Optimal Constraint Projection

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- Constraint violations often make it difficult to compute accurate numerical solutions to constrained evolution systems.
- Constraint projection is used to control the growth of constraints by solving the evolution equations until the constraints become too large, and then projecting back onto the constraint submanifold by re-solving the constraint equations.
- Outline of this talk:
  - General Discussion of Optimal Constraint Projection.
  - Example: Constraint Projection for the Scalar Field System.
  - Preliminary Analysis of the Einstein system.

General Discussion of Optimal Constraint Projection

- Numerical solutions to hyperbolic evolution systems

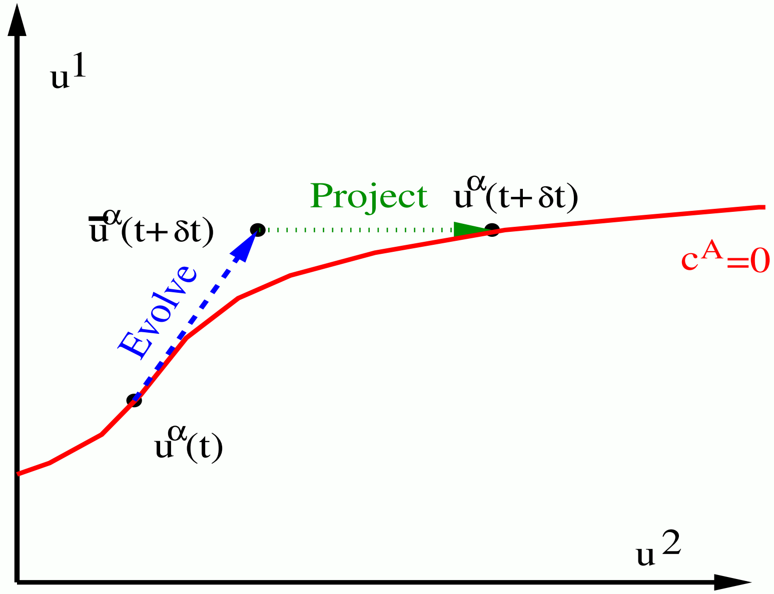
$$\partial_t u^\alpha + A^{k\alpha}{}_\beta(u)\partial_k u^\beta \quad = \quad F^\alpha(u),$$

that are subject to constraints (typically of the form)

$$0 = c^A \equiv K^{Ak}{}_\alpha(u)\partial_k u^\alpha + L^A(u),$$

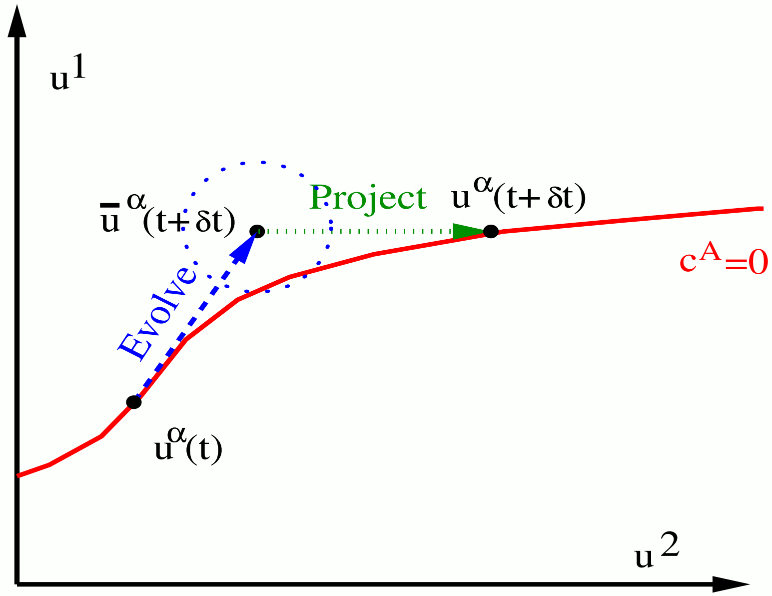
can be corrupted by the uncontrollable growth of the constraints.

- The idea of constraint projection is to evolve the dynamical fields using the free evolution system, and then project back into the constraint submanifold whenever the constraints become too large.



General Discussion of Optimal Constraint Projection II

- Unfortunately the projection into the constraint satisfying submanifold is not unique.



- We propose to use "optimal" constraint projection in which we minimize the distance between the field point $\bar{u}^\alpha$ and its projection u^α. We construct this optimal projection by insisting that the Lagrangian $\mathscr{L}$,

$$\mathscr{L} = S_{\alpha\beta}(u^\alpha - \bar{u}^\alpha)(u^\beta - \bar{u}^\beta) + \lambda_A c^A,$$

be stationary with respect to arbitrary variations in the fields u^α and the Lagrange multipliers λ_A.

- Optimal constraint projection depends on the choice of the metric $S_{\alpha\beta}$ which defines distances on the space of dynamical fields,

$$\mathscr{L} = S_{\alpha\beta}(u^\alpha - \bar{u}^\alpha)(u^\beta - \bar{u}^\beta) + \lambda_A c^A.$$

- Fortunately symmetric hyperbolic evolution systems,

$$\partial_t u^\alpha + A^{k\alpha}{}_\beta(u)\partial_k u^\beta \quad = \quad F^\alpha(u),$$

  have a natural positive definite metric on the space of fields. This is the "symmetrizer" matrix that makes the characteristic matrices of the fundamental evolution equations symmetric:

$$S_{\alpha\gamma} A^{k\gamma}{}_\beta \equiv A^k_{\alpha\beta} = A^k_{\beta\alpha}.$$

- We use this symmetrizer metric, which defines the "energy" norm for these systems, to define our optimal constraint projections.
- If $\mathscr{L}$ is stationary with respect to variations in u^α and λ_A,

$$\frac{\delta\mathscr{L}}{\delta u^\alpha} = 0 \text{ and } \frac{\delta\mathscr{L}}{\delta\lambda_A} = 0,$$

  then u^α represents the optimal projection of $\bar{u}^\alpha$.

