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ON MULTISYMPLECTICITY OF PARTITIONED RUNGE–KUTTA METHODS*

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Abstract. Previously, it has been shown that discretizing a multi-Hamiltonian PDE in space and time with partitioned Runge–Kutta methods gives rise to a system of equations that formally satisfy a discrete multisymplectic conservation law. However, these previous studies use the same partitioning of the variables into two parts in both space and time. This gives rise to a large number of cases to be considered, each with its own set of conditions to be satisfied. We present here a much simpler set of conditions, covering all of these cases, where the variables are partitioned independently in space and time into an arbitrary number of parts. In general, it is not known when such a discretization of a multi-Hamiltonian PDE will give rise to a well-defined numerical integrator. However, a numerical integrator that is explicit will typically be well defined. In this paper, we give sufficient conditions on a multi-Hamiltonian PDE for a Lobatto IIIA–IIIB discretization in space to give rise to explicit ODEs and an algorithm for constructing these ODEs.

Key words. partitioned Runge–Kutta, multisymplectic, multi-Hamiltonian, Lobatto IIIA-IIIB

AMS subject classifications. 37M15, 37K05, 35L05

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1. Introduction.

A multi-Hamiltonian PDE in one time and one space dimension is a PDE which can be written as a first order system in the form

$$\mathbf{K}\mathbf{z}_t + \mathbf{L}\mathbf{z}_x = \nabla_{\mathbf{z}} S(\mathbf{z}), \tag{1.1}$$

where $\mathbf{z} \in \mathbb{R}^n$, $\mathbf{K}$ and $\mathbf{L}$ are nonzero skew-symmetric matrices, and $S(\mathbf{z})$ is a smooth function [5].

Along solutions, $\mathbf{z}(t,x)$, to (1.1) the multisymplectic conservation law,

$$\omega_t + \kappa_x = 0, \tag{1.2}$$

holds, where $\omega = \frac{1}{2}\mathbf{K}\mathrm{d}\mathbf{z} \wedge \mathrm{d}\mathbf{z}$ and $\kappa = \frac{1}{2}\mathbf{L}\mathrm{d}\mathbf{z} \wedge \mathrm{d}\mathbf{z}$ are 2-forms and $\mathrm{d}\mathbf{z}$ satisfies the first variation of the PDE,

$$\mathbf{K}\mathrm{d}\mathbf{z}_t + \mathbf{L}\mathrm{d}\mathbf{z}_x = \mathbf{D}_{\mathbf{zz}} S(\mathbf{z})\mathrm{d}\mathbf{z}, \tag{1.3}$$

where $\mathbf{D}_{\mathbf{zz}} S(\mathbf{z})$ is a symmetric matrix.

One definition of a multisymplectic integrator is a numerical method that exactly preserves a discrete analogue of (1.2) (a so-called discrete multisymplectic conservation law) by applying a symplectic one-step method in space and time [11]. An important fact here is that multisymplectic integrators do not conserve (1.2) exactly, but rather different multisymplectic integrators preserve different discrete multisymplectic conservation laws, i.e., different discretizations of (1.2). This is in contrast

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to symplectic integrators for ODEs, which conserve symplecticity exactly. Some of the consequences of preserving a discrete multisymplectic conservation law are the following:

(i) exact preservation of some integrals, e.g., potential vorticity [14];
(ii) both energy and momentum are approximately locally conserved [5, 7, 18];
(iii) quasi-periodic orbits and chaotic regions are preserved (KAM theory) [22];
(iv) the ability to take comparatively large time-steps and retain long-time stability [12].

In the past several authors [7, 13, 17, 18] have given discretizations of (1.1) which they have shown to formally satisfy a discrete multisymplectic conservation law. What these authors typically fail to consider is whether the resulting system of equations forms a well-defined numerical integrator. Some problems that may occur in such discretizations are [20]

(i) there may be no obvious choice of dependent variables;
(ii) the discrete equations may not be well defined locally (i.e., there may not be one equation per dependent variable per cell);
(iii) the discrete equations may not be well defined globally (i.e., there may not be one equation per dependent variable across all spatial grid points when boundary conditions are imposed);
(iv) the discrete equations may not have a solution, or may not have a unique solution or isolated solutions.

Difficulties due to these problems already occur for the most popular multisymplectic integrator, the Preissman box scheme. With periodic boundary conditions in one space dimension, the discrete equations typically have only solutions with an odd number of grid points, while with an even number of grid points they have no solution (nonlinear problems) or an infinite number of solutions (linear problems). With higher order Runge–Kutta (RK) methods these problems are even worse [19].

Problems (iii) and (iv) will, in general, be avoided if a discretization method is used which gives rise to explicit multisymplectic integrators. In order to construct an explicit multisymplectic integrator, it is necessary for the discretization in each dimension to be explicit and symplectic. For PDEs in one space and one time dimension, this condition means that a symplectic spatial discretization must give rise to explicit ODEs in time (or vice versa, since space and time are treated on an equal footing). This rules out discretization by symplectic RK methods. However, for some partitioned Runge–Kutta (PRK) methods this is possible, e.g., the well-known 5-point method obtained by applying leapfrog in space and time to the nonlinear wave equation, $u_{tt} - u_{xx} = -V'(u)$, gives the explicit multisymplectic integrator [7]

$$\frac{1}{(\Delta t)^2}\begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} u - \frac{1}{(\Delta x)^2}\begin{bmatrix} 1 & -2 & 1 \end{bmatrix} u = -V'(u), \tag{1.4}$$

where we have used the notation of centered stencils.

Thus, in this paper we will be concerned with applying a PRK discretization in space to obtain explicit ODEs in time. In particular we will consider the Lobatto IIIA–IIIB class of PRK discretization, which, under certain requirements on the PDE, avoids problems (i) and (ii) and allows explicit ODEs to be obtained.

The remainder of this paper consists of four sections. In section 2 we will describe a PRK discretization with an arbitrary number of parts and show that such a discretization in time and space gives rise to a natural discrete multisymplectic

conservation law which is formally satisfied. In section 3 we give the conditions on the coefficients of a PRK discretization to be of Lobatto IIIA–IIIB type and specify our reasons for considering the Lobatto IIIA–IIIB class of PRK discretization. In section 4 we give the conditions on a multi-Hamiltonian PDE such that the application of a Lobatto IIIA–IIIB discretization in space allows one to construct explicit ODEs and then present an algorithm for constructing these ODEs. We follow this with several examples of PDEs that satisfy these conditions (such as the nonlinear wave equation and the nonlinear Schrödinger equation) and some examples of PDEs that do not. In section 5 we will discuss some properties of the ODEs formed through our construction algorithm and give a shortcut for constructing these ODEs. We will also discuss the discretization of these ODEs in time and their behavior with respect to boundary conditions.

2. PRK discretization. When a differential equation,

$$\mathbf{z}_t = f(\mathbf{z}), \tag{2.1}$$

is discretized with a PRK discretization, the vector of dependent variables $\mathbf{z} \in \mathbb{R}^n$ is partitioned into several parts, $\mathbf{z}^{(\gamma)} \in \mathbb{R}^{n_\gamma}$ with $\sum_\gamma n_\gamma = n$. Typically, the number of parts is two, but it is possible for the number of parts to be as high as n. A grid is then introduced where we take the grid points (or *nodes*) (for convenience only) to have equal spacing Δt, and we adopt the following notation: let cell i be the region in the domain defined by $t \in [i\Delta t, (i+1)\Delta t)$, let z^γ be the entry γ in $\mathbf{z}$, let $\mathbf{z}_i^{(\gamma)} \in \mathbb{R}^{n_\gamma}$ be the vector of variables in part γ at the node in cell i, let $\mathbf{Z}_{i,j}^{(\gamma)} \in \mathbb{R}^{n_\gamma}$ be the vector of variables in part γ at stage j in cell i, and let the lack of a raised index (γ) indicate the unpartitioned variable.

For an r-stage PRK discretization of (2.1) one obtains a set of equations coupling the node values $\mathbf{z}_i$ to the stage values $\mathbf{Z}_{i,j}$ at r internal stages given by

$$\begin{aligned} \mathbf{Z}_{i,j}^{(\gamma)} &= \mathbf{z}_i^{(\gamma)} + \Delta t \sum_{k=1}^{r} a_{jk}^{(\gamma)} \partial_t \mathbf{Z}_{i,k}^{(\gamma)}, \quad j = 1, \dots, r, \\ \mathbf{z}_{i+1}^{(\gamma)} &= \mathbf{z}_i^{(\gamma)} + \Delta t \sum_{j=1}^{r} b_j^{(\gamma)} \partial_t \mathbf{Z}_{i,j}^{(\gamma)}, \end{aligned} \tag{2.2}$$

for each γ, where the new variables $\partial_t \mathbf{Z}_{i,j}$ satisfy (2.1), i.e.,

$$\partial_t \mathbf{Z}_{i,j} = f(\mathbf{Z}_{i,j}), \tag{2.3}$$

and the coefficients $b_j^{(\gamma)}$ and $a_{jk}^{(\gamma)}$ are chosen to satisfy certain order conditions.

The conditions for a two-part PRK discretization of a canonical Hamiltonian ODE, with partitioning $\mathbf{z}^{(1)} = \mathbf{q}$ and $\mathbf{z}^{(2)} = \mathbf{p}$, to be symplectic are [1]

$$-a_{kj}^{(1)} b_k^{(2)} - b_j^{(1)} a_{jk}^{(2)} + b_j^{(1)} b_k^{(2)} = 0 \qquad \text{for all } j, k, \tag{2.4}$$

while the conditions for an RK discretization (i.e., a one-part PRK discretization with $\mathbf{z}^{(1)} = \mathbf{z}$, $n_1 = n$) of the same ODE to be symplectic are [21]

$$-a_{kj}^{(1)} b_k^{(1)} - b_j^{(1)} a_{jk}^{(1)} + b_j^{(1)} b_k^{(1)} = 0 \qquad \text{for all } j, k. \tag{2.5}$$

Generally, for a PRK discretization with coefficients satisfying (2.4), the coefficients will not satisfy (2.5).

