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Space-Time Primal-Dual Active Set Method: Benchmark for Collision of Elastic Bar with Discontinuous Velocity

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Abstract

The dynamic contact problem describing collision of an elastic bar with a rigid obstacle, prescribed by an initial velocity, is considered in a variational formulation. The non-smooth, piecewise-linear solution is constructed analytically using partition of a 2D rectangular domain along characteristics. Challenged by the discontinuous velocity after collision, full discretization of the problem is applied that is based on a space-time finite element method. For an iterative solution of the discrete variational inequality, a primal—dual active set algorithm is used. Computer simulation of the collision problem is presented on uniform triangle grids. The active sets defined in the 2D space-time domain converge in a few iterations after re-initialization. The benchmark solution at grid points is indistinguishable from the analytical solution. The discrete energy has no dissipation, it is free of spurious oscillations, and it converges super-linearly under mesh refinement.

Keywords: impact contact dynamics; variational inequality; discontinuous velocity; space-time finite element; primal-dual active set

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1. Introduction

In this paper, the research aims at solutions of dynamic contact problems, which model the time-dependent deformation of a solid body colliding a rigid obstacle. The moving body and the stationary obstacle have different velocities, therefore, an impact occurs. By using elementary physics concepts, some elastic properties of falling bars and springs that were suddenly released after being hung from one end were discussed in [1]. In experiments of body motion, a spring allowed larger deformations and slower wave propagation than an elastic bar. Highlighting broader relevance in variational mechanics, this work cites studies on nonlinear vibrations and micro-electro-mechanical systems (MEMSs) involving micro-beams and sensors [2]. The periodic motion of an MEMS is highly sensitive to operating conditions and may become unstable when reaching specific threshold values [3]. This makes it crucial to find an exact solution of the problem and to gain insight the property of dynamic stability, which is highly important for numerical solution.

Since responses by the impact demonstrate an oscillatory nature, proper solution methods of contact dynamics problems should follow its wave propagation characteristics. The mathematical analysis of solutions to variational and hemivariational inequalities describing contact problems can be found in [4,5]. The solvability to wave equations stated in half-space

under unilateral constraints imposed at the boundary was proved in [6]. This work refers to monographs [7,8] for the basic computational concepts used in the field, to [9,10] for finite element methods (FEM), and to [11,12] for boundary element methods (BEM). For some dynamic issues in physical modeling this work cites [13–19] for bio-mechanical models.

To illustrate properties of colliding bodies, this study performs theoretical analysis and numerical simulation of the dynamic contact problem in a two-dimensional (2D) setting. In our context, one dimension is time, and the second dimension is space. For benchmark, this work considers a 1D elastic bar of the prescribed initial position and initial velocity, for which an exact solution is derived. The bar undergoes a rigid body motion until its end collides with the rigid obstacle. Is stays in contact during elastic waves travel through the body and then moves back as the waves reach the bar end. This benchmark of collision is relevant to the considerations from [20,21], where an undeformed bar was dropped against a rigid ground surface with a given initial velocity. In the other relevant benchmark from [22–24], a rigid obstacle was impacted by an initially deformed elastic bar with zero initial velocity.

From the mathematical point of view, the impact of bodies is characterized by a discontinuous velocity; see [25]. For time integration, there are the well-established semi-discrete methods of Newmark [26] and Hilber–Hughes–Taylor [27]. For extension of the HHT method to dynamic contact problems within a semi-smooth Newton approach, the reader is referred to [28–30]. However, when determining the acceleration from an expansion in Taylor series, these numerical integration schemes assume continuity of velocity. The variational theory of discontinuous solutions to problems stated in non-smooth domains was elaborated in [31,32] and relevant works [33–36]. The reader is referred to proper numerical methods in [37–39] and to asymptotic methods using boundary layers in [40–42].

For efficient iterative solution of complementarity problems, there are well-known semi-smooth Newton (SSN) methods, which have a locally super-linear convergence rate. Moreover, the realization of SSN methods as a primal–dual active set (PDAS) iteration converges globally in a monotone way for stiffness matrices obeying the M-matrix property; see [43]. The a priori and a posteriori numerical analysis of PDAS algorithms for static unilaterally constrained problems in mechanics was given in [44,45]. In the theory of dynamic multi-body and discrete contact problems, for the realization of the PDAS strategy and corresponding numerical simulations, this work refers to [46,47].

To take the velocity discontinuity into account, in [48,49], we first realized a space-time PDAS approach, which is based on a full discretization of dynamic variational inequalities within space-time finite elements, referred to here as ST-PDAS for short. The reader can find studies of the space-time approximation for second-order hyperbolic equations in [50,51]. Unconditionally stable conforming finite element discretization with piecewise polynomial functions in space and time was studied in the literature performing continuous solutions for heat and wave equations. In constrast, this study's contribution to the field pays attention to solutions with discontinuous derivatives offering analytical–numerical synergy of impact phenomena. In this research's previous works, the dynamic contact condition was stated at a 1D boundary. In contrast, in the current contribution, this study presents contact sets over the whole 2D space-time domain. The novelty consists in developing the ST-PDAS algorithm for contact conditions imposed in two dimensions. This study constructs an analytical benchmark of non-smooth solutions of the wave equation, which is given by piecewise linear functions along characteristics on a suitable partition of rectangular domains.