Example System: Scalar Waves on a Fixed Background Spacetime

- Consider the scalar wave equation $\nabla^\mu\nabla_\mu\psi = 0$ where ψ is the scalar field, and ∇_μ is the covariant derivative on the background spacetime

$$ds^2 = -N^2dt^2 + g_{ij}(dx^i + N^idt)(dx^j + N^jdt).$$

- This equation can be written as a first-order hyperbolic evolution system for $u^\alpha = \{\psi, \Pi, \Phi_i\}$. For flat space these equations reduce to,

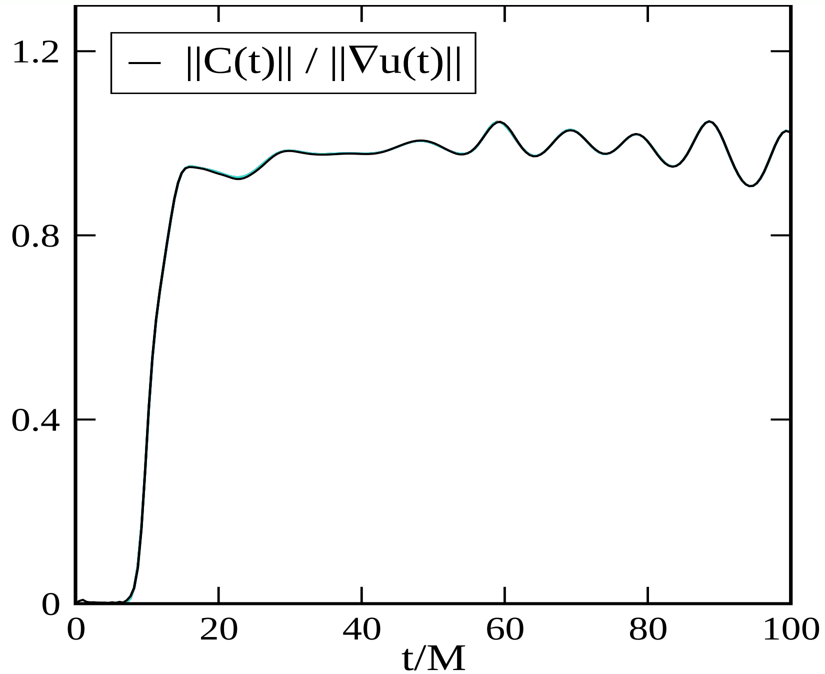
$$\begin{aligned} \partial_t\psi &= -\Pi, \\ \partial_t\Pi + g^{ki}\partial_k\Phi_i &= 0, \\ \partial_t\Phi_i + \partial_i\Pi &= 0. \end{aligned}$$

- This evolution system is subject to the constraints $0 = c^A = \{\mathscr{C}_i, \mathscr{C}_{ij}\}$:

$$\begin{aligned} \mathscr{C}_i &= \partial_i\psi - \Phi_i, \\ \mathscr{C}_{ij} &= \partial_{[i}\Phi_{j]}. \end{aligned}$$

  These constraints must be satisfied if the solutions to this first-order system also satisfy the original scalar wave equation.

Free Evolution with Freezing Boundary conditions



- Evolutions of the first-order scalar field system, using freezing boundary conditions, on a Schwarzschild background spacetime in Kerr-Schild coordinates.
- Constraint violations are measured using the norm $||C(t)||$ defined by

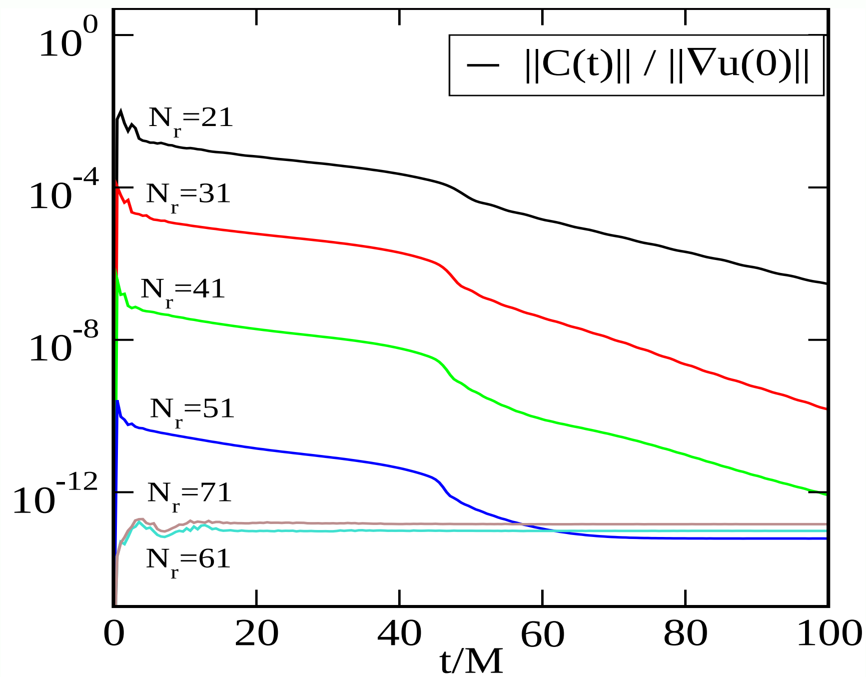
$$||C(t)||^2 = \int \left(\mathscr{C}_i \mathscr{C}^i + \mathscr{C}_{ij}\mathscr{C}^{ij}\right) \sqrt{g}\, d^3x.$$