When the PDE (1.1) is discretized in space with an r-stage PRK discretization, the set of equations that one obtains is given by

$$\begin{aligned} \mathbf{Z}_{i,j}^{(\gamma)} &= \mathbf{z}_i^{(\gamma)} + \Delta x \sum_{k=1}^{r} a_{jk}^{(\gamma)} \partial_x \mathbf{Z}_{i,k}^{(\gamma)}, \quad j = 1, \ldots, r, \\ \mathbf{z}_{i+1}^{(\gamma)} &= \mathbf{z}_i^{(\gamma)} + \Delta x \sum_{j=1}^{r} b_j^{(\gamma)} \partial_x \mathbf{Z}_{i,j}^{(\gamma)}, \end{aligned} \tag{2.6}$$

for each γ, where the new variables $\partial_x \mathbf{Z}_{i,j}$ satisfy (1.1), i.e.,

$$\mathbf{K}\partial_t \mathbf{Z}_{i,j} + \mathbf{L}\partial_x \mathbf{Z}_{i,j} = \nabla_{\mathbf{z}} S(\mathbf{Z}_{i,j}). \tag{2.7}$$

Equations (2.6) and (2.7) form a differential-algebraic equation (DAE) for $\mathbf{Z}_{i,j}$ and $\mathbf{z}_i$. However, in this DAE there are no ODEs for the node values, and the constraints apply only to $\mathbf{L}\mathbf{Z}_{i,j}$, not $\mathbf{Z}_{i,j}$. Furthermore, $\mathbf{L}$ may not have full rank, which may prevent one from obtaining a system of explicit ODEs for the $\mathbf{Z}_{i,j}$.

Previous studies of the PDE (1.1) discretized in space and time with PRK methods have concluded that such discretizations satisfy a natural discrete approximation of the multisymplectic conservation law (1.2) [13]. However, these studies use the same partitioning of the variables for both the space and time discretizations, which leads to a large number of cases to be considered, each with its own set of conditions to be satisfied. This choice of partitioning in each dimension is important, as the conditions for the discretized equations to satisfy the discrete multisymplectic conservation law depend upon $\mathbf{K}$ and $\mathbf{L}$.

For example, given a multi-Hamiltonian PDE and a two-part PRK discretization in time with coefficients satisfying (2.4), if the PDE has no time derivatives of the variables in the second part, then the discretization is in fact an RK discretization with the same coefficients as the first of the PRK pair, which will not in general satisfy (2.5).

To consider the most general case, we will now assume the finest possible partitioning of the variables, namely n parts, where for each entry γ in $\mathbf{z}$ we have that $n_\gamma = 1$ and the part $\mathbf{z}^{(\gamma)}$ consists simply of the variable z^γ. We will use the notation $\mathrm{d}Z_{i,j}^{\gamma,n,m}$ to represent the entry γ in $\mathbf{z}$ at stage j of cell i in space and stage m of cell n in time, where a lack of either the index j or m indicates the node variable of cell i in space or cell n in time, respectively. Also, let $b_j^{(\gamma)}$ and $a_{ij}^{(\gamma)}$ be the coefficients of the spatial PRK discretization associated with the variable z^γ, and let $B_m^{(\gamma)}$ and $A_{nm}^{(\gamma)}$ be the coefficients of the temporal PRK discretization associated with the variable z^γ.

The following theorem gives a much simpler set of conditions for PRK discretizations of (1.1) in space and time to satisfy a discrete multisymplectic conservation law. Since it immediately applies to any other partitioning of the variables by simply equating the $b_j^{(\gamma)}$ and $a_{ij}^{(\gamma)}$ coefficients of the appropriate parts in space or time, this set of conditions encompasses all of the cases considered in previous studies.

THEOREM 2.1. *A multi-Hamiltonian PDE* (1.1) *discretized by a PRK method in space and another PRK method in time has a discrete multisymplectic conservation law, given by*

$$\Delta x \sum_j b_j (\omega_{i,j}^{n+1} - \omega_{i,j}^n) + \Delta t \sum_m B_m (\kappa_{i+1}^{n,m} - \kappa_i^{n,m}) = 0, \tag{2.8}$$

where $\omega^n_{i,j} = \frac{1}{2}\sum_{\beta,\gamma} \mathbf{K}_{\beta\gamma} \mathrm{d}Z^{\gamma,n}_{i,j} \wedge \mathrm{d}Z^{\beta,n}_{i,j}$ *and* $\kappa^{n,m}_i = \frac{1}{2}\sum_{\beta,\gamma} \mathbf{L}_{\beta\gamma} \mathrm{d}Z^{\gamma,n,m}_i \wedge \mathrm{d}Z^{\beta,n,m}_i$ *when the following conditions hold:*

$$\begin{aligned} b^{(\gamma)}_j &= b_j, \\ -a^{(\gamma)}_{kj} b^{(\beta)}_k - b^{(\gamma)}_j a^{(\beta)}_{jk} + b^{(\gamma)}_j b^{(\beta)}_k &= 0 \end{aligned} \tag{2.9}$$

for all j, k *and pairs* (β, γ) *such that* $\mathbf{L}_{\beta\gamma} \neq 0$ *and*

$$\begin{aligned} B^{(\gamma)}_m &= B_m, \\ -A^{(\gamma)}_{nm} B^{(\beta)}_n - B^{(\gamma)}_m A^{(\beta)}_{mn} + B^{(\gamma)}_m B^{(\beta)}_n &= 0 \end{aligned} \tag{2.10}$$

for all m, n *and pairs* (β, γ) *such that* $\mathbf{K}_{\beta\gamma} \neq 0$.

Proof.

(2.11)

$$\begin{aligned}
&\left(\kappa^{n,m}_{i+1} - \kappa^{n,m}_i\right) \\
&= \frac{1}{2}\sum_{\beta,\gamma} \left(\mathbf{L}_{\beta\gamma} \mathrm{d}Z^{\gamma,n,m}_{i+1} \wedge \mathrm{d}Z^{\beta,n,m}_{i+1} - \mathbf{L}_{\beta\gamma} \mathrm{d}Z^{\gamma,n,m}_i \wedge \mathrm{d}Z^{\beta,n,m}_i \right) \\
&= \frac{1}{2}\sum_{\beta,\gamma} \mathbf{L}_{\beta\gamma} \Bigg(\left(\mathrm{d}Z^{\gamma,n,m}_i + \Delta x \sum_j b^{(\gamma)}_j \partial_x \mathrm{d}Z^{\gamma,n,m}_{i,j} \right) \wedge \Bigg(\mathrm{d}Z^{\beta,n,m}_i \\
&\qquad + \Delta x \sum_k b^{(\beta)}_k \partial_x \mathrm{d}Z^{\beta,n,m}_{i,k} \Bigg) - \mathrm{d}Z^{\gamma,n,m}_i \wedge \mathrm{d}Z^{\beta,n,m}_i \Bigg) \\
&= \frac{1}{2}\sum_{\beta,\gamma} \mathbf{L}_{\beta\gamma} \Bigg(\Delta x \Bigg(\mathrm{d}Z^{\gamma,n,m}_i \wedge \sum_k b^{(\beta)}_k \partial_x \mathrm{d}Z^{\beta,n,m}_{i,k} + \sum_j b^{(\gamma)}_j \partial_x \mathrm{d}Z^{\gamma,n,m}_{i,j} \wedge \mathrm{d}Z^{\beta,n,m}_i \Bigg) \\
&\qquad + (\Delta x)^2 \sum_{j,k} b^{(\gamma)}_j b^{(\beta)}_k \partial_x \mathrm{d}Z^{\gamma,n,m}_{i,j} \wedge \partial_x \mathrm{d}Z^{\beta,n,m}_{i,k} \Bigg) \\
&= \frac{1}{2}\sum_{\beta,\gamma} \mathbf{L}_{\beta\gamma} \Bigg(\Delta x \sum_k \left(\mathrm{d}Z^{\gamma,n,m}_{i,k} - \Delta x \sum_j a^{(\gamma)}_{kj} \partial_x \mathrm{d}Z^{\gamma,n,m}_{i,j} \right) \wedge b^{(\beta)}_k \partial_x \mathrm{d}Z^{\beta,n,m}_{i,k} \\
&\qquad + \Delta x \sum_j b^{(\gamma)}_j \partial_x \mathrm{d}Z^{\gamma,n,m}_{i,j} \wedge \left(\mathrm{d}Z^{\beta,n,m}_{i,j} - \Delta x \sum_k a^{(\beta)}_{jk} \partial_x \mathrm{d}Z^{\beta,n,m}_{i,k} \right) \\
&\qquad + (\Delta x)^2 \sum_{j,k} b^{(\gamma)}_j b^{(\beta)}_k \partial_x \mathrm{d}Z^{\gamma,n,m}_{i,j} \wedge \partial_x \mathrm{d}Z^{\beta,n,m}_{i,k} \Bigg) \\
&= \frac{1}{2}\sum_{\beta,\gamma} \mathbf{L}_{\beta\gamma} \Bigg(\Delta x \Bigg(\sum_k b^{(\beta)}_k \mathrm{d}Z^{\gamma,n,m}_{i,k} \wedge \partial_x \mathrm{d}Z^{\beta,n,m}_{i,k} + \sum_j b^{(\gamma)}_j \partial_x \mathrm{d}Z^{\gamma,n,m}_{i,j} \wedge \mathrm{d}Z^{\beta,n,m}_{i,j} \Bigg)
\end{aligned}$$

$$+ (\Delta x)^2 \sum_{j,k} \left(- a_{kj}^{(\gamma)} b_k^{(\beta)} - b_j^{(\gamma)} a_{jk}^{(\beta)} + b_j^{(\gamma)} b_k^{(\beta)} \right) \partial_x \mathrm{d}Z_{i,j}^{\gamma,n,m} \wedge \partial_x \mathrm{d}Z_{i,k}^{\beta,n,m} \Bigg)$$

$$= \Delta x \sum_{\beta,\gamma,j} b_j^{(\gamma)} \mathbf{L}_{\beta\gamma} \partial_x \mathrm{d}Z_{i,j}^{\gamma,n,m} \wedge \mathrm{d}Z_{i,j}^{\beta,n,m}$$

$$+ \frac{1}{2}(\Delta x)^2 \sum_{\beta,\gamma} \mathbf{L}_{\beta\gamma} \sum_{j,k} \big(- a_{kj}^{(\gamma)} b_k^{(\beta)} - b_j^{(\gamma)} a_{jk}^{(\beta)} + b_j^{(\gamma)} b_k^{(\beta)} \big) \partial_x \mathrm{d}Z_{i,j}^{\gamma,n,m} \wedge \partial_x \mathrm{d}Z_{i,k}^{\beta,n,m}.$$

When $\mathbf{L}_{\beta\gamma}$ is nonzero, the $(\Delta x)^2$ term above is zero if

$$-a_{kj}^{(\gamma)} b_k^{(\beta)} - b_j^{(\gamma)} a_{jk}^{(\beta)} + b_j^{(\gamma)} b_k^{(\beta)} = 0 \qquad \text{for all } j,k. \tag{2.12}$$

