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PRESERVING CONTINUUM SPACE-TIME SYMMETRIES ON THE LATTICE

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A.R., W. Horowitz and J. Nordström: arXiv:2404.18676

see also JCP 498 (2024) 112652



Norwegian Particle, Astroparticle
& Cosmology Theory network

The Broader Picture

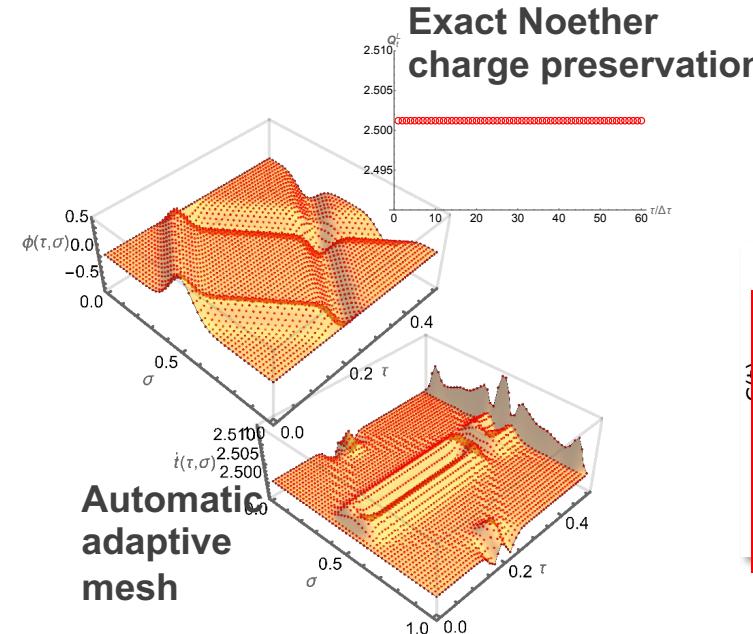
Quantum Boundary
Value Problems
Euclidean Lattice QCD

Anisotropic lattices

Absence of space-time
symmetries affects
spectral properties:
non-positive spectral
functions

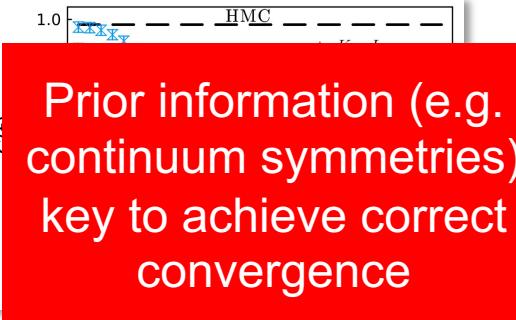
R. Larsen, G. Parkar, A.R. J. Weber
arXiv:2402.10819

R. Larsen, A.R. & HotQCD
PRD 109 (2024) 7, 074504



Novel SCL action
Classical Initial
Value Problems

Quantum Initial
Value Problems
Complex Langevin



D. Alvestad, A.R., D. Sexty
PRD 109 (2024) 3, L031502

Outline

- Motivation – The Broader Picture
- From the world-line formalism to a new action for classical fields (SCL)
- The discretized classical initial-boundary value problem
- Scalar wave propagation in (1+1)d as proof-of-principle
- Summary

Worldline Formalism in GR

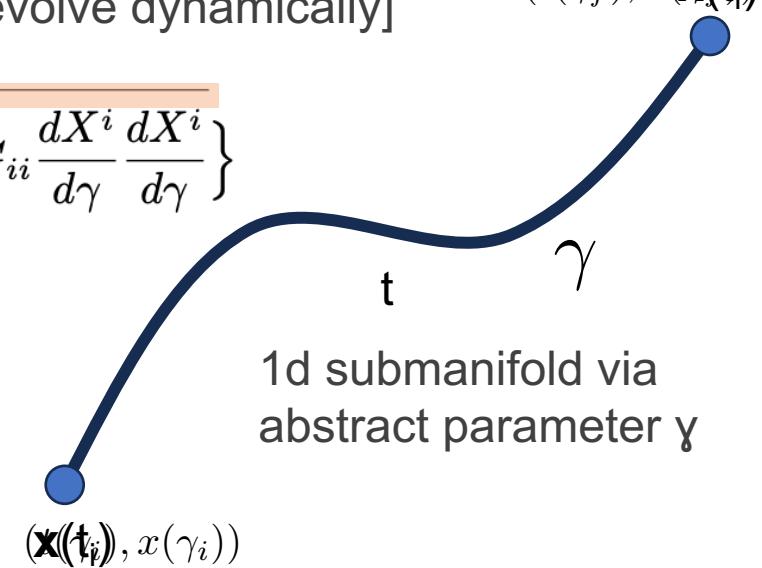
- Relativistic point particle motion: "shortest path in given space-time" = geodesic
- Equal treatment of space & time as **dynamic coordinate maps**:
from trajectory to world line [both $t(\gamma)$ and $\vec{x}(\gamma)$ evolve dynamically]

$$S_{\text{geo}} = \int d\gamma (-mc) \left\{ \sqrt{\left(G_{00} + \frac{V(\vec{x})}{2mc^2} \right) \frac{dX^0}{d\gamma} \frac{dX^0}{d\gamma} + G_{ii} \frac{dX^i}{d\gamma} \frac{dX^i}{d\gamma}} \right\}$$