Free Evolution with Constraint Preserving Boundary Conditions

- Constraint preserving boundary conditions for the scalar field system are imposed by setting conditions on the incoming characteristic fields which ensure that there are no incoming constraints:

$$\partial_t(\Pi - n^k\Phi_k) = 0, \qquad \partial_t\psi = N^k\Phi_k - N\Pi, \qquad (\delta^k{}_i - n^k n_i)\partial_t(\Phi_k - \partial_k\psi) = 0.$$

- Evolutions of the first-order scalar field system using these constraint preserving boundary conditions:



Modified Scalar Wave System

- The standard scalar wave system was transformed into a better model of the Einstein system by modifying the evolution equations. For the flat space equations, this modification is:

$$\partial_t \Phi_i + \partial_i \Pi \qquad\qquad = \gamma \mathscr{C}_i,$$
$$\partial_t \Phi_i + \partial_i \Pi \quad - \gamma \partial_i \psi \quad = -\gamma \Phi_i.$$

- This term changes the equation for the evolution of the constraints:

$$\partial_t \mathscr{C}_i - \mathscr{L}_{\vec{N}} \mathscr{C}_i = -\gamma N \mathscr{C}_i,$$

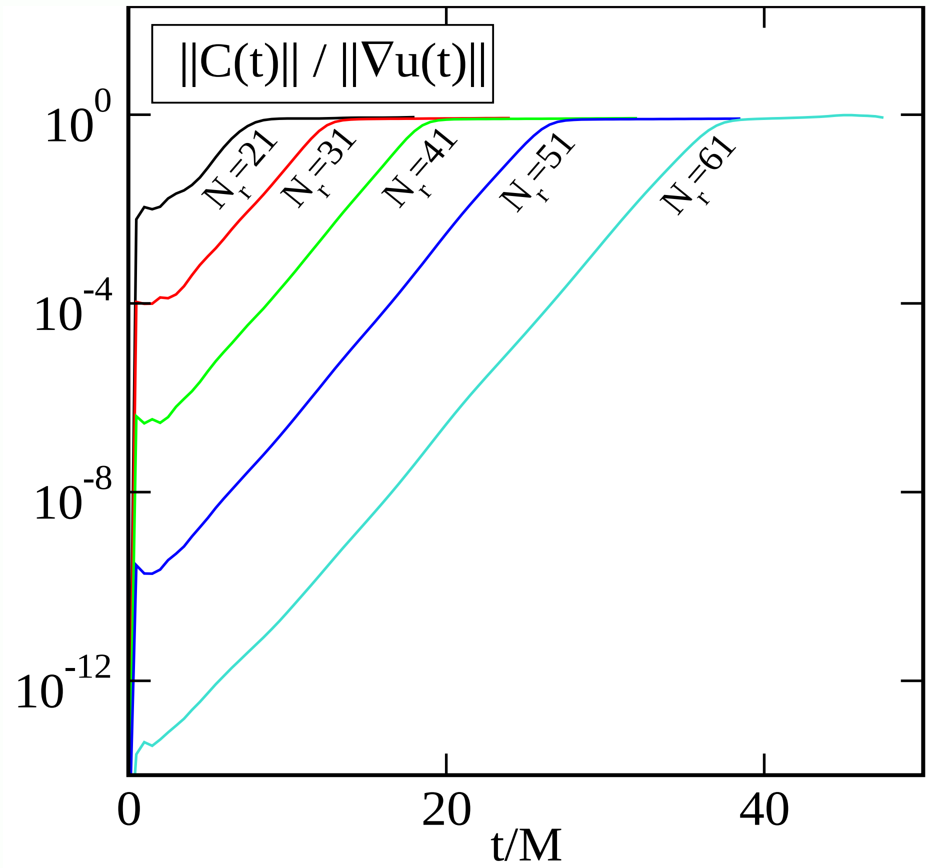
  causing them to grow exponentially when $\gamma < 0$.

- This modified scalar field system admits constraint violations that enter the computational domain through the boundaries, as well as constraint violations generated by this new bulk term. This system now suffers from constraint violation pathologies similar to those of the Einstein system.

Free Evolution of the Pathological Scalar Field System

- Evolutions of the pathological ($\gamma = -1$) scalar field system with constraint preserving boundary conditions.

- The constraints grow exponentially in the pathological scalar field system, even when constraint preserving boundary conditions are used.



- Constraint preserving boundary conditions alone are inadequate for controlling the growth of the constraints in this system.

Optimal Constraint Projection for the Scalar Field System

- The symmetrizer metric for the scalar field system is given by

$$\begin{aligned} dS^2 &= S_{\alpha\beta}\, du^\alpha du^\beta, \\ &= \Lambda^2 d\psi^2 - 2\gamma\, d\psi\, d\Pi + d\Pi^2 + g^{ij} d\Phi_i d\Phi_j. \end{aligned}$$

  This symmetrizer is positive definite whenever the arbitrary parameter Λ satisfies $\Lambda^2 - \gamma^2 > 0$.

