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Integral Preserving Numerical Methods on Moving Grids

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Abstract

Integral preservation for ordinary and partial differential equations is defined, and the integral preserving discrete gradient methods and discrete variational derivative methods on fixed grids are given, with a formal definiton for the latter in a general grid case.

General moving grid methods are presented, with special emphasis on grid movement strategies. The integral preserving modified discrete variational derivative methods for moving grids are introduced, and integral preserving projection methods are shown to be a subset of these. New interpolation techniques are introduced, and a general solution procedure for implementing the methods is presented. Two alternative integral preserving moving grids methods are briefly presented.

The modified discrete variational derivative methods are applied to two different partial differential equations, and numerical experiments are performed on moving grids. The integral preserving property of the methods is demonstrated and their advantages and applications are discussed.

Samandrag

Integralbevaring for ordinære og partielle differensiallikningar er definert, og integralbevarande metodar av diskrete gradientar og av diskrete variasjonsderiverte er gjevne, sistnemnde med ein formell definisjon på generelle faste gitter.

Generelle løysingsmetodar på flyttande gitter er presentert, med særskild vekt lagt på strategiar for å flytta gitteret. Modifiserte integralbevarande metodar av diskrete variasjonsderiverte på flyttande gitter er introdusert, og integralbevarande projeksjonsmetodar er vist å vera ei undermengd av desse. Nye interpolasjonsteknikkar er introdusert, og ein generell framgangsmåte for å implementera metodane er presentert. Korte presentasjonar av to alternative integralbevarande metodar på flyttande gitter er òg gjevne.

Dei modifiserte integralbevarande metodane av diskrete variasjonsderiverte er nytta på to ulike partielle differensiallikningar, og numeriske forsøk er utført på flyttande gitter. Den integralbevarande eigenskapen til metodane er demonstrert og nytteverdi og bruksområde er diskutert.

Preface

This master's thesis was written during my tenth and final semester of the Master's Degree Programme in Applied Physics and Mathematics, with specialization in Industrial Mathematics, at the Norwegian University of Science and Technology.

The thesis is a continuation of my work with the specialization project in the previous semester, and it has been inspiring to feel how my insight and understanding of the subject has grown over the last year. Although challenging and frustrating at times, I have found the work to be very rewarding.

I would like to thank my supervisor, Prof. Brynjulf Owren, for helpful ideas and guidance, as well as inspiring enthusiasm for the subject.

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Chapter 1

Introduction

Difference schemes with a conservation property was first introduced by Courant, Friedrichs and Lewy in [6], originally published in 1928, where a discrete conservation law for a finite difference approximation of the wave equation is deduced. Their method is often called *energy method* [11] or *energy-conserwing method* [18], although the conserved quantity is often not energy in the physical sense. The primary motivation for developing conservative methods was originally to devise a norm that can guarantee the global stability. This was still an objective, in addition to proving existence and uniqueness of solutions, when the energy method garnered newfound interest in the 1950s and 1960s, resulting in new developments like generalizations of the method and more difference schemes, summarized by Richtmyer and Morton in [23].

In the 1970s, the motivation behind studying schemes that preserve invariant quantities shifted to the conservation property itself. Li and Vu-Quoc present in [18] a historical survey of conservative methods developed up to the early 1990s. They state that this line of work is motivated by the fact that in some situations, the success of a numerical solution will depend on its ability to preserve one or more of the invariant properties of the original differential equation. In addition, as noted in [14] and [4], there is the general idea that transferring more of the properties of the original continuous dynamical system over to a discrete dynamical system, may lead to a more accurate numerical approximation of the solution, especially over longer periods of time.

In recent years, there has been a greater interest in developing completely systematic methods applicable to larger classes of differential equations. Hairer, Lubich and Wanner give in [14] a presentation of *geometric integrators* for differential equations, i.e. methods for solving ordinary differential equations (ODEs) that preserve a *geometric structure* of the system. Examples of such geometric structures are symplectic structures, symmetries, reversing symmetries, isospectrality, Lie group integrators, orthonormality, first integrals, and other integral invariants, like volume and invariant measure. Studies of numerical methods that preserve each of these structural properties are mentioned in [19].

In this thesis we will be concerned with the preservation of first integrals. The *discrete gradient methods*, first explicitly given by Gonzalez in [13], are among the most popular methods for preserving first integrals for ODEs. Recently, integral preserving methods for partial differential equations (PDEs) based on the discrete gradient methods have been developed on fixed, uniform grids. Different approaches to achieving this has been collected to a unified framework in [9], where these integral preserving methods for PDEs are called *discrete variational derivative methods*.

The primary object of this thesis is to extend the discrete variational derivative methods to non-uniform and moving grids. Non-uniform grids is of exceptional importance for multidimensional problems, since the use of uniform grids would greatly restricts the types of domains possible to discretize. Yaguchi, Matsuo and Sugihara present in [25] and [26] two different discrete variational derivative methods on fixed, non-uniform grids, specifically defined for certain classes of PDEs. In this thesis, we extend the theory of [9] to non-uniform grids, thus obtaining a framework for developing integral preserving methods on general fixed grids, corresponding to all existing discrete variational derivative methods on uniform grids.

Furthermore, the possibility of grid adaptivity can be of critical importance when solving PDEs numerically. Even for one-dimensional problems, the computational cost with a fixed grid can be extensive in cases where the solution has large variations occurring over small portions of the physical domain. Taking as an example a propagating wave, the sections of large variations in the solution, and hence the sections where the greatest number of grid points is needed, will move with time, making it difficult to create a good fixed non-uniform grid for a numerical discretization of the problem. To our knowledge, integral preserving methods on moving grids have not yet been studied in the literature. With basis in the discrete variational derivative methods on fixed grids, we develop such methods in this thesis.

The subsequent chapter begins with the definition of integral preserving methods for ODEs, before presenting the discrete gradient methods. Integral preserving methods for PDEs are then defined, before the discrete variational derivative methods on fixed grids are introduced, first for uniform and then for non-uniform grids. Chapter 3 gives a brief introduction to moving grid methods, mostly focusing on methods for redistributing the grid at every time step.

Integral preserving moving grid methods are then introduced in Chapter 4, in form of the *modified discrete variational derivative methods*. Furthermore, integral preserving projection methods on moving grids are introduced and shown to be a subset of the modified discrete variational derivative methods. The interpolation of the solution from one grid to another is discussed in the light of these methods, and general solution procedures are presented. The chapter concludes with a brief discussion of other possible integral preserving moving grid methods, not fitting into the framework of the modified discrete variational derivative methods.

In chapter 5, we present examples of the modified discrete variational derivative methods for two different nonlinear, dispersive PDEs, the KdV equation and the BBM equation. Numerical results are presented and discussed. The thesis ends with a conclusion in chapter 6.

Chapter 2

Integral Preserving Methods on Fixed Grids

The aim of this chapter is to give an introduction to the integral preserving discrete variational derivative methods for solving partial differential equations (PDEs). First however, we will give a short introduction to the integral preserving discrete gradient methods for ordinary differential equations (ODEs), since they are strongly connected to the discrete variational derivative methods for PDEs. We will furthermore state what is meant by integral preservation, both in the continuous and discrete case, and establish the properties of the PDE that leads to the integral preservation. The chapter concludes with a general framework for discrete variational derivative methods on general fixed grids, which to our knowledge is not previously presented in the literature.

2.1 Integral Preserving Methods for ODEs

We will now first define integral preserving methods for ODEs, and then introduce the concept of discrete gradients and discrete gradient methods, before presenting four different discrete gradients. A more thorough presentation of discrete gradient methods, with various properties of the discrete gradients and numerical examples, can be found in [9].

2.1.1 Preservation of First Integrals

For a given ordinary differential equation of the form

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = f(\mathbf{x}), \qquad \mathbf{x} \in \mathbb{R}^d, \tag{2.1}$$

a *first integral* is a function $I(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}$ that satisfies

$$\nabla I(\mathbf{x})^{\mathrm{T}} f(\mathbf{x}) = 0 \qquad \forall \mathbf{x}. \tag{2.2}$$

This implies that
$$\frac{\mathrm{d}I}{\mathrm{d}t} = \nabla I(\mathbf{x})^{\mathrm{T}} \left(\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \right) = 0,$$
and hence $I(\mathbf{x}(t)) = I(\mathbf{x}(t_0)) =$ *constant* for all solutions $\mathbf{x}$ of (2.1). Other terms used for the first integral $I(\mathbf{x})$ are *invariant*, *conserved quantity* and *constant of motion* [14].

As proven by McLachlan, Quispel and Robidoux in [19], the property (2.2) is satisfied, under some mild technical conditions, if and only if there exists some skew-symmetric matrix $S(x)$ such that
$$f(\mathbf{x}) = S(\mathbf{x})\nabla I(\mathbf{x}). \tag{2.3}$$
The fact that (2.2) follows from (2.3) is verified by
$$\nabla I(\mathbf{x})^{\mathrm{T}} f(\mathbf{x}) = \nabla I(\mathbf{x})^{\mathrm{T}} S(\mathbf{x})\nabla I(\mathbf{x}) = 0, \tag{2.4}$$
where the last equality is a result of the skew-symmetric property of $S(\mathbf{x})$. Utilizing (2.3), we may write (2.1) on the form
$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = S(\mathbf{x})\nabla I(\mathbf{x}), \tag{2.5}$$
representing any ODE with a preserved first integral $I(\mathbf{x})$.

A numerical method for solving (2.5) is said to be an *integral preserving method* if the numerical approximation $I(\mathbf{x}_n) \approx I(\mathbf{x}(t_n))$ satisfies $I(\mathbf{x}_n) = I(\mathbf{x}(t_0))$ for all values of $n \geq 0$.

2.1.2 Discrete Gradient Methods

A discrete gradient of the first integral $I(\mathbf{x})$ is defined in [14] as a continuous function $\overline{\nabla} I(\hat{\mathbf{x}}, \mathbf{x})$ of $(\hat{\mathbf{x}}, \mathbf{x})$ satisfying
$$\overline{\nabla} I(\hat{\mathbf{x}}, \mathbf{x})^{\mathrm{T}} (\hat{\mathbf{x}} - \mathbf{x}) = I(\hat{\mathbf{x}}) - I(\mathbf{x}), \tag{2.6}$$
$$\overline{\nabla} I(\mathbf{x}, \mathbf{x}) = \nabla I(\mathbf{x}). \tag{2.7}$$

When a discrete gradient is chosen, what remains is to find a skew-symmetric matrix $\overline{S}(\hat{\mathbf{x}}, \mathbf{x})$ approximating to $S(\mathbf{x})$. It is often required that $\overline{S}(\mathbf{x}, \mathbf{x}) = S(\mathbf{x})$ [14, 4]. We then have the discrete gradient method given by
$$\frac{\mathbf{x}_{n+1} - \mathbf{x}_n}{\Delta t} = \overline{S}(\mathbf{x}_{n+1}, \mathbf{x}_n)\overline{\nabla} I(\mathbf{x}_{n+1}, \mathbf{x}_n), \tag{2.8}$$
where Δt is the time step and $\mathbf{x}_n \approx \mathbf{x}(t_n)$ is the numerical approximation to $\mathbf{x}$ at time step number n, consistent with the ordinary differential equation (2.5). We have that the discrete gradient methods preserve the first integral, as by coupling (2.6) with (2.8), we get that
$$\begin{aligned} I(\mathbf{x}_{n+1}) - I(\mathbf{x}_n) &= \overline{\nabla} I(\mathbf{x}_{n+1}, \mathbf{x}_n)^{\mathrm{T}} \left(\Delta t \cdot \overline{S}(\mathbf{x}_{n+1}, \mathbf{x}_n)\overline{\nabla} I(\mathbf{x}_{n+1}, \mathbf{x}_n) \right) \\ &= \Delta t \cdot \overline{\nabla} I(\mathbf{x}_{n+1}, \mathbf{x}_n)^{\mathrm{T}} \overline{S}(\mathbf{x}_{n+1}, \mathbf{x}_n)\overline{\nabla} I(\mathbf{x}_{n+1}, \mathbf{x}_n) = 0, \end{aligned}$$
for all $n \geq 0$, and consequently we have $I(\mathbf{x}_n) = I(\mathbf{x}_0) = I(\mathbf{x}(t_0)) =$ *constant*, for all $n \geq 0$.

2.1.3 Examples of Discrete Gradients

If $d = 1$ in (2.1), then the unique discrete gradient of $I(x)$ is given by

$$\overline{\nabla} I(\hat{x}, x) = \frac{I(\hat{x}) - I(x)}{\hat{x} - x}. \tag{2.9}$$

For $d \geq 2$, there are infinitely many different discrete gradients. The *coordinate increment discrete gradient* introduced by Itoh and Abe in [17] is given by

$$\overline{\nabla}_{\mathrm{CI}} I(\hat{\mathbf{x}}, \mathbf{x}) := \begin{pmatrix} \frac{I(\hat{x}_1, x_2, x_3, \ldots, x_{d-1}, x_d) - I(x_1, x_2, x_3, \ldots, x_{d-1}, x_d)}{\hat{x}_1 - x_1} \\ \frac{I(\hat{x}_1, \hat{x}_2, x_3, \ldots, x_{d-1}, x_d) - I(\hat{x}_1, x_2, x_3, \ldots, x_{d-1}, x_d)}{\hat{x}_2 - x_2} \\ \vdots \\ \frac{I(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_{d-2}, \hat{x}_{d-1}, x_d) - I(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_{d-2}, x_{d-1}, x_d)}{\hat{x}_{d-1} - x_{d-1}} \\ \frac{I(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_{d-2}, \hat{x}_{d-1}, \hat{x}_d) - I(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_{d-1}, \hat{x}_{d-1}, x_d)}{\hat{x}_d - x_d} \end{pmatrix}, \tag{2.10}$$

where x_i and $\hat{x}_i$ denotes the i'th element, for $i = 1, 2, ..., d$, of $\mathbf{x}$ and $\hat{\mathbf{x}}$, respectively. As noted in [19], it is here understood that $0/0$ leads to $\frac{\partial I}{\partial x_i}$.

Gonzalez introduced in [13] what has been called the *midpoint discrete gradient*,

$$\overline{\nabla}_{\mathrm{M}} I(\hat{\mathbf{x}}, \mathbf{x}) := \nabla I\left(\frac{\hat{\mathbf{x}} + \mathbf{x}}{2}\right) + \frac{I(\hat{\mathbf{x}}) - I(\mathbf{x}) - \nabla I\left(\frac{\hat{\mathbf{x}}+\mathbf{x}}{2}\right)^{\mathrm{T}} (\hat{\mathbf{x}} - \mathbf{x})}{|\hat{\mathbf{x}} - \mathbf{x}|^2} (\hat{\mathbf{x}} - \mathbf{x}). \tag{2.11}$$

We remark that in the case that $\nabla I\left(\frac{\hat{\mathbf{x}}+\mathbf{x}}{2}\right)$ is itself a discrete gradient satisfying (2.6), the numerator in the second term of the midpoint discrete gradient is zero, and thus the midpoint discrete gradient is $\nabla I\left(\frac{\hat{\mathbf{x}}+\mathbf{x}}{2}\right)$.

The type which later has been labeled *mean value discrete gradient* [19] or *averaged vector field discrete gradient* [22, 7] was first introduced by Harten, Lax and van Leer in [15]. Henceforth it will be called the averaged vector field discrete gradient. It is defined by

$$\overline{\nabla}_{\mathrm{AVF}} I(\hat{\mathbf{x}}, \mathbf{x}) := \int_0^1 \nabla I\left((1 - \xi)\, \mathbf{x} + \xi \hat{\mathbf{x}}\right) \mathrm{d}\xi. \tag{2.12}$$

A new discrete gradient, based on the discrete variational derivative method presented by Furihata in [10] and expanded upon by Cohen and Raynaud in [5], is introduced in [9]. Assume that we can write the first integral $I(\mathbf{x})$ on the form

$$I(\mathbf{x}) = \sum_l c_l \prod_{i=1}^{d} f_i^l(x_i), \tag{2.13}$$

where c_l are constants, and x_i are the elements of $\mathbf{x}$, for $i = 1, 2, ..., d$. Then the *product discrete gradient* $\overline{\nabla}_{\mathrm{P}} I(\hat{\mathbf{x}}, \mathbf{x})$ is defined by its elements

$$\overline{\nabla}_{\mathrm{P}} I(\hat{\mathbf{x}}, \mathbf{x})_i = \sum_l \frac{c_l}{2} \frac{\mathrm{d} f_i^l}{\mathrm{d}(\hat{x}_i, x_i)} \left(\prod_{j=1}^{i-1} f_j^l(\hat{x}_j) + \prod_{j=1}^{i-1} f_j^l(x_j) \right) \prod_{k=i+1}^{d} \frac{f_k^l(\hat{x}_k) + f_k^l(x_k)}{2},$$

for $i = 1, 2, ..., d$, where

$$\frac{\mathrm{d}f}{\mathrm{d}(\hat{x}, x)} := \begin{cases} \frac{f(\hat{x})-f(x)}{\hat{x}-x} & \text{if} \quad \hat{x} \neq x \\ \frac{\mathrm{d}}{\mathrm{d}x} f(x) & \text{if} \quad \hat{x} = x. \end{cases} \tag{2.14}$$

The term (2.14) may be evaluated with help from the rule

$$\delta\left[(f \cdot g)\right] = \delta\left[f\right] \cdot \mu\left[g\right] + \delta\left[g\right] \cdot \mu\left[f\right], \tag{2.15}$$

where

$$\begin{aligned} \delta\left[f\right] &= f(\hat{x}) - f(x), \\ \mu\left[f\right] &= \frac{f(\hat{x}) + f(x)}{2}. \end{aligned}$$

In [9] it is shown that there exists an infinite number of discrete gradients for any first integral with $d \geq 2$. Given a discrete gradient $\overline{\nabla}_K I(\hat{\mathbf{x}}, \mathbf{x})$, any discrete gradient satisfying (2.6) and (2.7) is given by

$$\overline{\nabla}_N I(\hat{\mathbf{x}}, \mathbf{x}) := \overline{\nabla}_K I(\hat{\mathbf{x}}, \mathbf{x}) + N(\hat{\mathbf{x}}, \mathbf{x}),$$

for a function $N(\hat{\mathbf{x}}, \mathbf{x}) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ satisfying

$$N(\hat{\mathbf{x}}, \mathbf{x})^{\mathrm{T}}(\hat{\mathbf{x}} - \mathbf{x}) = 0, \tag{2.16}$$

$$N(\mathbf{x}, \mathbf{x}) = 0, \tag{2.17}$$

which there is an infinite number of functions that do, if $d \geq 2$.

