A Space-time Symmetry Preserving Discretization Scheme for IVPs

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A.R., J. Nordström: arXiv:2307.04490 (accepted in JCP), and JCP 477 (2023) 111942

Norwegian Particle, Astroparticle & Cosmology Theory network

Outline

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- Motivation: Challenges in treating IVPs
- Formulating IVPs on the level of the system action
- The world-line formalism from general relativity
- A discretization scheme preserving space-time symmetries
- Summary

Motivation

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- Intrinsic constraints not maintained in deriving governing equations (corrections need to be introduced aposteriori) M.C. Pinto, M. Mounier, E. Sonnendrücker, *Appl. Math. and Comp.* 272 (2016)

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Solution I: discretize IVPs directly on the level of the system action and obtain the classical solution from a optimization procedure.
(no need to derive governing equations)

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Solution II: borrow concepts from general relativity to disentangle discretization from space-time symmetries

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Formulating IVPs on the level of the system action

Towards initial value problems

- Starting point: Lagrangian formulation

$$\mathcal{S} = \int_{t_i}^{t_f} \mathcal{L}[x, \dot{x}]dt = \int_{t_i}^{t_f} \Big(\frac{1}{2}m\dot{x}^2(t) - V(x)\Big)dt$$

Towards initial value problems

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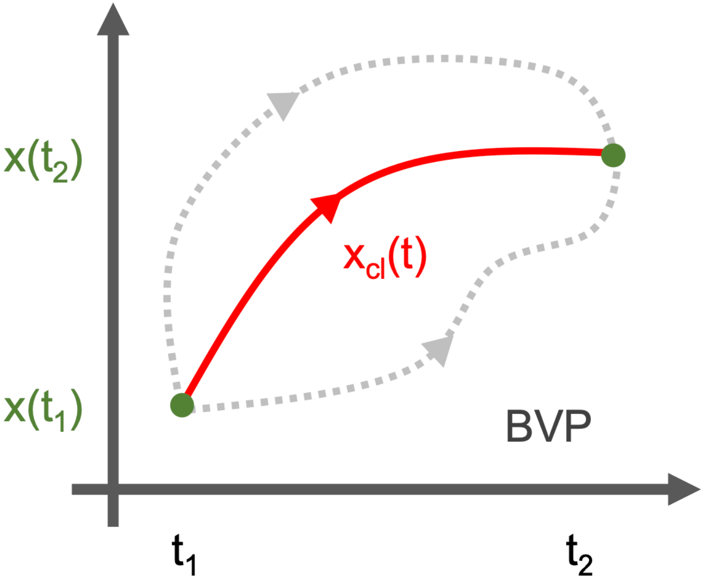
- Variational principle as boundary value problem

$$\delta\mathcal{S} = 0 \quad \Rightarrow \quad \frac{\partial\mathcal{L}}{\partial x} - \partial_t \frac{\partial\mathcal{L}}{\partial\dot{x}} = 0$$



both starting and end point of the trajectory must be known apriori

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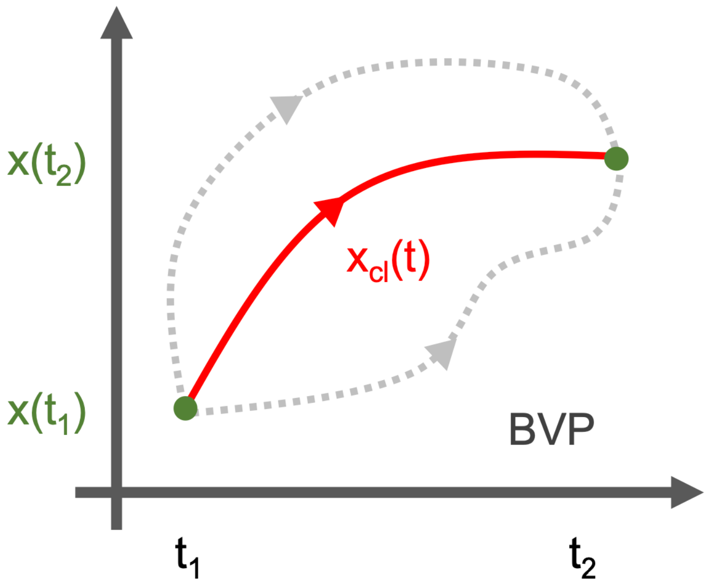
- Reinterpretation as initial value problem only after derivation of equation of motion



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A variational principle for IVPs

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Quantum: L. Keldysh Sov. Phys. JETP. 20: 1018, (1965)
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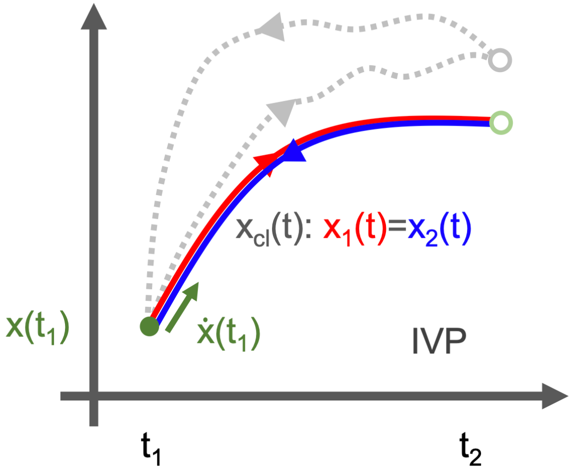

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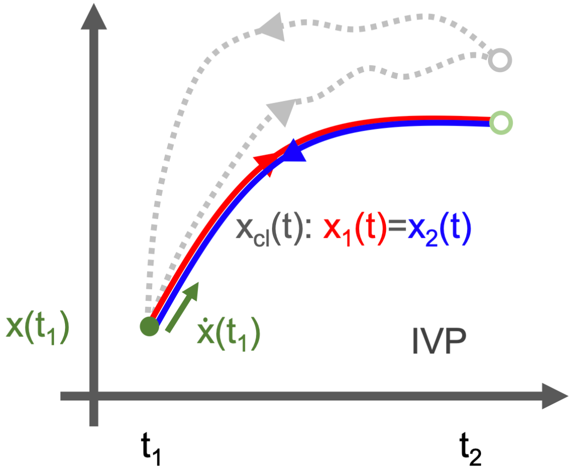

only initial value and derivatives need to be supplied.

