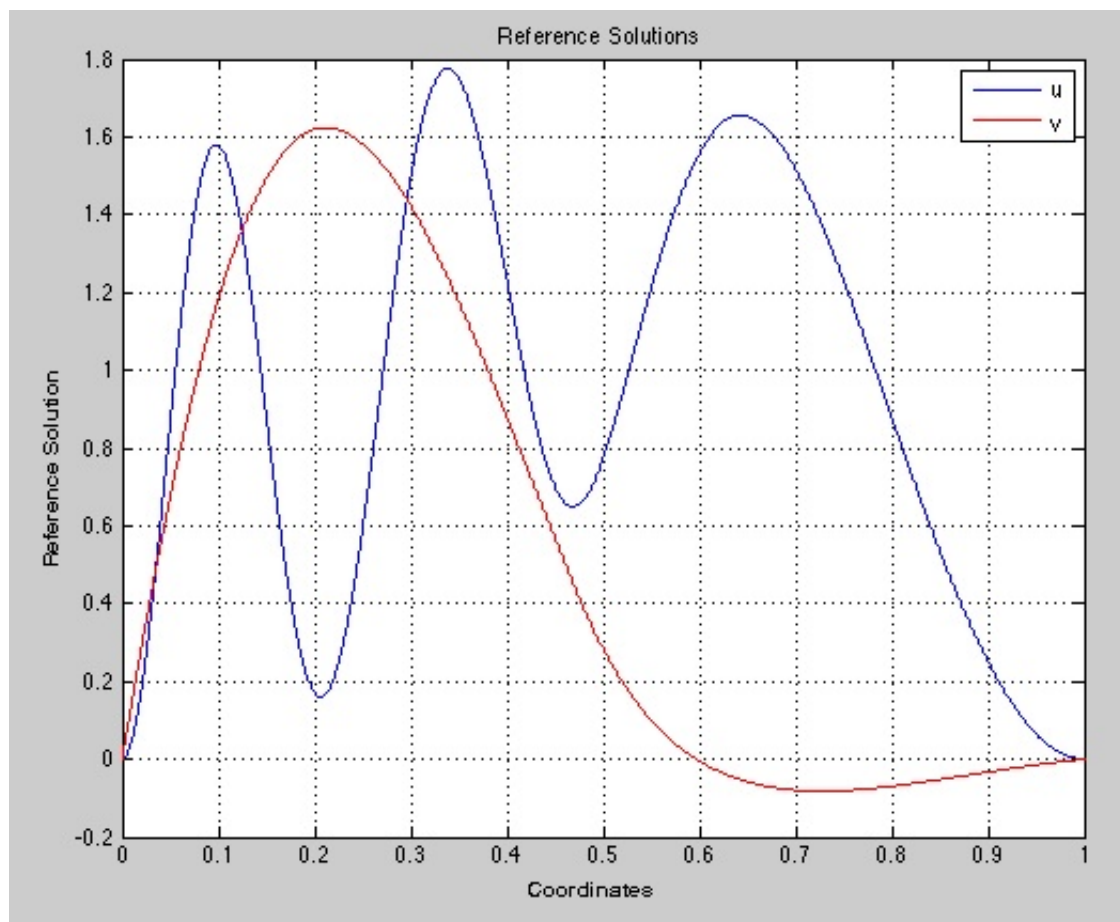


Figure 5.21: Reference solution $f(x, t) = xe^{-tx}$

Function c: $f(x, t) = xe^{-tx}$

see figure 5.21

5.2.2 Spatial Convergence

Function a: $f \equiv 1$

Weak Formulations (1.2)

Midpoint Rule:

Figure 5.22 shows the spatial convergence. The convergence was computed with $M = 2^{3:8}$ spatial dofs and $N = 10000$ temporal dofs.

Interpretation of the result:

The convergence rate is 4. Which means its converging very fast to the exact solution.

There is no theory regarding the convergence rate for this weak formulation.

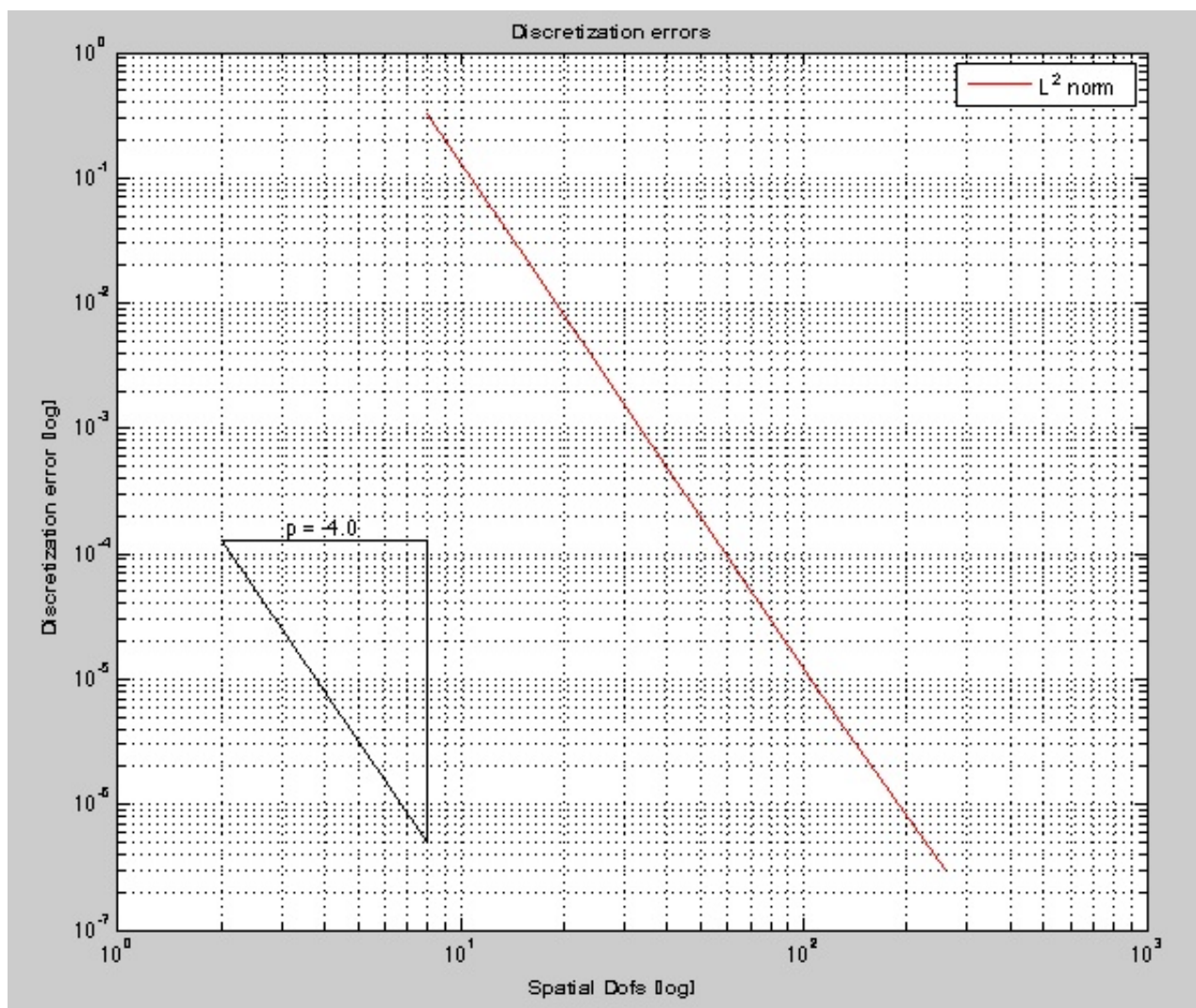


Figure 5.22: (1.2)-a - Spatial Convergence: $M = 2^{3:8}$ spatial dofs, $N = 10000$ temporal dofs (midpoint)

Leapfrog Scheme:

Figure 5.23 shows the spatial convergence. The convergence was computed with $M = 2^{3:7}$ spatial dofs and $N = 10000$ temporal dofs.

Interpretation of the result:

The convergence rate is even $4.2 \rightarrow 4$, so its converging very fast again. We repeat, that there is no theory of convergence rate for this weak formulatios and that we do not have any expected values to it.

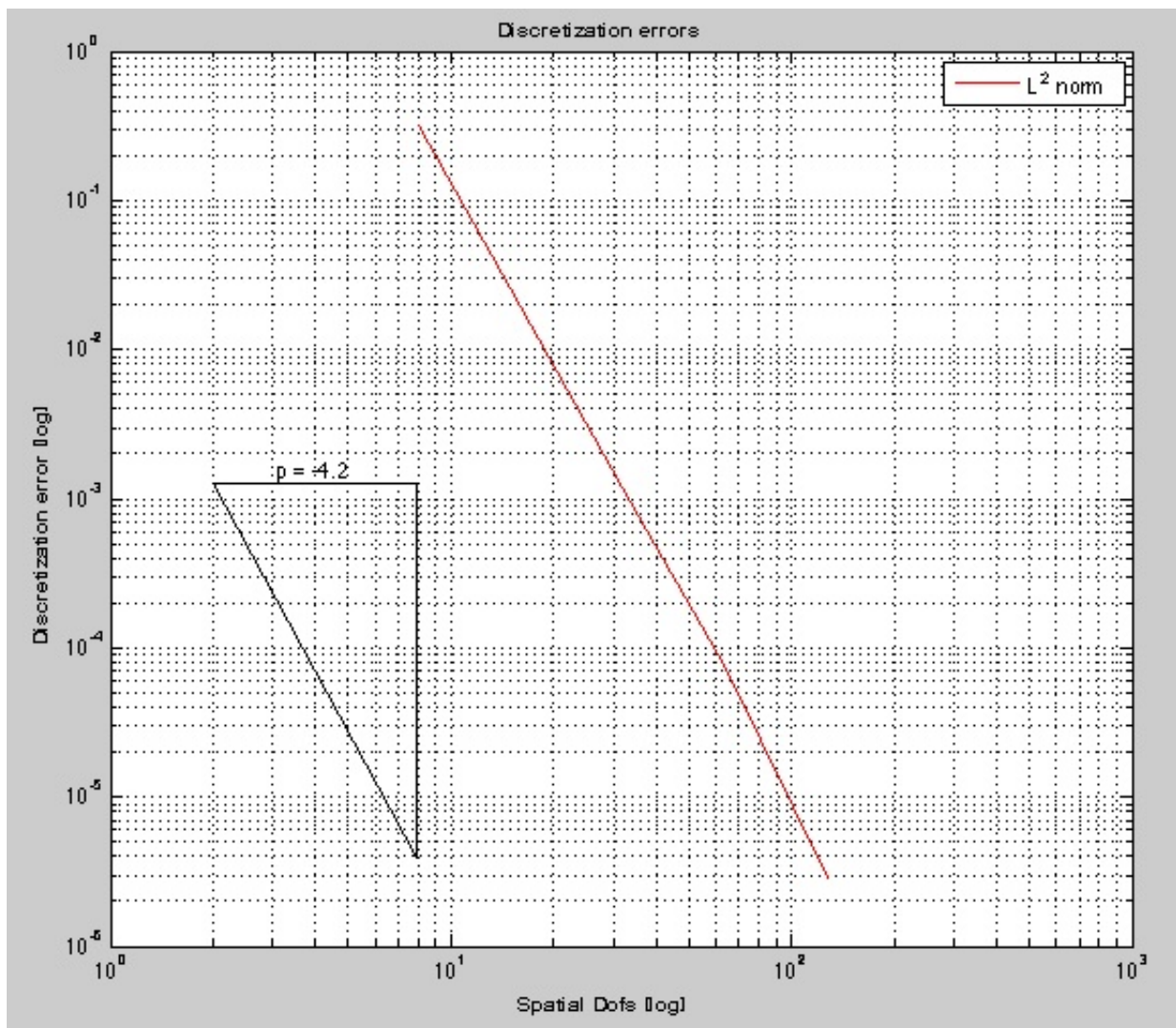


Figure 5.23: (1.2)-a - Spatial Convergence: $M = 2^{3:7}$ spatial dofs, $N = 10000$ temporal dofs (leapfrog)

Weak Formulations (1.3)

Midpoint Rule:

See figure 5.24.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

Leapfrog Scheme:

See figure 5.25.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

Weak Formulations (1.4)

Midpoint Rule:

See figure 5.26.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: $1.1 \rightarrow 1$

Leapfrog Scheme:

See figure 5.27.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: $1.1 \rightarrow 1$

Function b: $f(x) = xe^{-2x}$

Weak Formulations (1.2)

Midpoint Rule:

See figure 5.28.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 2

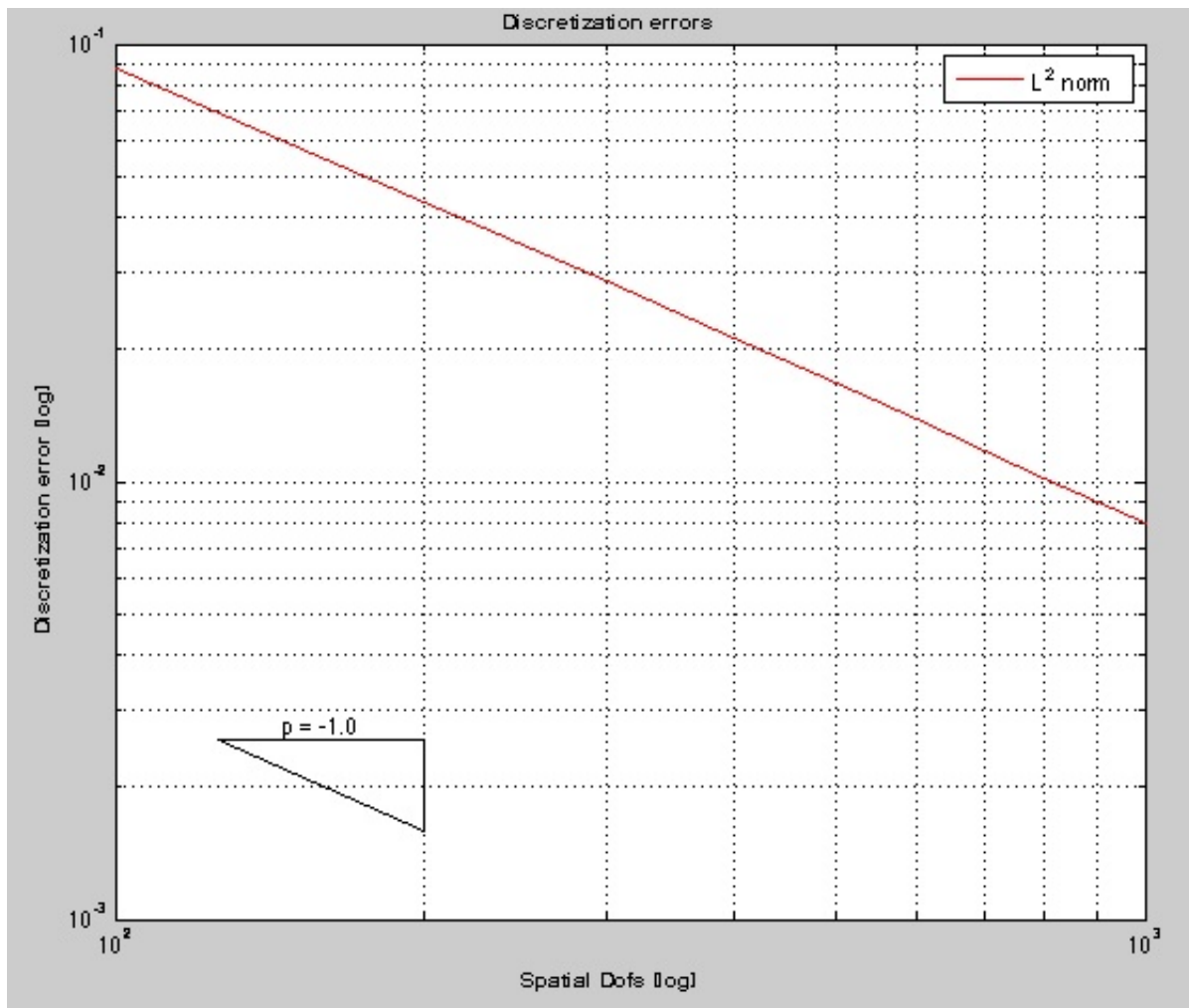


Figure 5.24: (1.3)-a - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (midpoint)