Example 2.1.1. Consider the double well system,

$$\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} = -2q(q^2 - 1), \tag{2.18}$$

which can be written on the form (2.3) with the first integral being the Hamiltonian

$$H(q, p) = \frac{1}{2}p^2 + \frac{1}{2}(q^2 - 1)^2. \tag{2.19}$$

and the skew-symmetric matrix being

$$S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The Hamiltonian (2.19) is a first integral of the from

$$I(\mathbf{x}) = \sum_{i=1}^{d} c_i f_i(x_i) + c_{d+1},$$

where $c_i \in \mathbb{R}$ are constants, and $f_i(x_i) : \mathbb{R} \to \mathbb{R}$ are functions, and hence, by Theorem 2 in [9], the coordinate increment, average vector field and product discrete gradients are identical for this problem. We get

$$\overline{\nabla}_{\mathrm{CI}} H(\hat{q}, \hat{p}, q, p) = \begin{pmatrix} \frac{1}{2}(\hat{q}+q)(\hat{q}^2+q^2-2) \\ \frac{1}{2}(\hat{p}+p) \end{pmatrix},$$

and the resulting integral preserving numerical scheme

$$\begin{pmatrix} q_{n+1}-q_n \\ p_{n+1}-p_n \end{pmatrix} = \frac{\Delta t}{2} \begin{pmatrix} p_{n+1}+p_n \\ -(q_{n+1}+q_n)(q_{n+1}^2+q_n^2-2) \end{pmatrix}$$

for solving (2.18). Furthermore,

$$\overline{\nabla}_{\mathrm{M}} H(\hat{q}, \hat{p}, q, p) = \begin{pmatrix} (\hat{q}+q)(\frac{1}{4}(\hat{q}+q)^2-1) \\ \frac{1}{2}(\hat{p}+p) \end{pmatrix} + \frac{1}{4}\frac{(\hat{q}-q)^3(\hat{q}+q)}{(\hat{q}-q)^2+(\hat{p}-p)^2} \begin{pmatrix} \hat{q}-q \\ \hat{p}-p \end{pmatrix},$$

and another scheme preserving (2.19) is given by

$$\begin{pmatrix} q_{n+1}-q_n \\ p_{n+1}-p_n \end{pmatrix} = \frac{\Delta t}{4} \begin{pmatrix} 2(p_{n+1}+p_n) + \frac{(q_{n+1}-q_n)^3(q_{n+1}+q_n)(p_{n+1}-p_n)}{(q_{n+1}-q_n)^2+(p_{n+1}-p_n)^2} \\ (q_{n+1}+q_n)(4-(q_{n+1}+q_n)^2) - \frac{(q_{n+1}-q_n)^4(q_{n+1}+q_n)}{(q_{n+1}-q_n)^2+(p_{n+1}-p_n)^2} \end{pmatrix}.$$

We have that

$$\overline{\nabla}_{\mathrm{CI}} H(\hat{q}, \hat{p}, q, p) = \overline{\nabla}_{\mathrm{M}} H(\hat{q}, \hat{p}, q, p) + N(\hat{q}, \hat{p}, q, p)$$

with

$$N(\hat{q}, \hat{p}, q, p) = \frac{1}{4}\frac{(\hat{q}-q)^2(\hat{q}+q)(\hat{p}-p)}{(\hat{q}-q)^2+(\hat{p}-p)^2} \begin{pmatrix} \hat{p}-p \\ q-\hat{q} \end{pmatrix},$$

satisfying (2.16)-(2.17).

2.2 Integral Preserving Methods for PDEs

We will now define first integrals of PDEs and numerical methods preserving an approximation of these. We will then introduce discrete variational derivative (DVD) methods, and establish their relationship to discrete gradient methods, first on uniform grids and then on general fixed grids.

2.2.1 First Integrals of PDEs

Consider now partial differential equations of the form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = f(\mathbf{x}, u^J) \qquad \mathbf{x} \in \mathbb{R}^d, u \in \mathcal{B}, \tag{2.20}$$

where we by u^J mean u itself and all its partial derivatives with respect to the independent variables $(x^1, ..., x^d)$, up to and including some degree ν. The function u belongs to the Hilbert space $\mathcal{B} \subseteq L^2$, where the inner product is the L^2 inner product $\langle \cdot, \cdot \rangle$, with values $u(\mathbf{x}, t) \in \mathbb{R}^l$. The precise definition of $\mathcal{B}$ will depend on the PDE (2.20), and we will not be discussing its technicalities in this thesis. We assume however that $\mathcal{B}$ consists of functions that are sufficiently regular for the purposes of the remains of this section. We then define a first integral of (2.20) to be a functional $\mathcal{I}[u]$ satisfying

$$\left\langle \frac{\delta \mathcal{I}}{\delta u}, f(\mathbf{x}, u^J) \right\rangle = 0 \qquad \forall \mathbf{x} \in \mathbb{R}^d, \quad \forall u \in \mathcal{B}, \tag{2.21}$$

where $\frac{\delta \mathcal{I}}{\delta u}$ is the *variational derivative* with respect to u defined by

$$\left\langle \frac{\delta \mathcal{I}}{\delta u}, v \right\rangle = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\bigg|_{\epsilon=0} \mathcal{I}[u + \epsilon v] \qquad \forall v \in \mathcal{B}. \tag{2.22}$$

By inserting (2.20) into (2.21), we get that

$$\frac{\mathrm{d}\mathcal{I}}{\mathrm{d}t} = \left\langle \frac{\delta \mathcal{I}}{\delta u}, \frac{\mathrm{d}u}{\mathrm{d}t} \right\rangle = 0,$$

and therefore $\mathcal{I}[u]$ is preserved in the sense that $\mathcal{I}[u(t)] = \mathcal{I}[u(t_0)] =$ *constant* for all solutions $u(\mathbf{x}, t)$ of (2.20).

We have that (2.21) is satisfied if there exists some differential operator $\mathcal{S}(u^J)$ that is antisymmetric with respect to the L^2-inner product such that we can write

$$f(\mathbf{x}, u^J) = \mathcal{S}(u^J) \frac{\delta \mathcal{I}}{\delta u}, \tag{2.23}$$

since we then will get

$$\left\langle \frac{\delta \mathcal{I}}{\delta u}, f(\mathbf{x}, u^J) \right\rangle = \left\langle \frac{\delta \mathcal{I}}{\delta u}, \mathcal{S}(u^J) \frac{\delta \mathcal{I}}{\delta u} \right\rangle = 0,$$

where the last equality is a property of the antisymmetric operator $\mathcal{S}(u^J)$.

In this thesis we will only consider integral preserving PDEs, i.e. PDEs where (2.23) is satisfied, and which therefore can be written on the form

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \mathcal{S}(u^J) \frac{\delta \mathcal{I}}{\delta u}, \tag{2.24}$$

where

$$\mathcal{I}[u] = \int_\Omega I(\mathbf{x}, u^J) \mathrm{d}x \qquad \Omega \subseteq \mathbb{R}^d, \tag{2.25}$$

with $\mathrm{d}x = \mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_d$. The class of PDEs of the form (2.24) contains the class of Hamiltonian PDEs, in which case $\mathcal{I}[u]$ would be the Hamiltonian $\mathcal{H}[u]$, and $\mathcal{S}(u^J)$ must satisfy the Jacobi identity [7, 21].

Since the exact value of the integral $\mathcal{I}[u]$ cannot be calculated numerically without knowing the function $u(\mathbf{x}, t)$, we define an *integral preserving numerical method* for solving (2.24) to be a method that preserves a consistent numerical approximation to $\mathcal{I}[u]$.

2.2.2 Discrete Variational Derivative Methods on Uniform Grids

There are published several different studies on how to develop the theory of dicrete gradient methods to partial differential equations. A method founded on developing discrete counterparts to the variational derivative is thoroughly reviewed by Furihata, Matsuo and coauthors in a large number of publications, see e.g. [10] and [12]. The average vector field method performed on the system of ordinary differential equations obtained by discretizing the PDE in spatial dimensions is presented, with examples for several different PDEs, in [3]. Dahlby and Owren present a method in [7] where they defer the spatial discretization and perform a semi-discrete variational derivative method on the system. However, as stated in [9], all these methods can be viewed as identical, in the sense that they lead to the same scheme, for a given discrete gradient and a given spatial discretization.

Following the definition in [9], a *discrete variational derivative method* for PDEs of the form (2.24), preserving the consistent approximation $\mathcal{I}_d(\mathbf{u}) : \mathbb{R}^M \to \mathbb{R}$ of the first integral $\mathcal{I}[u]$ on the uniform grid $X_h : x_0 < x_1 < ... < x_{M-1}$, represented by the vector $\mathbf{x} = (x_0, x_1, ..., x_{M-1})^{\mathrm{T}}$, is given by

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \mathcal{S}_d \frac{\delta \mathcal{I}_d}{\delta(\mathbf{u}^{n+1}, \mathbf{u}^n)}, \tag{2.26}$$

where $\mathbf{u}^n = (u_0^n, u_1^n, ..., u_{M-1}^n)^{\mathrm{T}}$ are vectors of approximations u_i^n to $u(x_i, t^n)$, $\mathcal{S}_d$ is a skew-symmetric matrix $\mathcal{S}_d(\mathbf{u}^{n+1}, \mathbf{u}^n)$ approximating the antisymmetric operator $\mathcal{S}(u)$, and the discrete variational derivative $\frac{\delta \mathcal{I}_d}{\delta(\hat{\mathbf{u}}, \mathbf{u})}$ is a continuous function of $(\hat{\mathbf{u}}, \mathbf{u})$ satisfying

$$\left\langle \frac{\delta \mathcal{I}_d}{\delta(\hat{\mathbf{u}}, \mathbf{u})}, \hat{\mathbf{u}} - \mathbf{u} \right\rangle = \mathcal{I}_d(\hat{\mathbf{u}}) - \mathcal{I}_d(\mathbf{u}), \tag{2.27}$$

$$\frac{\delta \mathcal{I}_d}{\delta(\mathbf{u}, \mathbf{u})} = \frac{\delta \mathcal{I}_d}{\delta \mathbf{u}}. \tag{2.28}$$

The inner product $\langle \cdot, \cdot \rangle$ in (2.27) is here meant to be the discrete analogue to the L^2-inner product in the continuous case, defined by

$$\langle \mathbf{u}, \mathbf{v} \rangle = \Delta x \cdot \mathbf{u}^{\mathrm{T}} \mathbf{v}, \tag{2.29}$$

where Δx is the spatial step size.

As proven in [9], by setting $\tilde{\mathcal{I}}_d(\mathbf{u}) = \frac{1}{\Delta x} \mathcal{I}_d(\mathbf{u})$, a discrete variational derivative satisfying (2.27)-(2.28) can be found by the relationship

$$\frac{\delta \mathcal{I}_d}{\delta(\hat{\mathbf{u}}, \mathbf{u})} = \overline{\nabla} \tilde{\mathcal{I}}_d(\hat{\mathbf{u}}, \mathbf{u}), \tag{2.30}$$

for any discrete gradient $\overline{\nabla} \tilde{\mathcal{I}}_d(\hat{\mathbf{u}}, \mathbf{u})$ satisfying (2.6)-(2.7).

Example 2.2.1. The well-known Korteweg–de Vries (KdV) equation is given by

$$u_t = -6 u u_x - u_{xxx}. \tag{2.31}$$

It can be written on the form (2.24) with

$$\begin{aligned} \mathcal{S}^{\mathrm{K}} &= \frac{\partial}{\partial x}, \\ \mathcal{H}^{\mathrm{K}}[u] &= \int \left(\frac{1}{2} u_x^2 - u^3 \right) \mathrm{d}x, \end{aligned} \tag{2.32}$$

where the first integral $\mathcal{H}^{\mathrm{K}}[u]$ is the Hamiltonian. We wish to discretize the equation on a uniform grid uniform grid $X_h : x_0 < x_1 < ... < x_{M-1}$ with spatial step size $h = x_{i+1} - x_i$. We let the approximation to $u(x_i, t)$ be denoted by u_i, and define the difference operators on the vector $\mathbf{u} = (u_0, u_1, ..., u_{M-1})^{\mathrm{T}}$ by

$$\begin{aligned} \delta_x^+ u_i &= \frac{u_{i+1} - u_i}{h}, \\ \delta_x^- u_i &= \frac{u_i - u_{i-1}}{h}, \\ \delta_x^{\mathrm{c}} u_i &= \frac{u_{i+1} - u_{i-1}}{2h} = \frac{1}{2} \delta_x^+ u + \delta_x^- u_i, \\ \delta_x^2 u_i &= \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2}. \end{aligned}$$

The Hamiltonian (2.32) can then be approximated by

$$\begin{aligned} \mathcal{H}_d^{\mathrm{K}}(\mathbf{u}) &= \sum_{i=0}^{M-1} h \left(\frac{1}{2} \left(\delta_x^+ u_i \right)^2 - (u_i)^3 \right) \\ &= \sum_{i=0}^{M-1} \left(\frac{1}{2h} \left(u_{i+1} - u_i \right)^2 - h (u_i)^3 \right). \end{aligned} \tag{2.33}$$

This is a first integral of the form

$$\mathcal{H}_d(\mathbf{u}) = \sum_{i=1}^{d} \left(c_i f_i(u_i) + \sum_{j=i+1}^{d} c_{ij} u_i u_j \right) + c_{d+1}, \tag{2.34}$$

where $c_i, c_{ij}, c_{d+1} \in \mathbb{R}$ are constants, and $f_i(u_i) : \mathbb{R} \to \mathbb{R}$ are functions. From Proposition 1 in [9], we then have that the average vector field and product discrete gradients are identical. By applying (2.30), we get the discrete variational derivative

$$\frac{\delta_{\mathrm{AVF}} \mathcal{H}_d^{\mathrm{K}}}{\delta(\hat{\mathbf{u}}, \mathbf{u})} = \frac{\delta_{\mathrm{P}} \mathcal{H}_d^{\mathrm{K}}}{\delta(\hat{\mathbf{u}}, \mathbf{u})} = -\frac{1}{2} \delta_x^2 (\hat{\mathbf{u}} + \mathbf{u}) - (\hat{\mathbf{u}}^2 + \hat{\mathbf{u}}\mathbf{u} + \mathbf{u}^2),$$

where the multiplication of two vectors is meant to be component-wise. Similarly, we get the coordinate increment discrete variational derivative

$$\frac{\delta_{\mathrm{CI}} \mathcal{H}_d^{\mathrm{K}}}{\delta(\hat{\mathbf{u}}, \mathbf{u})} = \frac{1}{h} \left(\delta_x^- \hat{\mathbf{u}} - \delta_x^+ \mathbf{u} \right) - (\hat{\mathbf{u}}^2 + \hat{\mathbf{u}}\mathbf{u} + \mathbf{u}^2),$$

and have then two different schemes for solving (2.31),

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \Delta t \cdot \delta_x^{\mathrm{c}} \left(\frac{1}{2} \delta_x^2 (\mathbf{u}^{n+1} + \mathbf{u}^n) + (\mathbf{u}^{n+1})^2 + \mathbf{u}^n \mathbf{u}^{n+1} + (\mathbf{u}^n)^2 \right)$$

and

$$\mathbf{u}^{n+1} = \mathbf{u}^n - \Delta t \delta_x^{\mathrm{c}} \left(\frac{1}{h} (\delta_x^+ \mathbf{u}^{n+1} - \delta_x^- \mathbf{u}^n) + (\mathbf{u}^{n+1})^2 + \mathbf{u}^n \mathbf{u}^{n+1} + (\mathbf{u}^n)^2 \right)$$

which both preserve the approximation (2.33) of the Hamiltonian (2.32). Although not presented here, a third, slightly more intricate scheme can be found by applying the midpoint discrete variational derivative.

2.2.3 Discrete Variational Derivative Methods on General Fixed Grids

Extending the discrete variational derivative methods to non-uniform grids is of great interest, both since it increases the possibility of getting precise results with a limited number og space points and because it makes it possible to solve multi-dimensional problems on complicated domains.

Yaguchi, Matsuo and Sugihara developed in [25] an extension of the discrete variational derivative method of Matsuo and Furihata, presenting a discrete variational derivative, for every PDE in a limited class, that is unique up to the spatial discretization. In [26], they have developed an integral preserving method for general fixed grids by combining the discrete differential forms of Bochev and Hyman [2] and the discrete variational derivative methods.

In this section, we will extend the theory of the previous section to non-uniform grids, thus obtaining integral preserving methods for general fixed grids, with infinitely many different discrete variational derivatives for a given first integral. Let us first give a formal definition of a discrete variational derivative on a general fixed grid.

Definition 1. Denote by κ_i, $i = 0, ..., M-1$, the positive weights defined such that $\sum_{i=0}^{M-1} \kappa_i$ approximates the integral operator. Let the function $\mathcal{I}_{\mathbf{x}}(\mathbf{u}) = \sum_{i=0}^{M-1} \kappa_i I_{\mathbf{x}}^i(\mathbf{u})$ of the vector $\mathbf{u} \in \mathbb{R}^M$ of approximations u_i to $u(x_i)$ be a consistent approximation to the first integral $\mathcal{I}[u]$ on the grid $X_h : x_0 < x_1 < ... < x_{M-1}$, whose grid points x_i are the elements of $\mathbf{x} \in \mathbb{R}^M$. Then the continuous function $\frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta(\hat{\mathbf{u}}, \mathbf{u})}$ of $(\hat{\mathbf{u}}, \mathbf{u})$ is a discrete variational derivative of $\mathcal{I}_{\mathbf{x}}(\mathbf{u})$ if it satisfies

$$\left\langle \frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta(\hat{\mathbf{u}}, \mathbf{u})}, \hat{\mathbf{u}} - \mathbf{u} \right\rangle_{\mathbf{x}} = \mathcal{I}_{\mathbf{x}}(\hat{\mathbf{u}}) - \mathcal{I}_{\mathbf{x}}(\mathbf{u}), \tag{2.35}$$

$$\frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta(\mathbf{u}, \mathbf{u})} = \frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta \mathbf{u}}, \tag{2.36}$$

where the inner product $\langle \cdot, \cdot \rangle_{\mathbf{x}}$ is the discrete analogue to the L^2-inner product, defined by

$$\langle \mathbf{u}, \mathbf{v} \rangle_{\mathbf{x}} = \sum_{i=0}^{M-1} \kappa_i u_i v_i. \tag{2.37}$$

Note that the weights κ_i depend on the grid points x_i, and are typically given by $\kappa_i = x_{i+1} - x_i$ or $\kappa_i = \frac{x_{i+1}-x_{i-1}}{2}$.

We now present a generalization of (2.30) that also holds for non-uniform grids.