\downarrow

$$\begin{aligned} V(\vec{x})/2mc^2 &\ll 1 \\ \frac{d|\vec{x}|/d\gamma}{dt/d\gamma}/c = v/c &\ll 1 \end{aligned} \quad X^\mu = (t, \vec{x})^\mu$$

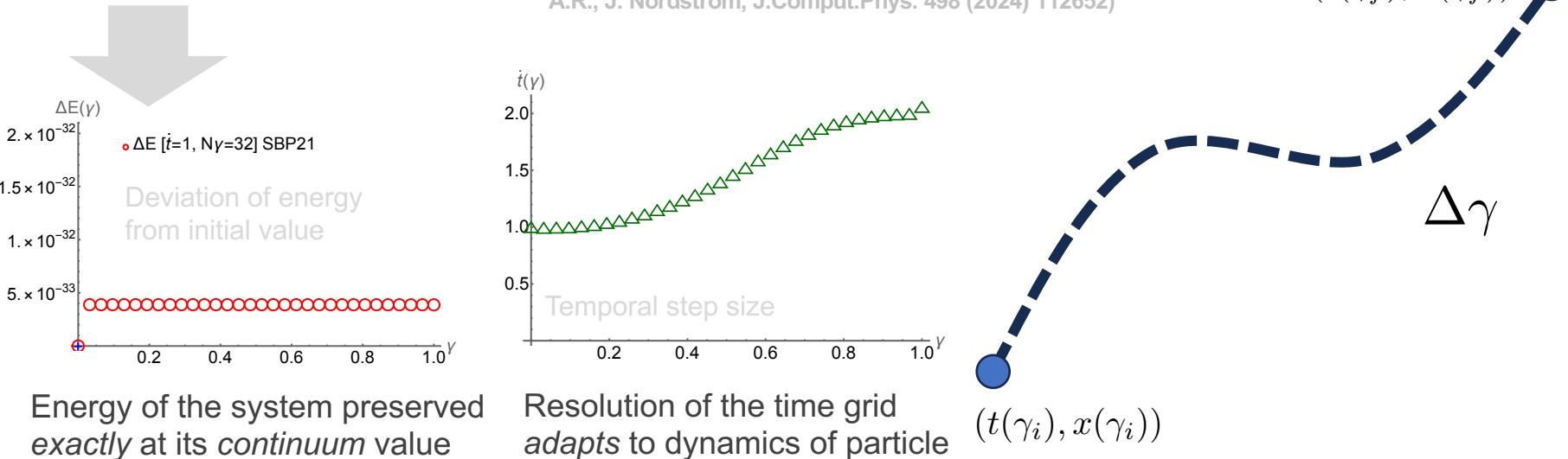
$$S_{\text{nr}} = \int dt \left\{ -mc^2 + \frac{1}{2} m \dot{\vec{x}}^2(t) - V(\vec{x}(t)) \right\}$$



- mc denotes scale where motion through space and time becomes inseparable

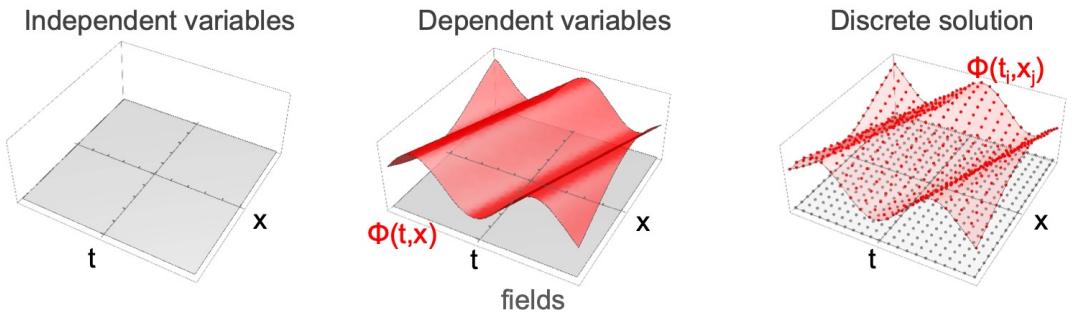
Advantages of the worldline formalism

- Discretizing the action in γ leaves space-time coordinates $X^\mu = (t, \vec{x})^\mu$ continuous
- Discretized world-line action invariant under infinitesimal coordinate transforms:
Noether's theorem holds!



A Field Theory Counterpart?

Conventional
field theory



Field theory with
dynamic coordinate
maps

Spacetime
symmetries
broken by
 Δt and Δx

Spacetime
symmetries
unaffected by
 $\Delta \tau$ and $\Delta \sigma$?

A world "volume" action for fields?

