Toward Spacetime Adaptive Variational Integrators

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1 Introduction

In this report we investigate numerical algorithms for structure-preserving integration of mechanical systems over irregular discretizations of spacetime. The ultimate goal is to develop integrators that *adapt* the discretization to the solution. In this report we take the first step by considering discretizations that are *fixed*, but arbitrary. The hope is that if we can develop algorithms that demonstrate good conservation properties on arbitrary meshes, then adaptive methods can be achieved via, e.g., simple adaptive refinement. Our approach to adaptation is in a way more naïve than other adaptive methods (in particular, the time adaptive method of Kharevych et al [2] and the r-adaptive method of Zielonka et al [5]) since we do not attempt to simultaneously solve for the evolution of the system *and* adapt the material and/or time coordinates.

When comparing our method to these "simultaneous" approaches, there are several important practical and theoretical issues to consider. Simultaneous methods tend to produce more accurate solutions for a given number of temporal and material nodes, since these nodes are placed judiciously. However, the resulting systems of equations can be more difficult to solve not just because they involve more *total* degrees of freedom (e.g., temporal coordinates and Lagrange multipliers), but also because these DOFs can be coupled in a way that makes the system dense or otherwise difficult to solve (cf. Kharevych et al [2]). More importantly, simultaneous methods require that the combinatorics of the spacetime mesh be fixed, since the resulting equations involve derivatives of material and temporal coordinates. In contrast, our approach could permit arbitrary refinement of the spacetime mesh. Further, we have more flexibility in choosing refinement criteria since we do not have to incorporate this refinement into a global framework. But it is not yet entirely clear how our method performs with respect to accuracy and momentum conservation; even worse, we do not even know how to formulate the method for an initial value problem! (These issues are discussed in greater detail in Section 4).

The main difference between the two approaches from a theoretical perspective is that our method directly integrates the original system, whereas the simultaneous methods augment the system with additional fields that govern mesh evolution. Both methods correspond to the evolution of *some* Hamiltonian system, but there is an interesting question of how closely the augmented system follows trajectories of the original system.

Finally, as noted in a paper by Zielonka et al [5], "*...in attempting a general implementation, an unexpected essential difficulty arises: A direct space-time discretization of the action results in unstable discrete systems in general. ... The instabilities that plague naive space-time discretizations may be traced to inaccuracies in the velocity field introduced by the motion of the mesh.*" In other words, it is already known that a compromise between the two approaches (i.e., a single-field theory of simultaneous adaptation) is not feasible.

2 Background

The fundamental variational principle governing mechanical systems is *d'Alembert's principle*, which says that *any system of forces is in equilibrium if we add to the impressed forces the forces of inertia* [3]. We can express this principle as

$$\delta w^e = 0$$

where w^e is the *effective virtual work*, i.e., the virtual work done by both impressed *and* interial forces and δ denotes variations in the configuration of our system around an equilibrium. *Hamilton's principle* reformulates this idea by requiring that d'Alembert's principle be satisfied at every moment in time, i.e., that

$$\int_{t_1}^{t_2} \delta w^e dt = 0$$

which can be expressed more explicitly as

$$\delta \int_{t_1}^{t_2} L dt - [p\delta q]_{t_1}^{t_2}$$

where L is the Lagrangian of the system, and p and q are the momentum and configuration of the system (expressed in generalized coordinates). In order to make this statement a true variational principle (i.e., the extremization of a scalar functional), we require that the variation δq be zero at the endpoints t_1 and t_2, yielding the typical statement of Hamilton's principle

$$\delta S = \delta \int_{t_1}^{t_2} L dt = 0.$$

(We will refer to the quantity S as the *action integral*.) We can subsequently write down the Euler-Lagrange equations corresponding to Hamilton's principle in order to get the equations of motion for the system in question. The standard approach to numerical time integration is to discretize the equations of motion directly (usually using finite differences to approximate derivatives). However, there is an alternative approach, namely to approximate the action integral S using numerical quadrature and derive the Euler-Lagrange equations corresponding to the resulting approximated action. Both procedures yield an update rule for a discrete system, but in general the two approaches do not commute. In fact, it can be shown that the latter, "variational" approach will produce integrators with good conservation properties [4], whereas the standard approach, in general, will not.