Theorem 1. *Given a discrete gradient $\overline{\nabla} I(\hat{\mathbf{u}}, \mathbf{u})$ satisfying (2.6)-(2.7), then for every function $\mathcal{I}_{\mathbf{x}}(\mathbf{u}) = \sum_{i=0}^{M-1} \kappa_i I_i(\mathbf{u}) : \mathbb{R}^M \to \mathbb{R}$ of the vector $\mathbf{u}$ of values u_i on the fixed grid $X_h : x_0 < x_1 < ... < x_{M-1}$, whose grid points x_i are the elements of the vector $\mathbf{x}$, a discrete variational derivative satisfying (2.35)-(2.36) is given by*

$$\frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta(\hat{\mathbf{u}}, \mathbf{u})} = D(\kappa)^{-1} \overline{\nabla} \mathcal{I}_{\mathbf{x}}(\hat{\mathbf{u}}, \mathbf{u}), \tag{2.38}$$

where the M-dimensional vector $\kappa := (\kappa_0, \kappa_1, ..., \kappa_{M-1})^{\mathrm{T}}$ and the $M \times M$-matrix $D(\kappa) :=$ $\mathrm{diag}\,(\kappa_0, \kappa_1, ..., \kappa_{M-1})$.

Proof. Applying (2.6), we get that, for the discrete variational derivative defined by (2.38),

$$\begin{aligned}
\left\langle \frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta(\hat{\mathbf{u}}, \mathbf{u})}, \hat{\mathbf{u}} - \mathbf{u} \right\rangle_{\mathbf{x}} &= \left\langle D(\kappa)^{-1} \overline{\nabla} \mathcal{I}_{\mathbf{x}}(\hat{\mathbf{u}}, \mathbf{u}), \hat{\mathbf{u}} - \mathbf{u} \right\rangle_{\mathbf{x}} \\
&= \sum_{i=0}^{M-1} \kappa_i \frac{1}{\kappa_i} \overline{\nabla} \mathcal{I}_{\mathbf{x}} \left(\hat{\mathbf{u}}, \mathbf{u}\right)_i \left(\hat{u}_i - u_i\right) = \overline{\nabla} \mathcal{I}_{\mathbf{x}} \left(\hat{\mathbf{u}}, \mathbf{u}\right)^{\mathrm{T}} \left(\hat{\mathbf{u}} - \mathbf{u}\right) \\
&= \mathcal{I}_{\mathbf{x}}(\hat{\mathbf{u}}) - \mathcal{I}_{\mathbf{x}}(\mathbf{u}),
\end{aligned}$$

and hence (2.35) is satisfied. Furthermore, applying (2.7),

$$\frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta(\mathbf{u}, \mathbf{u})} = D(\kappa)^{-1} \overline{\nabla} \mathcal{I}_{\mathbf{x}}(\mathbf{u}, \mathbf{u}) = D(\kappa)^{-1} \nabla \mathcal{I}_{\mathbf{x}} \left(\mathbf{u}\right). \tag{2.39}$$

Now, with the discrete inner product given by (2.37), we have from (2.22) that

$$\begin{aligned}
\left. \frac{\mathrm{d}}{\mathrm{d}\epsilon} \right|_{\epsilon=0} \mathcal{I}_{\mathbf{x}} \left(\mathbf{u} + \epsilon \mathbf{v}\right) &= \left\langle \frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta \mathbf{u}}, \mathbf{v} \right\rangle_{\mathbf{x}} = \sum_{i=0}^{M-1} \kappa_i \left(\frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta \mathbf{u}} \right)_i v_i \\
&= \left(D(\kappa) \frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta \mathbf{u}} \right)^{\mathrm{T}} \mathbf{v}, \quad \forall \mathbf{v} \in \mathbb{R}^M.
\end{aligned} \tag{2.40}$$

This can be compared to a property of the directional derivative of $\mathcal{I}_{\mathbf{x}}$ which says that

$$\left. \frac{\mathrm{d}}{\mathrm{d}\epsilon} \right|_{\epsilon=0} \mathcal{I}_{\mathbf{x}} \left(\mathbf{u} + \epsilon \mathbf{v}\right) = \nabla_{\mathbf{v}} \mathcal{I}_{\mathbf{x}}(\mathbf{u}) = \nabla \mathcal{I}_{\mathbf{x}}(\mathbf{u})^{\mathrm{T}} \mathbf{v}, \qquad \forall \mathbf{v} \in \mathbb{R}^M, \tag{2.41}$$

as long as $\mathcal{I}_{\mathbf{x}}$ is differentiable at $\mathbf{u}$. Since (2.40) and (2.41) holds for all vectors $\mathbf{v}$, we have that

$$\frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta \mathbf{u}} = D(\kappa)^{-1} \nabla \mathcal{I}_{\mathbf{x}}(\mathbf{u}), \tag{2.42}$$

and by coupling (2.39) and (2.42) we get

$$\frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta(\mathbf{u}, \mathbf{u})} = \frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta \mathbf{u}},$$

and (2.36) is also satisfied. □

Then we have that the discrete variational derivative methods for PDEs of the form (2.24), preserving the consistent approximation $\mathcal{I}_{\mathbf{x}}(\mathbf{u})$ of the first integral $\mathcal{I}[u]$ on the general grid $\mathbf{x} \in \mathbb{R}^M$, is given by

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \mathcal{S}_{\mathbf{x}} \frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta(\mathbf{u}^{n+1}, \mathbf{u}^n)}, \tag{2.43}$$

where $\mathcal{S}_{\mathbf{x}}$ is a matrix $\mathcal{S}_{\mathbf{x}}(\mathbf{u}^{n+1}, \mathbf{u}^n)$ that is an approximation to the antisymmetric operator $\mathcal{S}(u)$, and itself antisymmetic *with respect to the inner product* $\langle \cdot, \cdot \rangle_{\mathbf{x}}$ defined by (2.37). That is, $\mathcal{S}_{\mathbf{x}}$ must satisfy

$$\langle \mathbf{v}, \mathcal{S}_{\mathbf{x}} \mathbf{w} \rangle_{\mathbf{x}} = - \langle \mathcal{S}_{\mathbf{x}} \mathbf{v}, \mathbf{w} \rangle_{\mathbf{x}} \tag{2.44}$$

for two arbitrary vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^M$. Note that a matrix $\mathcal{S}_{\mathbf{x}}$ satisfying (2.44) is in general not antisymmetric by the standard definition in linear algebra, i.e. $\mathcal{S}_{\mathbf{x}}^{\mathrm{T}} \neq -\mathcal{S}_{\mathbf{x}}$. However,

$$\left(D(\kappa)\mathcal{S}_{\mathbf{x}}\right)^{\mathrm{T}} = -D(\kappa)\mathcal{S}_{\mathbf{x}}$$

is an equivalent definition to (2.44).

Chapter 3

Moving Grid Methods

In this chapter we will give a brief presentation of general methods for solving time-dependent PDEs on moving grids. The moving grid methods can roughly be described by three major components: A grid movement strategy, discretization of the PDE and the approach used to solve the coupled system of physical and grid equations [16]. The grid movement strategy and the discretization of the PDE can to a large extent be described separately from eachother. We will therefore mainly focus on the grid movement in this chapter, since it is independent of any integral preserving property of the method. Lastly we give a short summary of common approaches to discretizing the PDE and solving the coupled system.

3.1 Grid Movement

The motivation behind using a moving grid is a wish to minimize the number of grid-points necessary to achieve the desired accuracy of the numerical solution, thus minimizing the computational cost for the solver. The intuitive idea is that more grid-points are needed in the areas with the highest spatial activity. More formally, the grid-points should be clustered in the regions of the domain where the gradient of the solution u is largest at a time t.

3.1.1 Equidistribution

Most methods for distributing the grid are based on the *equidistribution principle*, first introduced by de Boor in [8]. Given a continuous function $\omega(x)$, typically depending on the first and/or second order derivatives of the underlying solution u to be adapted, the number of grid points $M+1$ and the bounded domain $[a,b]$ where u is defined, equidistribution entails finding a grid $X_h : x_0 = a < x_1 < ... < x_M = b$ such that

$$\int_{x_0}^{x_1} \omega(x)\mathrm{d}x = \int_{x_i}^{x_{i+1}} \omega(x)\mathrm{d}x, \qquad \text{for } i = 1, ..., M-1. \tag{3.1}$$

The function $\omega(x)$ is in most cases chosen out of a desire to minimize the error of the numerical approximation. It is called the monitor function in much of the literature, including [27] and [24], while it is labeled the mesh density function in [16], where its square, $\omega(x)^2$, is called the monitor function. We will follow the latter terminology here, renaming $\omega(x)$ the *grid density function*. To ensure that the equidistribution is unique, we will impose that the grid density function is by definition strictly positive, i.e.

$$\omega(x) > 0, \quad \forall x \in [a,b]\,.$$

A typical choice of $\omega(x)$ is the arc length grid density function

$$\omega(x) = \sqrt{1 + \frac{\partial u}{\partial x}}, \tag{3.2}$$

which is such that the integrals in (3.1) represent the arc length of the curve between adjacent nodes.

3.1.2 Coordinate Transformation

The grid X_h may be given by a one-to-one coordinate transformation from the computational domain $\Xi = [0,1]$ to the physical domain $X = [a,b]$, denoted by

$$x = x(\xi), \quad \xi \in [0,1]\,. \tag{3.3}$$

Given a uniform grid $\Xi_h : \xi_0 < \xi_1 < ... < \xi_M$ in the computational domain Ξ, defined by

$$\xi_i = \frac{i}{M}, \tag{3.4}$$

the transformation (3.3) should be defined such that

$$x_i = x(\xi_i), \quad i = 0, ..., M. \tag{3.5}$$

The equidistribution property (3.1) may be rewritten as

$$\int_{x_0}^{x_i} \omega(x)\mathrm{d}x = \frac{i}{M}\int_{x_0}^{x_M} \omega(x)\mathrm{d}x. \tag{3.6}$$

Defining $\sigma = \int_{x_0}^{x_M} \omega(x)\mathrm{d}x$ and inserting (3.4) and (3.5), the property (3.6) becomes

$$\int_{x_0}^{x(\xi_i)} \omega(x)\mathrm{d}x = \sigma\xi_i. \tag{3.7}$$

Generally, a continuous mapping (3.3) is called an *equidistributing coordinate transformation* for $\omega(x)$ if it satisfies the equidistribution principle given as

$$\int_{x_0}^{x(\xi)} \omega(x)\mathrm{d}x = \sigma\xi. \tag{3.8}$$

Differentiating (3.8) once or twice with respect to ξ yields two equivalent definitions,

$$\omega(x)\frac{\mathrm{d}x}{\mathrm{d}\xi} = \sigma$$

and

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\omega(x)\frac{\mathrm{d}x}{\mathrm{d}\xi}\right) = 0. \tag{3.9}$$

3.1.3 Computing the Equidistributing Grid

Although the equidistributing grid is uniquely given for a strictly positive grid density function, it can rarely be found exactly. Even if we know the function $u(x)$, the integral of $\omega(x)$ is often impossible to calculate analytically. Since, in most cases, it is impossible and also unnecessary to find a precise equidistributing grid, there exists several different methods for obtaining the grid by numerical computations, giving slightly different approximations to the equidistributing grid defined by (3.1). We will now give a brief presentation of some different methods for finding an approximately equidistributing grid X_h.

Zegeling presents in [27] a method for finding a system of $M-1$ semi-discrete grid equations for the implicit determination of the grid X_h. By applying the midpoint quadrature rule on the integrals in (3.1) and inserting semi-discrete variables, we get the system of $M-1$ equations

$$(x_1 - x_0)\omega_{\frac{1}{2}} = (x_{i+1} - x_i)\omega_{i+\frac{1}{2}}, \quad i = 1, ..., M-1$$

or equivalently

$$(x_i - x_{i-1})\omega_{i-\frac{1}{2}} = (x_{i+1} - x_i)\omega_{i+\frac{1}{2}}, \quad i = 1, ..., M-1, \tag{3.10}$$

which together with the boundary conditions

$$x_0 = a, \quad x_M = b,$$

can be solved to give an approximation to an equidistributing grid. In (3.10), $\omega_{i+\frac{1}{2}}$ represents a semi-discrete approximation to $\omega(\frac{x_i+x_{i+1}}{2})$. As an example, for the arc length grid density function (3.2), we may set

$$\omega_{i+\frac{1}{2}} = \sqrt{1 + \left(\frac{u_{i+1} - u_i}{x_{i+1} - x_i}\right)^2}.$$

If $u(x)$ in known, the u_i's can be found exactly. However, typically u is only given by numerical approximations evaluated on a previously evaluated grid. The u_i's can then be found by interpolation over on the the new grid, or the system of equations (3.10) can be coupled with the system of equations representing a step in time of the PDE solver.

The system of equations (3.10) can also be found by discretizing (3.9) on the computational grid ξ_h, obtaining

$$\frac{2}{\xi_{i+1} - \xi_{i-1}} \left(\omega_{i+\frac{1}{2}} \frac{x_{i+1} - x_i}{\xi_{i+1} - \xi_i} - \omega_{i-\frac{1}{2}} \frac{x_i - x_{i-1}}{\xi_i - \xi_{i-1}} \right) = 0, \tag{3.11}$$

which is equivalent to (3.10) when $\xi_{i+1} - \xi_i = \Delta\xi$ is constant. To avoid having to interpolate the u_i's over on the new grid, we may introduce an artificial time τ to (3.9) and solve a relaxed version of (3.11) with the ω's evaluated on a previous grid, as described in [24].

An alternative to the discrete moving grid equations given above is the so-called moving mesh PDEs, which explicitly involves the speed of the grid. A presentation of these methods is given in [16].

A direct approximation method for one-dimensional problems is proposed by de Boor in [8]. For this method, it is assumed that the grid density function is known on a given grid $X'_h : x'_0 = a < x'_1 < ... < x'_K = b$, typically the current approximate grid in an iterative process. The grid density function $\omega(x)$ is then approximated by the piecewise constant function

$$p(x) = \begin{cases} \frac{\omega(x'_0)+\omega(x'_1)}{2} & \text{for } x \in [x'_0, x'_1] \\ \frac{\omega(x'_1)+\omega(x'_2)}{2} & \text{for } x \in (x'_1, x'_2] \\ \vdots & \\ \frac{\omega(x'_{K-1})+\omega(x'_K)}{2} & \text{for } x \in \left(x'_{K-1}, x'_K\right]. \end{cases} \quad (3.12)$$

We will modify the algorithm slightly, by replacing $\frac{\omega(x'_i)+\omega(x'_{i+1})}{2}$ with $\omega(\frac{x'_i+x'_{i+1}}{2})$, or a discrete approximation of this, as in Zegeling's method.

De Boor's algorithm finds the equidistributing grid for the function $p(x)$. Denoting

$$P(x) = \int_{x_0}^{x} p(x)\mathrm{d}x,$$

we get

$$P(x'_i) = \sum_{j=1}^{i}(x'_j - x'_{j-1})\omega(\frac{x'_{j-1} + x'_j}{2}), \quad i = 1, ..., K.$$

After determining, for a given $i \in [1, M-1]$, the index k such that

$$P(x'_{k-1}) < \frac{i}{M}P(x_M) \leq P(x'_k),$$

we also get

$$P(x_i) = P(x'_{k-1}) + (x_i - x'_{k-1})\omega(\frac{x'_{k-1} + x'_k}{2}) \quad \text{for } i = 1, ..., M-1. \quad (3.13)$$

The property (3.7) can now be rewritten as

$$P(x_i) = \xi_i P(x_M),$$

and by inserting (3.4) and (3.13), we find that x_i can be directly calculated from

$$x_i = x'_{k-1} + \frac{\frac{i}{M}P(x_M) - P(x'_{k-1})}{\omega(x'_{k-1} + x'_k)}.$$

The drawback of de Boor's algorithm is that it does not extend easily to higher dimensions.

Note that all these methods only find the equidistributing grid for an approximation to $\omega(x)$. For a better approximation to the equidistributing grid of $\omega(x)$, an iteration procedure could be performed.

3.2 Discretization of the PDE

The effect of grid movement in the time discretization of the PDE is typically treated with either the Lagrangian approach or the rezoning approach [16].

3.2.1 The Lagrangian Approach

With the Lagrangian discretization approach, we assume that the grid points move continuously in time, so that the time-derivative term u_t in the PDE (2.20) can be transformed into a term along the grid trajectories $X_h(t) : x_0 = a < x_1(t) < ... < x_i(t) < ...x_M = b$. Denote the transformed variable $v(\xi, t) = u(x(\xi, t), t)$. By the chain rule, we then have

$$\frac{\partial v}{\partial t} = \frac{\partial u}{\partial t} + \frac{\partial x}{\partial t}\frac{\partial u}{\partial x},$$

which inserted into (2.20) results in the Lagrangian form

$$\frac{\partial v}{\partial t} = \frac{\partial x}{\partial t}\frac{\partial u}{\partial x} + f(\mathbf{x}, u^J). \tag{3.14}$$

Applying the differences operator δ_x to spatially discretize the convection term $\frac{\partial x}{\partial t}\frac{\partial u}{\partial x}$ and letting $F(\mathbf{u}, \mathbf{x}) = [f_0(\mathbf{u}, \mathbf{x}), ..., f_{M-1}(\mathbf{u}, \mathbf{x})]$ denote the discretization of $f(\mathbf{x}, u^J)$, we obtain the semi-discrete system of ODEs

$$\frac{\partial u_i}{\partial t} = \frac{\partial x_i}{\partial t}\delta_x u_i + f_i(\mathbf{u}, \mathbf{x}), \qquad i = 0, ..., M-1$$

where $u_i(t) \approx v(\xi_i, t) = u(x_i(t), t)$. Thus the temporal discretization can be performed in a standard manner.

3.2.2 The Rezoning Approach

When applying the rezoning approach, we assume that the grid moves in an intermittent manner in time. That is, the grid is considered to vary only at discrete time levels t^n. The PDE can then be integrated for the current time step at the fixed grid X_h^{n+1} : $x_0^{n+1} = a < x_1^{n+1} < ... < x_M^{n+1} = b$. The initial data $\tilde{u}_i^n \approx u(x_i^{n+1}, t^n)$ at the integration step from time t^n to t^{n+1} must then be interpolated from the solution data $u_i^n \approx u(x_i^n, t^n)$ from the integration over the previous time step.

3.3 Solution Procedure

There are two different approaches used to solve the coupled system of physical and grid equations: The alternate and the simultaneous solution procedure.

3.3.1 Alternate Solution Procedure

As its name suggests, the alternate solution procedure involves solving alternately for the physical solution and the grid. Given the grid X_h^n and numerical solution $\mathbf{u}^n$ at time t^n, the grid X_h^{n+1} is evaluated, before the solution $\mathbf{u}^{n+1}$ is obtained on this grid by a PDE solver. With this procedure, the grid at time t^{n+1} adapts only to the solution $\mathbf{u}^n$ at time t^n. This lagging in time will usually not create any trouble, as long as the time step is reasonable small. By design the rezoning approach can only be carried out this way. For higher dimensional problems, with accompanying increased complexity, the alternate solution approach is usually preferred.

