Applied Mathematics Letters 110 (2020) 106576

Contents lists available at ScienceDirect

Applied Mathematics Letters

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# Supplementary variable method for structure-preserving approximations to partial differential equations with deduced equations

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A R T I C L E I N F O

*Article history:*
Received 10 April 2020
Received in revised form 7 June 2020
Accepted 7 June 2020
Available online 15 June 2020

*Keywords:*
Supplementary variable method
Structural-preserving schemes
Partial differential equations with deduced equations
Energy-production-rate preserving schemes
Finite difference methods

A B S T R A C T

We present a supplementary variable method (SVM) for developing structure-preserving numerical approximations to a partial differential equation system with deduced equations. The PDE system with deduced equations constitutes an over-determined, yet consistent and structurally unstable system of equations. We augment a proper set of supplementary variables to the over-determined system to make it well-determined with a stable structure. We then discretize the modified system to arrive at a structure-preserving numerical approximation to the over-determined PDE system. We illustrate the idea using a dissipative network generating partial differential equation model by developing an energy-dissipation-rate preserving scheme. We then simulate the network generating phenomenon using the numerical scheme. This numerical method is so general that it applies literally to any PDE systems with deduced equations.



## 1. Introduction

Many partial differential equation systems have deduced equations that have significant physical, engineering, and application significance. For example, a thermodynamically consistent partial differential equation (TCPDE) system consists of a partial differential equation system, an energy functional and a deduced time evolutional equation of the energy functional that has a negative time rate of change. The energy functional and its time evolutionary equation have a profound physical and mathematical implication to the physical process that the TCPDE describes. All the nonequilibrium thermodynamical models derived from principles of nonequilibrium thermodynamics such as the second law of thermodynamics or principles like the Onsager

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https://doi.org/10.1016/j.aml.2020.106576
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principle belong to this class of equations [1–3]. Other potential deduced equations can include conservation equations for certain invariant quantities such as mass, momentum etc.

When we augment the PDE system by including the deduced equations, the extended/augmented system is over-determined and yet consistent since the number of equations exceeds the number of unknowns. A structure-preserving approximation to the extended system simply means that an approximation to the PDE system is consistent with a corresponding approximation to the deduced equations. If the approximations are carried out respectively on the PDE system and its deduced equations, the chance to arrive at consistent approximations to the two sets of equations is extremely small.

Traditionally, one relies on clever techniques meticulous attentions to details to achieve the desired consistency by exploiting the structure of each individual PDE system. So, the development of structure-preserving approximation becomes highly equation-type dependent and technically challenging. In this letter, we present a new idea to achieve the structure-preserving purpose for any PDE systems with deduced equations. We augment the over-determined system with a proper set of supplementary variables to make it well-determined and structurally stable in the meantime. We note that the modified system reduces to the original one when the supplementary variables taking on certain specific values. This can be viewed as an embedding of the original dynamical system into a modified dynamical system in a higher dimensional phase space whose solution set includes the solution of the original PDE system as a subset. Since the perturbation is done in such a way that the modified system is structurally stable. This requirement ensures the solution of the supplementary variable exists near the specific values and is unique locally. We illustrate the idea using the TCPDE as an example in this letter.

Assuming the unknown variables in the TCPDE system are denoted as $\Phi \in \mathbf{R}^n$, where $n$ is the dimension of the phase space, and the free energy of the system is described by a functional $F[\Phi]$. The TCPDE system, its energy definition and the deduced energy equation are given by the following:

$$\begin{cases} \dot{\Phi} = \mathbf{M}(\Phi, \nabla\Phi, \ldots), & \text{(a)} \\ F[\Phi] = \int_\Omega f(\Phi, \nabla\Phi, \ldots)\mathrm{d}\mathbf{x}, & \text{(b)} \\ \frac{\mathrm{d}F}{\mathrm{d}t} = \int_\Omega h(\Phi, \nabla\Phi, \ldots)\mathrm{d}\mathbf{x}, & \text{(c)} \end{cases} \tag{1.1}$$

where $\mathbf{M}$ is an operator, $f$ is the free energy density and $h$ is the energy-dissipation-rate density. The consistence among the equations means that (1.1a)+(1.1b) implies (1.1c). Then, the three equations constitute an over-determined and yet consistent system of differential–integral system, where the number of unknowns are $\Phi, F$ (n+1) while the number of equations is n+2.