In Section 2, the collision problem is formulated as a variational inequality for the wave equation given in a rectangle and subject to a one-sided inequality constraint. The analytical solution having discontinuous time and spatial derivatives is proven in Section 3. For its numerical realization, in Section 4, the problem within ST-FEM is approximated by

Computation 2025, 13, 210 3 of 15

piecewise linear polynomial functions on uniform triangular grids, and it is solved with the help of PDAS. In Section 5, numerical experiments of the benchmark are presented, and properties of the full approximation are discussed. Namely, the ST-PDAS algorithm converges in only few iterations; its numerical solution almost coincides with the analytical solution at grid points. The discrete energy is non-dissipative and converges super-linearly when the mesh size decreases.

2. Formulation of the Collision Problem

In the following, we neglect the force of gravity for simplicity. We consider a bar of length L>0 made of a linear elastic isotropic material of unit density and unit modulus of rigidity. In the undeformed configuration $x\in(0,L)$, where t=0, let the bar be posed below the origin at initial depth H>0 without initial deformation. Pushed with an initial velocity $v_0>0$, Figure 1 illustrates motion of the bar in the deformed configuration x+u(t,x).

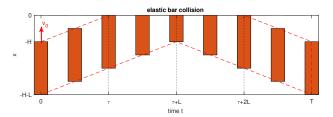


Figure 1. The collision benchmark in the deformed configuration x + u(t, x) for $(t, x) \in Q$.

Its displacement u(t, x) in the rectangle $Q = (0, T) \times (0, L)$ with the boundary ∂Q , defined for some fixed final time T > 0, is described by the inhomogeneous wave equation:

$$u_{tt}(t,x) - u_{xx}(t,x) = \lambda(t,x) \quad \text{for } (t,x) \in Q, \tag{1}$$

where λ is a contact force such that

$$\lambda(t,L) = u_x(t,L) \quad \text{for } t \in (0,T). \tag{2}$$

Here, u_{tt} stands for the second time derivative (the acceleration) u_x and u_{xx} for the first and second space derivatives, respectively. The equation of motion (1) is supported by the following initial conditions:

$$u(0,x) = 0, \quad u_t(0,x) = v_0 \quad \text{for } x \in (0,L),$$
 (3)

where u_t is the first time derivative (the velocity). Let the lower bar end x = 0 be free and defined as

$$u_x(t,0) = 0 \text{ for } t \in (0,T),$$
 (4)

where u_x denotes the first space derivative.

The upper end x = L collides with the rigid obstacle occupying the half-space $x \ge 0$. Therefore, the following complementarity conditions should hold for all space-time points:

$$u(t,x) \le L - x$$
, $\lambda(t,x) \le 0$, $\lambda(t,x) (u(t,x) - L + x) = 0$ for $(t,x) \in \widetilde{Q}$ (5)

on the set $\widetilde{Q}=Q\cup\Gamma$, where $\Gamma=\{t\in(0,T),\ x=L\}$. In (5), the former inequality yields non-penetration over the obstacle, that is, $u(t,L)\leq 0$ at the upper end x=L and $u(t,0)\leq L$ approaching the lower end x=0 of the bar. Under contact, the force should be non-expansive; hence, λ is non-positive. The non-penetration equations and inequalities (5) imply that $u(t,x)\leq L-x$ and $\lambda(t,x)=0$ before and after collision; otherwise, u(t,x)=L-x and $\lambda(t,x)\leq 0$ during the collision.

Computation 2025, 13, 210 4 of 15

Remark 1. By continuity, the non-penetration condition $u(t,x) \le L - x$ can be extended to the the closure $cl(Q) = Q \cup \partial Q$.

Remark 2. For comparison, if contact conditions (2) and (5) are stated at the boundary portion Γ only, then they turn into the complementarity relations:

$$\lambda(t,L) = u_x(t,L), \quad u(t,L) \le 0, \quad \lambda(t,L) \le 0, \quad \lambda(t,L)u(t,L) = 0 \quad \text{for } t \in (0,T).$$
 (6)

The particular case (6) can be treated as described in the previous works [48,49].

After integration by parts using Green's formula for smooth functions u, v in cl(Q), we have

$$\int_{Q} (u_{tt} - u_{xx}) v \, dx dt = \int_{Q} (-u_{t} v_{t} + u_{x} v_{x}) \, dx dt + \int_{0}^{L} u_{t} v \, dx \Big|_{t=0}^{T} - \int_{0}^{T} u_{x} v \, dt \Big|_{x=0}^{L}$$
 (7)

and we give a weak formulation to the initial boundary value problems (1)–(5). For this task, the following notation of linear sub-spaces from [50] is employed:

$$H_0^1(0,T) = \{v \in H^1(0,T), v(0) = 0\}, \quad H_0^1(0,T) = \{v \in H^1(0,T), v(T) = 0\}.$$

We look for a solution $u \in V_0$, from the trial space

$$V_{0,} = L^{2}(0,T; H_{0,}^{1}(0,L)) \cap H_{0,}^{1}(0,T; L^{2}(0,L))$$

such that $u(t, x) \leq L - x$ for $(t, x) \in \widetilde{Q}$, which satisfies the following variational inequality:

$$\int_{O} \left(-u_{t}(v_{t} - u_{t}) + u_{x}(v_{x} - u_{x}) \right) dxdt \ge \int_{0}^{L} v_{0}v \, dx \big|_{t=0} \tag{8}$$

for all functions $v - u \in V_0$ such that $v(t, x) \leq L - x$, for $(t, x) \in \widetilde{Q}$, from the test space

$$V_{,0} = L^2(0,T; H^1_{0,}(0,L)) \cap H^1_{,0}(0,T; L^2(0,L)).$$

Conversely, if the variational solution to (8) is smooth such that $u, u_x \in C(\operatorname{cl}(Q))$, then the Green Formula (7) justifies the initial boundary value problems (1)–(5).