3.3.2 Simultaneous Solution Procedure

With the simultaneous solution procedure, which is only relevant when a Lagrangian approach is used, the grid x_h^{n+1} is evaluated simultaneously with the solution $\mathbf{u}^{n+1}$ at the time t^{n+1}. That is, the grid equations and the physical PDE are coupled and solved as one large system of equations.

Chapter 4

Integral Preserving Methods on Moving Grids

In this chapter we will present integral preserving moving grid methods. As noted in the previous chapter for general moving grid methods, the grid movement strategy and the discretization of the PDE can to a large extent be described separately from eachother. We will propose methods where the integral preservation property is a consequence of the temporal discretization of the PDE, which thus is the part we will focus on in this chapter.

First we must clarify what is meant by integral preservation on moving grids, since the exact integral $\mathcal{I}[u]$ cannot be calculated without knowing the continuous function $u(x,t)$, and must therefore typically be approximated by a function of the vector $\mathbf{u}$ evaluated at a given grid X_h. Given such an approximation $\mathcal{I}_{\mathbf{x^0}}(\mathbf{u}^0)$ of $\mathcal{I}[u]$ at the initial time t^0 on the grid X_h^0 represented by $\mathbf{x}^0$, the methods introduced in this chapter are integral preserving in the sense that

$$\mathcal{I}_{\mathbf{x}^n}(\mathbf{u}^n) = \mathcal{I}_{\mathbf{x}^0}\left(\mathbf{u}^0\right), \qquad \text{for all } n \geq 0.$$

The methods will all be defined by a single step

$$\mathbf{u}^{n+1} = \Psi_{(\mathbf{x}_{n+1}, \mathbf{x}^n, \Delta t)}\mathbf{u}^n,$$

computing the approximated solution $\mathbf{u}^{n+1}$ at time $t^{n+1} = t^n + \Delta t$ on the grid $\mathbf{x}^{n+1}$, from the solution $\mathbf{u}^n$ at time t^n on the grid $\mathbf{x}^n$. To simplify notation and make the numerical schemes more perspicuous, we will use $\hat{\mathbf{u}} := \mathbf{u}^{n+1}$ and $\mathbf{u} := \mathbf{u}^n$, and likewise for $\mathbf{x}$ and t, in the subsequent sections.

4.1 The Modified Discrete Variational Derivative Methods on Moving Grids

We wish to further develop the discrete variational derivative methods to also be applicable to moving grids. Since the Lagrangian discretization approach involves the introduction of a convection term and subsequently discretization of a PDE not of the form (2.24), it is incompatible with the DVD methods. We will therefore focus on alternate solution procedures that utilize the rezoning approach, which requires the initial data at every time step to be evaluated at the new grid $\hat{X}_h$, represented by $\hat{\mathbf{x}}$. Therefore it is necessary to interpolate the solution approximation at time t from the old grid $\mathbf{x}$ to the new one, $\hat{\mathbf{x}}$.

Unless the interpolation procedure, given by the operator $\Phi_{(\hat{\mathbf{x}},\mathbf{x})}$ mapping a vector $\mathbf{v} \in \mathbb{R}^M$ from $\mathbf{x}$ to $\hat{\mathbf{x}}$, has integral preservation as a property, the approximation of the first integral will in general not be preserved, i.e.

$$\mathcal{I}_{\mathbf{x}}\left(\mathbf{u}\right) \neq \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}).$$

Hence applying a standard discrete variational derivative method, as given by (2.43), on $\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ will not preserve $\mathcal{I}_{\mathbf{x}}\left(\mathbf{u}\right)$, although it will give

$$\mathcal{I}_{\hat{\mathbf{x}}}\left(\hat{\mathbf{u}}\right) = \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}).$$

We will thus propose a method that adjusts the DVD method so that is does indeed preserve $\mathcal{I}_{\mathbf{x}}\left(\mathbf{u}\right)$, while still being a discrete analogue to the form (2.24) of the continuous equation.

Definition 2. Let the elements x_i of $\mathbf{x} \in \mathbb{R}^M$ be the first M points on the grid X_h : $x_0 = a < x_1 < ... < x_M = b$, and let $\mathbf{u} \in \mathbb{R}^M$ be a vector of approximations u_i to $u(x_i, t)$, for $i = 0, ..., M-1$. Let $\mathcal{I}_{\mathbf{x}}(\mathbf{u}) : \mathbb{R}^M \to \mathbb{R}$ be a consistent approximation to the first integral $\mathcal{I}\left[u\right]$ over the interval $[a, b]$, and $\frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta(\hat{\mathbf{u}},\mathbf{u})}$ any discrete variational derivative of $\mathcal{I}_{\mathbf{x}}(\mathbf{u})$, as given by Definition 1. Then, the *modified discrete variational derivative methods* on moving grids, for advancing the numerical solution $\mathbf{u}$ of (2.24) on $\mathbf{x}$ at time t to $\hat{\mathbf{u}}$ on $\hat{\mathbf{x}}$ at time $\hat{t}$, are given by

$$\hat{\mathbf{u}} = \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} + \frac{\mathcal{I}_{\mathbf{x}}\left(\mathbf{u}\right) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}\left(\hat{\mathbf{u}}\right)\right\rangle_{\hat{\mathbf{x}}}} \nabla \mathcal{I}_{\hat{\mathbf{x}}}\left(\hat{\mathbf{u}}\right) + \Delta t \cdot \mathcal{S}_{\hat{\mathbf{x}}} \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \tag{4.1}$$

where $\Phi_{(\hat{\mathbf{x}},\mathbf{x})}$ is any operator interpolating from $\mathbf{x}$ to $\hat{\mathbf{x}}$, $\Delta t = \hat{t} - t$, and $\mathcal{S}_{\hat{\mathbf{x}}} := \mathcal{S}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}, \mathbf{u})$ is an approximation to $\mathcal{S}(u)$ that is antisymmetric with respect to the scalar product $\langle \cdot, \cdot \rangle_{\hat{\mathbf{x}}}$.

Theorem 2. *The modified discrete variational derivative methods on moving grids, defined by (4.1), preserve an approximation to the integral $\mathcal{I}\left[u\right]$, in the sense that*

$$\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) = \mathcal{I}_{\mathbf{x}}(\mathbf{u}). \tag{4.2}$$

Proof. By inserting (4.1) into (2.35), we get

$$\begin{aligned}
\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) &= \left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \frac{\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\mathbf{x}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right. \\
&\quad \left. + \Delta t \cdot \mathcal{S}_{\hat{\mathbf{x}}} \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)} \right\rangle_{\hat{\mathbf{x}}} \\
&= \frac{\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} \left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}} \\
&\quad + \Delta t \left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \mathcal{S}_{\hat{\mathbf{x}}} \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)} \right\rangle_{\hat{\mathbf{x}}} \\
&= \mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}),
\end{aligned}$$

and hence (4.2) is statisfied. □

We will call the second term on the right hand side of (4.1) for the *adjustment term*, since it adjusts the solution $\hat{\mathbf{u}}$ to make it satisfy (4.2). Note that $\nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) = D(\hat{\kappa}) \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta \hat{\mathbf{u}}}$ in the adjustment term could be replaced by any vector field $\tilde{\nabla} \mathcal{I}_{\hat{\mathbf{x}}} : \mathbb{R}^M \times \mathbb{R}^M \to \mathbb{R}^M$ and (4.1) would still be integral preserving as defined by (4.2). However, $\tilde{\nabla} \mathcal{I}_{\hat{\mathbf{x}}}$ should be an approximation to $\nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})$, as this keeps the adjustment term small. We have chosen to only include $\nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})$ in the definition of the modified DVD method, whereas one step of the *alternate modified DVD methods* is given by

$$\begin{aligned}
\hat{\mathbf{u}} &= \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} + \frac{\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \tilde{\nabla} \mathcal{I}_{\hat{\mathbf{x}}}\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right) \right\rangle_{\hat{\mathbf{x}}}} \tilde{\nabla} \mathcal{I}_{\hat{\mathbf{x}}}\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right) \\
&\quad + \Delta t \cdot \mathcal{S}_{\hat{\mathbf{x}}} \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)},
\end{aligned} \tag{4.3}$$

where $\tilde{\nabla} \mathcal{I}_{\hat{\mathbf{x}}}\left(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)$ can be chosen to be different from $\nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})$.

4.2 Linear Projection Methods

An introduction to integral preserving projection methods for solving ODEs is given in [14]. By semi-discretizing the PDE (2.20) to obtain a set of ODEs, projection methods can thus be used to generate integral-preserving methods for PDEs on a fixed grid, as with discrete gradient methods. We will now introduce integral preserving projection methods on moving grids. For simplicity, only linear projection is regarded.

Definition 3. Let the function $f_{\mathbf{x}} : \mathbb{R}^M \times \mathbb{R}^M \to \mathbb{R}^M$ be such that

$$\frac{\hat{\mathbf{u}} - \mathbf{u}}{\Delta t} = f_{\mathbf{x}}(\hat{\mathbf{u}}, \mathbf{u}) \tag{4.4}$$

defines a step from time t to time $\hat{t} = t + \Delta t$ of an arbitrary one-step method applied to (2.20) on the fixed grid X_h represented by $\mathbf{x}$. Define the $(M-1)$-dimensional submanifold $\mathcal{M}_{(\hat{\mathbf{x}},\mathbf{x},\mathbf{u})}$ of $\mathbb{R}^M$ by

$$\mathcal{M}_{(\hat{\mathbf{x}},\mathbf{x},\mathbf{u})} = \left\{\hat{\mathbf{u}} \in \mathbb{R}^M : \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) = \mathcal{I}_{\mathbf{x}}(\mathbf{u})\right\}. \tag{4.5}$$

Then, we define one step of a linear projection method $\mathbf{u} \mapsto \hat{\mathbf{u}}$ from the grid $\mathbf{x}$ to the grid $\hat{\mathbf{x}}$ by

1. Interpolate $\mathbf{u}$ over on $\hat{\mathbf{x}}$ by computing $\mathbf{v} = \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ for an arbitrary interpolation operator $\Phi_{(\hat{\mathbf{x}},\mathbf{x})}$ interpolating from $\mathbf{x}$ to $\hat{\mathbf{x}}$,

2. Integrate $\mathbf{v}$ one time step by computing $\hat{\mathbf{w}} = \mathbf{v} + \Delta t f_{\hat{\mathbf{x}}}(\hat{\mathbf{w}}, \mathbf{v})$,

3. Compute $\hat{\mathbf{u}} \in \mathcal{M}_{(\hat{\mathbf{x}},\mathbf{x},\mathbf{u})}$ by solving the system of $M+1$ equations $\hat{\mathbf{u}} = \hat{\mathbf{w}} + \lambda\nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})$ and $\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) = \mathcal{I}_{\mathbf{x}}(\mathbf{u})$, for $\hat{\mathbf{u}} \in \mathbb{R}^M$ and $\lambda \in \mathbb{R}$.

The projection in the above definition is called *linear* projection because $\nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \parallel (\hat{\mathbf{u}} - \hat{\mathbf{w}})$. Note that $\nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})$ in point 3, which defines the direction of the projection, may be replaced by any vector field $\tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}} : \mathbb{R}^M \times \mathbb{R}^M \to \mathbb{R}^M$, but $\nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})$ is the choice that minimizes the Euclidean distance $\|\hat{\mathbf{u}} - \hat{\mathbf{w}}\|$.

By utilizing the fact that for a method defined by (4.4) there exists an implicitly defined map $\Psi_{\mathbf{x}} : \mathbb{R}^M \to \mathbb{R}^M$ such that $\hat{\mathbf{u}} = \Psi_{\mathbf{x}}\mathbf{u}$, we define

$$g_{\mathbf{x}}(\mathbf{u}) := \frac{\Psi_{\mathbf{x}}\mathbf{u} - \mathbf{u}}{\Delta t},$$

and may then write the tree points in Definition 3 in an equivalent, more compact form as: Compute $\hat{\mathbf{u}} \in \mathbb{R}^M$ and $\lambda \in \mathbb{R}$ such that

$$\hat{\mathbf{u}} = \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} + \Delta t g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) + \lambda\nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}), \tag{4.6}$$

$$\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) = \mathcal{I}_{\mathbf{x}}(\mathbf{u}), \tag{4.7}$$

for an arbitrary interpolation operator $\Phi_{(\hat{\mathbf{x}},\mathbf{x})}$ interpolating from $\mathbf{x}$ to $\hat{\mathbf{x}}$.

The following theorem and proof are reminiscent of Theorem 2 and its proof in [20], whose subsequent corollary shows how linear projection methods for solving ODEs are a subset of discrete gradient methods.

Theorem 3. *Let $g_{\hat{\mathbf{x}}} : \mathbb{R}^M \to \mathbb{R}^M$ be a consistent approximation of f in (2.20) and let $\frac{\delta\mathcal{I}_{\mathbf{x}}}{\delta(\hat{\mathbf{u}},\mathbf{u})}$ be an arbitrary discrete variational derivative of $\mathcal{I}$ in (2.24) on the grid X_h given by the elements of $\mathbf{x}$. If we set $\mathcal{S}_{\hat{\mathbf{x}}}$ in (4.1) to be*

$$\mathcal{S}_{\hat{\mathbf{x}}} = \frac{g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})\nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})^T - \nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})^T}{\left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})\right\rangle_{\hat{\mathbf{x}}}} D(\hat{\kappa}), \tag{4.8}$$

then the linear projection method for solving PDEs on a moving grid, given by Definition 3, is equivalent to the modified discrete variational derivative method on moving grids, given by Definition 2.

Proof. Assume that (4.6)-(4.7) are satisfied. By (4.7) and (2.35), we have that

$$\begin{aligned} \mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) &= \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) \\ &= \left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \hat{\mathbf{u}} - \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} \right\rangle_{\hat{\mathbf{x}}} \end{aligned} \tag{4.9}$$

and by applying (4.6), it follows that

$$\begin{aligned} \mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) &= \Delta t \left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) \right\rangle_{\hat{\mathbf{x}}} \\ &\quad + \lambda \left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}} \end{aligned}$$

and hence

$$\lambda = \frac{\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} - \Delta t \frac{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) \right\rangle_{\hat{\mathbf{x}}}}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}}. \tag{4.10}$$

Substituting this into (4.6), we get

$$\begin{aligned} \hat{\mathbf{u}} &= \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} + \frac{\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \\ &\quad + \Delta t \left(g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) - \frac{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) \right\rangle_{\hat{\mathbf{x}}}}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right) \\ &= \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} + \frac{\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \\ &\quad + \Delta t \left(\frac{\left(D(\hat{\kappa}) \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})} \right)^{\mathrm{T}} \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) \right. \\ &\quad \left. - \frac{\left(D(\hat{\kappa}) \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})} \right)^{\mathrm{T}} g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right) \\ &= \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} + \frac{\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \\ &\quad + \Delta t \left(\frac{g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})^{\mathrm{T}}}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} D(\hat{\kappa}) \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})} \right. \\ &\quad \left. - \frac{\nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})^{\mathrm{T}}}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) \right\rangle_{\hat{\mathbf{x}}}} D(\hat{\kappa}) \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})} \right), \end{aligned}$$

and hence (4.1) is satisfied, with $\mathcal{S}_{\hat{\mathbf{x}}}$ as given by (4.8). Conversely, if $\hat{\mathbf{u}}$ satisfies (4.1), we have from Theorem 2 that (4.7) is satisfied. Inserting (4.8) into (4.1) and following the above deduction backwards, we get (4.6), with λ defined by (4.10). □

Since defining $\mathcal{S}_{\hat{\mathbf{x}}}$ by (4.8) is a restriction, the linear projection methods on moving grids are a subset of all possible modified discrete variational derivative methods on moving grids. Note also that, since the linear projection methods are independent of the discrete variational derivative, each linear projection method defines an equivalence class of modified discrete variational derivative methods, uniquely defined by the choice of $g_{\hat{\mathbf{x}}}$.

If we allow for more generality in our projection methods, and replace $\nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})$ in the third step of the linear projection method by a different vector field $\tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}},\mathbf{v})$ as the direction of the projection, the linear projection method will be a subset of the alternate modified DVD methods (4.3), with

$$\mathcal{S}_{\hat{\mathbf{x}}} = \frac{g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})\tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})^{\mathrm{T}} - \tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})^{\mathrm{T}}}{\left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})\right\rangle_{\hat{\mathbf{x}}}} D(\hat{\kappa}).$$

We could also let $g_{\hat{\mathbf{x}}}$ depend on $\hat{\mathbf{u}}$ in addition to $\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$, thus obtaining the matrix

$$\mathcal{S}_{\hat{\mathbf{x}}} = \frac{g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u},\hat{\mathbf{u}})\tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})^{\mathrm{T}} - \tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u},\hat{\mathbf{u}})^{\mathrm{T}}}{\left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}},\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})\right\rangle_{\hat{\mathbf{x}}}} D(\hat{\kappa}).$$

4.3 Interpolation

Since the modified discrete variational derivative method defined by (4.1) utilizes the rezoning approach, the initial data at each time step must be interpolated over on the new grid from the solution data obtained on the old grid at the previous time step. The interpolation method may be chosen arbitrarily, but by choosing an integral preserving interpolation method, i.e. an operator $\Phi_{(\hat{\mathbf{x}},\mathbf{x})}$ dependent on $\mathcal{I}_{\mathbf{x}}$ that satisfies $\mathcal{I}_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) = \mathcal{I}_{\mathbf{x}}(\mathbf{u})$, the adjustment term on the right hand side of (4.1) vanishes, and thus (4.1) becomes identical to a standard DVD method on the non-uniform grid $\hat{\mathbf{x}}$, with $\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ as the initial solution data at each time step. We will therefore present two different ways of generating integral preserving interpolation methods.