- The Lagrangian that defines optimal constraint projections for the scalar field system is

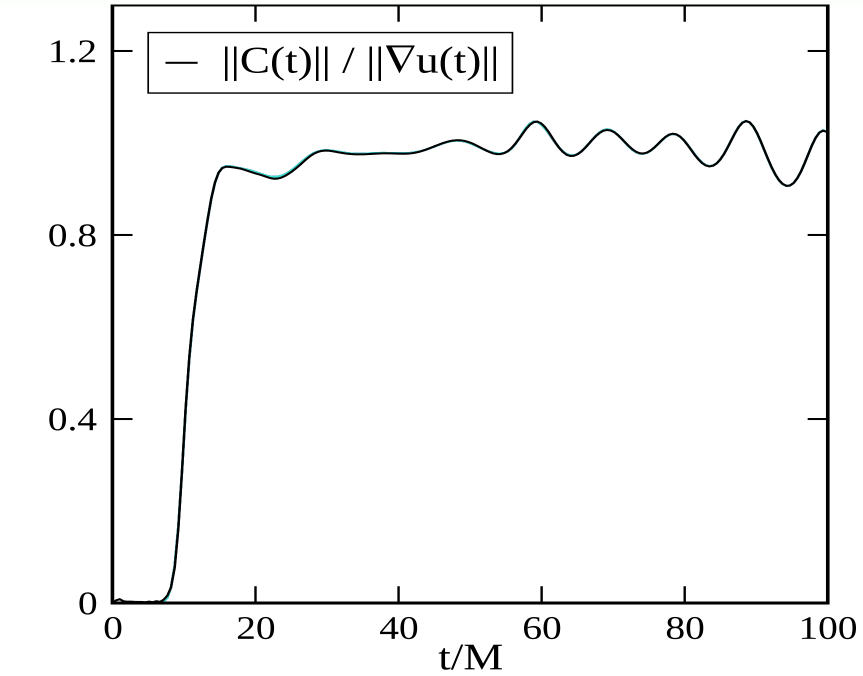
$$\begin{aligned} \mathscr{L} &= S_{\alpha\beta}(u^\alpha - \bar{u}^\alpha)(u^\beta - \bar{u}^\beta) + \lambda_A c^A, \\ &= \Lambda^2(\psi - \bar{\psi})^2 - 2\gamma(\Pi - \bar{\Pi})(\psi - \bar{\psi}) + (\Pi - \bar{\Pi})^2 \\ &\quad + g^{ij}(\Phi_i - \bar{\Phi}_i)(\Phi_j - \bar{\Phi}_j) + \lambda^i(\partial_i \psi - \Phi_i). \end{aligned}$$

- Making this Lagrangian stationary with respect to variations in ψ, Π, Φ_i, and λ^i, implies the following constraint projection equations:

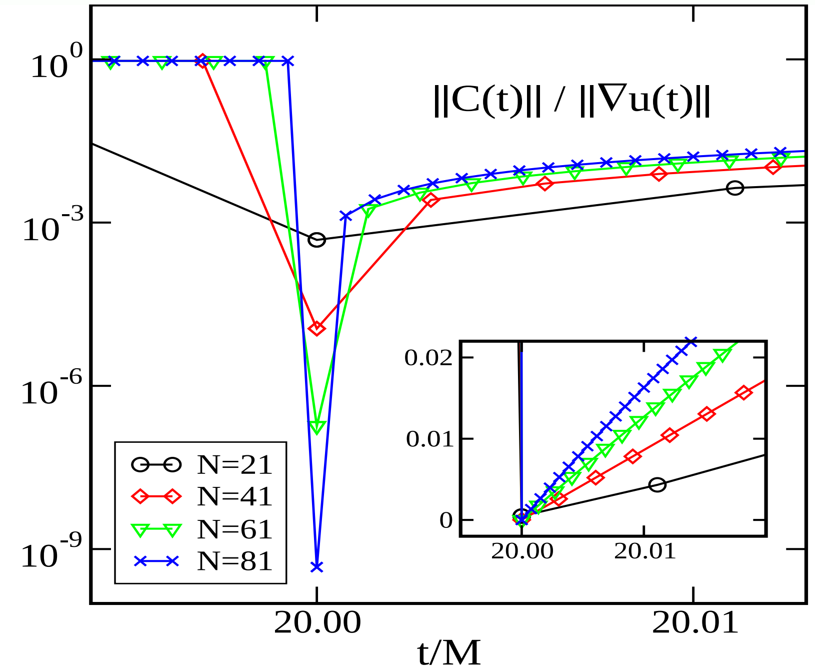
$$\begin{aligned} \nabla^i\nabla_i \psi - (\Lambda^2 - \gamma^2)\psi &= \nabla^i \bar{\Phi}_i - (\Lambda^2 - \gamma^2)\bar{\psi}, \\ \Pi &= \bar{\Pi} + \gamma(\psi - \bar{\psi}), \\ \Phi_i &= \partial_i \psi. \end{aligned}$$

Constraint Projection with Freezing Boundary Conditions

- Evolutions of the standard ($\gamma = 0$) scalar field system, with freezing boundary conditions, and a single constraint projection at $t = 20M$.



