Discrete Variational Derivative Method

one of structure preserving methods for PDEs

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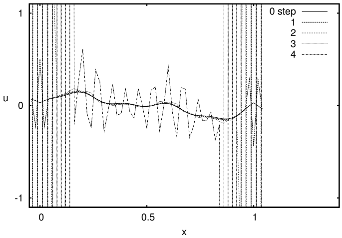
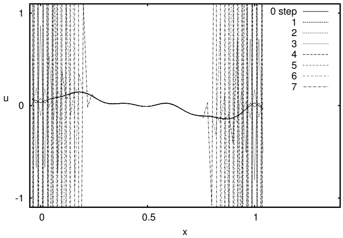
Introduction

Computation failure example without any criterion





$\Delta x = 1/50, \Delta t = 1/1200$ $\Delta x = 1/50, \Delta t = 1/12000$

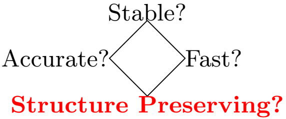
Numerical solutions blow up for the Cahn–Hilliard eq.

- We cannot apply usual, classical stability analysis/criterion to the Cahn–Hilliard equation since some small fluctuations around zero constant grow up spontaneously. This means that the equation looks unstable in the classical viewpoint.
- According to a nonlinear criterion(F, 1992), we may be able to obtain stable solution with very small $\Delta t \propto \Delta x^4$. But they are too small!
- We have to seek another approach for such problems.

Our answer: Structure preserving

"**Physics is characterized by conservation laws and by symmetry**" in "Conservative numerical methods for $\ddot{x} = f(x)$"(Greenspan 1984).

- First, studies of computations paid attention to conserve physical "local" quantities, such as mass, flux, charge and momentum.
- After 1970's there exist various studies which correspond one of current, global structure preserving methods.
- Don't seek stability directly, seek "inheritance of structure" on numerical solutions. We expect some stability when the inheritance is achieved.



4th criterion for computation

Recent structure preserving methods

Recently some "framework" studies for structure preserving method have been developed eagerly.

- Discrete gradient method (Quispel, McLachlan, McLaren,...)
- Average vector field method (above and Celledoni, Owren, Wright)
- Discrete variational integrator (Marsden, Patrick, Shkoller, West...)
- Lagrangian approach for Euler–Lagrange PDEs (Yaguchi, New Talent Award!)
- Discrete variational derivative method (**DVDM**)(F., Mori, Sugihara, Matsuo, Ide, Yaguchi, and ...)

1.2 History

In this section, we briefly mention the related studies on the main subject of this book.

First attempts on dissipative/conservative schemes, or more generally on structure-preserving algorithms, focused on ordinary differential equations such as Hamiltonian systems. For example, in the beginning of the 1970's Greenspan [77] considered strictly conservative discretization of some mechanical systems. The method was then extended to general mechanical systems by Gonzalez [74] and McLachlan–Quispel–Robidoux [126, 127] decades later. A strong alternative to these works is the so-called symplectic method, which is a specialized numerical method for Hamiltonian systems. Though symplectic schemes are not strictly conservative, they are nearly conservative, and provide us very effective ways to integrate Hamiltonian systems. For the symplectic method, see Hairer–Lubich–Wanner [83], Sanz-Serna–Calvo [151] and Leimkuhler–Reich [104]. Related interesting studies on nearly conservative numerical schemes include: Faou–Hairer–Pham [52] and Hairer [81].

After these successes on Hamiltonian ODEs, many other classes of ODEs that have some intrinsic geometric structure have been identified, and structure-preserving algorithms for these ODEs have been extensively studied. These activities for ODEs are now also referred to as the "geometric numerical integration of ODEs," and form a big trend in numerical analysis. Interested readers may refer to Hairer–Lubich–Wanner [83] and Budd–Piggott [23].

In the PDE context, a number of studies on dissipative/conservative schemes have been carried out on individual dissipative or conservative PDEs, since around the 1970's. Below are quite limited examples. Strauss–Vazquez [155] presented a conservative finite difference scheme for the nonlinear Klein–Gordon equation. Hughes–Caughey–Liu [89] presented a conservative finite element scheme for the nonlinear elastodynamics problem. Delfour–Fortin–Payre [35] presented a conservative finite difference scheme for the nonlinear Schrödinger equation, then Akrivis–Dougalis–Karakashian [8] presented a finite element version of the scheme and proved the convergence of the finite element scheme. Sanz–Serna [150] considered the nonlinear Schrödinger equation as well. Taha–Ablowitz [159, 160] presented conservative finite difference schemes for the nonlinear Schrödinger equation and the Korteweg–de Vries equation. Du–Nicolaides [39] presented a dissipative finite element scheme for the Cahn–Hilliard equation. Around the same time, in a completely different context from above, studies on soliton PDEs such as the KdV equation were done to find finite difference schemes that preserved discrete bilinear form or Wronskian form, corresponding to the original equations; see, for example, Hirota [85, 86]. They can be also regarded as structure-preserving methods.

Then during the 1990s, more general approaches that cover not only several individual PDEs but also a wide class of PDEs have been independently introduced by several groups. The discrete variational derivative method—the main subject of the present book—is one of such methods, proposed by Furihata–Mori [63, 64, 69, 65] around 1996 for PDEs with variational structure. The method has then been extended in various ways mainly by a Japanese group including Furihata, Matsuo, Ide, and Yaguchi [66, 67, 68, 90, 91, 116, 119, 120, 121, 122, 165, 166, 167], and succeeded in proving its effectiveness in various applications. At the same time, Gonzalez [75] proposed a conservative method for some general class of PDEs describing finite-deformation elastodynamics. There, the key is a special technique in time discretization devised for ODEs by Gonzalez [74]. Another excellent set of studies were given by McLachlan [129] and McLachlan–Robidoux [128], where a general method for designing conservative schemes for conservative PDEs based on their techniques on ODEs [126, 127] (and the related basic studies Quispel–Turner [145] and Quispel–Capel [144]) was developed (see also the recent related results: McLaren–Quispel [130], Quispel–McLaren [146], Celledoni *et al.* [26]). Jimenez [92] has also studied a systematic approach to obtain discrete conservation laws for certain finite difference schemes.

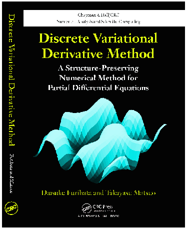
Aside from strictly conservative or dissipative methods, several interesting approaches for structure-preserving integration of PDEs have emerged as of the writing of the present book. For a very comprehensive review including these topics, see Budd–Piggot [23]. For Hamiltonian PDEs, a unique approach was proposed by Marsden–Patrick–Shkoller [112] (see also Marsden–West [113] for a good review), and it has been intensively studied by their group. Their method is based on the discretization of the variational principle. Its name "variational integrator" is quite close to the discrete variational derivative method, but these methods are quite different. For Hamiltonian PDEs, there is another interesting emerging method, the "multi-symplectic method," developed by Bridges–Reich [22]. In the method, Hamiltonian PDEs are transformed into a special "multi-symplectic form," and then integrated in such a way that the multi-symplecticity is conserved. This method can be regarded as a generalization of the symplectic method for ODEs (see also McLachlan [124]). For the recent literature in this context, see, for example, [27, 87, 88] and the references therein.