In general, one can only find the solution of (1.1a)–(1.1c) approximately. When one approximates (1.1a) numerically, the consistency among the equations is most likely to be broken so that the approximate solution of (1.1a) may not satisfy an approximate equation of (1.1c). This is known as structural instability conceptually. One way to deal with this is to modify or perturb the over-determined and structurally unstable equation system so that it is well-determined and structurally stable. To do so, we augment dynamical equation (1.1a) by a variable $\beta(t)$, called the supplementary variable, *without introducing any equation for it*

$$\dot{\Phi} = \mathbf{M}(\Phi, \nabla\Phi, \ldots) + \beta(t)g[\Phi], \tag{1.2}$$

where $g[\Phi]$ is a user supplied functional. The system consisting of (1.2), (1.1b) and (1.1c) is no longer over-determined, since its unknowns are now $\Phi, F, \beta$ (n+2), and it reduces to the original one when $\beta \equiv 0$. The supplementary variable not only makes the modified system well-determined, but also provides a mechanism to keep consistency of the equations in the system when they are approximated numerically, thereby, retains structural stability. This is the essence of the supplementary variable approach. It differs from the EQ and SAV strategies in that this methods do not introduce any additional equations governing the dynamics of the supplementary variable $\beta$.

If we set our goal as deriving numerical approximations to (1.2) that preserves energy-dissipation-rate, we approximate (1.1c) by a $k$th order approximation

$$F_{n+1} = F_n + \int_{\Omega} h^* \mathrm{d}\mathbf{x}, \tag{1.3}$$

where $h^*$ is an approximation to the energy dissipation rate function up to the desired accuracy and

$$F_n = \int_{\Omega} f(\Phi_n, \nabla \Phi_n, \ldots) \mathrm{d}\mathbf{x}. \tag{1.4}$$

We then approximate (1.2) using a commensurate (kth) order approximation

$$\Phi_{n+1} = \Phi_n + \Delta t(\mathbf{M}^* + \beta(t^*) g^*), \tag{1.5}$$

where $\beta(t^*), \mathbf{M}^*, g^*$ are $k$th order approximations to $\beta(t), \mathbf{M}, g$, respectively. The system consisting of (1.3), (1.4) and (1.5) has $n+2$ unknowns $(\Phi_{n+1}, \beta(t^*), F_{n+1})$ and $n+2$ equations, making it a well-determined system. If it has a solution for $\beta(t^*)$ close to 0, and the solution is unique, we obtain an approximate solution to $\Phi(t_{n+1})$. Of course, if we can show $\beta(t^*) \sim O(\Delta t^k)$ and solution $\Phi_{n+1}$ exists uniquely, we arrive at a $k$th order consistent approximation to the original TCPDE system, which preserves the energy dissipation rate at the discrete level [4,5].

Historically, there have been quite a number of methods proposed for developing energy stable algorithms for TCPDE systems. One popular one is the convex splitting technique [6,7] and another is the stabilizer technique [8,9]. In the past a few years, the energy quadratization (EQ) method and the subsequent scalar auxiliary variable (SAV) method have fueled the development for energy stable schemes [10–12]. Recently, a Lagrange multiplier method based on the SAV approach presented by Cheng, Liu and Shen [13] and a generalized SAV method proposed by Yang and Dong [14] aim at further extending the scope of searching strategies for energy stable numerical schemes. With the proper choice of discretization and the way that supplementary variables are added to the dynamical system, the SVM method recovers the Lagrange multiplier method and the generalized SAV method. Philosophically, SVM originates from a quite different perspective, where resolving system structural stability is the primary concern.

The purpose of this letter is to put the development of structure-preserving schemes in a new perspective using the concept of supplementary variable method (SVM) to shed light on the methodology for devising structure-preserving numerical approximations to any PDE systems with deduced equations. We next illustrate the SVM method using a network generating PDE system proposed and studied in [4,5,15–17].

