Term Project
(Mathematics, Computational Science & Engineering)

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Discretization of Linear Dirac Equations in 1D

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 $\mathbf{u} = \mathbf{u}(\boldsymbol{x}, t)$. $v = (v(\boldsymbol{x}, t))$ such that

$$\begin{aligned} \partial_t \mathbf{u} &= -if\,\mathbf{grad}\,v - \tfrac{i}{2}\,\mathbf{grad}\,f\,v\,, \\ \partial_t v &= if\,\mathrm{div}\,\mathbf{u} + \tfrac{i}{2}\,\mathbf{grad}\,f\cdot\mathbf{u}\,, \end{aligned} \quad \text{in } [0,T]\times\Omega\,,$$
$$v = 0 \quad \text{on } [0,T]\times\partial\Omega\,,$$
$$\mathbf{u}(\boldsymbol{x},0) = \mathbf{u}_0(\boldsymbol{x}) \quad , \quad v(\boldsymbol{x},0) = v_0(\boldsymbol{x})\,. \tag{1}$$

2 Weak Forms

- We may just test the two equation in (1) and integrate over Ω: seek $\mathbf{u} = \mathbf{u}(t, \mathbf{x})$. $v = (v(t, \mathbf{x}))$ such that

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

  where $(u,v)_0 := \int_\Omega u\bar{v}\,\mathrm{d}\mathbf{x}$.

- 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

$$\begin{aligned} (\partial_t \mathbf{u}, \mathbf{q})_0 &= \left(-if\,\mathbf{grad}\,v - \tfrac{i}{2}\,\mathbf{grad}\,f\,v, \mathbf{q}\right)_0 \quad \forall \mathbf{q} \in (L^2(\Omega))^d\,, \\ (\partial_t v, w)_0 &= -\frac{i}{2}\left(\mathbf{u}\cdot\mathbf{grad}\,f, w\right)_0 - i\int_\Omega f\mathbf{u}\cdot\mathbf{grad}\,\overline{w}\,\mathrm{d}\boldsymbol{x} \quad \forall w \in H_0^1(\Omega)\,. \end{aligned} \tag{3}$$

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

$$\begin{aligned} (\partial_t \mathbf{u}, \mathbf{q})_0 &= \int_\Omega \tfrac{i}{2}\,\mathbf{grad}\,f\cdot\mathbf{q}\,v + ivf\,\mathrm{div}\,\mathbf{q}\,\mathrm{d}\boldsymbol{x} \quad \forall \mathbf{q} \in \boldsymbol{H}(\mathrm{div}, \Omega)\,, \\ (\partial_t v, w)_0 &= \left(if\,\mathrm{div}\,\mathbf{u} + \tfrac{i}{2}\,\mathbf{grad}\,f\cdot\mathbf{u}, w\right)_0 \quad \forall w \in L^2(\Omega)\,. \end{aligned} \tag{4}$$

3 Conservation property

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

$$Q(t) := \int_{\Omega} |\mathbf{u}|^2 + |v|^2 \,\mathrm{d}\boldsymbol{x} \; . \tag{5}$$

4 Galerkin discretization

The variational formulations (2)- (4) allow a straightforward Galerkin discretization: We equip Ω with some mesh and choose $\boldsymbol{\mathcal{V}}$ and $\mathcal{W}$ as finite element subspaces of $L^2(\Omega)$, $\boldsymbol{H}(\mathrm{div},\Omega)$ and $H_0^1(\Omega)$, respectively. The simplest choice in 1D is piecewise linear/piecewise constant functions on some (non necessarily uniform) grid.

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

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

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

$$\frac{y^{k+1} - y^k}{\tau} = \mathbf{A}(t^k + \tfrac{1}{2}\tau)\left(\frac{y^{k+1} + y^k}{2}\right) \; . \tag{6}$$

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 $\langle \cdot, \cdot \rangle$, (6) involves

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

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

$$\|y(t)\| = \left\|y(t^0)\right\| \quad \forall t \; . \tag{7}$$

Then

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\|y(t)\|^2 = 2\,\mathrm{Re}\,\langle y(t), \mathbf{A}(t)y(t)\rangle \quad \forall t \; . \tag{8}$$

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

Apply these considerations to (2)-(4) with $y = \binom{\mathbf{u}}{v}$ and inner product $(\cdot,\cdot)_0$.

We also observe that for constant f (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].

6 Task

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

   Discretize the initial value problem based on (2)-(4) on an equidistant spatial mesh and lowest order finite elements. Timestepping should be done using the implicit midpoint rule (see Sect. 5) or an explicit leapfrog-type scheme (optional).
3. Investigate the convergence of the methods in terms of spatial and temporal resulution (meshwidth and timestep).

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References

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