Finally we would like to note that in this short summary we could by no means cover all of the related studies. We recommend that interested readers refer to several key reviews, such as Hairer–Lubich–Wanner [83], Budd–Piggott [23], Leimkuhler–Reich [104], and Lubich [110], and consult their references as well.

Short history:

From a dissipative scheme for the Cahn–Hilliard equation (F. 1991), we have been developed the discrete variational derivative method.
In the first few years we have paid attention to composing some structure preserving schemes on a case-by-case problems/techniques, but we slightly have moved to study "framework".
After obtaining some superior colleagues, such as Matsuo, Ide, Yaguchi, we have developed DVDM to wider problems and enhance their functionality.

"Discrete Variational Derivative Method",
F. and T.Matsuo,
CRC Press, 2010.
ISBN: 978-1-4200-9445-9



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DVDM Walk-through with an example: Cahn-Hilliard eq.

DVDM walk-through

"DVDM is a framework, methodology to design numerical schemes which inherit global properties from the original PDE based on variational derivative".

But it's hard to understand the DVDM by only this phrase, so we should start this talk with a walk-through.

- **Target:**

  Cahn–Hilliard eq. $\dfrac{\partial u}{\partial t} = \dfrac{\partial^2}{\partial x^2}\left(pu + ru^3 + q\dfrac{\partial^2 u}{\partial x^2} \right)$

  for $u = u(x,t)$ where $p, q < 0 < r$ are constants.

  This PDE is notorious since hardness to compute stable solutions...
- **Features:**

  Dissipation of energy and conservation of mass are important.
- **Main purpose:**

  Inheritance the above features (= Structure Preserving)
- **Hidden purpose:**

  We expect the designed scheme is stable and would like to check typical features in computation, i.e., solution existence, error evaluation, and ...

Dissipation property of the Cahn–Hilliard eq. (1)

Let us investigate the the dissipation property of the CH eq. Considering the local energy as $G(u, u_x) = (1/2)pu^2 + (1/4)ru^4 - q\left(\partial u/\partial x\right)^2$, we are able to treat the equation in the following form:

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\frac{\delta G}{\delta u}\right) \qquad \text{where } \frac{\delta G}{\delta u} \overset{\text{def}}{=} \frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x} = pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}.$$

The variational derivative $\delta G/\delta u$ is defined to satisfy the following equation

$$\begin{aligned} J[u+\delta u] - J[u] &= \int_0^L \left\{ \frac{\partial G}{\partial u}\delta u + \frac{\partial G}{\partial u_x}\delta u_x \right\} dx + \mathrm{O}(\delta u^2) \\ &= \int_0^L \left\{ \left(\frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x} \right)\delta u \right\} dx + (\text{b.t.}) + \mathrm{O}(\delta u^2) \\ &= \int_0^L \left\{ \frac{\delta G}{\delta u}\delta u \right\} dx + (\text{b.t.}) + \mathrm{O}(\delta u^2) \end{aligned}$$

where $J[u] = \int_0^L G(u, u_x)\, dx$. Note that “integration by parts” is used here to define the variational derivative.

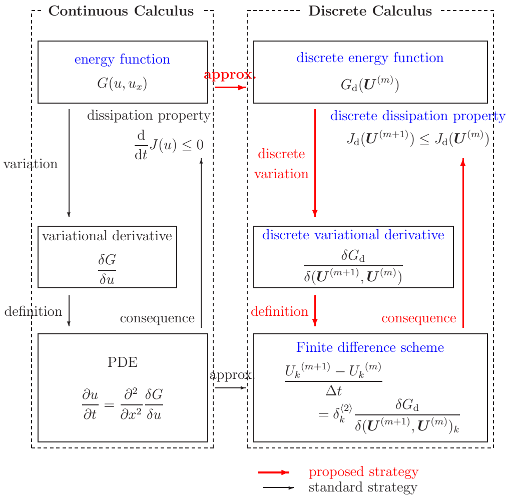
Dissipation property of the Cahn–Hilliard eq. (2)

Here, we can understand the dissipation property in the following inequality. The differentiation of total energy w.r.t. time,

$$
\begin{aligned}
&\frac{d}{dt}\int_0^L G(u,u_x)dx \\
&= \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}dx + \text{(b.t.)} \\
&= \int_0^L \frac{\delta G}{\delta u}\left(\frac{\partial}{\partial x}\right)^2 \frac{\delta G}{\delta u}dx + \text{(b.t.)} \\
&= (-1)\int_0^L \left\{\frac{\partial}{\partial x}\left(\frac{\delta G}{\delta u}\right)\right\}^2 dx + \text{(b.t.)} = \text{Negative } (= \text{dissipation}).
\end{aligned}
$$

We use the “integration by parts” twice above. First timing is the appearance of variational derivative, and the second one is to change the integration term to the negative one.
Note that the abstract form of the CH eq. (in the previous page) indicates the dissipation property naturally.

Relationship between PDE and variational derivative



DVDM basic concept is to mimic the continuous system in discrete context.
It means that we follow **the proposed strategy** in the left concept figure. When we follow the strategy completely, we will obtain the numerical scheme which has the discrete dissipation property.

Requirements: (detail in the next page)

- Some discrete operators,
- summation by parts,
- discrete variational derivative

Our Discrete Mathematical Tools

To implement the concept in the previous page, we need to prepare some discrete mathematical tools. They should be rigorous and consistent in discrete context. Here we prepare the following ones, which are simple and easy to use in finite difference context.

1. Discrete operators which correspond to differentiation, integration, ...

$$\delta_k^+ f_k \stackrel{\text{def}}{=} (f_{k+1} - f_k)/\Delta x, \quad \delta_k^- f_k \stackrel{\text{def}}{=} (f_k - f_{k-1})/\Delta x,$$

$$\delta_k^{\langle 1\rangle} \stackrel{\text{def}}{=} (\delta_k^+ + \delta_k^-)/2, \quad \delta_k^{\langle 2\rangle} \stackrel{\text{def}}{=} \delta_k^+ \delta_k^-,$$

$$\sum_{k=0}^{N}{}'' f_k \stackrel{\text{def}}{=} f_0/2 + \sum_{k=1}^{N-1} f_k + f_N/2, \ldots$$

2. **Summation by parts**. As you know, this is mathematical key to implement the concept because the integration by parts are key to indicate the dissipation property of the CH eq.

$$\sum_{k=0}^{N}{}'' (\delta_k^+ f_k) g_k \Delta x = -\sum_{k=0}^{N}{}'' f_k (\delta_k^- g_k) \Delta x + (\text{b.t.})$$

Now, try to implement the concept of DVDM (1)

For numerical solution $U_k^{(n)}$ corresponds $u(k\Delta x, n\Delta t)$, we implement the concept in the DVDM diagram.