- Starting point is the standard reparameterization invariant action

$$S = \int d^{(d+1)}X \sqrt{-\det[G]} \frac{1}{2} \left(G^{\mu\nu} \partial_\mu \phi(X) \partial_\nu \phi(X) - V(\phi) \right)$$

- Are we perhaps overlooking a constant term, just as in the non-relativistic action?

$$S = \int d^{(d+1)}X \sqrt{-\det[G]} \left\{ -T + \frac{1}{2} \left(G^{\mu\nu} \partial_\mu \phi(X) \partial_\nu \phi(X) + V(\phi) \right) \right\}.$$

- Consider as low energy limit of another more general action (κ = energy density/T)

$$\mathcal{S}_{\text{BVP}} \equiv \int d^{(d+1)}X \sqrt{-\det[G]} (-T) \left\{ 1 - \frac{1}{2T} \left(G^{\mu\nu} \partial_\mu \phi(X) \partial_\nu \phi(X) + V(\phi) \right) \right\} + \mathcal{O}(\kappa^2)$$

Towards the SCL action

- Crucial next step: elevate spacetime coordinates to dynamical coordinate maps

worldline: $t \rightarrow t(\gamma)$ here: $X^\mu \rightarrow X^\mu(\Sigma) \quad \Sigma^a = (\tau, \vec{\sigma})^a = (\tau, \sigma_1, \dots, \sigma_d)^a$

$$\mathcal{S}_{\text{BVP}} = \int d^{(d+1)}\Sigma (-T) \sqrt{\left(\frac{1}{T}V(\phi) - 1\right)\det[g] + \frac{1}{T}\partial_a\phi(\Sigma)\partial_b\phi(\Sigma)\text{adj}[g]_{ab}}.$$

$$\text{adj}[g] = g^{-1}\det[g]$$

- Can absorb the Jacobian into new *induced metric* g on the space of parameters

$$\sqrt{-\det[J]\det[G]\det[J]} = \sqrt{-\det[J^T]\det[G]\det[J]} = \sqrt{-\det[J^TGJ]} = \sqrt{-\det[g]}$$

- The scale T denotes where field and coordinate dynamics become inseparable

Next steps

$$\mathcal{S}_{\text{BVP}} = \int d^{(d+1)}\Sigma (-T) \sqrt{\left(\frac{1}{T}V(\phi) - 1\right)\det[g] + \frac{1}{T}\partial_a\phi(\Sigma)\partial_b\phi(\Sigma)\text{adj}[g]_{ab}}.$$

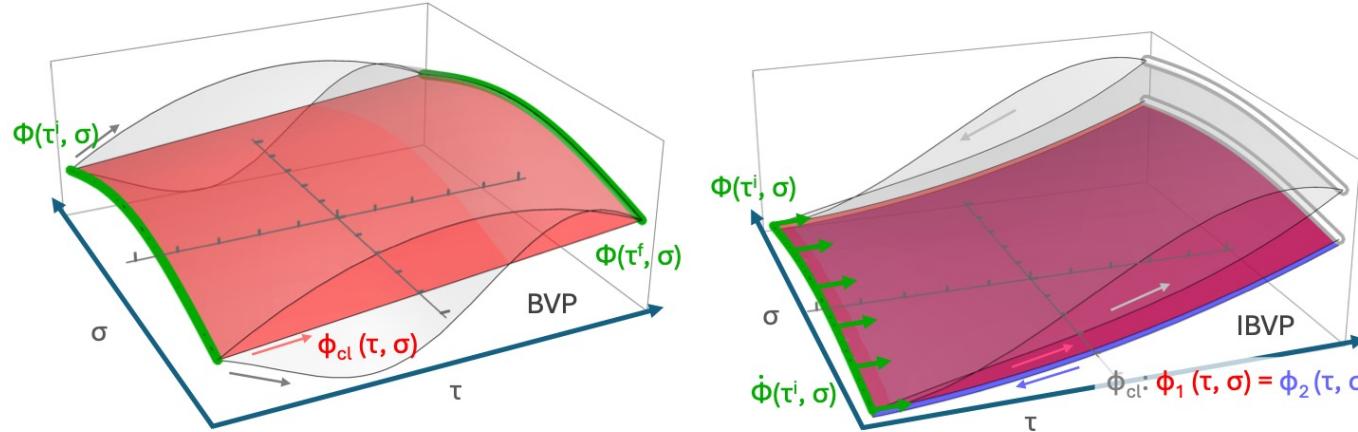
- Formulate an initial value problem version of the SCL action
- Discretize the action and show that Noether's theorem holds for Poincare group
- Demonstrate numerically feasibility of locating critical point of the action:
classical field solution without the need to solve Euler-Lagrange equations

$$\mathcal{E}_{\text{BVP}} = \int d^{(d+1)}\Sigma E_{\text{BVP}} = \int d^{(d+1)}\Sigma \frac{1}{2} \left\{ \left(\frac{1}{T}V(\phi) - 1\right)\det[g] + \frac{1}{T}\partial_a\phi(\Sigma)\partial_b\phi(\Sigma)\text{adj}[g]_{ab} \right\}$$

Classical Schwinger Keldysh (Galley)