4.3.1 A Direct Integral Preserving Interpolation Procedure

Assume that for the first integral $\mathcal{I}[u] = \int_a^b I\left(u^J\right) \mathrm{d}x$, we have a consistent approximation on the grid $\mathbf{x}$ given by

$$\mathcal{I}_{\mathbf{x}}(\mathbf{u}) = \sum_{i=0}^{M-1} \kappa_i \tilde{I}(\mathbf{x},\mathbf{u})_i,$$

which for any weight κ_i can be rewritten as

$$\mathcal{I}_{\mathbf{x}}(\mathbf{u}) = \sum_{i=0}^{M-1} (x_{i+1} - x_i) I(\mathbf{x}, \mathbf{u})_i = \int_{x_0}^{x_M} i(x) \mathrm{d}x,$$

where $i(x)$ is the piecewise constant function

$$i(x) = \begin{cases} I(\mathbf{x}, \mathbf{u})_0 & \text{for } x \in [x_0, x_1] \\ I(\mathbf{x}, \mathbf{u})_1 & \text{for } x \in (x_1, x_2] \\ \quad \vdots & \\ I(\mathbf{x}, \mathbf{u})_{M-1} & \text{for } x \in (x_{M-1}, x_M]\,. \end{cases}$$

Then the idea behind the integral preserving interpolation method $\tilde{\mathbf{u}} = \Phi^{\mathrm{D}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ is to find the vector $\tilde{\mathbf{u}} \in \mathbb{R}^M$ satisfying the system of M equations

$$(\hat{x}_{i+1} - \hat{x}_i) I(\hat{\mathbf{x}}, \tilde{\mathbf{u}})_i = \int_{\hat{x}_i}^{\hat{x}_{i+1}} i(x) \mathrm{d}x, \qquad i = 0, ..., M-1. \tag{4.11}$$

As an example, if for the grid point $\hat{x}_{i+1}$, there exists an integer k such that $\hat{x}_i \in (x_{k-1}, x_k]$ and $\hat{x}_{i+1} \in (x_k, x_{k+1}]$, then the i-th equation of (4.11) becomes

$$(\hat{x}_{i+1} - \hat{x}_i) I(\hat{\mathbf{x}}, \tilde{\mathbf{u}})_i = (x_k - \hat{x}_i) I(\mathbf{x}, \mathbf{u})_{k-1} + (\hat{x}_{i+1} - x_k) I(\mathbf{x}, \mathbf{u})_k.$$

4.3.2 A Two-Step Integral Preserving Interpolation Procedure

Given an approximation $\mathbf{u}'$ on $\hat{\mathbf{x}}$ found by an arbitrary interpolation method $\mathbf{u}' = \Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ which does not in general preserve the first integral $\mathcal{I}[u]$, an interpolant $\tilde{\mathbf{u}} = \Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ preserving the first integral can be found by linear projection, i.e. by solving

$$\tilde{\mathbf{u}} = \mathbf{u}' + \lambda \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\mathbf{u}') \tag{4.12}$$

$$\mathcal{I}_{\hat{\mathbf{x}}}(\tilde{\mathbf{u}}) = \mathcal{I}_{\mathbf{x}}(\mathbf{u}), \tag{4.13}$$

for $\tilde{\mathbf{u}} \in \mathbb{R}^M$ and $\lambda \in \mathbb{R}$. We have here replaced $\tilde{\mathbf{u}}$ with $\mathbf{u}'$ in the argument of $\nabla \mathcal{I}_{\hat{\mathbf{x}}}$ in order to save some evaluations of $\nabla \mathcal{I}_{\hat{\mathbf{x}}}$.

Proposition 1. *A step of the discrete variational derivative method on a moving grid with an antisymmetric matrix $\tilde{\mathcal{S}}_{\hat{\mathbf{x}}}$, and the initial solution data found by the two-step interpolation method $\tilde{\mathbf{u}} = \Phi^{TS}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$, is equivalent to a step of the alternate modified discrete variational method (4.3) with interpolation operator $\Phi^{A}_{(\hat{\mathbf{x}},\mathbf{x})}$, adjustment direction $\tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}}\left(\hat{\mathbf{u}}, \Phi^{A}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right) = \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\Phi^{A}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})$, and the antisymmetric matrix $\mathcal{S}_{\hat{\mathbf{x}}}$ given by*

$$\mathcal{S}_{\hat{\mathbf{x}}} = \frac{\left(\tilde{\mathcal{S}}_{\hat{\mathbf{x}}} \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}\right) \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})^T - \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) \left(\tilde{\mathcal{S}}_{\hat{\mathbf{x}}} \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}\right)^T}{\left\langle \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}}, \Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla \mathcal{I}_{\hat{\mathbf{x}}}\left(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right) \right\rangle_{\hat{\mathbf{x}}}} D(\hat{\kappa}). \tag{4.14}$$

Proof. Assume that $\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ satisfies (4.12)-(4.13), and that $\hat{\mathbf{u}}$ is found by (4.1) with $\tilde{\mathcal{S}}_{\hat{\mathbf{x}}}$ and $\tilde{\mathbf{u}} = \Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$. Inserting (4.12) and (4.13) into (4.1) yields

$$\hat{\mathbf{u}} = \Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} + \lambda\nabla\mathcal{I}_{\hat{\mathbf{x}}}(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) + \Delta t\cdot\tilde{\mathcal{S}}_{\hat{\mathbf{x}}}\frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)} \tag{4.15}$$

By applying (2.35), (4.13) and (4.15), we get that

$$\begin{aligned}
\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}\left(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right) &= \mathcal{I}_{\hat{\mathbf{x}}}\left(\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right) - \mathcal{I}_{\hat{\mathbf{x}}}\left(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)\\
&= \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) - \mathcal{I}_{\hat{\mathbf{x}}}\left(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right) + \mathcal{I}_{\hat{\mathbf{x}}}\left(\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right) - \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})\\
&= \left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \lambda\nabla\mathcal{I}_{\hat{\mathbf{x}}}(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})\right.\\
&\qquad \left. + \Delta t\cdot\tilde{\mathcal{S}}_{\hat{\mathbf{x}}}\frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}\right\rangle_{\hat{\mathbf{x}}}\\
&\qquad - \left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \Delta t\cdot\tilde{\mathcal{S}}_{\hat{\mathbf{x}}}\frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}\right\rangle_{\hat{\mathbf{x}}}\\
&= \lambda\left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \nabla\mathcal{I}_{\hat{\mathbf{x}}}(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})\right\rangle_{\hat{\mathbf{x}}}\\
&\qquad + \Delta t\left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}, \tilde{\mathcal{S}}_{\hat{\mathbf{x}}}\frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}\right\rangle_{\hat{\mathbf{x}}},
\end{aligned}$$

and hence

$$\lambda = \frac{\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}},\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})\right\rangle_{\hat{\mathbf{x}}}} - \Delta t\frac{\left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}},\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \tilde{\mathcal{S}}_{\hat{\mathbf{x}}}\frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)}\right\rangle_{\hat{\mathbf{x}}}}{\left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}},\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})\right\rangle_{\hat{\mathbf{x}}}}. \tag{4.16}$$

By substituting this into (4.15), and arguing as in the proof of Theorem 3, we then find that

$$\begin{aligned}
\hat{\mathbf{u}} &= \Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} + \frac{\mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \mathcal{I}_{\hat{\mathbf{x}}}(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left\langle \frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta(\hat{\mathbf{u}},\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}, \nabla\mathcal{I}_{\hat{\mathbf{x}}}\left(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)\right\rangle_{\hat{\mathbf{x}}}}\nabla\mathcal{I}_{\hat{\mathbf{x}}}\left(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)\\
&\quad + \Delta t\cdot\mathcal{S}_{\hat{\mathbf{x}}}\frac{\delta\mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\hat{\mathbf{u}},\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)},
\end{aligned}$$

with $\mathcal{S}_{\hat{\mathbf{x}}}$ as given by (4.14). To see the converse, follow this last deduction backwards to get (4.15), with λ as given by (4.16). For $\Phi^{\mathrm{TS}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ satisfying (4.12)-(4.13), the relation (4.15) is identical to (4.1). □

Discrete variational derivative methods on moving grids with the two-step interpolation method are thus a subset of the alternative modified DVD method with

$$\tilde{\nabla}\mathcal{I}_{\hat{\mathbf{x}}}\left(\hat{\mathbf{u}}, \Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right) = \nabla\mathcal{I}_{\hat{\mathbf{x}}}(\Phi^{\mathrm{A}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})$$

and an arbitrary interpolation method.

4.3.3 Standard Interpolation

The computation of $\tilde{\mathbf{u}} = \Phi^{\mathrm{D}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ typically consists of solving (4.11) numerically, which may be expensive. Thus it is often advantageous to use a simpler interpolation scheme. One of the simplest methods is the linear interpolation $\tilde{\mathbf{u}} = \Phi^{\mathrm{L}}_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$, where each element $\tilde{u}_i$, $i = 0, ..., M-1$, of $\tilde{\mathbf{u}}$ is found by

$$\tilde{u}_i = u_k + (u_{k+1} - u_k)\frac{\hat{x}_i - x_{k-1}}{x_k - x_{k-1}},$$

where k is the integer satisfying

$$x_k \leq \hat{x}_i \leq x_{k+1}.$$

Other choices can be polynomial or spline interpolation. These methods will in general not be integral preserving, but this will be made up for by the adjustment term in (4.1).

4.4 Solution Procedure

As remarked at the beginning of the chapter, the modified DVD methods on moving grids utilize the rezoning approach, and must be solved by an alternate solution procedure. That is, the solution at each new time t^{n+1} is calculated by three main steps. First, the grid X_h^{n+1} is computed based on the solution $\mathbf{u}^n$ on X_h^n, calculated in the previous time step. Then $\mathbf{u}^n$ is interpolated over on the new grid X_h^{n+1}, either by a procedure that preserves the approximation of the first integral or by a procedure that does not. Subsequently, the solution $\mathbf{u}^{n+1}$ at the time t^{n+1} can be found by the scheme (4.1). The two first steps can alternatively be repeated for a given number of iterations, or until convergence.

If the grid redistribution at each new time step is generated from the values at the old time step, with no further iterations, the solution procedure can be illustrated by the following flowchart.

1. Given a uniform fixed grid over the physical domain and an initial condition $u_0(x)$, use a suitable grid density function $\omega(x)$ and the equidistribution principle (3.1) to compute an (approximately) equidistributing initial grid $\mathbf{x}^0$. Then compute the initial solution data $\mathbf{u}^0 = \left\{u_0(x_i^0)\right\}_{i=0}^{M-1}$. Set $n = 0$.

2. Use one of the methods presented in section 3.1.3 to compute the approximately equidistributing grid $\mathbf{x}^{n+1}$ from $\mathbf{x}^n$ and $\mathbf{u}^n$.

3. Compute $\tilde{\mathbf{u}} = \Phi_{(\mathbf{x}^{n+1},\mathbf{x}^n)}\mathbf{u}^n$, for a given interpolation operator $\Phi_{(\mathbf{x}^{n+1},\mathbf{x}^n)}$ mapping from $\mathbf{x}^n$ to $\mathbf{x}^{n+1}$.

4. Solve

$$\begin{aligned}\mathbf{u}^{n+1} &= \tilde{\mathbf{u}} + \frac{\mathcal{I}_{\mathbf{x}^n}\left(\mathbf{u}^n\right) - \mathcal{I}_{\mathbf{x}^{n+1}}(\tilde{\mathbf{u}})}{\left\langle \frac{\delta \mathcal{I}_{\mathbf{x}^{n+1}}}{\delta(\mathbf{u}^{n+1},\tilde{\mathbf{u}})}, \nabla \mathcal{I}_{\mathbf{x}^{n+1}}\left(\mathbf{u}^{n+1}\right)\right\rangle_{\mathbf{x}^{n+1}}} \nabla \mathcal{I}_{\mathbf{x}^{n+1}}\left(\mathbf{u}^{n+1}\right) \\ &\quad + \Delta t \cdot \mathcal{S}_{\mathbf{x}^{n+1}} \frac{\delta \mathcal{I}_{\mathbf{x}^{n+1}}}{\delta\left(\mathbf{u}^{n+1},\tilde{\mathbf{u}}\right)},\end{aligned}$$

for a given discrete variational derivative $\frac{\delta \mathcal{I}_{\mathbf{x}^{n+1}}}{\delta(\mathbf{u}^{n+1},\tilde{\mathbf{u}})}$ and antisymmetric matrix $\mathcal{S}_{\mathbf{x}^{n+1}}$, to obtain $\mathbf{u}^{n+1}$.

5. If $t^{n+1} < t^{\max}$, increment $n \leftarrow n+1$, and go to step 2.

It may be desired to make several iterations of the grid redistribution process to achieve a better approximation of an equidistributing grid at every time step. Given a number of maximum iterations μ and a tolerance ϵ, the steps 2 and 3 of the above procedure can be replaced by the following steps.

a. Set $\tilde{\mathbf{x}}_0 := \mathbf{x}^n$ and $\tilde{\mathbf{u}}_0 := \mathbf{u}^n$. Set $l = 0$.

b. Use one of the methods presented in section 3.1.3 to compute the approximately equidistributing grid $\tilde{\mathbf{x}}_{l+1}$ from $\tilde{\mathbf{x}}_l$ and $\tilde{\mathbf{u}}_l$.

c. Compute $\tilde{\mathbf{u}}_{l+1} = \Phi_{(\tilde{\mathbf{x}}_{l+1},\tilde{\mathbf{x}}_l)}\tilde{\mathbf{u}}_l$. If $l+1 < \mu$ and $\|\tilde{\mathbf{x}}_{l+1} - \tilde{\mathbf{x}}_l\| > \epsilon$, increment $l \leftarrow l+1$ and go to step a. Otherwise, set $\tilde{\mathbf{u}} := \tilde{\mathbf{u}}_{l+1}$ and $\mathbf{x}^{n+1} := \tilde{\mathbf{x}}_{l+1}$ and proceed to step 4.

4.5 Alternative Methods

We will now briefly present two alternative integral preserving methods for PDEs on moving grids, neither of whom fits into the framework of the modified discrete variational derivative methods.

4.5.1 Method of Modified Discrete Variational Derivatives

The modified DVD methods utilize the discrete variational derivatives as defined on a fixed grid. Another way of developing the DVD methods to moving grids could be based on the idea of finding *modified discrete variational derivatives* $\frac{\delta \mathcal{I}_{(\hat{\mathbf{x}},\mathbf{x},\Phi)}}{\delta(\hat{\mathbf{u}},\mathbf{u})} : \mathbb{R}^M \times \mathbb{R}^M \to \mathbb{R}^M$, dependent on the grids $\mathbf{x}$ and $\hat{\mathbf{x}}$ and an interpolation operator $\Phi_{(\hat{\mathbf{x}},\mathbf{x})}$, satisfying

$$\left\langle \frac{\delta \mathcal{I}_{(\hat{\mathbf{x}},\mathbf{x},\Phi)}}{\delta(\hat{\mathbf{u}},\mathbf{u})}, \hat{\mathbf{u}} - \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u} \right\rangle_{\hat{\mathbf{x}}} = \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) - \mathcal{I}_{\mathbf{x}}(\mathbf{u}), \tag{4.17}$$

$$\frac{\delta \mathcal{I}_{(\mathbf{x},\mathbf{x},\Phi)}}{\delta(\mathbf{u},\mathbf{u})} = \frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta \mathbf{u}}, \tag{4.18}$$

so that one step of an integral preserving scheme advancing the numerical solution $\mathbf{u}$ of (2.24) on $\mathbf{x}$ at time t to $\hat{\mathbf{u}}$ on $\hat{\mathbf{x}}$ at time $\hat{t}$ can be given by

$$\frac{\hat{\mathbf{u}} - \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}}{\Delta t} = \mathcal{S}_{\hat{\mathbf{x}}} \frac{\delta \mathcal{I}_{(\hat{\mathbf{x}},\mathbf{x},\Phi)}}{\delta(\hat{\mathbf{u}},\mathbf{u})}, \tag{4.19}$$

where $\mathcal{S}_{\hat{\mathbf{x}}}$ as before is antisymmetric with respect to the inner product $\langle\cdot,\cdot\rangle_{\hat{\mathbf{x}}}$.

One example of a function satisfying (4.17)-(4.18) is the *modified coordinate increment discrete variational derivative*, defined by its i'th element

$$\left[\frac{\delta_{\mathrm{CI}} \mathcal{I}_{(\hat{\mathbf{x}},\mathbf{x},\Phi)}}{\delta(\hat{\mathbf{u}},\mathbf{u})}\right]_i := \frac{1}{\hat{\kappa}_i} \frac{\mathcal{I}_{\tilde{\mathbf{x}}^i}(\hat{u}_1,...,\hat{u}_i,u_{i+1},...,u_{M-1}) - \mathcal{I}_{\tilde{\mathbf{x}}^{i-1}}(\hat{u}_1,...,\hat{u}_{i-1},u_i,...,u_{M-1})}{\hat{u}_i - \Phi_{(\hat{\mathbf{x}},\mathbf{x})}u_i},$$

where we have set $\tilde{\mathbf{x}}^i := (\hat{x}_1,...,\hat{x}_i,x_{i+1},...,x_{M-1})^{\mathrm{T}}$. Another example is the *modified midpoint discrete variational derivative*, defined by

$$\frac{\delta_{\mathrm{M}} \mathcal{I}_{(\hat{\mathbf{x}},\mathbf{x},\Phi)}}{\delta(\hat{\mathbf{u}},\mathbf{u})} := \frac{\delta \mathcal{I}_{\hat{\mathbf{x}}}}{\delta\left(\left(\hat{\mathbf{u}} + \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)/2\right)} + D(\hat{\kappa})^{-1} \frac{\mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) - \mathcal{I}_{\mathbf{x}}(\mathbf{u}) - \nabla \mathcal{I}_{\hat{\mathbf{x}}}\left(\frac{\hat{\mathbf{u}}+\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}}{2}\right)^{\mathrm{T}}(\hat{\mathbf{u}} - \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u})}{\left|\hat{\mathbf{u}} - \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right|^2}(\hat{\mathbf{u}} - \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}).$$

A modified version of the product discrete variational derivative can also be found, but its explicit definition is quite intricate, and therefore omitted here.

Even if the consistency relation (4.18) is satisfied by the modified DVDs defined above, we generally have that

$$\frac{\mathcal{I}_{(\hat{\mathbf{x}},\mathbf{x},\Phi)}}{\delta(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u},\mathbf{u})} \neq \frac{\delta \mathcal{I}_{\mathbf{x}}}{\delta \mathbf{u}},$$

as long as $\hat{\mathbf{x}} \neq \mathbf{x}$. In fact, the modified DVDs generally diverge as $\hat{\mathbf{u}} \to \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ and $\hat{\mathbf{x}} \neq \mathbf{x}$, and hence (4.19) is often difficult to solve numerically. For this method to be successful, the implementation must ensure that the grid movement is sufficiently small where the variations in the solution are small.

4.5.2 Projection Method with Lagrangian Discretization

The main goal of this thesis is to extend the discrete variational derivative methods to moving grids, in which case the Lagrangian approach is not relevant, as noted in section

4.1. Considering projection methods however, the Lagrangian approach could be used to obtain a temporary solution at the new time step, which could then be projected over on the manifold $\mathcal{M}_{(\hat{\mathbf{x}},\mathbf{x},\mathbf{u})}$ defined by (4.5). One step of that particular projection method could then be given by the following: Compute $\hat{\mathbf{u}} \in \mathbb{R}^M$ and $\lambda \in \mathbb{R}$ such that

$$\begin{aligned} \hat{\mathbf{u}} &= \mathbf{u} + D(\hat{\mathbf{x}} - \mathbf{x})\delta_{\mathbf{x}}\mathbf{u} + \Delta t g_{\mathbf{x}}(\mathbf{u}) + \lambda \nabla \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}), \\ \mathcal{I}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) &= \mathcal{I}_{\mathbf{x}}(\mathbf{u}), \end{aligned}$$

where $g_{\mathbf{x}}$ is defined as in section 4.2, and the difference operator $\delta_{\mathbf{x}}$ approximates the spatial derivative on the grid $\mathbf{x}$. Coupling this system of equations with the equations for grid generations, we obtain an integral preserving method than can be solved by a simultaneous solution procedure.