Letting Q be the configuration space of the system, the standard approach to variational integrators is to first define a *discrete Lagrangian*

$$L_D : Q \times Q \to \mathbb{R}$$

that approximates the integral of the Lagrangian between time t_k and t_{k+1}. One then writes down the discrete action in terms of three consecutive configurations q_{k-1}, q_k, and q_{k+1}, and finds extrema of this action with respect to q_k while keeping q_{k-1} and q_{k+1} fixed:

$$\frac{\partial}{\partial q_k} \left(L(q_{k-1}, q_k) + L(q_k, q_{k+1}) \right) = 0.$$

This equation (or system of equations, in the case of PDEs) can then be solved for the next configuration of the system q_{k+1}. This procedure is then repeated ad nauseum to produce a series of configurations $q_1, q_2, q_3, ...$ In this report we adpot a slightly different perspective, which is to write down a discrete action

$$S_D = \sum_{k=1}^{N-1} L_D(q_k, q_{k+1})$$

in terms of *all* the DOFs in our discrete trajectory, and then solve the system of equations

$$\frac{\partial S_D}{\partial q_i} = 0$$

for all q_i not at the beginning or end of our trajectory. It is not hard to see (Section 3) that if the first two configurations q_1 and q_2 are known, these two formulations of variational integrators are completely equivalent in the case of ODEs. However, this perspective will be very useful in formulating integrators on irregular spacetime domains, and does not (yet) appear to reduce to something "obvious."

The main assumption that we make in this report (and it may be flawed) is stated below.

> MAIN ASSUMPTION: *extremization of the discrete action integral yields a discrete flow that is symplectic, independent of the choice of quadrature.*

In particular, if this assumption holds then we should be able to adapt our solution purely through choice of quadrature points between the initial and final configurations in our trajectory. In other words, we think of all the intermediate points in our trajectory as merely quadrature points for the action between q_1 and q_N.

3 Kepler problem

We first examine the behavior of our approach for ODEs using a mesh that is irregular in time (we will henceforth refer to our approach as the *global* approach, since we solve for all degrees of freedom simultaneously). In particular, we study the *Kepler problem*, which describes the motion of a particle with position q moving under the influence of the simple potential

$$U(q) = -\frac{mk}{||q||}$$

where m is the mass of the particle, $a \in \mathbb{R}$ is an arbitrary constant, and $\|\cdot\|$ denotes the Euclidean norm. For $a > 0$ and non-zero intial velocity, the trajectories of this system are generally ellipses around the origin. For simplicity, we will use $m = 1$ and $k = -1$. The Lagrangian for this system then becomes

$$\mathcal{L} = \frac{1}{2}\,||\dot{q}||^2 - \frac{1}{||q||}$$

where $\dot{q}$ is the time derivative of q.

3.1 Discretization

As discussed previously, the global method fixes the configuration q of the system at the initial and final times t_i and t_f, and seeks extrema of the corresponding action integral with respect to variations in the intermediate q. In particular, we discretize $\dot{q}$ via first-order finite differences and use midpoint quadrature for the potential. The discrete action is thus given by

$$S_d = \sum_{k=1}^{N} h_k \left(\frac{1}{2} \left\| \frac{q_{k+1} - q_k}{h_k} \right\|^2 - \frac{1}{\left\| \frac{q_k + q_{k+1}}{2} \right\|} \right)$$

where N is the number of time steps in the discrete trajectory and h_k is the length of the kth time step. We then solve the system

$$\frac{\partial S_d}{\partial q_k} = 0,\ 1 < k < N$$

for the unknown coordinates along the trajectory.

