A New Finite Volume Scheme for a Linear Schrödinger Evolution Equation

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Aim

The aim of the present contribution is to deal with some error estimates of an implicit finite volume scheme of a linear Schrödinger evolution equation with a time dependent potential in several space dimension on a general class of meshes has been recently used to approximate stationary equations.

Overview : References based on...

- Akrivis, G. D. , Dougalis, V. A.: On a class of conservative, highly accurate Galerkin methods for the Schrödinger equation. RAIRO, 25 /6, 643–670 (1991).
- Bradji, A. , Fuhrmann, J.: Some abstract error estimates of a finite volume scheme for a nonstationary heat equation on general nonconforming multidimensional spatial meshes. Applications of Mathematics, Praha, 58/1, 1–38, 2013.

Overview : References based on...(Suite)

- Eymard, R., Gallouët, T., Herbin, R.: Discretization of heterogeneous and anisotropic diffusion problems on general nonconforming meshes SUSHI. IMA J. Numer. Anal. 30/4, 1009–1043 (2010).
- Koprucki, T., Eymard, R., Fuhrmann, J.: Convergence of a finite volume scheme to the eigenvalues of a Schrödinger operator. WIAS-Preprint 1260 (2007).

Plan of the presentation

1. Motivation and statement of previous results
2. Problem to be discretized
3. Our main result
    1. Statement of the present result
    2. What advantages of our present contribution?
    3. Some idea on the proof of the present result
4. Some numerical tests
5. Conclusion and some perspectives

Linear Schrödinger evolution equation

We seek a complex valued function u defined on $\Omega \times [0, T]$ satisfying, for $(x, t) \in \Omega \times (0, T)$

$$i\, u_t(x, t) + \Delta u(x, t) - V(x, t) u(x, t) = f(x, t), \tag{1}$$

where Ω is an open bounded polyhedral subset in $\mathbb{R}^d$, with $d \in \mathbb{N} \setminus \{0\}$, $T > 0$, $i = \sqrt{-1}$, V is a time dependent potential, and f is a given function. Initial and homogeneous Dirichlet boundary conditions are given by:

$$u(x, 0) = u^0(x), \;\; x \in \Omega, \tag{2}$$

$$u(x, t) = 0, \;\; (x, t) \in \partial\Omega \times (0, T). \tag{3}$$

About Schrödinger equation?

1. (some physics): The form (1)–(3) of Schrödinger equation occurs, for example, when $d = 1$ in underwater acoustics,...
   The Schrödinger equation is also the fundamental equation of quantum mechanics.
2. (existence and uniqueness): existence and uniqueness can be found for instance in the book of "C. Sulem and P. L. Sulem (1999): The Nonlinear Schrödinger Equation. Self-focusing and wave collapse. Applied Mathematical Sciences. 139. New York, NY: Springer. equation."

Some literature

- The model of (1)–(3) is studied for instance in Akrivis and Dougalis (1991) when a Galerkin finite element method is used as discretization in space.
- The stationary case of Schrödinger equation is also considered using finite volume methods in Koprucki et *al.* (2007) where there are some interesting numerical tests

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Some facts to be taken in consideration to get a discretization scheme for the problem

- The exact solution is not a real valued function but a complex valued function. So, the discrete space and their norms should be slightly modified.
- Be Careful: Even the formulation of the Schrödiger equation is similar to the one Heat but the convergence results for the Schödinger equation are different from those of the Heat equation, e.g. the explicit finite scheme for the Heat equation is conditionally convergent but the corresponding scheme for the Schrödiger equation is not convergent

Some facts to be taken in consideration to get a discretization scheme for the problem (suite)

- The presence of a time dependent potential makes the techniques of previous work (Bradji and Fuhrmann, Applications of Mathematics, 2013) be not applied directly.

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A new finite volume mesh: any space dimension and orthogonality property is not required

A new mesh recently used in the following reference which deals with stationary equation:

1. Eymard, R., Gallouët, T., Herbin, R.: Discretization of heterogeneous and anisotropic diffusion problems on general nonconforming meshes. IMA J. Numer. Anal. 30/4, 1009–1043 (2010).

Some advantages of the new mesh

Advantages of this new spatial mesh

1. (mesh defined at any space dimension): $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$
2. (othogonality property is not required): the othogonality property is not required in this new mesh. But, additional discrete unknowns are required.
3. (convexity): the classical admissible mesh should satisfy that the control volumes are convexe, whereas the convexity property is not required in this new mesh.