- "Double shooting method":

$$x_{1,2}(t_i) = x_i \quad \dot{x}_1(t_i) = \dot{x}_i$$

initial conditions

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

connecting conditions

The world-line formalism from general relativity

General Relativity's Worldline Formalism

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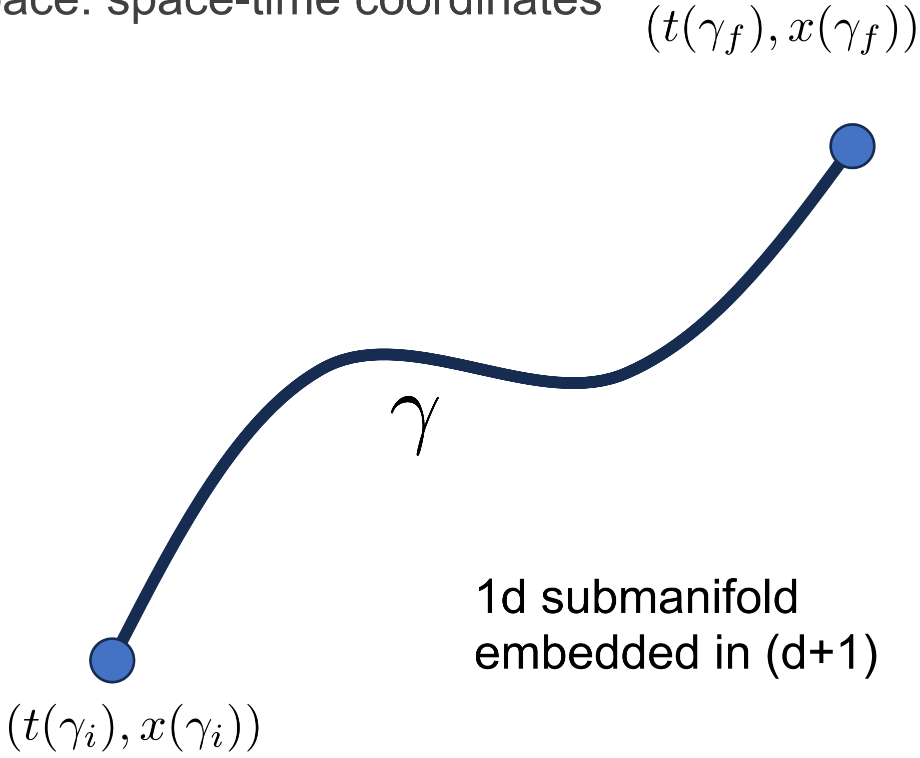
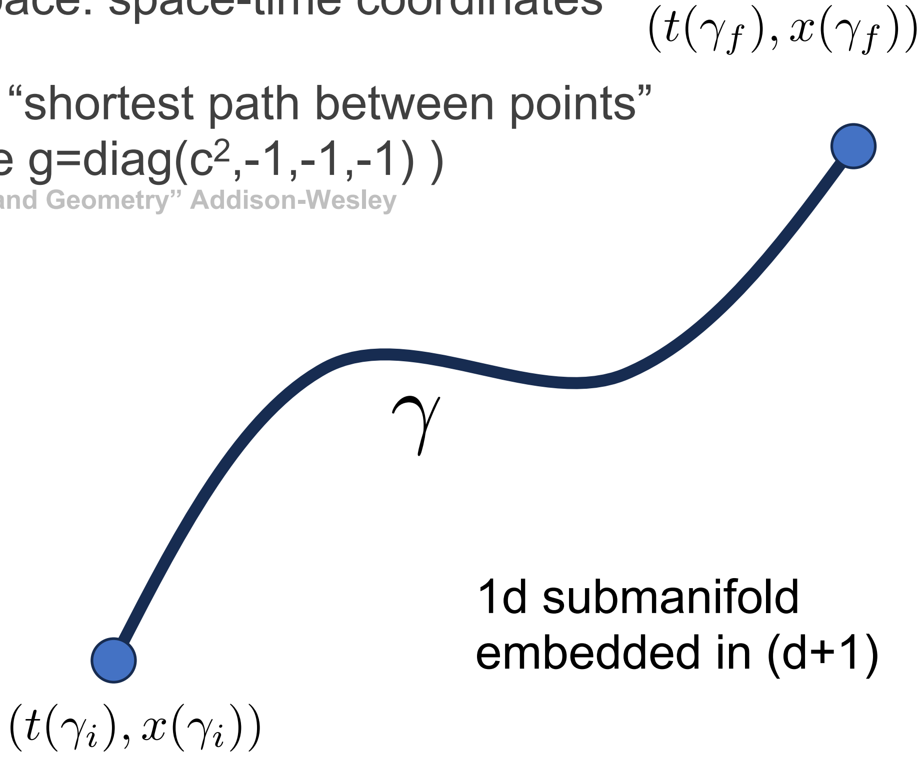
- Requires equal treatment of time and space: space-time coordinates