- **Definition the discrete local energy:**

$$G_{\mathrm{d},k}(\boldsymbol{U}) \stackrel{\text{def}}{=} \frac{1}{2}p(U_k)^2 + \frac{1}{4}r(U_k)^4 - \frac{1}{2}q\left(\frac{(\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2}{2}\right).$$

- **Derivation of the discrete variational derivative:**
For audience, here we derive it from the variation of the total energy (to be correct, the discrete variational derivative is defined explicitly for functions). For convenience, we separate the energy into a polynomial part and a non-polynomial one as $G_{\mathrm{d},k}(\boldsymbol{U}) = P_k(\boldsymbol{U}) + N_k(\boldsymbol{U})$.
First, variation of the polynomial part P is decomposed easily,

$$\begin{aligned}
&\sum_{k=0}^{N}{}'' P_k(\boldsymbol{U})\Delta x - \sum_{k=0}^{N}{}'' P_k(\boldsymbol{V})\Delta x \\
&= \sum_{k=0}^{N}{}'' \left\{ p\left(\frac{U_k + V_k}{2}\right) + r\left(\frac{(U_k)^3 + (U_k)^2 V_k + U_k (V_k)^2 + (V_k)^3}{4}\right)\right\} \\
&\qquad \times (U_k - V_k)\Delta x
\end{aligned}$$

Now, try to implement the concept of DVDM (2)

Variation of the non-polynomial part is indicated below using the summation by parts.

$$\sum_{k=0}^{N}{}'' N_k(\boldsymbol{U})\Delta x - \sum_{k=0}^{N}{}'' N_k(\boldsymbol{V})\Delta x$$

$$= -\frac{1}{4}q\sum_{k=0}^{N}{}'' \left((\delta_k^+ U_k)^2 + (\delta_k^- U_k)^2 - (\delta_k^+ V_k)^2 - (\delta_k^- V_k)^2\right)\Delta x$$

$$= -\frac{1}{2}q\sum_{k=0}^{N}{}'' \left\{\delta_k^+\left(\frac{U_k+V_k}{2}\right)\delta_k^+(U_k-V_k) + \delta_k^-\left(\frac{U_k+V_k}{2}\right)\delta_k^-(U_k-V_k)\right\}\Delta x$$

$$= \sum_{k=0}^{N}{}'' q\delta_k^{\langle 2\rangle}\left(\frac{U_k+V_k}{2}\right)(U_k-V_k)\Delta x + (\mathrm{b.t.})$$

Note that this equality correspond

$$\delta\left\{\int (\frac{-1}{2})q(u_x)^2\,\mathrm{d}x\right\} \cong -q\int u_x\delta u_x\,\mathrm{d}x = \int qu_{xx}\delta u\,\mathrm{d}x + (\mathrm{b.t.}).$$

Now, try to implement the concept of DVDM (3)

Obtaining the variation of the discrete total energy, we define the discrete variational derivative of energy function G_{d}.

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k} \stackrel{\mathrm{def}}{=} p\left(\frac{U_k+V_k}{2}\right)+r\left(\frac{(U_k)^3+(U_k)^2V_k+U_k(V_k)^2+(V_k)^3}{4}\right)+q\delta_k^{\langle 2\rangle}\left(\frac{U_k+V_k}{2}\right)$$

From the derivation, it is trivial that they satisfy the following relationship.

$$\sum_{k=0}^{N}{}'' G_{\mathrm{d},k}(\boldsymbol{U})\Delta x-\sum_{k=0}^{N}{}'' G_{\mathrm{d},k}(\boldsymbol{V})\Delta x=\sum_{k=0}^{N}{}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k}(U_k-V_k)\Delta x+(\mathrm{b.t.})$$

This relationship does not include any limit operation term and it means that this is consistent in the finite difference calculation context.

Now, try to implement the concept of DVDM (4)

- **Derivation of the DVDM scheme:**

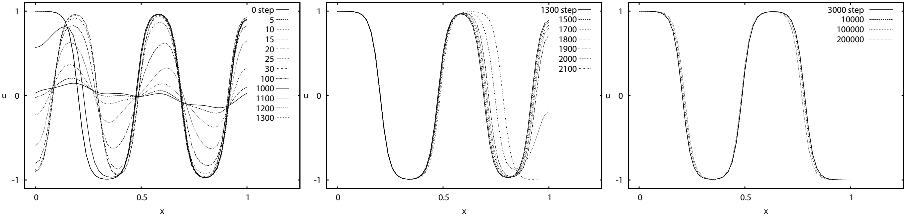
  Finally, using the discrete variational derivative, we are able to design a DVDM scheme which inherits the dissipation property.

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2 \rangle} \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \right)$$

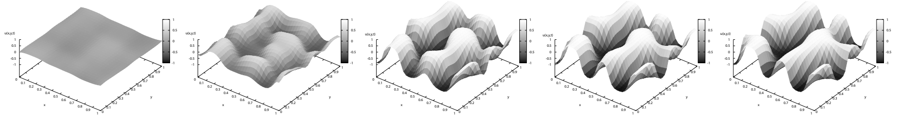
  We can guess/confirm the following features of the scheme easily.

  1. It has a dissipation property (described later)
  2. Does it has a conservation mass property? (described later)
  3. The scheme is a fully-implicit and hard to obtain numerical solutions by the nonlinearity.
  4. Accuracy should be 2nd order with Δx and Δt because all operations are symmetric (described later)

Here we have computation examples of the DVDM scheme in previous page.



Computation results by the scheme for 1 dim.



Computation results by the scheme for 2 dim.

Check: Is the main purpose accomplished? (1)

Let us recall our main purpose of DVDM design: "inheritance the features of the original PDE". Those features of the Cahn–Hilliard eq. are

- **Dissipation of the total energy:**
  We design the DVDM scheme such that it inherits the dissipation property. In fact, we can confirm that as

$$
\begin{aligned}
&\frac{1}{\Delta t}\left\{\sum_{k=0}^{N}{}'' \, G_{\mathrm{d},k}(\boldsymbol{U}^{(n+1)})\Delta x - \sum_{k=0}^{N}{}'' \, G_{\mathrm{d},k}(\boldsymbol{U}^{(n)})\Delta x\right\} \\
&= \sum_{k=0}^{N}{}'' \, \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})_k}\left(\frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t}\right)\Delta x + (\mathrm{b.t.}) \\
&= \sum_{k=0}^{N}{}'' \left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})_k}\right)\delta_k^{\langle 2\rangle}\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})_k}\right)\Delta x + (\mathrm{b.t.}) = \\
&-\frac{1}{2}\sum_{k=0}^{N}{}'' \left\{\left(\delta_k^{+}\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})_k}\right)^2 + \left(\delta_k^{-}\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})_k}\right)^2\right\}\Delta x + (\mathrm{b.t.})
\end{aligned}
$$

Check: Is the main purpose accomplished? (2)

- **Conservation of the total mass:**
  Our process of design is no concern of this property so far. Here we should confirm if it is inherited by the DVDM scheme or not.

$$
\begin{aligned}
&\frac{1}{\Delta t}\left\{\sum_{k=0}^{N}{}'' \, U_k^{(n+1)}\Delta x - \sum_{k=0}^{N}{}'' \, U_k^{(n)}\Delta x\right\} \\
&= \sum_{k=0}^{N}{}'' \left(\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t}\right)\Delta x \\
&= \sum_{k=0}^{N}{}'' \, \delta_k^{\langle 2\rangle}\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)},\boldsymbol{U}^{(n)})_k}\Delta x \\
&= (\text{b.t.}) = 0
\end{aligned}
$$

! This is a coincidence, anyway, the conservation of total mass property is inherited by the DVDM scheme in discrete context.

