A new discretization technique for initial value problems based on a variational principle

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Abstract
Motivated by the fact that both the classical and quantum description of nature rest on causality and a variational principle, we develop a novel and highly versatile discretization prescription for classical initial value problems (IVPs). It is based on an optimization functional with doubled degrees of freedom, which is discretized using a single regularized summation-by-parts (SBP) operator. The variational principle provides a straightforward recipe to formulate the corresponding optimization functional for a large class of differential equations. The novel regularization we develop here is inspired by the weak imposition of initial data, often deployed in the modern treatment of IVPs and is implemented using affine coordinates. We demonstrate numerically the stability, accuracy and convergence properties of our approach in systems with classical equations of motion featuring both first and second order derivatives in time.

Keywords: Initial Value Problem, Summation By Parts, Variational Principle

1 Introduction
The numerical treatment of dynamical phenomena in classical and quantum systems is at the core of progress in natural sciences and engineering. In computational fluid dynamics [1] or electrodynamics [2], a set of coupled partial differential equations is solved on a predefined geometric domain with boundary conditions, starting from an initial condition, in order to predict trajectories of point particles or configurations of fields. In the study of atomic properties, linear and non-linear variants of the Schrödinger equation or more generally Lindblad equations [3] of multiple entangled particles are solved as initial value problems. For an understanding of the nuclei of atoms on the other hand, an ensemble of fluctuating quantum fields of a non-linear variant of Maxwell’s equations (Yang-Mills theory) needs to be simulated on a hypercubic grid (lattice QCD) [4].

Much progress has been made in developing accurate and cost effective discretization schemes for partial differential equations over the past two decades. Due to their ease of implementation, finite difference schemes have long enjoyed popularity, but historically were challenged when confronted with intricate simulation geometries. It took the development of summation-by-parts (SBP) finite difference operators (for reviews see e.g. [5–7]), to elevate finite difference schemes to a similar level of
versatility as traditional functional basis approaches, such as Galerkin schemes [8]. The SBP approach both in spatial dimensions, as well as in time [7, 9, 10] provides proofs of stability for finite difference based discretization schemes via the so-called energy method and is easily extended to higher order approximations.

Implementing the integration-by-parts property of the underlying continuum IVP, summation-by-parts operators are an example of so-called mimetic discretizations. It has been shown that SBP operators form a versatile framework, which encompasses various other numerical approximation techniques besides finite differences [11], such as finite volume schemes [12], spectral element [13], flux reconstruction [14] and both continuous [15] and discontinuous Galerkin (dG) [16, 17] schemes.

A crucial development in the numerical treatment of differential equations is the concept of weak boundary or initial conditions. It acknowledges that the solution of a discretized PDE not only in the interior of the domain but also on the boundary (or initial time slice) need only be as accurate as the order of the discretization. By allowing the solution to deviate from the initial or boundary conditions within the tolerance of the discretization, one obtains a new lever, which one can exploit in the construction of discretization schemes. The simultaneous approximation term (SAT) approach [18] e.g. implements weak boundary or initial conditions by the addition of appropriately designed penalty terms to the differential equation of interest. In recent studies it has been shown how to absorb part of these penalty terms into a redefinition of the SBP operators, in order to reduce their null-space to the corresponding physical dimension, leading to so called null-space consistent SBP operators [19–22].

In this paper we develop a versatile discretization scheme for classical systems, based on a generalized variational principle. We will deploy the SBP technique to approximate derivatives occurring in the continuum formulation of the problem and will take inspiration by the SAT approach to regularize the resulting difference operators. To this end we deploy affine coordinates to absorb the whole penalty term including data into a redefined null-space consistent SBP operator.

The paper is structured as follows: In section 2 we review the continuum formulation of the conventional variational principle of classical physics for initial value problems, featuring equations of motion with second order derivatives in time. In the subsequent section 3 we introduce our discretization prescription, discuss the need for regularization and construct a regularized SBP operator based on initial value data. To extend the applicability of our discretization scheme to a more general class of systems, we consider a generalized variational principle in section 4 and show that our approach successfully captures differential equations of motion containing also first order derivatives. We close with a brief summary in section 5.

2 Continuum formalism for second order differential equations

The classical physics of closed systems (i.e. systems that are not in contact with their environment) is conveniently captured via their Lagrangian. In point mechanics the Lagrangian is a functional, which depends on the trajectory of the point mass \( x(t) \) and its velocity \( \dot{x}(t) \). In a field theory, such as in electromagnetism, it is formulated in terms of the vector fields \( A_\mu(x) \) and its derivatives \( \partial_\nu A_\mu(x) \). In the simple systems under consideration here, the Lagrangian can be written as the difference between
the kinetic energy of the system and its potential energy. Taking a point mass in a constant gravitational field as an explicit example we have

$$\mathcal{L} = T - V = \frac{1}{2} m \dot{x}^2(x) - mgx(t).$$  \hspace{1cm} (1)

In the 19th century, physicists discovered that the trajectory of a classical particle can be obtained from a variational principle (see e.g. ref. [23]). If a point mass starts out at position $x(t_1)$ at $t_1$ and ends up at position $x(t_2)$ at $t_2$ then the classical trajectory that is realized in nature between those points is given by the extremum of the classical action\footnote{More specifically, for short times, where the classical trajectory has not yet reached any turning point, the action exhibits an actual minimum. In the presence of turning points in the classical trajectory it in general represents a saddle point of the action. (see e.g. ref. [24])}

$$S[x(t), \dot{x}(t)] = \int_{t_1}^{t_2} dt \, \mathcal{L}[x(t), \dot{x}(t)].$$ \hspace{1cm} (2)

This observation is stated as a \textit{boundary value problem}, where the start and end point of the trajectory are specified. While it is of conceptual interest that such a formulation exists, we cannot use it to determine the classical trajectory itself in a causal fashion, since in order to formulate the variational principle, we already need to know where the point mass will end up at $t_2$. When setting up an experiment, we are of course only in control of the initial position and velocity.

To proceed, physicist conventionally convert the above boundary value problem into an \textit{initial value problem} using the following strategy: one derives a set of differential equations that are equivalent to the variational principle and which can be solved as initial value problem. These are the celebrated Euler-Lagrange equations. We wish to inspect the variation of the Lagrangian using a slightly deformed path $x(t, \epsilon) = x(t) + \delta x(t)$. Here $\delta x(t)$ is an arbitrary function with the only condition that it goes to zero at $t_1$ and $t_2$, as the points $x(t_1)$ and $x(t_2)$ are fixed. Varying the action we obtain

$$\delta S = \int_{t_1}^{t_2} dt \left\{ \frac{\partial \mathcal{L}}{\partial x} \delta x + \frac{\partial \mathcal{L}}{\partial \dot{x}} \dot{\delta x} \right\},$$ \hspace{1cm} (3)

$$= \int_{t_1}^{t_2} dt \left\{ \frac{\partial \mathcal{L}}{\partial x} + \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} \right\} \delta x,$$ \hspace{1cm} (4)

$$= \int_{t_1}^{t_2} dt \left\{ \frac{\partial \mathcal{L}}{\partial x} \right\} \delta x + \left[ \frac{\partial \mathcal{L}}{\partial \dot{x}} \right]_{t_1}^{t_2} \delta x.$$ \hspace{1cm} (5)

Since the variation $\delta x$ by construction vanishes on the boundary, the term in the square brackets also vanishes. If we inspect the extremum of the functional $S$, defined by $\delta S = 0$, we find that it is equivalent to the term in the curly brackets equalling zero, since $\delta x$ can be any (well behaved) function between $t_1$ and $t_2$.

