

Optimization Methods for One Dimensional Elastodynamics

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1 Introduction

We propose a new approach for solving systems of conservation laws that admit a variational formulation of the time-discretized form, and encompasses the p -system or the system of elastodynamics. The approach consists of using constrained gradient descent for solving an implicit scheme with variational formulation, while discontinuous Galerkin finite element methods is used for the spatial discretization. The resulting optimization scheme performs well, it has an advantage on how it handles oscillations near shocks, and a disadvantage in computational cost, which can be partly alleviated by using techniques on step selection from optimization methods.

The system of elastodynamics is a nonlinear system of hyperbolic conservation laws which describes the propagation of longitudinal (or of shear) waves in an elastic medium. The same system describes one-dimensional motions of a gas, and is widely used as a paradigm in the theory of conservation laws, then called as the p -system. It takes the form

$$\begin{aligned}u_t - v_x &= 0, \\v_t - \sigma(u)_x &= 0,\end{aligned}\tag{1}$$

where $(x, t) \in \mathbb{R} \times \mathbb{R}_+$, and in the elasticity context u is the strain, $v \in \mathbb{R}$ is the velocity, and $\sigma(u)$ is a strictly increasing function describing the stress. For longitudinal motions $u > 0$ ($u > 1$ corresponds to extension and $u < 1$ to compression), while for shear motions $u \in \mathbb{R}$. The system (1) is supplemented with initial data $u(x, 0) = u_0(x)$, $v(x, 0) = v_0(x)$.

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Smooth solutions of (1) generally develop discontinuities in finite time, reflecting the development of shock waves, and classical solutions cease to exist. Introducing the concept of weak solutions, global solutions are constructed using viscosity approximations [8, 13], relaxation approximations [12] and numerical schemes (see [9] and references therein). For the theory of shock waves we refer to [5].

Our objective is to introduce a new approach for the numerical approximation of (1) inspired by optimization methods. This approach is not expected to work for general systems of conservation laws, but applies to special systems that can be viewed as time-discretizations of Hamiltonian dynamics and includes in particular (1). It is motivated by an variational approximation developed in [7] that produces entropy weak solutions. A (nontrivial) variant of this variational scheme is available for the system of multi-dimensional elastodynamics with polyconvex energy, see [6] and [11], and our hope is to eventually extend the present methodology in this interesting context.

The numerical experiments performed here indicate that, when shocks are present in the solution and in the absence of any special techniques that handle oscillations, our method achieves better results compared to some classical DG methods, see Section 4. A disadvantage however is that the present method is computationally demanding; to mitigate this issue, we propose some novel computational techniques and mechanisms that significantly improve the convergence speed. We are working in implementing the scheme in multiple dimensions, where we expect further benefits.

2 The approximation framework

We work in a bounded domain, $(x, t) \in [0, 1] \times [0, T]$ with periodic boundary conditions. Let k be a time step, $\{t^j\}_{j=0}^M$ be a partition of $[0, T]$ with time step k , and we are interested in constructing an approximate solution of (1) as follows. We start with the initial data (u^0, v^0) periodic. At each time step $t^j = jk$ given (u^{j-1}, v^{j-1}) we solve the implicit problem

$$\frac{u^j - u^{j-1}}{k} = v_x^j, \quad \frac{v^j - v^{j-1}}{k} = \sigma(u^j)_x. \quad (2)$$

The solutions $(u^j(x), v^j(x))$ of problem (2) are obtained by variational minimization.

In [7] two such schemes have been developed; the first formulates the solution of the equivalent second order equation as an unconstrained minimization problem while the second, described below, as a constrained one. In particular, if $W(u)$ is the strain energy function (that is $W' = \sigma$), given (u^{j-1}, v^{j-1}) , (u^j, v^j) is the unique minimizer of the problem

$$\min J[u, v] = \min \int W(u) + \frac{(v - v^{j-1})^2}{2} dx, \quad (3a)$$

where minimization is done over the set of functions satisfying the affine constraint

$$\int \frac{u - u^{j-1}}{k} \phi + v \phi_x dx = 0, \quad \forall \phi \in C^1. \quad (3b)$$