The variational inequality (8) can be rewritten as the following system of primal and dual relations: Find solution pair $(u, \lambda) \in V_{0} \times L^2(Q) \cup L^2(\Gamma)$ such that

$$u \le L - x, \quad \lambda \le 0 \quad \text{in } \widetilde{Q}, \quad \int_{Q} \lambda (u - L + x) \, dx dt + \int_{0}^{T} \lambda u \, dt \big|_{x = L} = 0,$$

$$\int_{Q} (-u_{t}v_{t} + u_{x}v_{x}) \, dx dt = \int_{0}^{L} v_{0}v \, dx \big|_{t = 0} + \int_{Q} \lambda v \, dx dt + \int_{0}^{T} \lambda v \, dt \big|_{x = L}$$

$$(9)$$

for all test functions $v \in V_{,0}$. Indeed, introducing the contact force λ according to Equations (1) and (2) and using Green's Formula (7) for v - u yields

$$\begin{split} & \int_{Q} \lambda(v-u) \, dx dt = \int_{Q} (u_{tt} - u_{xx})(v-u) \, dx dt \\ & = \int_{Q} \left(-u_{t}(v_{t} - u_{t}) + u_{x}(v_{x} - u_{x}) \right) \, dx dt + \int_{0}^{L} u_{t}(v-u) \, dx \big|_{t=0}^{T} - \int_{0}^{T} u_{x}(v-u) \, dt \big|_{x=0}^{L} \\ & = \int_{Q} \left(-u_{t}(v_{t} - u_{t}) + u_{x}(v_{x} - u_{x}) \right) \, dx dt - \int_{0}^{L} v_{0} v \, dx \big|_{t=0} - \int_{0}^{T} \lambda(v-u) \, dt \big|_{x=L}. \end{split}$$

Computation **2025**, 13, 210 5 of 15

Through the variational inequality (8), it follows that

$$\int_{Q} \lambda \left(v - L + x - (u - L + x) \right) dx dt + \int_{0}^{T} \lambda (v - u) dt \big|_{x = L} \ge 0$$

for all functions such that $v \le L - x$ in \widetilde{Q} . These relations imply the primal–dual system (9). Conversely, testing (9) with $v - u \in V_{,0}$, we derive that

$$\begin{split} &\int_{Q} \left(-u_{t}(v_{t} - u_{t}) + u_{x}(v_{x} - u_{x}) \right) dxdt \\ &= \int_{0}^{L} v_{0}(v - u) dx \big|_{t=0} + \int_{Q} \lambda \left(v - L + x - \left(u - L + x \right) \right) dxdt + \int_{0}^{T} \lambda \left(v - u \right) dt \big|_{x=L} \\ &= \int_{0}^{L} v_{0}v dx \big|_{t=0} + \int_{Q} \lambda \left(v - L + x \right) dxdt + \int_{0}^{T} \lambda v dt \big|_{x=L}. \end{split}$$

It follows the variational inequality (8) if $\lambda(t,x) \leq 0$ and $v(t,x) \leq L - x$ for $(t,x) \in \widetilde{Q}$.

3. Analytical Solution to the Variational Inequality

Below, an analytical solution to the variational inequality (8) is provided drawn in three plots of Figure 2: the displacement u(t,x), velocity $u_t(t,x)$, and space derivative $u_x(t,x)$ for $(t,x) \in \operatorname{cl}(Q)$. The piecewise linear solution is constructed explicitly along characteristics x+t=const before collision, which begins at the time $\tau=H/v_0$ and along x-t=const afterwords. By this, the time and space derivatives are discontinuous across the characteristics $x+t=\tau+L$ and $x-t=-\tau-L$. The magnitudes of the velocity u_t and the gradient u_x discontinuities equal v_0 .

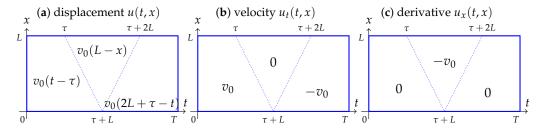


Figure 2. Analytical solution: displacement (a); velocity (b); space derivative (c).