- Doubling of all degrees of freedom by introducing forward and backward branches

see C. Galley PRL 110 (2013) 17, 174301 and A.R., J. Nordström JCP 477 (2023) 111942



$$\mathcal{E}_{\text{IBVP}} = \int d^{(d+1)}\Sigma \left\{ E_{\text{BVP}}[X_1, \partial_a X_1, \phi_1, \partial_a \phi_1] - E_{\text{BVP}}[X_2, \partial_a X_2, \phi_2, \partial_a \phi_2] \right\}$$

**connecting
conditions**

$$X_1^\mu(\tau = \tau^f, \vec{\sigma}) = X_2^\mu(\tau = \tau^f, \vec{\sigma}),$$

$$\partial_0 X_1^\mu|_{\tau=\tau^f} = \partial_0 X_2^\mu|_{\tau=\tau^f},$$

$$\phi_1(\tau = \tau^f, \vec{\sigma}) = \phi_2(\tau = \tau^f, \vec{\sigma})$$

$$\partial_0 \phi_1|_{\tau=\tau^f} = \partial_0 \phi_2|_{\tau=\tau^f}.$$

Summation-by-parts finite differences

- Derivation of Noether theorem or governing equations rely on integration by parts
- Mimetic discretization needed to preserve IBP in discrete setting:

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

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

quadrature rule



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

finite difference
stencil

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

$$= \text{diag}[-1, 0, \dots, 0, 1]$$

$$\Delta t \begin{bmatrix} \frac{1}{2} & & \\ & 1 & \\ & & 1 \end{bmatrix} \quad \frac{1}{\Delta t} \begin{bmatrix} -1 & 1 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

$\mathbb{H}^{[2,1]}$ $\mathbb{D}^{[2,1]}$



$$\begin{aligned} (\mathbb{D}\mathbf{u})^t \mathbb{H} \mathbf{v} = & -\mathbf{u}^t \mathbb{H} \mathbb{D} \mathbf{v} \\ & + \mathbf{u}_N \mathbf{v}_N \\ & - \mathbf{u}_0 \mathbf{v}_0 \end{aligned}$$

Avoiding the doubler problem

- Symmetric stencil leads to appearance of doubler modes when naïve SBP is used
- Wilson term trick not applicable: derivative acts on real-valued functions
- Modern approach in PDE community: weakly enforced boundary data

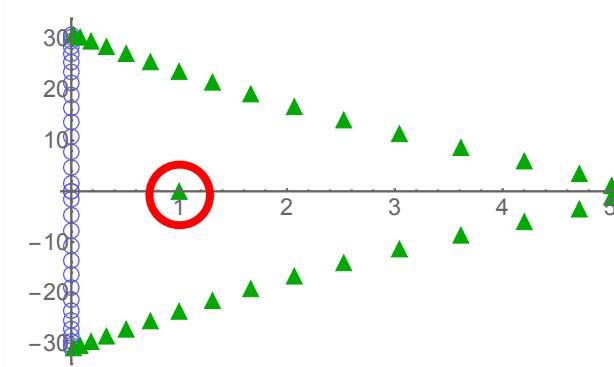
Affine coordinate formulation

$$S = \int dt (\dot{x}(t) \dot{x}(t)) \quad x(0) = x_i$$

$$S \approx (\mathbb{D}\mathbf{x})^t \mathbb{H} \mathbb{D}\mathbf{x}$$

$$\bar{\mathbb{D}}\mathbf{x} = \mathbb{D}\mathbf{x} + \mathbb{H}^{-1} \mathbb{E}_0 (\mathbf{x} - \mathbf{x}_i)$$

Modification acting on the path x itself
constant shift



- + all zero modes are lifted
- + physical constant mode with correct IC as unit EV

The discretized action

- Due to mimetic nature of SBP operator simply replace derivatives by $\bar{\mathbb{D}}$

$$\mathbb{E}_{\text{BVP}}[\mathbf{X}_1^\mu, \bar{\mathbb{D}}_a^\mu \mathbf{X}_1^\mu, \boldsymbol{\phi}_1, \bar{\mathbb{D}}_a^\phi \boldsymbol{\phi}_1] =$$

$$\frac{1}{2} \left\{ \left(\frac{1}{T} V(\boldsymbol{\phi}_1) - 1 \right) \circ \det[\mathbf{g}_1] + \frac{1}{T} (\bar{\mathbb{D}}_a^\phi \boldsymbol{\phi}_1) \circ (\bar{\mathbb{D}}_b^\phi \boldsymbol{\phi}_1) \circ \text{adj}[\mathbf{g}_1]_{ab} \right\}^T \mathbf{h}$$

$$\mathbf{g}_{ab} = G_{\mu\nu} (\bar{\mathbb{D}}_a^\mu \mathbf{X}^\mu) \circ (\bar{\mathbb{D}}_b^\nu \mathbf{X}^\nu), \quad \det[\mathbf{g}] = \sum_{i_0, \dots, i_d} \epsilon_{i_0 \dots i_d} \mathbf{g}_{0,i_0} \circ \dots \circ \mathbf{g}_{d,i_d}$$