Check: Is the hidden purpose accomplished? (1)

Next, let us recall the hidden purpose of DVDM design: "stability, solution existence, accuracy, ...", which are typical concerns in numerical computation. The numerical stability is crucial in the Cahn–Hilliard eq. problem, so we cannot ignore this hidden purpose.

- **Stability:**
  Before that we investigate the numerical stability, here we consider about the evaluation of the exact solutions of the original PDE.
  1. The Sobolev norm of the exact solutions is bounded above by a constant which is determined by the initial value. The energy dissipation property causes this result.
  2. If the space dim. is one, the Sup norm of functions is bounded above by the Sobolev norm. This is a part of the Sobolev lemma.
  3. From facts above, the exact solutions' Sup norm is bounded above by a constant which is independent of time.

  Remembering these facts, let us investigate the numerical stability.

Check: Is the hidden purpose accomplished? (2)

Here we know that those facts satisfied with the exact solutions (in the previous page) are fully satisfied with the numerical solutions.

1. Discrete Sobolev norm is bounded above because of the discrete dissipation property.

$$\left\| U^{(n)} \right\|_{\text{d-}(1,2)}^2 \leq \frac{1}{\min(-p, -\frac{q}{2})} \left\{ \sum_{k=0}^{N}{}'' G_{\text{d}}(\boldsymbol{U}^{(0)}) \Delta x + \frac{9p^2 |\Omega|}{4r} \right\}$$

2. There is a discrete Sobolev lemma when the space dim. is one. By the lemma we bound the max norm from above by the Sobolev norm.

$$\max_{0 \leq k \leq N} |f_k| \leq 2 \sqrt{\max(\frac{|\Omega|}{2}, \frac{1}{|\Omega|})} \, \|f\|_{\text{d-}(1,2)}$$

3. From the above facts, we can show the following inequality and it means that the DVDM scheme is unconditionally stable.

$$\max_{0 \leq k \leq N} \left| U_k^{(n)} \right| \leq 2 \left[\frac{\max(1/|\Omega|, |\Omega|/2)}{\min(-p, -q/2)} \left\{ \sum_{k=0}^{N}{}'' G_{\text{d}}(\boldsymbol{U}^{(0)}) \Delta x + \frac{9p^2 |\Omega|}{4r} \right\} \right]^{1/2}$$

Check: Is the hidden purpose accomplished? (3)

- **Numerical solutions existence:**

  The DVDM scheme is nonlinear and fully-implicit and they may not have numerical solutions. We have to check it has numerical solutions or not, or, seek some conditions to have solutions.
  We already know that the max norm of the numerical solutions are bounded above and it brings us the following result through some cumbersome Taylor expansion.

  When the following inequality is satisfied, the DVDM scheme has the next unique numerical solutions.

$$\Delta t < \min\left(\frac{-q(\Delta x)^2}{2\left(-p\Delta x + 82rM^2\right)^2}, \frac{-2q(\Delta x)^2}{\left(-p\Delta x + 226rM^2\right)^2} \right),$$

where $M \stackrel{\text{def}}{=} \|\boldsymbol{U}^{(n)}\|_2$.

Check: Is the hidden purpose accomplished? (4)

- **Accuracy:**

  As already noted, we can guess the error of numerical solutions is 2nd order of Δx and Δt because all of our operations are symmetric.
  Using the max norm evaluation and some cumbersome Taylor expansion, we can obtain the following results as expected.

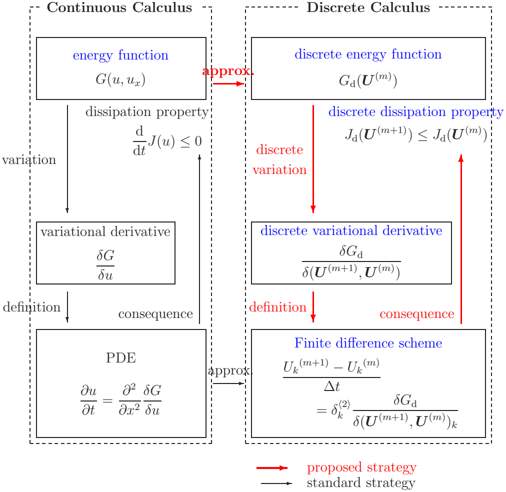
$$\|u(\bullet, T) - U_k^{(n)}\|$$
$$\leq \sqrt{C|\Omega|T} \exp\left[\left(1 + \frac{2\left\{-p + 3r(C_2)^2\right\}^2}{-q}\right)T\right]\left(\Delta x^2 + \Delta t^2\right),$$

where C is a constant which depends on exact solutions and $T = n\Delta t$.

General DVDM based on FDM

General DVDM based on finite difference

The basic idea of DVDM is already shown in the diagram below.



To generalize the story in walk-through,

1. We give more rigorous definition of the discrete variational derivative than one in the walk-through.
2. We would like to seek some classifications of target PDEs via the DVDM.

Definition of the discrete variational derivative (DVD)

To define the discrete variational derivative rigorously and explicitly, we assume that the discrete energy function is a polynomial of U, $\delta_k^+ U$, $\delta_k^- U$.

$$G_{\mathrm{d},k}(\boldsymbol{U}) = \sum_{l=1}^{m} f_l(U_k)\; g_l^+(\delta_k^+ U_k)\; g_l^-(\delta_k^- U_k)$$

For this function G_d, we define the discrete variational derivative in the following equation.

$$\frac{\delta G_\mathrm{d}}{\delta(\boldsymbol{U},\boldsymbol{V})_k} \stackrel{\mathrm{def}}{=} \sum_{l=1}^{m} \left(\frac{df_l}{d(U_k,V_k)} \frac{g_l^+(\delta_k^+ U_k) g_l^-(\delta_k^- U_k) + g_l^+(\delta_k^+ V_k) g_l^-(\delta_k^- V_k)}{2} \right.$$
$$\left. -\delta_k^+ W_l^-(\boldsymbol{U},\boldsymbol{V})_k - \delta_k^- W_l^+(\boldsymbol{U},\boldsymbol{U})_k \right),$$

where $W_l^\pm(\boldsymbol{U},\boldsymbol{V})_k \stackrel{\mathrm{def}}{=} \left(\frac{f_l(U_k) + f_l(V_k)}{2} \right) \left(\frac{g_l^\mp(\delta_k^\mp U_k) + g_l^\mp(\delta_k^\mp V_k)}{2} \right) \frac{dg_l^\pm}{d(\delta_k^\pm U_k, \delta_k^\pm V_k)}$

This definition looks cumbersome, but it is rigorous and explicit so that we can avoid vagueness that how to derive the discrete variational derivative.

What kind of PDEs are targets of DVDM?

From here, we show the wide classification of target PDEs of DVDM.

- **First order, real-valued PDEs:**
  This means that the time-differentiation is only 1st order and the solution $u = u(x,t)$ is a real-valued function.

  In this situation, we treat the following PDEs mainly as targets of DVDM.