3.2 Numerical Experiments

We implemented the algorithm described above in *Mathematica*. For comparison, we also implemented symplectic Euler, the time adaptive method of Kharevych et al [2], as well as the standard three-point variational integrator described in the previous section (again using midpoint quadrature for a fair comparison). The adaptive method, which we will henceforth refer to as the *Pontryagin approach*, represents the state-of-the-art in temporally adaptive variational integrators for ODEs. The basic idea is to specify a function $\sigma : Q \times Q \to \mathbb{R}$ that expresses the desired temporal spacing between consecutive configurations via the relationship

$$\frac{t_{k+1} - t_k}{h} = \sigma(q_k, q_{k+1}),$$

where h is a "fictitious" time step that determines the overall granularity of the solution. In order to enforce this relationship, the method adds a Lagrange multiplier term $\lambda_k\left((t_{k+1} - t_k) - h\sigma(q_k, q_{k+1})\right)$ to the discrete action and extremizes this action with respect to q, t, *and* λ. The Pontryagin method effectivly introduces an additional force that pushes the solution towards the desired time steps, but may also push the original system from its true trajectory (even if momenta are conserved).

Energy plots and the corresponding time steps are shown in figures (1), (2), and (3) for the trajectory shown in figure (1). Not surprisingly, the global method and the standard three-point method yielded identical results (and hence are not plotted independently). It is easy to see why this should be the case, since in both methods the solutions must satisfy

$$\frac{\partial}{\partial q_k} S_D = 0$$

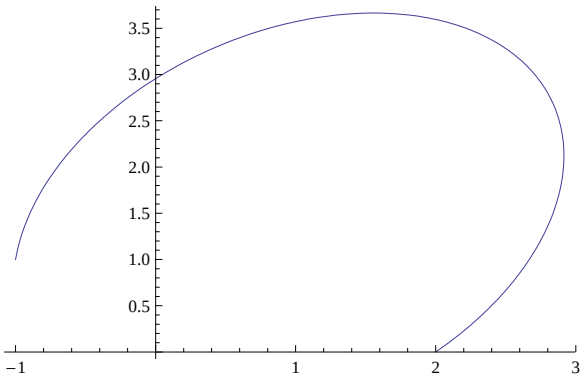


Figure 1: *Trajectory examined in this section (all trajectories look roughly the same).*

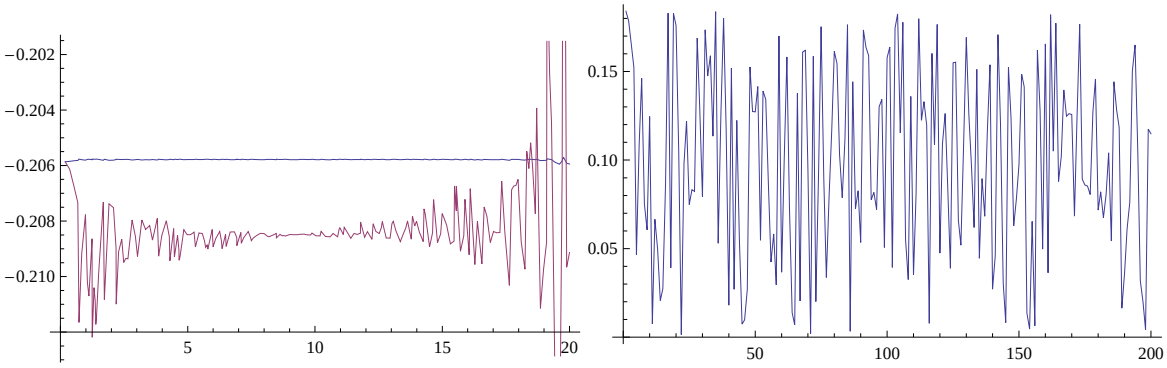


Figure 2: *Left: energy curves for a partial orbit in Kepler's problem using the global method (equivalent to a standard variational integrator with a midpoint evaluation of the potential) and standard symplectic Euler – the flatter curve corresponds to the global method. Right: time step magnitude as a function of step index.*

for all intermediate points q_k, regardless of how the actual computation is carried out. It is most interesting to note that this global/standard approach demonstrates much better energy behavior that standard symplectic Euler for variable time steps. This discrepancy is most likely due to the fact that we chose a *midpoint* discretization of the potential, resulting in a scheme that is not only symplectic, but also *symmetric* with respect to time – such integrators are well-known for their good long-term energy behavior [1], although it is not clear what the relationship is (if any) between symmetry and symplecticity. Finally, the Pontryagin approach and the symmetric approach behaved almost identically in terms of energy behavior. However, because the function σ which determines the time step in the Pontryagin approach can be written only in terms of q_k and q_{k+1}, we could not compare it directly with symplectic Euler and the symmetric method using truly random time steps.