Theorem 1. Let the final time be $T \ge \tau + 2L$ and the initial velocity be $v_0 \le 1$. Set the partition $cl(Q) = \bigcup_{i=1}^{3} K_i$, where

$$K_{1} = \{(t, x) \in cl(Q) : x + t \le \tau + L\},$$

$$K_{2} = \{(t, x) \in cl(Q) : x + t \ge \tau + L, x - t \ge -\tau - L\},$$

$$K_{3} = \{(t, x) \in cl(Q) : x - t \le -\tau - L\}.$$
(10)

A unique solution to the variational inequality (8) is given by

$$u(t,x) = \begin{cases} v_0(t-\tau) & \text{in } K_1, \\ v_0(L-x) & \text{in } K_2, \\ v_0(\tau+2L-t) & \text{in } K_3. \end{cases}$$
 (11)

Computation **2025**, 13, 210 6 of 15

Proof. For the elements K_1 – K_3 in the partition (10), let us denote by Γ_{12} the joint side between K_1 and K_2 with the normal $(1,1)/\sqrt{2}$ and by Γ_{23} the interface between K_2 and K_3 with the normal $(1,-1)/\sqrt{2}$. The jump of a discontinuous field w(t,x) is denoted by

$$[w] = w|_{\partial K_2 \cap \Gamma_{12}} - w|_{\partial K_1 \cap \Gamma_{12}}, \quad [w] = w|_{\partial K_3 \cap \Gamma_{23}} - w|_{\partial K_2 \cap \Gamma_{23}}.$$

We apply to the elements in partition the Green Formula (7) written for piecewise smooth functions u, v with discontinuous derivatives such that

$$\sum_{i=1}^{3} \int_{K_{i}} (u_{tt} - u_{xx}) v \, dx dt = \sum_{i=1}^{3} \int_{K_{i}} (-u_{t} v_{t} + u_{x} v_{x}) \, dx dt$$

$$- \int_{\Gamma_{12}} \left[(u_{t} - u_{x}) v \right] \frac{1}{\sqrt{2}} \, d\Gamma - \int_{\Gamma_{23}} \left[(u_{t} + u_{x}) v \right] \frac{1}{\sqrt{2}} \, d\Gamma$$

$$+ \int_{0}^{L} u_{t} v \, dx \Big|_{t=0}^{T} - \int_{0}^{T} u_{x} v \, dt \Big|_{x=0}^{L}.$$

$$(12)$$

The piecewise linear function in (11) is continuous and satisfies the following relations:

$$\begin{cases} u_{tt} = u_{xx} = 0 & \text{in } K_1 - K_3, \\ [u_t] = [u_x] = -v_0 & \text{on } \Gamma_{12}, \\ [u_t] = -v_0, & [u_x] = v_0 & \text{on } \Gamma_{23}, \\ u_t|_{t=0} = v_0, & u_x|_{x=0} = 0 & \text{on } \partial Q, \\ u(t, L) = v_0(t - \tau), & u_x(t, L) = 0 & \text{for } t \in [0, \tau], \\ u(t, L) = 0, & u_x(t, L) = -v_0 & \text{for } t \in [\tau, \tau + 2L], \\ u(t, L) = v_0(2L + \tau - t), & u_x(t, L) = 0 & \text{for } t \in [\tau + 2L, T]. \end{cases}$$

Inserting (13) into (12) with smooth functions v such that $[(u_t - u_x)v] = [u_t - u_x]v$ at Γ_{12} and $[(u_t + u_x)v] = [u_t + u_x]v$ at Γ_{23} yields the variational equation

$$\int_{Q} (-u_{t}v_{t} + u_{x}v_{x}) dxdt - \int_{0}^{L} v_{0}v dx \big|_{t=0} = \int_{0}^{T} u_{x}v dt \big|_{x=L}$$

$$= -\int_{\tau}^{\tau+2L} v_{0}v dt \big|_{x=L} \ge 0$$
(14)

for all functions $v \in V_{,0}$ such that $v(t,L) \le 0$ for $t \in (\tau,\tau+2L)$. In particular, testing (14) with $v = u\chi$, where a cutoff function $\chi(t)$ is compactly supported in (0,T) and $\chi(t) = 1$ for $t \in (0,T-\zeta)$ with small $\zeta > 0$, we get the identity

$$\int_{O} \left(-u_t(u\chi)_t + u_x u_x \chi \right) dx dt = \int_{0}^{T} u_x u\chi dt \big|_{x=L} = 0.$$
 (15)

The subtraction of (15) from (14) leads to the following variational inequality

$$\int_{O} \left(-u_{t}(v_{t} - u_{t}) + u_{x}(v_{x} - u_{x}) \right) dxdt \ge \int_{0}^{L} v_{0}v \, dx \big|_{t=0}$$
(16)

which holds for all test functions $v - u \in V_0$ such that $v(t, L) \le 0$ for $t \in (0, T)$.

Moreover, the function in (11) justifies the following equations on the partition:

$$\begin{cases} u - L + x = (v_0 - 1)(t - \tau) + x + t - \tau - L, & u_x(t, L) = 0 & \text{in } K_1, \\ u - L + x = (v_0 - 1)(L - x), & u_x(t, L) = -v_0 & \text{in } K_2, \\ u - L + x = (v_0 - 1)(2L + \tau - t) + x - t + \tau + L, & u_x(t, L) = 0 & \text{in } K_3. \end{cases}$$
 (17)

Computation **2025**, 13, 210 7 of 15

For $t \le \tau$, the position yields $u - L + x = v_0(t - \tau) - L + x \le 0$ in (11) for all points $x \le L$. Let $v_0 - 1 \le 0$ in (17). Then, $u - L + x = (v_0 - 1)(t - \tau) + x + t - \tau - L \le 0$ for $t \ge \tau$ and $x + t - \tau - L \le 0$ in K_1 . In K_2 , there holds $u - L + x = (v_0 - 1)(L - x) \le 0$ for all $x \le L$. If $t \le \tau + 2L$ and $x - t + \tau + L \le 0$, then $u - L + x = (v_0 - 1)(2L + \tau - t) + x - t + \tau + L \le 0$ in K_3 . For all $t \ge \tau + 2L$, we have $u - L + x = v_0(2L + \tau - t) \le 0$ in (11). Therefore, the non-penetration condition $u(t, x) \le L - x$ holds globally. To fulfill with (17) the complementarity conditions (5), we set a discontinuous contact force in the following form:

$$\lambda(t,x) = \begin{cases} 0 & \text{in } Q, \\ u_x & \text{on } \Gamma. \end{cases}$$
 (18)

The uniqueness of solution to the problem (8) follows by an energy method.