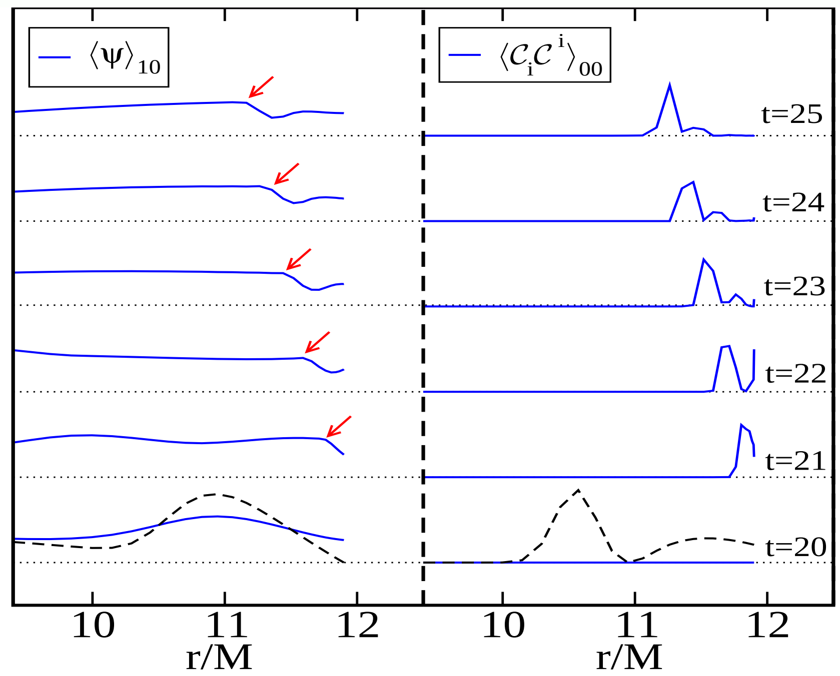
Without Projection

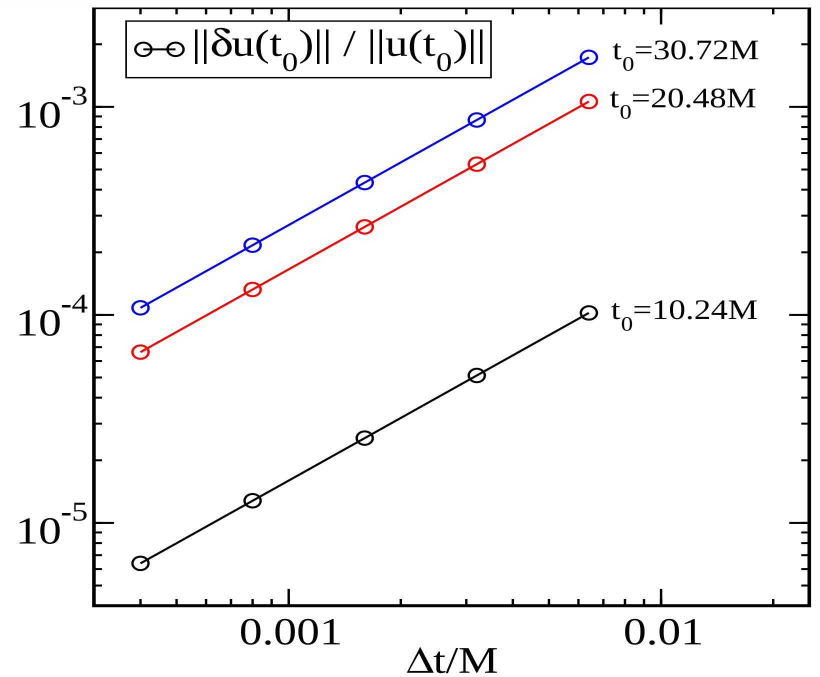


With Projection

- While the constraints are satisfied to truncation-error levels immediately after the constraint projection step, they grow by many orders of magnitude during the very next free evolution time step!
- There is a significant loss of numerical convergence during the free evolution which follows the constraint projection step.

