A variational approach to discretised initial value problems

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in collaboration with Jan Nordström
A.R., J. Nordström: arXiv:2307.04490,
see also JCP 477 (2023) 111942

Norwegian Particle, Astroparticle & Cosmology Theory network

Symmetries on a lattice

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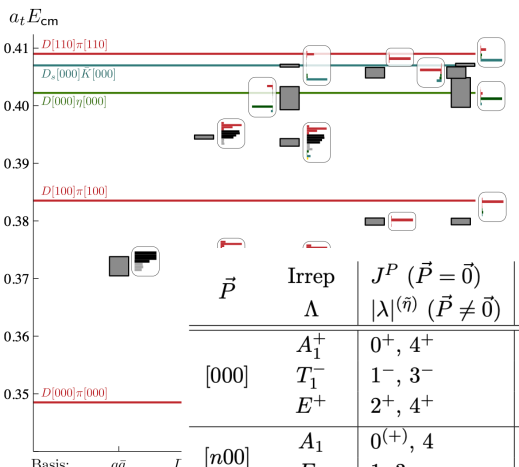
- **Internal symmetries** preserved through discrete formulation:
  local SU(N) via link variables, chiral symmetry via Overlap Dirac operator

- **Spacetime symmetries** explicitly broken:
  absence of continuous translation and rotation invariance modify physics of orbital angular momentum and spin (mixing of otherwise orthogonal states).

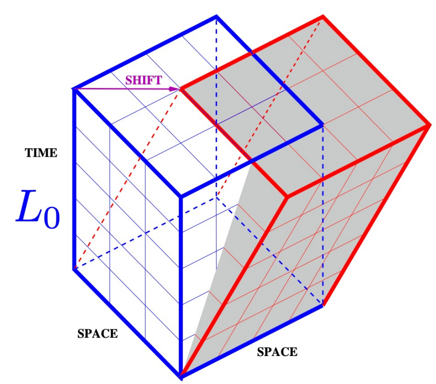


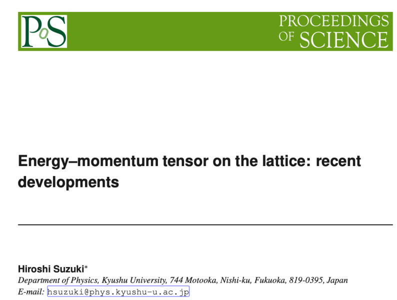
$\vec{P}$	Irrep Λ	J^P $(\vec{P}=\vec{0})$ $\lvert\lambda\rvert^{(\tilde{\eta})}$ $(\vec{P}\neq\vec{0})$	$D\pi$ $J^P_{[N]}$	$D^*\pi$ $J^P_{[N]}$
[000]	A_1^+	0^+, 4^+	$\mathbf{0^+}$, ...	...
	T_1^-	1^-, 3^-	$\mathbf{1^-}$, ...	...
	E^+	2^+, 4^+	$\mathbf{2^+}$, ...	...
$[n00]$	A_1	$0^{(+)}$, 4	$\mathbf{0^+}$, $\mathbf{1^-}$, 2^+, ...	...
	E_2	1, 3	$\mathbf{1^-}$, 2^+, ...	$\mathbf{1^+}$, ...
$[nn0]$	A_1	$0^{(+)}$, 2, 4	$\mathbf{0^+}$, $\mathbf{1^-}$, $2^+_{[2]}$, ...	...
	B_2, B_2	1, 3	$\mathbf{1^-}$, 2^+, ...	$\mathbf{1^+}$, ...
$[nnn]$	A_1	$0^{(+)}$, 3	$\mathbf{0^+}$, $\mathbf{1^-}$, 2^+, ...	...

