Relaxations of discrete gradients for differential equations

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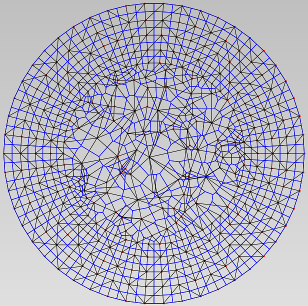
1. Introduction

Story of this talk

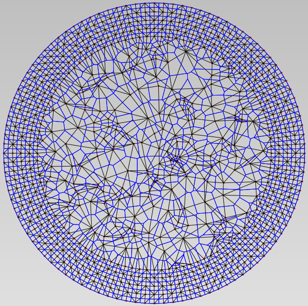
- Discrete gradients are approximations of (continuous) gradients
- "**Discrete gradients**" + "**discrete Green formula**"
  = some **structure-preserving methods for differential equations**.
- Conventional conditions derive symmetric discrete gradients and symmetric numerical schemes. Computation costs by symmetric schemes are too heavy for strongly nonlinear problems.
- If we relax those two conditions, we can derive flexible discrete gradients:
  examples:
  - symmetric/asymmetric linearized DVDM (Discrete Variational Derivative Methods that design ST-schemes for PDEs),
  - asymmetric (non-extra time step) DVDM .
- Via those flexible discrete gradients, we can design some structure-preserving schemes which has "weak nonlinearity".
- (In future) We would like to generalize discrete gradient to apply it for complex integralation in numerical analysis context... but how?

inner.

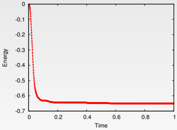
For the Cahn–Hilliard equation, randomly-located points.



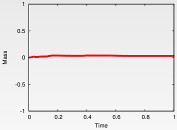
▸ 350 Points



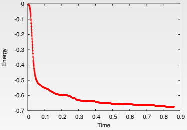
▸ 700 Points



Energy



Mass



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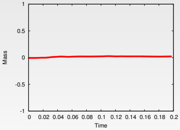

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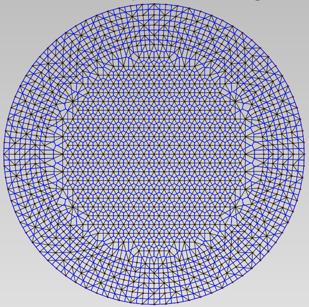
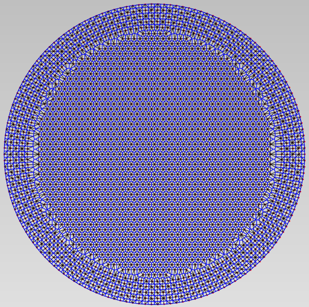
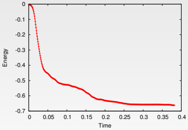
For the Cahn–Hilliard equation, hexagonal lattice points.





741 Points

2319 Points



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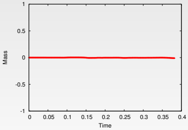

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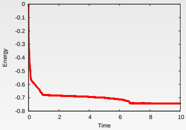
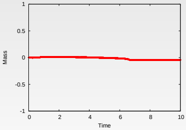


Energy



Mass

Conventional definition of discrete gradient

For a set U with an inner product $<,>$ and a map $V : U \to K$, typical discrete gradients $\overline{\nabla V} : U^2 \to U$ are defined to satisfy the following two conditions [Harten et al., 1983, etc.]:

$$\begin{cases} V(\boldsymbol{x}') - V(\boldsymbol{x}) &= \left\langle \overline{\nabla V}(\boldsymbol{x}', \boldsymbol{x}), (\boldsymbol{x}' - \boldsymbol{x}) \right\rangle, \\ \overline{\nabla V}(\boldsymbol{x}, \boldsymbol{x}) &= \nabla V(\boldsymbol{x}). \end{cases} \qquad \text{for any } \boldsymbol{x}, \boldsymbol{x}' \in U.$$

Note: Discrete gradients $\overline{\nabla V}$ which satisty these conditions are **not unique**.

So far we have satisfied this definition, however, we would like to relax these conditions to design more fast/nice numerical schemes for differential equations.

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Discrete gradients and structure-preserving methods: 1

- Discrete gradients are essential to inherit conservative or dissipative properties of some integrals in numerical approximations of differential equations.

- How to design discrete gradients is mathematical point.

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$$V(\boldsymbol{x}) \text{ is a conserved quantity in } \frac{d\boldsymbol{x}}{dt} = S(\boldsymbol{x})\,\nabla V(\boldsymbol{x}), \text{ where } S \text{ is skew,}$$

$$\text{since } \frac{dV(\boldsymbol{x})}{dt} = \left\langle \nabla V(\boldsymbol{x}), \frac{d\boldsymbol{x}}{dt} \right\rangle = \langle \nabla V(\boldsymbol{x}), S(\boldsymbol{x})\,\nabla V(\boldsymbol{x}) \rangle = 0.$$

An example of structure-preserving schemes for the above problem:

$$\frac{\boldsymbol{x}^{(n+1)} - \boldsymbol{x}^{(n)}}{\Delta t} = \overline{S}(\boldsymbol{x}^{(n+1)}, \boldsymbol{x}^{(n)})\,\overline{\nabla V}(\boldsymbol{x}^{(n+1)}, \boldsymbol{x}^{(n)}), \text{ where } \overline{S} \text{ is skew.}$$

$$\begin{aligned} \frac{V(\boldsymbol{x}^{(n+1)}) - V(\boldsymbol{x}^{(n)})}{\Delta t} &= \left\langle \overline{\nabla V}(\boldsymbol{x}^{(n+1)}, \boldsymbol{x}^{(n+1)}), \frac{\boldsymbol{x}^{(n+1)} - \boldsymbol{x}^{(n)}}{\Delta t} \right\rangle \\ &= \left\langle \overline{\nabla V}(\boldsymbol{x}^{(n+1)}, \boldsymbol{x}^{(n+1)}), \overline{S}(\boldsymbol{x}^{(n+1)}, \boldsymbol{x}^{(n)})\overline{\nabla V}(\boldsymbol{x}^{(n+1)}, \boldsymbol{x}^{(n+1)}) \right\rangle \\ &= 0. \end{aligned}$$

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$I = \int G(u)\,\mathrm{d}x$ is a conserved integral in

$$\frac{\partial u}{\partial t} = S\,\frac{\delta G}{\delta u}, \text{ where } S \text{ is skew,}$$

$$\text{since } \frac{d}{dt}\int G(u)\,\mathrm{d}x = \left\langle \frac{\delta G}{\delta u}, \frac{\partial u}{\partial t} \right\rangle = \left\langle \frac{\delta G}{\delta u}, S\frac{\delta G}{\delta u} \right\rangle = 0,$$

where the inner product is defined as $\langle f, g\rangle \stackrel{\text{def}}{=} \int f(x)g(x)\,\mathrm{d}x$.