In other words, if we assume the validity of the variational principle, i.e. that the classical trajectory follows from the extremum of the action, then this trajectory
Fig. 1 Differences between the variational principle as boundary value problem (left) and as initial value problem (right). In the BVP setting there may exist multiple paths that fulfill the boundary conditions, but only one of them, \( x_{cl}(t) \), represents an extremum of the action. In the IVP setting, a doubling of the degrees of freedom is required. For the true classical trajectory, the forward and backward path must agree. Figure adapted from ref. [25].

must fulfill the Euler-Lagrange equations, which are just the terms inside the curly brackets set to zero

\[
\left. \frac{\delta S[x, \dot{x}]}{\delta x} \right|_{x=x_{\text{classical}}} = 0 \quad \text{BVP} \quad \text{IVP} \quad \frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = 0. \tag{6}
\]

Since for more complex systems (with internal constraints etc.) it is often easier to formulate the action than to derive the Euler-Lagrange equations as initial value problem, our goal here is to formulate and solve the initial value problem as a variational problem on the level of the action. To this end we combine the reasoning of ref. [25] and ref. [26], which together establish the continuum formalism for the variational IVP.

Retracing the train of thought of ref. [25], we first note that the equivalence between the Euler-Lagrange equations (which provide the correct classical equations of motion) and the stationarity of the action requires that the variation of the path vanishes at initial \( t_1 \) and final time \( t_2 \) (see eq. (5)). Since we do not know \( x(t_2) \) apriori and we only know \( x(t_1) \) and \( \dot{x}(t_1) \), we must instead find a way how to formulate the variational principle in such a way that the value of \( x \) at \( t_2 \) does not need to be fixed. This can be accomplished by doubling the degrees of freedom with one trajectory \( x_1(t) \) describing a forward path and one trajectory \( x_2(t) \) describing a backward path.

The intuition here is that we follow the path forward in time from \( t_1 \) until we reach \( t_2 \) and for the true solution, which is invariant under time-reversal in a closed system, reversing and going back to \( t_1 \) along the backward path must lead us to the same initial point. I.e. only if forward and backward path agree will we have found the correct solution. This strategy is reminiscent of the shooting method, extended such that the aim is to find the trajectory which correctly returns to the starting point given by the initial conditions (see fig. 1 for a sketch of the difference in the approaches).

In order to achieve the cancellation of the variation terms between the forward and backward path at \( t_2 \), ref. [25] constructs a new joint action for the two degrees
of freedom $x_1(t)$ and $x_2(t)$ as

$$S_{IVP}[x_1(t), \dot{x}_1(t), x_2(t), \dot{x}_2(t)] = \int_{t_1}^{t_2} dt \left( \mathcal{L}[x_1(t), \dot{x}_1(t)] - \mathcal{L}[x_2(t), \dot{x}_2(t)] \right),$$  \hspace{1cm} (7)

$$= \int_{t_1}^{t_2} dt \left( L[x_1(t), \dot{x}_1(t), x_2(t), \dot{x}_2(t)] \right).$$  \hspace{1cm} (8)

The Lagrangian housing the backward path $x_2$ is introduced with a relative minus sign, which allows the boundary terms arising in the variation of $\mathcal{L}[x_1(t), \dot{x}_1(t)]$ and $\mathcal{L}[x_2(t), \dot{x}_2(t)]$ to cancel. Let’s carry out the variation of this new $S_{IVP}$, which yields twice as many terms

$$\delta S = \int dt \left( \left\{ \frac{\partial L}{\partial x_1} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_1} \right\} \delta x_1 - \left\{ \frac{\partial L}{\partial x_2} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_2} \right\} \delta x_2 \right)$$

$$+ \left. \left[ \frac{\partial L}{\partial \dot{x}_1} \delta x_1 \right] \right|_{t_1}^{t_2} - \left. \left[ \frac{\partial L}{\partial \dot{x}_2} \delta x_2 \right] \right|_{t_1}^{t_2}. \hspace{1cm} (9)$$

In order to see the cancellations explicitly, it is advantageous to change coordinates, going over to relative $x_- = x_1 - x_2$ and centered coordinates $x_+ = (x_1 + x_2)/2$. This change is not necessary, but expressed in $x_-$ and $x_+$ the new variational principle can be formulated in a very concise form and the relation between the functional and the resulting differential equation of motion becomes much more lucid.

We rewrite the action using $x_\pm(t, \epsilon) = x_\pm(t) + \delta x_\pm(t)$. The new path deformations $\delta x_\pm(t)$ vanish at the initial time $t_1$, as the original deformations are set to zero there $\delta x_1(t_1) = \delta x_2(t_1) = 0$. In order to correctly cancel the boundary contributions, the values of $x_1(t_2)$ and $x_2(t_2)$ have to agree, but it is important to note that they are not fixed to a certain value, since we do not know that value apriori. I.e. the two paths need to be connected, corresponding to the condition $x_1(t_2) = x_2(t_2)$.

Let us see how this works in more detail. As the action is now a functional of the newly introduced paths $S_{IVP}[x_+(t), \dot{x}_+(t), x_-(t), \dot{x}_-(t)]$, its variation produces the following expression

$$\delta S_{IVP} = \int dt \left( \left\{ \frac{\partial L}{\partial x_+} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_+} \right\} \delta x_+ + \left\{ \frac{\partial L}{\partial x_-} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_-} \right\} \delta x_- \right)$$

$$+ \left. \left[ \frac{\delta L}{\delta \dot{x}_+} \delta x_+ + \frac{\delta L}{\delta \dot{x}_-} \delta x_- \right] \right|_{t_1}^{t_2}. \hspace{1cm} (11)$$

Due to the identification of the paths at $t_2$, we have that $\delta x_-(t_2) = \delta x_1(t_2) - \delta x_2(t_2) = 0$ and thus $\delta x_-(t_2) = 0$. From it follows that the second boundary term proportional to $\delta x_-$ vanishes.