  1. Real-valued, dissipative PDEs:

  $$\frac{\partial u}{\partial t} = (-1)^{s+1}\left(\frac{\partial}{\partial x}\right)^{2s}\frac{\delta G}{\delta u},\ s = 0, 1, \ldots$$

  2. Real-valued, conservative PDEs:

  $$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{2s+1}\frac{\delta G}{\delta u},\ s = 0, 1, \ldots$$

Schemes and Properties of real-valued, dissipative PDEs

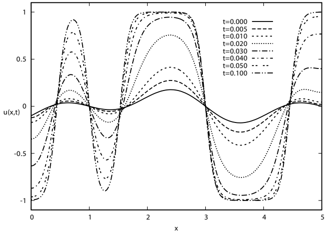
- **DVDM Scheme:**

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = (-1)^{s+1} \delta_k^{\langle 2s \rangle} \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}$$

- **Inherited property:**

$$\text{Decrease of } \sum_{k=0}^{N}{}'' \, G_{\mathrm{d},k}(\boldsymbol{U}^{(n)}) \Delta x$$

- **Target examples:**
  - $(s = 0)$ linear diffusion eq.
  - $(s = 0)$ Swift–Hohenberg eq.
  - $(s = 0)$ Fujita explosion eq.
  - $(s = 0)$ Allen–Cahn eq.
  - $(s = 0)$ extended Fisher–Kolmogorov eq.
  - $(s = 1)$ Prominence temperature eq.
  - $(s = 1)$ Cahn–Hilliard eq.

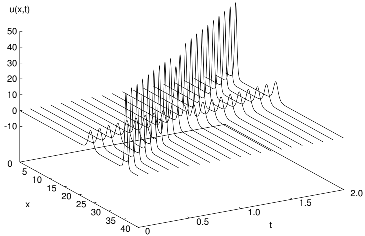


- **DVDM Scheme:**

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 2s+1\rangle} \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}$$

- **Inherited property:**

Conservation of $\sum_{k=0}^{N}{}'' \, G_{\mathrm{d},k}(\boldsymbol{U}^{(n)})\Delta x$



- **Target examples:**
  - $(s=0)$ linear convection eq.
  - $(s=0)$ Korteweg-de Vries eq.
  - $(s=0)$ Zakharov–Kuznetsov eq.

First order, complex-valued PDEs are also target

We have found another type PDEs, which is complex-valued, as targets of DVDM.

- **First order, complex-valued PDEs:**

  In this situation, we treat the following PDEs mainly as targets of DVDM.

  1. Complex-valued, dissipative PDEs: $\dfrac{\partial u}{\partial t} = -\dfrac{\delta G}{\delta \overline{u}}$
  2. Complex-valued, conservative PDEs: $i\dfrac{\partial u}{\partial t} = -\dfrac{\delta G}{\delta \overline{u}}$

For the complex-valued function $G(u, u_x)$ the variational derivative is

$$\frac{\delta G}{\delta u} \stackrel{\mathrm{def}}{=} \frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}, \qquad \frac{\delta G}{\delta \overline{u}} \stackrel{\mathrm{def}}{=} \frac{\partial G}{\partial \overline{u}} - \frac{\partial}{\partial x}\frac{\partial G}{\partial \overline{u_x}} = \overline{\frac{\delta G}{\delta u}},$$

and

$$\delta\left(\int G(u, u_x)\,\mathrm{d}x\right) = \int\left(\frac{\delta G}{\delta u}\delta u + \frac{\delta G}{\delta \overline{u}}\delta \overline{u}\right)\mathrm{d}x + (\text{b.t.}).$$

Schemes,Properties of complex-valued,dissipative PDEs

- **DVDM Scheme:**

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = -\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(n+1)}}, \overline{\boldsymbol{U}^{(n)}})_k}$$

  ... We omit the definition of the discrete variational derivative for the complex-valued function since it is too cumbersome.

- **Inherited property:**

  Decrease of $\displaystyle\sum_{k=0}^{N}{}'' \, G_{\mathrm{d},k}(\boldsymbol{U}^{(n)})\Delta x$

- **Target examples:**
  - (A variant of) Ginzburg–Landau eq.
  - Newell–Whitehead eq.

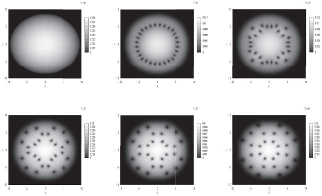
Schemes,Properties of complex-valued,conservative PDEs

- **DVDM Scheme:**

$$i\left(\frac{U_k^{(n+1)}-U_k^{(n)}}{\Delta t}\right)=-\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(n+1)}},\overline{\boldsymbol{U}^{(n)}})_k}$$

- **Inherited property:**

$$\text{Conservation of } \sum_{k=0}^{N}{}'' \, G_{\mathrm{d},k}(\boldsymbol{U}^{(n)})\Delta x$$



- **Target examples:**
  - Nonlinear Schrödinger eq.
  - Gross–Pitaevskii eq.

Systems of first order PDEs

There exist some targets that are systems of first order PDEs, but I omit the discussion and notation about them because they are too cumbersome (, we have written them in our book in detail).

- **Target examples:**
  - Zakharov eq.
  - good Boussinesq eq.
  - Eguchi–Oki–Matsumura eq.

  ... we omit their schemes too.

Second order PDEs

We found that there exist some target 2nd order PDEs. These are conservative and interesting because the conserved quantity is not the total of energy.

- **Second order PDEs:**

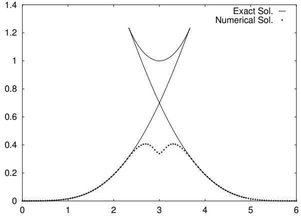
$$\frac{\partial^2 u}{\partial t^2} = -\frac{\delta G}{\delta u}$$

- **Conservation property:**

The integration $\int \left\{ \frac{1}{2} (u_t)^2 + G(u, u_x) \right\} \mathrm{d}x$ is conserved since

$$\frac{d}{dt} \int \left\{ \frac{1}{2} (u_t)^2 + G(u, u_x) \right\} \mathrm{d}x = \int \left(u_{tt} + \frac{\delta G}{\delta u} \right) u_t \ \mathrm{d}x + (\text{b.t.}) = 0.$$

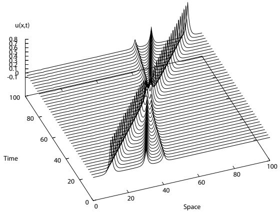
- **Target examples:**
  - linear wave eq.
  - Fermi–Pasta–Ulam eq. I and II.
  - nonlinear string vibration eq.
  - nonlinear Klein–Gordon eq.
  - Shimoji–Kawai eq.
  - Ebihara eq.



Other equations

There are some target PDEs that do not belong to the typical target PDEs. We think that we may treat them as systems of PDEs via generalizing of the systems target.

- **Target examples:**
  - Feng wave eq.
  - Keller–Segel eq.
  - Camassa–Holm eq.