Hadron spectroscopy

see e.g. HadSpec Collaboration JHEP 07 (2021) 123

$$T^{\mathrm{cont}}_{\mu\nu} \text{ vs. } T^{\mathrm{latt}}_{\mu\nu} = z_1 T^{[6]}_{\mu\nu} + z_2 T^{[3]}_{\mu\nu} + z_3 T^{[1]}_{\mu\nu}$$




PoS PROCEEDINGS OF SCIENCE

Energy–momentum tensor on the lattice: recent developments

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Energy Momentum Tensor

see e.g. H. Suzuki PoS LATTICE2016 (2017) 002 and references therein

The conventional lattice approach

- Simplest case: non-relativistic point particle under the influence of a potential

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

- Proving time translational invariance involved: replacement of x(t) by derivative and bounds of integral are affected. Due to infinitesimal δt Noether theorem holds

$$x(t+\delta t) = x(t) + \delta t\, \dot{x}(t) \qquad \mathcal{S} \overset{t+\delta t}{\longrightarrow} \mathcal{S}$$

- After discretization: Δt finite, requires infinite sum for translation – unclear substitution at final time step. Noether theorem does not hold, i.e. energy not conserved

$$\mathbb{S} = \sum_{k=1}^{N_t} \Big(\frac{1}{2} m (\mathbb{D}\mathbf{x})_i^2 - V(\mathbf{x}_i)\Big) \Delta t_i$$

- Usual way out: go over to Hamiltonian picture where time remains continuous and implement symplectic time stepping for e.o.m. (energy conserved on average/staggering)

The worldline picture of GR

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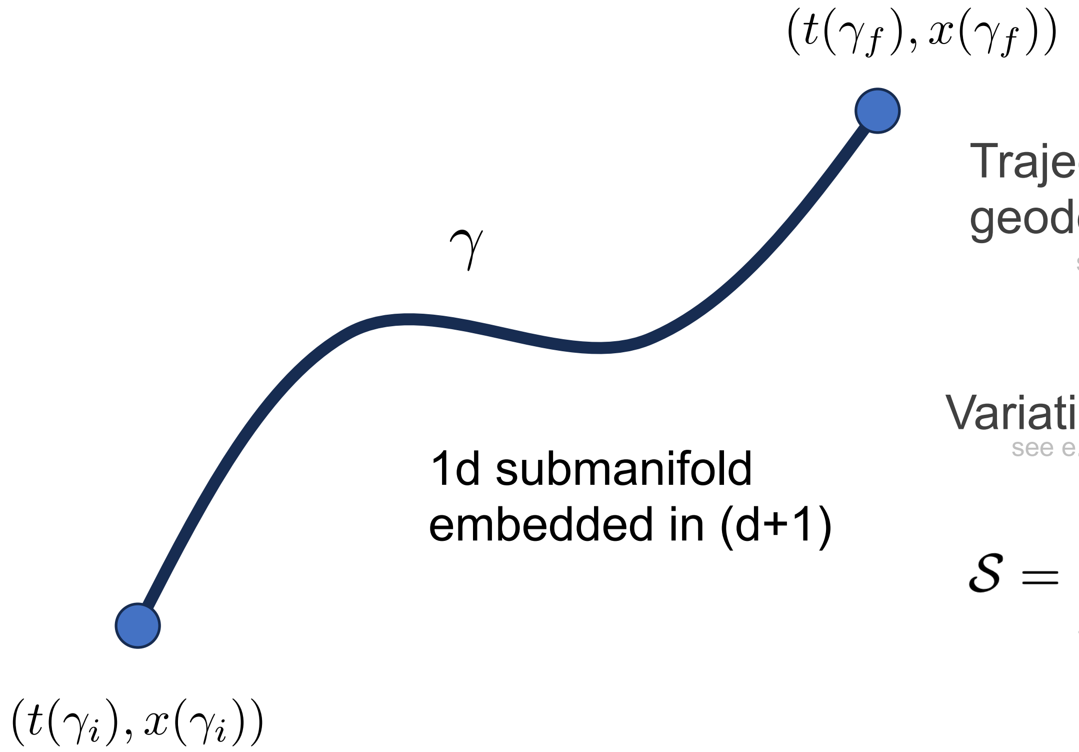
- Simplest case: free point particle in spacetime described by metric g



Trajectory of particle given by geodesic: “shortest path between points”

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

Variational principle via geodesic action

see e.g. J. Jost, X. Li-Jost ” Calculus of Variations” Cam.Uni.Press

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

$$\mathbf{x}(\gamma_i) = \mathbf{x}_i, \;\; \mathbf{x}(\gamma_f) = \mathbf{x}_f$$

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

- Reparameterization invariant ɣ->ɣ’. Time and position dependent on ɣ.