An example of structure-preserving schemes (DVDM) for the above problem:

$$\frac{U_k^{(n+1)} - U_k^{(n)}}{\Delta t} = \overline{S}\left(\frac{\delta G_{\mathsf{d}}}{\delta(U^{(n+1)}, U^{(n)})}\right)_k, \text{ where } \overline{S} \text{ is skew.}$$

$$\begin{aligned}
\frac{\langle G_{\mathsf{d}}(U^{(n+1)}), 1\rangle - \langle G_{\mathsf{d}}(U^{(n)}), 1\rangle}{\Delta t} &= \left\langle \frac{\delta G_{\mathsf{d}}}{\delta(U^{(n+1)}, U^{(n)})}, \frac{U^{(n+1)} - U^{(n)}}{\Delta t} \right\rangle \\
&= \left\langle \frac{\delta G_{\mathsf{d}}}{\delta(U^{(n+1)}, U^{(n)})}, \overline{S}\frac{\delta G_{\mathsf{d}}}{\delta(U^{(n+1)}, U^{(n)})} \right\rangle = 0,
\end{aligned}$$

where $\langle f, g\rangle = \sum_k{}'' f_k g_k \Delta x$.

One example of discrete gradients: Harten, Lax and van Leer 1983

For $(\nabla V)_i = \dfrac{\partial}{\partial x_i} V$, they defined as

$$\left(\overline{\nabla V}\right)_i (\boldsymbol{x}', \boldsymbol{x}) \stackrel{\text{def}}{=} \int_0^1 (\nabla V)_i \, (\gamma \boldsymbol{x}' + (1-\gamma)\boldsymbol{x}) \mathrm{d}\gamma.$$

We can confirm the first condition is satisfied as:

$$\begin{aligned}
\langle \overline{\nabla V}, \boldsymbol{x}' - \boldsymbol{x} \rangle &= \sum_i \left(\overline{\nabla V}\right)_i (x_i' - x_i) \\
&= \int_0^1 \sum_i (\nabla V)_i \, (\gamma \boldsymbol{x}' + (1-\gamma)\boldsymbol{x})(x_i' - x_i) \mathrm{d}\gamma \\
&= \int_0^1 \frac{d}{d\gamma} V(\gamma \boldsymbol{x}' + (1-\gamma)\boldsymbol{x}) \mathrm{d}\gamma \\
&= V(\boldsymbol{x}') - V(\boldsymbol{x}).
\end{aligned}$$

Note: This is in virtually the same definition as "Average Vector Field (AVF)" for PDEs [Celledoni et al., 2012].

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One example discrete gradients: Ito and Abe 1988

A difference approximation on the path from $\boldsymbol{x}$ to $\boldsymbol{x}'$.

Note: This definition is **not symmetric**.

For example, in $\mathbf{R}^3$, they define it as

$$\overline{\nabla V}(\boldsymbol{x}', \boldsymbol{x}) \stackrel{\text{def}}{=} \begin{pmatrix} \frac{V(x',y,z)-V(x,y,z)}{x'-x} \\ \frac{V(x',y',z)-V(x',y,z)}{y'-y} \\ \frac{V(x',y',z')-V(x',y',z)}{z'-z} \end{pmatrix}.$$

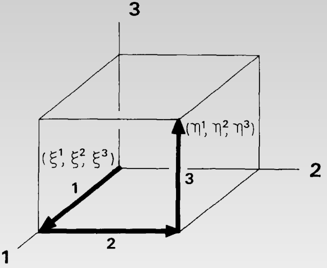

FIG 1. Illustration of $\Delta_{\xi'} G(\xi)|_\eta$ when $\mu = 3$

From Ito and Abe 1988.

Note: Of course, we can define a symmetric discrete gradient taking an average of all paths. However, the combinations become enormous for large dimension cases.

One example discrete gradients: Gonzalez 1996

The discrepancy between the continuous gradient and discrete one is recovered via addition of it.

Note: This discrete gradient is always "nonlinear."

$$\overline{\nabla V}(\boldsymbol{x}', \boldsymbol{x}) \stackrel{\text{def}}{=} \nabla V(\boldsymbol{z}) + \frac{V(\boldsymbol{x}') - V(\boldsymbol{x}) - \langle \nabla V(\boldsymbol{z}), \boldsymbol{x}' - \boldsymbol{x} \rangle}{\|\boldsymbol{x}' - \boldsymbol{x}\|^2} (\boldsymbol{x}' - \boldsymbol{x}),$$

where $\boldsymbol{z} = (\boldsymbol{x}' + \boldsymbol{x})/2$.

We can confirm that the first condition is satisfied as:

$$\begin{aligned} \left\langle \overline{\nabla V}, \boldsymbol{x}' - \boldsymbol{x} \right\rangle &= \left\langle \nabla V(\boldsymbol{z}), \boldsymbol{x}' - \boldsymbol{x} \right\rangle + \frac{V(\boldsymbol{x}') - V(\boldsymbol{x}) - \langle \nabla V(\boldsymbol{z}), \boldsymbol{x}' - \boldsymbol{x} \rangle}{\|\boldsymbol{x}' - \boldsymbol{x}\|^2} \left\|\boldsymbol{x}' - \boldsymbol{x}\right\|^2 \\ &= V(\boldsymbol{x}') - V(\boldsymbol{x}). \end{aligned}$$

Note: There is a higher-order definition [Furihata and Matsuo 2011, p.251].

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One example discrete gradients: DVDM, Furihata 1996

Discrete derivatives as "**discrete varitional derivatives**", based on discrete varitiaonal computatons.