## 2. Second order energy-dissipation-rate preserving algorithms for network generating PDEs

We briefly recall the dissipative, network-generating PDE model proposed in [4,5]. Consider a bounded domain $\Omega$ with a smooth boundary $\partial\Omega$ and a time-independent source term $S(\mathbf{x})$. Here we use $p$ to represent the scalar pressure of the fluid transported within the network and $\mathbf{m}$ for the vector-valued conductance. The dissipative network-generating PDE system given in [5,18] consists of two equations

$$\begin{cases} -\nabla \cdot \Big( (r\mathbf{I} + \mathbf{m}\mathbf{m}) \nabla p \Big) = S, & \text{(a)} \\ \mathbf{m}_t - K\Delta \mathbf{m} - a^2 (\mathbf{m} \cdot \nabla p) \nabla p + \alpha |\mathbf{m}|^{2(\gamma-1)} \mathbf{m} = 0, & \text{(b)} \end{cases} \tag{2.1}$$

subject to homogeneous Dirichlet boundary conditions for $\mathbf{m}$ and $p$ at $\partial\Omega$:

$$\mathbf{m}(t, \mathbf{x}) = 0, \quad p(t, \mathbf{x}) = 0, \quad \forall\, \mathbf{x} \in \partial\Omega, \quad t \geq 0. \tag{2.2}$$

Here the model parameters are diffusivity $K \geq 0$, $r, \gamma, \alpha > 0$, and activation parameter $a > 0$.

One deduces from model (2.1a)–(2.1b) the following energy production rate equation

$$\frac{\mathrm{d}\mathscr{E}}{\mathrm{d}t} = -(\partial_t \mathbf{m}, \partial_t \mathbf{m}) + \int_{\partial\Omega} [K\mathbf{n}\mathbf{m} : \nabla \mathbf{m}_t + a^2 \mathbf{n} \cdot (r\mathbf{I} + \mathbf{m}\mathbf{m}) \cdot \nabla p p_t] \mathrm{d}s, \tag{2.3}$$

where $(\bullet, \bullet)$ is the inner product defined in $L_2(\Omega)$ and the energy functional $\mathscr{E}$ is defined by

$$\mathscr{E} = \frac{1}{2} \int_\Omega \Big( K|\nabla \mathbf{m}|^2 + \frac{\alpha}{\gamma} |\mathbf{m}|^{2\gamma} + a^2 |\mathbf{m} \cdot \nabla p|^2 + a^2 r |\nabla p|^2 \Big) \mathrm{d}\mathbf{x} \geq 0, \tag{2.4}$$

We note that the prescribed homogeneous Dirichlet boundary conditions given in (2.2) annihilate the boundary contribution to the energy dissipation rate. In fact, the following boundary conditions all annihilate the energetic contribution from the boundary:

$$\begin{cases} p = p_0(\mathbf{x}),\ \mathbf{m} = \mathbf{m}_0(\mathbf{x}); \quad \mathbf{n} \cdot \nabla \mathbf{m}_t = 0,\ p = p_0(\mathbf{x}); \\ \mathbf{n} \cdot (r\mathbf{I} + \mathbf{m}\mathbf{m}) \cdot \nabla p = 0,\ \mathbf{m} = \mathbf{m}_0(\mathbf{x}); \quad \mathbf{n} \cdot \nabla \mathbf{m}_t = 0,\ \mathbf{n} \cdot (r\mathbf{I} + \mathbf{m}\mathbf{m}) \cdot \nabla p = 0. \end{cases} \tag{2.5}$$

Among these boundary conditions, some require additional consistency conditions. For simplicity, we adopt the following boundary conditions in this study

$$\mathbf{n} \cdot \nabla p = 0, \mathbf{m} = 0.$$

Then, the energy production rate equation reduces to

$$\frac{\mathrm{d}\mathcal{E}}{\mathrm{d}t} = -(\partial_t \mathbf{m}, \partial_t \mathbf{m}) \leq 0,$$

and the additional consistency condition is $\int_\Omega S \mathrm{d}\mathbf{x} = 0$. Under the following boundary conditions:

$$\mathbf{m} = 0,\ p = 0, \quad \text{or } \mathbf{n} \cdot \nabla p = 0,$$

we have

$$r\|\nabla p\|^2 + \|\mathbf{m} \cdot \nabla p\|^2 = (p, S).$$

Thus, the energy functional (2.4) can be written equivalently into the following form

$$\mathcal{E} = \frac{1}{2} \int_\Omega \Big( K|\nabla \mathbf{m}|^2 + \frac{\alpha}{\gamma} |\mathbf{m}|^{2\gamma} + a^2 p S \Big) \mathrm{d}\mathbf{x}, \tag{2.6}$$

In what follows, we will adopt the energy functional given in (2.6) to devise structure-preserving algorithms for this model.