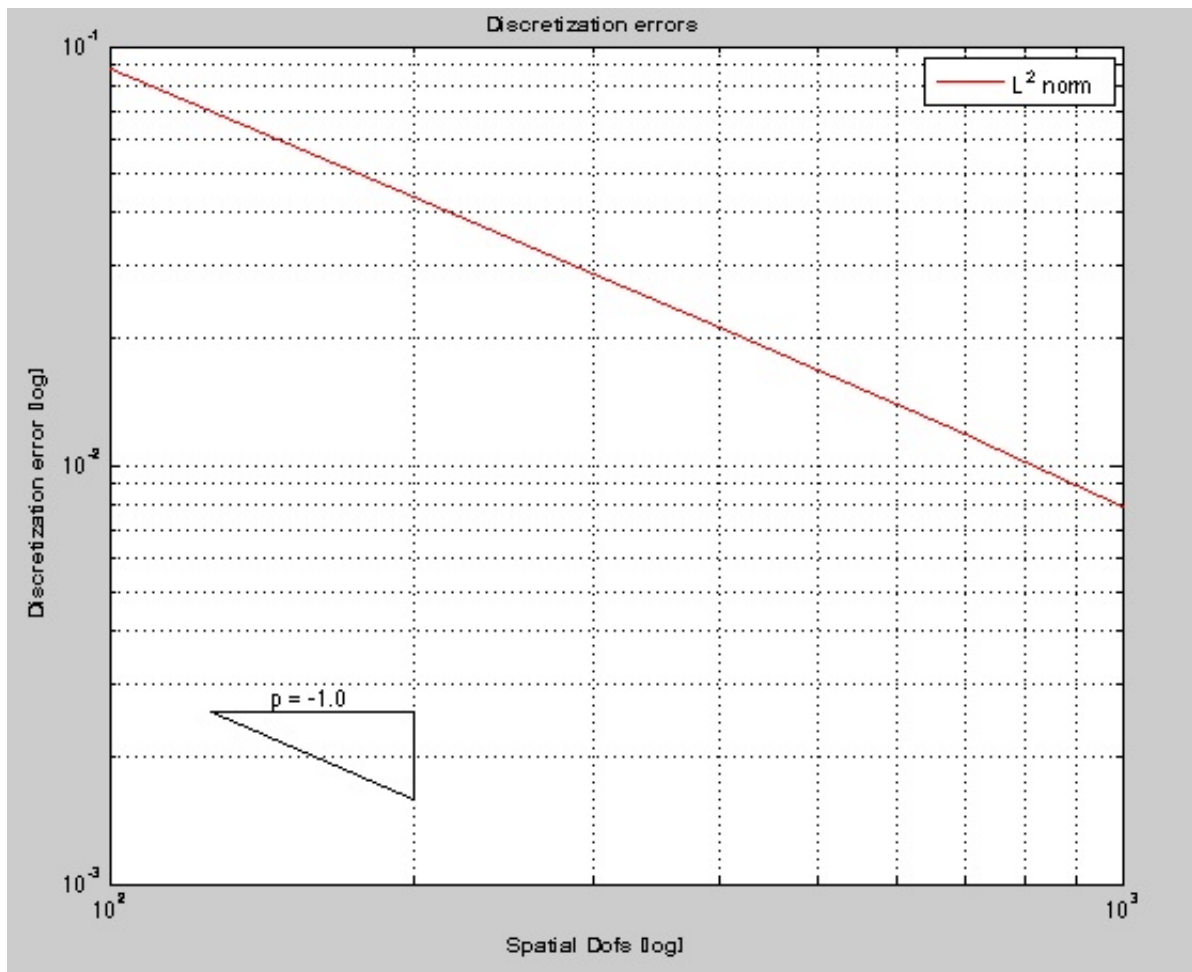


Figure 5.25: (1.3)-a - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (leapfrog)

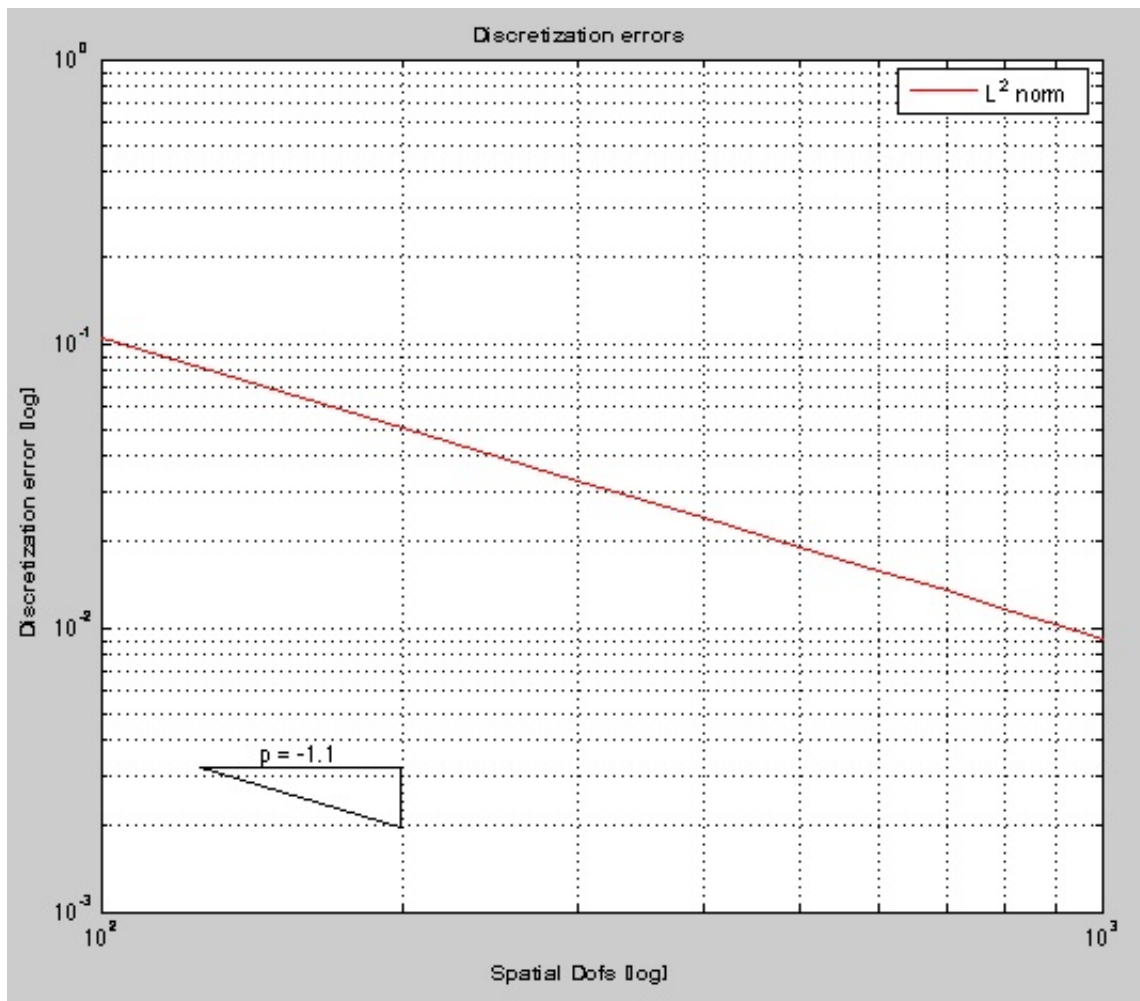


Figure 5.26: (1.4)-a - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (midpoint)

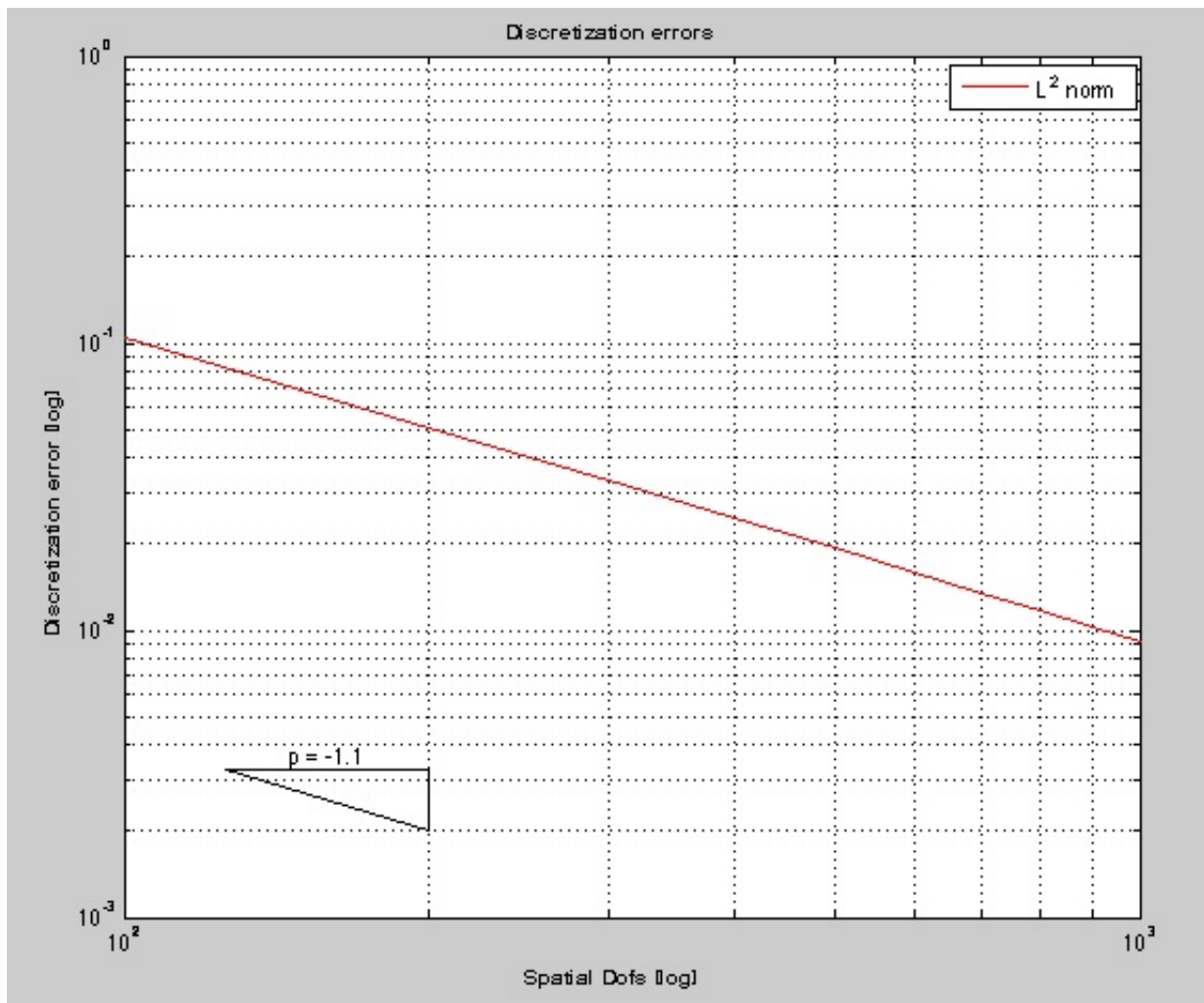


Figure 5.27: (1.4)-a - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (leapfrog)

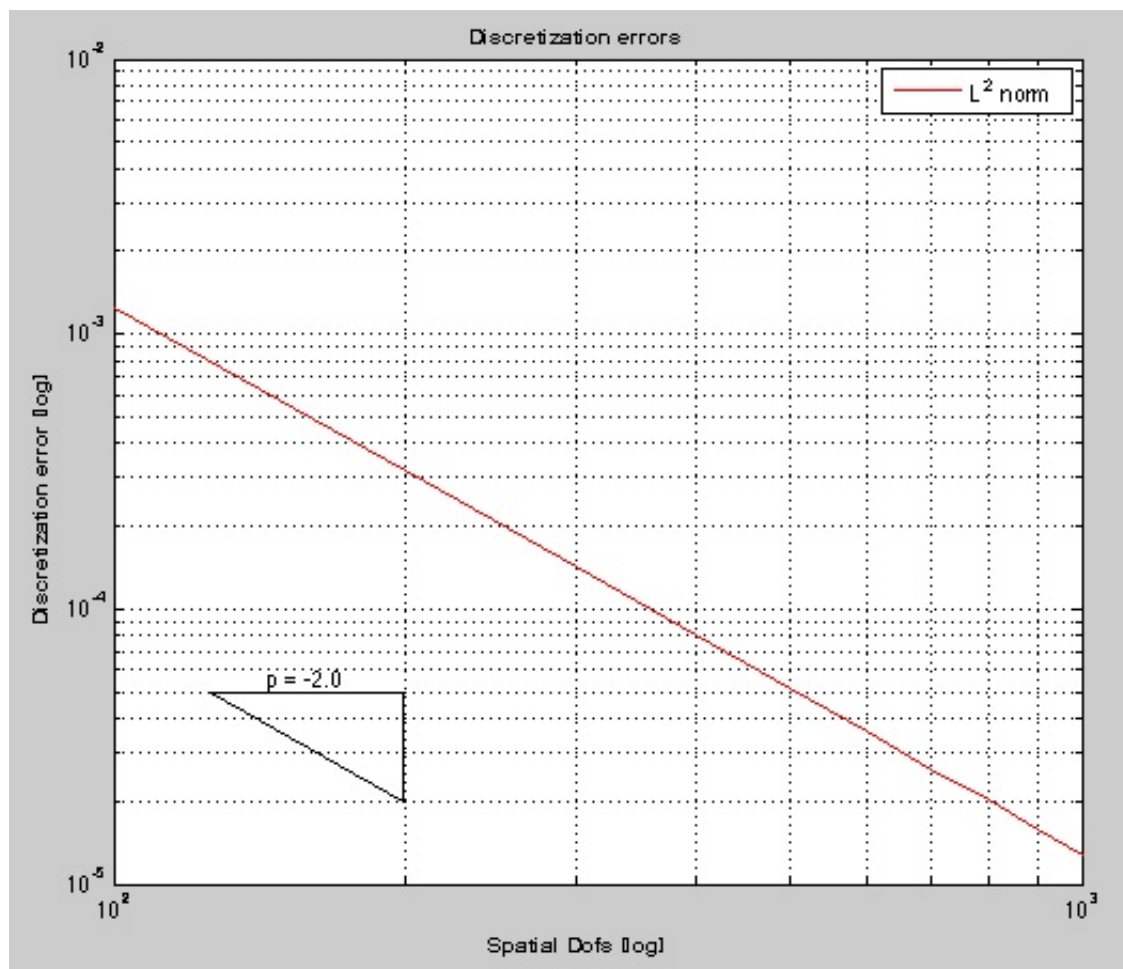


Figure 5.28: (1.2)-b - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (midpoint)