For example, $\dfrac{\delta G_{\mathsf{d}}}{\delta(U^{(n+1)}, U^{(n)})}$ for G_{d} which satistis the following equality:

$$\left\langle G_{\mathsf{d}}(U^{(n+1)}), 1 \right\rangle - \left\langle G_{\mathsf{d}}(U^{(n)}), 1 \right\rangle = \left\langle \frac{\delta G_{\mathsf{d}}}{\delta(U^{(n+1)}, U^{(n)})}, U^{(n+1)} - U^{(n)} \right\rangle$$

where $\langle f, g \rangle = \sum_k{}'' f_k g_k \Delta x.$

Note: This talk is to relax/genralize this "discrete variational derivative" from the viewpoint of discrete gradients.

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2. Relaxation of Discrete Gradient

Relaxations of discrete gradients

We relax the two conditions for discrete gradient:

1. **Extra time steps, symmetric:** (we obtain multi-step numerical schemes)

$$\begin{cases} V(\boldsymbol{x}^{(n)}, \boldsymbol{x}^{(n-1)}, \cdots, \boldsymbol{x}^{(m+1)}) - V(\boldsymbol{x}^{(n-1)}, \boldsymbol{x}^{(n-2)}, \cdots, \boldsymbol{x}^{(m)}) \\ \qquad = \left\langle \overline{\nabla V}(\boldsymbol{x}^{(n)}, \boldsymbol{x}^{(n-1)}, \cdots, \boldsymbol{x}^{(m)}), \dfrac{(\boldsymbol{x}^{(n)} - \boldsymbol{x}^{(m)})}{n-m} \right\rangle, \\ \overline{\nabla V}(\boldsymbol{x}, \cdots, \boldsymbol{x}) = \nabla V(\boldsymbol{x}). \end{cases}$$

2. **Extra time steps, asymmetric:** (we obtain multi-step numerical schemes)

$$\begin{cases} V(\boldsymbol{x}^{(n)}, \boldsymbol{x}^{(n-1)}, \cdots, \boldsymbol{x}^{(m+1)}) - V(\boldsymbol{x}^{(n-1)}, \boldsymbol{x}^{(n-2)}, \cdots, \boldsymbol{x}^{(m)}) \\ \qquad = \left\langle \overline{\nabla V}(\boldsymbol{x}^{(n)}, \boldsymbol{x}^{(n-1)}, \cdots, \boldsymbol{x}^{(m)}), \delta U(\boldsymbol{x}^{(n)}, \cdots, \boldsymbol{x}^{(m)}) \right\rangle, \\ \overline{\nabla V}(\boldsymbol{x}, \cdots, \boldsymbol{x}) = \nabla V(\boldsymbol{x}), \\ \delta U(\boldsymbol{x}^{(m)} + (n-m)\delta\boldsymbol{x}, \boldsymbol{x}^{(m)} + (n-m-1)\delta\boldsymbol{x}, \cdots, \boldsymbol{x}^{(m)}) \\ \qquad = \delta\boldsymbol{x} + O(\delta\boldsymbol{x}^2). \end{cases}$$

3. **No-extra time steps, asymmetric:** (we obtain single-step numerical schemes)

$$\begin{cases} V(\boldsymbol{x}') - V(\boldsymbol{x}) = \left\langle \overline{\nabla V}(\boldsymbol{x}', \boldsymbol{x}), \delta U(\boldsymbol{x}', \boldsymbol{x}) \right\rangle, \\ \overline{\nabla V}(\boldsymbol{x}, \boldsymbol{x}) = \nabla V(\boldsymbol{x}), \\ \delta U(\boldsymbol{x} + \delta\boldsymbol{x}, \boldsymbol{x}) = \delta\boldsymbol{x} + O(\delta\boldsymbol{x}^2). \end{cases}$$

1.1 The Normal DVDM:
what happens for strongly nonlinear problems
using conventional discrete gradient

What are problems in conventional, symmetric DVDM

To see the computation cost to solve numerical schemes for nonlinear PDE problems, consider the following two typical target nonlinear PDEs.

$\boxed{\text{Nonlinear PDE type 1}}$ High order polynomial problem.

Example: $$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}(u^7)$$

$\boxed{\text{Nonlinear PDE type 2}}$ Non-polynomial problem.

Example: $$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}(e^u)$$

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The conventional DVDM story (1)

Via the conventional DVDM for equations like $\dfrac{\partial u}{\partial t} = (\dfrac{\partial^2}{\partial x^2})\dfrac{\delta G}{\delta u}$, we propose the following scheme

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

where $\dfrac{\delta G}{\delta u}$ is the variational derivative and $\dfrac{\delta G_{\mathsf{d}}}{\delta(\boldsymbol{U}, \boldsymbol{V})_k}$ is the discrete varitaional derivative. They are defined via

$$\int G(u + \delta u) - G(u)\,\mathsf{d}x \longrightarrow \int \frac{\delta G}{\delta u} \delta u\,\mathsf{d}x \qquad \text{as } \delta u \to 0,$$

$$\sum_{k=0}^{N}{}'' \, G_{\mathsf{d}}(\boldsymbol{U})_k - G_{\mathsf{d}}(\boldsymbol{V})_k \Delta x = \sum_{k=0}^{N}{}'' \, \frac{\delta G_{\mathsf{d}}}{\delta(\boldsymbol{U}, \boldsymbol{V})_k}(U_k - V_k)\Delta x.$$

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The conventional DVDM story (2)

For the example equation $\dfrac{\partial u}{\partial t} = \dfrac{\partial^2}{\partial x^2}(u^7) = \dfrac{\partial^2}{\partial x^2}\left(\dfrac{\delta\left(u^8/8\right)}{\delta u}\right)$ where $G(u) = \dfrac{u^8}{8}$, via

$$\sum_{k=0}^{N}{}'' \left(\frac{(U_k)^8}{8} - \frac{(V_k)^8}{8}\right)\Delta x = \sum_{k=0}^{N}{}'' \frac{\delta G_{\mathsf{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k}(U_k - V_k)\Delta x,$$

we obtain the discrete variational derivative

$$\frac{\delta G_{\mathsf{d}}}{\delta(\boldsymbol{U},\boldsymbol{V})_k} = \frac{u^7 + u^6 v + u^5 v^2 + u^4 v^3 + u^3 v^4 + u^2 v^5 + u v^6 + v^7}{8},$$

where $u = U_k, v = V_k$,

and we will obtain the DVDM shceme (in the next page).