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Figure for the mesh

Definition (New mesh of Eymard et *al.*(2010))

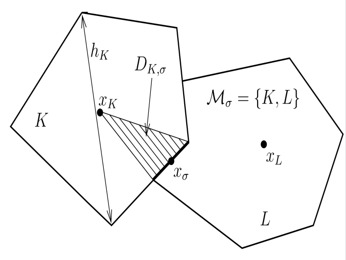

Figure: Notations for two neighbouring control volumes in $d = 2$

Discretization of the domain Ω and time interval $(0, T)$

Discretization is performed as:

1. Spatial domain $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$, is discretized using the new class of meshes.
2. The time interval $(0, T)$ constant step $k = T/(N+1)$, $N \in \mathbb{N}$.

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Principles of our scheme

Principles of our scheme

1. discretization of Schrödinger equation: the discretization of $i\,u_t + \Delta u - Vu = f$ stems from weak formulation (like in finite element method), for all $v \in H_0^1(\Omega)$

$$i\int_\Omega u_t(x,t)v(x)dx + \int_\Omega \nabla u(x,t)\cdot\nabla v(x)dx - \int_\Omega u(x,t)V(x,t)v(x)dx = \int_\Omega f(x,t)v(x)dx. \qquad (4)$$

2. (discretization of initial condition $u(x,0) = u^0(x)$): will be given later

Discretization of the equation $i\, u_t + \Delta u - Vu = f$

Recall $i \int_\Omega u_t(x,t) v(x) dx - \int_\Omega \nabla u(x,t) \cdot \nabla v(x) dx - \int_\Omega u(x,t) V(x,t) v(x) dx = \int_\Omega f(x,t) v(x) dx$, for all $v \in H_0^1(\Omega)$

1. (Discrete unknowns): the space of solution as well as the space of test functions are in

$$\mathcal{X}_{\mathcal{D},0} = \left\{ \left((v_K)_{K\in\mathcal{M}}, (v_\sigma)_{\sigma\in\mathcal{E}} \right), \; v_K, v_\sigma \in \mathbb{C}, \; v_\sigma = 0, \forall \sigma \in \mathcal{E}_{\text{ext}} \right\}$$

2. (discretization of the gradient): the discretization of ∇ can be performed using a stabilized discrete gradient denoted by $\nabla_{\mathcal{D}}$, see EGH (IMAJNA).

Discretization of $i\, u_t + \Delta u - Vu = f$ (suite)

Recall $i \int_\Omega u_t(x,t) v(x) dx - \int_\Omega \nabla u(x,t) \cdot \nabla v(x) dx - \int_\Omega u(x,t) V(x,t) v(x) dx = \int_\Omega f(x,t) v(x) dx$, for all $v \in H_0^1(\Omega)$.
So a discretization can be done as : For any $n \in [\![0, N]\!]$, find $u_{\mathcal{D}}^n \in \mathcal{X}_{\mathcal{D},0}$ such that, for all $v \in \mathcal{X}_{\mathcal{D},0}$

$$i \left(\partial^1 \Pi_{\mathcal{M}} u_{\mathcal{D}}^{n+1}, \Pi_{\mathcal{M}} v \right)_{\mathbb{L}^2} + \left(\nabla_{\mathcal{D}} u_{\mathcal{D}}^{n+1}, \nabla_{\mathcal{D}} v \right)_{(\mathbb{L}^2)^d} - \left(V(t_{n+1}) \Pi_{\mathcal{M}} u_{\mathcal{D}}^{n+1}, \Pi_{\mathcal{M}} v \right)_{\mathbb{L}^2} = \left(\frac{1}{k} \int_{t_n}^{t_{n+1}} f(t) dt, \Pi_{\mathcal{M}} v \right)_{\mathbb{L}^2}.$$

Discretization boundary condition and initial condition

- (discretization of initial condition $u(x,0) = u^0(x)$): as follows (it is discrete projection for u^0): find $u^0_{\mathcal{D}} \in \mathcal{X}_{\mathcal{D},0}$ such that

$$\left(\nabla_{\mathcal{D}} u^0_{\mathcal{D}}, \nabla_{\mathcal{D}} v\right)_{(\mathbb{L}^2)^d} + \left(V(0)\Pi_{\mathcal{M}} u^0_{\mathcal{D}}, \Pi_{\mathcal{M}} v\right)_{\mathbb{L}^2} = \left(-\Delta u^0 + V(0)u^0, \Pi_{\mathcal{M}} v\right)_{\mathbb{L}^2}, \quad \forall v \in \mathcal{X}_{\mathcal{D},0}, \tag{5}$$

where

$$\partial^1 v^n = \frac{v^n - v^{n-1}}{k}$$

Remark on the discretization of the initial condition

1. The discretization of initial condition $u(x, 0) = u^0(x)$ can be also performed as

$$u_K^0 = u^0(x_K), \; \forall K, \tag{6}$$

but this choice seems not optimal in the point of view of the error estimate.