Leapfrog Scheme:

See figure 5.29.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 2

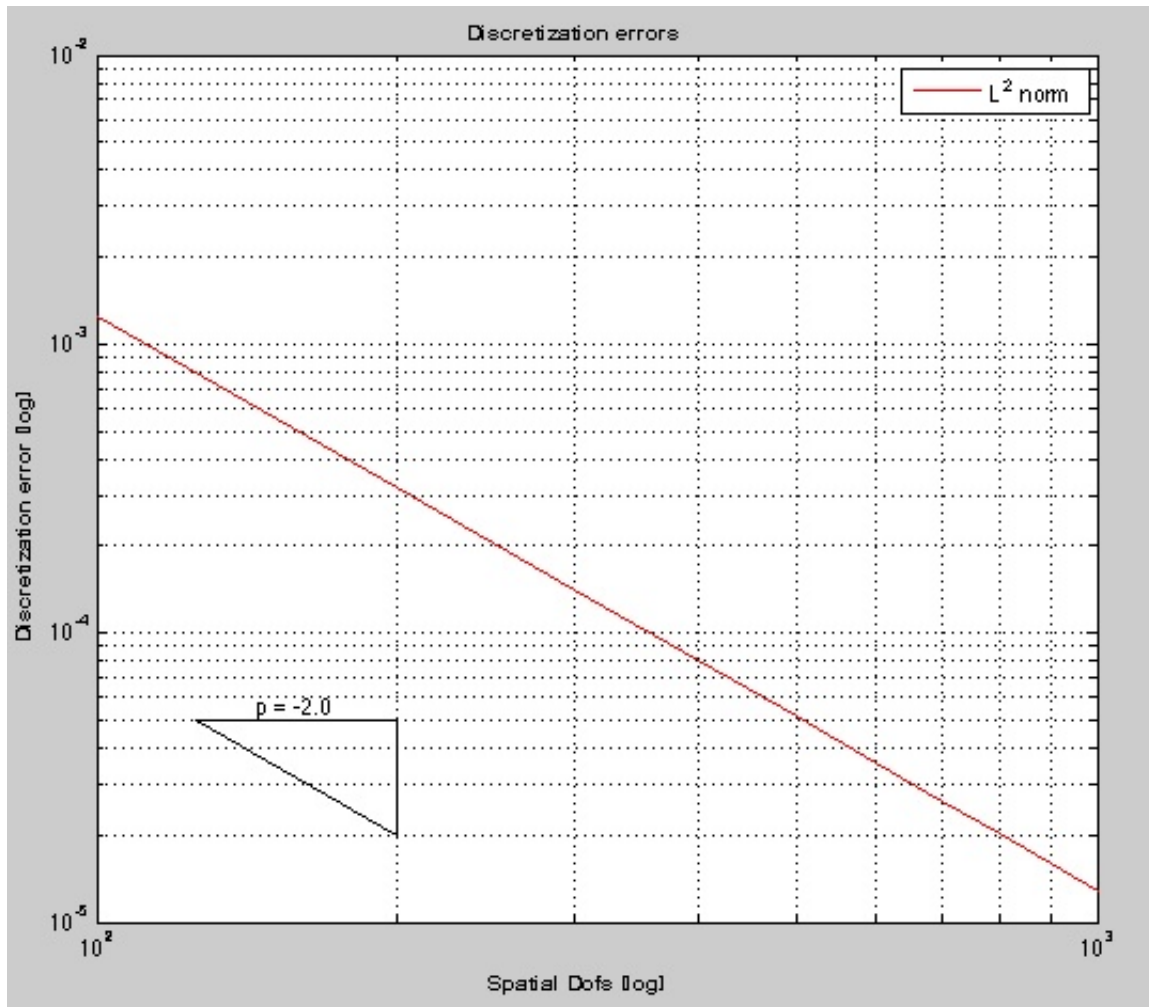


Figure 5.29: (1.2)-b - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (leapfrog)

Weak Formulations (1.3)

Midpoint Rule:

See figure 5.30.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

Leapfrog Scheme:

See figure 5.31.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

Weak Formulations (1.4)

Midpoint Rule:

See figure 5.32.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

Leapfrog Scheme:

See figure 5.33.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

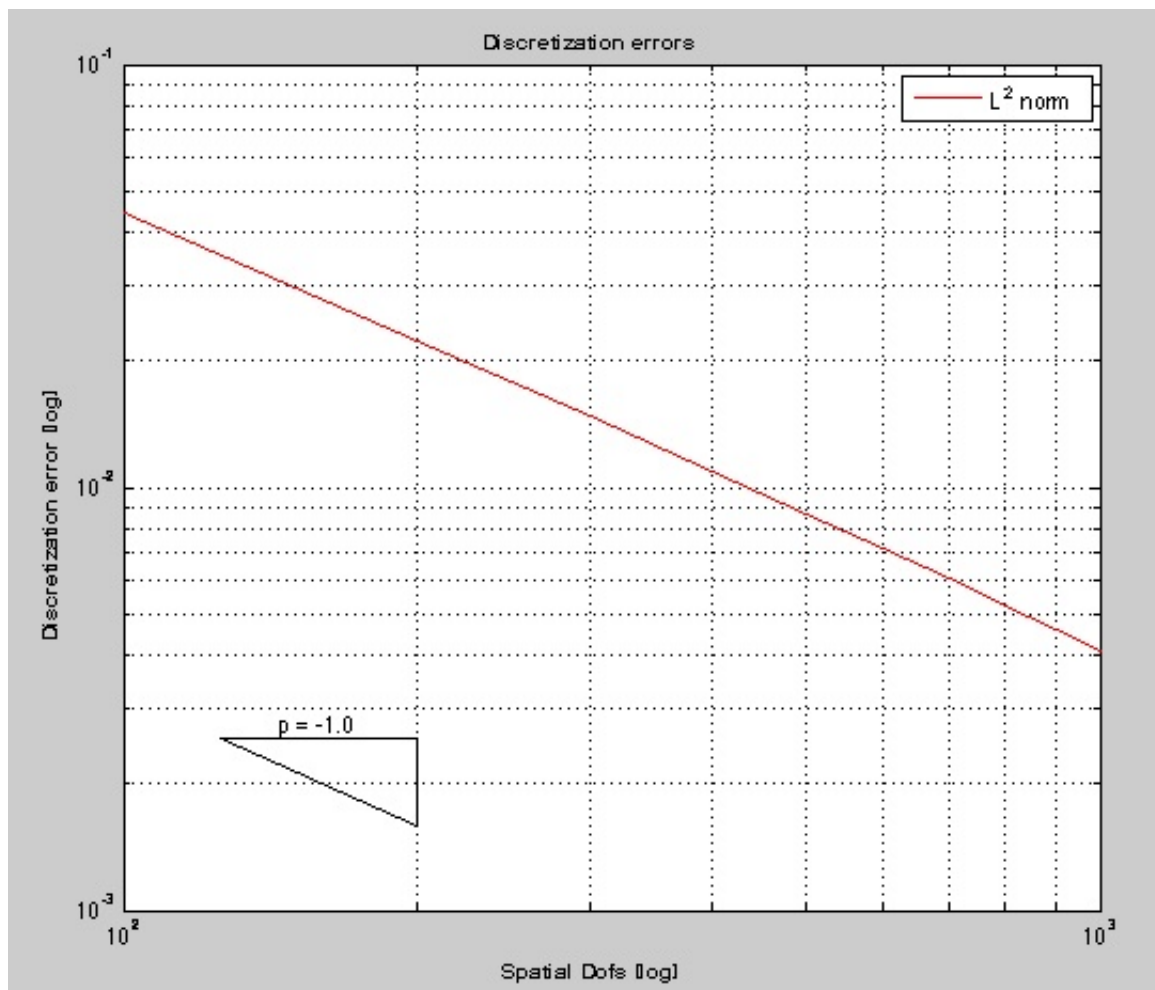


Figure 5.30: (1.3)-b - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (midpoint)

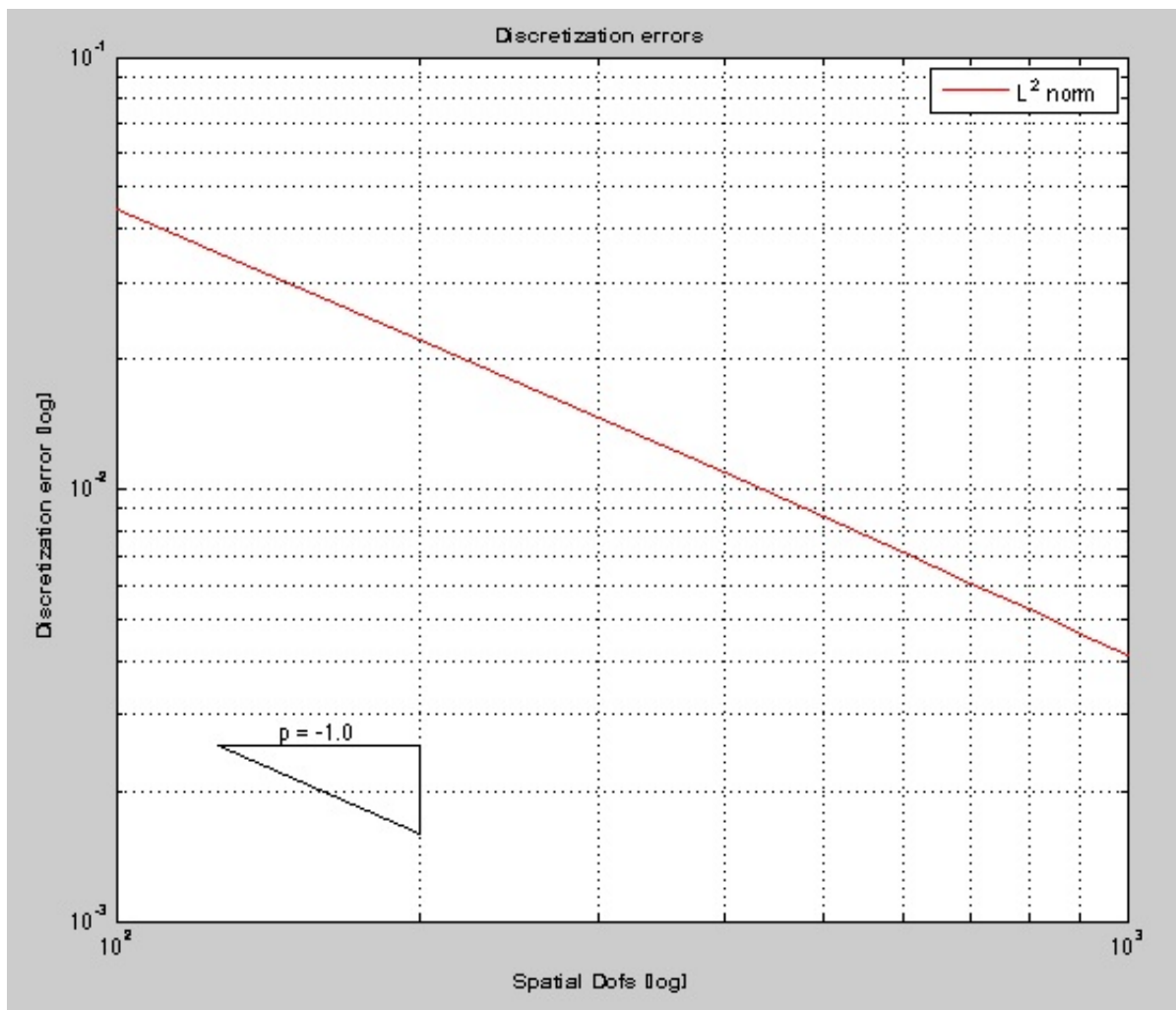


Figure 5.31: (1.3)-b - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (leapfrog)

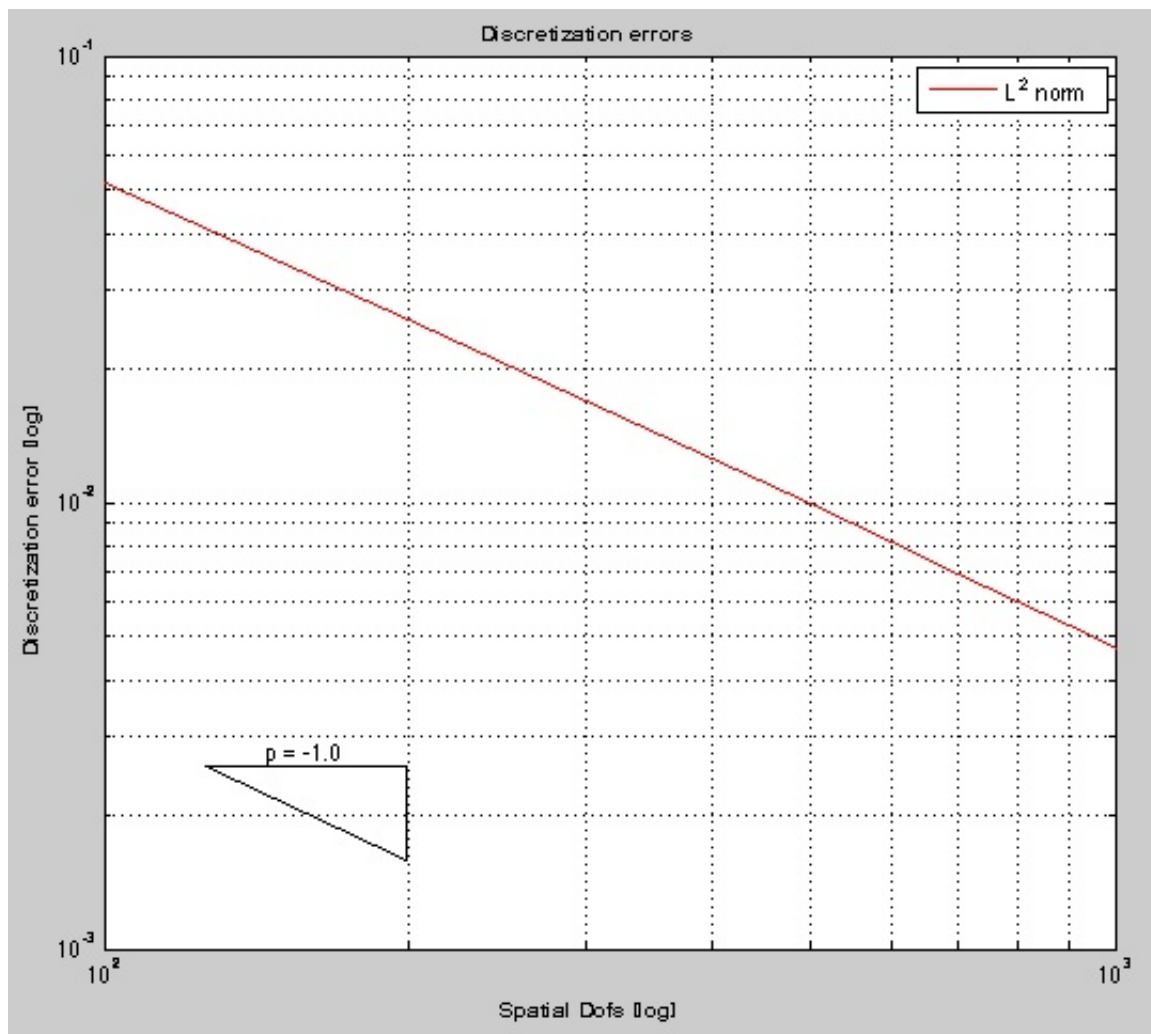


Figure 5.32: (1.4)-b - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (midpoint)