- Discrete action remains manifest **invariant under Poincare transformations**
- Integration by parts exactly mimicked: Noether current & charge as in continuum

$$\mathbf{q}^L = \frac{\partial \mathbb{E}_{\text{BVP}}^L}{\partial (\mathbb{D}_0 \mathbf{X}^\mu)} \delta \mathbf{X}^\mu = \left(\frac{\partial \mathbb{E}_{\text{BVP}}}{\partial (\mathbb{D}_0 \mathbf{X}^\mu)} + \tilde{\boldsymbol{\lambda}}_\mu \circ \mathfrak{d}^0[0] + \tilde{\boldsymbol{\gamma}}_\mu \circ \mathfrak{d}^0[N_0] \right) \delta \mathbf{X}^\mu.$$

$$\mathbf{Q}^L = \left(\mathbb{H}_\sigma \frac{\partial \mathbb{E}_{\text{BVP}}}{\partial (\mathbb{D}_0 \mathbf{X}^\mu)} + (\mathbf{h}_\sigma^T \tilde{\boldsymbol{\lambda}}_\mu) \mathfrak{d}^0[0] + (\mathbf{h}_\sigma^T \tilde{\boldsymbol{\gamma}}_\mu) \mathfrak{d}^0[N_0] \right) \delta \mathbf{X}^\mu.$$

Proof-of-principle in (1+1)d

- Scalar wave propagation is numerically challenging (stability, accuracy)

$$\begin{aligned}
 S_{\text{BVP}} &= \int d\tau d\sigma (-T) \sqrt{-\det[g] + \frac{1}{T} \partial_a \phi(\Sigma) \partial_b \phi(\Sigma) \text{adj}[g]_{ab}} \\
 &= \int d\tau d\sigma (-T) \left\{ c^2 (\dot{t}x' - \dot{x}t')^2 \right. \\
 &\quad \left. + \frac{1}{T} \left(\dot{\phi}^2 (c^2(t')^2 - (x')^2) + 2\dot{\phi}\phi'(\dot{x}x' - c^2\dot{t}t') + (\phi')^2(c^2\dot{t}^2 - \dot{x}^2) \right) \right\}^{1/2}
 \end{aligned}$$

- Simplify by considering only time as dynamical mapping (trivial $x[\tau, \sigma] = \sigma$)

$$\mathcal{E}_{\text{BVP}} \stackrel{x=\sigma}{=} \int d\tau d\sigma \frac{1}{2} \left\{ (\dot{t})^2 + \frac{1}{T} \left(\dot{\phi}^2 ((t')^2 - 1) - 2\dot{\phi}\phi'\dot{t}t' + (\phi')^2(\dot{t}^2) \right) \right\}$$

Discretized IBVP action

- Introduce forward and backward branch (classical Schwinger-Keldysh)

$$\begin{aligned} \mathbb{E}_{\text{IBVP}}^L = & \frac{1}{2} \left\{ (\bar{\mathbb{D}}_\tau^t \mathbf{t}_1)^2 + \frac{1}{T} \left((\bar{\mathbb{D}}_\tau^\phi \boldsymbol{\phi}_1)^2 \circ ((\mathbb{D}_\sigma \mathbf{t}_1)^2 - 1) \right. \right. \\ & \quad \left. \left. - 2(\bar{\mathbb{D}}_\sigma^\phi \boldsymbol{\phi}_1) \circ (\bar{\mathbb{D}}_\tau^\phi \boldsymbol{\phi}_1) \circ (\bar{\mathbb{D}}_\tau^t \mathbf{t}_1) \circ (\mathbb{D}_\sigma^t \mathbf{t}_1) + (\bar{\mathbb{D}}_\sigma^\phi \boldsymbol{\phi}_1)^2 \circ (\bar{\mathbb{D}}_\tau^t \mathbf{t}_1)^2 \right) \right\}^T \mathbf{h} \\ & - \frac{1}{2} \left\{ (\bar{\mathbb{D}}_\tau^t \mathbf{t}_2)^2 + \frac{1}{T} \left((\bar{\mathbb{D}}_\tau^\phi \boldsymbol{\phi}_2)^2 \circ ((\mathbb{D}_\sigma \mathbf{t}_2)^2 - 1) \right. \right. \\ & \quad \left. \left. - 2(\bar{\mathbb{D}}_\sigma^\phi \boldsymbol{\phi}_2) \circ (\bar{\mathbb{D}}_\tau^\phi \boldsymbol{\phi}_2) \circ (\bar{\mathbb{D}}_\tau^t \mathbf{t}_2) \circ (\mathbb{D}_\sigma^t \mathbf{t}_2) + (\bar{\mathbb{D}}_\sigma^\phi \boldsymbol{\phi}_2)^2 \circ (\bar{\mathbb{D}}_\tau^t \mathbf{t}_2)^2 \right) \right\}^T \mathbf{h} \end{aligned}$$