We denote

$$(\bullet)^{n+\frac{1}{2}} = \frac{(\bullet)^{n+1} + (\bullet)^n}{2},\ \widetilde{(\bullet)}^{n+\frac{1}{2}} = \frac{\widetilde{(\bullet)}^{n+1} + (\bullet)^n}{2},\ \overline{(\bullet)}^{n+\frac{1}{2}} = \frac{3(\bullet)^n - (\bullet)^{n-1}}{2},\ \overline{(\bullet)}^{n+1} = 2(\bullet)^n - (\bullet)^{n-1}.$$

To derive energy-dissipation-rate preserving numerical approximations, we firstly approximate the energy-dissipation-rate equation of the system with a second order scheme as follows:

$$\begin{cases} -\nabla \cdot \Big( (r\mathbf{I} + \overline{\mathbf{m}}^{n+1} \overline{\mathbf{m}}^{n+1}) \nabla \widetilde{p}^{n+1} \Big) = S, \\ \dfrac{\widetilde{\mathbf{m}}^{n+\frac{1}{2}} - \mathbf{m}^n}{\tau/2} - K\Delta \widetilde{\mathbf{m}}^{n+\frac{1}{2}} - a^2 (\overline{\mathbf{m}}^{n+\frac{1}{2}} \cdot \nabla \widetilde{p}^{n+\frac{1}{2}}) \nabla \widetilde{p}^{n+\frac{1}{2}} + \dfrac{\alpha}{\gamma} \mathbf{h}(\overline{\mathbf{m}}^{n+\frac{1}{2}}) \widetilde{q}^{n+\frac{1}{2}} = 0, \\ \dfrac{\widetilde{q}^{n+\frac{1}{2}} - q^n}{\tau/2} = \mathbf{h}(\overline{\mathbf{m}}^{n+\frac{1}{2}}) \dfrac{\widetilde{\mathbf{m}}^{n+\frac{1}{2}} - \mathbf{m}^n}{\tau/2}. \end{cases} \tag{2.7}$$

where $\mathbf{h}(\mathbf{m}) = \gamma \|\mathbf{m}\|^{\gamma-2} \mathbf{m}$ and $q = \|\mathbf{m}\|^\gamma$. This yields a discrete energy dissipation rate approximation as follows

$$\frac{\widetilde{\mathcal{E}}^{n+1} - \mathcal{E}[p^n, \mathbf{m}^n]}{\tau} = -\Big\| \frac{\widetilde{\mathbf{m}}^{n+1} - \mathbf{m}^n}{\tau} \Big\|^2, \tag{2.8}$$

$\widetilde{\mathcal{E}}^{n+1}$ is an intermediate variable, and

$$\mathcal{E}[p^n, \mathbf{m}^n, q^n] = \frac{K}{2}\|\nabla \mathbf{m}^n\|^2 + \frac{\alpha}{2\gamma}\|q^n\|^2 + \frac{a^2}{2}(p^n, S). \tag{2.9}$$

This is a 2th order approximation to the energy-dissipation-rate equation with a truncation error in the order of $\mathcal{O}(\tau^2)$.

Secondly, we impose (2.8) as a constraint for (2.1a)–(2.1b), i.e.,

$$\mathcal{E}[p(t^{n+1}), \mathbf{m}(t^{n+1})] = \widetilde{\mathcal{E}}^{n+1}. \tag{2.10}$$

Note that system (2.1a)–(2.1b) with constraint (2.10) constitutes an over-determined system, which may not have a solution. To resolve the issue, we perturb (2.1a)–(2.1b) by a supplementary variable $\beta(t)$ as follows

$$\begin{cases} -\nabla\cdot\Big((r\mathbf{I}+\mathbf{m}\mathbf{m})\nabla p\Big) = S, \\ \mathbf{m}_t - K\Delta\mathbf{m} - a^2(\mathbf{m}\cdot\nabla p)\nabla p + \dfrac{\alpha}{\gamma}\mathbf{h}(\mathbf{m})q = \beta(t)\mathbf{f}[p,\mathbf{m},q], \end{cases} \tag{2.11}$$

where $\mathbf{f}[p, \mathbf{m}]$ is a prescribed functional. In this study, we use

$$\mathbf{f} = -K\Delta\mathbf{m}, \tag{2.12}$$

Clearly, $\beta = 0$, the system reduces to system (2.1a)–(2.1b).