Symmetries in General Relativity

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- Comparing of quantities at different space-time points non-trivial for non-flat metric
- Systematically identify conserved quantities via Killing vectors K:

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

$$\Big(\frac{\partial K_\mu}{\partial x^\nu} - \Gamma^\alpha_{\mu\nu} K_\alpha\Big) + \Big(\frac{\partial K_\nu}{\partial x^\mu} - \Gamma^\alpha_{\nu\mu} K_\alpha\Big) = 0$$

- Conserved quantities associated with K, constructed such that their dependence on the world-line parameter vanishes on the geodesic (c.f. Noether theorem on-shell)

$$Q_K = g_{\alpha\beta} K^\alpha \dot{x}^\beta$$

relativistic Noether charge

- Interestingly involves only a single derivative in case of translations, rotations or boosts.

Geometrizing the interactions

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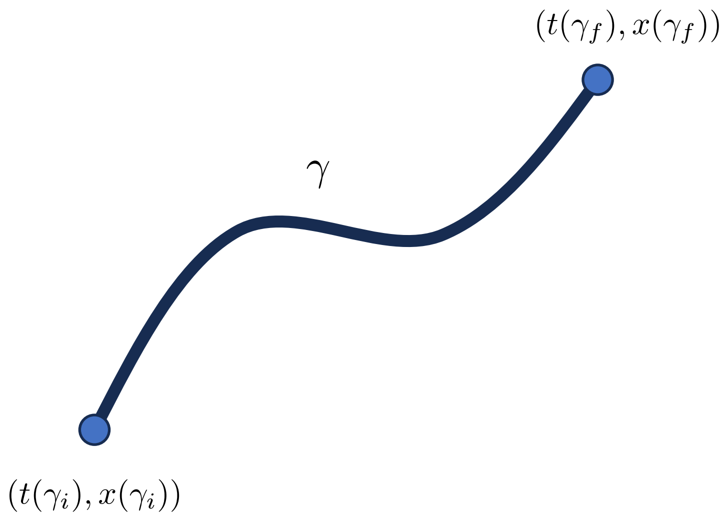
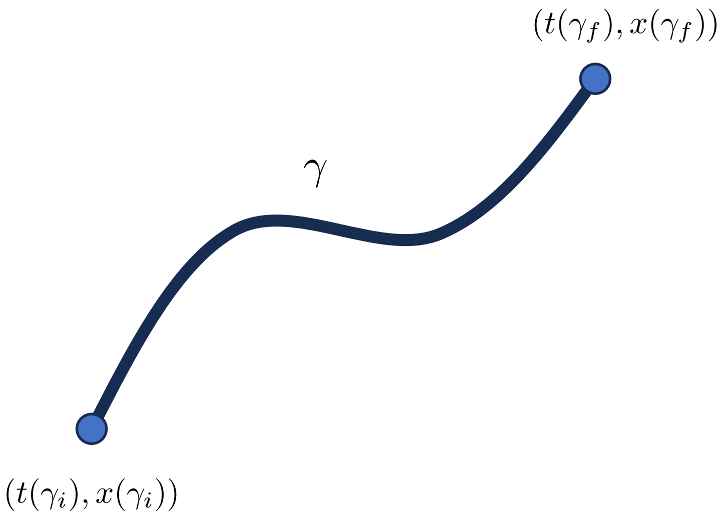
- Can one modify metric so that same trajectory ensues for non-interacting particle in a non-flat spacetime as for interacting particle in flat spacetime?



$$\approx$$

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



g=diag(c^2, -1)

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

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

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

- Yes: follows same logic as when deriving Newtons law in the weak gravity limit

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

Modified geodesic action

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- Reparameterization invariance is cumbersome for numerical optimization. Take instead the square of the integrand, which leaves extremum unchanged.