Remark 3. The function pair (u, λ) defined in (11) and (18) solves the primal–dual problem (9).

Remark 4. The global solution in (11) holds true when restricted for smaller values $T < \tau + 2L$, also for larger velocities $v_0 > 1$ within the time $t \in (0, \tau)$, when $u - L + x \le 0$ in (17).

Next, we consider the time-dependent energy of the bar as

$$E(t) = \frac{1}{2} \int_0^L (u_t^2 + u_x^2) \, dx, \quad t \in [0, T].$$
 (19)

Since the collision is supposed to be elastic, the energy is conserved, as justified below.

Corollary 1. *Under the assumptions of Theorem 1, the energy defined in* (19) *remains constant in time as*

$$E(t) = E(0) = \frac{1}{2}Lv_0^2 \quad \text{for } t \in [0, T].$$
 (20)

Proof. Consider the intersection of elements K_1 – K_3 from (10) with the rectangle $[0, s] \times [0, L]$ at fixed $s \in [0, T]$. We test with the discontinuous function $v = u_t$ the Green Formula (12) and skip integration by parts over time to calculate the following expression:

$$\sum_{i=1}^{3} \int_{K_{i} \cap \{t < s\}} (u_{tt} - u_{xx}) u_{t} dx dt = \frac{1}{2} \sum_{i=1}^{3} \int_{K_{i} \cap \{t < s\}} (u_{t}^{2} + u_{x}^{2})_{t} dx dt
+ \int_{\Gamma_{12} \cap \{t < s\}} [[u_{x} u_{t}]] \frac{1}{\sqrt{2}} d\Gamma - \int_{\Gamma_{23} \cap \{t < s\}} [[u_{x} u_{t}]] \frac{1}{\sqrt{2}} d\Gamma - \int_{0}^{s} u_{x} u_{t} dt \Big|_{x=0}^{L} .$$
(21)

Using properties (13) and zero product $u_x u_t = 0$ in $K_1 - K_3$, integration of (21) by parts over time yields

$$0 = \frac{1}{2} \sum_{i=1}^{3} \int_{K_{i} \cap \{t < s\}} (u_{t}^{2} + u_{x}^{2})_{t} dx dt = E \Big|_{t=0}^{s} - \frac{1}{2} \int_{(\Gamma_{12} \cup \Gamma_{23}) \cap \{t < s\}} [\![u_{t}^{2} + u_{x}^{2}]\!] \frac{1}{\sqrt{2}} d\Gamma$$
$$= E \Big|_{t=0}^{s}$$

due to $u_t^2 + u_x^2 = v_0^2$ in K_1 – K_3 . This identity and $E(0) = Lv_0^2/2$ prove the assertion (20).

In the next section, we discretize the primal–dual problem (9) by using ST-FEM approach on a uniform triangular mesh, and we adapt PDAS for its numerical solution.

Computation **2025**, 13, 210 8 of 15

4. ST-PDAS Approximation

Let $\operatorname{cl}(Q) = \bigcup_{i \in I} T_i$ be divided into equal triangles T_i indexed by a set I comprising a uniform grid of size h > 0, where h = 1/(N-1) for prescribed $N \in \mathbb{N}$. The grid nodes $(t_h, x_h) = \{(t_j, x_j)\}$ account for the number of degrees of freedom DOF = (T/h+1)(L/h+1), with the number M = (T/h-1)L/h of nodes $(t_h, x_h) \in \widetilde{Q}$. For T = 4 and L = 1, an example grid with h = 0.25 constituting DOF=85 and M = 60 is shown in Figure 3: before deformation in the left plot (a) and after deformation in the right plot (b). A full space-time discretization of the variational problem in the space of continuous piecewise linear functions is introduced below:

$$V^h = \{v_h \in C(\operatorname{cl}(Q)), v_h|_{T_i} \in \mathbb{P}_1(T_i)^2 \text{ for } i \in I\},$$

where the trial V_{0} , and the test $V_{,0}$ spaces are respectively,

$$V_{0}^{h} = \{v_{h} \in V^{h}, v_{h}(0, \cdot) = 0\}, \quad V_{0}^{h} = \{v_{h} \in V^{h}, v_{h}(T, \cdot) = 0\}.$$

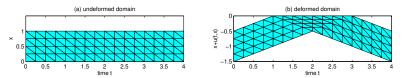


Figure 3. The diagonal triangle grid for N=5 before deformation (a) and after deformation (b).