Thirdly, we apply a special second-order implicit–explicit scheme in time to solve (2.11).

**Scheme 2.1.**

$$\begin{cases} -\nabla\cdot\Big((r\mathbf{I}+\overline{\mathbf{m}}^{n+1}\overline{\mathbf{m}}^{n+1})\nabla\widetilde{p}^{n+1}\Big) = S, \\ \delta_t^+\mathbf{m}^n - K\Delta\mathbf{m}^{n+\frac12} - a^2(\overline{\mathbf{m}}^{n+\frac12}\cdot\nabla\widetilde{p}^{n+\frac12})\nabla\widetilde{p}^{n+\frac12} + \dfrac{\alpha}{\gamma}\mathbf{h}(\overline{\mathbf{m}}^{n+\frac12})\widetilde{q}^{n+\frac12} = \beta^{n+\frac12}\mathbf{f}[\widetilde{p}^{n+\frac12}, \widetilde{\mathbf{m}}^{n+\frac12}], \\ q^{n+1} = \widetilde{q}^{n+1} + \tau\beta^{n+\frac12}\widetilde{q}^{n+\frac12}, \quad p^{n+1} = \widetilde{p}^{n+1} + \tau\beta^{n+\frac12}a^2 S, \\ \mathcal{E}[p^{n+1}, \mathbf{m}^{n+1}, q^{n+1}] = \widetilde{\mathcal{E}}^{n+1}, \end{cases} \tag{2.13}$$

where $\delta_t^+\mathbf{m}^n = (\mathbf{m}^{n+1} - \mathbf{m}^n)/\tau$. Next, we show how to implement Scheme 2.1 efficiently. Let

$$S_p = \tau a^2 S, \quad \boldsymbol{\omega}_{\mathbf{m}}^n = \big(1 - \frac{\tau}{2}K\Delta\big)^{-1}\big(\mathbf{f}[\widetilde{p}^{n+\frac12}, \widetilde{\mathbf{m}}^{n+\frac12}]\big), \quad \delta_q^n = \tau\widetilde{q}^{n+\frac12}.$$

Combining (2.7) and (2.13), it is easy to derive that $\mathbf{m}^{n+1} = \widetilde{\mathbf{m}}^{n+1} + \tau\beta^{n+\frac12}\boldsymbol{\omega}_{\mathbf{m}}^n$. Then, substituting the above results into (2.10) leads to

$$\mathcal{E}[\widetilde{p}^{n+1} + \beta^{n+\frac12}S_p, \widetilde{\mathbf{m}}^{n+1} + \beta^{n+\frac12}\boldsymbol{\omega}_{\mathbf{m}}^n, \widetilde{q}^{n+1} + \beta^{n+\frac12}\delta_q^n] = \widetilde{\mathcal{E}}^{n+1}.$$

This is a quadratic equation for $\beta^{n+\frac12}$ whose two roots can be expressed explicitly. One of the roots that approximates zero as $\tau \to 0$ is what we need. After obtaining $\beta^{n+\frac12}$, we update $p^{n+1}$ and $\mathbf{m}^{n+1}$. The solvability and uniqueness condition of the solution is given by

$$\left(\frac{\delta\mathcal{E}}{\delta p}, S_p\right) + \left(\frac{\delta\mathcal{E}}{\delta\mathbf{m}}, \boldsymbol{\omega}_{\mathbf{m}}^n\right) + \left(\frac{\delta\mathcal{E}}{\delta q}, \delta_q^n\right) \neq 0. \tag{2.14}$$

The semi-discrete Scheme 2.1 is further discretized in space via a second order finite-difference method on staggered grids. For more details of the spacial discretization on staggered grids, please refer to some existing literatures [19–21]. For simplicity, the resulting fully-discrete scheme is named by **SVM-CN**.