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The conventional DVDM story (3)

Through the previous consideration, we obtain the following DVDM schemes for the previous examples. From these schemes, we can understand the difficulties to solve them.

For the $\boxed{\text{Nonlinear PDE type 1}}$ example:

$$\frac{u-v}{\Delta t} = \delta_k^{\langle 2\rangle} \left\{ \frac{u^7 + u^6 v + u^5 v^2 + u^4 v^3 + u^3 v^4 + u^2 v^5 + u v^6 + v^7}{8} \right\}$$

where $u \overset{\text{def}}{=} U_k^{(n+1)}, v \overset{\text{def}}{=} U_k^{(n)}$.

This means that we have to solve a sysmtem of high-order polynomial equations to obtain new time step solutions.

For the $\boxed{\text{Nonlinear PDE type 2}}$ example:

$$\frac{u-v}{\Delta t} = \delta_k^{\langle 2\rangle} \left(\frac{e^u - e^v}{u-v} \right)$$

... have to solve a system of non-polynomial nonlinear equations ...

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2.2 The first example of relaxation: extra time steps and symmetric definition

For the $\boxed{\text{Nonlinear PDE type 1}}$ example:

On the linearization technique, via the following **"symmetric"** decomposition.

For u^8, we define the discrete approximation: $u^2 v^2 w^2 \zeta^2$,

where $u \stackrel{\text{def}}{=} U_k^{(n+4)}, v \stackrel{\text{def}}{=} U_k^{(n+3)}, w \stackrel{\text{def}}{=} U_k^{(n+2)}, \zeta \stackrel{\text{def}}{=} U_k^{(n+1)}, \xi \stackrel{\text{def}}{=} U_k^{(n)}$.

(unknown variable and known variables)

Then, we obtain the following linearized scheme:

$$\frac{u - \xi}{4\Delta t} = \delta_k^{\langle 2 \rangle} \left\{ \frac{v^2 w^2 \zeta^2 (u + \xi)}{2} \right\}$$

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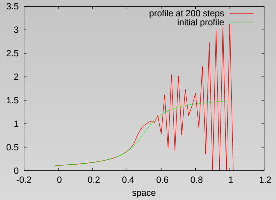
This is a "linear-implicit" system and easy-to-obtain new time step solutions, but this scheme is unstable because "extra 3" timesteps may be too many for this problem.



$\Delta x = 0.02$, $\Delta t = 5.0 \times 10^{-7}$.

How about is it for the type2?

For the $\boxed{\text{Nonlinear PDE type 2}}$ ...

We **cannot apply** the linearization technique to nonpolynomial problems.

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2.3 The 2nd example of relaxation: extra time steps and asymmetric definition

idea

Nonlinear term $\xrightarrow[\text{decomposition}]{\text{discrete}}$ $\begin{pmatrix}\text{unknown variables}\\ \text{polynomial}\end{pmatrix} \times \begin{pmatrix}\text{known variables}\\ \text{nonlinear term}\end{pmatrix}$

on multi-timestep numerical schemes by DVDM.

Examples for polynomial terms:

$$u^8 \longrightarrow \underbrace{U_k^{(n+1)}}_{\text{unknown}} \underbrace{(U_k^{(n)})^7}_{\text{known}} :$$ the obtained schemes are "explicit."

$$u^8 \longrightarrow \underbrace{(U_k^{(n+1)})^2}_{\text{unknown}} \underbrace{(U_k^{(n)})^6}_{\text{known}} :$$ the obtained schemes are "quadratic."

Originally, solvers in numerical schemes are systems of new timestep solutions. This means that the computation difficulty of solver depends on only the nonlinearity of new timestep solutions. This idea is to decrease the nonlinarity of new timestep solutions in those solvers.

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Extra time steps, asymmetric discrete gradient (2)

We can apply this idea to "non-polynomial problems."

Examples for non-polynomial terms: (unknown, known)

$$e^u \longrightarrow U_k^{(n+1)} \left(\frac{e^{U_k^{(n)}} - 1}{U_k^{(n)}} \right) + 1, \text{ or,}$$

$$e^u \longrightarrow (U_k^{(n+1)})^2 \left(\frac{e^{U_k^{(n)}} - 1 - U_k^{(n)}}{(U_k^{(n)})^2} \right) + 1 + U_k^{(n)}, \cdots$$

$$\log(u) \longrightarrow (U_k^{(n+1)} - 1) \left(\frac{\log(U_k^{(n)})}{U_k^{(n)} - 1} \right), \text{ or,}$$

$$\log(u) \longrightarrow (U_k^{(n+1)} - 1)^2 \left(\frac{\log(U_k^{(n)}) - (U_k^{(n)} - 1)}{(U_k^{(n)} - 1)^2} \right) + (U_k^{(n)} - 1),$$

Note: The above known variable terms are smooth and continuous.

To satisfy the first condition for discrete gradient (1)

We would like to apply the orthodox DVDM using the previous idea, but the story of orthodox DVDM is not applicable when the nonlinear term is non-polynomial one.

Example: Considering decomposition of a function $G(u)$ as $\tilde{G}(u,v,w) \stackrel{\text{def}}{=} u\,f(v)\,w$, the variation of $\tilde{G}$ is

$$\begin{aligned}\tilde{G}(u,v,w) - \tilde{G}(v,w,\zeta) &= uf(v)w - vf(w)\zeta \\ &= \left(\frac{f(v)w + vf(w)}{2}\right)(u-\zeta) + \left(\frac{u+\zeta}{2}\right)(f(v)w - vf(w)).\end{aligned}$$

If the function f is non-polynomial, we cannot extract the term "$u-\zeta$" ($\propto \delta u$) straightforwardly from this equation. This means that we cannot define any discrete variational derivative based on the orthodox DVDM.

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To satisfy the first condition for discrete gradient (2)

Seeing the previous example variation:

$$\delta\tilde{G} = \left(\frac{f(v)w + vf(w)}{2}\right)(u-\zeta) + \left(\frac{u+\zeta}{2}\right)(f(v)w - vf(w)),$$

we can find that the red term corresponds/resembles the variational derivative $\delta G/\delta u$ because it is a coefficient term of $(u-\zeta) \propto \delta u$.