The minimizing scheme produces iterates $(u^j(x), v^j(x))$, with $j = 1, \dots, Mk$, $Mk = T$. We then define approximate solutions $(u^k(x, t), v^k(x, t))$, $\forall t \in [0, T]$, to (1); this is done using the aforementioned iterates $(u^j(x), v^j(x))$ of (2) and interpolating in time via piecewise constant or piecewise linear interpolation. It is shown in [7] using the theory of compensated compactness that (u^k, v^k) converge to (u, v) almost everywhere (both piecewise constant and piecewise linear interpolations yield the same limit) and that (u, v) satisfies (1) and the following form of entropy inequalities: For any entropy pair (η, q) such that $\nabla\eta\nabla f = \nabla q$ with $f(u, v) = (-v, -\sigma(u))^T$ the solution $(u(x, t), v(x, t))$ satisfies

$$\partial_t \eta(u, v) + \partial_x q(u, v) \leq 0, \quad (4)$$

in distributions for any entropy $\eta(u, v)$ convex. Observe that (4) is the same admissibility condition that artificial viscosity would produce for the system (1).

3 Numerical method

3.1 Constrained Gradient Descent

Consider the constrained minimization problem

$$\min_{x \in \mathcal{A}} F(x) \quad (5a)$$

where X is a Banach space, $F : X \rightarrow \mathbb{R}$ is a convex functional, and the minimization is done over an affine subspace \mathcal{A}

$$\mathcal{A} = \{x \in X : A[x] = c\} \quad (5b)$$

defined by linear functionals $A = (A_1, \dots, A_n) : X \rightarrow \mathbb{R}^n$ with $c \in \mathbb{R}^n$. This problem consists of minimizing a convex function F over an affine subspace. Under fairly general conditions: X is reflexive, F is convex, coercive and weakly lower semicontinuous on X , while the linear functionals A_i determine a weakly closed subspace of X , this minimization problem has a solution [3, Cor. 3.23]. Moreover, when F is strictly convex the solution is unique. The associated Euler-Lagrange equations define the minimizer x implicitly.

We propose to compute the minimizer via gradient descent taking also into account the affine constraint (5b). (The method is expected to work when the constraint is affine, and it would lead in general to nonconvex problems when the constraint is nonlinear.) Given an iteration step λ and $x_l \in \mathcal{A}$, the gradient descent method computes the next iterate x_{l+1} by

$$x_{l+1} - x_l = \lambda \frac{\delta F}{\delta x}(x_l), \quad x_{l+1} \in \mathcal{A}. \quad (6)$$

The variational derivative $\frac{\delta F}{\delta x}$ for the constrained problem (5a) is computed by

$$\left\langle \frac{\delta F}{\delta x}(x), \varphi \right\rangle := \lim_{\varepsilon \rightarrow 0, \substack{x \in \mathcal{A} \\ x + \varepsilon \varphi \in \mathcal{A}}} \frac{F(x + \varepsilon \varphi) - F(x)}{\varepsilon}. \quad (7)$$

where φ is a test function. Equation (7) precisely defines the variational derivative of the constrained minimization problem (5a)-(5b). In applications it will be expressed by introducing a basis function on the constraint subspace \mathcal{A} .

3.2 Adaptation to the specific minimization problem

Given (u^{j-1}, v^{j-1}) , the j -th iterate (u^j, v^j) is constructed as the solution of the constrained minimization problem (3a) subject to the affine constraint (3b).

To implement gradient descend (GD) we first have to calculate the variational derivative of (3a). If we let $\varepsilon P := (\varepsilon p, \varepsilon q)^\top$ be the variation of $U := (u, v)^\top$ in the direction of $(p, q)^\top$, and $j(\varepsilon) := J(U + \varepsilon P)$, the derivative is

$$\left\langle \frac{\delta J}{\delta U}, (p, q) \right\rangle = \int (v - v^{j-1}) q + W'(u) p \, dx = \int (v - v^{j-1}) q + W'(u) k q_x \, dx, \quad (8)$$

where we've substituted $p = k q_x$ that comes from the constraint (3b).

Given some approximation u_l, v_l to u, v , the gradient descent method (GD) will decrease the value of (3a) by finding $v_{l+1} \in H_{\text{per}}^1(0, 1)$ such that

$$(v_{l+1}, \phi) = (v_l, \phi) - \lambda((v_l - v^{j-1}, \phi) + k(W'(u_l), \phi_x)), \quad \forall \phi \in H_{\text{per}}^1(0, 1), \quad (9a)$$

where λ is the GD iteration step. Let $A : H_{\text{per}}^1 \times H_{\text{per}}^1 \rightarrow \mathbb{R}$ stand for the bilinear form $A(v, \phi) = (v, \phi)$, and let $G_1(\phi) = G_1(\phi; \lambda, u_l, v_l, v^{j-1})$ denote the right hand side of (9a), which is then expressed as $A(v_{l+1}, \phi) = G_1(\phi)$.