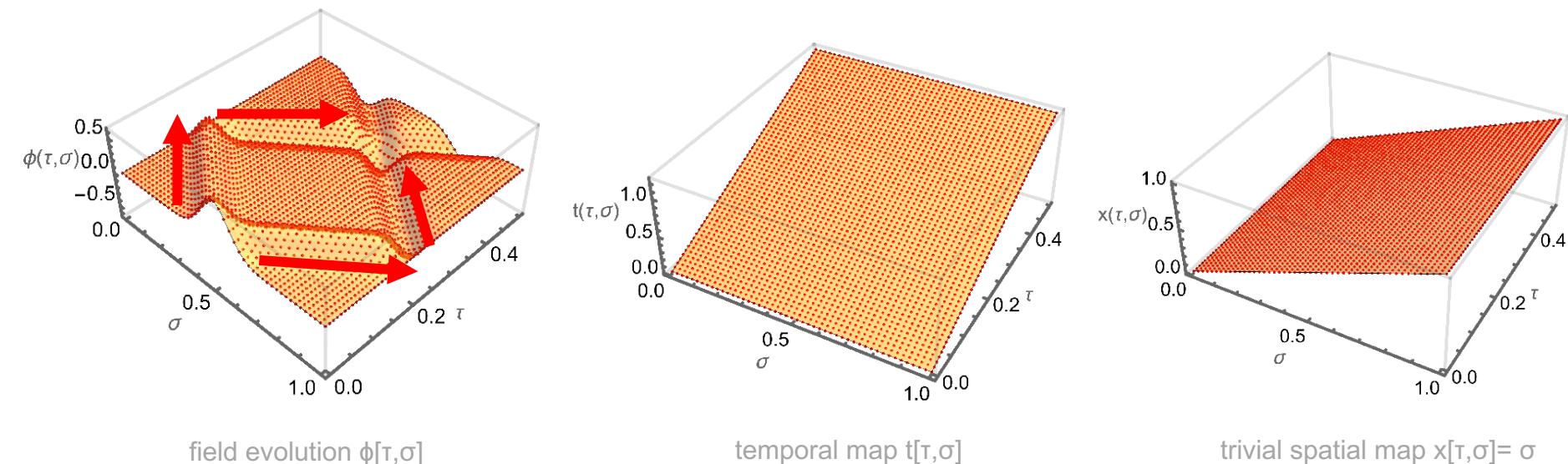
- Enforce initial (temporal), Dirichlet boundary (spatial) and connecting conditions

$$\begin{aligned} & + (\boldsymbol{\lambda}^t)^T \mathbb{h}_\sigma (\mathbb{P}_\tau^0[\mathbf{t}_1] - \mathbf{t}_{\text{IC}}) + (\boldsymbol{\lambda}^\phi)^T \mathbb{h}_\sigma (\mathbb{P}_\tau^0[\boldsymbol{\phi}_1] - \boldsymbol{\phi}_{\text{IC}}) \\ & + (\tilde{\boldsymbol{\lambda}}^t)^T \mathbb{h}_\sigma (\mathbb{P}_\tau^0[(\mathbb{D}_\tau \mathbf{t}_1)] - \dot{\mathbf{t}}_{\text{IC}}) + (\tilde{\boldsymbol{\lambda}}^\phi)^T \mathbb{h}_\sigma (\mathbb{P}_\tau^0[(\mathbb{D}_\tau \boldsymbol{\phi}_1)] - \dot{\boldsymbol{\phi}}_{\text{IC}}) \\ & + (\boldsymbol{\gamma}^t)^T \mathbb{h}_\sigma (\mathbb{P}_\tau^{N_\tau}[\mathbf{t}_1] - \mathbb{P}_\tau^{N_\tau}[\mathbf{t}_2]) + (\boldsymbol{\gamma}^\phi)^T \mathbb{h}_\sigma (\mathbb{P}_\tau^{N_\tau}[\boldsymbol{\phi}_1] - \mathbb{P}_\tau^{N_\tau}[\boldsymbol{\phi}_2]) \\ & \quad + (\tilde{\boldsymbol{\gamma}}^t)^T \mathbb{h}_\sigma (\mathbb{P}_\tau^{N_\tau}[(\mathbb{D}_\tau \mathbf{t}_1)] - \mathbb{P}_\tau^{N_\tau}[(\mathbb{D}_\tau \mathbf{t}_2)]) \\ & \quad + (\tilde{\boldsymbol{\gamma}}^\phi)^T \mathbb{h}_\sigma (\mathbb{P}_\tau^{N_\tau}[(\mathbb{D}_\tau \boldsymbol{\phi}_1)] - \mathbb{P}_\tau^{N_\tau}[(\mathbb{D}_\tau \boldsymbol{\phi}_2)]) \\ & \quad + (\boldsymbol{\kappa}^\phi)^T \mathbb{h}_\tau (\mathbb{P}_\sigma^0[\boldsymbol{\phi}_1] - \mathbf{0}) + (\tilde{\boldsymbol{\kappa}}^\phi)^T \mathbb{h}_\tau (\mathbb{P}_\sigma^{N_\sigma}[\boldsymbol{\phi}_1] - \mathbf{0}) \\ & \quad + (\boldsymbol{\xi}^\phi)^T \mathbb{h}_\tau (\mathbb{P}_\sigma^0[\boldsymbol{\phi}_2] - \mathbf{0}) + (\tilde{\boldsymbol{\xi}}^\phi)^T \mathbb{h}_\tau (\mathbb{P}_\sigma^{N_\sigma}[\boldsymbol{\phi}_2] - \mathbf{0}). \end{aligned}$$