Recall that $\delta G \cong \dfrac{\delta G}{\delta u}\delta u$.

So, we can decompose this equation to

$$= \left\{C(v,w)\left(\frac{f(v)w + vf(w)}{2}\right)\right\} \cdot \frac{1}{C(v,w)}\left\{(u-\zeta) + (u+\zeta)\frac{f(v)w - vf(w)}{f(v)w + vf(w)}\right\}$$

and define

$$\frac{\delta\tilde{G}}{\delta(v,w)} \stackrel{\text{def}}{=} C(v,w)\left(\frac{f(v)w + vf(w)}{2}\right),$$

$$\delta U(u,v,w,\zeta) \stackrel{\text{def}}{=} \frac{1}{C(v,w)}\left\{(u-\zeta) + (u+\zeta)\frac{f(v)w - vf(w)}{f(v)w + vf(w)}\right\}$$

where $C(v,w)$ is a correction function.

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We can design some structure-preserving schemes based on new discrete gradients

Based on those new ideas and new definitions, we can design new DVDM schemes for nonlinear PDE problems.

Example: For the typical PDE $u_t = \partial_x^2(\delta G/\delta u)$, if we decompose the energy function as $\tilde{G}(\boldsymbol{u}, \tilde{\boldsymbol{u}}_+, \tilde{\boldsymbol{u}}_-) = uf(v)w + \tilde{u}_+ g_+(\tilde{v}_+)\tilde{w}_+ + \tilde{u}_- g_-(\tilde{v}_-)\tilde{w}_-$, then we can propose the following new DVDM scheme:

$$
\left\{
\begin{aligned}
&\frac{1}{\Delta t\, C(v,w)} \left\{ (u-\zeta) + (u+\zeta)\frac{f(v)w - vf(w)}{f(v)w + vf(w)} \right\} \\
&\qquad\qquad\qquad = \delta_k^{\langle 2\rangle} \left\{ \tilde{G}_{\boldsymbol{u}} - \delta_k^- \tilde{G}_{\tilde{\boldsymbol{u}}_+} - \delta_k^+ \tilde{G}_{\tilde{\boldsymbol{u}}_-} \right\}, \\
&\frac{1}{\Delta t\, \tilde{C}(\tilde{v}_+, \tilde{w}_+)} \left\{ (\tilde{u}_+ - \tilde{\zeta}_+) + (\tilde{u}_+ + \tilde{\zeta}_+)\frac{g_+(\tilde{v}_+)\tilde{w}_+ - \tilde{v}_+ g_+(\tilde{w}_+)}{g_+(\tilde{v}_+)\tilde{w}_+ + \tilde{v}_+ g_+(\tilde{w}_+)} \right\} \\
&\qquad\qquad\qquad = \delta_k^+ \delta_k^{\langle 2\rangle} \left\{ \tilde{G}_{\boldsymbol{u}} - \delta_k^- \tilde{G}_{\tilde{\boldsymbol{u}}_+} - \delta_k^+ \tilde{G}_{\tilde{\boldsymbol{u}}_-} \right\},
\end{aligned}
\right.
$$

where $\boldsymbol{u} = (u, v, w, \zeta)$, $\tilde{\boldsymbol{u}}_+ = (\tilde{u}_+, \tilde{v}_+, \tilde{w}_+, \tilde{\zeta}_+) \cong \delta_k^+ \boldsymbol{u}$, $\tilde{\boldsymbol{u}}_- = s_k^- \tilde{\boldsymbol{u}}_+$, $g_-(a_-) = s_k^- g_+(a_+)$, $\tilde{G}_{\boldsymbol{u}}$ is the (new) discrete variational derivative with $\boldsymbol{u}$ and $\tilde{G}_{\tilde{\boldsymbol{u}}_\pm}$ is one with $\tilde{\boldsymbol{u}}_\pm$.

0478-E

Properties of the new scheme in the previous page

The previous scheme is based on the symmetric-linear decomposition $G(u,v,w) = uf(v)w$ and it's properties are...

- It is a 4-timestep scheme.
- It is Explicit! ... so, it is probably unstable.
- It is structure-preserving.

$$
\begin{aligned}
\delta_n^+ G(\boldsymbol{u}, \tilde{\boldsymbol{u}}_\pm) &= \frac{1}{\Delta t}\left(\tilde{G}_{\boldsymbol{u}}\,\delta U(\boldsymbol{u}) + \tilde{G}_{\tilde{\boldsymbol{u}}_+}\delta U(\tilde{\boldsymbol{u}}_+) + \tilde{G}_{\tilde{\boldsymbol{u}}_-}\delta U(\tilde{\boldsymbol{u}}_-)\right)\\
&= \tilde{G}_{\boldsymbol{u}}\,\delta_k^{\langle 2\rangle}\left(\tilde{G}_{\boldsymbol{u}} - \delta_k^-\tilde{G}_{\tilde{\boldsymbol{u}}_+} - \delta_k^+\tilde{G}_{\tilde{\boldsymbol{u}}_-}\right)\\
&\quad + \tilde{G}_{\tilde{\boldsymbol{u}}_+}\,\delta_k^+\delta_k^{\langle 2\rangle}\left(\tilde{G}_{\boldsymbol{u}} - \delta_k^-\tilde{G}_{\tilde{\boldsymbol{u}}_+} - \delta_k^+\tilde{G}_{\tilde{\boldsymbol{u}}_-}\right)\\
&\quad + \tilde{G}_{\tilde{\boldsymbol{u}}_-}\,\delta_k^-\delta_k^{\langle 2\rangle}\left(\tilde{G}_{\boldsymbol{u}} - \delta_k^-\tilde{G}_{\tilde{\boldsymbol{u}}_+} - \delta_k^+\tilde{G}_{\tilde{\boldsymbol{u}}_-}\right)\\
&= \left(\tilde{G}_{\boldsymbol{u}} - \delta_k^-\tilde{G}_{\tilde{\boldsymbol{u}}_+} - \delta_k^+\tilde{G}_{\tilde{\boldsymbol{u}}_-}\right)\delta_k^{\langle 2\rangle}\left(\tilde{G}_{\boldsymbol{u}} - \delta_k^-\tilde{G}_{\tilde{\boldsymbol{u}}_+} - \delta_k^+\tilde{G}_{\tilde{\boldsymbol{u}}_-}\right)\\
&\leq 0 \qquad \text{(in summation context, by summation by parts)}
\end{aligned}
$$