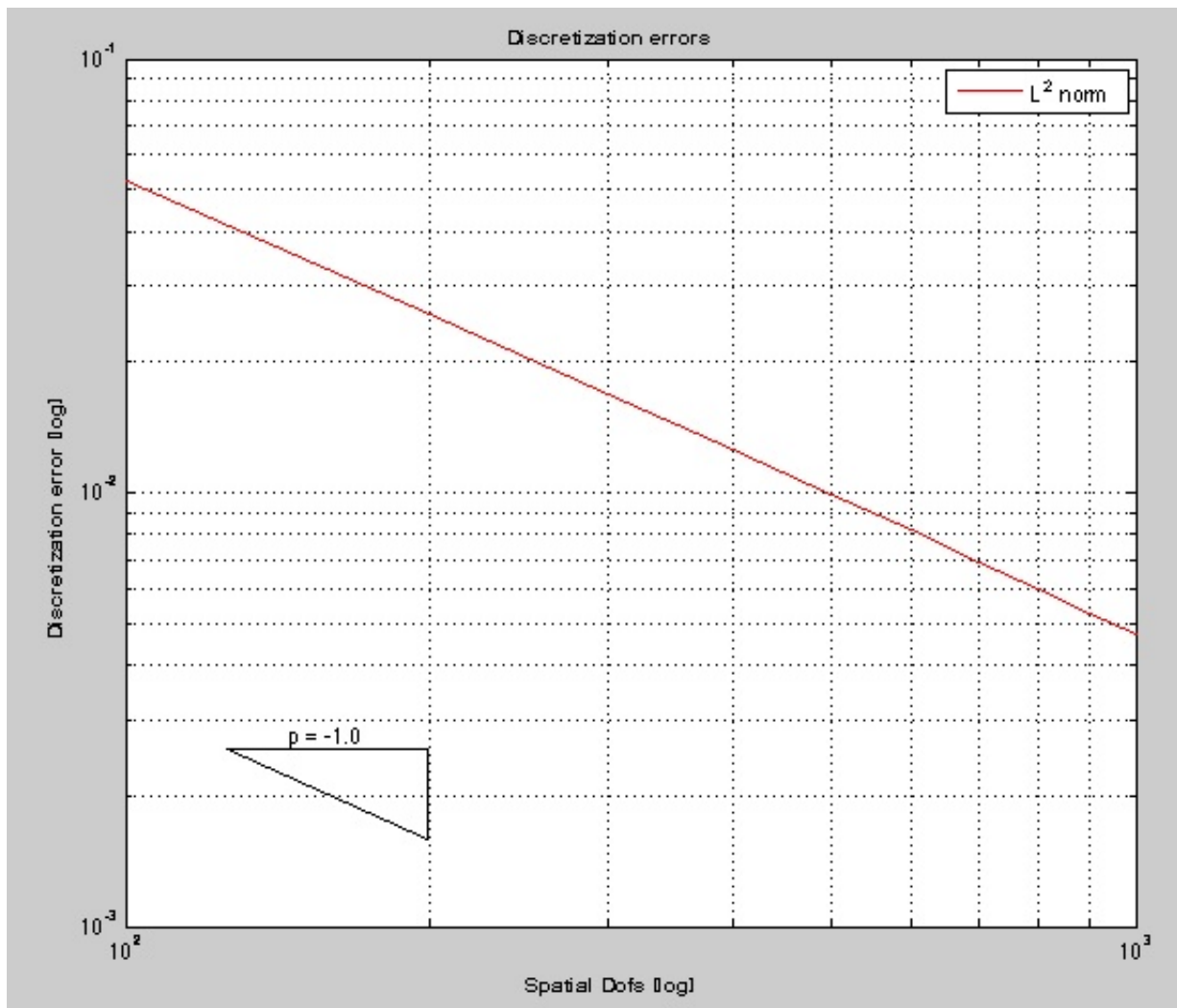


Figure 5.33: (1.4)-b - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (leapfrog)

Function c: $f(x, t) = xe^{-tx}$

Weak Formulations (1.2)

Midpoint Rule:

See figure 5.34.

Spatial dofs: $M = 2^{4:10}$

Temporal dofs: $N = 10000$

Result:

Convergence rate: 2

Leapfrog Scheme:

See figure 5.35.

Spatial dofs: $M = 10:10:100$

Temporal dofs: $N = 10000$

Result:

Convergence rate: 2

Weak Formulations (1.3)

Midpoint Rule:

See figure 5.36.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

Leapfrog Scheme:

See figure 5.37.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

Weak Formulations (1.4)

Midpoint Rule:

See figure 5.38.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

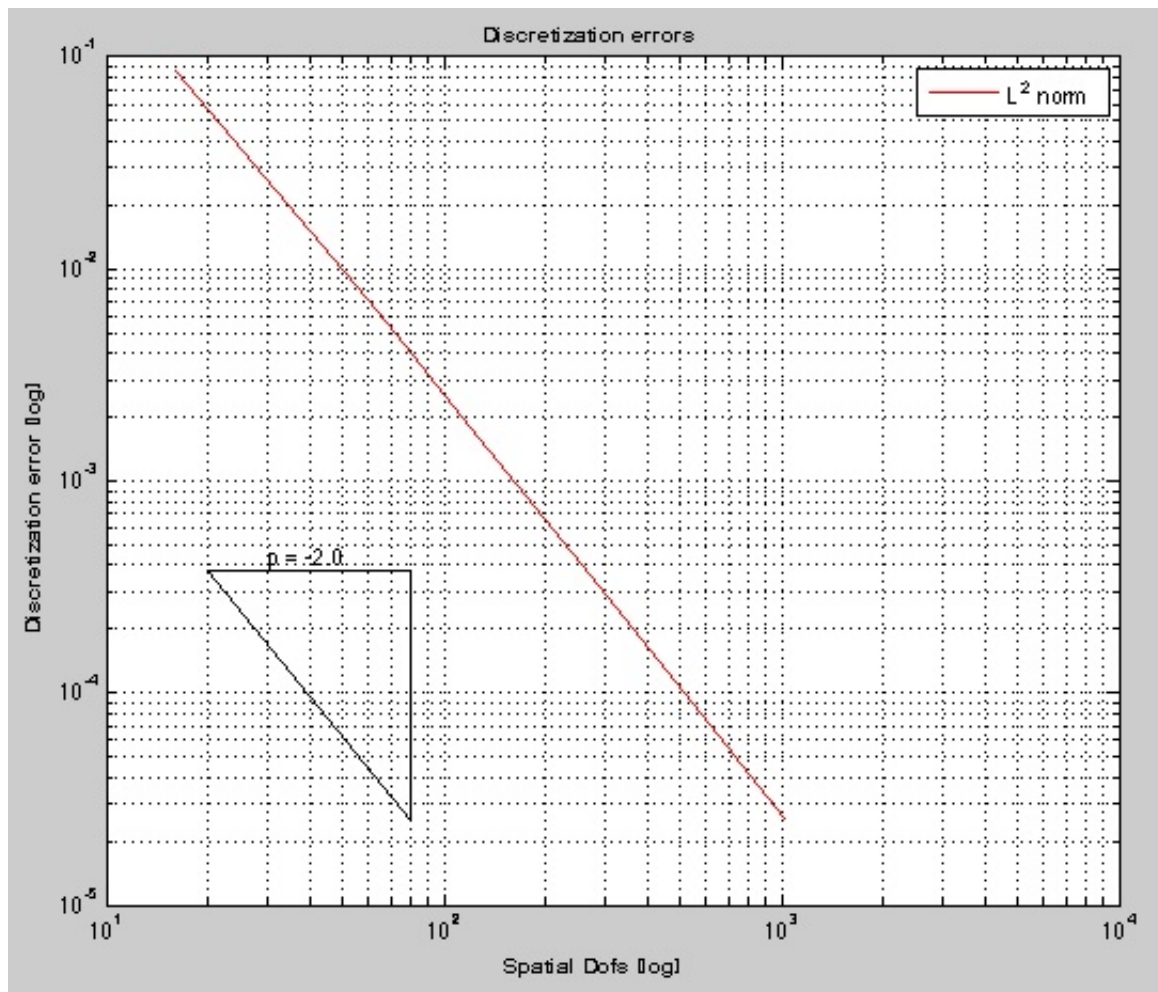


Figure 5.34: (1.2)-c - Spatial Convergence: $M = 2^{4:10}$ spatial dofs, $N = 10000$ temporal dofs (midpoint)

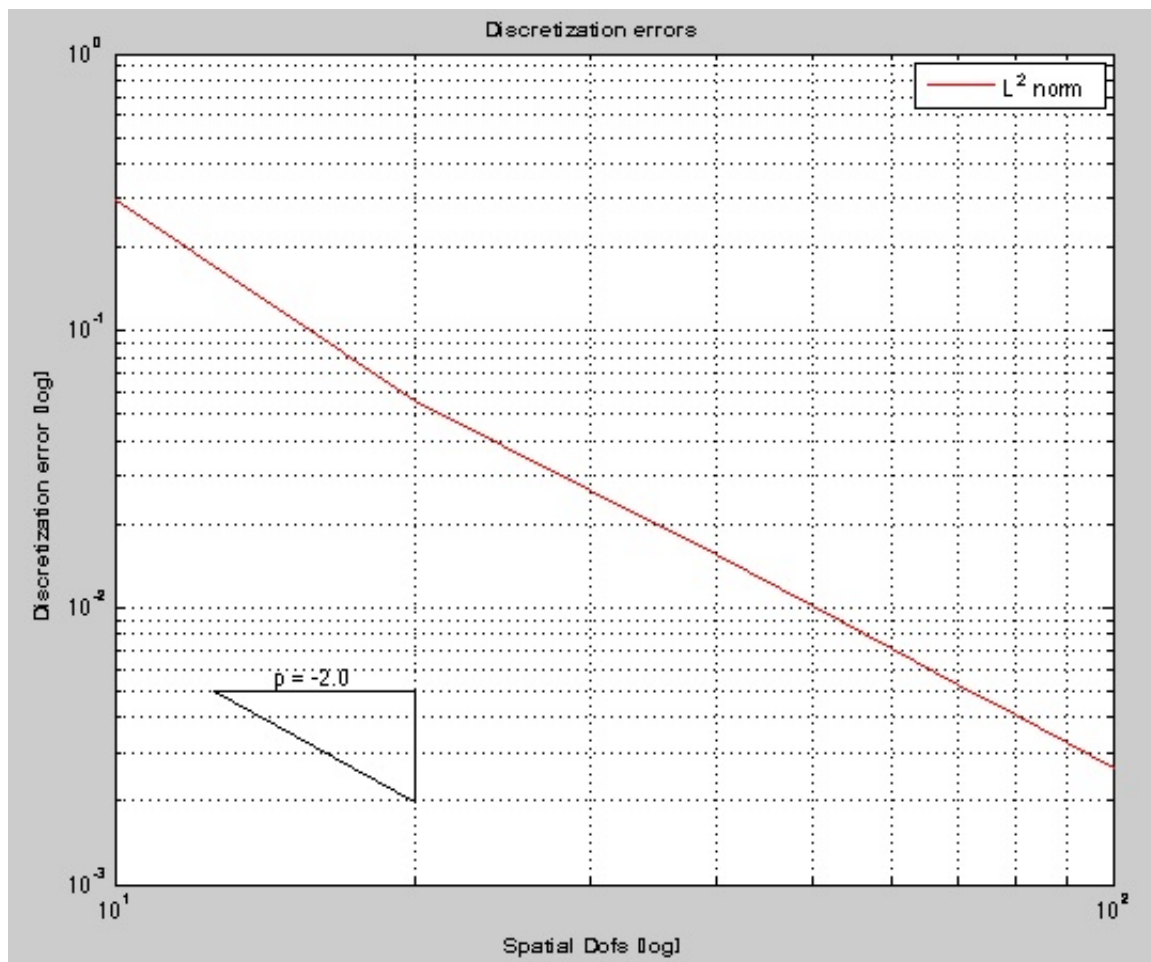


Figure 5.35: (1.2)-c - Spatial Convergence: $M = 10:10:100$ spatial dofs, $N = 10000$ temporal dofs (leapfrog)

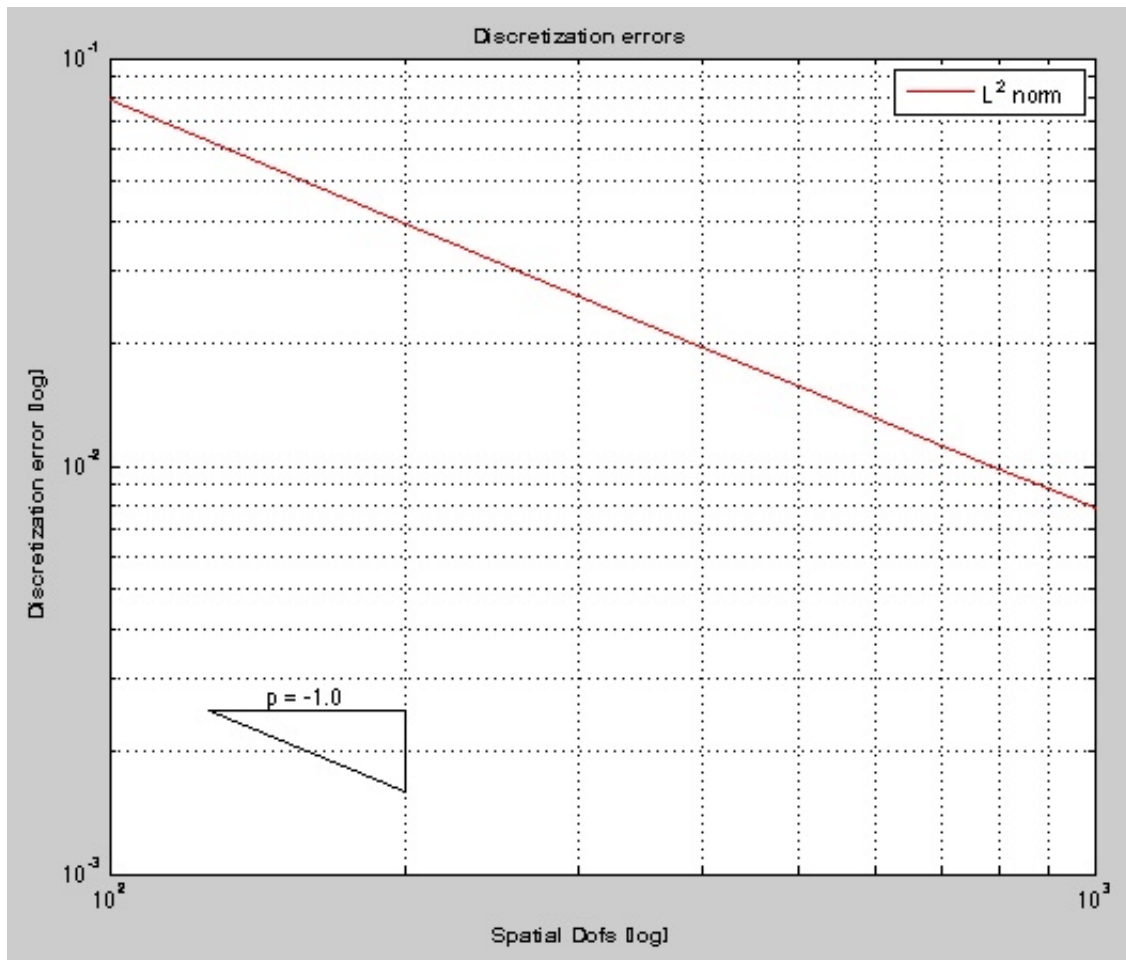


Figure 5.36: (1.3)-c - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (midpoint)