General Relativity's Worldline Formalism

- Requires equal treatment of time and space: space-time coordinates
- Trajectory of particle given by geodesic: "shortest path between points" for a given space-time metric (flat space g=diag(c^2,-1,-1,-1))

see e.g. S. Carroll "Spacetime and Geometry" Addison-Wesley



1d submanifold embedded in (d+1)

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- Variational principle via reparameterization invariant geodesic action
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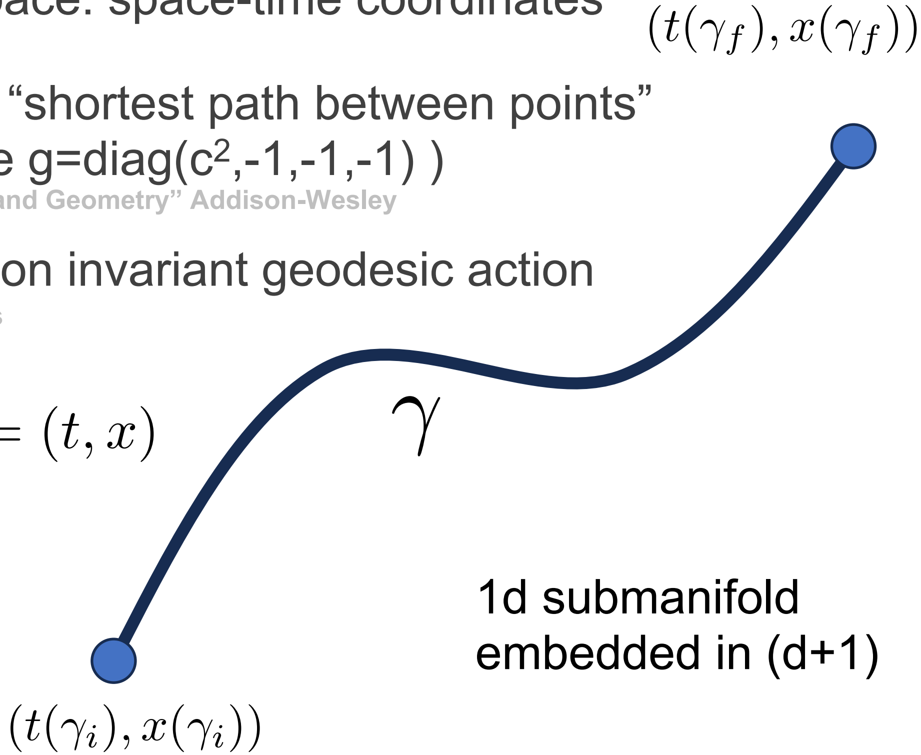
$$\mathcal{S} = \int_{\gamma_i}^{\gamma_f} d\gamma \, (-mc) \sqrt{g_{\mu\nu} \frac{dx^\mu}{d\gamma} \frac{dx^\nu}{d\gamma}} \qquad x^\mu = (t, x)$$



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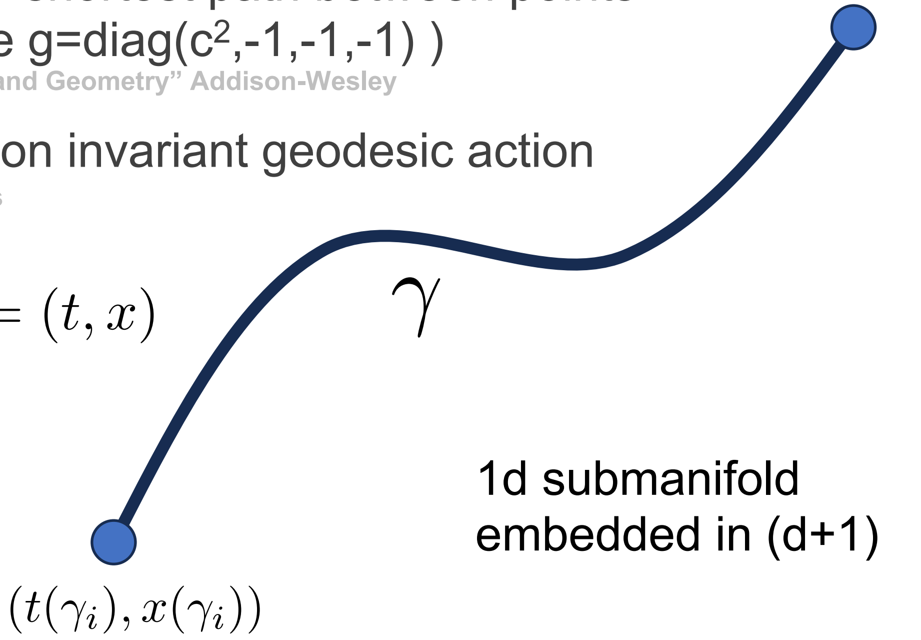
$$(t(\gamma_i),x(\gamma_i)) = (t_i,x_i)$$
$$(t(\gamma_f),x(\gamma_f)) = (t_f,x_f)$$

$$\frac{d^2x^\alpha}{d\gamma^2} + \Gamma^\alpha_{\mu\nu}\frac{dx^\mu}{d\gamma}\frac{dx^\nu}{d\gamma} = 0$$