Let us denote by $\phi_h = \{\phi_j\}$, $j = 1, \ldots$, DOF, standard hat functions spanning the nodal basis in V^h such that each $\phi_j = 1$ at the corresponding node (t_j, x_j) and zero otherwise. For the discrete initial velocity $v_{0h} \in V^h$, we approximate the system of primal and dual relations (9): Find a solution pair $(u_h, \lambda_h) \in V_0^h \times \mathbb{R}^M$ such that

$$u_h(t_h, x_h) \le L - x_h, \quad \lambda_h \le 0, \quad \lambda_h \left(u_h(t_h, x_h) - L + x_h \right) = 0 \quad \text{for } (t_h, x_h) \in \widetilde{Q},$$

$$\int_{Q} \left(-u_{ht} \phi_{ht} + u_{hx} \phi_{hx} \right) dx dt = \int_{0}^{L} v_{0h} \phi_h dx \big|_{t=0} + \lambda_h$$
(22)

for all basis functions $\phi_h \in V_0^h$. In contrast to an integral approach providing for non-penetration within whole elements, the nodal enforcement of constraints in (22) imposes for non-penetrating both on an individual element as well as at the boundary. Here, λ_h is referred to as a Lagrange multiplier compared to the contact force λ in (1) and (2).

Theorem 2. Let the complementary sets of active and inactive nodes be defined as

$$\mathcal{A}(u_h, \lambda_h) = \{ (t_h, x_h) \in \widetilde{Q} : r\lambda_h - u_h(t_h, x_h) + L - x_h < 0 \},$$

$$\mathcal{I}(u_h, \lambda_h) = \{ (t_h, x_h) \in \widetilde{Q} : r\lambda_h - u_h(t_h, x_h) + L - x_h \ge 0 \},$$
(23)

for r > 0. Using (23), system (22) can be realized as an implicit variational equation for the primal variable on a linear subspace: Find $u_h \in V_0^h$ such that

$$u_h(t_h, x_h) = L - x_h \text{ on } \mathcal{A}(u_h, \lambda_h), \quad \int_{\mathcal{Q}} (-u_{ht}\phi_{ht} + u_{hx}\phi_{hx}) \, dxdt = \int_0^L v_{0h}\phi_h \, dx \big|_{t=0}$$
 (24)

for all test functions $\phi_h \in V_0^h$ with $\phi_h(t_h, x_h) = 0$ on $\mathcal{A}(u_h, \lambda_h)$. In contrast, a dual variable (the Lagrange multiplier) $\lambda_h \in \mathbb{R}^M$ is defined such that

$$\lambda_h = \begin{cases} r_h & \text{on } \mathcal{A}(u_h, \lambda_h), \\ 0 & \text{on } \mathcal{I}(u_h, \lambda_h), \end{cases}$$
 (25)

can be determined from the residual $r_h \in \mathbb{R}^{DOF}$ as

$$r_{h} = \int_{O} \left(-u_{ht}\phi_{ht} + u_{hx}\phi_{hx} \right) dxdt - \int_{0}^{L} v_{0h}\phi_{h} dx \big|_{t=0}.$$
 (26)

Proof. According to the definition of active–inactive sets in (23) and complementarity conditions in (22), we have two options:

$$\begin{cases} u_h(t_h, x_h) - L + x_h = 0, & \lambda_h < 0 & \text{on } \mathcal{A}(u_h, \lambda_h), \\ u_h(t_h, x_h) - L + x_h \le 0, & \lambda_h = 0 & \text{on } \mathcal{I}(u_h, \lambda_h). \end{cases}$$

Therefore, relations (22) turns into (23)–(26) and vice versa. \Box

As a consequence of Theorem 2, we derive space-time iteration of the problems (23)–(26) over active sets, yielding a solution to the discretized primal–dual variational problem (22).

Some heuristics for stable implementation of Algorithm 1 are given, avoiding numerical instabilities and cycling.

Algorithm 1: (ST-PDAS).

Initialization: set iteration number k = 0 and initialize active set $A^0 = \emptyset$.

Iteration: *solve the linear system: Find* $u_h^k \in V_0^h$ *such that*

$$u_h^k(t_h, x_h) = L - x_h \text{ on } \mathcal{A}_h^k, \quad \int_Q (-u_{ht}^k \phi_{ht} + u_{hx}^k \phi_{hx}) \, dx dt = \int_0^L v_{0h} \phi_h \, dx \big|_{t=0} \quad (27)$$

for all $\phi_h \in V_{,0}^h$ with $v_h = 0$ on A_h^k : compute the residual $r_h^k \in \mathbb{R}^{DOF}$:

$$r_h^k = \int_{Q} (-u_{ht}^k \phi_{ht} + u_{hx}^k \phi_{hx}) \, dx dt - \int_{0}^{L} v_{0h} \phi_h \, dx \big|_{t=0}$$
 (28)

and the Lagrange multiplier $\lambda_h^k \in \mathbb{R}^M$:

$$\lambda_h^k = \begin{cases} r_h^k & \text{on } \mathcal{A}_h^k, \\ 0 & \text{on } \mathcal{I}_h^k. \end{cases}$$
 (29)

update the active and inactive sets:

$$\mathcal{A}_{h}^{k+1} = \{ (t_{h}, x_{h}) \in \widetilde{Q} : r\lambda_{h}^{k} - u_{h}^{k}(t_{h}, x_{h}) + L - x_{h} < -\text{tol} \},
\mathcal{T}_{h}^{k+1} = \{ (t_{h}, x_{h}) \in \widetilde{Q} : r\lambda_{h}^{k} - u_{h}^{k}(t_{h}, x_{h}) + L - x_{h} \ge -\text{tol} \}.$$
(30)