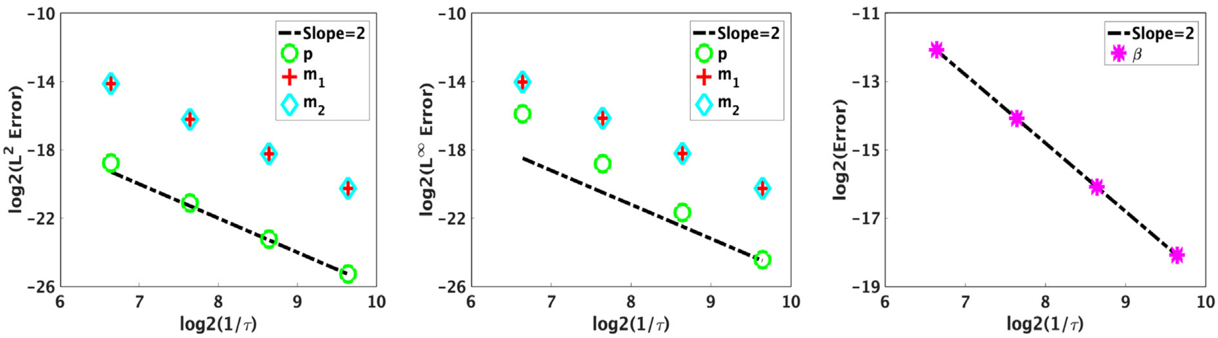



**Fig. 1.** Mesh refinement test for **SVM-CN**. The second order accuracy in time is achieved. The slope of the supplementary variable $\beta$ error curve is close to 2.

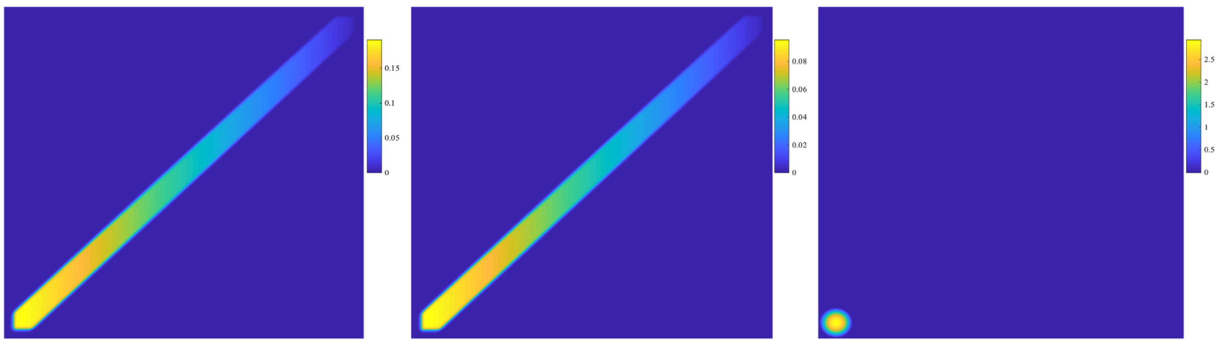


**Fig. 2.** The initial profiles of $m_1(x, y, 0)$ (left), $m_2(x, y, 0)$ (middle) and the source $S(x, y)$ (right) for Example 2.

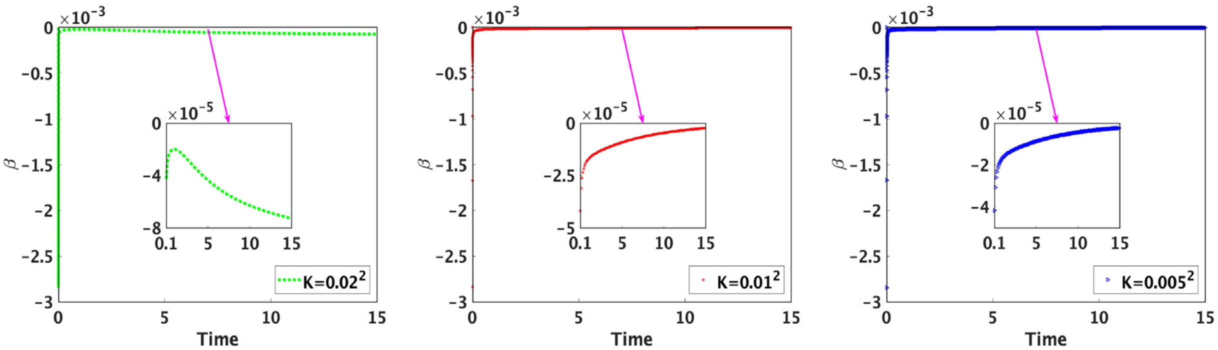
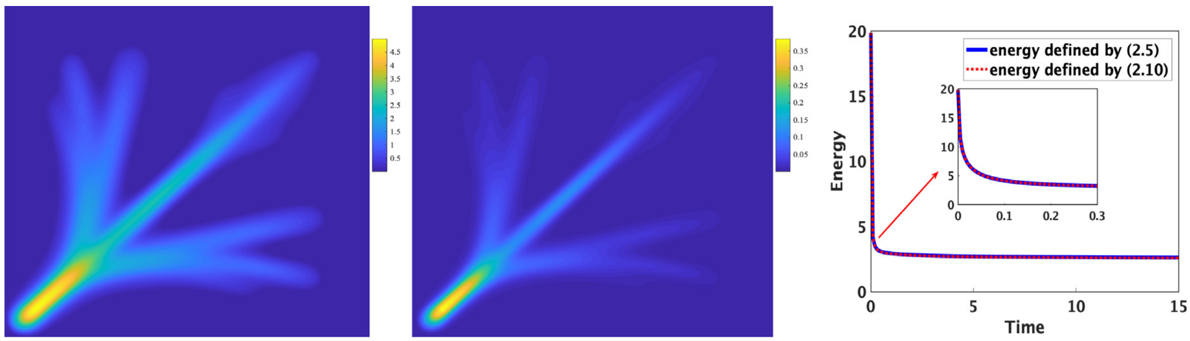