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

- Same geodesic equations ensure for S and E:

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

Summation by parts discretization

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- Consistent discretization of integration and derivatives: summation-by-parts

$$\langle x, y\rangle = \int d\gamma x(\gamma)y(\gamma) \rightarrow (\mathbf{x},\mathbf{y}) = \mathbf{x}^{\mathrm{T}}\mathbb{H}\mathbf{y}$$

$$\mathbb{D} = \mathbb{H}^{-1}\mathbb{Q}, \qquad \mathbb{Q}^{\mathrm{T}} + \mathbb{Q} = \mathbb{E}_N - \mathbb{E}_0 = \mathrm{diag}[-1, 0, \ldots, 0, 1]$$

$$\mathbb{H}^{[2,1]} = \Delta\gamma \begin{bmatrix} 1/2 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1/2 \end{bmatrix}, \quad \mathbb{D}^{[2,1]} = \frac{1}{2\Delta\gamma}\begin{bmatrix} -2 & 2 & & & \\ -1 & 0 & 1 & & \\ & & \ddots & & \\ & & -1 & 0 & 1 \\ & & & -2 & 2 \end{bmatrix}$$

- Straight forward to go to higher order schemes, available up to 20th order

Discretizing the geodesic action

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- We discretize in the world-line parameter, not in the time variable:

$$\mathbb{E}_{\rm BVP} = \frac{1}{2}\Big\{\Big(\big(c^2 + \frac{2V(\mathbf{x})}{m}\big) \circ \mathbb{D}\mathbf{t}\Big)^{\rm T} \mathbb{H}\,(\mathbb{D}\mathbf{t}) - (\mathbb{D}\mathbf{x})^{\rm T}\mathbb{H}\,(\mathbb{D}\mathbf{x})\Big\}$$
$$+ \lambda_1(\mathbf{t}[1] - t_i) + \lambda_2(\mathbf{t}[N_\gamma] - t_f)$$
$$+ \lambda_3(\mathbf{x}[1] - t_i) + \lambda_4(\mathbf{x}[N_\gamma] - x_f)$$

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

- Metric and action are both invariant under shifts in t-direction: $K_t = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Schwinger-Keldysh for IVPs

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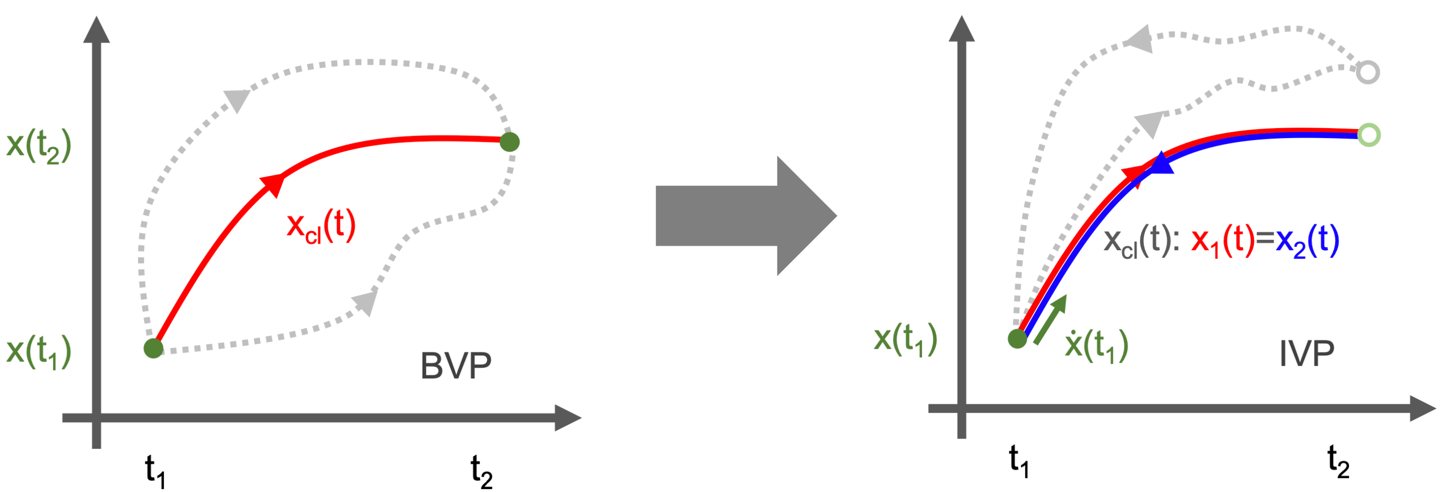
- So far everything as boundary value problem: not causal, need to know the final point of the trajectory to formulate variational principle.
  (for a detailed discussion see A.R. J.N. JCP 477 (2023) 111942)