- Locate extremum via numerical optimization (Interior Point Optimization)

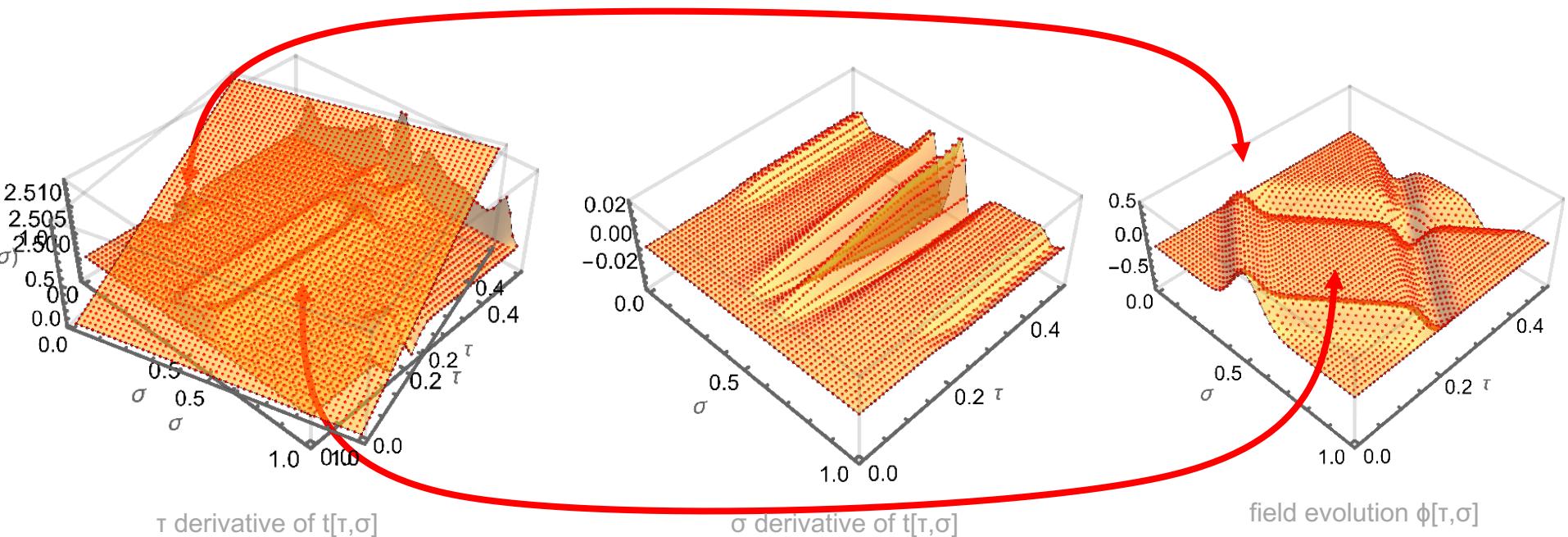
Proof-of-principle in (1+1)d

- Left- and right propagating wave-packages bouncing off a stiff wall



- Here $T=10.000$, choice to obtain effects on the coordinate maps on percent level

Automatic spacetime mesh refinement



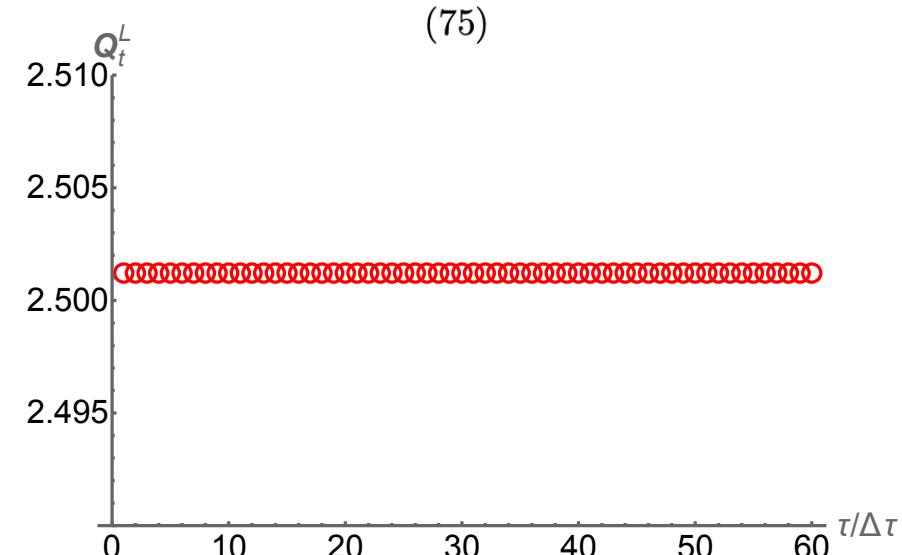
- Temporal map automatically adapts resolution according to wave dynamics