Chapter 5

Numerical Examples

In this chapter, we will develop the integral preserving modified discrete variational derivative methods presented in the previous chapter for two different initial-boundary value problems. The schemes will be evaluated in the form (4.1) for the concrete examples, and numerical results are subsequently presented.

5.1 The Test Problems

We will test the integral preserving moving grid methods on two different nonlinear, dispersive partial differential equations which both model waves on shallow water surfaces and have exact analytical solutions for certain initial conditions. The first such equation is the KdV equation from Example 2.2.1, given by (2.20). It is a popular choice of equation for testing numerical schemes. We will impose a given initial condition

$$u(x,0) = u_0(x), \tag{5.1}$$

and periodic boundary conditions,

$$u(-L,t) = u(L,t). \tag{5.2}$$

5.1.1 The BBM Equation

We will furthermore consider the Benjamin–Bona–Mahony (BBM) equation introduced in [1],

$$u_t - u_{xxt} + u_x + uu_x = 0, \tag{5.3}$$

with a given initial function (5.1) and periodic boundary conditions (5.2). The BBM equation describes surface waves in a channel. It belongs to a class of equations defined by the generalized hyperelastic-rod wave equations [5].

By introducing $m(x,t) = u(x,t) - u_{xx}(x,t)$, the equation (5.3) can be rewritten on the form (2.24) as

$$m_t = \mathcal{S}(m)\frac{\delta\mathcal{H}}{\delta m},$$

for two different pairs of a antisymmetric differential operator $\mathcal{S}(m)$ and a Hamiltonian $\mathcal{H}[m]$,

$$\begin{aligned}\mathcal{S}^1(m) &= -(\frac{2}{3}u+1)\partial_x - \frac{1}{3}u_x,\\ \mathcal{H}^1[m] &= \frac{1}{2}\int (u^2+u_x^2)\mathrm{d}x,\end{aligned} \tag{5.4}$$

and

$$\begin{aligned}\mathcal{S}^2(m) &= -\partial_x + \partial_{xxx},\\ \mathcal{H}^2[m] &= \frac{1}{2}\int (u^2+\frac{1}{3}u^3)\mathrm{d}x.\end{aligned} \tag{5.5}$$

Discrete variational derivative methods on uniform grids, preserving either $\mathcal{H}^1$ or $\mathcal{H}^2$, are derived for the problem in [9]. We will here develop corresponding schemes on moving grids.

5.2 Modified Discrete Variational Derivative Methods

We will now systematically derive integral preserving schemes of the form (4.1) for the KdV and BBM equations.

5.2.1 Spatial Discretization

We wish to discretize $\mathcal{H}^{\mathrm{K}}$, $\mathcal{H}^1$ and $\mathcal{H}^1$ in space using finite differences on the grid X_h : $x_0 = a < x_1 < ... < x_M = b$, from which we get the vector $\mathbf{x} = (x_0, x_1, ..., x_{M-1})^{\mathrm{T}}$. We let the approximation to $u(x_i, t)$ be denoted by u_i, and set $\mathbf{u} = (u_0, u_1, ..., u_{M-1})^{\mathrm{T}}$.

The difference operators δ^+, δ^- and δ on an element v_i of the vector $\mathbf{v}$ are defined by

$$\begin{aligned}\delta^+ v_i &= v_{i+1} - v_i,\\ \delta^- v_i &= v_i - v_{i-1},\\ \delta^{\mathrm{c}} v_i &= v_{i+1} - v_{i-1},\end{aligned}$$

and accordingly, the right, left and central discrete derivatives of $\mathbf{u}$ at x_i are given by

$$\begin{aligned}\delta^+_{\mathbf{x}} u_i &= \frac{\delta^+ u_i}{\delta^+ x_i} = \frac{u_{i+1}-u_i}{x_{i+1}-x_i}\\ \delta^-_{\mathbf{x}} u_i &= \frac{\delta^- u_i}{\delta^- x_i} = \frac{u_i-u_{i-1}}{x_i-x_{i-1}},\\ \delta^{\mathrm{c}}_{\mathbf{x}} u_i &= \frac{\delta^{\mathrm{c}} u_i}{\delta^{\mathrm{c}} x_i} = \frac{u_{i+1}-u_{i-1}}{x_{i+1}-x_{i-1}}.\end{aligned}$$

Furthermore, we define the discrete double derivative as

$$\begin{aligned}\delta_{\mathbf{x}}^2 u_i &= \frac{1}{2}\frac{1}{\delta^c x_i}\left(\delta^- \frac{\delta^c x_i}{(\delta^+ x_i)^2}\delta^+ + \delta^+ \frac{\delta^c x_i}{(\delta^- x_i)^2}\delta^-\right) u_i \\ &= \frac{1}{2(x_{i+1}-x_{i-1})}\left(\frac{x_{i+2}+x_{i+1}-x_i-x_{i-1}}{(x_{i+1}-x_i)^2}(u_{i+1}-u_i)\right. \\ &\quad \left. -\frac{x_{i+1}+x_i-x_{i-1}-x_{i-2}}{(x_i-x_{i-1})^2}(u_i-u_{i-1})\right),\end{aligned}$$

and set

$$\mathbf{m} := (1-\delta_{\mathbf{x}}^2)\mathbf{u}.$$

Utilizing the difference operators, we get a discrete approximation of $\mathcal{H}^{\mathrm{K}}[u]$ by

$$\begin{aligned}\mathcal{H}_{\mathbf{x}}^{\mathrm{K}}(\mathbf{u}) &= \sum_{i=0}^{M-1}\frac{\delta^c x_i}{2}\left(\frac{1}{4}\left(\left(\delta_{\mathbf{x}}^+ u_i\right)^2 + \left(\delta_{\mathbf{x}}^- u_i\right)^2\right) - (u_i)^3\right) \\ &= \sum_{i=0}^{M-1}\frac{x_{i+1}-x_{i-1}}{2}\left(\frac{1}{4}\left(\left(\frac{u_{i+1}-u_i}{x_{i+1}-x_i}\right)^2 + \left(\frac{u_i-u_{i-1}}{x_i-x_{i-1}}\right)^2\right) - (u_i)^3\right).\end{aligned}$$

For the BBM equation, we have a discrete approximation of the first Hamiltonian given by

$$\begin{aligned}\mathcal{H}_{\mathbf{x}}^1(\mathbf{m}) &= \sum_{i=0}^{M-1}\frac{\delta^c x_i}{4}\left((u_i)^2 + \frac{1}{2}\left(\left(\delta_{\mathbf{x}}^+ u_i\right)^2 + \left(\delta_{\mathbf{x}}^- u_i\right)^2\right)\right) \\ &= \sum_{i=0}^{M-1}\frac{x_{i+1}-x_{i-1}}{4}\left((u_i)^2 + \frac{1}{2}\left(\left(\frac{u_{i+1}-u_i}{x_{i+1}-x_i}\right)^2 + \left(\frac{u_i-u_{i-1}}{x_i-x_{i-1}}\right)^2\right)\right),\end{aligned}$$

while the second Hamiltonian is approximated by

$$\mathcal{H}_{\mathbf{x}}^2(\mathbf{m}) = \sum_{i=0}^{M-1}\frac{\delta^c x_i}{4}\left((u_i)^2 + \frac{1}{3}(u_i)^3\right) = \sum_{i=0}^{M-1}\frac{x_{i+1}-x_{i-1}}{4}\left((u_i)^2 + \frac{1}{3}(u_i)^3\right).$$

5.2.2 The Discrete Variational Derivatives

As in the case of a uniform grid, the approximation $\mathcal{H}_{\mathbf{x}}^{\mathrm{K}}(\mathbf{u})$ of (2.32) is of the form (2.34), and the average vector field and product discrete variational derivatives are therefore identical. We find it in the general grid case to be

$$\frac{\delta_{\mathrm{AVF}}\mathcal{H}_{\mathbf{x}}^{\mathrm{K}}}{\delta(\hat{\mathbf{u}},\mathbf{u})} = \frac{\delta_{\mathrm{P}}\mathcal{H}_{\mathbf{x}}^{\mathrm{K}}}{\delta(\hat{\mathbf{u}},\mathbf{u})} == -\frac{1}{2}\delta_{\mathbf{x}}^2\left(\hat{\mathbf{u}}+\mathbf{u}\right) - \left(\hat{\mathbf{u}}^2 + \hat{\mathbf{u}}\mathbf{u} + \mathbf{u}^2\right), \tag{5.6}$$

Here, and in the following, the multiplication of two column vectors is meant to be componentwise. We will utilize this DVD in the following experiments.

The variational derivatives with respect to m, $\frac{\delta\mathcal{H}^j}{\delta m}$ for $j = 1, 2$, can be found by first deriving the variational derivatives with respect to u, $\frac{\delta\mathcal{H}^j}{\delta u}$, using the definition (2.22), and then utilize the relation $\frac{\delta}{\delta m} = (1 - \partial_{xx})^{-1}\frac{\delta}{\delta u}$ to get $\frac{\delta\mathcal{H}^j}{\delta m}$. Using this approach, we get

$$\begin{aligned}\frac{\delta\mathcal{H}^1}{\delta m} &= u,\\ \frac{\delta\mathcal{H}^2}{\delta m} &= (1 - \partial_{xx})^{-1}(u + \frac{1}{2}u^2).\end{aligned}$$

Similarly, we use $\frac{\delta}{\delta \mathbf{m}} = (1 - \delta_{\mathbf{x}}^2)^{-1}\frac{\delta}{\delta \mathbf{u}}$ to get

$$\begin{aligned}\frac{\delta\mathcal{H}_{\mathbf{x}}^1}{\delta \mathbf{m}} &= \mathbf{u},\\ \frac{\delta\mathcal{H}_{\mathbf{x}}^2}{\delta \mathbf{m}} &= (1 - \delta_{\mathbf{x}}^2)^{-1}(\mathbf{u} + \frac{1}{2}\mathbf{u}^2).\end{aligned}$$

Corresponding to the variational derivative case, we define the discrete variational derivatives with respect to $\mathbf{m}$ by the relation

$$\frac{\delta\mathcal{H}_{\mathbf{x}}^j}{\delta(\hat{\mathbf{m}}, \mathbf{m})} = (1 - \delta_{\mathbf{x}}^2)^{-1}\frac{\delta\mathcal{H}_{\mathbf{x}}^j}{\delta(\hat{\mathbf{u}}, \mathbf{u})}. \tag{5.7}$$

We observe that $\frac{\delta\mathcal{H}_{\mathbf{x}}^1}{\delta \mathbf{m}}$ is a linear function of $\mathbf{m}$, and hence, by Theorem 3 in [9] and Theorem 1 in this thesis, the midpoint, average vector field and product discrete variational derivatives are identical for $\mathcal{H}^1$, and they are given by $\frac{\delta\mathcal{H}^1}{\delta((\hat{\mathbf{m}}+\mathbf{m})/2)}$. Thus we have a discrete variational derivative on the grid X_h represented by the elements of $\mathbf{x}$ given by

$$\frac{\delta_{\mathrm{M}}\mathcal{H}_{\mathbf{x}}^1}{\delta(\hat{\mathbf{m}}, \mathbf{m})} = \frac{\delta_{\mathrm{AVF}}\mathcal{H}_{\mathbf{x}}^1}{\delta(\hat{\mathbf{m}}, \mathbf{m})} = \frac{\delta_{\mathrm{P}}\mathcal{H}_{\mathbf{x}}^1}{\delta(\hat{\mathbf{m}}, \mathbf{m})} = \frac{\hat{\mathbf{u}} + \mathbf{u}}{2}, \tag{5.8}$$

which we will employ in the subsequent experiments.

Furthermore, since $\mathcal{H}_{\mathbf{x}}^2(\mathbf{m})$ is of the form

$$\mathcal{H}_{\mathbf{x}}(\mathbf{m}) = \sum_{i=0}^{M-1} c_i f_i(u_i) + c_M,$$

where $c_i \in \mathbb{R}$ are constants and $f_i(u_i) : \mathbb{R} \to \mathbb{R}$ are functions, we have from Theorem 2 in [9] that the coordinate increment, average vector field and product discrete variational derivatives are identical. We find

$$\begin{aligned}\overline{\nabla}_{\mathrm{CI}}\mathcal{H}_{\mathbf{x}}^2(\hat{\mathbf{u}}, \mathbf{u})_i &= \frac{\delta^{\mathrm{c}}x_i}{4}\frac{(\hat{u}_i)^2 + \frac{1}{3}(\hat{u}_i)^3 - (u_i)^2 - \frac{1}{3}(u_i)^3}{\hat{u}_i - u_i}\\ &= \frac{\delta^{\mathrm{c}}x_i}{4}\left(\hat{u}_i + u_i + \frac{1}{3}\left((\hat{u}_i)^2 + \hat{u}_i u_i + (u_i)^2\right)\right),\end{aligned}$$

and accordingly, we get

$$\frac{\delta_{\mathrm{CI}}\mathcal{H}^2_{\mathbf{x}}}{\delta(\hat{\mathbf{m}},\mathbf{m})} = \frac{\delta_{\mathrm{AVF}}\mathcal{H}^2_{\mathbf{x}}}{\delta(\hat{\mathbf{m}},\mathbf{m})} = \frac{\delta_{\mathrm{P}}\mathcal{H}^2_{\mathbf{x}}}{\delta(\hat{\mathbf{m}},\mathbf{m})} = \left(1-\delta^2_{\mathbf{x}}\right)^{-1} D\left(\frac{1}{2}\delta^{\mathrm{c}}\mathbf{x}\right)^{-1} \overline{\nabla}_{\mathrm{CI}}\mathcal{H}^2_{\mathbf{x}}(\hat{\mathbf{u}},\mathbf{u}) \qquad (5.9)$$

$$= \left(1-\delta^2_{\mathbf{x}}\right)^{-1}\left(\frac{1}{2}\left(\hat{\mathbf{u}}+\mathbf{u}\right)+\frac{1}{6}\left(\hat{\mathbf{u}}^2+\hat{\mathbf{u}}\mathbf{u}+\mathbf{u}^2\right)\right),$$

which we will use as the discrete variational derivative of $\mathcal{H}^2$ in the following experiments.

5.2.3 Approximation of the Antisymmetric Matrix

The choice of an approximation of $\mathcal{S}^{\mathrm{K}}(u)$ or $\mathcal{S}^j(m)$, for $j=1,2$, is not unique. For $\mathcal{S}^{\mathrm{K}}(u)$, it is natural to choose the central difference operator $\delta^{\mathrm{c}}_{\hat{\mathbf{x}}}$, which is indeed antisymmetric with respect to the inner product $\langle\cdot,\cdot\rangle_{\hat{\mathbf{x}}}$.

In the BBM case, we will use two different choices for each Hamiltonian. First we use the central difference operator, and apply the fact that

$$\mathcal{S}_1(m)v = -(\frac{2}{3}u+1)\partial_x v - \frac{1}{3}u_x v = -(\frac{1}{3}u+1)\partial_x v - \frac{1}{3}\partial_x(uv)$$

to find the antisymmetric operator

$$\mathcal{S}^1_{\hat{\mathbf{x}}}(\hat{\mathbf{m}},\mathbf{m}) = -\left(\frac{1}{6}\left(\hat{\mathbf{u}}+\mathbf{u}\right)+1\right)\delta^{\mathrm{c}}_{\hat{\mathbf{x}}} - \frac{1}{6}\delta^{\mathrm{c}}_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}+\mathbf{u}), \qquad (5.10)$$

where we emphasize that an operator $(\delta_{\mathbf{x}}\mathbf{u})$ is defined such that $(\delta_{\mathbf{x}}\mathbf{u})\mathbf{v} = \delta_{\mathbf{x}}(\mathbf{u}\mathbf{v})$. As an alternative choice, we have

$$\tilde{\mathcal{S}}^1_{\hat{\mathbf{x}}}(\hat{\mathbf{m}},\mathbf{m}) = \frac{-\left((1+\tilde{\mathbf{u}})\,\delta^{\mathrm{c}}_{\hat{\mathbf{x}}}\tilde{\mathbf{u}}\right)\left(D(\delta^{\mathrm{c}}\hat{\mathbf{x}})\hat{\mathbf{u}}\right)^{\mathrm{T}} + \left(D(\delta^{\mathrm{c}}\hat{\mathbf{x}})\hat{\mathbf{u}}\right)\left((1+\tilde{\mathbf{u}})\,\delta^{\mathrm{c}}_{\hat{\mathbf{x}}}\tilde{\mathbf{u}}\right)^{\mathrm{T}}}{\langle\hat{\mathbf{u}}+\tilde{\mathbf{u}}, D(\delta^{\mathrm{c}}\hat{\mathbf{x}})\hat{\mathbf{u}}\rangle_{\hat{\mathbf{x}}}} D(\delta^{\mathrm{c}}\hat{\mathbf{x}}), \qquad (5.11)$$

where we for convenience have set $\tilde{\mathbf{u}} := \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$. The matrix (5.11) is of the form (4.8), where we have set

$$g_{\hat{\mathbf{x}}}(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}) = -\left(1+\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right)\delta^{\mathrm{c}}_{\hat{\mathbf{x}}}\left(\Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}\right), \qquad (5.12)$$

and hence, for the BBM problem, the modified DVD method with the approximation to $\mathcal{S}^1(m)$ given by (5.11) is equivalent to a linear projection method with the temporal integration step given by the Euler method.