Constraint Projection with Freezing Boundary Conditions II

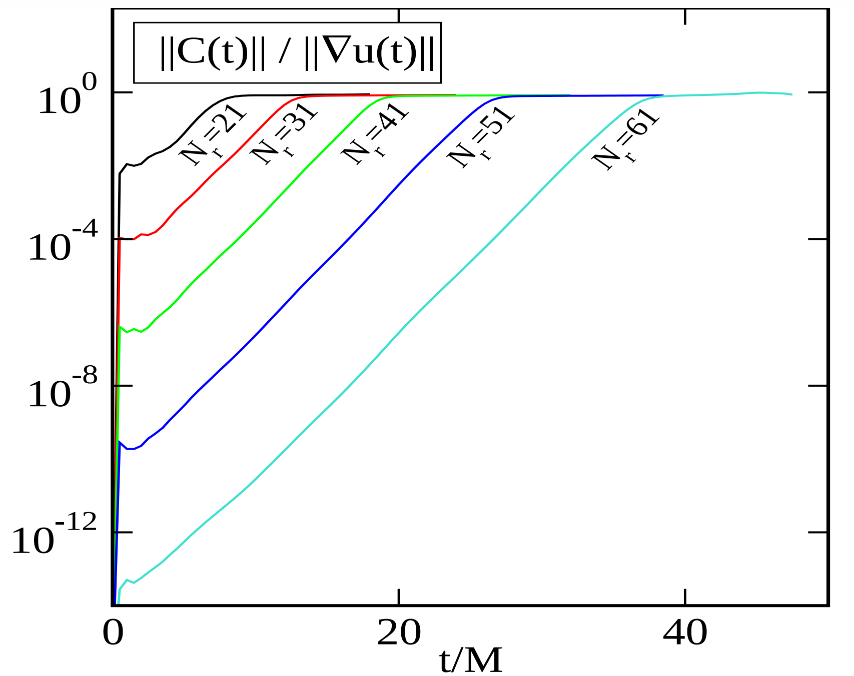




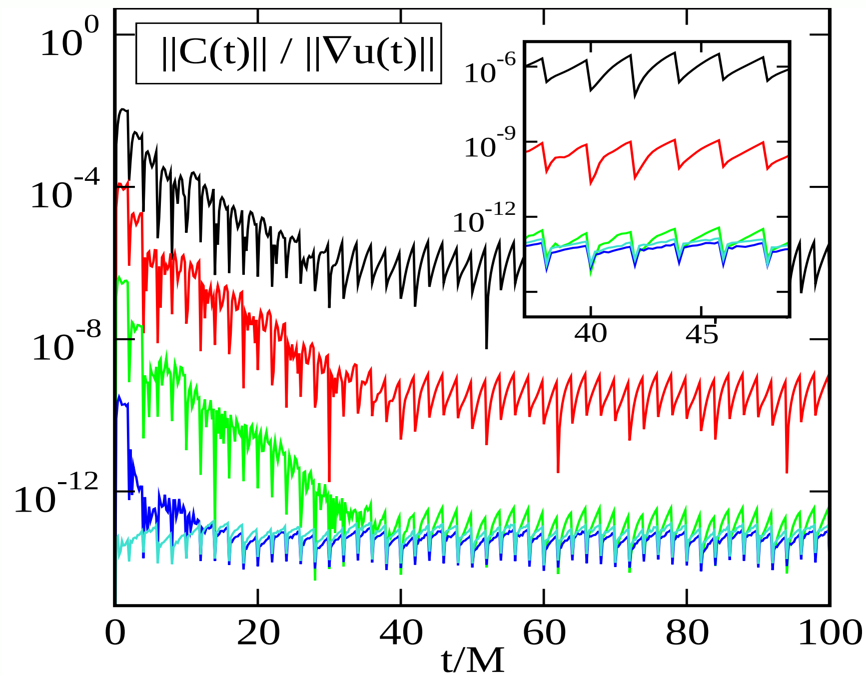
- Constraint projection causes the scalar field ψ to be non-zero at the boundary following the constraint projection step. Freezing boundary conditions force the incoming fields ψ and $(\delta^k{}_i - n^i n_i)\Phi_k$ to develop kinks as they propagate into the computational domain. These kinks in ψ generate spikes in $\mathcal{C}_i = \partial_i\psi - \Phi_i$.
- Constraint projection (even performed after every evolution time step) does not converge properly when freezing boundary conditions are used during the free evolution steps.

Constraint Projection with Constraint Preserving Boundary Conditions

- Evolutions of the pathological ($\gamma = -1$) scalar field system, with constraint preserving boundary conditions, and constraint projection (with $\Lambda = \sqrt{2}$) every $\Delta t = 2M$.



Without Projection

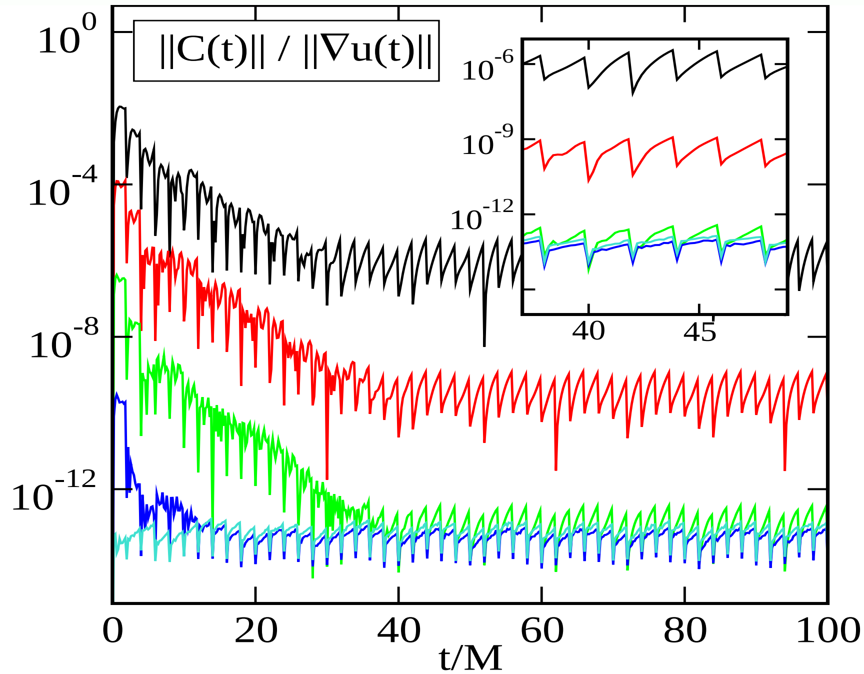


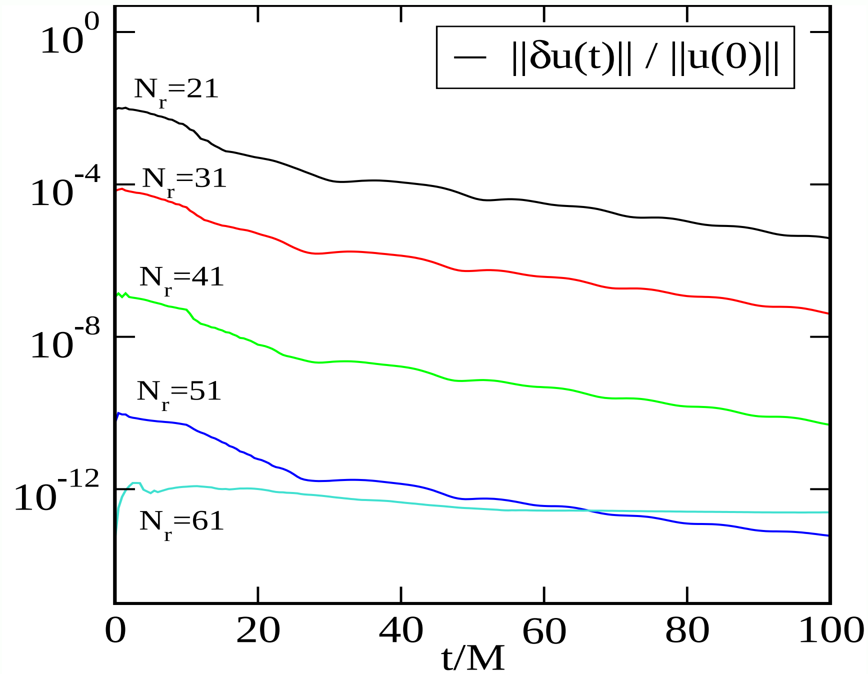
With Projection

- Optimal constraint projection does control the magnitudes of constraint violations, even in the pathological scalar fields system.