Similarly,

$$\big(\omega_{i,j}^{n+1} - \omega_{i,j}^{n}\big) = \Delta t \sum_{\beta,\gamma,m} B_m^{(\gamma)} \mathbf{K}_{\beta\gamma} \partial_t \mathrm{d}Z_{i,j}^{\gamma,n,m} \wedge \mathrm{d}Z_{i,j}^{\beta,n,m} \tag{2.13}$$

$$+ \frac{1}{2}(\Delta t)^2 \sum_{\beta,\gamma} \mathbf{K}_{\beta\gamma} \sum_{m,l} \big(- A_{lm}^{(\gamma)} B_l^{(\beta)} - B_m^{(\gamma)} A_{ml}^{(\beta)} + B_m^{(\gamma)} B_l^{(\beta)} \big) \partial_t \mathrm{d}Z_{i,j}^{\gamma,n,m} \wedge \partial_t \mathrm{d}Z_{i,k}^{\beta,n,m}$$

and when $\mathbf{K}_{\beta\gamma}$ is nonzero, the $(\Delta t)^2$ term is zero if

$$-A_{nm}^{(\gamma)} B_n^{(\beta)} - B_m^{(\gamma)} A_{mn}^{(\beta)} + B_m^{(\gamma)} B_n^{(\beta)} = 0 \qquad \text{for all } m,n. \tag{2.14}$$

Now, writing (1.3) in components and taking its wedge product with $\mathrm{d}z^\beta$ gives

$$\sum_{\gamma} \big(\mathbf{K}_{\beta\gamma} \partial_t \mathrm{d}z^\gamma \wedge \mathrm{d}z^\beta + \mathbf{L}_{\beta\gamma} \partial_x \mathrm{d}z^\gamma \wedge \mathrm{d}z^\beta \big) = 0 \qquad \text{for all } \beta \tag{2.15}$$

since $\mathbf{D}_{\mathbf{zz}} S(\mathbf{z})$ is symmetric. Thus, in general

$$\sum_{\gamma,j,m} b_j^{(\gamma)} B_m^{(\gamma)} \mathbf{L}_{\beta\gamma} \big(\partial_x \mathrm{d}Z_{i,j}^{\gamma,n,m} \wedge \mathrm{d}Z_{i,j}^{\beta,n,m} \big) \tag{2.16}$$

$$= - \sum_{\gamma,j,m} b_j^{(\gamma)} B_m^{(\gamma)} \mathbf{K}_{\beta\gamma} \big(\partial_t \mathrm{d}Z_{i,j}^{\gamma,n,m} \wedge \mathrm{d}Z_{i,j}^{\beta,n,m} \big)$$

when $b_j^{(\gamma)} = b_j$ and $B_m^{(\gamma)} = B_m$ for all j, m, and γ.

Therefore, if (2.9) and (2.10) hold, then we can see from (2.11) and (2.13) that the discrete multisymplectic conservation law (2.8) holds. ∎

The discrete multisymplectic conservation law (i.e., (2.8)) is an approximation to the integral

$$\int_{i\Delta x}^{(i+1)\Delta x} (\omega(x,(n+1)\Delta t) - \omega(x,n\Delta t))\,\mathrm{d}x \tag{2.17}$$

$$+ \int_{n\Delta t}^{(n+1)\Delta t} (\kappa((i+1)\Delta x,t) - \kappa(i\Delta x,t))\,\mathrm{d}t = 0,$$

which is the integral of (1.2) over the cell with one corner at $(i\Delta x, n\Delta t)$.

Now, suppose we have a two-part PRK discretization in space where the coefficients satisfy (2.4) but not (2.5); then for (2.12) to be satisfied the partitioning of the variables in space must be chosen such that κ has terms only of the form $\mathrm{d}z^{(1)} \wedge \mathrm{d}z^{(2)}$. Similarly, given a two-part PRK discretization in time where the coefficients satisfy (2.4) but not (2.5), for (2.14) to be satisfied the partitioning of the variables in time must be chosen such that ω has only terms of the form $\mathrm{d}z^{(1)} \wedge \mathrm{d}z^{(2)}$.

Theorem 2.1 shows that if the partitioning in space and time is chosen appropriately, then a PRK discretization in space and time with coefficients satisfying (2.4) will result in an integrator that formally satisfies a multisymplectic conservation law given by (2.8). However, this does not guarantee that the integrator is well defined. The approach we take to obtaining a well-defined multisymplectic integrator is to apply an explicit symplectic PRK discretization in each dimension.

We define an *explicit discretization* in space as a discretization for which the time derivatives of the dependent variables may be written explicitly in terms of the dependent variables. Their derivation may involve solving linear systems, but these must be independent of the PDE. An *explicit local discretization* is an explicit discretization for which these ODEs depend only on nearby values of the dependent variables.

In section 4 we will give the conditions on a multi-Hamiltonian PDE such that one can obtain an explicit local symplectic PRK discretization in space based on Lobatto IIIA–IIIB, and we will give an algorithm for obtaining the explicit ODEs in time.

3. Lobatto IIIA–IIIB. The particular class of PRK discretization that we consider in this paper is a two-part discretization known as Lobatto IIIA–IIIB. For these methods, the coefficients $a_{ij}^{(1)}$, $a_{ij}^{(2)}$ and $b_j^{(1)} = b_j^{(2)} = b_j$ are determined by [8]

$$
\begin{aligned}
B(r): &\quad \sum_{i=1}^{r} b_i c_i^{k-1} = \frac{1}{k} && \text{for } k \le r,\\
C(r): &\quad \sum_{j=1}^{r} a_{ij}^{(1)} c_j^{k-1} = \frac{1}{k} c_i^k && \text{for } i = 1,\dots,r \text{ and } k \le r,\\
D(r): &\quad \sum_{i=1}^{r} b_i c_i^{k-1} a_{ij}^{(2)} = \frac{1}{k} b_j (1 - c_j^k) && \text{for } j = 1,\dots,r \text{ and } k \le r,
\end{aligned}
\tag{3.1}
$$

where the c_i are zeros of the Lobatto quadrature polynomial

$$
\frac{\mathrm{d}^{r-2}}{\mathrm{d}x^{r-2}} \left(x^{r-1}(x-1)^{r-1} \right). \tag{3.2}
$$

While the Lobatto IIIA and Lobatto IIIB classes of RK methods have each been known since the mid 1960s, their coefficients do not satisfy (2.5), and it was discovered only relatively recently that the Lobatto IIIA–IIIB class of PRK methods formed by combining Lobatto IIIA and Lobatto IIIB has coefficients that satisfy (2.4) [16, 23]. Thus for a discretization of (1.1), if the partitioning of the variables in each of the space and time dimensions can be chosen such that the 2-form associated with each dimension has terms only of the form $\mathrm{d}z^{(1)} \wedge \mathrm{d}z^{(2)}$, then the resulting integrator will satisfy a discrete multisymplectic conservation law.

The reason we consider the Lobatto IIIA–IIIB class of PRK discretizations is because their coefficients are related in the following way:

$$a^{(1)}_{1j} = 0, \quad a^{(1)}_{rj} = b_j \qquad \text{for all } j, \tag{3.3}$$

$$a^{(2)}_{ir} = 0, \quad a^{(2)}_{i1} = b_1 \qquad \text{for all } i, \tag{3.4}$$

and the $(r-2)\times(r-2)$ matrix $\mathbf{C}$ with entries

$$\mathbf{C}_{i-1,j-1} = \sum_{k,l} a^{(1)}_{ik}(b_l - \delta_{kl})a^{(2)}_{lj} \quad \text{for } 2 \le i,j \le r-1 \tag{3.5}$$

is invertible.

The relations given in (3.3) and (3.4) are a direct consequence of (3.1) and (3.2) and give us three properties which will be required in our algorithm for constructing explicit ODEs in the next section. First, from (3.3) we can see that, for $\gamma = 1$, a node value is equal to the first stage value associated with that node and also equal to the last stage value associated with the previous node. Second, (3.4) gives us that both $\sum_j b_j a^{(2)}_{jr}$ and $b_1 - \sum_j b_j a^{(2)}_{j1}$ are zero. Lastly, (3.3) and (3.4) together give

$$\sum_{k,l} a^{(1)}_{ik}(b_l - \delta_{kl})a^{(2)}_{lj} = 0 \qquad \text{if either } i \in \{1,r\} \text{ or } j \in \{1,r\}, \tag{3.6}$$

where δ_{kl} is the Kronecker delta. The invertibility of $\mathbf{C}$ can then be shown via the Frobenius inequality and will be used directly in the construction algorithm.

The coefficients for Lobatto IIIA–IIIB methods can be written succinctly as pairs of Butcher tableaux; we give below the coefficients for $r = 2$, 3, and 4:

$$r = 2: \qquad \text{IIIA:} \quad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}, \qquad \text{IIIB:} \quad \begin{array}{c|cc} 0 & \frac{1}{2} & 0 \\ 1 & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}. \tag{3.7}$$

Second order Lobatto IIIA–IIIB is often referred to as generalized leapfrog:

$$r = 3: \qquad \text{IIIA:} \quad \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}, \qquad \text{IIIB:} \quad \begin{array}{c|ccc} 0 & \frac{1}{6} & -\frac{1}{6} & 0 \\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3} & 0 \\ 1 & \frac{1}{6} & \frac{5}{6} & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}, \tag{3.8}$$

(3.9)

$$r = 4: \qquad \text{IIIA:} \quad \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ \frac{5-\sqrt{5}}{10} & \frac{11+\sqrt{5}}{120} & \frac{25-\sqrt{5}}{120} & \frac{25-13\sqrt{5}}{120} & \frac{-1+\sqrt{5}}{120} \\ \frac{5+\sqrt{5}}{10} & \frac{11-\sqrt{5}}{120} & \frac{25+13\sqrt{5}}{120} & \frac{25+\sqrt{5}}{120} & \frac{-1-\sqrt{5}}{120} \\ 1 & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \\ \hline & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \end{array},$$

$$\text{IIIB:} \quad \begin{array}{c|cccc} 0 & \frac{1}{12} & \frac{-1-\sqrt{5}}{24} & \frac{-1+\sqrt{5}}{24} & 0 \\ \frac{5-\sqrt{5}}{10} & \frac{1}{12} & \frac{25+\sqrt{5}}{120} & \frac{25-13\sqrt{5}}{120} & 0 \\ \frac{5+\sqrt{5}}{10} & \frac{1}{12} & \frac{25+13\sqrt{5}}{120} & \frac{25-\sqrt{5}}{120} & 0 \\ 1 & \frac{1}{12} & \frac{11-\sqrt{5}}{24} & \frac{11+\sqrt{5}}{24} & 0 \\ \hline & \frac{1}{12} & \frac{5}{12} & \frac{5}{12} & \frac{1}{12} \end{array}.$$

4. Explicit ODEs. In the one dimensional situation (i.e., time integration), the dependent variables are the $\mathbf{z}_i$; (2.2) determines the stage variables $\mathbf{Z}_{i,j}$ and defines a map from $\mathbf{z}_i$ to $\mathbf{z}_{i+1}$. In contrast, for situations where the dimension is greater than one (e.g., for PDEs of the form of (1.1)), if one applies a PRK discretization in space, then the dependent variables will typically be the stage variables $\mathbf{Z}_{i,j}$, while the node variables $\mathbf{z}_i$ and the new variables $\partial_x \mathbf{Z}_{i,j}$ will be eliminated using the PDE to yield a set of ODEs in time for the $\mathbf{Z}_{i,j}$. As we shall see in the following theorem, this elimination depends upon the structure not only of $\mathbf{K}$ and $\mathbf{L}$, but also of $S(\mathbf{z})$.