Termination: *stop if the iteration cycles, or the stopping condition holds:*

$$\mathcal{A}_h^{k+1} = \mathcal{A}_h^k. \tag{31}$$

- The factors are r = 1 and to 10^{-5} in the definition of active and inactive sets (30).
- The computational domain Q is extended to $(0, T + 2h) \times (0, L)$ to fit the final time in the trial V_0^h and the test V_0^h spaces.
- At the contact boundary Γ , for extended grid points $\{t = T + h, x = L\}$, $\{t = T + 2h, x = L\}$, and for $t^* \in (0, T)$, where the inactive set meets the active

set (here $t^* = \tau$), we realize the Neumann condition $\lambda_h^k = u_{hx}^k = 0$ in (18) by using the finite difference defined as

$$u_h^k(t,L) - u_h^k(t,L-h) = 0 \quad \text{for } t \in \{t^*, T+h, T+2h\}.$$
 (32)

The finite difference approximation (32) for $t = t^*$ preserves iterates from instabilities happening near discontinuities.

• To avoid the instability of iteration (30) that becomes possible after collision for $k \ge 2$, we use re-initialization of the inactive set \mathcal{I}_h^k with $\mathcal{I}_h^{k'}$, satisfying the monotony condition

$$\lambda_j^k = 0$$
 for $j = 1, \dots, \text{DOF}$ such that $\mathcal{I}_j^{k-1} = \mathcal{I}_j^{k-2}$. (33)

The heuristic re-initialization (33) remedies the M-property of the stiffness matrix and prevents iterates from cycling without it during contact transitions.

• If the stopping condition (31) is attained, then $r\lambda_h^k < -\text{tol}$ on \mathcal{A}_h^k and $u_h^k(t_h, x_h) - L + x_h \le \text{tol}$ on \mathcal{I}_h^k are guaranteed by (30). In the case of $\text{tol} \ge 0$ and $u_h^k(t_h, x_h) \le L - x_h$ on \mathcal{I}_h^k , the iteration (u_h^k, λ_h^k) solves the reference problems (23)–(26) exactly.

We justify the ST-PDAS algorithm on the analytical benchmark from Theorem 1.

5. Numerical Benchmark

For numerical tests, this study set the parameters of bar length L=1, initial depth H=0.5, and velocity $v_0=0.5$ such that the collision time $\tau=1$ and the final time T=4, as shown in Figure 3. According to Theorem 1 and Remark 3, the analytical solution to the primal–dual problem (9) is given for the displacement as

$$u(t,x) = \frac{1}{2} \begin{cases} t-1 & \text{in } K_1 = \{0 \le t \le 4, \ 0 \le x \le 1 : \ x+t \le 2\}, \\ 1-x & \text{in } K_2 = \{0 \le t \le 4, \ 0 \le x \le 1 : \ x+t \ge 2, \ x-t \ge -2\}, \\ 3-t & \text{in } K_3 = \{0 \le t \le 4, \ 0 \le x \le 1 : \ x-t \le -2\}, \end{cases}$$
(34)

and for the Lagrange multiplier as

$$\lambda(t,x) = \begin{cases} 0 & \text{in } Q = \{0 < t < 4, \ 0 < x < 1\}, \\ \begin{cases} -0.5 & \text{if } 1 < t < 3 \\ 0 & \text{otherwise} \end{cases} & \text{on } \Gamma = \{0 < t < 4, \ x = 1\}. \end{cases}$$
(35)

After discretization of the collision problem in the finite element space V^h , the choice of the integer number N determines the discrete parameters used in the following numerical tests. They are presented in Table 1: the mesh size h, the number of DOF in the closure $\operatorname{cl}(Q)$, the number M of constrained nodes in $\widetilde{Q} = Q \cup \Gamma$, and the M/DOF ratio.

Tab	le 1.	Disc	rete j	parame	ters d	ete	ermir	ned	by	the	num	ber	N	•
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N	h	DOF	M	M/DOF
11	0.1	451	390	0.86
21	0.05	1701	1580	0.92
31	0.033	3751	3570	0.95
41	0.025	6601	6360	0.96
51	0.02	10,251	9950	0.97

According to Theorem 2, numerical solution to the corresponding discrete problem is computed with the help of Algorithm 1. For N=5, an example solution is drawn

in Figure 4. Here, the displacement $u_h(t,x)$, velocity $u_{ht}(t,x)$, and gradient $u_{hx}(t,x)$ are presented over the uniform triangle grid in the left (a), middle (b), and right (c) plots, respectively, where the color of triangles varies according to its heights. The time and space derivatives in the latter two plots are discontinuous. The numerical solution u_h computed at nodes x_h is almost equal to the exact solution $u(x_h)$, with the error being less then 10^{-14} . Indeed, the exact solution is given by a piecewise linear function on the partition K_1 – K_3 . Then, the piecewise linear interpolation differs only with respect to the elements crossing the interface Γ_{23} , which does not coincide with the diagonal grid.

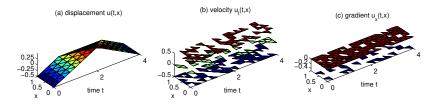


Figure 4. Example solution for N=5: displacement u_h (a), velocity u_{ht} (b), and gradient u_{hx} (c).