Constraint Projection with Constraint Preserving BC II

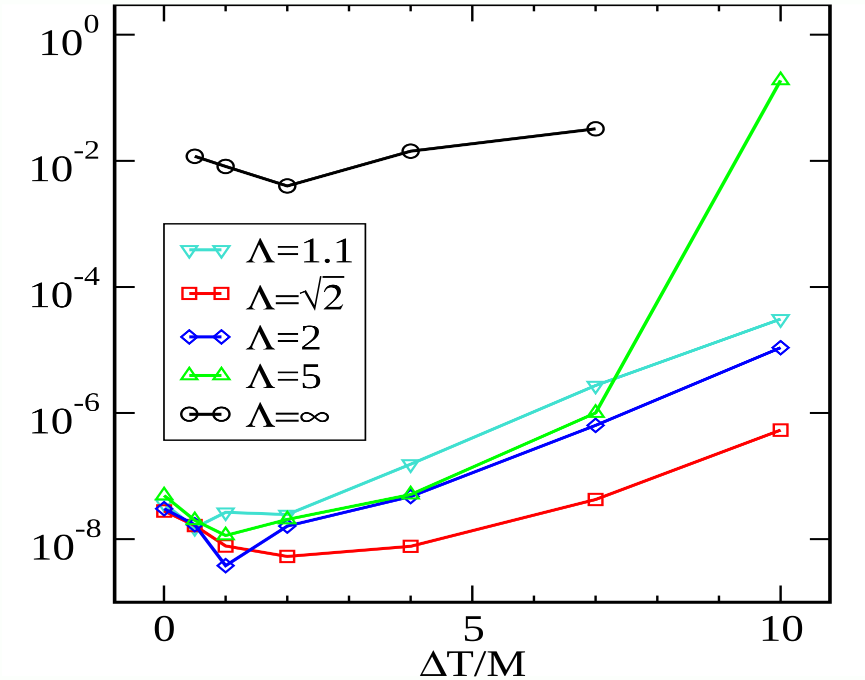
- The projected solutions have small constraint violations, but do they represent the correct solution to the evolution problem?



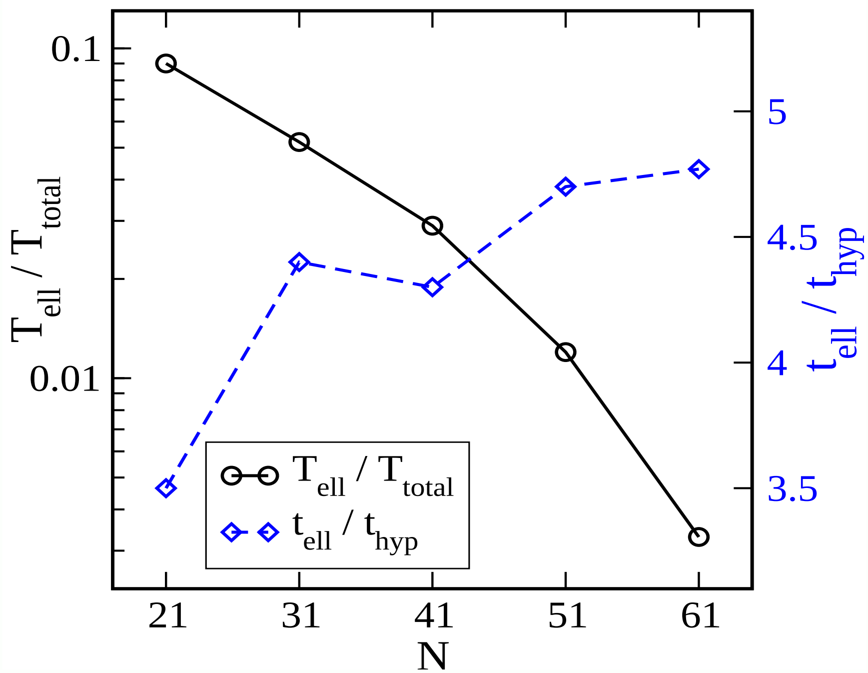


- The projected solutions also converge to the numerical solution of the standard scalar wave evolution system ($\gamma = 0$) with constraint preserving boundary conditions, in the sense that the difference norm $||\delta u(t)||$ converges to machine roundoff error levels.

Optimizing Constraint Projection



- Convergence of constraint projections for various values of the symmetrizer parameter Λ and the time between projections ΔT.



- Efficiency of constraint projection measured as the fraction of the total computational cost used by the elliptic solve $T_{\rm ell}/T_{\rm total}$; and the relative cost of one elliptic solve compared to one evolution time step $t_{\rm ell}/t_{\rm hyp}$.

Lessons Learned From the Toy Constraint Projection Problem

- Optimal constraint projection produces numerically stable constraint preserving evolutions which converge to the true numerical solutions.

- Simple constraint projection methods converge much more slowly (or not at all) compared to optimal constraint projection methods.

- Constraint projection is not convergent unless constraint preserving boundary conditions are also used during the free evolution steps.

- Constraint projection is not expensive using state-of-the-art elliptic solvers, accounting for only a fraction of a percent of the total computational cost in the highest resolution cases.

Preliminary Analysis of Optimal Projection for the Einstein System

- The Einstein system provides evolution equations for the dynamical fields,

$$u^\alpha = \{g_{ij}, K_{ij}, D_{kij}\},$$

  and also constraints that must be satisfied:

$$c^A = \{\mathcal{C}, \mathcal{C}_i, \mathcal{C}_{kij}\}$$

  where

$$\begin{aligned}
\mathcal{C} &= \frac{1}{2}(R^{(3)} - K^{ij}K_{ij} + K^2),\\
\mathcal{C}_i &= \nabla^j K_{ij} - \nabla_i K,\\
\mathcal{C}_{kij} &= \partial_k g_{ij} - 2D_{kij}.
\end{aligned}$$

- Many representations of the Einstein system are symmetric hyperbolic, so we propose to use the symmetrizer metric to construct the optimal projection Lagrangian:

$$\mathcal{L} = S_{\alpha\beta}(u^\alpha - \bar{u}^\alpha)(u^\beta - \bar{u}^\beta) + \lambda_A c^A.$$

- This Lagrangian (and the resulting optimal projection equations) are very complicated for the general Einstein system. So we first examined a simplified version of the Einstein system.