THEOREM 4.1. *Consider a multi-Hamiltonian PDE* (1.1)*, where the* $\mathbf{K}$ *and* $\mathbf{L}$ *matrices have the following structure:*

$$\mathbf{K} = \begin{bmatrix} & -\mathbf{I}_{\frac{1}{2}(d_1+d_2)} & \\ \mathbf{I}_{\frac{1}{2}(d_1+d_2)} & & \\ & & \mathbf{0}_{d_1} \end{bmatrix}, \qquad \mathbf{L} = \begin{bmatrix} & & \mathbf{I}_{d_1} \\ & \mathbf{0}_{d_2} & \\ -\mathbf{I}_{d_1} & & \end{bmatrix}, \tag{4.1}$$

where $d_1 = n - \operatorname{rank}(\mathbf{K})$*,* $d_2 = n - 2d_1 \le d_1$*,* $\mathbf{I}_d$ *is the* $d \times d$ *identity matrix, and* $\mathbf{0}_d$ *is the* $d \times d$ *zero matrix.*

Let the variables $\mathbf{z}$ *be partitioned into two parts* $\mathbf{z}^{(1)} \in \mathbb{R}^{d_1+d_2}$ *and* $\mathbf{z}^{(2)} \in \mathbb{R}^{d_1}$*, where we denote the first* d_1 *components of* $\mathbf{z}^{(1)}$ *by* $\mathbf{q}$*, the last* d_2 *components of* $\mathbf{z}^{(1)}$ *by* $\mathbf{v}$*, and the components of* $\mathbf{z}^{(2)}$ *by* $\mathbf{p}$ *such that the PDE may be written as*

$$\begin{bmatrix} & -\mathbf{I}_{\frac{1}{2}(d_1+d_2)} & \\ \mathbf{I}_{\frac{1}{2}(d_1+d_2)} & & \\ & & \mathbf{0}_{d_1} \end{bmatrix} \begin{bmatrix} \mathbf{q} \\ \mathbf{v} \\ \mathbf{p} \end{bmatrix}_t + \begin{bmatrix} & & \mathbf{I}_{d_1} \\ & \mathbf{0}_{d_2} & \\ -\mathbf{I}_{d_1} & & \end{bmatrix} \begin{bmatrix} \mathbf{q} \\ \mathbf{v} \\ \mathbf{p} \end{bmatrix}_x = \begin{bmatrix} \nabla_{\mathbf{q}} S(\mathbf{z}) \\ \nabla_{\mathbf{v}} S(\mathbf{z}) \\ \nabla_{\mathbf{p}} S(\mathbf{z}) \end{bmatrix}. \tag{4.2}$$

If the function $S(\mathbf{z})$ *can be written in the form*

$$S(\mathbf{z}) = T(\mathbf{p}) + V(\mathbf{q}) + \widehat{V}(\mathbf{v}), \tag{4.3}$$

where $T(\mathbf{p}) = \frac{1}{2}\mathbf{p}^t\beta\mathbf{p}$ *and* $\widehat{V}(\mathbf{v}) = \frac{1}{2}\mathbf{v}^T\alpha\mathbf{v}$ *such that* $|\beta| \neq 0$ *and* $|\alpha| \neq 0$*, then applying an* r*-stage Lobatto IIIA–IIIB PRK discretization in space to the PDE leads to a set of explicit local ODEs in time in the stage variables associated with* $\mathbf{q}$.

Proof. A general outline of the proof of this theorem is as follows. We first make use of the form of $S(\mathbf{z})$ to rewrite (4.2) by eliminating the $\mathbf{v}$ variables. The r-stage Lobatto IIIA–IIIB discretization is then applied to the resulting PDE. Next, we make use of the requirements of the theorem in order to eliminate the node variables and the stage variables associated with $\mathbf{p}$ and to rearrange the resulting equations to obtain explicit local ODEs in time in the stage variables associated with $\mathbf{q}$. This elimination and rearrangement is carried out by way of a five-step construction algorithm.

Due to the form of $S(\mathbf{z})$, the central d_2 rows of (4.2) allow us to write entry i in $\mathbf{v}$ as

$$v_i = \sum_{j=1}^{d_2} (\alpha^{-1})_{i,j}\partial_t q_{j+\frac{1}{2}(d_1-d_2)} \tag{4.4}$$

and hence

$$\partial_t v_i = \sum_{j=1}^{d_2} (\alpha^{-1})_{i,j}\partial_t^2 q_{j+\frac{1}{2}(d_1-d_2)}. \tag{4.5}$$

Substituting (4.5) into (4.2), we can eliminate the $\mathbf{v}$ variables in favor of higher order derivatives in time of the $\mathbf{q}$ variables. This lets us write (4.2) as

$$\mathbf{K}\mathbf{z}_t + \mathbf{L}\mathbf{z}_x - \mathcal{E}\mathbf{z}_{tt} = \nabla_{\mathbf{z}} S(\mathbf{z}), \tag{4.6}$$

where $\mathbf{z}$, $\mathbf{K}$, $\mathbf{L}$, $\mathcal{E}$, and $S(\mathbf{z})$ are the new vectors, matrices, and functions given below:

$$\mathbf{z} = \begin{bmatrix} \mathbf{q} \\ \mathbf{p} \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} & & -\mathbf{I}_{\frac{1}{2}(d_1-d_2)} & \\ & \mathbf{0}_{d_2} & & \\ \mathbf{I}_{\frac{1}{2}(d_1-d_2)} & & & \\ & & & \mathbf{0}_{d_1} \end{bmatrix},$$

$$\mathbf{L} = \begin{bmatrix} & \mathbf{I}_{d_1} \\ -\mathbf{I}_{d_1} & \end{bmatrix}, \quad \mathcal{E} = \begin{bmatrix} \mathbf{0}_{\frac{1}{2}(d_1-d_2)} & & & \\ & \alpha^{-1} & & \\ & & \mathbf{0}_{\frac{1}{2}(d_1-d_2)} & \\ & & & \mathbf{0}_{d_1} \end{bmatrix}, \tag{4.7}$$

and $S(\mathbf{z}) = T(\mathbf{p}) + V(\mathbf{q})$.

Note that if $d_2 = 0$, then (4.2) and (4.6) are identical; i.e., $\widehat{V}(\mathbf{v}) \equiv 0$ and $\mathcal{E}$ is a $d_1 \times d_1$ matrix of zeros.

We shall now give a five-step algorithm for constructing explicit local ODEs in time from an r-stage Lobatto IIIA–IIIB PRK discretization of (4.6). However, before we begin, it is necessary to introduce the following notation which will be used throughout the remainder of this text:

(i) z_i^η is the node variable in cell i for the entry η in $\mathbf{z}$,
(ii) $Z_{i,j}^\eta$ is the stage variable at stage j in cell i for the entry η in $\mathbf{z}$,
(iii) $\mathbf{Z}_i^\eta$ is the vector of stage variables in cell i for the entry η in $\mathbf{z}$,

(iv) $\mathbf{Z}_i$ is the tensor of stage variables for all values of η in cell i,
(v) $\partial_t^n Z_{i,j}^\eta$ is a variable representing the first ($n = 1$) and second ($n = 2$) time derivatives of $Z_{i,j}^\eta$,
(vi) $\partial_{z^\eta} S(\mathbf{Z}_i)$ is the vector of stage values at cell i obtained by taking the derivative of the function $S(\mathbf{z})$ with respect to the entry η in $\mathbf{z}$,
(vii) $\mathbf{A}^{(1)}$ is the $r \times r$ matrix of a_{ij} values for Lobatto IIIA,
(viii) $\mathbf{A}^{(2)}$ is the $r \times r$ matrix of a_{ij} values for Lobatto IIIB,
(ix) $\mathbf{b}$ is the common vector of length r of b_j values for Lobatto IIIA and IIIB,
(x) $\mathbf{1}$ is a vector of length r with all entries equal to 1.

Now, (4.6) discretized in space by an r-stage Lobatto IIIA–IIIB PRK discretization results in the following system of implicit ODEs:

$$\mathbf{Q}_i^\eta = q_i^\eta \mathbf{1} + \Delta x \mathbf{A}^{(1)}(-\partial_{p^\eta} T(\mathbf{P}_i)), \tag{4.8}$$

$$q_{i+1}^\eta = q_i^\eta + \Delta x \mathbf{b}^T(-\partial_{p^\eta} T(\mathbf{P}_i)), \tag{4.9}$$

$$\mathbf{P}_i^\eta = p_i^\eta \mathbf{1} + \Delta x \mathbf{A}^{(2)}(\partial_{q^\eta} V(\mathbf{Q}_i) + g_i^\eta), \tag{4.10}$$

$$p_{i+1}^\eta = p_i^\eta + \Delta x \mathbf{b}^T(\partial_{q^\eta} V(\mathbf{Q}_i) + g_i^\eta), \tag{4.11}$$

for $1 \le \eta \le d_1$, where

$$g_i^\eta = \begin{cases} \partial_t \mathbf{Q}_i^{\eta + \frac{1}{2}(d_1+d_2)}, & 1 \le \eta \le \frac{1}{2}(d_1 - d_2), \\ -\partial_t \mathbf{Q}_i^{\eta - \frac{1}{2}(d_1+d_2)}, & \frac{1}{2}(d_1+d_2) < \eta \le d_1, \\ \sum_{\theta=1}^{d_2} (\alpha^{-1})_{\eta - \frac{1}{2}(d_1-d_2),\theta} \partial_t^2 \mathbf{Q}_i^{\theta + \frac{1}{2}(d_1-d_2)}, & \frac{1}{2}(d_1-d_2) < \eta \le \frac{1}{2}(d_1+d_2). \end{cases} \tag{4.12}$$

It should be noted that for the simpler case where $d_2 = 0$, the third option for g_i^η vanishes.