2. The choice used in our contribution is based on some kind of a discrete orthogonal projection.

A main result: error estimates

Theorem

For each $n \in [\![0, N+1]\!]$, *let us define the error* $e_{\mathcal{M}}^n \in H_{\mathcal{M}}(\Omega)$ *by:*

$$e_{\mathcal{M}}^n = \mathcal{P}_{\mathcal{M}}\, u(\cdot, t_n) - \Pi_{\mathcal{M}}\, u_{\mathcal{D}}^n. \tag{7}$$

Then, the following error estimates hold

- *discrete* $\mathbb{L}^\infty(0, T; H_0^1(\Omega))$*–estimate: for all* $n \in [\![0, N+1]\!]$

$$\| e_{\mathcal{M}}^n \|_{1,2,\mathcal{M}} \le C(h_{\mathcal{D}} + k) \| u \|_{\mathcal{C}^2([0,T];\mathcal{C}^2(\overline{\Omega}))}. \tag{8}$$

A main result: error estimates (Suite)

Theorem

- $\mathcal{W}^{1,\infty}(0,T;\mathbb{L}^2(\Omega))$*–estimate: for all* $n \in [\![1, N+1]\!]$

$$\| \partial^1 e^n_{\mathcal{M}} \|_{\mathbb{L}^2(\Omega)} \le C(h_{\mathcal{D}} + k) \| u \|_{\mathcal{C}^2([0,T];\mathcal{C}^2(\overline{\Omega}))}. \tag{9}$$

- *error estimate in the gradient approximation: for all* $n \in [\![0, N+1]\!]$

$$\| \nabla_{\mathcal{D}} u^n_{\mathcal{D}} - \nabla u(\cdot, t_n) \|_{\left(\mathbb{L}^2(\Omega)\right)^d} \le C(h_{\mathcal{D}} + k) \| u \|_{\mathcal{C}^2([0,T];\mathcal{C}^2(\overline{\Omega}))}. \tag{10}$$

Theorem is useful

1. Estimate (9) allows us to approximate (the time derivative) $u_t(x_K, t_n)$, all K and n
2. Estimate (10) allows us to approximate the first spatial derivatives $\frac{\partial u}{\partial x_i}(x_K, t_n)$, all K and n.

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An idea on the proof

- Comparison with the scheme: for any $n \in [\![0, N+1]\!]$, find $\hat{u}^n_{\mathcal{D}} \in \mathcal{X}_{\mathcal{D},0}$ such that, for all $v \in \mathcal{X}_{\mathcal{D},0}$
$$\begin{aligned} &\langle \hat{u}^n_{\mathcal{D}}, v \rangle_F + \left(V(t_n) \Pi_{\mathcal{M}} \hat{u}^n_{\mathcal{D}}, \Pi_{\mathcal{M}} v \right)_{\mathbb{L}^2(\Omega)} \\ &= \left(-\Delta u(t_n) + V(t_n) u(t_n), \Pi_{\mathcal{M}} v \right)_{\mathbb{L}^2(\Omega)} . \end{aligned} \tag{11}$$
We will use mainly the two facts: $(\bar{u}^n_{\mathcal{D}})_{n \in [\![0, N+1]\!]}$ is an usual approximation for u (for each n, it is like an approximation of elliptic equation) and $u^0_{\mathcal{D}} = \bar{u}^0_{\mathcal{D}}$.
- An a priori estimate for the discrete problem.

Some numerical tests

We consider $\Omega = (0,1)^2$ meshed with the rectangular meshes with mesh size h. We consider $V \equiv 0$ and the exact solution is $u(x,y,t) = \frac{1}{2\pi^2}\sin(\pi x)\sin(\pi y)(1-\exp(-2i\pi^2 t))$, where $(x,y,t) \in (0,1)^2 \times (0,1)$. We take $k = h/50$ (k is the time step)

h	$\frac{\lvert \text{Error} \rvert_{L^\infty(H^1)}}{k+h}$	$\frac{\lvert \text{Error} \rvert_{W^{1,\infty}(L^2)}}{k+h}$	$\frac{\lvert \text{Gradient of Error} \rvert_{L^\infty(L^2)}}{k+h}$
1/25	0.552551471	1.8051691	0.5738725
1/30	0.560476471	1.8190118	0.5783265
1/35	0.566433824	1.8297348	0.5817892

Conclusion

We considered the linear Schrödinger evolution equation. A convergence analysis of a new finite volume scheme is provided in several discrete norms. We plan to consider:

- The case when the spatial spatial domain is not bounded.
- High order finite volume schemes for the Schrödinger evolution equation. In progress
- Nonlinear case of Schrödinger evolution equation.