Noether Charge

- Due to mimetic SBP discretization: continuum expression with

$$\begin{aligned}
 Q_t^L = & \mathbb{H}_\sigma \left\{ (\mathbb{D}_\tau t_1) + \underbrace{\frac{1}{T} \left((\mathbb{D}_\sigma \phi_1)^2 \circ (\mathbb{D}_\tau t_1) - (\mathbb{D}_\tau \phi_1) \circ (\mathbb{D}_\sigma \phi_1) \circ (\mathbb{D}_\sigma t_1) \right)}_{J^0 \in \mathbb{R}^{N_\tau \times N_\sigma}} \right\} \\
 & + \underbrace{\left\{ (\mathbf{h}_\sigma^T \tilde{\lambda}^t) \mathfrak{d}^\tau[0] + (\mathbf{h}_\sigma^T \tilde{\gamma}^t) \mathfrak{d}^\tau[N_\tau] \right\}}_{\text{Lagr. mult. contrib.}},
 \end{aligned}$$

- Exact conservation of the Noether charge associated with time translations.



Summary

- World-line formalism suggests dynamical coordinate maps are essential
- SCL action incorporates **dynamical coordinate maps** with field d.o.f.s
- Discretization via **summation-by-parts** mimetic finite difference scheme
- Discretization of abstract parameter action **retains space-time symmetries**
- **Dynamical** emergence of **time-mesh** & **exact conservation** of Noether charge

Inclusion of initial & boundary conditions

- In contrast to implicit analytic treatment make explicit via Lagrange multipliers
see also A.R., J. Nordström JCP 511 (2024) 113138

$$\mathcal{E}_{\text{IBVP}}^{\text{L}} = \int d^{(d+1)\Sigma} \left\{ E_{\text{BVP}}[X_1, \partial_a X_1, \phi_1, \partial_a \phi_1] - E_{\text{BVP}}[X_2, \partial_a X_2, \phi_2, \partial_a \phi_2] \right\}$$

$$+ \int \prod_{a=1}^d d\Sigma_a \left\{ \lambda_\mu (X_1^\mu(\tau^i, \vec{\sigma}) - X_{\text{IC}}^\mu) + \lambda_\phi (\phi_1(\tau^i, \vec{\sigma}) - \phi_{\text{IC}}) \right.$$

$$+ \tilde{\lambda}_\mu (\partial_0 X_1^\mu(\tau^i, \vec{\sigma}) - \dot{X}_{\text{IC}}^\mu) + \tilde{\lambda}_\phi (\partial_0 \phi_1(\tau^i, \vec{\sigma}) - \dot{\phi}_{\text{IC}})$$

$$+ \gamma_\mu (X_1^\mu(\tau^f, \vec{\sigma}) - X_2^\mu(\tau^f, \vec{\sigma})) + \gamma_\phi (\phi_1(\tau^f, \vec{\sigma}) - \phi_2(\tau^f, \vec{\sigma}))$$

$$\left. + \tilde{\gamma}_\mu (\partial_0 X_2^\mu(\tau^f, \vec{\sigma}) - \partial_0 X_2^\mu(\tau^f, \vec{\sigma})) + \tilde{\gamma}_\phi (\partial_0 \phi_1(\tau^f, \vec{\sigma}) - \partial_0 \phi_2(\tau^f, \vec{\sigma})) \right\}$$

$$+ \sum_{j=1}^d \int \prod_{\substack{a=0 \\ a \neq j}}^d d\Sigma_a \left\{ \kappa_\mu^j (X_1^\mu(\sigma_j^i) - X_{\text{sBCL}}^\mu(\sigma_j^i)) + \xi_\mu^j (X_2^\mu(\sigma_j^i) - X_{\text{sBCL}}^\mu(\sigma_j^i)) \right.$$

$$+ \tilde{\kappa}_\mu^j (X_1^\mu(\sigma_j^f) - X_{\text{sBCR}}^\mu(\sigma_j^f)) + \tilde{\xi}_\mu^j (X_2^\mu(\sigma_j^f) - X_{\text{sBCR}}^\mu(\sigma_j^f))$$

$$+ \kappa_\phi^j (\phi_1(\sigma_j^i) - \phi_{\text{sBCR}}(\sigma_j^i)) + \xi_\phi^j (\phi_2(\sigma_j^i) - \phi_{\text{sBCR}}(\sigma_j^i))$$

$$\left. + \tilde{\kappa}_\phi^j (\phi_1(\sigma_j^f) - \phi_{\text{sBCL}}(\sigma_j^f)) + \tilde{\xi}_\phi^j (\phi_2(\sigma_j^f) - \phi_{\text{sBCL}}(\sigma_j^f)) \right\},$$

$$= \int d^{(d+1)\Sigma} \left\{ E_{\text{BVP}}^{\text{L}}[X_1, \partial_a X_1, \phi_1, \partial_a \phi_1] - E_{\text{BVP}}^{\text{L}}[X_2, \partial_a X_2, \phi_2, \partial_a \phi_2] \right\}$$

Forward & backward branch
Lagrangian

Initial conditions for coordinate maps and fields

Connecting conditions for maps and fields
from classical Schwinger-Keldysh

Spatial boundary conditions for the coordinate
maps and fields

Redefined Lagrangians
including Lagrange mult.