CONSTRUCTION ALGORITHM.

Step 1. A special property of the Lobatto IIIA discretization is that the first row of the coefficient matrix $\mathbf{A}^{(1)}$ is zero and the last row of $\mathbf{A}^{(1)}$ is $\mathbf{b}^T$.

Due to this property, we can see that the first row of (4.8) gives $q_i^\eta = Q_{i,1}^\eta$, and comparing the last row of (4.8) with (4.9) gives $q_{i+1}^\eta = Q_{i,r}^\eta$. Furthermore, from these two identities we can conclude that $Q_{i,r}^\eta = Q_{i+1,1}^\eta$, $\partial_t Q_{i,r}^\eta = \partial_t Q_{i+1,1}^\eta$, and $\partial_t^2 Q_{i,r}^\eta = \partial_t^2 Q_{i+1,1}^\eta$.

Step 2. Since $T(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T \beta \mathbf{p}$ and $|\beta| \neq 0$ we have that $\mathbf{P}_i = \beta^{-1} \nabla_{\mathbf{p}} T(\mathbf{P}_i)$. Also a property of all RK and PRK discretizations is that $\mathbf{b}^T \mathbf{1} = 1$. Therefore we can substitute $\mathbf{P}_i^\eta$ from (4.10) into (4.9) and rearrange to get

$$p_i^\eta = -\frac{1}{\Delta x} \sum_{\zeta=1}^{d_1} \left((\beta^{-1})_{\eta,\zeta} (Q_{i+1,1}^\zeta - Q_{i,1}^\zeta) \right) - \Delta x \mathbf{b}^T \mathbf{A}^{(2)} (\partial_{q^\eta} V(\mathbf{Q}_i) + g_i^\eta). \tag{4.13}$$

Note that this rearrangement is possible since β operates on the index η, while $\mathbf{b}$ and $\mathbf{A}^{(2)}$ operate on the index j as given in the notation scheme.

Step 3. Substituting $\mathbf{P}_i^\eta$ from (4.10) into (4.8) and then substituting p_i^η from (4.13) into the resulting equation gives

$$\begin{aligned}\mathbf{Q}_i^\eta &= Q_{i,1}^\eta \mathbf{1} - \Delta x \mathbf{A}^{(1)} \left(\sum_{\zeta=1}^{d_1} \beta_{\eta,\zeta}(\mathbf{P}_i^\zeta) \right) \\ &= Q_{i,1}^\eta \mathbf{1} - \Delta x \mathbf{A}^{(1)} \left(\sum_{\zeta=1}^{d_1} \beta_{\eta,\zeta}(p_i^\zeta \mathbf{1} + \Delta x \mathbf{A}^{(2)}(\partial_{q^\zeta} V(\mathbf{Q}_i) + g_i^\zeta)) \right) \\ &= Q_{i,1}^\eta \mathbf{1} - \Delta x \mathbf{A}^{(1)} \Bigg(\sum_{\zeta=1}^{d_1} \beta_{\eta,\zeta} \Bigg(\Bigg[- \frac{1}{\Delta x} \sum_{\xi=1}^{d_1} \Big((\beta^{-1})_{\zeta,\xi} (Q_{i,r}^\xi - Q_{i,1}^\xi) \Big) \\ &\qquad - \Delta x \mathbf{b}^T \mathbf{A}^{(2)} (\partial_{q^\zeta} V(\mathbf{Q}_i) + g_i^\zeta) \Bigg] \mathbf{1} + \Delta x \mathbf{A}^{(2)} (\partial_{q^\zeta} V(\mathbf{Q}_i) + g_i^\zeta) \Bigg) \Bigg).\end{aligned} \tag{4.14}$$

Rearranging and applying β^{-1} gives

$$\begin{aligned}&\frac{1}{(\Delta x)^2} \sum_{\zeta=1}^{d_1} (\beta^{-1})_{\eta,\zeta} \left[\mathbf{Q}_i^\zeta - Q_{i,1}^\zeta \mathbf{1} - \mathbf{A}^{(1)} (Q_{i,r}^\zeta - Q_{i,1}^\zeta) \mathbf{1} \right] \\ &\qquad = \mathbf{A}^{(1)} \left[(\mathbf{b}^T \mathbf{A}^{(2)} (\partial_{q^\eta} V(\mathbf{Q}_i) + g_i^\eta)) \mathbf{1} - \mathbf{A}^{(2)} (\partial_{q^\eta} V(\mathbf{Q}_i) + g_i^\eta) \right] \\ &\qquad = \mathbf{A}^{(1)} (\mathbf{1}\mathbf{b}^T - \mathbf{I}) \mathbf{A}^{(2)} (\partial_{q^\eta} V(\mathbf{Q}_i) + g_i^\eta).\end{aligned} \tag{4.15}$$

Now, the first and last rows of the left-hand side of (4.15) are zero, as are the first and last rows and columns of $\mathbf{A}^{(1)}(\mathbf{1}\mathbf{b}^T - \mathbf{I})\mathbf{A}^{(2)}$. Therefore, we denote rows 2 to $r-1$ of $[\mathbf{Q}_i^\zeta - Q_{i,1}^\zeta \mathbf{1} - \mathbf{A}^{(1)}(Q_{i,r}^\zeta - Q_{i,1}^\zeta)\mathbf{1}]$ by $\mathbf{d}_i^\zeta$, the block of $\mathbf{A}^{(1)}(\mathbf{1}\mathbf{b}^T - \mathbf{I})\mathbf{A}^{(2)}$ from $(2,2)$ to $(r-1, r-1)$ by $\mathbf{C}$, and rows 2 to $r-1$ of $\partial_{q^\eta} V(\mathbf{Q}_i) + g_i^\eta$ by $\mathbf{e}_i^\eta$.

Then, noting that $\mathbf{C}$ has full rank due to (3.5), we can write

$$\frac{1}{(\Delta x)^2} \sum_{\zeta=1}^{d_1} (\beta^{-1})_{\eta,\zeta} \mathbf{C}^{-1} \mathbf{d}_i^\zeta = \mathbf{e}_i^\eta. \tag{4.16}$$

Recalling the definition of g_i^η, (4.16) immediately allows us to write down explicit formulas for $\partial_t Q_{i,k}^\eta$ in terms of $\mathbf{Q}_i$ for $1 < k < r$ and $1 \le \eta \le \frac{1}{2}(d_1 - d_2)$ or $\frac{1}{2}(d_1 + d_2) < \eta \le d_1$ and for $\partial_t^2 Q_{i,k}^\eta$ in terms of $\mathbf{Q}_i$ for $1 < k < r$ and $\frac{1}{2}(d_1 - d_2) < \eta \le \frac{1}{2}(d_1 + d_2)$.

Step 4. Substituting p_i^η from (4.13) into (4.11) for both p_i^η and p_{i+1}^η gives

$$\begin{aligned}&- \frac{1}{(\Delta x)^2} \sum_{\zeta=1}^{d_1} (\beta^{-1})_{\eta,\zeta} (Q_{i+2,1}^\zeta - 2Q_{i+1,1}^\zeta + Q_{i,1}^\zeta) \\ &\qquad = \mathbf{b}^T \mathbf{A}^{(2)} (\partial_{q^\eta} V(\mathbf{Q}_{i+1}) + g_{i+1}^\eta) + (\mathbf{b}^T - \mathbf{b}^T \mathbf{A}^{(2)}) (\partial_{q^\eta} V(\mathbf{Q}_i) + g_i^\eta)\end{aligned} \tag{4.17}$$

for each η.

Of importance here is that (4.17) does not involve the variables $\partial_t Q_{i+1,r}^\eta$ or $\partial_t^2 Q_{i+1,r}^\eta$ since the last entry of $\mathbf{b}^T \mathbf{A}^{(2)}$ is zero. Neither does it involve the variables $\partial_t Q_{i,1}^\eta$ or $\partial_t^2 Q_{i,1}^\eta$ since the first entry of $\mathbf{b}^T - \mathbf{b}^T \mathbf{A}^{(2)}$ is also zero.

Step 5. Substituting the formulas for $\partial_t Q^\eta_{i,k}$ and $\partial_t^2 Q^\eta_{i,k}$ found in Step 3 into (4.17) and recalling that $\partial_t Q^\eta_{i,r} = \partial_t Q^\eta_{i+1,1}$ and $\partial_t^2 Q^\eta_{i,r} = \partial_t^2 Q^\eta_{i+1,1}$, we can obtain explicit formulas for $\partial_t Q^\eta_{i+1,1}$ in terms of $\mathbf{Q}_i$ and $\mathbf{Q}_{i+1}$ for $1 \le \eta \le \frac{1}{2}(d_1 - d_2)$ and $\frac{1}{2}(d_1 + d_2) < \eta \le d_1$ and for $\partial_t^2 Q^\eta_{i+1,1}$ in terms of $\mathbf{Q}_i$ and $\mathbf{Q}_{i+1}$ for $\frac{1}{2}(d_1 - d_2) < \eta \le \frac{1}{2}(d_1 + d_2)$.

Thus, for each cell i in our grid, we have a system of explicit ODEs for either the first or second time derivatives of the stage variables $\mathbf{Q}_i$ in terms of local values of $\mathbf{Q}_i$. ∎

While the conditions on $\mathbf{K}$, $\mathbf{L}$, and $S(\mathbf{z})$ in the above theorem may at first appear restrictive, they allow several important equations such as the nonlinear wave and nonlinear Schrödinger equations. A notable exception is the Korteweg–de Vries equation for which $S(\mathbf{z})$ is not separable. It is also worth noting that the conditions on $\mathbf{K}$, $\mathbf{L}$, and $S(\mathbf{z})$ are the same as those required for the continuous system to be written as a system of PDEs in the variables $\mathbf{q}$ and are similar to those required for a separable Hamiltonian system to be written as a system of second order ODEs.