**Fig. 3.** Evolution of supplementary variable $\beta(t)$ for Example 2. The figure displays the supplementary variable $\beta$ will change rapidly at the beginning, but eventually, settles down close to zero.

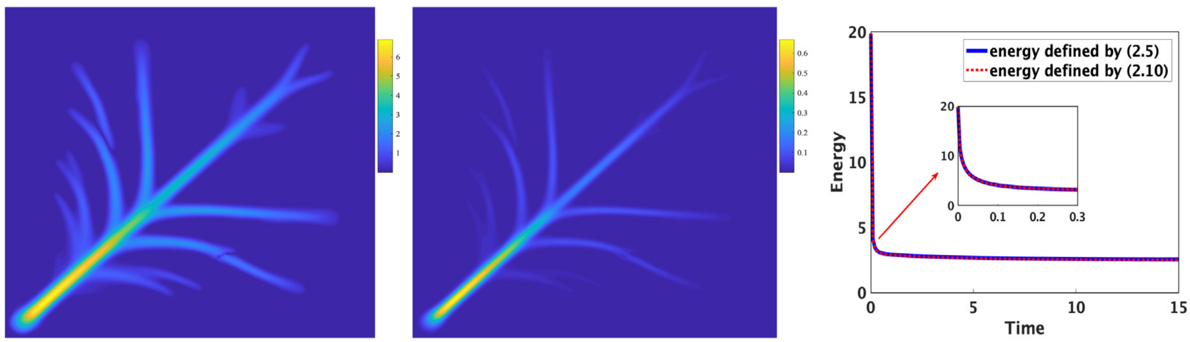
## 3. Numerical results

We confirm the accuracy of the scheme numerically and then present a numerical example to illustrate energy dissipation rate preserving property of the proposed scheme and its ability to generate networks numerically.

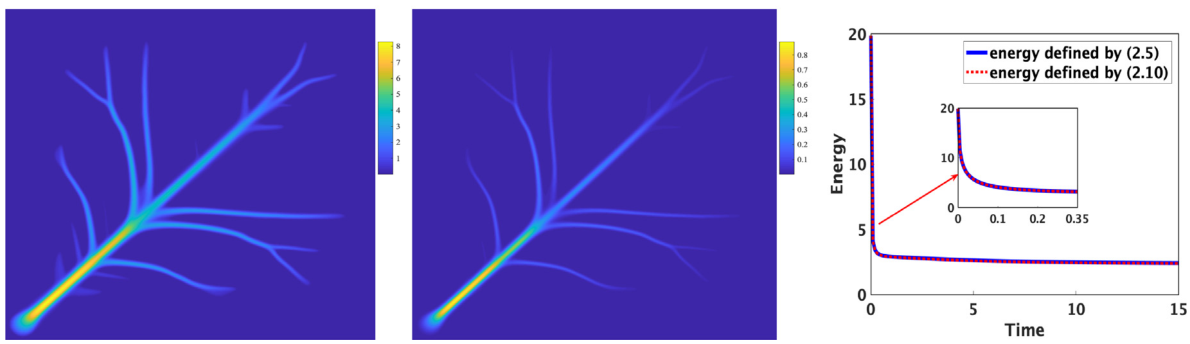
**Example 1** (*Mesh Refinement Test*)**.** We first conduct the time mesh refinement test to confirm the order of accuracy of the **SVM-CN** scheme in a 2D domain $\Omega = [0, 2\pi]^2$. In this test, we use the following initial




(a) The norm of conductance vector $\|\mathbf{m}\|$, fluid velocity $\|\mathbf{v}\|$ and the energy with $K = 0.02^2$ at $t = 15$.