Geometrizing the interactions

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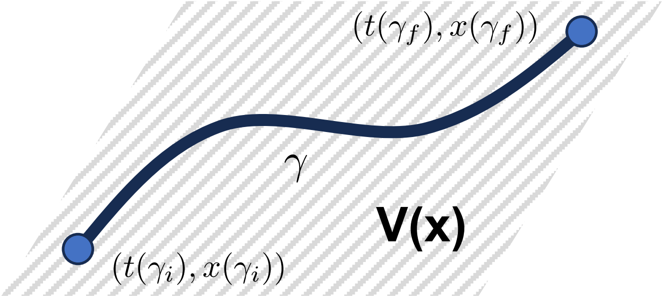
- Modify the metric so that the same trajectory ensues for interacting particle in flat spacetime and non-interacting particle in a non-flat spacetime

see e.g. S. Carlip: General Relativity: A Concise Introduction. OUP Oxford



g=diag(c^2, -1)

$$\mathcal{S}_{\rm flat} = \int_{\gamma_i}^{\gamma_f} d\gamma(-mc)\sqrt{c^2\Big(\frac{dt}{d\gamma}\Big)^2 - \Big(\frac{dx}{d\gamma}\Big)^2} + V(x)$$

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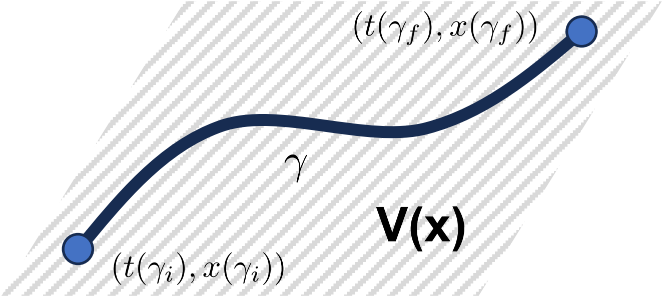

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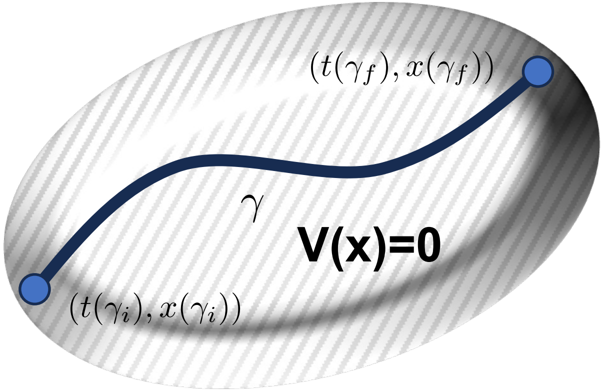

g=diag(c^2, -1)

$$\frac{V(x)}{2mc^2} \ll 1$$

g=diag(c^2 + V(x)/2m , -1)

$$\mathcal{S}_{\text{flat}} = \int_{\gamma_i}^{\gamma_f} d\gamma(-mc)\sqrt{c^2\left(\frac{dt}{d\gamma}\right)^2 - \left(\frac{dx}{d\gamma}\right)^2} + V(x)$$

$$\mathcal{S} = \int_{\gamma_i}^{\gamma_f} d\gamma\,(-mc)\sqrt{g_{00}\left(\frac{dt}{d\gamma}\right)^2 - \left(\frac{dx}{d\gamma}\right)^2}$$

Equation of motion

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- Reparameterization invariance will impede numerical search for critical point

$$\mathcal{S} = \int_{\gamma_i}^{\gamma_f} d\gamma \, (-mc) \sqrt{g_{\mu\nu} \frac{dx^\mu}{d\gamma} \frac{dx^\nu}{d\gamma}}$$

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$$\mathcal{E}_{\rm BVP} = \int_{\gamma_i}^{\gamma_f} d\gamma E_{\rm BVP}[t,\dot{t},x,\dot{x}] = \int_{\gamma_i}^{\gamma_f} d\gamma \frac{1}{2}\Big(g_{00}\Big(\frac{dt}{d\gamma}\Big)^2 + g_{11}\Big(\frac{dx}{d\gamma}\Big)^2\Big)$$

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- The following geodesic equations ensue from the action E:

$$\frac{d}{d\gamma}\Big(g_{00}\frac{dt}{d\gamma}\Big) = 0, \qquad \frac{d}{d\gamma}\Big(\frac{dx}{d\gamma}\Big) + \frac{1}{2}\frac{\partial g_{00}}{\partial x}\Big(\frac{dt}{d\gamma}\Big)^2 = 0$$

A discretization scheme preserving space-time symmetries

Discretizing the Worldline as BVP

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- Discretize in the world-line parameter using summation-by-parts finite differences:

for a review of SBP operators see D. Fernández, J. E. Hicken, and D. W. Zingg, Comp. & Fluids 95 171 (2014)