Intuition tells us that in order for the forward and backward path to agree, in case of the true classical trajectory, we also should identify the derivatives of the paths at the time $t_2$. Let us show explicitly that this identification makes the remaining boundary term vanish. Since $\dot{x}_1(t) = \dot{x}_+(t) + \frac{1}{2} \dot{x}_-(t)$ and $\dot{x}_2(t) = \dot{x}_+(t) - \frac{1}{2} \dot{x}_-(t)$, we find the following expression for the derivative of the joint Lagrangian $L$

$$\frac{\delta L}{\delta \dot{x}_+} = \frac{\delta L}{\delta \dot{x}_1} \frac{\partial x_1}{\partial \dot{x}_+} + \frac{\delta L}{\delta \dot{x}_2} \frac{\partial x_2}{\partial \dot{x}_+} = \delta \frac{\partial L}{\partial \dot{x}_1} - \delta \frac{\partial L}{\partial \dot{x}_2} = \pi_1 - \pi_2. \hspace{1cm} (12)$$
In the second equality we have explicitly written $L$ as the difference between the individual Lagrangians $\mathcal{L}$ for the forward path $x_1$ and backward path $x_2$. In the last step we furthermore introduced the conjugate momenta of the paths, defined as $\pi_{1,2} = \frac{\delta L}{\delta \dot{x}_{1,2}}$.

If we construct our paths such that the difference between the momenta $\pi_1(t_2) - \pi_2(t_2) = 0$ vanishes at time $t_2$, then the one remaining boundary term in eq. (11) will also be zero. For the systems considered here, which exhibit second order derivatives in their equation of motion we have the kinetic term $T = \frac{1}{2} \dot{x}^2$ in the Lagrangian $\mathcal{L}$. This term leads to the identification $\pi_{1,2} = \dot{x}_{1,2}$. In turn we find that if we require that in addition to the values of the paths at $t_2$ also the derivatives are identified $\dot{x}_1(t_2) = \dot{x}_2(t_2)$, both boundary terms in eq. (11) will vanish. This establishes the necessary conditions for joining the forward and backward path

$$x_1(t_2) = x_2(t_2), \quad \dot{x}_1(t_2) = \dot{x}_2(t_2),$$

in order to relate the extremum of the joint functional $L$ to the Euler-Lagrange equation expressions in the curly brackets in eq. (11). So far the reasoning of ref. [25] is impeccable, having arrived at eq. (11), where the boundary terms vanish and two separate Euler-Lagrange like terms remain in curly brackets.

As next step, the authors invoke the concept of the physical limit, which amounts to identifying the forward and backward path, or equivalently to let $x_- \to 0$. This step may appear ad hoc to the reader, which is why we here motivate it by considering how the classical variational principle follows from the underlying quantum field theory, as laid out in detail in ref. [26]. Starting from the path integral, in which an ensemble of paths is considered, the classical limit of taking $\hbar \to 0$ must collapse all of these paths onto the unique classical trajectory. It turns out that the relative path $x_- \equiv x_1 - x_2$ is related to the quantum contributions and taking $x_- \to 0$ is therefore intimately related to the classical limit. Ref. [26] shows that the variation of the joint action with respect to $x_-$ is the relevant expression that describes how the quantum paths collapse onto the classical trajectory and the classical trajectory indeed emerges after taking the limit $x_- \to 0$.

Combining the variation of the joint action of the forward and backward path with the physical limit, we arrive at the following concise formulation of the variational principle for a classical initial value problem

$$\frac{\delta S_{IVP}[x_\pm]}{\delta x_-} \bigg|_{x_- = 0, x_+ = x_{\text{class}}} = 0.$$  \hspace{1cm} (14)

Take as explicit example the point mass in a constant gravitational field. Its Lagrangian is $\mathcal{L} = \frac{1}{2} m \dot{x}^2(t) - mgx(t)$ and the Euler-Lagrange equation reads

$$\ddot{x}_{\text{class}}(t) = -g, \quad x_{\text{class}}(t) = -\frac{1}{2} gt^2 + \dot{x}(0)t + x(0),$$

which is nothing but Newton’s law in terms of acceleration and can be solved in a straight forward manner. We will take $g$ to be positive to indicate that gravity is acting downwards.
Using the formalism based on the doubled degrees of freedom we have instead

\[ S_{\text{IVP}} = \int dt \left( \frac{1}{2} m(\dddot{x}_1^2(t) - \dddot{x}_2^2(t)) - mg(x_1(t) - x_2(t)) \right), \]  

(16)

\[ = \int dt \left( m\ddot{x}_+(t)\ddot{x}_-(t) - mgx_-(t) \right). \]  

(17)

In computing the variation of the action, we carried out one integration by parts, which, in effect, allows us to reexpress \( S \) as a functional solely of the paths and not of their derivatives (see the step between eq. (4) and eq. (5)). Similarly we can integrate by parts here to move the time derivative on \( x_- \) in the kinetic term to \( x_+ \)

\[ S_{\text{IVP}} = \int dt \left( -m\dddot{x}_+(t)x_-(t) - mgx_-(t) \right). \]  

(18)

Since we identify both the values and derivatives of the paths at \( t_2 \) no boundary terms contribute. Taking the functional derivative of eq. (18) with respect to \( x_- \), setting the result to zero and identifying \( x_+ = x_{\text{class}} \) in the \textit{physical limit} yields exactly the conventional Euler-Lagrange equation

\[ \dddot{x}_+(t) = \dddot{x}_{\text{class}}(t) = -g. \]  

(19)

Note that eq. (14) and the example in eq. (17) and eq. (18) provide us with a first intuition on how to formulate the corresponding functional for a large variety of differential equations of motion of the form \( \dddot{x} + f(x) = 0 \). Since only terms linear in \( x_- \) survive the variation, we can write

\[ S_{\text{IVP}} = \int dt \left( m\dddot{x}_+(t)\dot{x}_-(t) - f(x_+)x_-(t) \right). \]  

(20)

In section 4, after having established the discrete formalism for systems with a second order equation of motion in time, we will consider a generalized variational principle also derived in ref. [25], which will allow us to extend the discrete treatment to systems with differential equations of motion containing also single derivatives in time.

3 Variational IVP based on SBP operators in time

3.1 A naive SBP discretization of the boundary value problem

As a first step, let us formulate the discretized variational principle in its conventional form as boundary value problem. The point mass in a constant gravitational field will again serve as an explicit example.

Our goal here is to discretize the action for the single forward path \( x(t) \)

\[ S = \int dt \left( \frac{1}{2} mx^2(t) - mgx(t) \right), \]  

(21)

with Dirichlet boundary conditions \( x(0) = x_i \) and \( x(1) = x_f \). To this end we introduce the path \( x = (x(0), x(\Delta t), x(2\Delta t), \ldots)^T \) resolved at \( N_t \) points with time
step $\Delta t = 1/(N_t - 1)$. The integral can be approximated by a quadrature rule, whose particular form is captured in a (diagonal) positive definite matrix $H$ and which defines an inner product on discretized paths $(x, x') = x^T H x'$. In order to retain as many of the continuum properties of the theory as possible, we discretize the time derivative with a summation by parts operator $D = H^{-1} Q$, compatible with our choice of $H$, where $Q^T + Q = \text{diag}[-1, 0, \ldots, 0, 1]$.