The constraint (3b) is enforced by defining $u_{l+1} \in H_{\text{per}}^1(0, 1)$ via

$$(u_{l+1}, \phi) = (u^{j-1}, \phi) + k(v_{x,l+1}, \phi), \quad \forall \phi \in H_{\text{per}}^1(0, 1). \quad (9b)$$

Similarly (9b) can be expressed via $A(u_{l+1}, \phi) = G_2(\phi; v_{l+1}, u^{j-1})$.

Notice that, in view of (6), GD only updates the velocity v_{l+1} in (9a) at each iteration, while u_{l+1} is updated by (9b) so that the solution (u_{l+1}, v_{l+1}) remains in the subspace \mathcal{A} .

3.3 Discontinuous solutions

The aforementioned scheme (9) maintains optimal order of convergence for smooth solutions, however is not suitable for solutions containing shocks since spurious oscillations are formed near discontinuities. We, therefore, will work in the framework of Discontinuous Galerkin methods (DG). The original system is a conservation law; conservation laws, in the setting of DG, have been studied by Cockburn and Shu in the series of papers [4], from which we will borrow various tools.

We seek a solution in the space of piecewise polynomial functions of order K with periodic b.c., $V_h = \{\phi \in L^1(0, 1) : \phi|_{I_i} \in \mathbb{P}^K(I_i), i = 1, \dots, N, \phi(0) = \phi(1)\}$, where I_i denotes the i -th cell, and use the usual Legendre pol. as basis functions.

Having defined the general GD step in (9) we now proceed in finding v^j, u^j , the solution at the next time step, in the setting of the now discontinuous finite element space V_h . Let $\{u_l^j\}_{l=0}^{L_j}, \{v_l^j\}_{l=0}^{L_j}$ represent the sequence generated by GD to approximate u^j, v^j . A sensible initial guess, to kickstart the method, is the solution

in the previous time step, $v_0^j = v^{j-1}$, $u_0^j = u^{j-1}$. Having calculated the first l iterates, v_{l+1}^j is the unique function in V_h that satisfies

$$A(v_{l+1}^j, \phi) + \int_{\Gamma} \frac{\mu}{h} \llbracket v_{l+1} \rrbracket \cdot \llbracket \phi \rrbracket ds = G_1(\phi; u_l^j, v_l^j, v^{j-1}), \quad \forall \phi \in V_h, \quad (10a)$$

where Γ is the elements boundary, h the minimum cell length, and $\mu > 0$ the penalty. A term that penalizes jumps across cell interfaces is required; this is motivated by the theory of DG methods for elliptic equations, see [1], where it plays the role of stabilization term; for given μ large enough, it ensures that the corresponding bilinear form is coercive. We enforce the constraint by updating u_{l+1}^j as

$$A(u_{l+1}^j, \phi) = G_2(\phi; v_{l+1}^j, u^{j-1}), \quad \forall \phi \in V_h, \quad (10b)$$

where an integration by part has to take place in G_2 resulting in a *numerical flux*. The above procedure is repeated until the solution converges and the integral to be minimized stops decreasing

$$I_l = I[v_l, u_l] := \int_0^1 \left(\frac{(v_l^j - v^{j-1})^2}{2} + W(u_l) \right) dx. \quad (11)$$

3.4 Implementation details

To handle the term that arises by the integration by parts in (10b) we will employ the Local Lax Friedrich (LLF) numerical flux. This flux is simple to implement and computationally efficient, but introduces a significant amount of numerical diffusion. Note that the choice of the numerical flux does not have a significant impact as the polynomial degree increases. We refer to [14] for a study about numerical fluxes.

A technique to combat spurious oscillations near discontinuities is limiting the slope of the solution based on its value in adjacent cells. To this end we have used *minmod* limiter, [4], for up to quadratic polynomials and *moments* limiter, [2], for higher order ones.

The number of iterations of GD play a significant role in the computational complexity of the method. We control the convergence of the algorithm using three quantities: the difference between (a) two successive evaluations of the integral-to-be-minimized (11), $|I_{l+1} - I_l| < c_I$, with default tolerance $c_I = 10^{-14}$; (b) two successive approximations of u , $\|u_{l+1} - u_l\| < c_u$, with default tolerance $c_u = 10^{-14}$; and (c) the number of actual iterations performed, c_i , with default value $c_i = 250$. The method is said to have converged when both conditions (a) and (b) are satisfied.