What can we conclude from these experiments? Standard symplectic Euler *is* a symplectic method for fixed time steps, but its energy behavior is not fantastic for variable time steps. Is this because symplecticity is not an absolute guarantee of good *energy* behavior, or is it an indicator that our main assumption is flawed? Conversely, if our main assumption holds, then symplectic Euler must be symplectic even for variable time steps, since it will be equivalent to a "global" variational method for some choice of quadrature.

It is also worth noting that we used a very short trajectory used in this experiment, rather than the long, looping trajectories typically seen in numerical tests of structure-preserving integrators. The global method was our limitation here: since we are only able to specify the initial and final configurations (and not initial velocities), we are likely to find the *shortest* among all trajectories satisfying these conditions.[1] This is a general limitation of our DMOC-like approach to time integration.

[1]Of course, now that we see that the global method is equivlaent to the standard approach, we could easily perform experiments of longer duration.

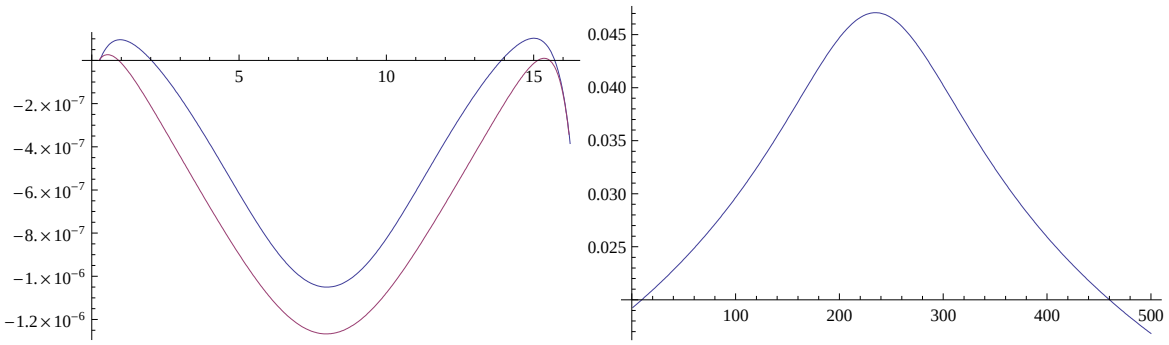


Figure 3: *Left: energy curves for a partial orbit in Kepler's problem using the global and standard methods (top) and the method of Kharevych et al [2] (bottom). Both trajectories use identical timesteps, adapted to generate equispaced poses. Right: time step magnitude as a function of time step index.*