The lowest order SBP discretization scheme of order two in the interior and order one on the boundary ensues when choosing the trapezoid rule for integration

$$H^{[2,1]} = \Delta t \begin{bmatrix} 1/2 & 1 & \cdots & 1 \\ 1 & \ddots & & \\ & & 1 \\ & & & 1/2 \end{bmatrix}, \quad D^{[2,1]} = \frac{1}{2\Delta t} \begin{bmatrix} -2 & 2 \\ -1 & 0 & 1 \\ & \ddots & \ddots \\ -1 & 0 & 1 \\ -2 & 2 \end{bmatrix}.$$ 

The next higher order SBP scheme is fourth order in the interior and second order on the boundary

$$H^{[4,2]} = \Delta t \begin{bmatrix} 17/48 & 59/48 & & & \\ & 43/48 & & \\ & & 49/48 & \\ & & & 1 \\ & & & & \end{bmatrix}.$$

$$D^{[4,2]} = \frac{1}{\Delta t} \begin{bmatrix} -24/17 & 59/34 & -4/17 & -3/34 \\ -1/2 & 0 & 1/2 & 0 \\ 1/2 & 0 & -59/86 & 0 \\ -1/2 & 0 & 59/86 & 0 \\ -1/2 & 0 & 32/49 & -4/49 \\ 1/12 & -2/3 & 0 & 2/3 & -1/12 \\ & \ddots & \ddots & \ddots & \ddots \end{bmatrix}. \quad (22)$$

In this section we will show explicit results based on the $[2,1]$ approximation and include the outcomes from the $[4,2]$ approximation in our scaling tests.

The discretized action, on which the variational boundary value problem rests, reads

$$S_{\text{BVP}} = \frac{1}{2} m (Dx)^T H (Dx) - mg x^T H x - \lambda_1 (x(0) - x_i) - \lambda_2 (x(1) - x_f). \quad (23)$$

We have added two Lagrange multipliers that are treated as additional dynamical degrees of freedom of our system and in turn enforce the boundary conditions of the numerical solution. This procedure may appear to introduce the boundary conditions strongly, however it does not amount to an a priori replacement of $x(t_1)$ and $x(t_2)$ by $x_i$ and $x_f$. During the procedure to locate the extremum of $S_{\text{BVP}},$
Figure 2: Numerical solution of the classical trajectory (red dots) by finding the discretized path $x$ ($N_t = 64$) that optimizes the functional eq. (23) using naive [2, 1] order summation-by-parts operators in time. Continuum solution of the Euler-Lagrange equation $\ddot{x}(t) = -g$ is shown as solid gray line.

we find that the minimization algorithms approach the extremum of the functional globally. I.e. the boundary conditions are fulfilled to machine precision for the actual solution, while deviations are possible at intermediate steps. We therefore consider our use of Lagrange multipliers in conjunction with a global optimization strategy as a weak imposition of the boundary conditions.

Note that when adding Lagrange multipliers to introduce constraints to an optimization functional, the relevant extremum may become a saddle point. If only algorithms are available that locate the minima of a functional, one can circumvent this issue by optimizing the norm of the gradient of the functional instead, for which the saddle point becomes a local minimum.

Having derived the continuum Euler-Lagrange equations for the point mass in a constant gravitational field before in eq. (15), we compute the explicit solution for the classical trajectory in the time interval $t \in [0, 1]$, based on a value of $g = 1$ and initial conditions $x(0) = 1$, $\dot{x}(0) = 0.3$. In that case the point mass reaches the position $x(1) = 0.8$ at time $t_2 = 1$. Supplying these values to eq. (23), we can solve for the extremum and, as shown in fig. 2, obtain a solution (red dots) that recovers the correct solution of the Euler-Lagrange equations (gray solid line).

While we succeed in recovering the correct solution, this approach, as mentioned before, is conceptually not satisfactory, since the formulation of the BVP relied on information about $x(1)$ obtained from the prior solution of the Euler-Lagrange equations as initial value problem.

3.2 A naive SBP discretization of the initial value problem
Let us continue by turning our attention to discretizing the continuum formulation of the variational principle for initial value problems, which is based on two paths. Introducing discretized paths $\mathbf{x}_1 = (x_1(0), x_1(\Delta t), x_1(2\Delta t), \ldots)^T$ and correspondingly $\mathbf{x}_2$ and using the same symbols as before for the integration $\mathbf{H}$ and
summation-by-parts difference operators $D$, we arrive at the following action

$$S_{IVP} = \left\{ \frac{1}{2} (Dx_1)^T H (Dx_1) - g^T H x_1 \right\} - \left\{ \frac{1}{2} (Dx_2)^T H (Dx_2) - g^T H x_2 \right\} + \lambda_1 (x_1(0) - x_i) + \lambda_2 ((Dx_1)(0) - \dot{x}_i) + \lambda_3 (x_1(N_t) - x_2(N_t)) + \lambda_4 ((Dx_1)(N_t) - (Dx_2)(N_t)).$$

(24)

Here we have introduced four Lagrange multipliers to both enforce the initial conditions for position $x_i$ and derivative $\dot{x}_i$ of the forward path ($\lambda_1, \lambda_2$), as well as to enforce the correct identification of the position and derivatives at the last point of the forward and backward path ($\lambda_3, \lambda_4$). We consider all $\lambda_i$’s as dynamical degrees of freedom, such that the constraints are enforced exactly on the final solution of the optimization problem, while permitting deviations from the constraints at intermediate steps.

When we determine the optimal paths $x_1$ and $x_2$ that minimize $S_{IVP}$ using $H^{[2,1]}$ and $D^{[2,1]}$ on $N_t = 64$ discrete points, we find the solution shown in fig. 3. We plot the values of the forward path as blue dots, while those of the backward path are given in red. The fact that only red points are visible (i.e. they lie on top of the blue points) tells us that the optimal solution fulfills the physical limit condition $x_1 = x_2$. On the other hand we also immediately see that only around half of the points on each path agree with the correct solution from the Euler-Lagrange equations (gray solid line). The other half lies significantly below the correct solution, forming a highly oscillatory structure.

We have identified the origin of these oscillatory structures to arise from the particular structure of the null-space of the finite difference operator. In the kinetic terms of $S_{IVP}$ both $D$ and $D^T$ appear. The study of null-space consistency of the lowest order SBP operator considered here, reveals that it contains exactly two zero eigenvalues. The space of right eigenvectors of $D$, associated with this doubly
degenerate eigenvalue, is only one-dimensional. Both eigenvectors are proportional to the constant function.

However when we study the form of the left eigenvectors of $D$, or equivalently the right eigenvectors of $D^T$, we find that those projecting into the null space are not at all constant but but highly oscillatory, reminiscent of the so-called $\pi$-mode. An example of these eigenvectors is shown in fig. 4.

Such unphysical oscillatory solutions have recently been identified to also interfere in determining the solutions of differential equations with non-trivial boundary conditions in one- and multiple dimensions in [27]. In the context of the variational problem considered here, the oscillatory solutions did not affect the solution when formulated as a boundary value problem in section 3.1. The fixing of the boundary at $t_2$ in the BVP formulation apparently prevents the oscillatory solution. On the other hand the IVP action eq. (24) clearly accommodates these oscillatory paths.

