Solving the scalar wave equation using spacetime discretization

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A. Discretized Lagrangian Approach

Consider the Lagrangian density $\mathcal{L}$ for a free scalar wave equation, that is used to extremize the action $\mathcal{S}$

$$S = \int \mathrm{d}x\,\mathrm{d}t\;\mathcal{L} = \int \left[\frac{1}{2}\eta^{\alpha\beta}\,\partial_\alpha u\,\partial_\beta u\right]\,\mathrm{d}x\,\mathrm{d}t. \tag{1}$$

We wish to find a solution vector $\mathbf{u}$ over a $N \times N$ spacetime grid. Thus $\mathbf{u}$ is a vector of length $N \times N$. Now, we write the discretized version of Eq. (1), by first replacing the continous integral with a summation, and replacing the derivatives by derivative operators. Note, that the summation is over spacetime points.

$$S_d = \frac{1}{2}\sum_{p=0}^{N\times N}\sum_{q=0}^{N\times N} w^{pq}\,\eta_{ab}\,D^a_{pk}u^k\,D^b_{ql}u^l \tag{2}$$

The matrix w^{pq} (an outer product of one-dimensional Curtis-Clenshaw weights) corresponds to the integration weights at each point on the spacetime grid. Further, the derivative operator D^a_{pk} corresponds to the derivative of the vector u^k evaluated at p. Concretely, the operator can be expressed as

$$\eta_{ab}\,D^a_{pk}\,D^b_{ql} = -\mathrm{I}\otimes\mathrm{D}^2_{\mathrm{t}} + \mathrm{D}^2_{\mathrm{x}}\otimes\mathrm{I} \tag{3}$$

for a (1+1) dimensionsal case, which gives a square matrix of dimension $(N \times N)$.

Eq. (2), therefore, can be written in terms of a quadratic form as

$$S_d = \frac{1}{2}\mathbf{u}^T\mathbf{C}\,\mathbf{u};\qquad \mathbf{C} = w^{pq}\,\eta^{ab}\,D^p_{ak}\,D^q_{bl}. \tag{4}$$

Now, given the method of integration, and the choice of basis functions we can construct the matrix C. It's a quadratic form, i.e. S_d is a scalar. Therefore, our problem reduces to finding the vector u^l, such that the scalar S_d is extremum. This is done by requiring

$$\frac{\partial S_d}{d\mathbf{u}} = 0 = \frac{1}{2}\mathbf{u}^T(\mathbf{C}+\mathbf{C}^T) \tag{5}$$

where the last equality is a standard result applicable to quadratic forms. Therefore, to get the solution, we solve the homogenous system of linear equations given by Eq. (5).

For imposing boundary conditions, we use the method of Lagrange multipliers, since this seems the most general and intiutive way to do this.

Appendix A: Finite Element Approach

1. Introduction

We are interested in finding solutions to the scalar wave equation using a finite element approach using spacetime discretization. Specifically, we want to find solutions $u(x,t)$ to

$$u_{tt} - c^2\,\triangle\,u = 0,\qquad \text{in}\quad \Omega\times(0,T], \tag{A1}$$

with boundary and initial conditions (we will check if these are necessary and/or sufficient below)

$$u = 0,\quad \partial_n u = 0 \quad \text{in}\quad \partial\Omega, \tag{A2}$$

$$u(\cdot,0) = f,\quad u_t(\cdot,0) = 0\quad \text{in}\quad \Omega, \tag{A3}$$

where Eq. (A2) enforces a reflecting boundary condition at the spatial boundaries, and Eq. (A3) specifies the initial data in terms of the wave profile and it's derivative at $t = 0$.