0478-E

Scheme obtained by one of quadratic approximations

Using a quadratic approximation $G(u, v, w) = u^2 f(v) w^2$, we can design a new DVDM scheme in similar form with the following definitions.

$$\begin{aligned} \delta U(\boldsymbol{u}) &\overset{\text{def}}{=} \frac{1}{C(v,w)} \left\{ (u - \zeta) + \left(\frac{u^2 + \zeta^2}{u + \zeta} \right) \left(\frac{f(v)w^2 - v^2 f(w)}{f(v)w^2 + v^2 f(w)} \right) \right\}, \\ \frac{\delta \tilde{G}}{\delta(\boldsymbol{u})} &\overset{\text{def}}{=} C(v,w)(u + \zeta) \left(\frac{f(v)w^2 + v^2 f(w)}{2} \right) \end{aligned}$$

The properties of the new scheme obtained from these definitions are:

- It is a 4-timestep scheme.
- The solver is nonlinear-implicit, but just quadratic. So, to obtain new timestep solutions is much easier than one for orthodox DVDM scheme.
- It is also structure-preserving.

0478-E

Scheme obtained by other asymmetric approximations

We can also adopt some asymmetric approximations, for example, $G(u,v) = uf(v)$, $G(u,v) = u^2 f(v)$, and so on. Of course we can desinze new DVDM scheme from those decompositions.
For example, the definitions of discrete mathematical terms for $G(u,v) = u^2 f(v)$ are the followin ones.

$$\begin{aligned}
\delta U(\boldsymbol{u}) &\stackrel{\text{def}}{=} \frac{1}{C(v,w)} \left\{ (u-v) + \left(\frac{u^2+v^2}{u+v} \right) \left(\frac{f(v)-f(w)}{f(v)+f(w)} \right) \right\}, \\
\frac{\delta \tilde{G}}{\delta(\boldsymbol{u})} &\stackrel{\text{def}}{=} C(v,w)(u+v) \left(\frac{f(v)+f(w)}{2} \right)
\end{aligned}$$

The properties of those new schemes obtained from above definitions are:

- They are 3-timestep scheme.
- The solver is explicit!(for linear decomposition) / just quadratic (for quadratic one).
- They are also structure-preserving.

0478-E

Now, we can try to design schemes for concrete problems. Here we try to design a new asymmetric-quadratic DVDM scheme for the higher Cahn–Hilliard equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\frac{\delta G}{\delta u}, \qquad G(u, u_x) = \frac{u^8}{8} - \frac{u^2}{2} - \frac{q}{2}(u_x)^2,\ q < 0,$$

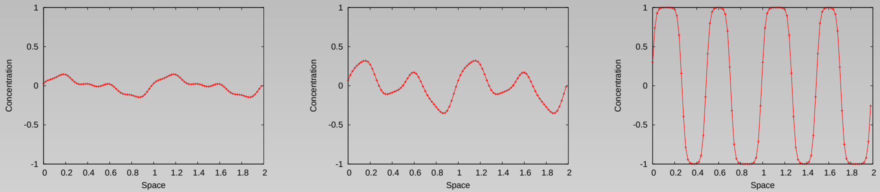
based the following asymmetric-quadratic decompositions:

$$\begin{aligned} \frac{u^8}{8} - \frac{u^2}{2} \quad &\rightarrow \quad u^2\left(\frac{v^6}{8} - \frac{1}{2}\right), \\ -\frac{q}{2}(u_x)^2 \quad &\rightarrow \quad -\frac{q}{2}\left(\frac{(\tilde{u}_+)^2 + (\tilde{v}_+)^2 + (\tilde{u}_-)^2 + (\tilde{v}_-)^2}{4}\right), \end{aligned}$$

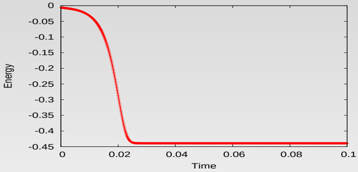
and the correction coefficient $C(v, w) = 4\left(\dfrac{v^6 + w^6 - 2}{v^6 + w^6 - 8}\right)$ and $\tilde{C}(\tilde{v}_\pm, \tilde{w}_\pm) = 1/2$.

0453-E

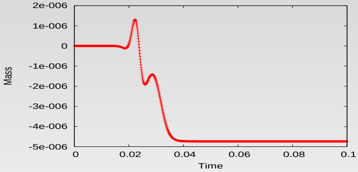
Numerical solutions by the new scheme for the higher Cahn–Hilliard eq.



Time Step $= 0$ $\qquad$ 10000 $\qquad$ 100000



Energy

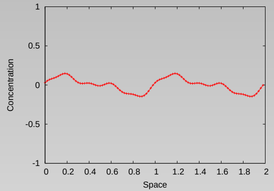


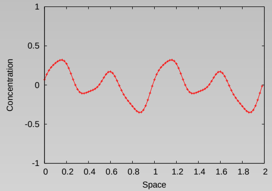
Mass

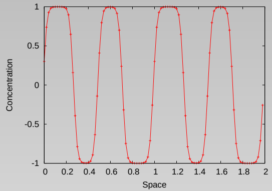
where $q = -0.001$, $\Delta x = 0.02$, $\Delta t = 1.0 \times 10^{-6}$.

Comp. time is 6.03 sec. with an Euler method guidance for 10000 time steps.

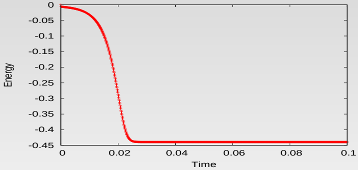
Numerical solutions by the Predictor–Corrector DVDM method for the higher Cahn–Hilliard eq.