An accurate discretization scheme for the IVP system action must therefore be able to avoid the appearance of unphysical oscillatory modes and several strategies to do so have been explored in the literature. One class of strategies consists of modifying the first order derivative operator $D$ by adding higher order derivative operators to it. A conventional SBP finite difference operator of order $p$ needs to fulfil the derivative property $D^{(p)}x^n = (n-1)x^{n-1}$ exactly only on monomials up to order $n = p-1$. Therefore, adding a higher derivative operator $\Delta t D^{(2p)}$, scaled by the grid spacing does not affect this property, as it annihilates all lower order monomials. In addition, this correction term vanishes in the limit of taking $\Delta t \to 0$. In the context of upwind schemes one e.g. adds the symmetric second derivative operator to the SBP first derivative, turning it into an upwind derivative. If one deals with complex functions one may instead add the symmetric second derivative multiplied with the imaginary unit. This modification is known as adding a Wilson term [28] in the physics literature. Wilson understood that in the absence of the modification term unphysical oscillatory solutions may contribute, which he identified as unphysical poles of the Green’s-function of the differential equation of motion.
Both of these approaches present challenges, which we wish to avoid here. By turning the central stencil into an upwind stencil, we loose the symmetry of the system, which adversely affects the accuracy of the solutions. Introducing a purely imaginary modification on the other hand requires the difference operator to act on complex functions to be meaningful. One may contemplate the possibility to complexify the functions involved in the variational problem, which while only cumbersome in the classical case will lead to conceptual problems when trying to use the discretization in the context of quantum path integrals (c.f. sign problem).

We therefore wish to explore a different route to remove the unphysical zero modes of the operator $D$, taking inspiration from more recent works on null-space consistent SBP operators, such as in refs. [19–22]. The central ingredient in these approaches is to exploit the weak formulation of boundary and initial conditions. Concretely, when boundary conditions are enforced weakly via a penalty term, this penalty term can be partially absorbed into the derivative operator to remove its zero modes. On the level of differential equations, the strategy works as follows. Consider the discretized differential equation for the exponential function

$$D u = \lambda u + \sigma_0 H^{-1} E_0 (u - g).$$

(25)

Here we have added a so-called SAT penalty term on the RHS, which includes the matrix $E_0 = \text{diag}[1,0,\ldots,0]$ that singles out the first entry in the discretized functions $u$ and $g$. The former $u$ refers to the solution of the differential equation and the latter $g$ contains the initial value as its first entry. Note that $H^{-1}$ contains $\Delta t^{-1}$, which contributes with increasing weight as $\Delta t \to 0$. The parameter $\sigma_0$ can be tuned to satisfy stability properties. The standard approach developed in the conventional SBP-SAT treatment of IVPs consists of absorbing the penalty term proportional to $u$ into a redefined $\tilde{D} = D - \sigma_0 H^{-1} E_0$, which does not feature any zero modes anymore. That operator is now nonsingular [29] and may be inverted to obtain the solution $u$. In the next section we will develop a similar strategy applicable to the variational problem.
3.3 Regularized SBP discretization of the initial value problem

Taking inspiration from the work on regularizing SBP operators in differential equations, we set out to absorb information about the initial conditions into the SBP operator as means of regularization. In the functional eq. (24) we do not have an equality sign, such as in our example (25), to rearrange terms. Instead we must find a way to incorporate the whole penalty term in $D$. Note that the penalty term contains one expression that is proportional to the function that the SBP operator acts on and one expression proportional to a constant. I.e. we have to modify the difference operator to include a shift. In other words, we are dealing with an affine transformation.

There exists an elegant way to express affine transformations using so-called affine coordinates. One defines $\bar{A}[b] \bar{x} = A x + b$, where $\bar{A}[b]$ refers to the matrix $A$ amended by one more row and column with 1 placed in the lower right corner. The additional column available in $\bar{A}[b]$ is filled with the values of $b$. The vector $\bar{x}$ is just $x$ amended by one more entry with value one. For our application to the variational formulation of the IVP we therefore define a new $\bar{D}$ using the vector of initial values $g$ to construct the shift $b$. For the $[2, 1]$ order SBP operator the explicit expression we obtain using $g = \text{diag}[x_i, x_i + \Delta t \dot{x}_i, 0, \cdots, 0]$ reads

$$\bar{D}^{[2,1]} = \begin{bmatrix}
-\frac{1}{\Delta t} - \sigma_0 \frac{2}{\Delta t} & \frac{1}{\Delta t} & 0 & \sigma_0 \frac{\Delta t}{\Delta t} x_i \\
\frac{1}{\Delta t} & 0 & \frac{1}{\Delta t} & 0 \\
\vdots & 0 & \frac{1}{\Delta t} & 0 \\
-\frac{1}{\Delta t} & 0 & \frac{1}{\Delta t} & 0 \\
0 & \cdots & -\frac{1}{\Delta t} & 0 & 1
\end{bmatrix}.$$  \hspace{1cm} \text{(26)}$$

In the remainder of this paper we choose the free parameter $\sigma_0 = -1$, whenever a penalty term is incorporated in $\bar{D}$. This choice is motivated by the fact that in the conventional treatment of IVPs using the SBP-SAT approach, this value leads to a minimal discretization error (see e.g. ref. [7]).

All zero modes of the original operator $D^{[2,1]}$ have been lifted in $\bar{D}^{[2,1]}$ and the resulting spectrum of eigenvalues $\nu$ is shown in fig. 5. Note that $\bar{D}^{[2,1]}$ still correctly annihilates the constant function, as long as it is compatible with the initial conditions $x_i = 1$. In affine coordinates this annihilation does not lead to a resulting zero vector, but a vector that contains vanishing entries, except for the final one associated with the single real eigenvalue of value one, shown in fig. 5.

When formulating the action with the modified SBP operator, we obtain

$$S_{IVP} = \left\{ \frac{1}{2} (\bar{D}x_1)^T \bar{H}(\bar{D}x_1) - g^T \bar{H}x_1 \right\} + \left\{ \frac{1}{2} (\bar{D}x_2)^T \bar{H}(\bar{D}x_2) - g^T \bar{H}x_2 \right\}$$
$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((Dx_1)(0) - \dot{x}_i)$$
$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((Dx_1)(N_t) - (Dx_2)(N_t)).$$  \hspace{1cm} \text{(27)}$$

In order to implement the inner product in affine coordinates, we define $\bar{H}$, which denotes the matrix $H$, amended by one extra row and column of values zero.

[2] For a higher order SBP operator, the values of $g$ need to be chosen, so that $\left[ Dg \right](0) = \dot{x}_i$ and $\left[ g \right](0) = x_i$. 
Figure 6 Numerical solution (red dots) of the discretized path $x$ ($N_t = 64$) that optimizes the functional eq. (27) corresponding to the discretized and regularized SIVP using $[2, 1]$ order summation-by-parts operator in time. Continuum solution of the Euler-Lagrange equation $\ddot{x}(t) = -g$ is shown as solid gray line. Note that the solution successfully avoids oscillatory contamination.