$$\mathbb{E}_{\rm BVP} = \frac{1}{2}\Big\{\Big(\big(c^2 + \frac{2V(\mathbf{x})}{m}\big)\circ \mathbb{D}\mathbf{t}\Big)^{\rm T}\mathbb{H}\,(\mathbb{D}\mathbf{t}) - (\mathbb{D}\mathbf{x})^{\rm T}\mathbb{H}\,(\mathbb{D}\mathbf{x})\Big\}$$
$$+ \lambda_1(\mathbf{t}[1] - t_i) + \lambda_2(\mathbf{t}[N_\gamma] - t_f)$$
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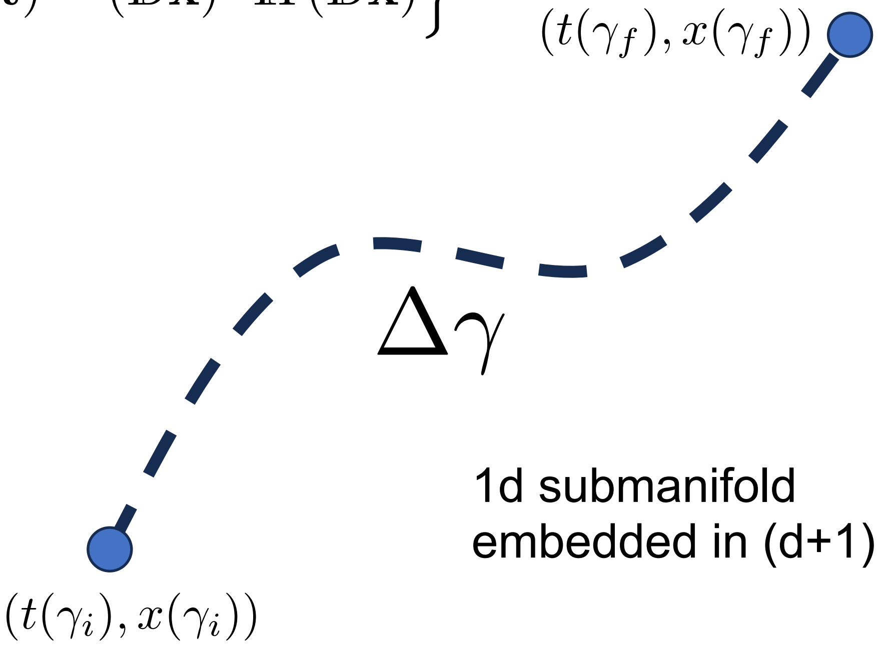

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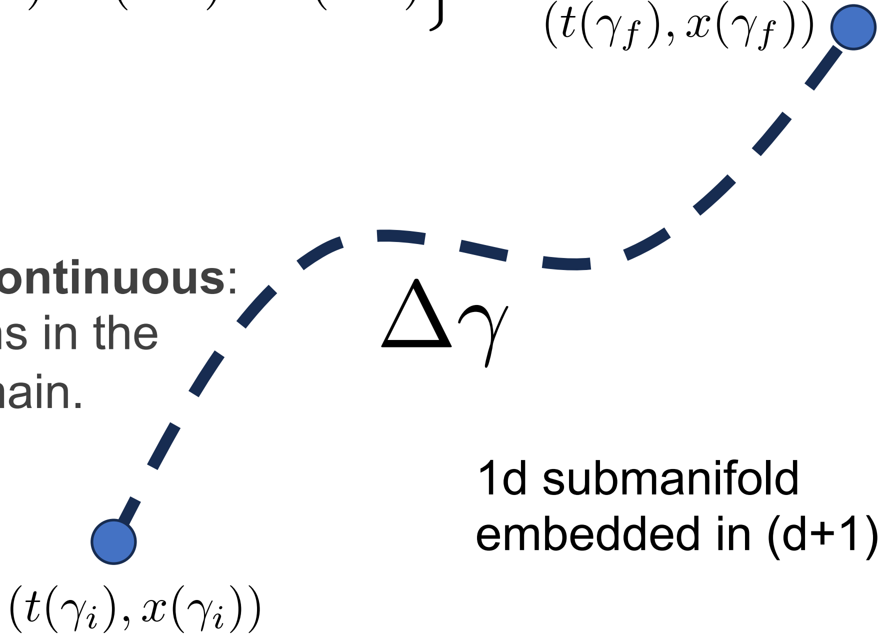
$$+ \lambda_1(\mathbf{t}[1] - t_i) + \lambda_2(\mathbf{t}[N_\gamma] - t_f)$$
$$+ \lambda_3(\mathbf{x}[1] - t_i) + \lambda_4(\mathbf{x}[N_\gamma] - x_f)$$

- Note that the values of **t** and **x** remain **continuous**: explicit invariance under time translations in the discrete setting. No issue with finite domain.



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$$\mathbb{E}_{\mathrm{BVP}} = \frac{1}{2}\Big\{\Big(\Big(c^2 + \frac{2V(\mathbf{x})}{m}\Big)\circ \mathbb{D}\mathbf{t}\Big)^{\mathrm{T}}\mathbb{H}\,(\mathbb{D}\mathbf{t}) - (\mathbb{D}\mathbf{x})^{\mathrm{T}}\mathbb{H}\,(\mathbb{D}\mathbf{x})\Big\}$$
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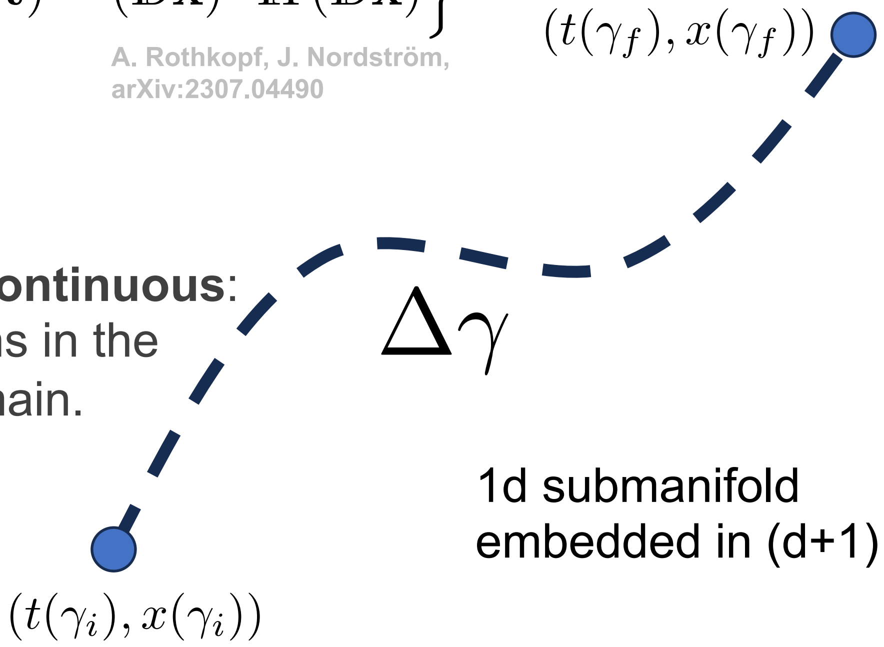
A. Rothkopf, J. Nordström, arXiv:2307.04490