Similarly, for the approximation of $\mathcal{S}^2(\mathbf{m})$, we use the central difference operator to find

$$\mathcal{S}^2_{\hat{\mathbf{x}}}(\hat{\mathbf{m}},\mathbf{m}) = -\delta^{\mathrm{c}}_{\hat{\mathbf{x}}}(1-\delta^{\mathrm{c}}_{\hat{\mathbf{x}}}\delta^{\mathrm{c}}_{\hat{\mathbf{x}}}), \qquad (5.13)$$

and from (4.8) and the Euler method, we obtain

$$\tilde{\mathcal{S}}^2_{\hat{\mathbf{x}}}(\hat{\mathbf{m}},\mathbf{m}) = \frac{g_{\hat{\mathbf{x}}}(\tilde{\mathbf{u}})\nabla\mathcal{H}^2_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})^{\mathrm{T}} + \nabla\mathcal{H}^2_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})\,g_{\hat{\mathbf{x}}}(\tilde{\mathbf{u}})^{\mathrm{T}}}{\left\langle\left(1-\delta^2_{\hat{\mathbf{x}}}\right)^{-1}\left(\hat{\mathbf{u}}+\tilde{\mathbf{u}}+\frac{1}{3}\left(\hat{\mathbf{u}}^2+\hat{\mathbf{u}}\tilde{\mathbf{u}}+\tilde{\mathbf{u}}^2\right)\right), \nabla\mathcal{H}^2_{\hat{\mathbf{x}}}(\hat{\mathbf{u}})\right\rangle_{\hat{\mathbf{x}}}} D(\delta^{\mathrm{c}}\hat{\mathbf{x}}), \qquad (5.14)$$

where $g_{\hat{\mathbf{x}}}(\tilde{\mathbf{u}})$ is given by (5.12), and

$$\nabla\mathcal{H}^2_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}) = \frac{1}{2}D(\delta^{\mathrm{c}}\hat{\mathbf{x}})\left(1-\delta^2_{\hat{\mathbf{x}}}\right)\left(\hat{\mathbf{u}}+\frac{1}{2}\hat{\mathbf{u}}^2\right).$$

5.2.4 An Integral Preserving Scheme for the KdV Equation

Applying the modified discrete variational derivative method with the DVD (5.6), and defining the operator δ^{b} on a vector $\mathbf{v}$ by

$$\delta^{\mathrm{b}} v_i = v_i + v_{i-1},$$

we get the scheme

$$\begin{aligned} \hat{\mathbf{u}} \; = \; & \tilde{\mathbf{u}} \\ & - \frac{(\delta^{\mathrm{c}}\mathbf{x}^n)^{\mathrm{T}} \left(\frac{1}{4}\delta^{\mathrm{b}} \left(\delta^{+}_{\mathbf{x}^n}\mathbf{u}^n\right)^2 - (\mathbf{u}^n)^3\right) - (\delta^{\mathrm{c}}\hat{\mathbf{x}})^{\mathrm{T}} \left(\frac{1}{4}\delta^{\mathrm{b}} \left(\delta^{+}_{\hat{\mathbf{x}}}\tilde{\mathbf{u}}\right)^2 - \tilde{\mathbf{u}}^3\right)}{\left(\frac{1}{2}\delta^2_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}+\tilde{\mathbf{u}}) + \hat{\mathbf{u}}^2 + \hat{\mathbf{u}}\tilde{\mathbf{u}} + \tilde{\mathbf{u}}^2\right)^{\mathrm{T}} \left(D\left((\delta^{\mathrm{c}}\hat{\mathbf{x}})^2\right)\left(\delta^2_{\hat{\mathbf{x}}}\hat{\mathbf{u}} + 3\hat{\mathbf{u}}^2\right)\right)} \\ & \cdot D(\delta^{\mathrm{c}}\hat{\mathbf{x}})\left(\delta^2_{\hat{\mathbf{x}}}\hat{\mathbf{u}} + 3\hat{\mathbf{u}}^2\right) \\ & -\Delta t \cdot \delta^{\mathrm{c}}_{\hat{\mathbf{x}}}\left(\frac{1}{2}\delta^2_{\hat{\mathbf{x}}}(\hat{\mathbf{u}}+\tilde{\mathbf{u}}) + \hat{\mathbf{u}}^2 + \hat{\mathbf{u}}\tilde{\mathbf{u}} + \tilde{\mathbf{u}}^2\right), \end{aligned} \tag{5.15}$$

where we have set $\hat{\mathbf{x}} := \mathbf{x}^{n+1}$, $\hat{\mathbf{u}} := \mathbf{u}^{n+1}$ and $\tilde{\mathbf{u}} := \Phi_{(\mathbf{x}^{n+1},\mathbf{x}^n)}\mathbf{u}^n$, for any interpolation operator $\Phi_{(\mathbf{x}^{n+1},\mathbf{x}^n)}$ mapping from the grid given by $\mathbf{x}^n$ to the grid given by $\mathbf{x}^{n+1}$. The scheme preserves the Hamiltonian (2.32) in the sense that

$$\mathcal{H}^{\mathrm{K}}_{\mathbf{x}^n}\left(\mathbf{u}^n\right) = \mathcal{H}^{\mathrm{K}}_{\mathbf{x}^0}\left(\mathbf{u}^0\right), \qquad \text{for all } n \geq 0.$$

5.2.5 Integral Preserving Schemes for the BBM Equation

Utilizing the discrete variational derivative (5.8), we obtain the numerical scheme

$$\begin{aligned} \mathbf{u}^{n+1} \; = \; & \tilde{\mathbf{u}} + \left(1 - \delta^2_{\mathbf{x}^{n+1}}\right)^{-1} \Bigg\{ \\ & \frac{(\delta^{\mathrm{c}}\mathbf{x}^n)^{\mathrm{T}} \left((\mathbf{u}^n)^2 + \frac{1}{2}\delta^{\mathrm{b}}\left(\delta^{+}_{\mathbf{x}^n}\mathbf{u}^n\right)^2\right) - \left(\delta^{\mathrm{c}}\mathbf{x}^{n+1}\right)^{\mathrm{T}} \left(\tilde{\mathbf{u}}^2 + \frac{1}{2}\delta^{\mathrm{b}}\left(\delta^{+}_{\mathbf{x}^{n+1}}\tilde{\mathbf{u}}\right)^2\right)}{(\mathbf{u}^{n+1} + \tilde{\mathbf{u}})^{\mathrm{T}} \left(D((\delta^{\mathrm{c}}\mathbf{x}^{n+1})^2)\mathbf{u}^{n+1}\right)} \\ & \cdot D(\delta^{\mathrm{c}}\mathbf{x}^{n+1})\mathbf{u}^{n+1} + \frac{\Delta t}{2}\mathcal{S}^1_{\mathbf{x}^{n+1}}(\mathbf{m}^{n+1}, \tilde{\mathbf{m}})\left(\mathbf{u}^{n+1} + \tilde{\mathbf{u}}\right)\Bigg\}, \end{aligned} \tag{5.16}$$

where still $\tilde{\mathbf{u}} = \Phi_{(\mathbf{x}^{n+1},\mathbf{x}^n)}\mathbf{u}^n$, and $\mathcal{S}^1_{\mathbf{x}}(\mathbf{m}^{n+1}, \tilde{\mathbf{m}})$ can be given by (5.10) or (5.11). The scheme preserves the Hamiltonian (5.4) in the sense that

$$\mathcal{H}^1_{\mathbf{x}^n}\left(\mathbf{m}^n\right) = \mathcal{H}^1_{\mathbf{x}^0}\left(\mathbf{m}^0\right), \qquad \text{for all } n \geq 0.$$

Similarly, by using the DVD (5.9), we get the scheme

$$\begin{aligned}
\mathbf{u}^{n+1} \; = \; & \tilde{\mathbf{u}} + \left(1 - \delta^2_{\mathbf{x}^{n+1}}\right)^{-1} \Bigg\{ \\
& \left[(\delta^c \mathbf{x}^n)^{\mathrm{T}} \left((\mathbf{u}^n)^2 + \frac{1}{3} (\mathbf{u}^n)^3 \right) - \left(\delta^c \mathbf{x}^{n+1}\right)^{\mathrm{T}} \left(\tilde{\mathbf{u}}^2 + \frac{1}{3} \tilde{\mathbf{u}}^3 \right) \right] \Big/ \\
& \left[\left(\left(1 - \delta^2_{\mathbf{x}^{n+1}}\right)^{-1} \left(\mathbf{u}^{n+1} + \tilde{\mathbf{u}} + \frac{1}{3} \left((\mathbf{u}^{n+1})^2 + \mathbf{u}^{n+1} \tilde{\mathbf{u}} + \tilde{\mathbf{u}}^2 \right) \right) \right)^{\mathrm{T}} \right. \\
& \left. \left(D((\delta^c \mathbf{x}^{n+1})^2) \left(1 - \delta^2_{\mathbf{x}^{n+1}}\right)^{-1} \left(\mathbf{u}^{n+1} + \frac{1}{2} (\mathbf{u}^{n+1})^2 \right) \right) \right] \qquad (5.17) \\
& \cdot D(\delta^c \mathbf{x}^{n+1}) \left(1 - \delta^2_{\mathbf{x}^{n+1}}\right)^{-1} \left(\mathbf{u}^{n+1} + \frac{1}{2} (\mathbf{u}^{n+1})^2 \right) \\
& + \frac{\Delta t}{2} \mathcal{S}^2_{\mathbf{x}^{n+1}} (\mathbf{m}^{n+1}, \tilde{\mathbf{m}}) \left(1 - \delta^2_{\mathbf{x}^{n+1}}\right)^{-1} \\
& \left(\mathbf{u}^{n+1} + \tilde{\mathbf{u}} + \frac{1}{3} \left((\mathbf{u}^{n+1})^2 + \mathbf{u}^{n+1} \tilde{\mathbf{u}} + \tilde{\mathbf{u}}^2 \right) \right) \Bigg\},
\end{aligned}$$

where $\mathcal{S}^2_{\mathbf{x}}(\mathbf{m}^{n+1}, \tilde{\mathbf{m}})$ can be given by either (5.13) or (5.14). This scheme preserves the second Hamiltonian (5.5), i.e. it satisfies

$$\mathcal{H}^2_{\mathbf{x}^n}(\mathbf{m}^n) = \mathcal{H}^2_{\mathbf{x}^0}(\mathbf{m}^0), \qquad \text{for all } n \geq 0.$$

5.3 Solution Procedure

For these one-dimensional problems we will use our slightly modified version of the straightforward de Boor's algorithm to compute an approximately equidistributing grid at each step of time. We choose the arc-length function (3.2) as our grid density function, and obtain the piecewise constant function

$$p^n(x) = \begin{cases}
\sqrt{1 + \left(\frac{u_1^n - u_0^n}{x_1^n - x_0^n} \right)^2} & \text{for } x \in [x_0^n, x_1^n] \\
\sqrt{1 + \left(\frac{u_2^n - u_1^n}{x_2^n - x_1^n} \right)^2} & \text{for } x \in (x_1^n, x_2^n] \\
\quad \vdots & \\
\sqrt{1 + \left(\frac{u_{M-1}^n - u_{M-2}^n}{x_{M-1}^n - x_{M-2}^n} \right)^2} & \text{for } x \in \left(x_{M-2}^n, x_{M-1}^n\right] \\
\sqrt{1 + \left(\frac{u_0^n - u_{M-1}^n}{L - x_{M-1}^n} \right)^2} & \text{for } x \in \left(x_{M-1}^n, L\right]
\end{cases}$$

at time t^n, used in the generation of the grid X_h^{n+1} represented by $\mathbf{x}^{n+1}$. We set $x_0^{n+1} = x_0^n = -L$ and find the remaining $M-1$ elements of $\mathbf{x}^{n+1}$ by first determining, for each

$i \in [1, M-1]$, the index k such that

$$P^n(x_{k-1}^n) < \frac{i}{M} P^n(L) \leq P^n(x_k^n),$$

where

$$\begin{aligned} P^n(x_k^n) &= \sum_{j=1}^{k} (x_j^n - x_{j-1}^n) p^n(x_j^n) \\ &= \sum_{j=1}^{k} \sqrt{(x_j^n - x_{j-1}^n)^2 + (u_j^n - u_{j-1}^n)^2}, \text{ for } k = 1, ..., M-1, \\ P^n(L) &= P^n(x_{M-1}^n) + (L - x_{M-1}^n) p^n(L) \\ &= P^n(x_{M-1}^n) + \sqrt{(L - x_{M-1}^n)^2 + (u_0^n - u_{M-1}^n)^2}, \end{aligned}$$

and then calculate

$$x_i^{n+1} = x_{k-1}^n + \frac{\frac{i}{M} P^n(L) - P^n(x_{k-1}^n)}{p^n(x_k^n)}. \tag{5.18}$$

For the calculation of the initial grid X_h^0 represented by $\mathbf{x}^0$, we use a background grid X_h^{-1} with grid points

$$x_i^{-1} = \frac{2iL}{M} - L, \text{ for } i = 0..., M-1, \tag{5.19}$$

and define the piecewise constant function $p^{-1}(x)$ by

$$p^{-1}(x) = \frac{1}{2} \left(\sqrt{1 + \left(\frac{\mathrm{d}}{\mathrm{d}x} u_0(x_i^{-1}) \right)^2} + \sqrt{1 + \left(\frac{\mathrm{d}}{\mathrm{d}x} u_0(x_{i+1}^{-1}) \right)^2} \right) \tag{5.20}$$

for $x \in \left(x_i^{-1}, x_{i+1}^{-1} \right]$, which we use to calculate $\mathbf{x}^0$ by (5.18).

For the interpolation over on the new grid, we use either linear interpolation, cubic Hermite interpolation or the two-step integral preserving interpolation procedure presented in section 4.3.2. We only regenerate the grid and interpolate $\mathbf{u}$ over on it once every time step, i.e. with no further iterations.

The solutions $\mathbf{u}^{n+1}$ at every new time step t^{n+1} are subsequently found by the schemes presented in the previous section. Note that when the integral preserving interpolation procedure is applied, the adjustment term vanishes from the schemes, and they are hence reduced to standard discrete variational derivative methods on the grid $\mathbf{x}^{n+1}$, with the initial solution at every time step being the solution from the previous time step, $\mathbf{u}^n$, interpolated over on $\mathbf{x}^{n+1}$.

The solution procedure can then be illustrated by the following flowchart.

1. Given the initial solution (5.1) and the background grid $\mathbf{x}^{-1}$ defined by (5.19), compute $\mathbf{x}^0$ by (5.18) with (5.20), and compute $\mathbf{u}^0 = \left\{ u_0(x_i^0) \right\}_{i=0}^{M-1}$. Set $n = 0$.

2. Generate $\mathbf{x}^{n+1}$ by (5.18), and compute $\tilde{\mathbf{u}} = \Phi_{(\mathbf{x}^{n+1},\mathbf{x}^n)}\mathbf{u}^n$, for a given interpolation method $\Phi_{(\mathbf{x}^{n+1},\mathbf{x}^n)}$ mapping from $\mathbf{x}^n$ to $\mathbf{x}^{n+1}$.

3. Compute the numerical approximation $\mathbf{u}^{n+1}$ at time t^{n+1} by one of the integral preserving schemes presented above.

4. If $t^{n+1} < t^{\max}$, increment $n \leftarrow n+1$, and go to step 2.

5.4 Numerical Results

We now present numerical results obtained with the scheme (5.15) for solving the KdV equation and the schemes (5.16) and (5.17) for solving the BBM equation, implemented as described above.

5.4.1 The KdV Equation

An exact solution of the KdV equation (2.31) with initial condition

$$u_0(x) = \frac{1}{2}c\,\mathrm{sech}^2\left(\frac{\sqrt{c}}{2}x\right) \tag{5.21}$$

and periodic boundary conditions (5.2) is given by

$$u(x,t) = \frac{1}{2}c\,\mathrm{sech}^2\left(\frac{\sqrt{c}}{2}l(x,t)\right), \tag{5.22}$$

where

$$l(x,t) = \min_{j\in\mathbb{Z}} |x - ct + 2jL|\,. \tag{5.23}$$

This is a soliton solution, traveling with a constant speed c in x-direction while maintaining its initial shape.

We set $\mathbf{u}^n_{\text{exact}}$ to be the vector of the exact solution at every space step x_i, $i = 0, ..., M-1$, at time t_n,

$$\mathbf{u}^n_{\text{exact}} = \left(u(x_0,t_n), ..., u(x_{M-1},t_n)\right)^{\mathrm{T}},$$

and have then that the global error at time step t_n is given by

$$\varepsilon^n_{\text{global}} = \|\mathbf{e}^n\|_2 = \|\mathbf{u}^n_{\text{exact}} - \mathbf{u}^n\|_2\,.$$

For a better indication of the long time behaviour of the presented schemes, we define the vector $\mathbf{u}^n_s(\eta) = (u_s(x^n_0,\eta), u_s(x^n_1,\eta), ..., u_s(x^n_{M-1},\eta))^{\mathrm{T}}$ of functions

$$u_s(x^n_i,\eta) = \frac{1}{2}c\,\mathrm{sech}^2\left(\frac{\sqrt{c}}{2}(x-\eta)\right), \quad \text{for } i = 0, ..., M-1,$$

and can then define the *shape error*

$$\varepsilon^n_{\text{shape}} = \min_{\eta} \|\mathbf{u}^n - \mathbf{u}^n_s(\eta)\|_2 \,, \tag{5.24}$$

measuring the extent to which the numerical methods are able to preserve the shape of the wave, and the *distance error*

$$\varepsilon^n_{\text{distance}} = \min_{j\in\mathbb{Z}} \left| \arg\min_{\eta} \|\mathbf{u}^n - \mathbf{u}^n_s(\eta)\|_2 - ct^n + 2jL \right| \tag{5.25}$$

measuring to what extent the methods preserve the phase speed c of the exact solution.

The global, shape and distance errors, as well as the Hamiltonian error

$$\varepsilon^n_{\mathcal{H}^{\text{K}}} = \left\| \mathcal{H}^{\text{K}}_{\mathbf{x}^n}(\mathbf{u}^n) - \mathcal{H}^{\text{K}}_{\mathbf{x}^0}(\mathbf{u}^0) \right\|_2 ,$$

is plotted for various implementations of the scheme (5.15) in Figure 5.1. The moving grid solution procedure described in the previous section is tested, with both the integral preserving two-step interpolation procedure and linear interpolation, and compared to the same scheme evaluated on a uniform grid.

In Figure 5.1a we see how the scheme preserves the Hamitonian, up to a small computational error that can be attributed to the round-off error in Matlab's numerical solver of systems of linear equations. From Figure 5.1b, we see that the global error of the moving grid implementations can be compared to the global error of the uniform grid implementation, although the graph seems to indicate that the error of the moving grid implementations will get considerably higher than the error of the uniform grid implementation over longer time periods. This assumption is supported by Figure 5.1d, where we see that the shape error of the moving grid methods grows steadily with time, while it seems to stay within a certain limit in the uniform grid case. The phase speed is however better preserved by the moving grid methods.

The choice between linear interpolation and the two-step interpolation procedure seems to make only a small difference in this case. We remark that for the initial interpolation step $\mathbf{u}' = \Phi_{(\hat{\mathbf{x}},\mathbf{x})}\mathbf{u}$ in the two-step procedure, we used linear interpolation. Thus the small difference between the methods makes sense in the view of Proposition 1, which states that they are then different types of the alternate modified DVD method, but with the same interpolation operator.