- One can show that using a classical Schwinger-Keldysh contour allows to set up a variational principle for initial value problems (C.R. Galley, PRL 110(17), 174301)



Non-linear potential example

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- Challenging non-harmonic V(x)= k x^4 as IVP with k=1/4 and v_0=1/10 x_0=1 t_0=0
  (A.R. Jan Nordström arXiv:2307.04490)

$$
\begin{aligned}
\mathbb{E}^{\rm qrt}_{\rm IVP} =& \frac{1}{2}\Big\{(\bar{\mathbb{D}}^{\rm R}_t\mathbf{t}_1)^{\rm T}\mathbb{d}\left[1+2\kappa\mathbf{x}_1^4\right]\bar{\mathbb{H}}(\bar{\mathbb{D}}^{\rm R}_t\mathbf{t}_1)-(\bar{\mathbb{D}}^{\rm R}_x\mathbf{x}_1)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}^{\rm R}_x\mathbf{x}_1)\Big\} && \text{Forward branch } x_1,t_1\\
&-\frac{1}{2}\Big\{(\bar{\mathbb{D}}^{\rm R}_t\mathbf{t}_2)^{\rm T}\mathbb{d}\left[1+2\kappa\mathbf{x}_2^4\right]\bar{\mathbb{H}}(\bar{\mathbb{D}}^{\rm R}_t\mathbf{t}_2)-(\bar{\mathbb{D}}^{\rm R}_x\mathbf{x}_2)^{\rm T}\bar{\mathbb{H}}(\bar{\mathbb{D}}^{\rm R}_x\mathbf{x}_2)\Big\} && \text{Backward branch } x_2,t_2\\
&+\lambda_1\big(\mathbf{t}_1[1]-t_i\big)+\lambda_2\big((\mathbb{D}\mathbf{t}_1)[1]-\dot{t}_i\big) && \text{Initial cond. forward t}\\
&+\lambda_3\big(\mathbf{x}_1[1]-x_i\big)+\lambda_4\big((\mathbb{D}\mathbf{x}_1)[1]-\dot{x}_i\big) && \text{Initial cond. forward x}\\
&+\lambda_5\big(\mathbf{t}_1[N_\gamma]-\mathbf{t}_2[N_\gamma]\big)+\lambda_6\big(\mathbf{x}_1[N_\gamma]-\mathbf{x}_2[N_\gamma]\big) && \\
&+\lambda_7\big((\mathbb{D}\mathbf{t}_1)[N_\gamma]-(\mathbb{D}\mathbf{t}_2)[N_\gamma]\big)+\lambda_8\big((\mathbb{D}\mathbf{x}_1)[N_\gamma]-(\mathbb{D}\mathbf{x}_2)[N_\gamma]\big) && \text{SK connecting at } \gamma_f
\end{aligned}
$$

- Note both x and t treated as IVP: no fixed end time of simulation set!

- Freedom to choose v_0= dx/dt = dx/dγ / dt/dγ we go with dt/dγ = 1

- Technical aspect: need to lift unphysical zero mode of the SBP symmetric finite difference operator (for details see A.R. J.N. JCP 477 (2023) 111942)

Numerical results (Nɣ=32)