For physical consistency, the discrete energy is calculated from Formula (19) on the grid at equidistant time points $t_i = (j-1)h$ for j = 1, ..., 4(N-1) + 1 such that

$$E_h(t_j) = \frac{1}{2} \sum_{i=1}^{3} \int_{K_i \cap \{t=t_j, x \in (0,1)\}} (u_{ht}^2 + u_{hx}^2) \, dx. \tag{36}$$

According to Corollary 1, the exact energy E = 0.125 is constant at all times. We measure the relative error with respect to the discrete L^2 -norm as

$$\operatorname{Err}_{h} = \left\| \frac{E_{h} - E}{E} \right\| \times 100 \text{ (\%)}.$$
 (37)

The numerical energy E_h computed from (36) and the relative energy error Err_h obtained by (37) are portrayed in the left (a) and right (b) plots of Figure 5, respectively. Here, one can observes piecewise constant values of E_h with jumps at the times t=2 and t=3. These times correspond to the interface between regions K_2 and K_3 in the partition (37), which does not coincide with the diagonal grid. In contrary, the interface between regions K_1 and K_2 coincides with the diagonal grid, and energy at the time t=1 is continuous without jump. The curves E_h are visually indistinguishable from E for E0 and E1 of the visually indistinguishable from E2 and E3; otherwise, they tend to E3 when decreasing the step size E4. The order of accuracy is estimated to be 1.5. The convergence rate is super-linear, that is, inherent for SSN methods.

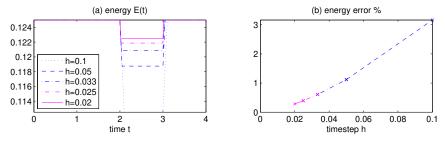


Figure 5. The discrete energy E_h (a) and relative energy error Err_h (b).

Finally, the convergence behavior of the ST-PDAS algorithm is demonstrated. For N=51, implying about 10^4 constrained nodes, Algorithm 1 terminates successfully with $\mathcal{A}_h^{k+1}=\mathcal{A}_h^k$ at the final k=4 iterate. The iteration history of active sets $\mathcal{A}_h^0-\mathcal{A}_h^{k+1}$ is shown in the dark color over \widetilde{Q} in Figure 6. Here, we realize the Neumann condition (32) and apply the monotony condition (33) by re-initializing the inactive set \mathcal{I}_h^2 with $\mathcal{I}_h^{2'}$. Namely,

 $\lambda_j^2 = 0$ is set for the nodes j where the both previous iterates $\mathcal{I}_j^1 = \mathcal{I}_j^0$ were inactive. Here, one can observe at iterates 1 and 2 that the active sets \mathcal{A}_h^1 and \mathcal{A}_h^2 are bounded by lines x + t = 3 and x + t = 2, where the latter is characteristic, but the former is not.

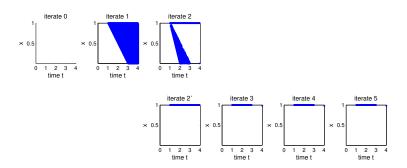


Figure 6. ST-PDAS iterates $\mathcal{A}_h^0 - \mathcal{A}_h^5$ of the active set as N = 51.

We have observed the same behavior of active sets for all numbers N tested. For illustration purposes, the iterates of the displacement $u_h^0 - u_h^4$ in $\mathrm{cl}(Q)$ are shown in Figure 7 as N=3. For N=5, the iterates of the Lagrange multiplier $\lambda_h^0 - \lambda_h^4$ over \widetilde{Q} are presented in Figure 8. Here various colors are used for visualization reason to distinguish between portions of the reference rectangle Q.

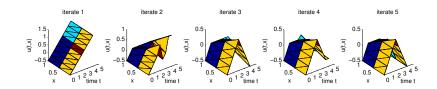


Figure 7. ST-PDAS iterates $u_h^0 - u_h^4$ of the displacement as N = 3.

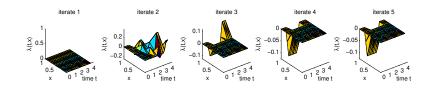


Figure 8. ST-PDAS iterates $\lambda_h^0 - \lambda_h^4$ of the Lagrange multiplier as N = 5.

6. Concluding Remarks

A space-time method of finite-element approximation has been developed and endowed with a primal–dual active set iteration treating unilateral constraints in two dimensions. The ST-PDAS algorithm has been tested for an analytical benchmark of a rigid obstacle collided by an elastic bar, which is characterized by a discontinuous velocity. The numerical tests on a uniform triangular grid converge in few iterations when processing some heuristic conditions before and after collision and provided by re-initialization. On grid points, the numerical solution is visually indistinguishable from the exact solution, and the energy converges super-linearly under grid refinement. If the initial velocity of the bar is $v_0 \leq 1$, then the analytical solution is given by a piecewise linear function.

From the physical point of view, at time $t = \tau$, the bar collides with the obstacle at its upper end. An elastic wave propagates through the bar with a velocity 1 and reaches its opposite end when moving with a kinematic velocity $v_0 \le 1$. Otherwise, the bar lower end

Computation 2025, 13, 210 13 of 15

reaches the obstacle before then at the elastic wave. For $v_0 > 1$, there is a known bounce effect, which might be a subject of future research.

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