The last entry of the vector $\bar{D}x_{1,2}$ serves only to implement the shift in affine coordinates, hence it can be discarded via $\bar{H}$ since the regularized SBP operator has already acted on the path. Note that here we again add Lagrange multipliers as dynamical degrees of freedom, to fulfil the initial conditions. One may ask whether enforcing the initial conditions in this way neutralizes the effect of the regularization. We emphasize that this is not the case. Minimization algorithms approach the extremum of the functional globally, allowing the regulator to remain effective and to avoid the oscillatory solutions.

Another question of both conceptual and practical relevance is whether the functional eq. (27) houses one or multiple extrema. For the case of the point particle in a constant gravitational field, we find that the answer is that the functional is convex and thus a unique extremum is present, if it exists. This fact can be established via the curvature of eq. (27) with respect to the individual entries of the paths $x_{1,2}$.

I.e. the matrix $A_{ij} = \frac{\partial^2 S_{IVP}}{\partial x_i \partial x_j} = [\bar{D}^T \bar{H} \bar{D}]_{ij}$ is indeed positive semi-definite, as can be checked explicitly using a computer algebra system. However, in general convexity is not automatic and needs to be checked on a case-by-case basis [3].

For the point particle in a constant gravitational field, the solution $x_1$ obtained with eq. (27) and the regularized $[2, 1]$ SBP operator is shown in fig. 6 as red dots. The regularization has successfully removed the contamination by an unphysical oscillatory mode and we are able to reproduce the correct classical solution.

The combination of a penalty term based on the initial conditions, together with Lagrange multipliers enforcing the initial conditions and expressed in a variational formulation, has provided us with a novel discretization prescription for a wide

[3] None of the functionals treated in this study suffered from multiple extrema, allowing the Newton and Quasi-Newton methods implemented in Mathematica [30] to arrive at a single solution independent of starting point.
range of classical systems with differential equations of motion containing second order derivatives.

Let us take a look at the accuracy and convergence properties of the discretization scheme constructed in this section. The simple model of a point mass in a constant gravitational field again serves as explicit example. To this end we compute the optimal path $x_1$ according to the appropriately regularized eq. (27) using both the $[2, 1]$ and $[4, 2]$ order regularized SBP operator on different grids using $N_t \in [16, \ldots, 512]$ points. We compare the values of the path at the final step $t_2 = 1$ to the analytically known solution and compute the absolute error between them. These errors are shown in fig. 7.

The lowest order SBP approximation $[2, 1]$ (blue points) exhibits steady improvement in the residual deviation from the true solution, as the grid spacing is reduced. In fig. 8 we zoom in on the $[2, 1]$ errors and fit them with a power-law ansatz, which on the log-log plot appears as a straight line. The best fit exponent $\Delta t^{2.03}$ we obtain, tells us that our discretization scheme achieves second order accuracy in the solution values. Interestingly, when considering the $[4, 2]$ order SBP operator, we find that irrespective of the grid spacing we are able to reproduce the true solution down to machine precision (which in our case, using the Mathematica software package, was
Figure 8 Deviation of the value between the optimal numerical solution of eq. (27) and the true solution at the final time $t_2 = 1$ (blue points). The best power law fit to the behavior is shown as the gray solid line which corresponds to $\Delta t^{2.03}$.

set to $10^{-30}$). This result is reassuring, as by construction the SBP operator and the corresponding quadrature rule are able to differentiate and integrate polynomials up to second order exactly. Since the solution of the point mass in the constant gravitational field is a parabola, we do not find any residual dependence on the grid spacing.

While instructive, our first example described a very simple linear system. Let us use the formalism established in eq. (20) to apply our discretization prescription to a highly non-linear differential equation of motion instead. To realize

$$\ddot{x}(t) + 20x^3(t) = 0,$$

we must discretize the corresponding continuum functional

$$S_{IVP} = \int dt \left( \dot{x}_+(t)\dot{x}_-(t) - 20x_+^3(t)x_-(t) \right),$$

which is equivalent to the following optimization functional

$$S_{IVP} = \left\{ \frac{1}{2}(\bar{D}\bar{x}_1)^T\bar{H}(\bar{D}\bar{x}_1) \right\} - \left\{ \frac{1}{2}(\bar{D}\bar{x}_2)^T\bar{H}(\bar{D}\bar{x}_2) \right\}$$

$$- 20 \left( (x_1 + x_2)/2 \right)^3 \bar{H}(x_1 - x_2)$$

$$+ \lambda_1(x_1(0) - x_i) + \lambda_2((Dx_1)(0) - \dot{x}_i)$$

$$+ \lambda_3(x_1(N_t) - x_2(N_t)) + \lambda_4((Dx_1)(N_t) - (Dx_2)(N_t)).$$

The third power in the second line is understood as acting element-wise on the entries of $(x_1 + x_2)/2$. The continuum trajectory is given as the gray solid line in fig. 9 together with the [2, 1] order numerical solution using $N_t = 64$ grid points as red dots.

Let us consider how the new discretization prescription performs on this second order non-linear problem. The continuum solution is given in terms of the Jacobi
elliptic function and its inverse, i.e. it is not polynomial. Thus neither the [2, 1] nor the [4, 2] SBP operator are able to reproduce it exactly. The deviation of the numerical solution $x_1$ from the true solution is shown in the top panel of fig. 10 as blue points for the [2, 1] order SBP operator and as red points for the [4, 2] one. One finds that compared to the linear system, the error made in the non-linear system is around one order of magnitude larger at the same lattice spacing for the [2, 1] operator. However the order of convergence remains close to quadratic with a best fit $\Delta t^{2.12}$ shown by the gray lines in fig. 10. For the the [4, 2] operator we find that the error compared to the [2, 1] case is one order of magnitude lower at $N_t = 16$ and converges to the continuum limit with $\Delta t^{3.35}$.

In line with established results for the conventional numerical treatment of differential equations, we see in fig. 10 that the error in the derivative $\dot{x} = [Dx_1](N_t)$ of the numerical solution shows convergence with one full order less than the values of the solution itself. As plotted in the lower panel of fig. 10 we obtain for the regularized [2, 1] SBP operator convergence for the derivative according to $\Delta t^{1.06}$, while the [4, 2] operator exhibits $\Delta t^{1.87}$.

Having established the applicability and convergence properties of our novel discretization approach for both a linear and non-linear second order differential equation of motion, let us continue to treat systems with equations of motion that feature different orders of time derivatives.

4 Discretization of first order derivative terms
So far we have considered the simplest case of physical systems with classical equations of motion that contain a second derivative in time. These follow naturally from the conventional formulation of the continuum variational principle, based on an action that is written in terms of a Lagrangian. As has been shown in [25], the variational principle is able to accommodate a much larger variety of systems, in-
Figure 10 Deviation of the value (top plot) and the derivative (bottom plot) between the optimal numerical solution of eq. (30) and the true solution at the final time $t_f = 1$. The deviation for the [2, 1] order regularized SBP operator is given as blue points, the one for the [4, 2] operator as red points. Note that at both orders the solution improves steadily with diminishing $\Delta t \sim 1/N_t$. The best power law fit to the data is shown as gray lines. We find that our approach exhibits convergence in the values with one higher power in the grid spacing than for the derivative.