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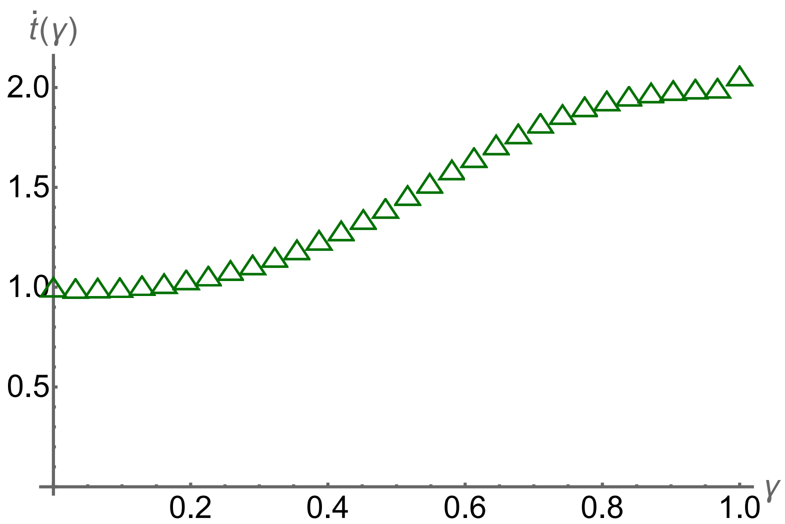
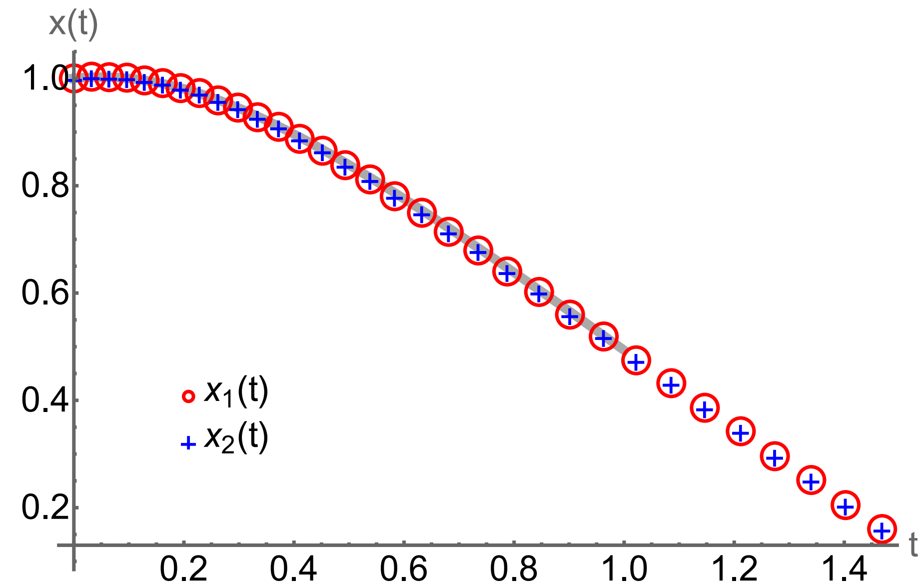
- Find the critical point of E^{qrt}_{IVP} using Quasi-Newton, Newton, Interior Point minimizer
  (A.R. Jan Nordström arXiv:2307.04490)





- Excellent agreement with direct solution of geodesic equation (gray solid)

- Note that time is not linearly dependent on the world-line parameter

- Times pacing adapts to the curvature of the position (automatic mesh refinement)