The structure of $\mathbf{K}$ is known as the "Darboux normal form" of $\mathbf{K}$ and a change of coordinates will allow any skew-symmetric matrix to be written this way. If putting $\mathbf{K}$ in Darboux normal form gives $\mathbf{L}$ the structure

$$\mathbf{L} = \begin{bmatrix} & & \Lambda \\ & 0_{d_2} & \\ -\Lambda^T & & \end{bmatrix} \tag{4.18}$$

for some $d_1 \times d_1$ matrix Λ with $|\Lambda| \neq 0$, then the following change of coordinates in the $\mathbf{p}$ variables can put $\mathbf{L}$ in the form given in (4.1). Let $\hat{\mathbf{p}} = \Lambda \mathbf{p}$ and $\widehat{T}(\hat{\mathbf{p}}) = T(\Lambda^{-1}\hat{\mathbf{p}}) = T(\mathbf{p})$; then $\nabla_{\hat{\mathbf{p}}} S(\mathbf{z}) = \nabla_{\hat{\mathbf{p}}} \widehat{T}(\hat{\mathbf{p}}) = \Lambda \nabla_{\mathbf{p}} T(\mathbf{p}) = \Lambda \beta \mathbf{p} = \Lambda \beta \Lambda^{-1} \hat{\mathbf{p}}$ and $S(\mathbf{z})$ still has the desired structure $S(\mathbf{z}) = V(\mathbf{q}) + \frac{1}{2}\hat{\mathbf{p}}^T (\Lambda \beta \Lambda^{-1}) \hat{\mathbf{p}}$.

The upper left $(d_1 + d_2) \times (d_1 + d_2)$ block of $\mathbf{L}$ being all zeros is fulfilled for PDEs which, when written as a first order system with $\mathbf{K}$ in Darboux normal form, have no equations involving both a time and space derivative of the same variable; i.e., $z^\eta_t + z^\eta_x = f(\mathbf{z})$ does not appear for any η.

4.1. Examples. Here we give several examples of common multi-Hamiltonian PDEs. For the PDEs that satisfy the requirements of Theorem 4.1 we give the ODEs that one obtains by applying the construction algorithm to those PDEs. For PDEs that do not satisfy the requirements of Theorem 4.1 we show why they fail and where the construction algorithm breaks down. We also give a PDE constructed so as to require the full use of Theorem 4.1.

4.1.1. Nonlinear wave equation. Our first example is the nonlinear wave equation,

$$u_{tt} = u_{xx} - V'(u), \tag{4.19}$$

which can be written as a multi-Hamiltonian PDE in the form of (4.2) with [5]

$$\mathbf{z} = \begin{bmatrix} u \\ v \\ w \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \tag{4.20}$$

and $S(\mathbf{z}) = V(u) + \frac{1}{2}v^2 - \frac{1}{2}w^2$.

Here, $d_1 = d_2 = 1$ with $\mathbf{z}^{(1)} = \{u, v\}$ and $\mathbf{z}^{(2)} = \{w\}$. We also have $\alpha = -\beta = 1$; thus we can see that $\mathbf{K}$, $\mathbf{L}$, and $S(\mathbf{z})$ satisfy the requirements of Theorem 4.1. Upon eliminating the variable v, we obtain the PDE (4.6) with

$$\mathbf{z} = \begin{bmatrix} u \\ w \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \mathcal{E} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \tag{4.21}$$

and $S = V(u) - \frac{1}{2}w^2$.

Applying the construction algorithm for $r = 2$ gives the following pair of ODEs for each cell i:

$$\begin{aligned} \partial_t^2 U_{i,1} &= \frac{1}{(\Delta x)^2}(U_{i-1,1} - 2U_{i,1} + U_{i+1,1}) - V'(U_{i,1}), \\ \partial_t^2 U_{i,2} &= \partial_t^2 U_{i+1,1}. \end{aligned} \tag{4.22}$$

Recalling from Step 1 that $\mathbf{q}_i = \mathbf{Q}_{i,1}$ and noting that the last ODE is simply the first ODE of the next cell, it is convenient to drop the second ODE and rewrite the first ODE in terms of the node variable u_i:

$$\partial_t^2 u_i = \frac{1}{(\Delta x)^2}(u_{i-1} - 2u_i + u_{i+1}) - V'(u_i). \tag{4.23}$$

Applying the construction algorithm for $r = 3$ gives the following triplet of ODEs for each cell i:

$$\begin{aligned} \partial_t^2 U_{i,1} &= \frac{1}{(\Delta x)^2}(-U_{i-1,1} + 8U_{i-1,2} - 14U_{i,1} + 8U_{i,2} - U_{i+1,1}) - V'(U_{i,1}), \\ \partial_t^2 U_{i,2} &= \frac{1}{(\Delta x)^2}(4U_{i,1} - 8U_{i,2} + 4U_{i+1,1}) - V'(U_{i,2}), \\ \partial_t^2 U_{i,3} &= \partial_t^2 U_{i+1,1}, \end{aligned} \tag{4.24}$$

which cannot be written in terms of the node variables alone.

4.1.2. NLS equation. Our second example is the famous cubic-potential nonlinear Schrödinger (NLS) equation,

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0, \tag{4.25}$$

where $\psi \in \mathbb{C}$. Taking $\psi = p + iq$ and separating the real and imaginary components of NLS allows the PDE to be written in the form of (4.2) with [15]

$$\mathbf{z} = \begin{bmatrix} p \\ q \\ v \\ w \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} \tag{4.26}$$

and $S = -\frac{1}{2}(p^2 + q^2)^2 - \frac{1}{2}(v^2 + w^2)$.

Here we have $d_1 = 2$ and $d_2 = 0$ with $\mathbf{z}^{(1)} = \{p, q\}$ and $\mathbf{z}^{(2)} = \{v, w\}$. $S(\mathbf{z})$ can be written as (4.3) with $V(\mathbf{q}) = -\frac{1}{2}(p^2 + q^2)$ and $T(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T\beta\mathbf{p}$, where

$$\beta = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \quad \text{and} \quad \mathbf{p} = \begin{bmatrix} v \\ w \end{bmatrix}, \tag{4.27}$$

and thus the NLS equation also satisfies the requirements of Theorem 4.1.

Applying the construction algorithm for an r-stage discretization gives r ODEs for each element of $\mathbf{z}^{(1)}$ at cell i. As with the nonlinear wave equation, if we use the 2-stage discretization, then for each element of $\mathbf{z}^{(1)}$ at cell i we can drop the ODE for the second stage variable and write the ODE for the first stage variable in terms of the node variables. The resulting ODEs are

$$\begin{aligned} \partial_t p_i &= -\frac{1}{(\Delta x)^2}(q_{i-1} - 2q_i + q_{i+1}) - 2(p_i^2 + q_i^2)q_i, \\ \partial_t q_i &= \frac{1}{(\Delta x)^2}(p_{i-1} - 2p_i + p_{i+1}) + 2(p_i^2 + q_i^2)p_i. \end{aligned} \tag{4.28}$$

These are precisely the ODEs one obtains by applying second order finite differences in space to (4.25). The same statement applies for other PDEs that satisfy the conditions of Theorem 4.1; thus we note that 2-stage Lobatto IIIA–IIIB discretization in space is equivalent to second order finite differences in space up to second order differences when applied to such a PDE.

For $r = 3$ we obtain a triplet of ODEs for each element of $\mathbf{z}^{(1)}$ at cell i:

$$\begin{aligned} \partial_t P_{i,1} &= -\frac{1}{(\Delta x)^2}(-Q_{i-1,1} + 8Q_{i-1,2} - 14Q_{i,1} + 8Q_{i,2} - Q_{i+1,1}) \\ &\qquad - 2(P_{i,1}^2 + Q_{i,1}^2)Q_{i,1}, \\ \partial_t P_{i,2} &= -\frac{1}{(\Delta x)^2}(4Q_{i,1} - 8Q_{i,2} + 4Q_{i+1,1}) - 2(P_{i,2}^2 + Q_{i,2}^2)Q_{i,2}, \\ \partial_t P_{i,3} &= \partial_t P_{i+1,1}, \\ \partial_t Q_{i,1} &= \frac{1}{(\Delta x)^2}(-P_{i-1,1} + 8P_{i-1,2} - 14P_{i,1} + 8P_{i,2} - P_{i+1,1}) \\ &\qquad + 2(P_{i,1}^2 + Q_{i,1}^2)P_{i,1}, \\ \partial_t Q_{i,2} &= \frac{1}{(\Delta x)^2}(4P_{i,1} - 8P_{i,2} + 4P_{i+1,1}) + 2(P_{i,2}^2 + Q_{i,2}^2)P_{i,2}, \\ \partial_t Q_{i,3} &= \partial_t Q_{i+1,1}. \end{aligned} \tag{4.29}$$

4.1.3. Boussinesq equation. Our third example is the "good" Boussinesq equation,

$$p_{tt} = (\varepsilon p_{xx} + V'(p))_{xx}, \tag{4.30}$$

which, when written as a multi-Hamiltonian PDE, shares the same $\mathbf{z}$, $\mathbf{z}^{(1)}$, $\mathbf{z}^{(2)}$, $\mathbf{K}$, and $\mathbf{L}$ as the NLS equation above [9]. The only difference is the function $S(\mathbf{z})$ which is given by $S(\mathbf{z}) = -V(p) + \frac{1}{2}(w^2 - \frac{1}{\varepsilon}v^2)$. (The class of Boussinesq equations includes a broad range of PDEs, some of which satisfy the conditions of Theorem 4.1.)

As before, the requirements of Theorem 4.1 are satisfied, and applying the construction algorithm gives r ODEs for each element of $\mathbf{z}^{(1)}$ at cell i. For $r = 2$, we once again drop the ODEs for the second stage variables and write the first ODEs in

terms of the node variables as

$$\begin{aligned}\partial_t p_i &= \frac{1}{(\Delta x)^2}(q_{i-1} - 2q_i + q_{i+1}),\\ \partial_t q_i &= \frac{\varepsilon}{(\Delta x)^2}(p_{i-1} - 2p_i + p_{i+1}) + V'(p).\end{aligned} \tag{4.31}$$

For $r = 3$ we get

$$\begin{aligned}\partial_t P_{i,1} &= \frac{1}{(\Delta x)^2}(-Q_{i-1,1} + 8Q_{i-1,2} - 14Q_{i,1} + 8Q_{i,2} - Q_{i+1,1}),\\ \partial_t P_{i,2} &= \frac{1}{(\Delta x)^2}(4Q_{i,1} - 8Q_{i,2} + 4Q_{i+1,1}),\\ \partial_t P_{i,3} &= \partial_t P_{i+1,1},\\ \partial_t Q_{i,1} &= \frac{\varepsilon}{(\Delta x)^2}(-P_{i-1,1} + 8P_{i-1,2} - 14P_{i,1} + 8P_{i,2} - P_{i+1,1}) + V'(P_{i,1}),\\ \partial_t Q_{i,2} &= \frac{\varepsilon}{(\Delta x)^2}(4P_{i,1} - 8P_{i,2} + 4P_{i+1,1}) + V'(P_{i,2}),\\ \partial_t Q_{i,3} &= \partial_t Q_{i+1,1}.\end{aligned} \tag{4.32}$$

4.1.4. Korteweg–de Vries (KdV) equation. Our fourth example is the KdV equation,

$$u_t = V'(u)_x + \nu u_{xxx}, \tag{4.33}$$

which can be written in the form of (4.2) with [6]

$$\mathbf{z} = \begin{bmatrix} u\\ \phi\\ v\\ w\end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} 0 & -1 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ -1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\end{bmatrix} \tag{4.34}$$

and with $S(\mathbf{z}) = -\frac{1}{2}uw - V(u) - \frac{1}{2\nu}v^2$. Here, $d_1 = 2$, $d_2 = 0$ and $\mathbf{z}$ is partitioned into $\mathbf{z}^{(1)} = \{u, \phi\}$ and $\mathbf{z}^{(2)} = \{v, w\}$.