Figure 11 Deviation of the value (top plot) and the derivative (bottom plot) between the optimal numerical solution of eq. (30) and the true solution at the final time $t_f = 1$. The deviation for the [2, 1] order regularized SBP operator is given as blue points, the one for the [4, 2] operator as red points. Note that at both orders the solution improves steadily with diminishing $\Delta t \sim 1/N_t$. The best power law fit to the data is shown as gray lines. We find that our approach exhibits convergence in the values with one higher power in the grid spacing than for the derivative.

including those with dissipative forces, which are not time-reversal invariant\cite{4}. Such systems lead to equations of motion, which contain also first order derivatives in time. The crucial step is to realize that in analogy with the Feynman-Vernon influence functional formalism in quantum field theory, we may generalize the classical variational principle by adding to the Lagrangian $L$ another functional that may depend on both the forward and backward path and their derivatives as follows

$$S_{GIVP}[x_1(t), \dot{x}_1(t), x_2(t), \dot{x}_2(t)] = \int_{t_1}^{t_2} dt \left( L[x_1(t), \dot{x}_1(t)] - L[x_2(t), \dot{x}_2(t)] + \Lambda[x_1(t), \dot{x}_1(t), x_2(t), \dot{x}_2(t)] \right). \quad (31)$$

Ref.\cite{25}, aided by ref.\cite{26}, shows in detail that the classical equations of motion also for this generalized variational principle are obtained by going over to relative

\footnote{Note that the concept of time-reversal invariance only served as guide for our intuition in section 2, the formalism applies also to dissipative systems, as discussed in detail in ref.\cite{25}.}
Figure 11 Numerical solution (red dots) of the discretized path $x$ ($N_t = 64$) that optimizes the functional eq. (36) corresponding to the discretized and regularized $S_{GIVP}$ using $[2, 1]$ order summation-by-parts operators in time. Continuum solution of the Euler-Lagrange equation $\dot{x}(t) - \frac{1}{2}x(t) = 0$ is shown as solid gray line.

$x_\pm = x_1 - x_2$ and centered coordinates $x_\pm = (x_1 + x_2)/2$ with the defining equation

$$\frac{\delta S_{GIVP}[x_\pm]}{\delta x_-} \bigg|_{x_-=0, x_+=x_{class}} = 0. \quad (32)$$

This immediately invites us to apply the discretization prescription developed in the previous section to two systems often considered in the literature, the differential equation of motion for an exponential function and the damped harmonic oscillator. By considering these two examples, we will acquire intuition in how to construct the appropriate continuum functional $\Lambda$ of eq. (31), in order to describe a differential equation of motion also containing first order derivatives.

4.1 The exponential function

Our goal here is to reproduce the defining equation of the exponential function

$$\dot{x}(t) - \xi x(t) = 0. \quad (33)$$

Since there are no second order derivatives present in eq. (33) we do not need to supply the standard kinetic term to $L$ in (31). The term linear in $x(t)$ can be thought of as arising from a potential contribution in $L$, which must contain one power of $x_+$ and one power of $x_-$ similar to our argument in eq. (20). The new ingredient is the term that features a single time derivative. It has to emerge from $S_{GIVP}$ after functional differentiation with respect to $x_-$. This behavior is achieved by choosing the following Lagrangian and $\Lambda$ functional

$$\mathcal{L} = -\frac{1}{2}\xi x^2(t), \quad \Lambda = \dot{x}_+ x_-, \quad (34)$$

which amounts to the joint Lagrangian

$$L = -\xi x_+(t)x_-(t) + \dot{x}_+ x_- \quad (35)$$
Best fit $\Delta t = 2.03$

Best fit $\Delta t = 2.95$

$SBP[2,1]$

$SBP[4,2]$

0.005 0.010 0.020 0.050 $1/N_t$

10^{-6} 10^{-5} 10^{-4}

0.001 0.010 0.100

$|x-x_{\text{true}}| (1)$

Best fit $\Delta t = 1.06$

Best fit $\Delta t = 1.99$

$SBP[2,1]$

$SBP[4,2]$

0.005 0.010 0.020 0.050 $1/N_t$

0.001 0.010 0.100

$|x-x_{\text{true}}| (1)$

Figure 12 Deviation of the value (top plot) and the derivative (bottom plot) between the optimal numerical solution of eq. (36) and the true solution at the final time $t_2 = 1$. The deviation for the [2, 1] order regularized SBP operator is given as blue points, the one for the [4, 2] operator as red points. Note that at both orders the solution improves steadily with diminishing $\Delta t \sim 1/N_t$. The best power law fit to the data is shown as gray lines. We find that our approach exhibits convergence in the values with one higher power in the grid spacing than for the derivative.

Note that if one rewrites eq. (34) explicitly in terms of $x_1$ and $x_2$, the contribution from $\Lambda$ indeed does not factorize into terms that depend $x_1$ or $x_2$ separately.

Using the strategy developed in the previous section, let us write down the discretized action functional, keeping in mind that for a first order equation only the initial position needs to be supplied at the beginning of $x_1$. Correspondingly only the position information needs to be matched at the end of the paths

$$S_{\text{GIVP}} = \left\{ -\frac{1}{2} (x_1)^T H x_1 \right\} - \left\{ -\frac{1}{2} (x_2)^T H x_2 \right\}$$

$$+ \xi \frac{1}{2} \left( D (\bar{x}_1 + \bar{x}_2) \right)^T \bar{H} (x_1 - x_2)$$

$$+ \lambda_1 (x_1(0) - x_i) + \lambda_3 (x_1(N_t) - x_2(N_t)).$$

The solution to this equation on the interval $t \in [0, 1]$ discretized with $N_t = 64$ equidistant steps $\Delta t$ and a $\xi = \frac{3}{2}$ with initial condition $x_1 = 1$ produces the data shown in fig. 11.

In fig. 12 we plot the difference between the optimal numerical solution of eq. (36) and the true solution at the final time $t_2 = 1$ focusing on the value itself in the top plot and the derivative in the bottom plot. The results for the [2, 1] order regularized SBP operator are given as blue points, those for the [4, 2] operator as red points. Since the solution is not a simple polynomial, the [4, 2] order SBP operator cannot
exactly integrate it. Both the $[2, 1]$ and $[4, 2]$ case show the same convergence rates, as observed in the conventional formulation of IVPs (c.f. ref. [21]). We find again that the convergence is one order higher in the values of the solution than in the derivative of the solution. The $[2, 1]$ SBP operator yields a $\Delta t^{2.03}$ improvement for the values of $x_1(t)$, while the $[4, 2]$ operator exhibits $\Delta t^{2.95}$.