Naïve discretize geodesic equations

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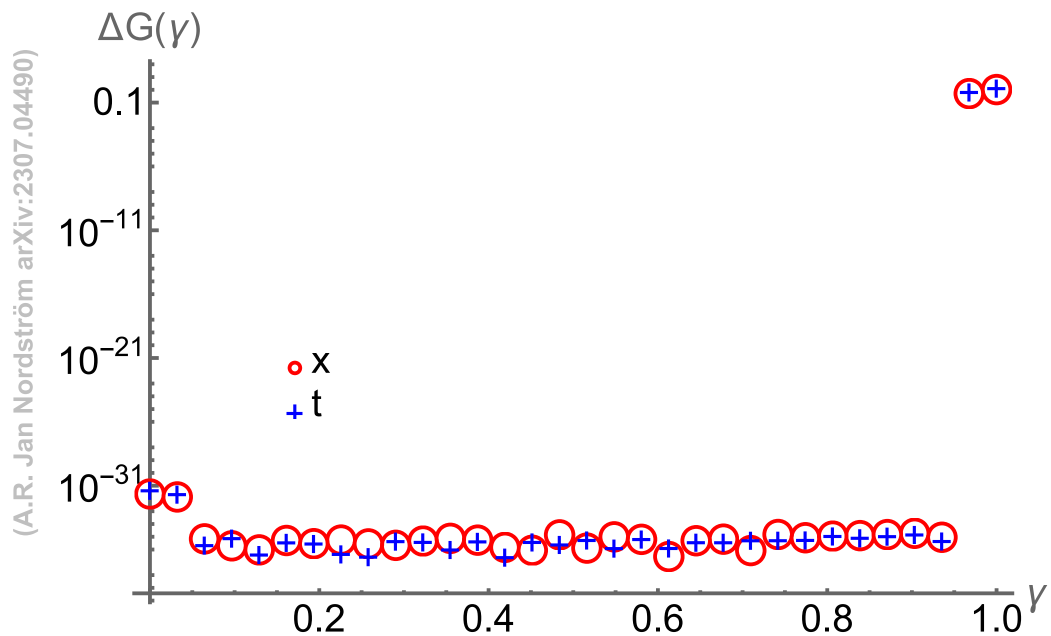
$$\frac{d}{d\gamma}\Big(g_{00}\frac{dt}{d\gamma}\Big) = \frac{d}{d\gamma}\Big((1+2\kappa x^4)\frac{dt}{d\gamma}\Big) = 0,$$
$$\frac{d}{d\gamma}\Big(\frac{dx}{d\gamma}\Big) + \frac{1}{2}\frac{\partial g_{00}}{\partial x}\Big(\frac{dt}{d\gamma}\Big)^2 = \frac{d^2x}{d\gamma^2} + 4\kappa x^3\Big(\frac{dt}{d\gamma}\Big)^2 = 0$$

$$\mathbb{D}\big((1+2\kappa\mathbf{x}^4)\circ\mathbb{D}\mathbf{t}\big) = \mathbf{\Delta G}^t,$$
$$\mathbb{D}\mathbb{D}\mathbf{x} + (4\kappa\mathbf{x}^3)\circ(\mathbb{D}\mathbf{t})\circ(\mathbb{D}\mathbf{t}) = \mathbf{\Delta G}^x$$



- Exactly follows the continuum geodesic equation except for the last two points

Naïve discretize Noether Charge

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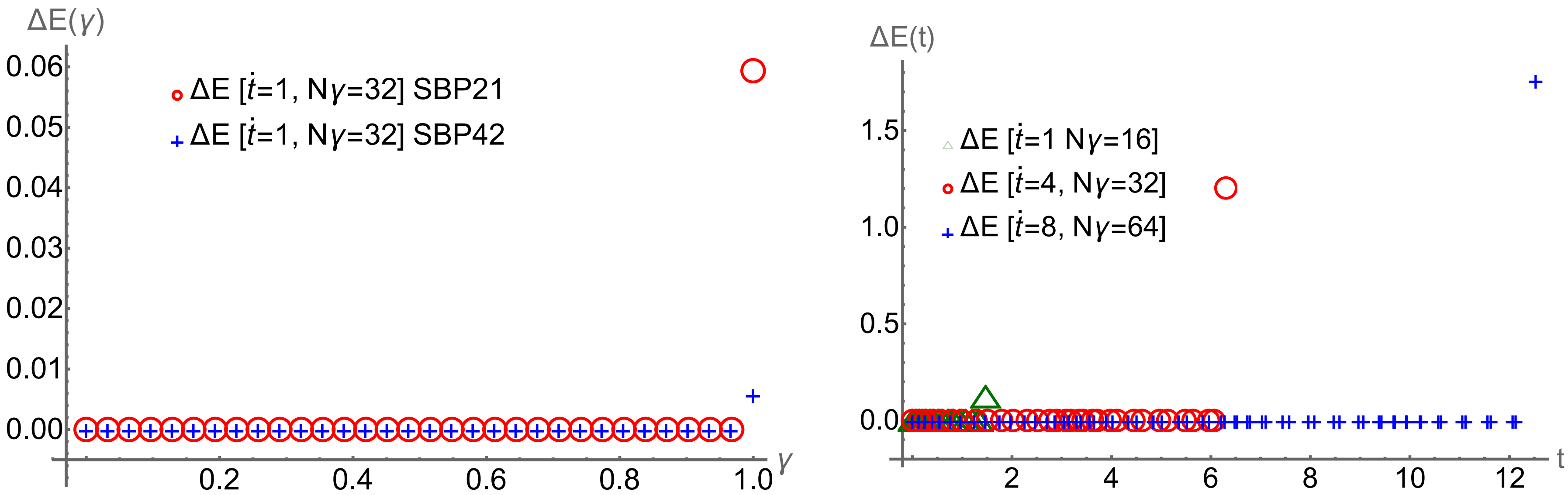
$$Q_K = g_{\alpha\beta} K^\alpha \dot{x}^\beta \quad \& \quad K_t = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow \mathbb{Q}_\mathbf{t} = (\mathbb{D}\mathbf{t}) \circ (\mathbf{1} + 2\kappa \mathbf{x}^4)$$