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- Noether charge:

$$\mathbb{Q}_{\mathbf{t}} = 2(\mathbb{D}\mathbf{t})\circ(\mathbf{1}+2\mathbf{V}(\mathbf{x})/m)$$

Now reformulate as IVP

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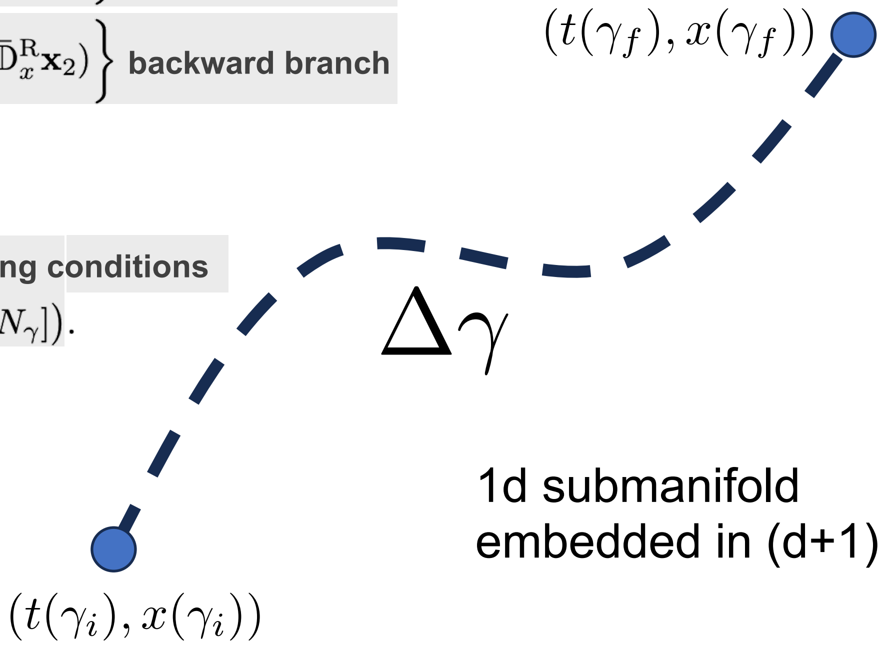
- Forward-backward construction for both time and space coordinate

$$
\begin{aligned}
\mathbb{E}_{\rm IVP} =& \frac{1}{2}\left\{(\bar{\mathbb{D}}_t^{\rm R}\mathbf{t}_1)^{\rm T}\mathbb{d}\left[c^2 + \frac{2\mathbf{V}(\mathbf{x}_1)}{m}\right]\bar{\mathbb{H}}(\bar{\mathbb{D}}_t^{\rm R}\mathbf{t}_1) - (\bar{\mathbb{D}}_x^{\rm R}\mathbf{x}_1)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}_x^{\rm R}\mathbf{x}_1)\right\} \quad \text{forward branch}\\
&-\frac{1}{2}\left\{(\bar{\mathbb{D}}_t^{\rm R}\mathbf{t}_2)^{\rm T}\mathbb{d}\left[c^2 + \frac{2\mathbf{V}(\mathbf{x}_2)}{m}\right]\bar{\mathbb{H}}(\bar{\mathbb{D}}_t^{\rm R}\mathbf{t}_2) - (\bar{\mathbb{D}}_x^{\rm R}\mathbf{x}_2)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}_x^{\rm R}\mathbf{x}_2)\right\} \quad \text{backward branch}\\
&+\lambda_1\big(\mathbf{t}_1[1] - t_i\big) + \lambda_2\big((\mathbb{D}\mathbf{t}_1)[1] - \dot{t}_i\big) + \lambda_3\big(\mathbf{x}_1[1] - x_i\big)\\
&+\lambda_4\big((\mathbb{D}\mathbf{x}_1)[1] - \dot{x}_i\big) \quad \text{initial conditions}\\
&+\lambda_5\big(\mathbf{t}_1[N_\gamma] - \mathbf{t}_2[N_\gamma]\big) + \lambda_6\big(\mathbf{x}_1[N_\gamma] - \mathbf{x}_2[N_\gamma]\big) \quad \text{connecting conditions}\\
&+\lambda_7\big((\mathbb{D}\mathbf{t}_1)[N_\gamma] - (\mathbb{D}\mathbf{t}_2)[N_\gamma]\big) + \lambda_8\big((\mathbb{D}\mathbf{x}_1)[N_\gamma] - (\mathbb{D}\mathbf{x}_2)[N_\gamma]\big).
\end{aligned}
$$