The Camassa–Holm equation $u_t - u_{txx} = 2u_x u_{xx} + u u_{xxx} - 3uu_x$ is able to be treated as various conservative abstract forms. For example, this equation can be written as

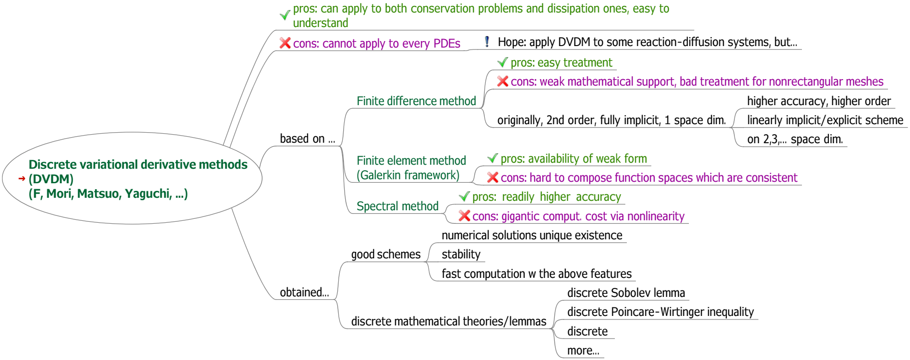
$$(1 - \partial_x^2)u_t = -\partial_x \frac{\delta G}{\delta u}, \quad \text{where } G(u, u_x) = \frac{1}{2} u \left(u^2 + (u_x)^2\right).$$

In this viewpoint, the total energy $\int G(u, u_x)\,\mathrm{d}x$ is conserved and we can design some DVDM schemes along this description.

Advanced Topic: Overview

Overview

Before stepping into some advanced topics, let us look the overview of topics about the DVDM.



Advanced Topic:
Design of High-Order Schemes

Design of High-Order Schemes

- The DVDM schemes shown are second order accurate w.r.t. the space mesh size Δx and the time mesh size Δt so far. This means that the computation error is $\mathrm{O}(\Delta x^2, \Delta t^2)$.
- We would like to develop some "higher order accurate schemes" in the DVDM framework.
- There exist some studies to treat this issues, here I introduce three of them.
  - Spatially high-order schemes (to spectral differentiation)
  - Temporally high-order schemes via composition method
  - Temporally high-order schemes with high-order discrete variational derivative

Spatially High-Order Schemes (1)

Our method to obtain spatially high-order schemes is relatively simple.

- **Basic idea:** We substitute higher order difference operators for the second order ones. Higher order difference operators are widely known. For example, most typical high order first difference is written as

  $$\delta_k^{\langle 1 \rangle, 2p} U_k = \frac{1}{\Delta x} \sum_{j=-p}^{p} \alpha_{p,j} U_{k+j},$$

  and the operator $\delta_k^{\langle 1 \rangle, 2p}$ is skew-symmetric, it means $\alpha_{p,j} = -\alpha_{p,-j}$. When we take the limit of $p \to \infty$, the operator becomes a spectral differentiation operator.

- **Math tools:** We can reconstruct almost our mathematical tools with high order operators which are needed for the DVDM, e.g., we obtain the summation by parts as

  $$\sum_{k=0}^{N}{}'' (\delta_k^{\langle 1 \rangle, 2p} f_k) g_k \Delta x = - \sum_{k=0}^{N}{}'' f_k (\delta_k^{\langle 1 \rangle, 2p} g_k) \Delta x + \text{(b.t.)}$$

  since the operator $\delta_k^{\langle 1 \rangle, 2p}$ is skew-symmetric.

Spatially High-Order Schemes (2)

- **Discrete variational derivative:** Assuming that the discrete energy function G_{d} is a polynomial function of U_k and $\delta_k^{\langle 1 \rangle, 2p} U_k$, we can extend the definition of the discrete variational derivative to spatially high order ones.
- **DVDM scheme:** Now, operators, energy and discrete variational derivatives are extended to high order ones and it is straightforward to design of schemes. For example, we design the spatially high order DVDM scheme for the real-valued, dissipative PDEs as

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = (-1)^{s+1} \left(\delta_k^{\langle 1 \rangle, 2p} \right)^{2s} \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k}$$

This extension is easy to understand and easy to use, but the obtained schemes has heavy computation cost for nonlinear problems.

Temporally High-Order Schemes: Composition Method

Recall that schemes are ideal when the following conditions are satisfied,

1. It is stable
2. It has low computation cost
3. It is high order accurate
4. It is a kind of structure preserving method
5. It is a linear scheme for linear problems

At the present moment, we do not have any ideal method to extend the DVDM in temporally high order ones, but I'd like to introduce some results.

- **Composition method:**
  This methodology, which is widely known in astronomy, is to design high order time evolution operators by composition of lower order ones. For example, when $I_{\Delta t}$ denotes the 2nd order time evolution operators, $I_{1.351\Delta t} I_{-1.702\Delta t} I_{1.351\Delta t}$ becomes a 4th order one.
  This method is easy to use, but always includes some "negative time evolution step". This prevents the composition scheme from becoming a structure preserving method for dissipation problems.

Temporally High-Order Schemes: DVDM (1)

The another approach to this problem is to extend the DVDM with temporally high order operators. Concept is simple but there exist a difficulty in definition of the discrete variational derivative.

- **What is so difficult?**
  With high order operators, it is hard to mimic the "chain rule" of differentiation, which appears in the DVDM process. For example, the chain rule of differentiation appears in

  $$\frac{\partial}{\partial t}\int G(u,u_x)\,\mathrm{d}x = \int\left(\frac{\partial G}{\partial u}u_t + \frac{\partial G}{\partial u_x}u_{xt}\right)\mathrm{d}x,$$

  included in the process to define the discrete variational derivative.

  In the 2nd order context, it is attained simply as

  $$\frac{f(U^+)-f(U)}{\Delta t} = \frac{f(U^+)-f(U)}{U^+-U}\,\frac{U^+-U}{\Delta t},$$

  but this idea has some mathematical problems in higher order context, e.g., they are not well-defined in some situations.

Temporally High-Order Schemes: DVDM (2)

- **Matsuo's idea:**
  For this difficulty, Matsuo defined the following discrete gradient with high order operators which is extension of Gonzalez's one.

$$\left(\frac{\partial f}{\partial U}\right)^{,q} \stackrel{\text{def}}{=} \frac{\partial f}{\partial U} + \left(\frac{\delta^{\langle 1\rangle,q} f - \frac{\partial f}{\partial U}\delta^{\langle 1\rangle,q} U}{\|\text{numerator}\|^2}\right)\delta^{\langle 1\rangle,q} U.$$

  This definition is well-defined and satisfy the following discrete chain rule.

$$\delta^{\langle 1\rangle,q} f(U) = \left(\frac{\partial f}{\partial U}\right)^{,q} \delta^{\langle 1\rangle,q} U.$$

  With this definition we are able to define the discrete variational derivative on multi time steps and design the DVDM schemes which are temporally high order accurate.

- **Features:**

  1. (Pros) Obtained DVDM schemes are structure preserving.
  2. (Cons) Obtained schemes always become nonlinear.
  3. (Cons) Usually, stability is not guaranteed

Advanced Topic:
Design of Linearly Implicit Schemes

Design of Linearly Implicit Schemes

The basic linearization technique may have long history and it has been studied in structure preserving method by various researchers, e.g., Matsuo, F. (2001), Dahlby, Owren (2010).