While the $\mathbf{K}$ and $\mathbf{L}$ matrices have the required structure for Theorem 4.1, the function $S(\mathbf{z})$ does not. Specifically, the $-uw$ term in $S(\mathbf{z})$ prevents us from writing $T(\mathbf{p}) = \frac{1}{2}\mathbf{p}^T\beta\mathbf{p}$, and so step 2 of the construction algorithm cannot be carried out.

For example, discretizing the KdV equation with two-stage Lobatto IIIA–IIIB gives

$$\begin{aligned}v_{i+\frac{1}{2}} &= v_{i-\frac{1}{2}} + \Delta x(\partial_t\phi_i - V'(u_i) - \frac{1}{4}(w_{i+\frac{1}{2}} + w_{i-\frac{1}{2}})),\\ w_{i+\frac{1}{2}} &= w_{i-\frac{1}{2}} - \Delta x\partial_t u_i,\\ -u_{i+1} &= -u_i - \Delta x\frac{1}{\nu}v_{i+\frac{1}{2}},\\ -\phi_{i+1} &= -\phi_i - \Delta x\frac{1}{4}(u_i + u_{i+1}),\end{aligned} \tag{4.35}$$

where $u_i = U_{i,1}$, $u_{i+1} = U_{i,2}$, $\phi_i = \Phi_{i,1}$, $\phi_{i+1} = \Phi_{i,2}$, $v_{i+\frac{1}{2}} = V_{i,1} = V_{i,2}$, and $w_{i+\frac{1}{2}} = W_{i,1} = W_{i,2}$.

Introducing the operators D and M, where $Du_i = \frac{1}{\Delta x}(u_{i+1} - u_i)$ and $Mu_i = \frac{1}{2}(u_{i+1} + u_i)$, allows us to write this system as

$$\begin{aligned} Dv_{i-\frac{1}{2}} &= \partial_t \phi_i - V'(u_i) - \frac{1}{2} M w_{i-\frac{1}{2}}, \\ Dw_{i-\frac{1}{2}} &= -\partial_t u_i, \\ -Du_i &= -\frac{1}{\nu} v_{i+\frac{1}{2}}, \\ -D\phi_i &= -\frac{1}{2} M u_i. \end{aligned} \tag{4.36}$$

Eliminating all the variables other than the original variable u gives the implicit ODE

$$M\partial_t u_i = DV'(u_i) + \nu D^3 u_{i-1}. \tag{4.37}$$

In general, M is not invertible; thus further conditions are required (e.g., periodic boundary conditions with an odd number of grid points) to form a well-defined integrator from this implicit ODE.

This is none other than the *narrow box scheme*, introduced in [2] and derived as a finite volume scheme (and shown to be more accurate than the box scheme) in [3]. Thus, we have shown that the narrow box scheme is multisymplectic.

4.1.5. Benjamin–Bona–Mahony (BBM) equation. Our fifth example is the BBM equation [4],

$$u_t - \alpha u_{xxt} = V'(u)_x. \tag{4.38}$$

This equation can be written in the form of (1.1) [19] with $\mathbf{z} = [u,\ \theta,\ \phi,\ w,\ \rho]^T$,

$$\mathbf{K} = \begin{bmatrix} 0 & \frac{\alpha}{2} & -\frac{1}{2} & 0 & 0 \\ -\frac{\alpha}{2} & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{\alpha}{2} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ -\frac{\alpha}{2} & 0 & 0 & 0 & 0 \end{bmatrix} \tag{4.39}$$

and $S(\mathbf{z}) = uw - V(u) - \frac{\alpha}{2}\theta\rho$.

Putting $\mathbf{K}$ into its Darboux normal form results in an $\mathbf{L}$ of the form

$$\mathbf{L} = \begin{bmatrix} \mathbf{0}_3 & \Lambda \\ -\Lambda^T & \mathbf{0}_2 \end{bmatrix}, \tag{4.40}$$

where Λ is a 3×2 matrix. The matrix $\mathbf{L}$ does not have the form of (4.18), and so it cannot be written in the form of (4.1) by applying a change of variables. Thus, the BBM equation does not satisfy the requirements of Theorem 4.1.

However, partitioning $\mathbf{z}$ into $\mathbf{z}^{(1)} = \{u, \theta, \phi\}$ and $\mathbf{z}^{(2)} = \{w, \rho\}$, then discretizing the BBM equation with two-stage Lobatto IIIA–IIIB using the D and M notation

gives

$$
\begin{aligned}
\frac{\alpha}{2}D\rho_{i-\frac{1}{2}} &= Mw_{i-\frac{1}{2}} - V'(u_i) - \frac{\alpha}{2}\partial_t\theta_i + \frac{1}{2}\partial_t\phi_i,\\
0 &= -\frac{\alpha}{2}M\rho_{i-\frac{1}{2}} + \frac{\alpha}{2}\partial_t u_i,\\
-Dw_{i-\frac{1}{2}} &= -\frac{1}{2}\partial_t u_i,\\
D\phi_i &= Mu_i,\\
-\frac{\alpha}{2}Du_i &= -\frac{\alpha}{2}M\theta_i.
\end{aligned}
\tag{4.41}
$$

Eliminating θ, ϕ, w, and ρ gives the implicit ODE

$$
(M^2 - \alpha D^2)\partial_t u_i = MDV'(u_i). \tag{4.42}
$$

As with the KdV equation, the operator on the left-hand side cannot be *locally* inverted, although it is at least typically invertible.

4.1.6. Padé–II equation. Our sixth example is the equation

$$
u_t - \alpha u_{xxt} = V'(u)_x + \nu u_{xxx}, \tag{4.43}
$$

which contains a mixture of the third order derivatives found in the KdV and BBM equations. This equation is referred to as the Padé–II equation in [10] when $\nu = \frac{9}{10}$, $\alpha = \frac{19}{10}$, and $V(u) = -\frac{1}{2}u^2 - \frac{1}{6}u^3$. It can be written in the form of (1.1) [19] with $\mathbf{z} = [u,\ \theta,\ \phi,\ w,\ \rho,\ v]^T$,

$$
\mathbf{K} = \begin{bmatrix}
0 & \frac{\alpha}{2} & -\frac{1}{2} & 0 & 0 & 0\\
-\frac{\alpha}{2} & 0 & 0 & 0 & 0 & 0\\
\frac{1}{2} & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}, \quad
\mathbf{L} = \begin{bmatrix}
0 & 0 & 0 & 0 & \frac{\alpha}{2} & \nu\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & -1 & 0 & 0\\
0 & 0 & 1 & 0 & 0 & 0\\
-\frac{\alpha}{2} & 0 & 0 & 0 & 0 & 0\\
-\nu & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\tag{4.44}
$$

and $S(\mathbf{z}) = uw - V(u) - \frac{\nu}{2}v^2 - \frac{\alpha}{2}\theta\rho$.

Putting $\mathbf{K}$ into its Darboux normal form results in an $\mathbf{L}$ of the form

$$
\mathbf{L} = \begin{bmatrix} 0_3 & \Lambda \\ -\Lambda^T & 0_3 \end{bmatrix}, \tag{4.45}
$$

where Λ is a 3×3 matrix with $\operatorname{rank}(\Lambda) = 2$. Thus, we cannot write $\mathbf{L}$ in the form of (4.1), and so the Padé–II equation does not satisfy the requirements of Theorem 4.1.

However, partitioning $\mathbf{z}$ into $\mathbf{z}^{(1)} = \{u, \theta, \phi\}$ and $\mathbf{z}^{(2)} = \{w, \rho, v\}$, then discretizing the Padé–II equation with two-stage Lobatto IIIA–IIIB using the D and M notation

gives

$$
\begin{aligned}
\frac{\alpha}{2} D\rho_{i-\frac{1}{2}} + \nu D v_{i-\frac{1}{2}} &= M w_{i-\frac{1}{2}} - V'(u_i) - \frac{\alpha}{2}\partial_t \theta_i + \frac{1}{2}\partial_t \phi_i, \\
0 &= -\frac{\alpha}{2} M \rho_{i-\frac{1}{2}} + \frac{\alpha}{2}\partial_t u_i, \\
-D w_{i-\frac{1}{2}} &= -\frac{1}{2}\partial_t u_i, \\
D\phi_i &= M u_i, \\
-\frac{\alpha}{2} D u_i &= -\frac{\alpha}{2} M \theta_i, \\
-\nu D u_i &= -\nu v_{i-\frac{1}{2}}.
\end{aligned} \tag{4.46}
$$

Eliminating θ, ϕ, w, ρ, and v gives the implicit ODE

$$
(M^2 - \alpha D^2)\partial_t u_i = MDV'(u_i) + \nu M D^3 u_{i-1}. \tag{4.47}
$$

As in the previous two examples, the operator on the left-hand side of (4.47) cannot be locally inverted.