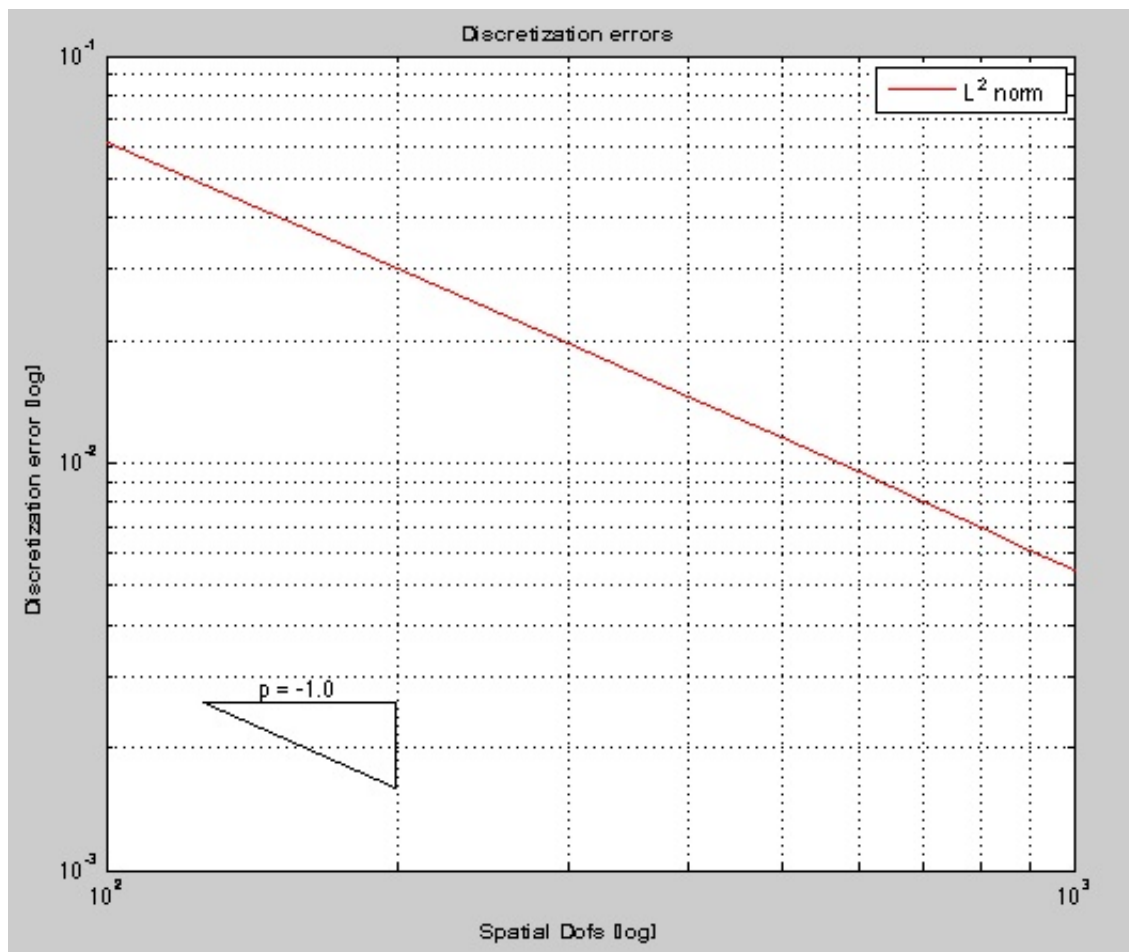


Figure 5.37: (1.3)-c - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (leapfrog)

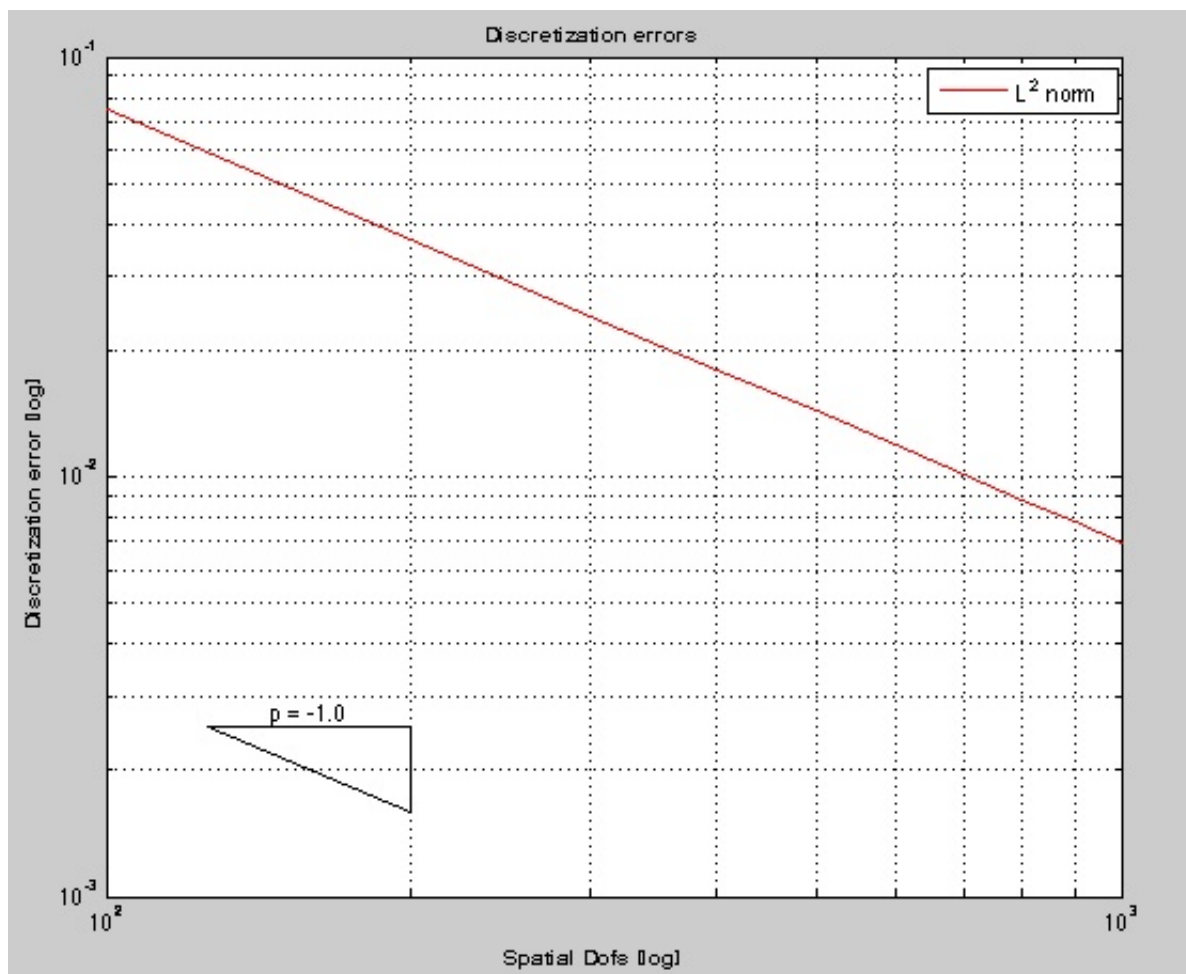


Figure 5.38: (1.4)-c - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (midpoint)

Leapfrog Scheme:

See figure 5.39.

Spatial dofs: $M = 100:100:1000$

Temporal dofs: $N = 2000$

Result:

Convergence rate: 1

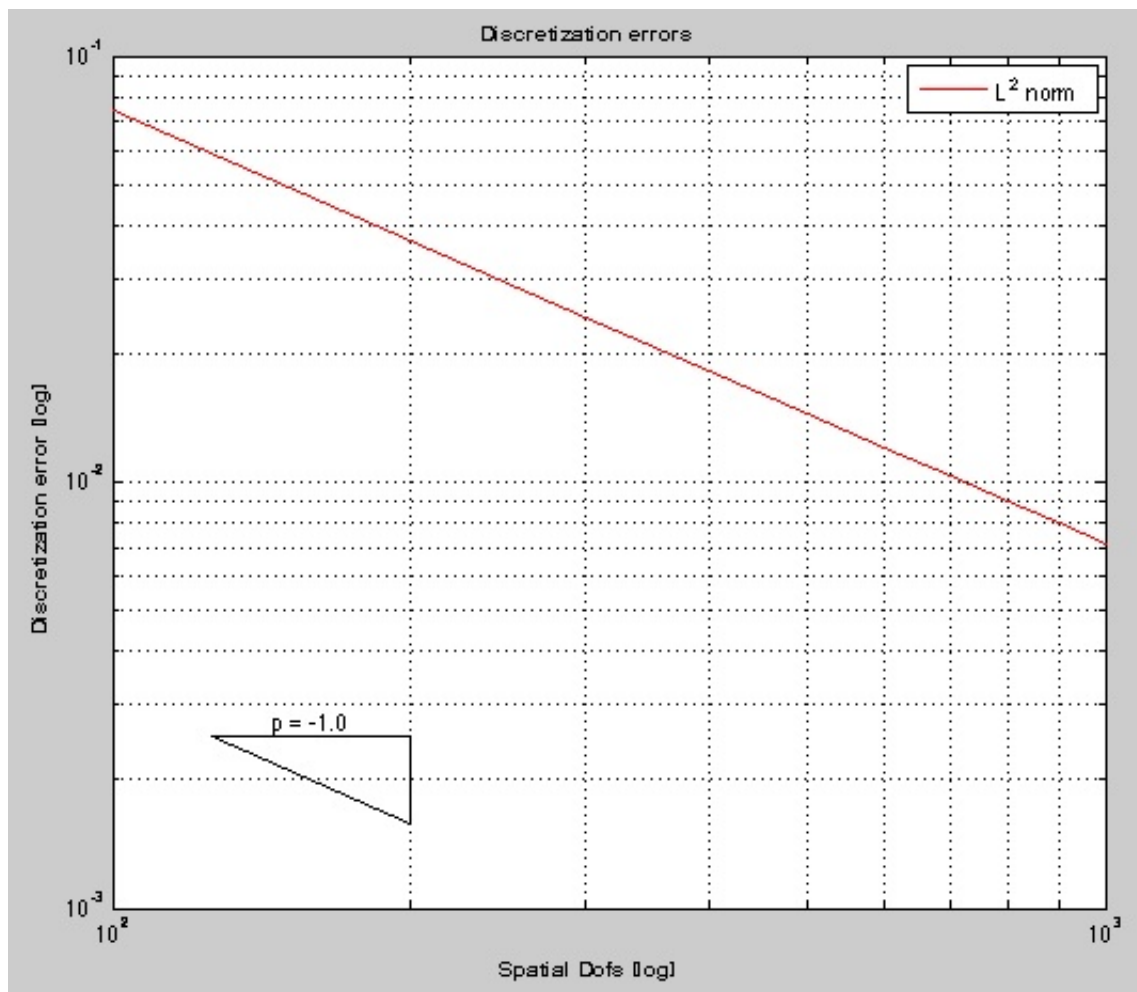


Figure 5.39: (1.4)-c - Spatial Convergence: $M = 100:100:1000$ spatial dofs, $N = 2000$ temporal dofs (leapfrog)

5.2.3 Temporal Convergence

The temporal convergence cannot be computed for the leapfrog algorithm. It is not possible to choose the temporal and spatial degree of freedoms such that we get stability.

Function a: $f \equiv 1$

Weak Formulations (1.2)

Midpoint Rule:

See figure 5.40.

Spatial dofs: $M = 200$

Temporal dofs: $N = 1000:100:2000$

Result:

Convergence rate: 2

Weak Formulations (1.3)

Midpoint Rule:

See figure 5.41.

Spatial dofs: $M = 8000$

Temporal dofs: $N = 2^{4:9}$

Result:

Convergence rate: 2

Weak Formulations (1.4)

Midpoint Rule:

See figure 5.42.

Spatial dofs: $M = 8000$

Temporal dofs: $N = 2^{4:9}$

Result:

Convergence rate: 2

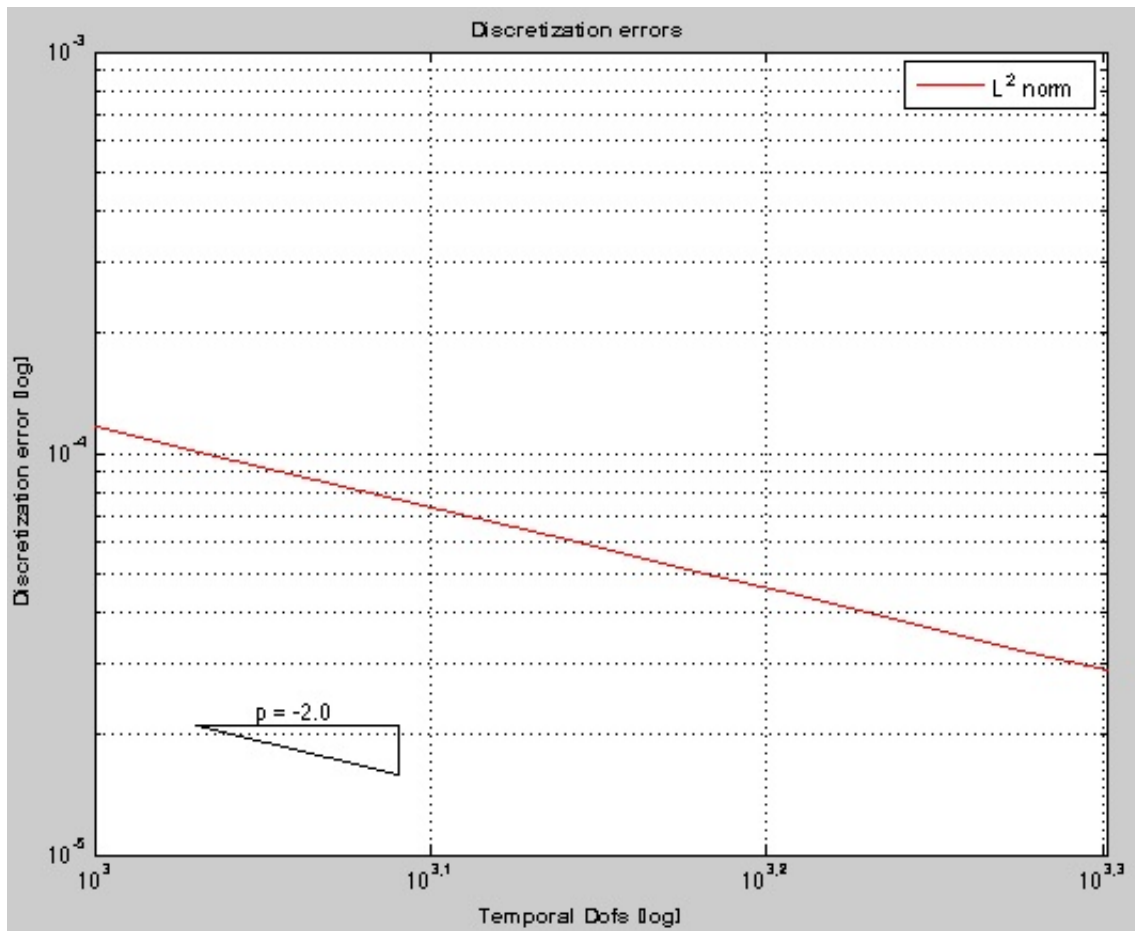


Figure 5.40: (1.2)-a - Temporal Convergence: $M = 200$ spatial dofs, $N = 1000:100:2000$ temporal dofs (midpoint)