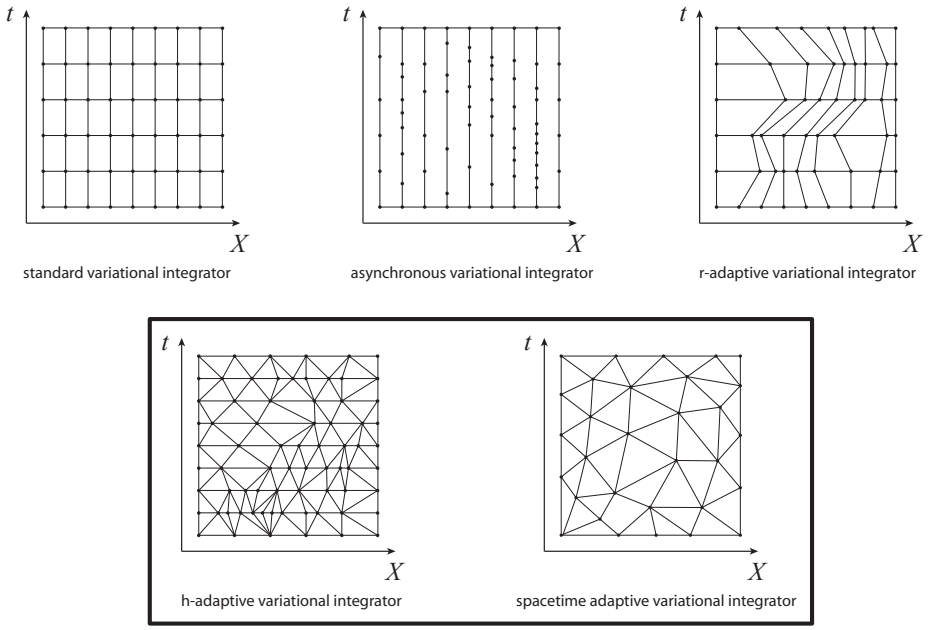


Figure 4: *Cartoon of effective spacetime discretizations used by different variational methods for the 1D elasticity problem. Mesh types not used by existing variational methods are highlighted in the bottom row.*

4 1D Elasticity

We now consider a mechanical PDE using a mesh that is irregular in both time *and* space. Notably, the number of degrees of freedom is not required to be fixed over the course of the simulation.

4.1 Lagrangian

Consider a 1D elastic body immersed in $\mathbb{R}^3$ with reference configuration $\mathcal{B} = [0, 1]$ and uniform mass density $\rho = 2$. The immersion $q : \mathcal{B} \to \mathbb{R}^3$ gives the configuration of the body at time t. The total kinetic energy at time t can therefore be written as

$$K = \int_{\mathcal{B}} \frac{\rho}{2} \left\| \frac{\partial q}{\partial t} \right\|^2 dV.$$

We use a simple elastic potential

$$U = \frac{1}{2} \int_{\mathcal{B}} \rho \left(\left\| \frac{\partial q}{\partial X} \right\| - 1 \right)^2 dV$$

where the leading factor $1/2$ is merely for convenience. The resulting Lagrangian is then simply

$$L = -\mathcal{V}_{\mathcal{B}} + \int_{\mathcal{B}} \left\| \frac{\partial q}{\partial t} \right\|^2 - \left\| \frac{\partial q}{\partial X} \right\|^2 + 2 \left\| \frac{q}{X} \right\| dV$$

where in the final expression $\mathcal{V}_{\mathcal{B}}$ is the volume of the body.

4.2 Discrete Lagrangian

Consider a spacetime domain with coordinates X and t along the material and temporal axes, respectively. Let V, E, and F be the sets of vertices, edges, and faces in a simplicial mesh of this domain. For the moment, assume that we are only interested in configurations in $\mathbb{R}$ (instead of $\mathbb{R}^3$). We can then describe the discrete configuration of the body via the map $q_D : \mathsf{V} \to \mathbb{R}$. Suppose that we interpolate $\hat{q}$ piecewise linearly over each simplex to get a map $\hat{q} : \mathcal{B} \to \mathbb{R}^3$. We can then express a *discrete* action $\mathcal{S}_D$ as the sum over each simplex of the action of the interpolated configuration:

$$\mathcal{S}_D = \sum_{f \in \mathsf{F}} \int_f L.$$

Note that the integral over f is actually an integral over space *and* time. In fact, this integral is very straightforward to compute. Let A_{qX}, A_{qt} and A_{Xt} be the signed, *projected* areas of f along the t, X, and q axes, respectively. It is easy to show that on f