4.1.7. A made-up example. Our last example is contrived to satisfy the requirements of Theorem 4.1 and demonstrates the case when $d_2 \neq d_1$ and $d_2 \neq 0$. We have chosen $d_1 = 3$, $d_2 = 1$, and a multi-Hamiltonian PDE (1.1) with $\mathbf{z} = [q^1,\ q^2,\ q^3,\ v,\ p^1,\ p^2,\ p^3]^T$,

$$
\mathbf{K} = \begin{bmatrix}
0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}, \quad
\mathbf{L} = \begin{bmatrix}
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & 0
\end{bmatrix} \tag{4.48}
$$

and $S(\mathbf{z}) = V(\mathbf{q}) + \frac{1}{2}\mathbf{p}^T\beta\mathbf{p} + \frac{\alpha}{2}v^2$, where α is a constant and

$$
\beta = \begin{bmatrix}
1 & 1 & -\frac{1}{2} \\
1 & 1 & 0 \\
-\frac{1}{2} & 0 & 1
\end{bmatrix}. \tag{4.49}
$$

This corresponds to the PDE

$$
\begin{aligned}
\partial_t q^1 &= -2q^1_{xx} + 2q^2_{xx} + \partial_{q^3} V(\mathbf{q}), \\
\frac{1}{\alpha}\partial_t^2 q^2 &= -4q^1_{xx} + 3q^2_{xx} - 2q^3_{xx} - \partial_{q^2} V(\mathbf{q}), \\
\partial_t q^3 &= 4q^1_{xx} - 4q^2_{xx} + 2q^3_{xx} - \partial_{q^1} V(\mathbf{q}).
\end{aligned} \tag{4.50}
$$

Eliminating the variable v in favor of higher derivatives in time of q^2 gives (4.6) with

(4.51)
$$\mathbf{z} = \begin{bmatrix} q^1 \\ q^2 \\ q^3 \\ p^1 \\ p^2 \\ p^3 \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{L} = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \end{bmatrix},$$

$S(\mathbf{z}) = V(\mathbf{q}) + \frac{1}{2}\mathbf{p}^T\beta\mathbf{p}$, and the only nonzero entry of $\mathcal{E}$ given by $\mathcal{E}_{2,2} = \frac{1}{\alpha}$.

If we apply the construction algorithm for $r = 2$, then once again we can drop the ODEs for the second stage variables and write the ODEs for the first stage variables in terms of the node variables giving the following ODEs at cell i:

(4.52)
$$\partial_t q_i^1 = \frac{1}{(\Delta x)^2}(-2q_{i-1}^1 + 2q_{i-1}^2 + 4q_i^1 - 4q_i^2 - 2q_{i+1}^1 + 2q_{i+1}^2) + \partial_{q^3}V(\mathbf{q}_i),$$

$$\partial_t^2 q_i^2 = \frac{\alpha}{(\Delta x)^2}(-4q_{i-1}^1 + 3q_{i-1}^2 - 2q_{i-1}^3 + 8q_i^1 - 6q_i^2 + 4q_i^3 - 4q_{i+1}^1 + 3q_{i+1}^2 - 2q_{i+1}^3) - \alpha\partial_{q^2}V(\mathbf{q}_i),$$

$$\partial_t q_i^3 = \frac{1}{(\Delta x)^2}(4q_{i-1}^1 - 4q_{i-1}^2 + 2q_{i-1}^3 - 8q_i^1 + 8q_i^2 - 4q_i^3 + 4q_{i+1}^1 - 4q_{i+1}^2 + 2q_{i+1}^3) - \partial_{q^1}V(\mathbf{q}_i).$$

5. Discussion. We would like to point out that the discretization in space by Lobatto IIIA–IIIB in the above examples only modifies the linear component of the multi-Hamiltonian PDE, i.e., the discrete approximation of $\mathbf{L}\mathbf{z}_x$. The reason for this is that, throughout the construction algorithm, the nonlinear components of the multi-Hamiltonian PDE always appear coupled to the time derivatives as the expression $\partial_{q^\eta}V(\mathbf{Q}_i) + g_i^\eta$.

Furthermore, we note that, in the examples above, the same pattern of coefficients arises from discretizing different PDEs with the same order Lobatto IIIA–IIIB discretization. For example, with $r = 2$ the coefficients in the approximation of $\mathbf{q}_{xx}$ have a weighting proportional to $[1,\ -2,\ 1]$, while for $r = 3$ these coefficients are proportional to $[-1,\ 8,\ -14,\ 8,\ -1]$ for the first ODE and $[4,\ -8,\ 4]$ for the second ODE. This behavior continues for higher values of r; e.g., for $r = 4$ the approximation of $\mathbf{q}_{xx}$ in the first ODE has coefficients proportional to $[1,\ \frac{1}{2}(25 - 15\sqrt{(5)}),\ \frac{1}{2}(25 + 15\sqrt{(5)}),\ -52,\ \frac{1}{2}(25+15\sqrt{(5)}),\ \frac{1}{2}(25-15\sqrt{(5)}),\ 1]$, the second ODE has coefficients proportional to $[5+3\sqrt{(5)},\ -20,\ 10,\ 5-3\sqrt{(5)}]$, and the third ODE has coefficients proportional to $[5-3\sqrt{(5)},\ 10,\ -20,\ 5+3\sqrt{(5)}]$. For higher values of r these patterns of the coefficients in the approximation of $\mathbf{q}_{xx}$ become increasingly complicated, yet for a given value of r these patterns remain the same regardless of the PDE under consideration.

The reason these patterns of coefficients occur for different PDEs is due to (4.16) and (4.17). For a given value of r, $\mathbf{C}$ and $\mathbf{d}_i^\zeta$ are fixed regardless of the PDE. Similarly, the coefficients $\mathbf{b}^T\mathbf{A}^{(2)}$ and $\mathbf{b}^T - \mathbf{b}^T\mathbf{A}^{(2)}$ in (4.17) are completely determined by r.

Thus, when solving (4.16) and (4.17) for g_i^η, the same weighting of the nearby stage variables occurs for $\mathbf{q}_{xx}$ for different PDEs.

For an r stage discretization, the approximation to q_{xx}^ζ at stage j of cell i is given by

$$-\frac{1}{(\Delta x)^2}(\mathbf{C}^{-1}\mathbf{d}_i^\zeta)_{j-1} = \frac{1}{(\Delta x)^2}\sum_{k=2}^{r-1}(\mathbf{C}^{-1})_{j-1,k-1}((1-c_k)Q_{i,1}^\zeta - Q_{i,k}^\zeta + c_k Q_{i,r}^\zeta) \tag{5.1}$$

for $2 \le j \le r-1$ and $1 \le \zeta \le r$, where $\mathbf{C}$ and c_k are given by (3.5) and (3.2), respectively. The approximation to q_{xx}^ζ at stage 1 of cell $i+1$ is given by

$$\frac{1}{2b_1(\Delta x)^2}\left(\sum_{k=2}^{r-1}\Big((\mathbf{b}^T\mathbf{A}^{(2)})_k(\mathbf{C}^{-1}\mathbf{d}_{i+1}^\zeta)_{k-1} + (\mathbf{b}^T - \mathbf{b}^T\mathbf{A}^{(2)})_k(\mathbf{C}^{-1}\mathbf{d}_i^\zeta)_{k-1}\Big) + (Q_{i+2,1}^\zeta - 2Q_{i+1,1}^\zeta + Q_{i,1}^\zeta)\right), \tag{5.2}$$

where b_1 is the first entry in $\mathbf{b}$.

This suggests the following shortcut:

1. Write the PDE with only terms of the form $\mathbf{z}_{xx}$ (no $\mathbf{z}_x$).
2. Replace the $\mathbf{z}_{xx}$ terms with the PRK finite differences of the desired order.

Now, the system of ODEs that one obtains from applying Theorem 4.1 to an appropriate PDE can be written as a Hamiltonian system; e.g., for the Boussinesq equation and $r = 2$, the system of ODEs at node i can be written as

$$\partial_t \mathbf{z}_i = \mathbf{J}^{-1}\nabla_{\mathbf{z}_i} H_i, \tag{5.3}$$

where

$$\mathbf{z}_i = \begin{bmatrix} q_i \\ p_i \end{bmatrix}, \quad \mathbf{J}^{-1} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \tag{5.4}$$

and

$$H_i = \frac{1}{(\Delta x)^2}(-q_{i-1}q_i + q_i^2 - q_i q_{i+1} + \varepsilon p_{i-1}p_i - \varepsilon p_i^2 + \varepsilon p_i p_{i+1}) + V(p_i). \tag{5.5}$$

If the nonlinear terms in such a Hamiltonian system are separable, then one can apply an explicit symplectic PRK discretization in time to obtain an explicit (and hence well defined) high order local multisymplectic integrator. If the nonlinear terms are not separable, then other explicit time integrators may be applied, e.g., symplectic splitting methods [20], which may give superior performance (in terms of speed and stability) over implicit integrators. Even if no explicit time integrator can be applied to the Hamiltonian system, there may be some benefits to having a spatial discretization that gives rise to explicit ODEs; e.g., the ODEs may be less stiff than those obtained from an implicit discretization.

In the examples in the previous section, the systems of ODEs arising from the nonlinear wave equation and the Boussinesq equation both have separable Hamiltonians and thus allow for a high order explicit symplectic PRK discretization to be applied in time. The NLS equation is not so fortunate, however; its nonlinearity is

only quadratic, and thus for an r-stage Lobatto IIIA–IIIB discretization in time it is necessary to solve a system of $r-1$ coupled quadratic equations for each update of $\mathbf{P}_i$ or $\mathbf{Q}_i$. For $r=2$, this quadratic equation can be solved explicitly (in particular, the same root of the quadratic is always taken) and an explicit (and hence well defined), local, high order in space, multisymplectic integrator can be formed.

Another point that we would like to make is about how the ODEs that one obtains from our construction algorithm handle boundary conditions. Many other discretization schemes (e.g., implicit midpoint, higher order Gaussian Runge–Kutta) either do not remain well defined or require extra conditions to be so [2, 19]. However, our ODEs remain well defined under periodic, Dirichlet, and Neumann boundary conditions without any further restrictions. For example, 3-stage Lobatto IIIA–IIIB applied to the NLS equation with Neumann boundary conditions, $\psi_x = 0$, applied to the left boundary as $v_1 = w_1 = 0$ leads to the following ODEs:

$$\begin{aligned} \partial_t P_{1,1} &= -\frac{1}{(\Delta x)^2}(-14Q_{1,1} + 16Q_{1,2} - 2Q_{2,1}) - 2(P_{1,1}^2 + Q_{1,1}^2)Q_{1,1}, \\ \partial_t Q_{1,1} &= \frac{1}{(\Delta x)^2}(-14P_{1,1} + 16P_{1,2} - 2P_{2,1}) + 2(P_{1,1}^2 + Q_{1,1}^2)P_{1,1}, \end{aligned} \tag{5.6}$$

which are equivalent to the first and fourth lines of (4.29), where the points outside the domain are treated as phantom points, i.e., $Q_{0,1} = Q_{2,1}$ and $Q_{0,2} = Q_{1,2}$.

Finally, we would like to point out that although Theorem 4.1 is stated for the Lobatto IIIA–IIIB class of PRK discretizations, it applies equally well to any PRK discretization satisfying (3.3), (3.4), and (3.5). We leave it as an open question whether there are any other PRK discretizations that satisfy (3.3), (3.4), and (3.5).

In this paper we have deliberately restricted our attention to the structural properties of PRK discretization, namely its multisymplecticity and explicitness. Results on its dynamical properties, such as order and dispersion, will be reported elsewhere.

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