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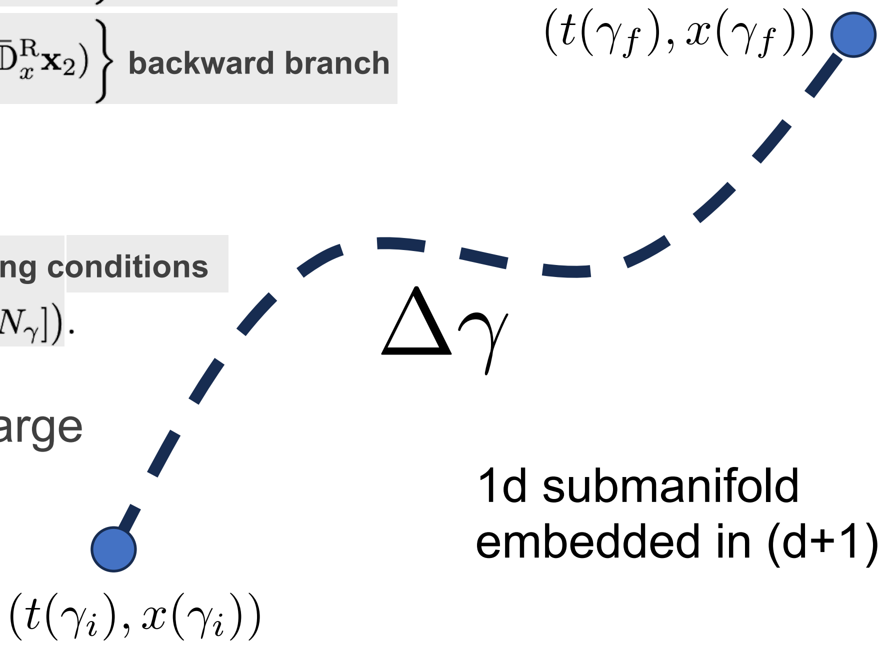
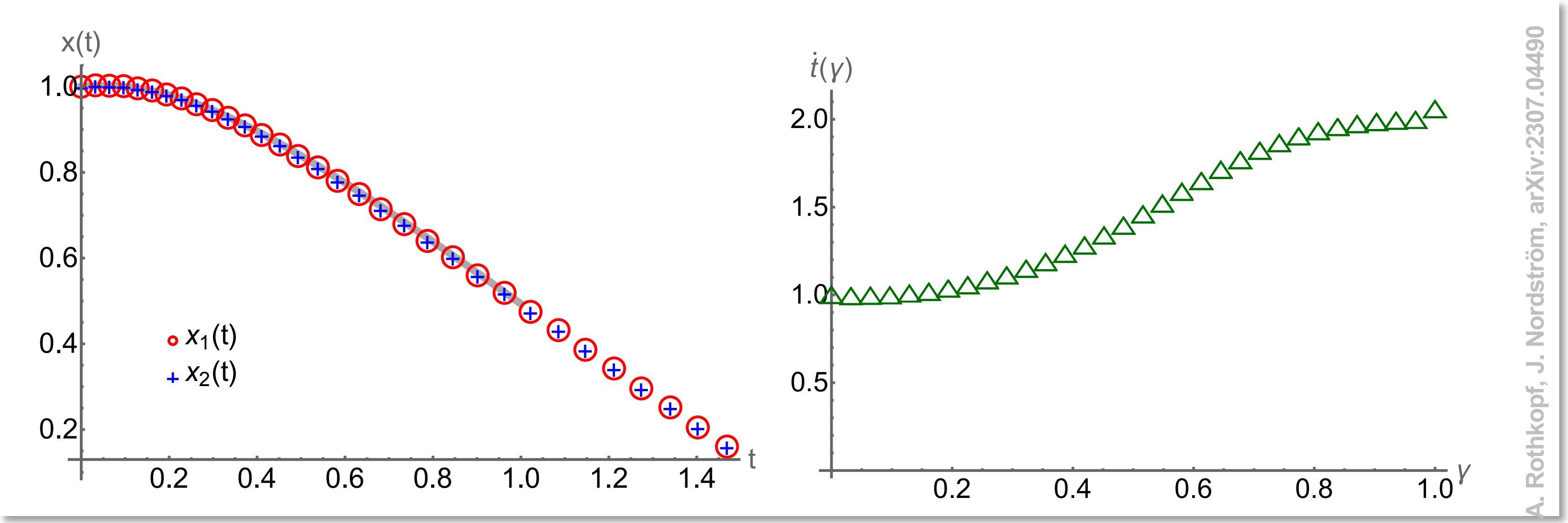
- Lagrange multipliers modify Noether charge

$$\mathbb{Q}_{\mathbf{t}} = 2(\mathbb{D}\mathbf{t})\circ(\mathbf{1}+2\mathbf{V}(\mathbf{x})/m) + \lambda_2\delta(\gamma-\gamma_i)+\lambda_7\delta(\gamma-\gamma_f)$$



Nonlinear potential case V(x)=kx⁴

- End of simulation now emerges dynamically, as time is dynamical on worldline
- Temporal grid spacing adapts to the dynamics of the position coordinate: a form of **automatic adaptive mesh refinement**



Discretized Noether charge

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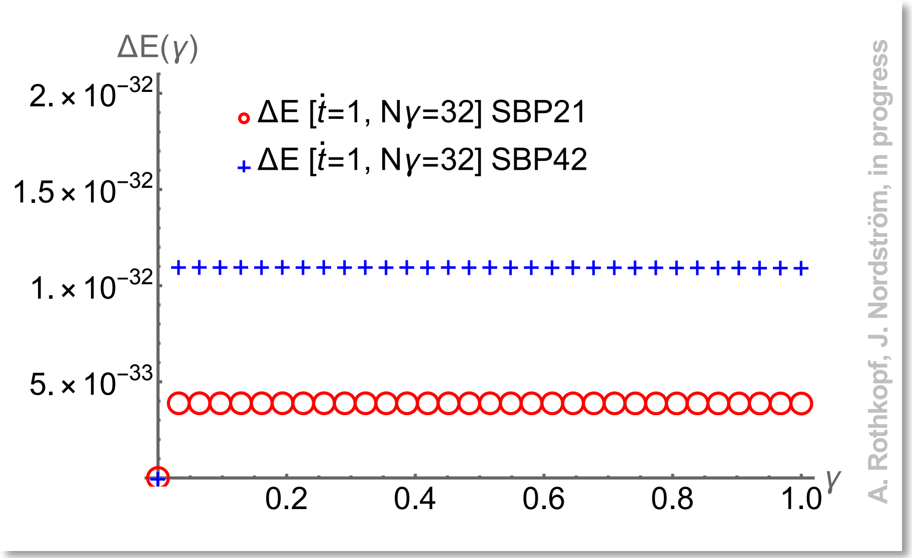
- Manifest time-translation invariance of action: **exactly preserved Noether charge**