$$\frac{\partial \hat{q}}{\partial t} = \frac{A_{qX}}{A_{tX}}$$

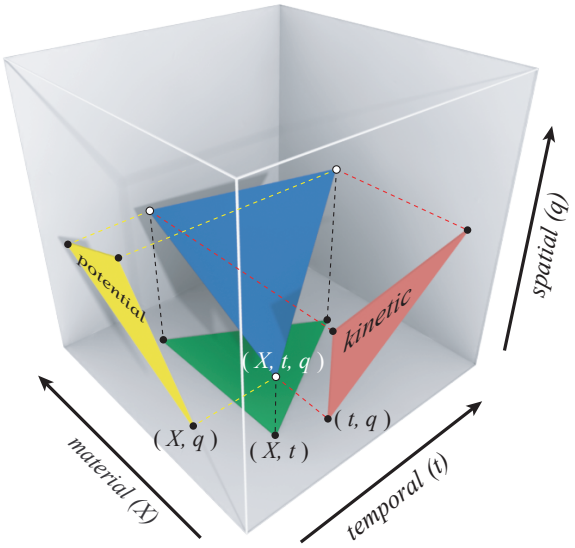
and

$$\frac{\partial \hat{q}}{\partial X} = \frac{A_{tq}}{A_{tX}},$$

hence integrating these quantities over f (which we assume has signed area $A_{tX} > 0$ in the material/time domain) gives us

$$\mathcal{S}_D(f) = A_{qX}^2 - A_{tq}^2 + 2A_{tq} - A_{tX},$$

where the final term accounts for $\mathcal{V}_{\mathcal{B}}$ in the continuous Lagrangian.



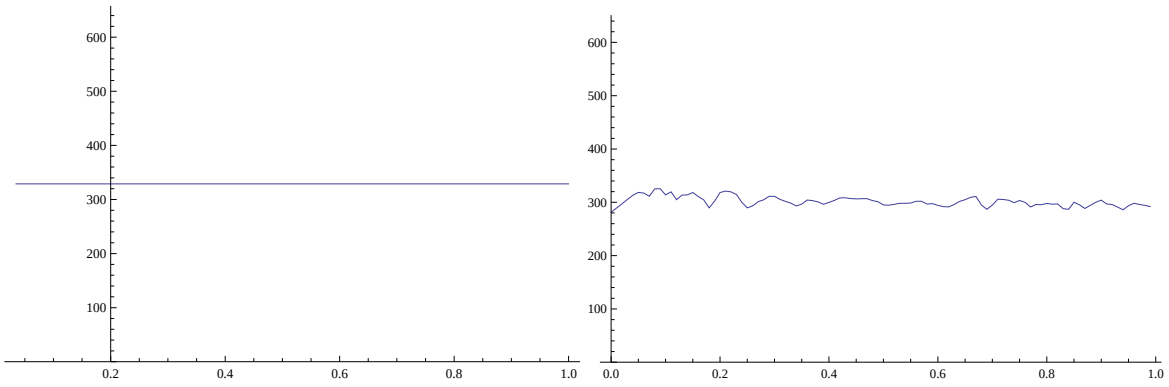


Figure 5: *Energy curves for uniform (left) and variable (right) discretizations.*

4.3 Numerical Implementation

Our discrete action is quadratic in q, hence the system expressing extremization of this action with respect to q is linear. We implemented this system in *Mathematica*, again specifying the initial and final configurations of the body as boundary conditions. For reference, we also implemented a standard (non-adaptive) variational integrator using the same midpoint discretization of the potential. Trajectories produces by these two integrators are shown in figures (4.3) and (6); the corresponding energy curves are given in figure (5).

Although the energy in the irregular case is not preserved as well as in the reference integrator, it does not appear to drift. Again, the inability to perform long-term integration makes it difficult to truly understand the energy behavior of this method. However, it does give hope that adaptivity on arbitrary meshes may be possible.[2]

Practically speaking, the main obstruction to turning the existing integrator into a initial value-type integrator is that (unlike the ODE case) we may not have the same number of material degrees of freedom at the beginning and the end of the action. Hence we cannot merely "swap out" known degrees of freedom at the end for known degrees of freedom near the beginning. We speculate that this situation may reflect the fact that if we lose (or gain) information from the beginning to the end of the integration, it makes it very difficult to conserve momenta in a meaningful way. Clearly there are many more questions to be answered!

References

[1] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration*. Springer-Verlag, 2002.

[2] L. Kharevych, P. Mullen, S. Leyendecker, Y. Tong, J. Marsden, and M. Desbrun. Time adaption strategies for variational integrators. In *to appear*, 2009.