(b) The norm of conductance vector $\|\mathbf{m}\|$, fluid velocity $\|\mathbf{v}\|$ and the energy with $K = 0.01^2$ at $t = 15$.




(c) The norm of conductance vector $\|\mathbf{m}\|$, fluid velocity $\|\mathbf{v}\|$ and the energy with $K = 0.005^2$ at $t = 15$.

**Fig. 4.** Effect of diffusion coefficient $K$ on the network formation and time evolution of the energy for Example 2. The first two sub-figures in each row indicate the smaller diffusion coefficient $K$ is, the more detailed structure the network tends to exhibit. The last column sub-figures show that two types of energy decay with time using the **SVM-CN** scheme.

conditions

$$\mathbf{m}(x, y, 0) = (\sin(x)\sin(y), \sin(x)\sin(y))^T,$$

where $= (m_1, m_2)^T$. We set following parameter values as $r = a = \alpha = 1$, $\gamma = 0.75$, $K = 0.01^2$, and the source term $S$ is defined as

$$S(x,y) = \begin{cases} \exp\left(-\frac{1}{1-((x-0.1)/0.1)^2-((y-0.1)/0.1)^2}\right), & \textit{when } ((x-0.1)/0.1)^2 + ((y-0.1)/0.1)^2 < 1, \\ 0, & \textit{otherwise.} \end{cases}$$

Here, we conduct the test with spatial mesh size $256 \times 256$ and time steps $\tau = 0.02, 0.01, 0.005, 0.0025, 0.00125$, respectively. At the final time $t = 1$, the discrete $L^2$ and $L^\infty$ errors are calculated as the difference between the solution of the coarse mesh and that of the adjacent finer mesh. The numerical results are list in Fig. 1, where the approximately second order convergence rates in time for all variables are observed. Moreover, the second-order accuracy of supplementary variable $\beta$ is attained as well. Thus, the numerical results validate the correct order of **SVM-CN** scheme.

**Example 2** (*Network Formation*)**.** In this test, we demonstrate the capability of **SVM-CN** scheme to capture dynamics of network formation in space–time. The initial condition and source term are depicted in Fig. 2. The flux, $\mathbf{v}$, in this model is defined by $\mathbf{v} = -(r\mathbf{I} + \mathbf{mm})\nabla p$. We set the parameter as $r = 0.1$, $a = 50$, $\alpha = 1$ and $\gamma = 0.75$. The computational domain is chosen as $[0, 2] \times [0, 2]$ with $256 \times 256$ grids.

The profiles of the network and its structure are influenced significantly by diffusion coefficient $K$. Here, we choose $K = 0.02^2$, $0.01^2$ and $0.005^2$ to verify the effect. The simulation results are shown in Fig. 4, where we clearly observe networks exhibit tree-like structures and emergence of more detailed structures at smaller diffusion coefficients. The numerically simulated phenomena agree qualitatively well with those in the published literature [15,17]. Fig. 4 also shows the energy functional defined in (2.4) and (2.9) as functions of time, which all decay in time. We thus conclude that **SVM-CN** scheme provides a good approximation to the solution and the original energy at the discrete level since the original energy (2.4) and the energy given by (2.9) exhibit nearly indistinguishable behavior. From Fig. 3, we found that the supplementary variable $\beta(t)$ varies rapidly at the beginning of the computation and gradually settle down to a near zero steady state value. Thus, the numerical results clearly demonstrate the capability of **SVM-CN** scheme in capturing fine network structures.

## Acknowledgment

Research is partially supported by the Foundation of Jiangsu Key Laboratory for Numerical Simulation of Large Scale Complex Systems (Grand No. 202001), the National Natural Science Foundation of China (award 11801269 and NSAF-U1930402) and National Science Foundation (award DMS-1815921 and OIA-1655740) and a GEAR award from SC EPSCoR/IDeA Program. Jun Li's work is supported by Tianjin Normal University Foundation for the introduction of talent (5RL154).

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