2. Variational Formulation

We start by computing the variational formulation of Eq. (A1). If $u(x,t)$ is a solution to Eq. (A1), then for any reasonable test function $v \in \Omega \times (0,T]$

$$u_{tt}\, v - c^2(\triangle u)\, v = 0. \tag{A4}$$

Integrating over the domain $\mathcal{M} = \Omega \times (0,T]$, and using integration by parts for converting the second order derivatives to first order derivatives, we get

$$\int\limits_{\mathcal{M}} u_{tt}\, v \,\mathrm{d}t\, \mathrm{d}\Omega - c^2 \int\limits_{\mathcal{M}} \nabla \cdot (\nabla u)\, v \,\mathrm{d}t\, \mathrm{d}\Omega = 0, \tag{A5}$$

$$\int\limits_{\Omega} [u_t v]_0^T \;\mathrm{d}\Omega - \int\limits_{\Omega} \mathrm{d}\Omega \int\limits_{T} u_t v_t \,\mathrm{d}t + c^2 \int\limits_{T} \mathrm{d}t \int\limits_{\Omega} \nabla u \cdot \nabla v \;\mathrm{d}\Omega - c^2 \int\limits_{T} \mathrm{d}t \int\limits_{\Omega} \nabla \cdot (v\, \nabla u) \;\mathrm{d}\Omega = 0. \tag{A6}$$

Applying Gauss law to the fourth term in the right hand side of Eq. (A6), we get

$$\int\limits_{\Omega} [u_t v]_0^T \;\mathrm{d}\Omega - \int\limits_{\mathcal{M}} u_t v_t \;\mathrm{d}t\mathrm{d}\Omega + c^2 \int\limits_{\mathcal{M}} \nabla u \cdot \nabla v \;\mathrm{d}t\mathrm{d}\Omega - c^2 \int\limits_{T} \mathrm{d}t \oint\limits_{\partial\Omega} v\; (\nabla u \cdot \mathbf{n}) \;\mathrm{d}\Gamma = 0. \tag{A7}$$

The above equation is the intial weak form of the scalar wave equation. We now apply the boundary conditions to set some of the terms to zero[1]. Consider the fourth term in Eq. (A7). We set this to zero, since our boundary conditions demand that the flux $(\nabla u \cdot \mathbf{n})$ at the boundary is zero; see Eq. (A2).The first term can also be (partially) eliminated using using the initial condtions. However, the term $u_t v|_T$ remains, since we do not have a boundary condition there. We could, however, choose a function v, which vanishes at the final time slice, but I'm not sure if that's allowed. For the time, we assume that the first term can also be set to zero in Eq. (A2).

Therefore, we have, together with the Dirichlet boundary conditions

$$-\int\limits_{\mathcal{M}} u_t v_t \,\mathrm{d}t\mathrm{d}\Omega + c^2 \int\limits_{\mathcal{M}} \nabla u \cdot \nabla v \;\mathrm{d}t\mathrm{d}\Omega = 0, \quad \text{in } \Omega, \tag{A8}$$

$$u = 0, \quad \text{in } \partial\Omega. \tag{A9}$$

3. Spacetime discretization

For the sake of simplicity, we consider Eq. (A8) in 1D, where Eq. (A8) becomes much simpler, and reduces to

$$-\int\limits_{\mathcal{M}} u_t v_t \,\mathrm{d}t\mathrm{d}x + c^2 \int\limits_{\mathcal{M}} u_x v_x \;\mathrm{d}t\mathrm{d}x = 0. \tag{A10}$$

The above equation has been derived directly in [1]. We now discretize Eq. (A10) using a spacetime discretization approach, and express u in terms of M basis functions in time $\tilde{\psi}_l(t)$, and N basis functions in space $\tilde{\phi}_i(x)$ as

$$u = \sum_{l=0}^{M} \sum_{i=0}^{N} \tilde{u}_i^l\, \tilde{\phi}_i(x)\, \tilde{\psi}_l(t), \tag{A11}$$

and choose the test function as any of the basis functions

$$v = \tilde{\phi}_j(x)\, \tilde{\psi}_m(t), \tag{A12}$$

as we are free to choose any (reasonable) function in Ω. Plugging these into Eq. (A10), we arrive at (setting $c = 1$ for convinience)

$$-\sum_{i=0}^{N} \sum_{l=0}^{M} u_i^l \int\limits_{x} \mathrm{d}x\, \tilde{\phi}_i(x) \tilde{\phi}_j(x) \int\limits_{T} \mathrm{d}t\, \partial_t \tilde{\psi}_l(t) \partial_t \tilde{\psi}_m^0(t) + \sum_{i=0}^{M} \sum_{l=0}^{N} u_i^l \int\limits_{T} \mathrm{d}t\, \tilde{\psi}_l(t) \tilde{\psi}_m(t) \int\limits_{x} \partial_x \tilde{\phi}_i(x) \partial_x \tilde{\phi}_j(x) = 0. \tag{A13}$$

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[1] How we apply these boundary conditions explicitly in the code is something I'm still working on.