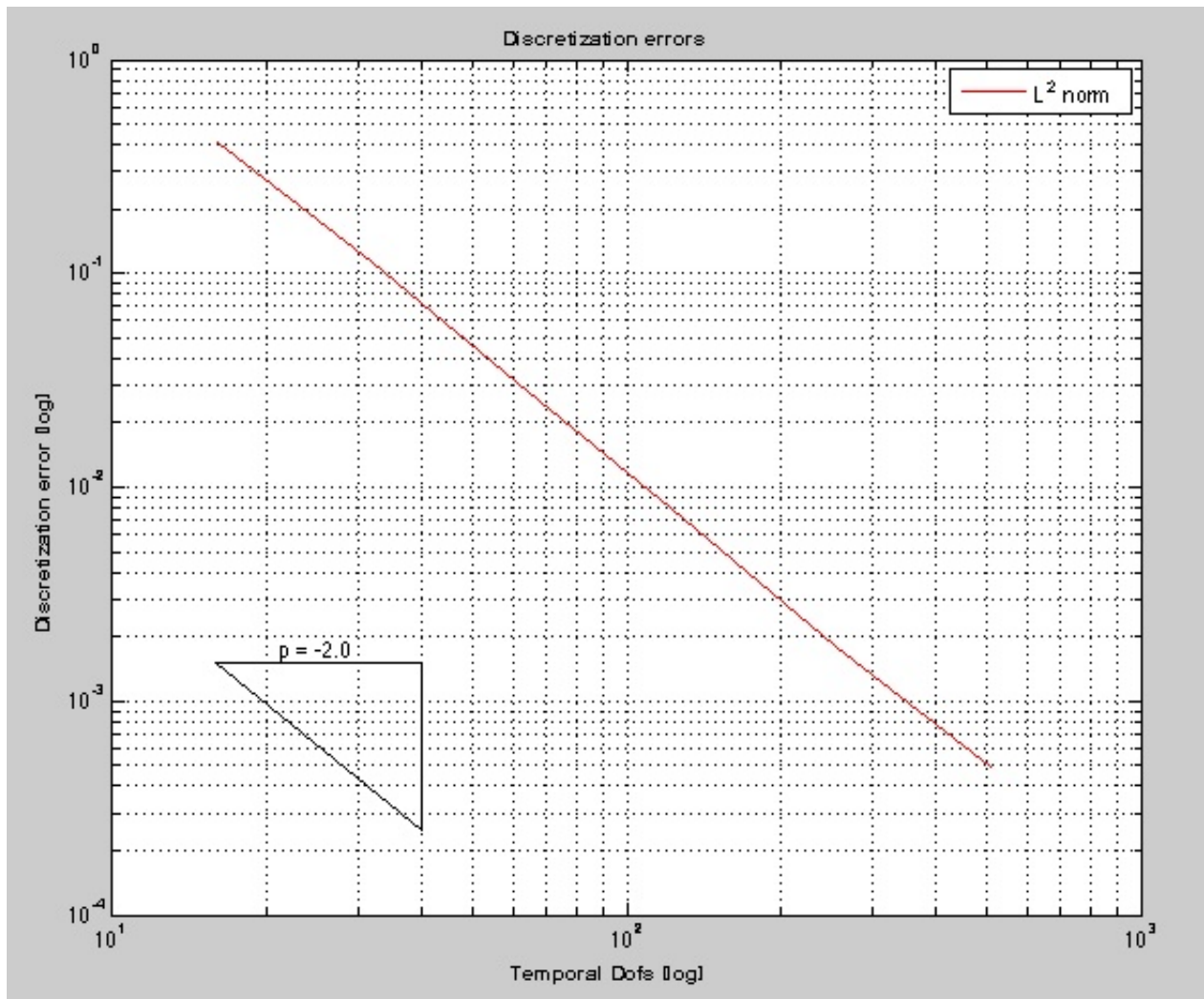


Figure 5.41: (1.3)-a - Temporal Convergence: $M = 8000$ spatial dofs, $N = 2^{49}$ temporal dofs (midpoint)

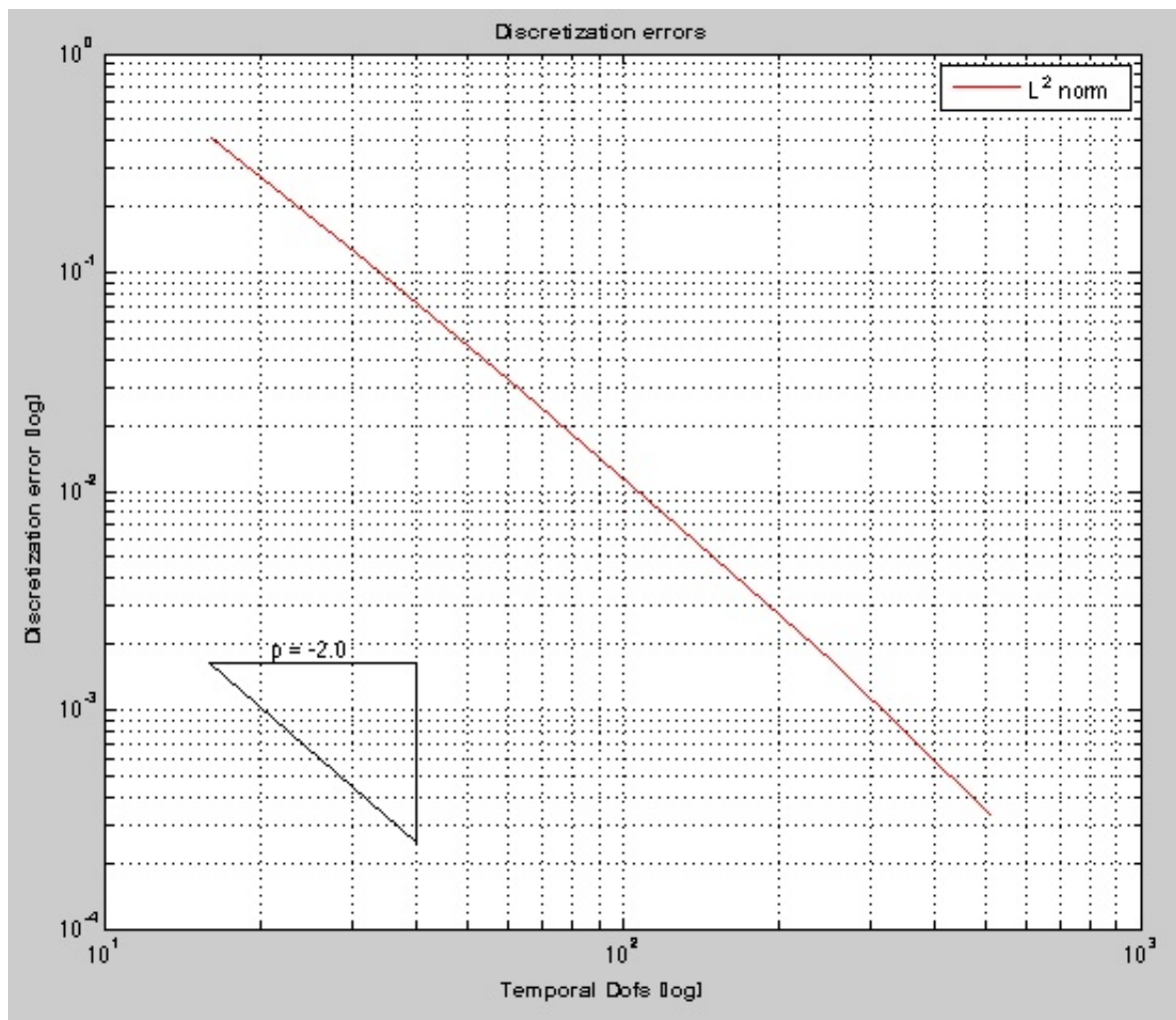


Figure 5.42: (1.4)-a - Temporal Convergence: $M = 8000$ spatial dofs, $N = 2^{14}$ temporal dofs (midpoint)

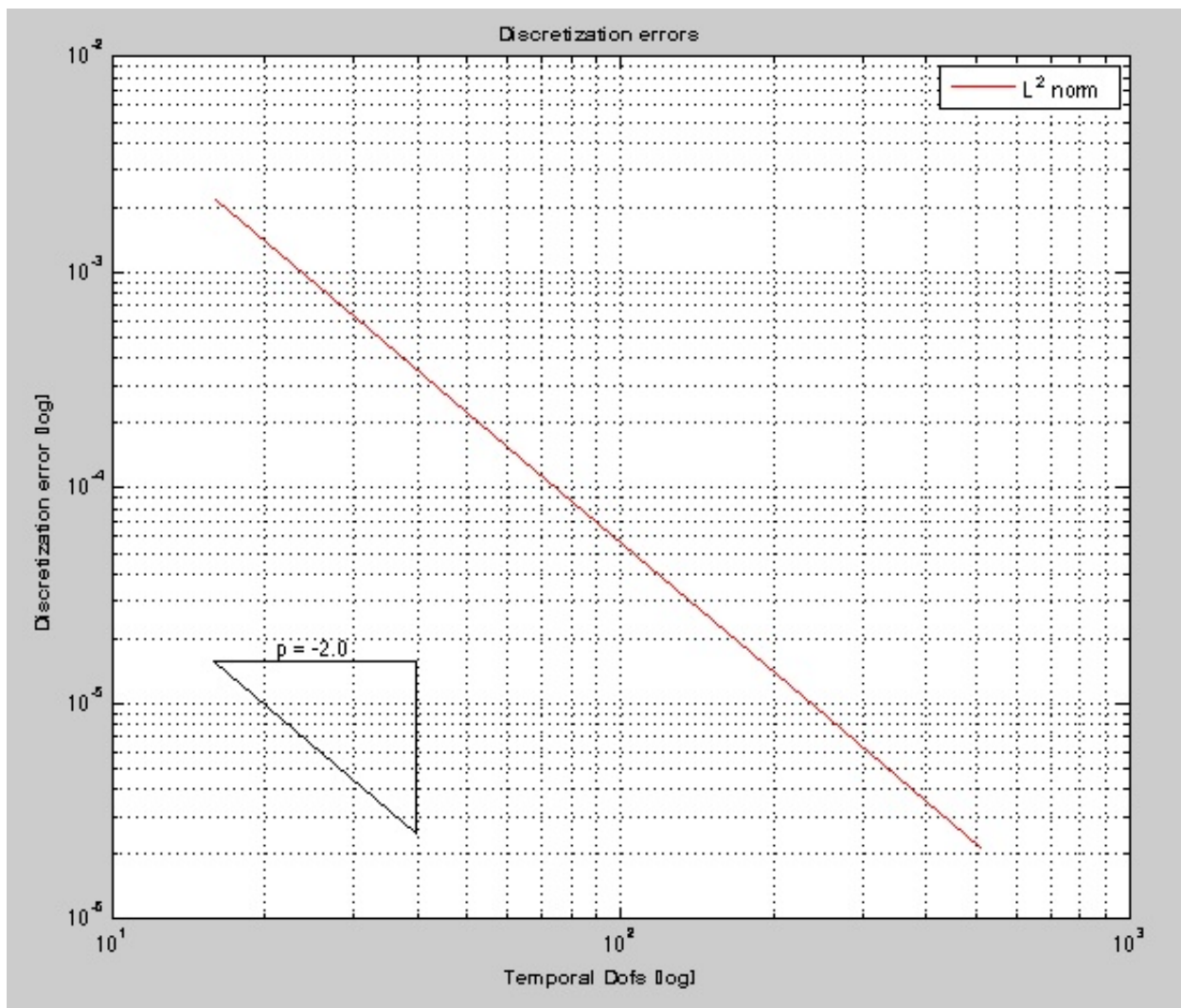


Figure 5.43: (1.2)-b - Temporal Convergence: $M = 8000$ spatial dofs, $N = 2^{4:9}$ temporal dofs (midpoint)

Function b: $f(x) = xe^{-2x}$

Weak Formulations (1.2)

Midpoint Rule:

See figure 5.43.

Spatial dofs: $M = 8000$

Temporal dofs: $N = 2^{4:9}$

Result:

Convergence rate: 2

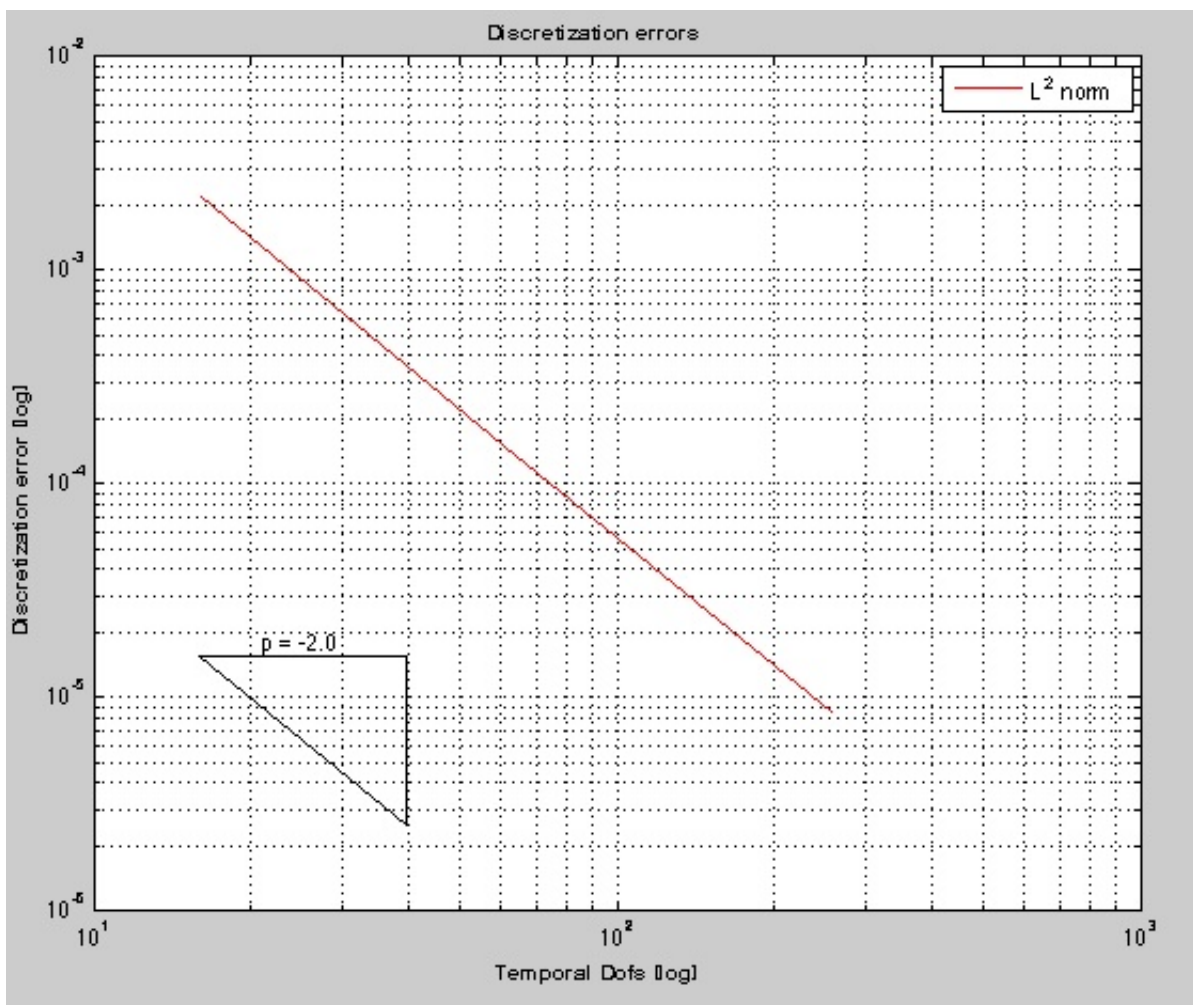


Figure 5.44: (1.3)-b - Temporal Convergence: $M = 10000$ spatial dofs, $N = 2^{4:8}$ temporal dofs (midpoint)

Weak Formulations (1.3)

Midpoint Rule:

See figure 5.44.