4.2 The damped harmonic oscillator

As final challenge let us now turn to one iconic physics system, which combines both first and second order derivatives in its equation of motion: the damped harmonic oscillator. The damped harmonic oscillator is characterized by an Euler-Lagrange equation that reads

$$\mu \ddot{x}(t) + \xi \dot{x}(t) + \kappa x(t) = 0.$$  \hspace{1cm} (37)

Even though this system underlies a wealth of experimentally relevant phenomena, the conventional formulation of classical mechanics is unable to accommodate it in terms of a classical Lagrangian. In the generalized approach of ref. [25] the kinetic and conservative force term are captured by the Lagrangian and the dissipative term is included via the $\Lambda$ functional. Remembering that only terms linear in $x_-$ survive the stationarity condition and using the intuition we built in the preceding sections, we can now write down the corresponding expressions for the functionals of the damped harmonic oscillator

$$\mathcal{L} = \frac{1}{2} \mu \dot{x}^2(t) - \kappa x^2(t), \quad \Lambda = -\xi \dot{x}_+ x_-,$$  \hspace{1cm} (38)

which correspond to the joint Lagrangian

$$L = \mu \dot{x}_+ (t) \dot{x}_- - 2 \kappa x_+(t) x_-(t) - \xi \dot{x}_+ x_-.$$  \hspace{1cm} (39)
Inserting the above into eq. (32) immediately yields eq. (37). The discretized joint action functional based on eq. (39) reads

\[
S_{GIVP} = \left\{ \frac{1}{2} \mu ( \overline{D} \overline{x}_1 )^T \overline{H} ( \overline{D} \overline{x}_1 ) - \frac{1}{2} \kappa ( \overline{x}_1 )^T \overline{H} \overline{x}_1 \right\} - \left\{ \frac{1}{2} \mu ( \overline{D} \overline{x}_2 )^T \overline{H} ( \overline{D} \overline{x}_2 ) - \frac{1}{2} \kappa ( \overline{x}_2 )^T \overline{H} \overline{x}_2 \right\} \\
- \frac{\xi}{2} ( \overline{D} ( \overline{x}_1 + \overline{x}_2 ) )^T \overline{H} ( \overline{x}_1 - \overline{x}_2 ) \\
+ \lambda_1 ( x_1(0) - x_i ) + \lambda_2 ( (Dx_1)(0) - \dot{x}_i ) \\
+ \lambda_3 ( x_1(N_t) - x_2(N_t) ) + \lambda_4 ((Dx_1)(N_t) - (Dx_2)(N_t)) \right). \tag{40}
\]

Searching for the extremum of this functional numerically using the parameters \( \mu = 0.5, \kappa = 1, \xi = 0.00071 \) with initial conditions \( x_i = 1, \dot{x}_i = 0 \) on discretized paths with \( N_t = 64 \) steps and \([2, 1]\) regularized SBP operators leads to the results shown as red points in fig. 13.

In the top panel of fig. 14 we present the deviation between the numerically determined extremum of eq. (36) and the true solution at the final time \( t_2 = 1 \). The deviation of the derivative is given in the bottom plot. Blue points denote the \([2, 1]\) order case while red points refer to the \([4, 2]\) operator. The power law fits show that also for the damped harmonic oscillator the convergence order agrees with the expectations from the conventional formulation of IVPs [21] and is one order higher in the values of the solution than in the derivative of the solution. The \([2, 1]\)
Figure 15 (Top panel) Numerical solution (red dots) of the discretized path $x_1$ ($N_t = 2048$, $\Delta t = 0.1$) that optimizes the functional eq. (40) corresponding to the discretized and regularized $S_{GIVP}$ using summation-by-parts in time. Continuum solution of the Euler-Lagrange equation $\mu \ddot{x}(t) + \xi \dot{x}(t) + \kappa x(t) = 0$ is shown as solid gray line. (Bottom panel) Comparison of the optimal solutions at a different number of grids points $N_t = 512$ (red), $N_t = 1024$ (blue) and $N_t = 2048$ (green) at late times.

SBP operator yields a $\Delta t^{2.03}$ improvement for the values of $x_1(1)$, while the [4,2] operator exhibits $\Delta t^{3.04}$.

So far we have only investigated the short time behavior. However it is late-time stability that plays the most important role for the utility of a discretization scheme to the description of physical processes in practice. For initial boundary value problems this calls for so-called error-bounded schemes [31–33]. In the literature the damped harmonic oscillator is often used as a non-trivial test-bed to evaluate the late-time stability and accuracy of numerical solvers. Let us therefore determine the numerical solution to eq. (40) up to $t_2 = 204.8$, which is shown in the upper panel of fig. 15, based on the [4,2] regularized SBP operator at $\Delta t = 0.1$. This choice of $t_2$ allows the system to pass through multiple oscillations and to show a visible reduction of the oscillation amplitude. As our SBP in time discretization is inherently implicit, we find numerically that while the solution degrades in accuracy as we increase the grid spacing $\Delta t \in \{0.1, 0.133, 0.2, 0.4\}$ it remains bounded for all times. The behavior of the discrete solution for different grid spacings $\Delta t$ at late times, is shown in the lower panel of fig. 15. One finds that the solution converges as the grid spacing is decreased. The most pertinent error introduced by the discretization procedure appears to be an artificial phase shift, the dispersion error, which however vanishes as the continuum limit $\Delta t \to 0$ is approached.
A common quality criterion for numerical solvers in the physical sciences is the reproduction of the system energy. We consider here as energy the following Hamiltonian $\mathcal{H} = T + V = \frac{1}{2} \mu \dot{x}^2(t) + \kappa x^2(t)$, which is plotted for different grid spacings in fig. 16. One can clearly see that the discretization procedure leads to an overall shift in the value of the energy. However, that shift vanishes with grid refinement and no artificial energy deviation or late-time instability is present.

5 Summary
We have presented a new unified discretization strategy for a wide range of initial value problems, formulated in terms of a generalized variational problem. Our approach is based on summation-by-parts finite difference operators, which are regularized through a penalty term, associated with the initial conditions using affine coordinates. We derived a weak formulation of the variational IVP in section 3.3 using Lagrange multipliers and subsequently applied the prescription to systems with purely second order, first order and mixed time derivatives in their equations of motion. Explicit scaling tests for each of these systems confirmed that our prescription converges to the true solution under grid refinement, with the same convergence rates, as expected from the conventional formulation of IVPs. Convergence in the values of the solution occurs with one higher order in the grid spacing $\Delta t$ compared to the derivative of the solution. Our approach is based on a single realization of the first order SBP finite difference operator and does not require a separate treatment of systems with equations of motion containing first or second order derivatives in time.

Our study describes a genuinely novel and versatile approach to the discretization of IVPs. Its extension to higher dimensions for the treatment of partial differential equations is the natural next step and is work in progress. We are looking forward to applying the formalism presented here to the discretization of theories with intrinsic constraints, in particular gauge theories, such as classical electromagnetism and Yang-Mills theory.
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Competing interests
The authors declare that they have no competing interests.

Author’s contributions
• A. Rothkopf: project inception, development of the discretization and regularization prescription, scaling tests, writing and editing
• J. Nordström: guidance on the SBP-SAT formalism, development of the discretization formalism, literature review, writing and editing

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