The basic idea is decomposition of a nonlinear polynomial term into a multiplied term by quadratic/linear terms w.r.t. various time steps.

For example, consider a PDE $u_t = (u^4)_x$ and a typical symmetric scheme

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \delta_k^{\langle 1 \rangle} \left(\frac{\left(U_k^{(n+1)}\right)^4 + \left(U_k^{(n)}\right)^4}{2} \right).$$

If we decompose the nonlinear polynomial term, it becomes linearly-implicit

$$\frac{U_k^{(n+2)} - U_k^{(n-1)}}{3\Delta t} = \delta_k^{\langle 1 \rangle} \left(U_k^{(n+2)} U_k^{(n+1)} U_k^{(n)} U_k^{(n-1)} \right).$$

Note that the linearized schemes are "strongly unstable" in general. So, we hope the stabilization effect/expectation by structure preserving overcome this adverse affect.

Linearly Implicit Schemes: Cahn–Hilliard eq.

Here we show an example of linearly-implicit DVDM schemes. The target is the Cahn–Hilliard eq. and the obtained scheme is superior...

- **Linearly-implicit DVDM scheme:**
  With one extra time step and decompose the biquadratic term in the energy function and obtain a linearly-implicit DVDM scheme:

$$\frac{U_k^{(n+1)} - U_k^{(n-1)}}{\Delta t}$$
$$= \delta_k^{\langle 2 \rangle} \left\{ p U_k^{(n)} + r \left(\frac{U_k^{(n+1)} + U_k^{(n-1)}}{2} \right) \left(U_k^{(n)} \right)^2 + q \delta_k^{\langle 2 \rangle} \left(\frac{U_k^{(n+1)} + U_k^{(n-1)}}{2} \right) \right\}$$

- **Features:**
  1. The scheme inherits the dissipation property.
  2. It is unconditionally stable and this stability is proved via discrete Poincaré–Wirtinger inequality.

Linearly Implicit Schemes: Other Examples

We designed linearly-implicit schemes for other problems and some of them are such efficient that we can compute by them.
The followings are those examples

- nonlinear Schödinger eq.
- Ginzburg–Landau eq.
- Zakharov eq.
- Newell–Whitehead eq.

Overview of linearly-implicit schemes:
Design of them is easy but it is difficult to obtain stable schemes. Choice of decomposition is essential but this methodology is too flexible so far.

Advanced Topic: Switch to Galerkin Framework

Switch to Galerkin Framework

If we able to use the Galerkin framework/context on DVDM for the finite difference one, we can expect the following features.

1. More flexible mesh generation is available and this feature is especially preferable in the 2D problems and higher ones.
2. Lower differentiation of functions are needed then ones in FDM.
3. Galerkin framework brings the L^2 structure naturally and this structure will assist to obtain numerical solution evaluation, error evaluation, etc. by function analysis context.

Matsuo has developed studies about this issue and from here let us introduce a part of results.

The Galerkin Framework in the DVDM context (1)

Originally, a variational derivative satisfies the following something like a weak form with variation function δu,

$$\left(\frac{\delta G}{\delta u}, \delta u\right) = \left(\frac{\partial G}{\partial u}, \delta u\right) + \left(\frac{\partial G}{\partial u_x}, \delta u_x\right) - \left[\frac{\partial G}{\partial u_x}\,\delta u\right]_{\partial\Omega}$$

- **Re-definition of variational derivative:**
  Based on above form we can re-define the variational derivative in the Galerkin framework as "a function $P = P(u)$ which satisfies the following weak form for ${}^{\forall} w \in W$"

$$(P, w) = \left(\frac{\partial G}{\partial u}, w\right) + \left(\frac{\partial G}{\partial u_x}, w_x\right) - \left[\frac{\partial G}{\partial u_x}\,w\right]_{\partial\Omega}$$

- **Re-definition of discrete variational derivative:**
  When the weak form is extended in the discrete context, we also can re-define the discrete variational derivative as "a function $P = P(u, v)$ which satisfies the following weak form for ${}^{\forall} w \in W$"

$$(P, w) = \left(\frac{\partial G}{\partial (u, v)}, w\right) + \left(\frac{\partial G}{\partial (u_x, v_x)}, w_x\right) - \left[\frac{\partial G}{\partial (u_x, v_x)}\,w\right]_{\partial\Omega},$$

(continue to the next page...)

(... continued from the previous page) where

$$\frac{\partial G}{\partial(u,v)} \stackrel{\text{def}}{=} \sum_{l=1}^{m} \frac{df_l}{d(u,v)} \left(\frac{g_l(u_x)+g_l(v_x)}{2} \right),$$

$$\frac{\partial G}{\partial(u_x,v_x)} \stackrel{\text{def}}{=} \sum_{l=1}^{m} \left(\frac{f_l(u)+f_l(v)}{2} \right) \frac{dg_l}{d(u_x,v_x)}, \text{ for } G(u,u_x) = \sum_{l=1}^{m} f_l(u) g_l(u_x).$$

Here we show one example of schemes.

- **Galerkin Scheme for** $\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\frac{\delta G}{\delta u}\right)$**:**

  $$\left(\frac{u^{(n+1)} - u^{(n)}}{\Delta t}, v \right) = \left((P^{(n+\frac{1}{2})})_x, v \right),$$

  for $^{\forall} v$ where the discrete variational derivative $P^{(n+\frac{1}{2})}$ for $(u^{(n+1)}, u^{(n)})$ is defined by the re-definition weak form in the previous page.

The Galerkin Framework: Korteweg-de Vries eq.

Since the KdV eq. is one of PDEs $\partial u/\partial t = \partial_x(\delta G/\delta u)$, we are able to apply the Galerkin scheme in the previous page.

The energy function G of the equation is $(1/6)u^3 - (1/2)(u_x)^2$ and we obtain from it

$$\frac{\partial G}{\partial(u,v)} = \frac{u^2+uv+v^2}{6},$$
$$\frac{\partial G}{\partial(u_x,v_x)} = -\frac{u_x+v_x}{2}.$$

Of course this scheme is strictly conservative.

Advanced Topic:
Design for 2D Problems

Advanced Topic: Design for 2D Problems

There exist some studies to apply the DVDM to 2D (or 3D) problems and the methodologies are able to be classified as

1. **Mapping** (mainly by Yaguchi)

   In this procedures, first we prepare virtual, orthogonal mesh region and a mapping from it to the real region. Essential calculation is done on the virtual region and we use the mapped scheme for computation.

   - (Pros) Flexible and comprehensive.
   - (Pros) Arbitrary dimension, 2D, 3D, 4D,...
   - (Cons) By just one mapping for complicated region, it will be difficult...

2. **Galerkin framework** (mainly by Matsuo)

   We already introduced that.

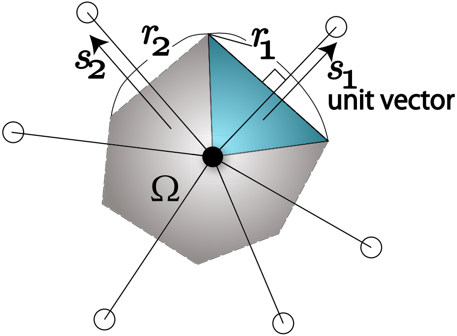
3. **Using special mesh: Voronoi mesh** (mainly by F.)