4 Numerical results

4.1 Effective order of convergence

In numerical simulations we will use $\sigma(u) = u^3 + u$ and penalty constant $\mu = 1$, also in this and the next subsection we use a fixed $\lambda = 1/4$ and the GD stop criteria described in the previous section. To verify the convergence rate of the method we consider the following smooth initial conditions

$$u(x, 0) = u_0(x) = 2 - \exp(-0.5(x - 4)^4), \quad v(x, 0) = v_0(x) = u_0'(x), \quad (12)$$

for $x \in [0, 8]$ and $T = 1/40$ (so that the solution remains smooth for the duration of the simulation). We consider piecewise linear polynomials and a uniform partition in space. To attain the optimum rate of convergence, we employ a multistep method for time discretization (BDF2); we set the time step to be $k = c_{\text{cfl}}h$, where $c_{\text{cfl}} = c_{\text{RK}}/\max_{x,t} \sqrt{\sigma'(u)}$ and $c_{\text{RK}} = 1/8$ is a constant that depends on the degree of polynomials used. Convergence rates are as expected, and can be seen in Table 1.

N	$\ u - u_{\text{ex}}\ $	rate	$\ u - u_{\text{ex}}\ _{\infty}$	rate	$\ v - v_{\text{ex}}\ $	rate	$\ v - v_{\text{ex}}\ _{\infty}$	rate
20	2.979e-02	-	3.844e-02	-	1.086e-01	-	1.193e-01	-
40	9.961e-03	1.58	1.605e-02	1.26	2.419e-02	2.17	3.278e-02	1.86
80	2.580e-03	1.95	4.258e-03	1.91	5.471e-03	2.14	7.806e-03	2.07
160	6.303e-04	2.03	1.041e-03	2.03	1.339e-03	2.03	1.920e-03	2.02
320	1.555e-04	2.02	2.591e-04	2.01	3.436e-04	1.96	5.045e-04	1.93

Table 1: DG-IP, LLF flux, convergence rates. $T = 0.025$. Smooth solution. Linear polynomials.

4.2 Evolution of discontinuous initial profile

In case of discontinuous solution, and in the absence of any special treatment, i.e. slope limiting, some spurious oscillations are generated near discontinuities. An analogous phenomenon is also observed in the standard discretization of the system as a conservation law using DG methods. Oscillations grow larger as the rate k/h gets smaller.

Consider the following discontinuous initial conditions

$$u_0(x) = 2 - \mathbf{1}_{[2,6]}, \quad v_0(x) = 2. \quad (13)$$

The solution for piecewise linear polynomials and $k/h = 1/8$ at time $T = 1/4$ can be seen in Figure 1a, where the presence of oscillations is evident. The amplitude of oscillations decreases as the degree of polynomials increases. For example, in Figure 1b we consider cubic polynomials and $k/h = 1/28$.

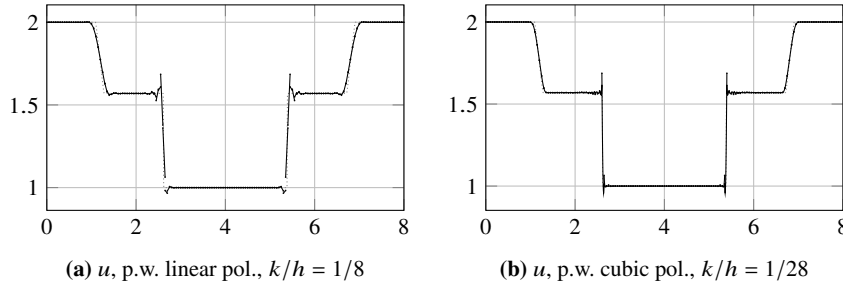


Fig. 1: DG-IP, $N = 160$, $T = 0.25$, no slope limiter. Discontinuous solution.

It is worth mentioning that, compared to the standard discretization of the system as a conservation law using DG and Euler method in time, the optimization method has significantly less oscillations near discontinuities. This does not hold though when a TVD Runge-Kutta (for example Osher's 3rd order RK) time discretization is

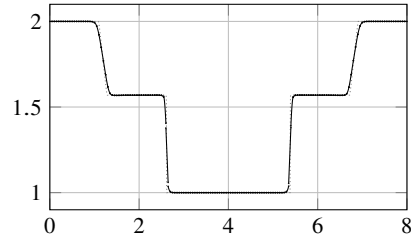
used. This can be seen in Table 2, where the exact value of total variation for u is 2 and for v is 5.6. Oscillations can be eliminated if a slope limiter is applied.