$$\Delta\mathbf{E} = \mathbb{Q}_\mathbf{t} - Q_t = (\mathbb{D}\mathbf{t})\circ(\mathbf{1}+2\kappa\mathbf{x}^4) + \lambda_2\mathfrak{d}_1 + \lambda_7\mathfrak{d}_{N_\gamma} - \dot{t}_i(1+2\kappa x_i^4)$$



- Noether charge not only conserved but exhibits correct **continuum value**

Convergence properties

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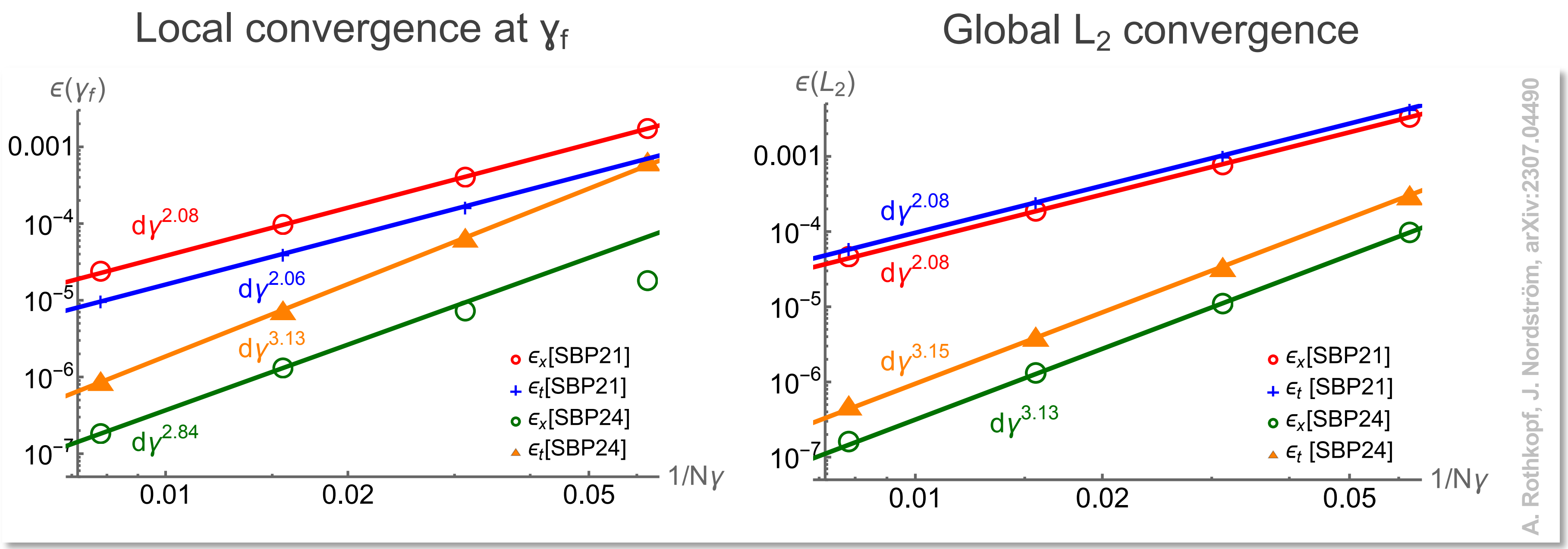

- Global convergence en-par with expectations for stable SBP schemes

Summary

- IVPs directly formulated on the action level using forward-backward construction
- General Relativity offers alternative action formulation in terms of world-lines
- Discretization on action level via a single type of SBP finite difference operator
- Discretization of world-line action retains continuum symmetries
- **Dynamical** emergence of **time-mesh** & **exact conservation** of Noether charge

Summation-by-parts finite differences

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- Derivation of Noether theorem or governing equations rely on integration by parts

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$$\int_{t_i}^{t_f} dt\, u(t)\, v(t) \approx \mathbf{u}^t\, \mathbb{H}\, \mathbf{v}$$

quadrature rule

⟷

$$\mathbb{D} = \mathbb{H}^{-1}\mathbb{Q}$$ finite difference

$$\mathbb{Q} + \mathbb{Q}^t = \mathbb{E}_N - \mathbb{E}_0$$

$$= \mathrm{diag}[-1, 0, \ldots, 0, 1]$$

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$$\mathbb{H}^{[2,1]} = \Delta t \begin{bmatrix} \frac{1}{2} & & & \\ & 1 & & \\ & & 1 & \\ & & & \frac{1}{2} \end{bmatrix} \qquad \mathbb{D}^{[2,1]} = \frac{1}{\Delta t}\begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

$$(\mathbb{D}\mathbf{u})^t\, \mathbb{H}\, \mathbf{v} = -\mathbf{u}^t\, \mathbb{H}\, \mathbb{D}\mathbf{v} + \mathbf{u}_N \mathbf{v}_N - \mathbf{u}_0 \mathbf{v}_0$$