Spatial dofs: $M = 10000$

Temporal dofs: $N = 2^{4:8}$

Result:

Convergence rate: 2

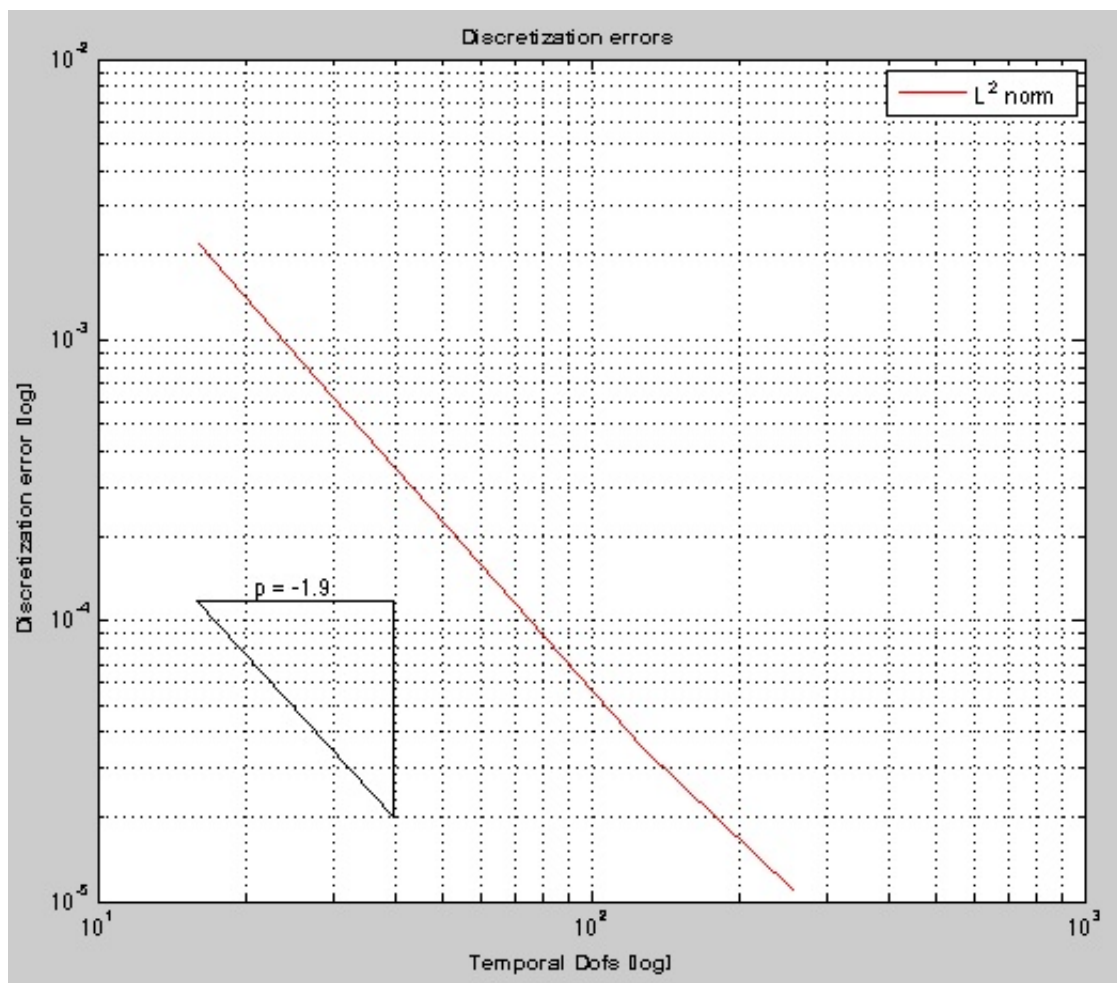


Figure 5.45: (1.4)-b - Temporal Convergence: $M = 10000$ spatial dofs, $N = 2^{4:8}$ temporal dofs (midpoint)

Weak Formulations (1.4)

Midpoint Rule:

See figure 5.45.

Spatial dofs: $M = 10000$

Temporal dofs: $N = 2^{4:8}$

Result:

Convergence rate: $1.9 \rightarrow 2$

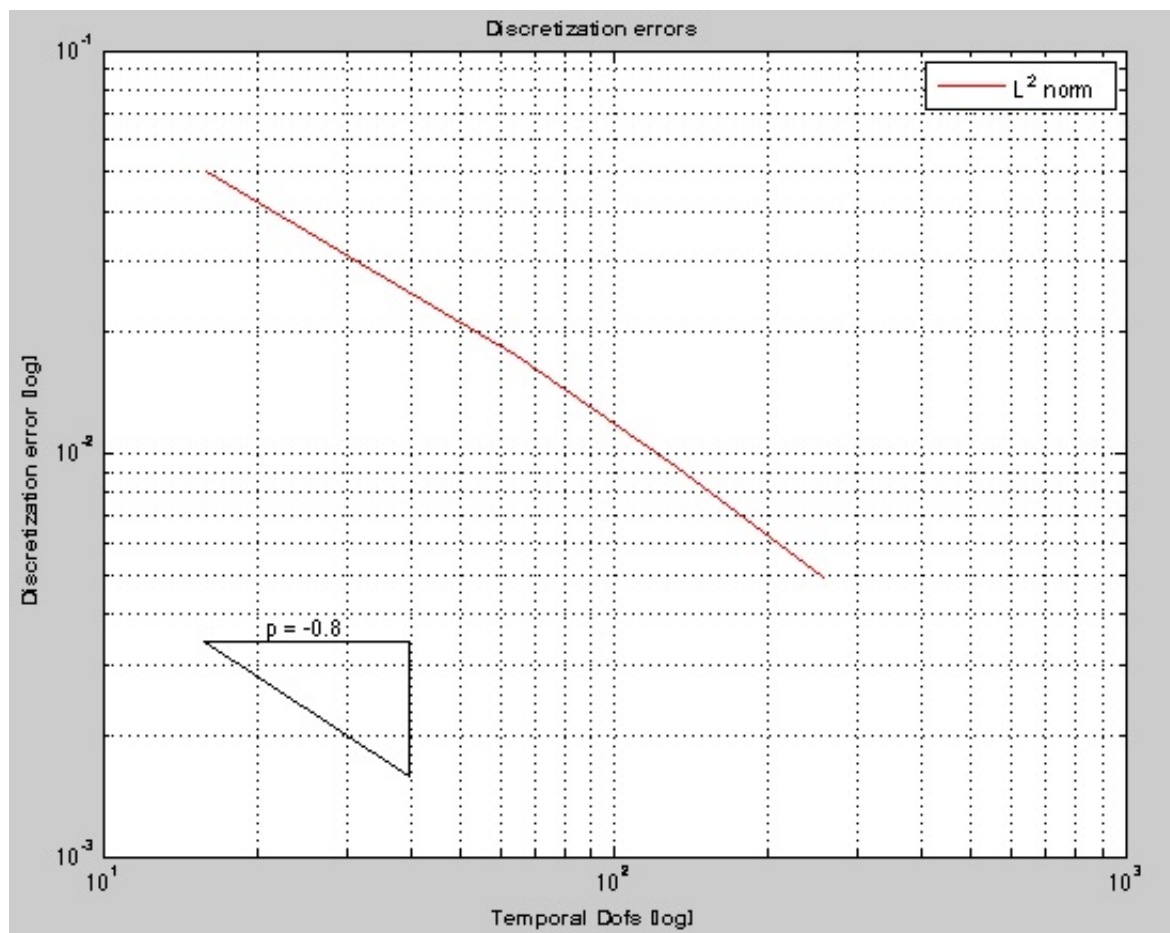


Figure 5.46: (1.2)-c - Temporal Convergence: $M = 10000$ spatial dofs, $N = 2^{3:8}$ temporal dofs (midpoint)

Function c: $f(x, t) = xe^{-tx}$

Weak Formulations (1.2)

Midpoint Rule:

See figure 5.46.

Spatial dofs: $M = 10000$

Temporal dofs: $N = 2^{4:9}$

Result:

Convergence rate: $0.8 \rightarrow 1$

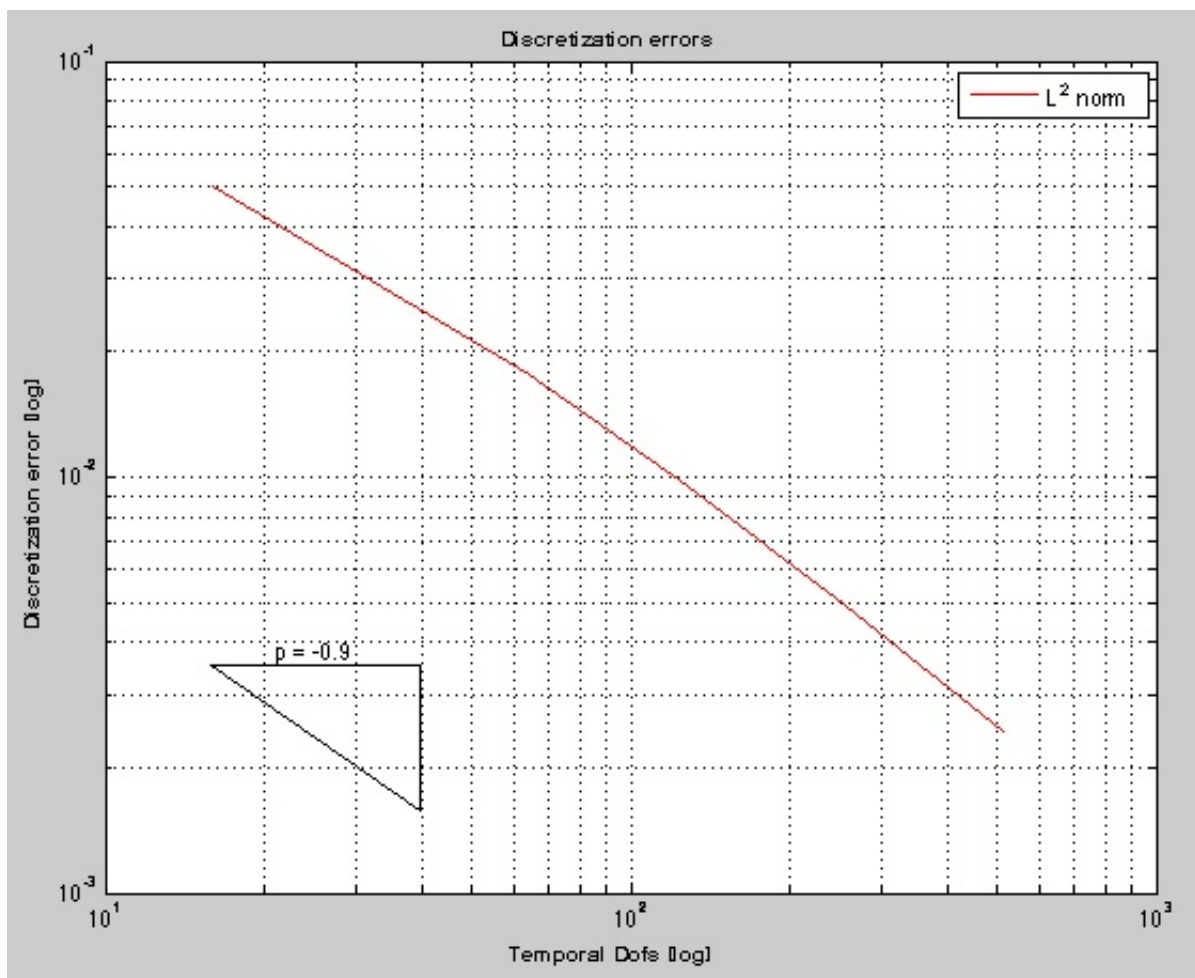


Figure 5.47: (1.3)-c - Temporal Convergence: $M = 8000$ spatial dofs, $N = 2^{4:9}$ temporal dofs (midpoint)

Weak Formulations (1.3)

Midpoint Rule:

See figure 5.47.