Table 2 DG-IP, LLF flux, comparison of total variation. $T = 0.25$, $k/h = 1/12$, $\lambda = 0.25$, $\mu = 1$. Discontinuous solution. Linear polynomials.

N	optimization		DG Euler		RKDG Osher	
	TV u	TV v	TV u	TV v	TV u	TV v
40	2.269	6.601	2.627	7.301	2.369	6.509
80	2.338	6.601	2.918	8.135	2.446	6.669
160	2.339	6.559	3.443	9.657	2.529	6.845
320	2.294	6.416	3.858	11.00	2.522	6.883

To address the formation of oscillations we employ a slope limiting technique, the resulting solution for piecewise cubic polynomials can be seen in Figure 3.

Fig. 3 u , DG-IP, $N = 160$, $T = 0.25$, $k/h = 1/28$, p.w. cubic pol., moments limiter.

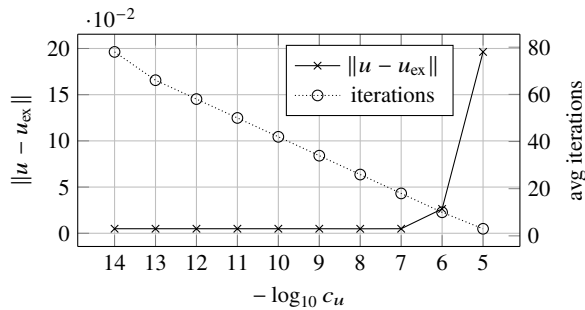


4.3 Optimization iteration convergence criteria

Suitable stop criteria for GD are necessary to avoid excessive iterations that will slow down the code and possibly introduce roundoff errors.

Consider for example the smooth initial conditions (12); errors and average GD iterations count per time step, in relation to convergence tolerances, can be seen in Figure 4. We see that 78 iterations are required for the strictest tolerances, while only 14 iterations are needed when we set $c_I = c_u = 10^{-6}$ with insignificant increase in approximation error. Similar results hold for the discontinuous solution (13).

Fig. 4 GD iterations count and errors w.r.t. c_u . $T = 0.25$, $N = 160$, $k/h = 1/12$, $\lambda = 0.25$, $\mu = 1$. Smooth solution.



4.4 GD step selection

GD step plays an important role in convergence speed of the method and can lead to significant acceleration if selected adaptively within each time step. Many methods exist in optimization literature for this purpose, such as e.g. adagrad, adam, etc., see [10]) and may be adapted for our setting. Here, for illustrative purposes, we have

implemented a simple heuristic algorithm that modifies λ according to the decrease rate of I_ℓ , starting with λ small and gradually increasing its value.

As a typical example to highlight the performance benefits, we consider the smooth solution example, (12), with parameters $c_I = 1e-14$, $c_u = 1e-14$, $T = 0.25$, $N = 80$, $k/h = 1/12$. This algorithm reduces the average number of iterations from 73 to 26.

Another significant measure for the performance of the algorithm is the approximation error given a fixed amount of computational resources. Using the aforementioned parameters we investigate the approximation error for various N given that the maximum amount of iterations is limited, i.e. $c_i = 10$. Errors, as well as the difference between the last two iterations of GD (that is 9th and 10th) of the integral under minimization and the value of u can be seen in Table 3.

Finally we notice that the order of convergence is still maintained.

Table 3 DG-IP, LLF flux, fixed versus adaptive λ . $T = 0.25$, $c_i = 10$. Smooth solution. Linear polynomials.

N	$\ u - u_{\text{ex}}\ $	$\ v - v_{\text{ex}}\ $	$ I_\ell - I_{\ell-1} $	$\ u_\ell - u_{\ell-1}\ $
80 (λ fixed)	1.832e-2	1.072e-1	6.1e-07	5.5e-07
80 (λ adapt)	1.033e-2	2.664e-2	4.4e-10	1.8e-08
320 (λ fixed)	1.864e-2	9.989e-2	4.0e-08	4.0e-08
320 (λ adapt)	2.355e-3	6.842e-3	1.5e-09	1.6e-08

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