Optimal Projection for the Simplified Einstein System

- Consider solutions to the Einstein system that represent small perturbations of flat space,

$$u^\alpha = \{\,\delta_{ij} + \delta g_{ij},\, \delta K_{ij},\, \delta D_{kij}\,\}.$$

- The constraints simplify in this case to,

$$\begin{aligned}
\delta\mathscr{C} &= 2\partial_{[k}\delta D^{ik}{}_{i]}, \\
\delta\mathscr{C}_i &= 2\partial_{[k}\delta K_{i]}{}^{k}, \\
\delta\mathscr{C}_{kij} &= \partial_k \delta g_{ij} - 2\delta D_{kij}.
\end{aligned}$$

- Simplify the optimal projection Lagrangian further by using the trivial metric on the space of fields $S_{\alpha\beta} = \delta_{\alpha\beta}$:

$$\begin{aligned}
\mathscr{L} = {} & (\delta g^{ij} - \delta\bar{g}^{ij})(\delta g_{ij} - \delta\bar{g}_{ij}) + (\delta K^{ij} - \delta\bar{K}^{ij})(\delta K_{ij} - \delta\bar{K}_{ij}) \\
& + (\delta D^{kij} - \delta\bar{D}^{kij})(\delta D_{kij} - \delta\bar{D}_{kij}) \\
& + 2\lambda\,\partial_{[k}\delta D^{ik}{}_{i]} + 2\lambda^i \partial_{[k}\delta K_{i]}{}^{k} + \lambda^{kij}(\partial_k \delta g_{ij} - 2\delta D_{kij}).
\end{aligned}$$

- The variations of this Lagrangian produce a set of linear equations for δg_{ij}, δK_{ij}, δD_{kij}, λ, λ^i, and λ^{kij}.

Optimal Projection for the Simplified Einstein System II

- The optimal projection equations for the simplified Einstein system reduce to algebraic equations for δK_{ij}, δD_{kij}, and λ_{kij}:

$$\begin{aligned}
\delta K_{ij} &= \delta\bar{K}_{ij} + \frac{1}{2}\partial_{(i}\lambda_{j)} - \frac{1}{2}\delta_{ij}\partial_k\lambda^k,\\
\delta D_{kij} &= \frac{1}{2}\partial_k\delta g_{ij},\\
\lambda_{kij} &= -\delta\bar{D}_{kij} + \frac{1}{2}\delta_{ij}\partial_k\lambda - \frac{1}{2}\delta_{k(i}\partial_{j)}\lambda + \frac{1}{2}\partial_k\delta g_{ij},
\end{aligned}$$

  plus a system of differential equations for the fields δg_{ij}, λ^i, and λ:

$$\begin{aligned}
\partial^k\partial_{(i}\lambda_{k)} + \partial_i\partial_k\lambda^k &= -2\partial^k\delta\bar{K}_{ik} + 2\delta^{jk}\partial_i\delta\bar{K}_{jk},\\
\partial^k\partial_k\delta g_{ij} - \partial_i\partial_j\lambda + \delta_{ij}\partial^k\partial_k\lambda - 4\delta g_{ij} &= 2\partial^k\delta\bar{D}_{kij} - 4\delta\bar{g}_{ij},\\
\partial^i\partial^j\delta g_{ij} - \delta^{ij}\partial^k\partial_k\delta g_{ij} &= 0.
\end{aligned}$$

- This system of differential equations is elliptic. However, the equations that determine δg_{ij}, and λ are badly coupled and may be difficult to solve numerically.

Optimal Projection for the Simplified Einstein System III

- The system of equations for δg_{ij} and λ can be decoupled by decomposing δg_{ij} into transverse and longitudinal parts:

$$\delta g_{ij} = \delta\tau_{ij} + \partial_i \delta w_j + \partial_j \delta w_i + \frac{1}{3}\delta_{ij}\,\delta\tau,$$

where $0 = \delta\tau^k{}_k = \partial^k \delta\tau_{ki}$.

- Using this decomposition, the differential equations for δg_{ij} and λ can be written as a larger but decouped system of elliptic differential equations for $\delta\tau$, $\delta\mu_i$, δw_i, λ and $\delta\tau_{ij}$:

$$\begin{aligned}
\partial^k\partial_k\delta\tau &= 0,\\
\partial^k\partial_k\delta\mu_i - 4\delta\mu_i &= 2\partial^k\partial^j\delta\bar{D}_{kij} - 4\partial^k\delta\bar{g}_{ki},\\
\partial^k\partial_k\delta w_i + \partial_i\partial_k\delta w^k &= \delta\mu_i - \frac{1}{3}\partial_i\delta\tau,\\
\partial^k\partial_k\lambda &= 2\partial^k\delta\bar{D}_{ki}{}^i - \delta\bar{g}^i{}_i - \partial^k\partial_k\partial_i\delta w^i + 4\partial_k\delta w^k + 2\delta\tau,\\
\partial^k\partial_k\delta\tau_{ij} - 4\delta\tau_{ij} &= 2\partial^k\delta\bar{D}_{kij} - 4\delta\bar{g}_{ij} + \partial_i\partial_j\lambda - \delta_{ij}\,\partial^k\partial_k\lambda + \frac{4}{3}\delta_{ij}\delta\tau\\
&\quad -\partial^k\partial_k(\partial_i\delta w_j + \partial_j\delta w_i) + 4(\partial_i\delta w_j + \partial_j\delta w_i),
\end{aligned}$$

where $\delta\mu_i = \partial^k\delta g_{ki}$.