[3] C. Lanczos. *The Variational Principles of Mechanics*. University of Toronto Press, February 1971.

[4] Jerrold E. Marsden, George W. Patrick, and Steve Shkoller. Multisymplectic geometry, variational integrators, and nonlinear pdes. *Comm. Math. Phys*, 199:351–395, 1997.

[5] M. Zielonka, M. Ortiz, and J. Marsden. Variational r-adaption in elastodynamics. In *International Journal for Numerical Methods in Engineering*, 2007.

[2] In the spirit of full disclosure, I will note that my implementation of the integrator for irregular meshes is fairly erratic, and it is possible that the current incarnation of the code does not reflect the true behavior of the algorithm.

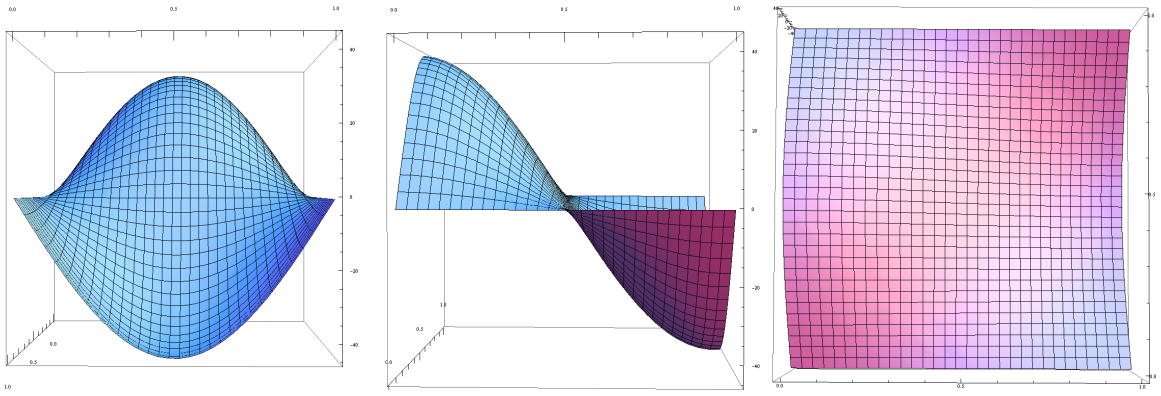


Figure 6: *Spacetime solution of 1D elasticity problem using uniform discretization projected along X (left), t (middle) and q (right) axes.*

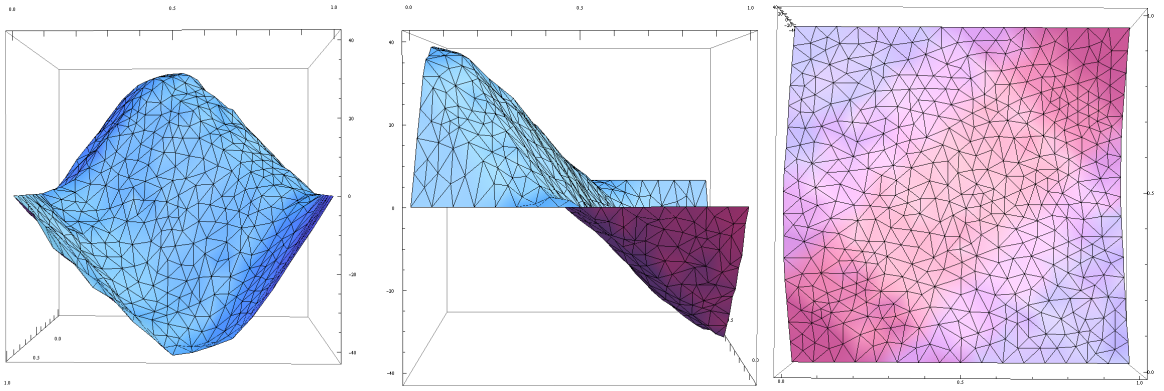


Figure 7: *Spacetime solution of 1D elasticity problem using variable discretization projected along X (left), t (middle) and q (right) axes.*