5.4.2 The BBM Equation

We have that

$$u(x,t) = 3(c-1)\,\text{sech}^2\left(\frac{1}{2}\sqrt{1-\frac{1}{c}}\,l(x,t)\right), \tag{5.26}$$

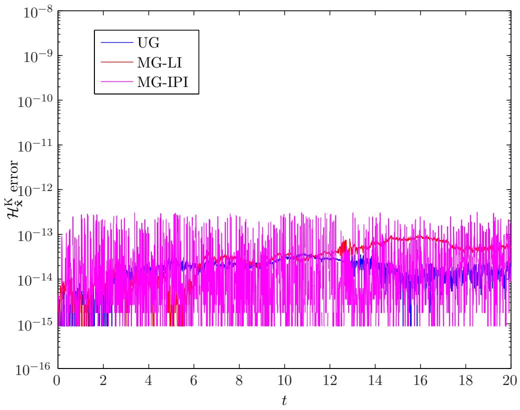
with $l(x,t)$ as given by (5.23), is a solution of (5.3) with the periodic boundary conditions (5.2) and the initial value

$$u_0(x) = 3(c-1)\,\text{sech}^2\left(\frac{1}{2}\sqrt{1-\frac{1}{c}}\,x\right). \tag{5.27}$$

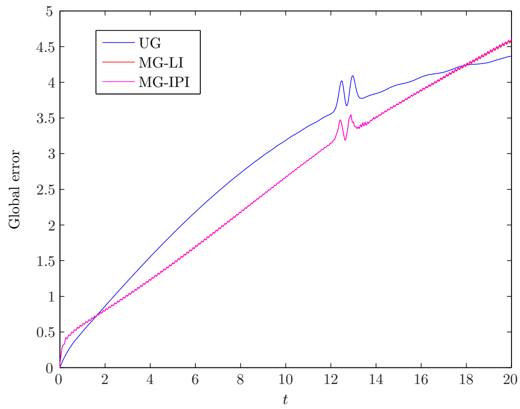
This is a soliton solution of the BBM equation which travels with a constant speed c in x-direction while maintaining its initial shape.

We define the vector of exact solutions $\mathbf{u}^n_{\text{exact}} = (u(x_0,t_n),...,u(x_{M-1},t_n))^{\mathrm{T}}$, the global error $\varepsilon^n_{\text{global}} = \|\mathbf{u}^n_{\text{exact}} - \mathbf{u}^n\|_2$ and the Hamiltonian errors

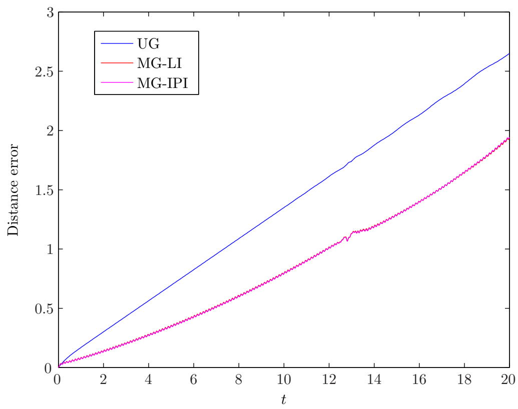
$$\varepsilon^n_{\mathcal{H}^j} = \left\| \mathcal{H}^j_{\mathbf{x}^n}(\mathbf{u}^n) - \mathcal{H}^j_{\mathbf{x}^0}(\mathbf{u}^0) \right\|_2$$



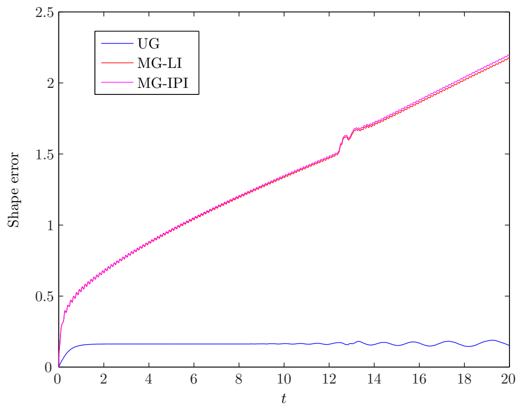
(a) The Hamiltoninan error $\varepsilon^n_{\mathcal{H}^{\mathrm{K}}}$ at different time steps t^n.



(b) The global error $\varepsilon^n_{\text{global}}$ at different time steps t^n.



(c) The distance error $\varepsilon^n_{\text{distance}}$ at different time steps t^n.



(d) The shape error $\varepsilon^n_{\text{shape}}$ at different time steps t^n.

Figure 5.1: Error plots for variants of the integral preserving numerical scheme (5.15) applied to the KdV equation (2.31), with initial-value conditions (5.1)-(5.2), u_0 given by (5.21) with $c = 4$, $L = 20$, the number of grid points $M = 200$, time step $\Delta t = 0.1$ and $t_{\max} = 20$. UG: DVD method on a fixed uniform fixed grid. MG-LI: Modified DVD method on moving grid, with linear interpolation. MG-LI: DVD method on moving grid, with integral preserving interpolation.

as for the KdV equation. For this problem we set the elements of $\mathbf{u}_s^n(\eta)$ to be

$$u_s(x_i^n, \eta) = 3(c-1)\,\mathrm{sech}^2\left(\frac{1}{2}\sqrt{1-\frac{1}{c}}(x-\eta)\right), \quad \text{for } i = 0, ..., M-1$$

and have the shape error given by (5.24) and the distance error given by (5.25).

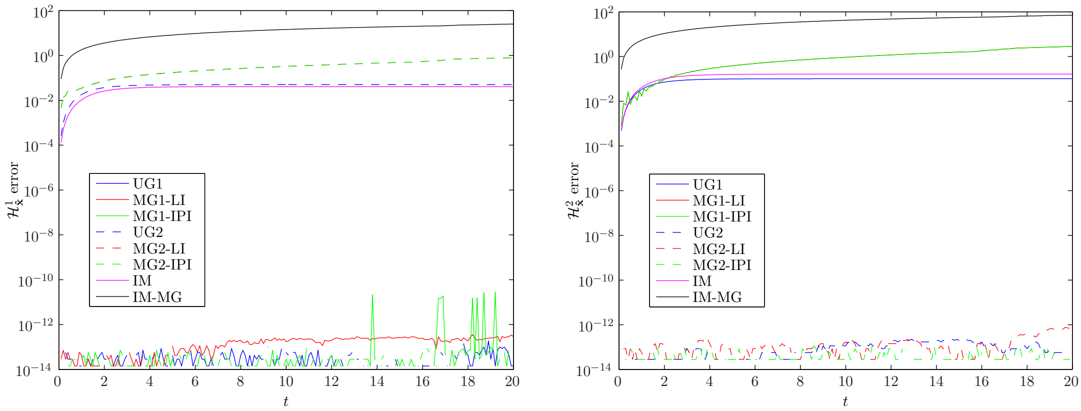
The schemes (5.16) and (5.17) are tested on the interval $[-50, 50]$, with initial solution (5.27) and various choices of the grid, the antisymmetric matrix and the interpolation method. The schemes are also compared to the implicit midpoint method, evaluated both on a fixed uniform grid and a moving grid.

First we note that the variants of the schemes (5.16) and (5.17) with the alternative antisymmetric matrices (5.11) and (5.14), i.e. the schemes equivalent to projection methods, perform consistently worse than the schemes with the antisymmetric matrices (5.10) and (5.13). Still, they generally express similar behaviour as the schemes with (5.10) and (5.13) when compared to eachother and the implicit midpoint method. Therefore we refrain from showing plots of the numerical results of the schemes with the alternative antisymmetric matrices, focusing on the similar plots for the schemes with (5.10) and (5.13).

We first present the results when the schemes are implemented with a linear interpolation method, either as the whole interpolation procedure or as part of the integral preserving two-step interpolation procedure. The Hamiltonian errors are presented for these methods in Figure 5.2. We observe how all the variants of the scheme (5.16) preserve an approximation of $\mathcal{H}^1$, while the variants of the scheme (5.16) preserve an approximation of $\mathcal{H}^2$.

In Figure 5.3a we see that the integral preserving methods give good results compared to both implementations of the implicit midpoint method. As in the KdV case, the choice between the direct and two-step interpolation methods have only a small impact on the results. We also observe that the difference in the results of the scheme (5.16) and (5.17) are small. In the figures 5.3b and 5.3c we observe results similar to the results in the KdV case. That is, the moving grid implementation of the modified discrete variational derivative methods preserves the phase speed better than the fixed grid implementation, while the opposite is true for the shape of the wave. In this case, it is reasonable to claim that the moving grid implementation of the DVD methods preserve the phase speed quite well.

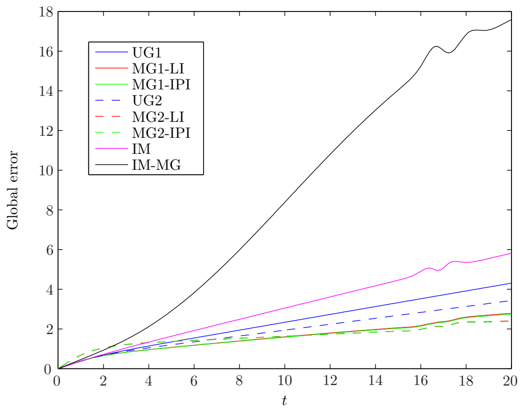
In Figure 5.4 we present the errors of the schemes when implemented on a moving grid with a cubic interpolation method instead of a linear interpolation method. The most evident result is how greatly the implicit midpoint method benefits from this change. However, we can also observe how the integral preserving schemes, especially (5.16), in this case preserves the shape of the wave much better than in the cases with linear interpolation. The global error and distance error are on the other hand larger when cubic interpolation is used.



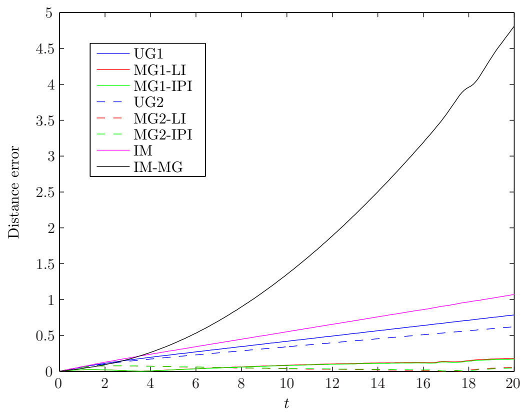
(a) The error $\varepsilon^n_{\mathcal{H}^1}$ in the discrete approximation of the Hamiltonian $\mathcal{H}^1$.

(b) The error $\varepsilon^n_{\mathcal{H}^2}$ in the discrete approximation of the Hamiltonian $\mathcal{H}^2$.

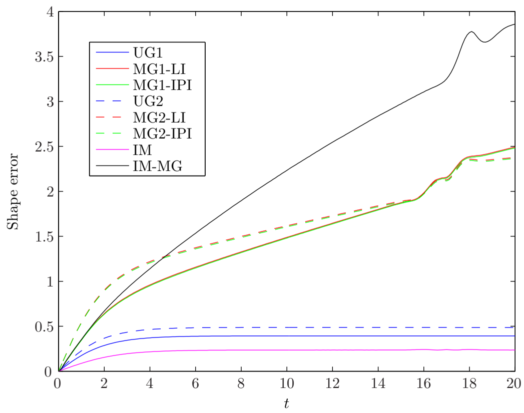
Figure 5.2: The Hamiltonian errors for the different numerical schemes, when applied to the BBM equation (5.3), with initial-boundary value conditions (5.1)-(5.2), u_0 given by (5.27) with $c = 3$, $L = 50$, the number of grid points $M = 200$, time step $\Delta t = 0.1$ and $t_{\max} = 20$. UG1: Scheme (5.16) on a fixed uniform grid. MG1-LI: (5.16) on a moving grid, with linear interpolation. MG1-IPI: (5.16) on a moving grid, with the integral preserving two-step interpolation procedure. UG2: Scheme (5.17) on a fixed uniform grid. MG2-LI: (5.17) on a moving grid, with linear interpolation. MG2-IPI: (5.17) on a moving grid, with the two-step interpolation procedure. IM: Implicit midpoint method on a fixed uniform grid. IM-MG: Implicit midpoint method on a moving grid, with linear interpolation.



(a) The global error $\varepsilon^n_{\text{global}}$ at different time steps t^n.

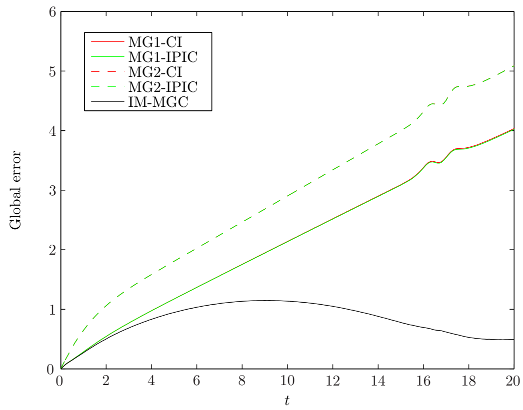


(b) The distance error $\varepsilon^n_{\text{distance}}$ at different time steps t^n.

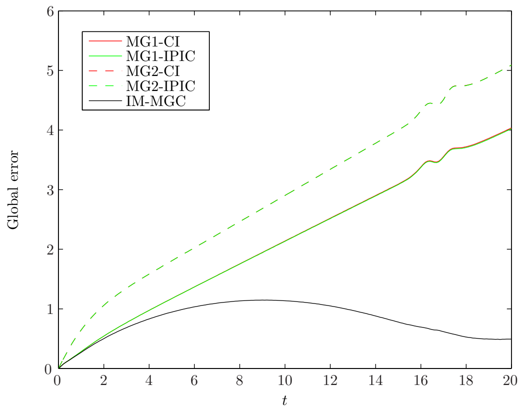


(c) The shape error $\varepsilon^n_{\text{shape}}$ at different time steps t^n.

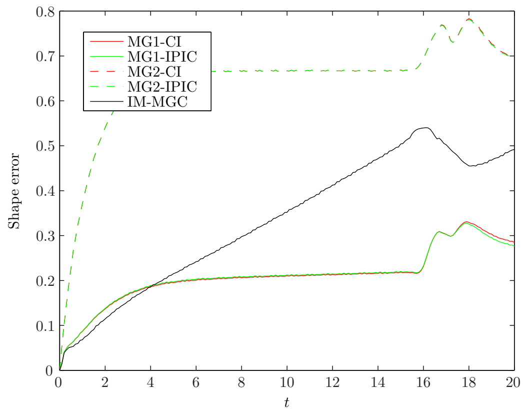
Figure 5.3: Error plots for the different numerical schemes applied to the BBM equation (5.3), with initial-boundary value conditions (5.1)-(5.2), u_0 given by (5.27) with $c = 3$, $L = 50$, number of grid points $M = 200$, time step $\Delta k = 0.1$ and $t_{\max} = 20$. UG1: Scheme (5.16) on a fixed uniform grid. MG1-LI: (5.16) on a moving grid, with linear interpolation. MG1-IPI: (5.16) on a moving grid, with the integral preserving two-step interpolation procedure. UG2: Scheme (5.17) on a fixed uniform grid. MG2-LI: (5.17) on a moving grid, with linear interpolation. MG2-IPI: (5.17) on a moving grid, with the two-step interpolation procedure. IM: Implicit midpoint method on a fixed uniform grid. IM-MG: Implicit midpoint method on a moving grid, with linear interpolation.



(a) The global error $\varepsilon^n_{\text{global}}$ at different time steps t^n.



(b) The distance error $\varepsilon^n_{\text{distance}}$ at different time steps t^n.



(c) The shape error $\varepsilon^n_{\text{shape}}$ at different time steps t^n.

Figure 5.4: Error plots for the different numerical schemes applied to the BBM equation (5.3), with initial-boundary value conditions (5.1)-(5.2), u_0 given by (5.27) with $c = 3$, $L = 50$, the number of grid points $M = 200$, time step $\Delta t = 0.1$ and $t_{\max} = 20$. MG1-CI: (5.16) on a moving grid, with cubic interpolation. MG1-IPIC: (5.16) on a moving grid, with the integral preserving two-step interpolation procedure with cubic interpolation. MG2-CI: (5.17) on a moving grid, with cubic interpolation. MG2-IPIC: (5.17) on a moving grid, with the two-step interpolation procedure with cubic interpolation. IM-MGC: Implicit midpoint method on a moving grid, with cubic interpolation.

Chapter 6

Conclusion and Discussion

We have presented the integral preserving discrete gradient methods for solving ODEs and the related discrete variational derivative methods for solving PDEs on uniform grids, before defining the discrete variational derivative methods on general fixed grids. We have subsequently given a short introduction to general moving grid methods, and introduced the modified discrete variational derivative methods for solving PDEs on moving grids while preserving an approximation to a first integral. Integral preserving linear projection methods on moving grids were also presented and proven to be a subset of the modified discrete variational derivative methods. We presented various methods for interpolating a numerical solution from one grid to another, including a new, integral preserving procedure, and we showed their different properties as a part of the modified discrete variational derivative methods. A brief presentation of two alternate integral preserving methods on moving grids was also given.

Although some variants of the discrete variational derivative methods have been proposed on non-uniform grids previously in the literature, e.g. in [25, 26], the unified method presented in this thesis adds to what is already presented in that it is a completely generic approach valid for all discrete variational derivatives and general grids, so that all known methods for constructing integral preserving methods for PDEs based on the discrete gradient methods fits into this new framework. In addition and most importantly, this thesis presents, as far as we know, the first integral preserving methods on moving grids.

Numerical experiments confirm that the modified discrete variational derivative methods preserve an approximation of the first integral. When tested on soliton solutions of the KdV and BBM equations with linear interpolation, we see that the moving grid implementations preserve the speed of the waves better than the uniform grid implementation, while the shape error is larger in the moving grid case. However, for the BBM equation, we observe how the shape error can be significantly reduced, at the expense or larger distance error, by choosing cubic interpolation instead of linear. This indicates that the results of the discrete variational derivative methods will have large variations for different choices of interpolation methods.

Our primary concern in this thesis has been to develop integral preserving methods for PDEs on moving grid and show that they do indeed preserve an approximation of the first integral while otherwise giving good numerical results. We have therefore not put much effort into optimizing the solvers. In general, the discrete variational derivative methods, as implemented in our examples, perform well when compared to the implicit midpoint method, but we expect that more accurate numerical solutions can be achieved by improving the implementation of the methods, e.g. by using higher order spatial discretization or by iterate the grid redistribution procedure to produce more accurate approximations of equidistributing grids. This can be a subject for further studies.

We have in this thesis only considered PDEs with a conservation property. The variational derivative methods can however, with a small alteration, also be applied to PDEs with a constant dissipative structure, generating schemes that preserve the correct monotonic decrease of energy, as shown for the average vector field DVD method in [3]. We remark that the generalization in this thesis of the discrete variational derivative methods to moving grids also holds for the dissipative variant, replacing the antisymmetric matrix $\mathcal{S}_{\mathbf{x}}$ in (4.1) with a matrix $\mathcal{N}_{\mathbf{x}}$ approximating the semi-definite operator $\mathcal{N}$ of the dissipative PDE and being itself semi-definite with respect to the discrete inner product $\langle \cdot, \cdot \rangle_{\hat{\mathbf{x}}}$.

For simplicity, we have only considered one-dimensional problems in this thesis. The framework we have presented can however be generalized to multiple dimensions, in which case a moving grid implementation can be of especially great use.

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