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



(A.R. Jan Nordström arXiv:2307.04490)

- **Exactly preserved in the interior** of the domain, irrespective of time interval
- Preserved value is actually the **continuum value**!

Convergence

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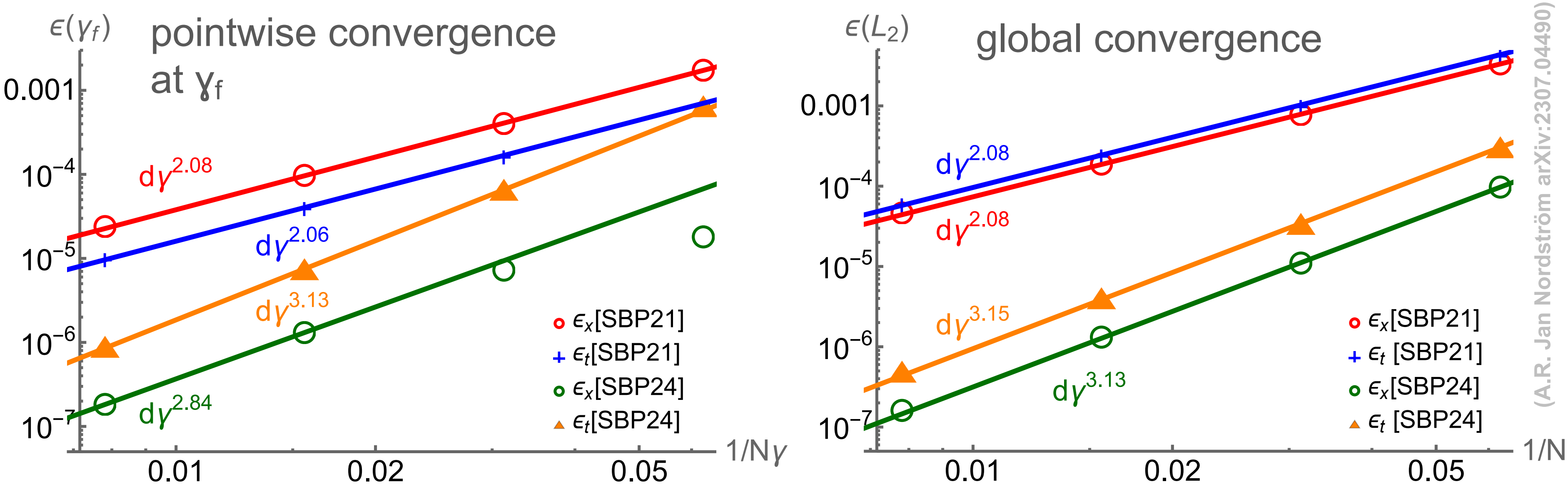
- Does the last point spoil the approach to correct solution in the continuum?



- Correct continuum limit reached with competitive scaling behavior.

Summary

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- Novel geometric variational principle for IVPs, adopting the world-line formalism of a point particle in general relativity

- Both time and position are dependent variables on world-line parameter γ geodesic action is manifestly invariant under space-time translations & boosts

- Discretizing in γ leaves time and position continuous and thus discretized action retains its continuum space-time symmetries

- Numerical implementation with summation-by-parts operators: exact conservation of relativistic Noether charge at continuum value in the interior of simulated domain

- Even though last point deviates, competitive scaling towards the continuum limit

- Future Goal: generalize to initial boundary value problems in d+1 dimensions for systems such as the wave equation and Maxwell electrodynamics