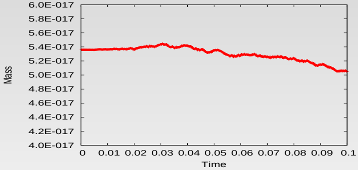




Time Step $= 0$ $\quad 10000 \quad 100000$



Energy



Mass

where $q = -0.001$, $\Delta x = 0.02$, $\Delta t = 1.0 \times 10^{-6}$.

For 10000 steps, PC DVDM scheme: 1.375 sec. Normal DVDM: 43.296 sec.

Example for an exponential heat equation

Here we try to design a new asymmetric DVDM scheme for a non-polynomial heat equation.

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\frac{\delta G}{\delta u}, \qquad G(u, u_x) = \exp(u)\,(= \frac{\delta G}{\delta u}),$$

based the following asymmetric-linear / quadratic approximations:

$$\text{For an explicit DVDM scheme} \quad : \quad e^u \to u\left(\frac{e^v - 1}{v}\right) + 1,$$

$$\text{For an quadratic DVDM scheme} \quad : \quad e^u \to u^2\left(\frac{e^v - 1 - v}{v^2}\right) + 1 + v.$$

where $u = U_k^{(n+1)}$, $v = U_k^{(n)}$ and $w = U_k^{(n-1)}$.

The designed DVDM scheme will be shown in the next page...

0454-E

We obtain the following asymmetric DVDM schemes:

[Explicit DVDM scheme]

$$\frac{h(v)u - h(w)v}{\Delta t} = \left(\frac{e^{v} + e^{w}}{2}\right) \delta_k^{\langle 2 \rangle} \left(\frac{e^{v} + e^{w}}{2}\right)$$

where $h(a) = (\exp(a) - 1)/a$, $u = U_k^{(n+1)}$, $v = U_k^{(n)}$ and $w = U_k^{(n-1)}$.

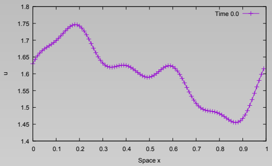
[Quadratic DVDM scheme]

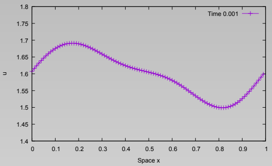
$$\frac{\phi(v)u^2 - \phi(w)v^2 + v - w}{\Delta t} = \varphi(v, w)(u + v)\ \delta_k^{\langle 2 \rangle}(\varphi(v, w)(u + v))$$

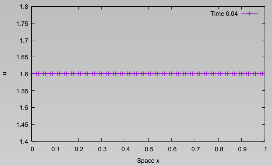
where $\phi(a) = (\exp(a) - 1 - a)/(a^2)$ and
$\varphi(a, b) = (e^a + e^b)\left\{\phi(a) + \phi(b)\right\} / \left[4\left\{a\phi(a) + b\phi(b)\right\}\right]$.

0454-E

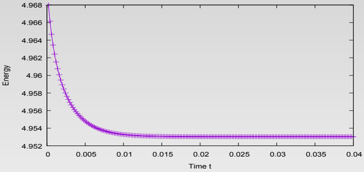
Numerical solutions by the quadratic scheme for the exponential heat eq.

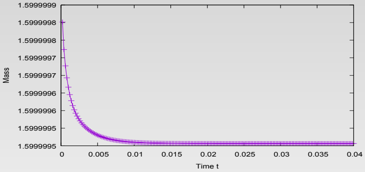






Time Step $= 0$ $\qquad$ 100 $\qquad$ 4000





Energy $\qquad$ Mass

where B.C. is periodic, $\Delta x = 0.01$, and $\Delta t = 1.0 \times 10^{-5}$. The scheme is implemented as a predictor-corrector scheme, an Euler method is the predictor.

Misc. of schemes

We designed and implemented the following schemes for this problem:

1. an Euler scheme:
   works well. $\max \Delta t = 9.84862 \cdots \times 10^{-6}$.
2. a Crank–Nicolson scheme (w Euler predictor):
   works well. $\max \Delta t = 9.31789 \cdots \times 10^{-6}$.
3. the explicit DVDM scheme:
   works, **but makes weird solutions**. $\max \Delta t = 5.51849 \cdots \times 10^{-6}$.
4. the quadratic DVDM scheme (w Euler predictor):
   works well. $\max \Delta t = 1.02707 \cdots \times 10^{-5}$.
5. a normal DVDM scheme (GSL solver):
   does not work because the solver failed.
6. a normal DVDM scheme (w Euler predictor):
   works well. $\max \Delta t = 9.29992 \cdots \times 10^{-6}$.
7. a normal DVDM scheme (w the explicit DVDM predictor):
   works well. $\max \Delta t = 8.96001 \cdots \times 10^{-6}$.

0454-E

2.4 The 3rd example of relaxation: no-extra time steps and asymmetric definition

$\boxed{\textbf{idea}}$ **: For PDE numerical schemes, most of computation cost comes from the terms mixed by space-derivatives. So ...**

We decompose the following variation without any extra time step:

$$G(u) - G(v) \xrightarrow[\text{decomposition}]{\text{discrete}} \left(\text{nice approx. of } \frac{\delta G}{\delta u}\right) \times (\text{approx. of } u - v)$$

Example:

$$\begin{aligned} u^8 - v^8 &= (8v^7) \left\{ \frac{u^7 + u^6 v + u^5 v^2 + u^4 v^3 + u^3 v^4 + u^2 v^5 + u v^6 + v^7}{8v^7} \right\} (u - v) \\ &=: \frac{\delta G_d}{\delta v} \qquad dU \end{aligned}$$

$$\begin{aligned} e^u - e^v &= e^v \left(e^{u-v} - 1\right) \\ &=: \frac{\delta G_d}{\delta v} \quad dU \end{aligned}$$

0479-E

Re-define the discrete variational derivative

For a function $f(u)$, from the following equation:

$$f(U^+) - f(U) = f'(U) \cdot \frac{\frac{f(U^+)-f(U)}{U^+-U}}{f'(U)} (U^+ - U),$$

we obtain the following new definitions:

$$\frac{\delta \tilde{G}}{\delta(U^+, U)} \overset{\text{def}}{=} f'(U),$$

$$\delta U(U^+, U) \overset{\text{def}}{=} \frac{\frac{f(U^+)-f(U)}{U^+-U}}{f'(U)} (U^+ - U)$$

where $U^+ = U_k^{(n+1)}$, $U = U_k^{(n)}$.