Spatial dofs: $M = 8000$

Temporal dofs: $N = 2^{4:9}$

Result:

Convergence rate: $0.9 \rightarrow 1$

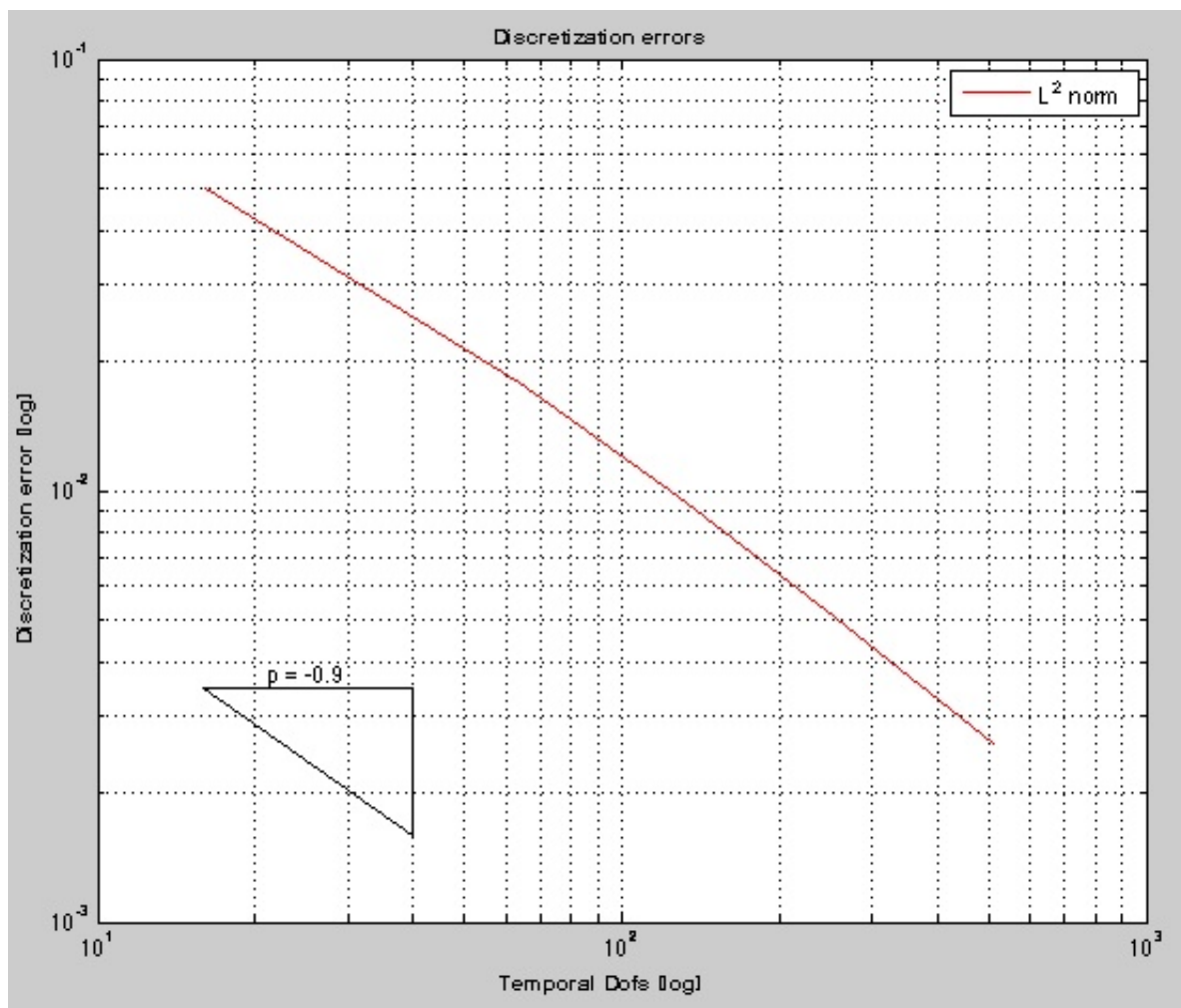


Figure 5.48: (1.4)-c - Temporal Convergence: $M = 8000$ spatial dofs, $N = 2^{4.9}$ temporal dofs (midpoint)

Weak Formulations (1.4)

Midpoint Rule:

See figure 5.48.

Spatial dofs: $M = 8000$

Temporal dofs: $N = 2^{4.9}$

Result:

Convergence rate: $0.9 \rightarrow 1$

5.2.4 Conclusions

The convergence rates do not depend on the timestepping schemes very much. For the weak formulation (1.2) there is no theory about convergence, the discretized solution converges faster than with the other two weak formulations in terms of spatial degrees of freedom. For the spatial convergence in weak formulations (1.3) and (1.4), the theory says, that it should be 1 and for the temporal convergence that the convergence should be 2. We got all the expected values, except for the function c , where we got 1 for the temporal convergence instead of the expected value 2.

Chapter 6

Summary

In this term project the "Linear Dirac Equations in 1D" were examined. We tested it on three different functions and weak formulations. We showed that the total charge stays constant over the time for the midpoint rule (implicit), for the explicit leapfrog timestepping the total charge fluctuates around a constant value over the time. We found out that the convergence rates are better for the weak formulation (1.2) than for the other ones. For weak formulations (1.3) and (1.4) we got the expected convergence rates 1 in terms of spatial convergence and 2 in terms of temporal convergence. The exception was only in the function c) for the temporal convergence, there we got the rate 1.

Appendix A

References

1. P. DEUFLHARD and F. BORNEMANN, Numerische Mathematik II, DeGruyter, Berlin, 2 ed., 2002.
2. R. HIPTMAIR, Numerics of hyperbolic partial differential equations. Online lecture notes, 2007.
http://www.sam.math.ethz.ch/hiptmair/tmp/NUMHYP_07.pdf

Appendix B

Source Code Descriptions

B.1 Time-Independent Problem

The function a: $f \equiv 1$ and b: $f(x) = x e^{-2x}$ are time-independent functions and so the whole problem to it gets for all three weak formulations time-independent.

add_Slope

function [] = add_Slope(axes_handle, loc, rate)

ADD_SLOPE(AXES_HANDLE, LOC, RATE) adds a slope triangle with convergence rate P at the location LOC to the plot specified by AXES_HANDLE.

assemLoad_1D_u

function L = assemLoad_1D_u(Coordinates, EHandle, varargin)

L = ASSEMLOAD_1D_U(COORDINATES, EHANDLE) assembles the global load vector U from the local element contributions given by the function handle EHANDLE.

assemLoad_1D_v

function L = assemLoad_1D_v(Coordinates, EHandle, varargin)

L = ASSEMLOAD_1D_V(COORDINATES, EHANDLE) assembles the global load vector V from the local element contributions given by the function handle EHANDLE.

assemMat_1D_A

function A = assemMat_1D_A(Coordinates, EHandle, varargin)

A = ASSEMMAT_1D_A(COORDINATES, EHANDLE) assembles the global matrix A from the local element contributions given by the function handle EHANDLE.

assemMat_1D_B

function A = assemMat_1D_B(Coordinates, EHandle, varargin)

A = ASSEMMAT_1D_B(COORDINATES, EHANDLE) assembles the global matrix B from the local element contributions given by the function handle EHANDLE.

assemMat_1D_CE

function A = assemMat_1D_CE(Coordinates, EHandle, varargin)

A = ASSEMMAT_1D_CE(COORDINATES, EHANDLE) assembles the global matrix CE from the local element contributions given by the function handle EHANDLE.

assemMat_1D_DF

function A = assemMat_1D_DF(Coordinates, EHandle, varargin)

A = ASSEMMAT_1D_DF(COORDINATES, EHANDLE, H, QUADRULE, FHANDLE, GHANDLE) assembles the global matrix DF from the local element contributions given by the function handle EHANDLE.

constant_1D

function shap = constant_1d(x)

SHAP = CONSTANT_1D(X) computes the values of the shape functions for constant finite elements at the quadrature points X.

euler

function [x_new,Q] = euler(x_old, A_glo, M_glo, tau, NSTEPS, n, varargin)

[x_new,Q] = EULER(X_OLD, A_GLO, M_GLO, TAU, NSTEPS, N) solves the time-independent problem with the explicit euler timestepping scheme and computes the total charge Q for every time point.

gauleg

function QuadRule = gauleg(a, b, n, tol)

QUADRULE = GAULEG(A, B, N, TOL) computes the N-point Gauss-Legendre quadrature rule on the interval [A,B] up to the prescribed tolerance TOL. If no tolerance is prescribed GAULEG uses the machine precision EPS.

global_idx

function k = global_idx(n, loc)

k = GLOBAL_IDX(N, LOC) computes the entry of a local matrix into the global matrix.

grad_constant_1d

function grad_shap = grad_constant_1d(x)

GRAD_SHAP = GRAD_CONSTANT_1D(X) computes the values of the derivatives of the shape functions for constant finite elements.

grad_hat_1d

function grad_shap = grad_hat_1d(x)

GRAD_SHAP = GRAD_HAT_1D(X) computes the values of the derivatives of the shape functions for linear finite elements.

hat_1d

function shap = hat_1d(x)

SHAP = HAT_1D(X) computes the values of the shape functions for linear finite elements at the quadrature points X.

L2Err_uv

function err = L2Err_uv(Vertices, u_fem, v_fem, QuadRule, varargin)

ERR = L2ERR_UV(VERTICES, U_FEM, V_FEM, QUADRULE) computes the discretization error between the reference solution and the finite element solution U_FEM and V_FEM.

leap_frog

function [x_new,Q] = leap_frog(x_old, A_glo, M_glo, A, B, CE, DF, tau, NSTEPS, varargin)

[x_new, Q] = LEAP_FROG(X_OLD, A_GLO, M_GLO, A, B, CE, DF, TAU, NSTEPS) solves the time-independent problem with the explicit leapfrog timestepping scheme and computes the total charge for every time point. The initial values are computed with the explicit euler scheme.

main_Dirac_cha_leap

Computes and plots the total charge for Linear Dirac Equations in 1d with the explicit leapfrog scheme.

main_Dirac_cha_mid

Computes and plots the total charge for Linear Dirac Equations in 1d with the implicit midpoint rule.

main_Dirac_spa_leap

Computes and plots the spatial convergence rates for Linear Dirac Equations in 1d with the explicit leapfrog scheme.

main_Dirac_spa_mid

Computes and plots the spatial convergence rates for Linear Dirac Equations in 1d with the implicit midpoint rule.

main_Dirac_tmp_mid

Computes and plots the temporal convergence rates for Linear Dirac Equations in 1d with the implicit midpoint rule

MASS_Dirac_A

function MlocA = MASS_Dirac_A(Vertices, QuadRule, varargin)

MLOCA = MASS_DIRAC_A(VERTICES, QUADRULE) computes the element mass ma-

trix using linear finite elements.

MASS_Dirac_B

function MlocB = MASS_Dirac_B(Vertices, QuadRule, varargin)

MLOCB = MASS_DIRAC_B(VERTICES, QUADRULE) computes the element mass matrix using linear finite elements.

midpoint_rule

function [x_new,Q] = midpoint_rule(x_old, A, M, tau, NSTEPS, varargin)

[x_new, Q] = MIDPOINT_RULE(x_old, A, M, tau, NSTEPS) solves the time-independent problem with the implicit midpoint rule scheme and computes the total charge for every time point.

progress_bar

function [] = progress_bar(i)

PROGRESS_BAR(PER) displays the progress percentage PER as a progress bar inside the command window.

STIMA_Dirac_CE

function AlocCE = STIMA_Dirac_CE(Vertices, QuadRule, FHandle, GFHandle, varargin)

ALOCCE = STIMA_DIRAC_CE(VERTICES, QUADRULE, FVAL, GFVAL) computes the element stiffness matrix using linear finite elements.

STIMA_Dirac_DF

function AlocDF = STIMA_Dirac_DF(Vertices, QuadRule, FHandle, GFHandle, varargin)

ALOCDF = STIMA_DIRAC_DF(VERTICES, QUADRULE, FVAL, GFVAL) computes the element stiffness matrix using linear finite elements.

u_init

function u0 = u_init(x,varargin)

U0 = U_INIT(X) computes the function $u(x) = 1 - \cos((2 * \pi) * x)^2$.

v_init

function v0 = v_init(x,varargin)

V0 = V_INIT(X) computes the function $v(x) = \sin(\pi * x)$.

B.2 Time-Dependent Problem

The function $c: f(x, t) = x e^{-tx}$ is a time-dependent function and so the whole problem to it gets for all three weak formulations time-dependent. This induces changes in the timestepping methods.

add_Slope

See above.

assemLoad_1D_u

See above.

assemLoad_1D_v

See above.

assemMat_1D_A

function [A_row,A_col,A_val,sA] = assemMat_1D_A(Coordinates, EHandle, h, QuadRule, varargin)

[A_row, A_col, A_val, sA] = ASSEMMAT_1D_A(COORDINATES, EHANDLE, H, QUADRULE) assembles the global matrix A from the local element contributions given by the function handle EHANDLE and returns the matrix in a sparse representation.

assemMat_1D_B

function [A_row,A_col,A_val] = assemMat_1D_B(Coordinates,EHandle,h,QuadRule,varargin)
[A_row, A_col, A_val] = ASSEMMAT_1D_B(COORDINATES, EHANDLE, H, QUADRULE) assembles the global matrix B from the local element contributions given by the function handle EHANDLE and returns the matrix in a sparse representation.

assemMat_1D_CE

function [A_row,A_col,A_val,sCE] = assemMat_1D_CE(Coordinates, EHandle, h, QuadRule, FHandle, GFHandle, varargin)
[A_row, A_col, A_val, sCE] = ASSEMMAT_1D_CE(COORDINATES, EHANDLE, H, QUADRULE, FHANDLE, GHANDLE) assembles the global matrix CE from the local element contributions given by the function handle EHANDLE and returns the matrix in a sparse representation.

assemMat_1D_DF

function [A_row,A_col,A_val, sDF] = assemMat_1D_DF(Coordinates, EHandle, h, QuadRule, FHandle, GFHandle, varargin)
[A_row, A_col, A_val, sDF]= ASSEMMAT_1D_DF(COORDINATES, EHANDLE, H, QUADRULE, FHANDLE, GHANDLE) assembles the global matrix DF from the local element contributions given by the function handle EHANDLE and returns the matrix in a sparse representation.

constant_1D

See above.

euler_time

function [x_new,Q] = euler_time(Coordinates, x_old, A_glo, M_glo, tau, NSTEPS, h, QuadRule, n, Fu, GF, varargin)
[x_new, Q] = EULER_TIME(COORDINATES, X_OLD, A_GLO, M_GLO, TAU, NSTEPS, H, QUADRULE, N, FU, GF) solves the time-dependent problem with the explicit euler timestepping scheme and computes the total charge for every time point.

gauleg

See above.

grad_constant_1d

See above.

grad_hat_1d

See above.

hat_1d

See above.

L2Err_uv

See above.

leap_frog_time

function [x_new,Q] = leap_frog_time(Coordinates, x_old, A_glo, M_glo, A, B, CE, DF, tau, NSTEPS, h, QuadRule, Fu, GF, varargin)

[x_new,Q] = LEAP_FROG_TIME(COORDINATES, X_OLD, A_GLO, M_GLO, A, B, CE, DF, TAU, NSTEPS, H, QUADRULE, FU, GF) solves the time-dependent problem with the explicit leapfrog timestepping scheme and computes the total charge for every time point. The initial value are computed with the explicit euler scheme.

main_Dirac_cha_leap

See above.

main_Dirac_cha_mid

See above.

main_Dirac_spa_leap

See above.

main_Dirac_spa_mid

See above.

main_Dirac_tmp_mid

See above.

MASS_Dirac_A

function MlocA = MASS_Dirac_A(h, N, QuadRule, varargin)

MLOCA = MASS_DIRAC_A(H, N, QUADRULE) computes the element mass matrix using linear finite elements.

MASS_Dirac_B

function MlocB = MASS_Dirac_B(h, S, QuadRule, varargin)

MLOCB = MASS_DIRAC_B(H, S, QUADRULE) computes the element mass matrix using linear finite elements.

midpoint_rule_time

function [x_new,Q] = midpoint_rule_time(Coordinates, x_old, A_glo, M_glo, tau, h, QuadRule, NSTEPS, Fu, GF, varargin)

[x_new,Q] = MIDPOINT_RULE_TIME(COORDINATES, X_OLD, A_GLO, M_GLO, TAU, H, QUADRULE, NSTEPS, Fu, GF) solves the time-dependent problem with the implicit midpoint rule scheme and computes the total charge for every time point.

progress_bar

See above.

STIMA_Dirac_CE

function AlocCE = STIMA_Dirac_CE(S, gS, h, QuadRule, FVal, GFVal, varargin)

ALOCCE = STIMA_DIRAC_CE(S, gS, H, QUADRULE, FVAL, GFVAL) computes the element stiffness matrix using linear finite elements.

STIMA_Dirac_DF

function AlocDF = STIMA_Dirac_DF(N, gN, h, QuadRule, FVal, GFVal, varargin)

ALOCDF = STIMA_DIRAC_DF(N, gN, H, QUADRULE, FVAL, GFVAL) computes the element stiffness matrix using linear finite elements.

u_init

See above.

v_init

See above.