Defining the mass matrix M and stiffness matrix A in the spatial dimension,

$$M := m_{ij} = \int\limits_x \mathrm{dx}\, \tilde{\phi}_i(x)\tilde{\phi}_j(x), \tag{A14}$$

$$A := a_{ij} = \int\limits_x \partial_x\tilde{\phi}_i(x)\partial_x\tilde{\phi}_j(x), \tag{A15}$$

and two additional matrices

$$k_{lm} = \int\limits_T \mathrm{dt}\, \tilde{\psi}_l(t)\tilde{\psi}_m(t), \tag{A16}$$

$$p_{lm} = \int\limits_T \mathrm{dt}\, \partial_t\tilde{\psi}_l(t)\partial_t\tilde{\psi}_m(t), \tag{A17}$$

we can express Eq. (A13) as

$$-\sum_{l=0}^{M}\sum_{i=0}^{N} u_i^l\, m_{ij}\, p_{lm} + \sum_{l=0}^{M}\sum_{i=0}^{N} u_i^l\, a_{ik}\, k_{lm} = 0. \tag{A18}$$

Notice that we have two free indices (j, m) and hence $(j \times m)$ independent equations, the same number as the number of unknowns $(i \times l)$, so things look consistent till now. However, we have boundary conditions, and how many degrees of freedom do they take away?. If we use hat functions as basis functions for both space and time basis dimensions Eqs. (A14–A16), the integrals are simple to evaluate. We will discuss the case for k_{lm} and p_{lm}, since it will give us an implicit time-stepping equation. Let

$$\psi_j(t) = \begin{cases} 0 & \text{if } t \in [t_{l-1}, t_{l+1}] \\ \dfrac{t - t_{l-1}}{t_l - t_{l-1}} & \text{if } t \in [t_{l-1}, t_l] \\ \dfrac{t_{l+1} - t}{t_{l+1} - t_l} & \text{if } t \in [t_l, t_{l+1}] \end{cases}. \tag{A19}$$

Then, we immediately notice that the product of two functions (or their derivatives) would only be non-zero, if there are in the same element, i.e. $[t_{l-1}, t_{l+1}]$. Thus, Eq. (A13) now reduces to (localized in a single element in time)

$$-\sum_{l=0}^{M}\sum_{i=0}^{N} u_i^l\, m_{ij} \int\limits_{t_{l-1}}^{t_{l+1}} \mathrm{dt}\, \partial_t\tilde{\psi}_l(t)\partial_t\tilde{\psi}_m^0(t) + \sum_{l=0}^{M}\sum_{i=0}^{N} u_i^l\, a_{ik} \int\limits_{t_{l-1}}^{t_{l+1}} \mathrm{dt}\, \tilde{\psi}_l(t)\tilde{\psi}_m(t) = 0. \tag{A20}$$

The only surviving elements in k_{lm} and p_{lm}

$$k_{l-1,l} = h_0/6, \quad k_{ll} = 2h_0/3, \quad k_{l,l+1} = h_0/6, \tag{A21}$$

$$p_{l-1,l} = -1/h_0, \quad p_{ll} = 2/h_0, \quad p_{l,l+1} = -1/h_0, \tag{A22}$$

where $h_0 = t_l - t_{l-1}$ is the unform spacing in time. Finally, plugging Eq. (A21) into Eq. (A20), gives us an implicit step in time, as