   Here we introduce it.

DVDM on Voronoi Mesh

- On Voronoi mesh, there exist some natural discrete Green formula. These correspond the summation by parts in 2D (or 3D...).
  So, we can extend the whole story of the DVDM on 1D to 2D or higher dimensional problems without much effort.

- Originally, Voronoi mesh has a kind of "flatness property" and it causes the Green formula.



flatness condition:
$r_1 \boldsymbol{s}_1 + r_2 \boldsymbol{s}_2 + \cdots\cdots = \mathbf{0}$

Discrete Green formula on Voronoi Mesh

We have some discrete Green formula on the Voronoi mesh.

- **Discrete Green formula 1:**

$$\sum_i \left\{ \sum_{j\in S_i} u_i \left(\frac{w_j - w_i}{l_{ij}} \right) \boldsymbol{s}_{ji} \Delta\Omega_{ij} \right\}$$
$$= -\sum_i \left\{ \sum_{j\in S_i} w_i \left(\frac{u_j - u_i}{l_{ij}} \right) \boldsymbol{s}_{ji} \Delta\Omega_{ij} \right\} + \sum_{i\in\partial\Omega_d} u_i w_i \boldsymbol{R}_i,$$

where $\partial\Omega_d$ is the boundary,$\Delta\Omega_{ij} \stackrel{\text{def}}{=} \frac{1}{4} r_{ij} l_{ij}$, and $\boldsymbol{R}_i \stackrel{\text{def}}{=} -\sum_{j\in S_i} r_{ij} \boldsymbol{s}_{ji}$. The proof is readily straightforward using the flatness property.

- **Discrete Green formula 2:**

$$\sum_i \left\{ \sum_{j\in S_i} \left(\frac{u_j - u_i}{l_{ij}} \right) \left(\frac{w_j - w_i}{l_{ij}} \right) \Delta\Omega_{ij} \right\} = -\sum_i (\Delta_d u)_i w_i \Omega_i + \sum_{i\in\partial\Omega_d} (D_{out} u)_i w_i,$$

where Δ_d is discrete Laplacian and $(D_{out} u)_i$ are correction terms on boundary.

Example on Voronoi Mesh: Cahn–Hilliard eq.

We have necessary discrete Green formula and can use whole DVDM story. Here we show the example for the Cahn–Hilliard eq.

- **DVDM Scheme:**

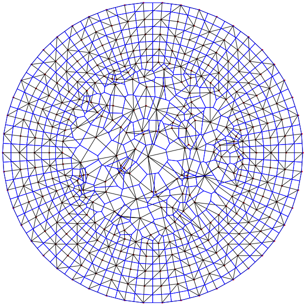
$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \Delta_d \left(\frac{\delta G_\mathrm{d}}{\delta(\boldsymbol{U}^{(n+1)}, \boldsymbol{U}^{(n)})_k} \right)$$

where the discrete energy is

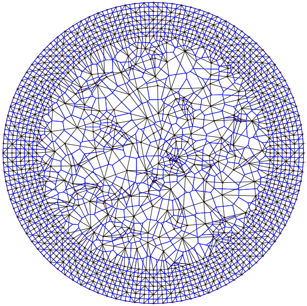
$$G_\mathrm{d}(\boldsymbol{U})_k \stackrel{\mathrm{def}}{=} \frac{1}{2} p U_k^2 + \frac{1}{4} r U_k^4 - \frac{1}{2} q \sum_{j \in S_k} \left(\frac{U_j - U_k}{l_{kj}} \right)^2 \frac{\Delta\Omega_{kj}}{\Omega_k}$$

- **Inherited properties:**
  1. The total mass $\sum_k U_k^{(n)} \Omega_k$ is conserved,
  2. The total energy $\sum_k G_\mathrm{d}(\boldsymbol{U}^{(n)})_k \Omega_k$ is dissipated.

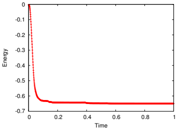
Computation Example: Random Points



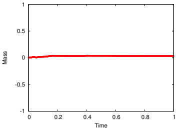
▸ 350 Points



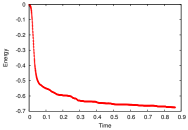
▸ 700 Points



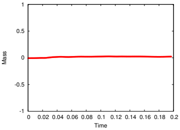
Energy



Mass

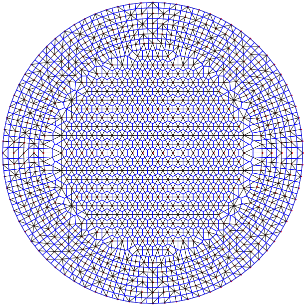


Energy

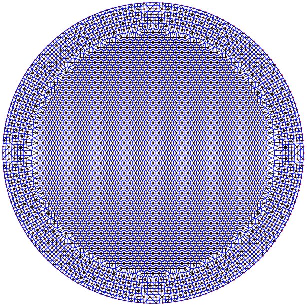


Mass

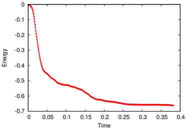
Computation Example: Hexagonal Lattice Points



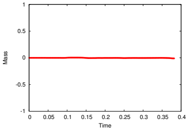
▸ 741 Points



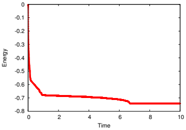
▸ 2319 Points



Energy



Mass



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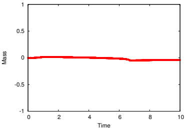

Mass

Appendix

Appendix: Discrete Mathematics

Through studies about the DVDM, we have found or made some discrete mathematical lemmas.

- **Discrete Sobolev Lemma:**

$$\max_{0\le k\le N} |f_k| \le 2\sqrt{\max(\frac{|\Omega|}{2}, \frac{1}{|\Omega|})}\|f\|_{H^1}$$

- **Discrete Poincaré–Wirtinger inequality:**

$$\frac{1}{|\Omega|}\left(u_k - \frac{\overline{u}}{|\Omega|}\right)^2 \le \sum_{k=0}^{N-1} |\delta_k^+ u_k|^2 \Delta x$$

- **Discrete Gagliardo–Nirenberg inequality:**

$$\|\boldsymbol{u}\|_4^4 \le 2\|\boldsymbol{u}_x\|\|\boldsymbol{u}\|^3 \text{ where } \|\boldsymbol{u}_x\|^2 \stackrel{\text{def}}{=} \textstyle\sum_{k=0}^{N-1} |\delta_k^+ u_k|^2 \Delta x,$$

$$\|\boldsymbol{u}\|_4^4 \le b\|\boldsymbol{u}\|_{H^1}\|\boldsymbol{u}\|^3.$$

Conclusion

Conclusion

- Through the "discrete variational derivative" concept, we've been developed the discrete variational derivative method (DVDM) as one of structure preserving methods. This method is available to both conservative problems and dissipative ones, it means that this is relatively comprehensive.
- DVDM is based on finite difference context originally, but we have stepped into the Galerkin framework.
- We also have tried to extend the DVDM and obtained some results – such as spatially high order schemes, temporally ones, linearly implicit schemes and some methods on 2D or 3D, etc.

Thank you for listening!!