Note that this $\frac{\delta \tilde{G}}{\delta(U^+, U)}$ is explicit. So, we can design some "light" schemes based on these definitions.

0479-E

New schemes based on those new defintions

Example: For the typical PDE $u_t = \partial_x^2(\delta G/\delta u)$, if we define the discrete energy function as $\tilde{G}(u, \tilde{u}_+, \tilde{u}_-) = f(u) + g_+(\tilde{u}_+) + g_-(\tilde{u}_-)$, where $\tilde{u}_\pm \cong \delta_k^{\pm} u$, then we can derive the following equality:

$$\begin{aligned} &\tilde{G}(u, \tilde{u}_+, \tilde{u}_-) - \tilde{G}(v, \tilde{v}_+, \tilde{v}_-) \\ &\quad = \quad f'(v) dU(u, v) + g'_+(\tilde{v}_+) d\tilde{U}_+(\tilde{u}_+, \tilde{v}_+) + g'_-(\tilde{v}_-) d\tilde{U}_-(\tilde{u}_-, \tilde{v}_-), \end{aligned}$$

So, we can define the disrete varitional derivative for $\tilde{G}$:

$$\text{discrete variational derivative } H(v, v_\pm) \stackrel{\text{def}}{=} f'(v) - \delta_k^- g'_+(\tilde{v}_+) - \delta_k^+ g'_-(\tilde{v}_-)$$

Now we can desing the following new DVDM scheme:

$$\begin{cases} \dfrac{dU(u, v)}{\Delta t} = \delta_k^{\langle 2 \rangle} H(v, v_\pm), \\ \dfrac{d\tilde{U}_+(\tilde{u}_+, \tilde{v}_+)}{\Delta t} = \delta_k^+ \delta_k^{\langle 2 \rangle} H(v, v_\pm), \end{cases}$$

where $u = U_k^{(n+1)}$, $v = U_k^{(n)}$, $\tilde{u}_\pm \cong \delta_k^{\pm} U_k^{(n+1)}$, $\tilde{v}_\pm \cong \delta_k^{\pm} U_k^{(n)}$.

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For example, the scheme in the previous page has the following properties:

- It is explicit in essence $\cdots$ nonlinear terms exist in the left-hand-side. So, the scheme is NOT a system of equations.
- Of course, the scheme is structure-preserving.

$$
\begin{aligned}
\sum_{k=0}^{N}{}'' \, \delta_n^+ G(u, \tilde{u}_\pm)\Delta x
&= \sum_{k=0}^{N}{}'' \, \frac{1}{\Delta t}\left(f'(v)\,\delta U + g'_+(\tilde{v}_+)d\tilde{U}_+ + g'_-(\tilde{v}_-)d\tilde{U}_-\right)\Delta x \\
&= \sum_{k=0}^{N}{}'' \, \left(f'(v)\delta_k^{\langle 2\rangle} H + g'_+(\tilde{v}_+)\delta_k^+\delta_k^{\langle 2\rangle} H + g'_-(\tilde{v}_-)\delta_k^-\delta_k^{\langle 2\rangle} H\right)\Delta x \\
&= \sum_{k=0}^{N}{}'' \, \left\{f'(v) - \delta_k^- g'_+(\tilde{v}_+) - \delta_k^+ g'_-(\tilde{v}_-)\right\}\delta_k^{\langle 2\rangle} H\Delta x \\
&= \sum_{k=0}^{N}{}'' \, H\delta_k^{\langle 2\rangle} H\Delta x \qquad \leq 0
\end{aligned}
$$

0479-E

Here we try to design a new asymmetric DVDM scheme for a non-polynomial heat equation.

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\frac{\delta G}{\delta u}, \qquad G(u, u_x) = \exp(u)\,(= \frac{\delta G}{\delta u}),$$

based the following asymmetric decomposition:

$$e^u - e^v = e^v\left(e^{u-v} - 1\right).$$

where $u = U_k^{(n+1)}$, $v = U_k^{(n)}$.

The following new scheme is obtained.

[A single step, almost explicit DVDM scheme]

$$u = v + \log\left\{1 + \Delta t \delta_k^{\langle 2\rangle}\left(e^v\right)\right\}$$

0471-E

Misc. of schemes

We designed and implemented the following schemes for this problem:

1. an Euler scheme:
   works well. $\max \Delta t = 9.84862 \cdots \times 10^{-6}$.
2. a Crank–Nicolson scheme (w Euler predictor):
   works well. $\max \Delta t = 9.31789 \cdots \times 10^{-6}$.
3. a single-step, almost explicit DVDM scheme:
   works well. $\max \Delta t = 1.250000 \cdots \times 10^{-5}$ (the largest value).
4. the two-step explicit DVDM scheme:
   works, **but makes weird solutions**. $\max \Delta t = 5.51849 \cdots \times 10^{-6}$.
5. the two-step quadratic DVDM scheme (w Euler predictor):
   works well. $\max \Delta t = 1.02707 \cdots \times 10^{-5}$.
6. a normal nonlinear DVDM scheme (GSL solver):
   does not work because the solver failed.
7. a normal nonlinear DVDM scheme (w Euler predictor):
   works well. $\max \Delta t = 9.29992 \cdots \times 10^{-6}$.
8. a normal nonlinear DVDM scheme (w the explicit DVDM predictor):
   works well. $\max \Delta t = 8.96001 \cdots \times 10^{-6}$.

0471-E

Summary

Summary

- Discrete gradients are approximations of (continuous) gradients
- "**Discrete gradients**" + "**discrete Green formula**"
  = some **structure-preserving methods for differential equations**.
- Conventional conditions derive symmetric discrete gradients and symmetric numerical schemes. Computation costs by symmetric schemes are too heavy for strongly nonlinear problems.
- If we relax those two conditions, we can derive flexible discrete gradients:
  examples:
  - symmetric/asymmetric linearized DVDM (Discrete Variational Derivative Methods that design ST-schemes for PDEs),
  - asymmetric (non-extra time step) DVDM .
- Via those flexible discrete gradients, we can design some structure-preserving schemes which has "weak nonlinearity".
- (In future) We would like to generalize discrete gradient to apply it for complex integralation in numerical analysis context... but how?

inner.

Thank you for listening !!

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