$$-\sum_{i=0}^{N} m_{ij}\, \left(u_i^{l-1}p_{l-1,l} + u_i^l p_{l,l} + u_i^{l+1}p_{l,l+1}\right) + \sum_{i=0}^{N} a_{ij}\, \left(u_i^{l-1}k_{l-1,l} + u_i^l k_{l,l} + u_i^{l+1}k_{l,l+1}\right) = 0, \tag{A23}$$

$$M\left(\frac{1}{h_0}\mathbf{u}^{l+1} - \frac{2}{h_0}\mathbf{u}^l + \frac{1}{h_0}\mathbf{u}^{l-1}\right) = -A\left(\frac{h_0}{6}\mathbf{u}^{l+1} + \frac{2h_0}{3}\mathbf{u}^l + \frac{h_0}{6}\mathbf{u}^{l-1}\right) \tag{A24}$$

Therfore, given $\mathbf{u}^r$ and $\mathbf{u}^{r-1}$, both vectors of length N, we can solve for $\mathbf{u}^{k+1}$, using the equation

$$M\left(\mathbf{u}^{r+1} - 2\mathbf{u}^r + \mathbf{u}^{r-1}\right) = -Ah_0^2\left(\frac{1}{6}\mathbf{u}^{r+1} + \frac{2}{3}\mathbf{u}^r + \frac{1}{6}\mathbf{u}^{r-1}\right), \tag{A25}$$

which can be cast in the form of $\tilde{A}\, x = b$, where

$$\tilde{A} = M + \frac{h_0^2}{6} A, \tag{A26}$$

$$x = \mathbf{u}^{r+1}, \tag{A27}$$

$$b = 2\,\mathbf{u}^r \left(M - \frac{2h_0^2}{3} A \right) - \mathbf{u}^{r-1} \left(M + \frac{h_0^2}{6} A \right) \tag{A28}$$

Appendix B: Discretized Euler-Lagrange Equations Approach

In the previous section, we started with the equations of motion followed by a spacetime discretization to arrive at the numerical implementation of the problem. However, we can instead start by discretizing the Lagrangian to arrive at a similar implicit time-stepping scheme, which is the focus of this section. For a discrete formulation of the action princple, we begin by discretizing in time (t_n), and approximating the discrete Lagrangian for a time interval (t_n, t_{n+1})

$$L_d(q_n, q_{n+1}) \approx \int_{t_n}^{t_{n+1}} L(q, \dot{q})\, \mathrm{d}t, \tag{B1}$$

where $q_n = q(t_n)$ is a sequence of configuations in time. We can then approximate the action integral as

$$S_d(q_0, q_1, ..., q_N) = \sum_{n=0}^{N-1} L_d(q_n, q_{n+1}) \approx \int_0^T L(q, \dot{q})\, \mathrm{d}t. \tag{B2}$$

Now, if we deman that the variation $\delta S_d(q_0, q_1, ..., q_N) = 0$, for the true configuration at each time level, then the variation of the discrete action can be written as

$$\delta S_d(q_0, q_1, ..., q_N) = \sum_{n=0}^{N-1} \left[D_1\, L_d(q_n, q_{n+1}) \cdot \delta q_n + D_2\, L_d(q_n, q_{n+1}) \cdot \delta q_{n+1} \right]. \tag{B3}$$

Using summation by parts on the second term in Eq. (B3), and the fact that the variation at the end points vanish ($\delta q_0 = \delta q_N = 0$), we get

$$\delta S_d(q_0, q_1, ..., q_N) = \sum_{n=1}^{N-1} \left[D_1\, L_d(q_n, q_{n+1}) \cdot \delta q_n + D_2\, L_d(q_{n-1}, q_n) \right] \cdot \delta q_n, \tag{B4}$$

which gives us

$$\left[D_1\, L_d(q_n, q_{n+1}) \cdot \delta q_n + D_2\, L_d(q_{n-1}, q_n) \right] = 0, \quad n = 1, 2, ..., N-1, \tag{B5}$$

which gives an implicit time-stepping scheme to go from (q_{n-1}, q_n) to $(q_n, q_n + 1)$ at each time level n.

[1] G. Zumbusch, Classical and Quantum Gravity **26**, 175011 (2009), arXiv:0901.0851 [gr-qc].