Numerical Treatment of Differential Constraints in Evolution Systems

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The Evolution Systems with Differential Constraints

Some physical processes require equations two types for their description: the equations that contain both time and space derivatives, called the evolution equations and the equations that only contain spatial derivatives, called the constraint equations.

The constraint equations play an important role in the system. Among other things they

- *guarantee that the obtained solutions is physical,*
- *enable transitions from the current process to some other processes with possibly more general descriptions and*
- *influence properties of the solution, including the stability property.*

Usually, treatment of constraints in numerical calculations is a challenging task.

The Maxwell's Equations

The evolution equations

$$\begin{aligned} \mu_0\varepsilon_0\partial_t E &= \mathbf{curl}\, B - \mu_0 J && \text{(Ampere's Circuital law)} \\ \partial_t B &= -\mathbf{curl}\, E && \text{(Faraday's law of induction)} \end{aligned}$$

The constraint equations

$$\begin{aligned} \mathbf{div}\, E &= \frac{\rho}{\varepsilon_0} && \text{(Gauss law)} \\ \mathbf{div}\, B &= 0 && \text{(absence of magnetic monopoles)} \end{aligned}$$

- the divergence constraints guarantee that a solution is physical;
- the divergence constraints enable transition from the wave equation to the Maxwell's equations.

The Incompressible Navier-Stokes Equations

Evolution equations

$$\rho\Big(\partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}\Big) = -\nabla p + \mu\Delta\mathbf{v} + f, \qquad \text{(conservation of momentum)}$$

The constraint equation

$$\mathbf{div}\,\mathbf{v} = 0 \qquad \text{(the mass continuity equation)}$$

- in the case of compressible fluid, the mass continuity equation completes the conservation of momentum equation to a closed system;
- unless the continuity equation is satisfied, transition to the incompressible Navier-Stokes equations is not possible.

The BSSN Formulation of General Relativity

Evolution equations

$$
\begin{aligned}
\partial_0 \varphi &= -\frac{1}{6} a k + \ldots, \\
\mathbf{e}^{4\varphi} \partial_0 k &= -6 a \partial^p \partial_q \varphi + \ldots, \\
\partial_0 \tilde{h}_{ij} &= -2 a \tilde{A}_{ij} + \ldots, \\
\mathbf{e}^{4\varphi} \partial_0 \tilde{A}_{ij} &= -\frac{1}{2} a \partial^p \partial_p \tilde{h}_{ij} + a \partial^p \tilde{h}_{p(i} (\tilde{\Gamma}_{j)} - 8 \partial_{j)} \varphi) + \ldots, \\
\partial_0 \tilde{\Gamma}_i &= -\frac{4}{3} a \partial_i k + \ldots,
\end{aligned}
$$

The constraint equations

$$
\partial^p \partial^q \tilde{h}_{pq} - 8 \partial^p \partial_p \varphi = \ldots, \qquad \partial^l A_{il} - \frac{2}{3} \partial_i k = \ldots,
$$

$$
\tilde{\Gamma}_j = \tilde{h}^{pq} \partial_p \tilde{h}_{qj} \,.
$$

- the constraints are used to derive the BSSN system form the Einstein equation,
- constraints are necessary to distinguish physical solutions from all solutions,
- constraints are important to the stability properties of the formulation.

The Generalized Harmonic Formulation

Evolution equations

$$\begin{aligned} \frac{1}{2}\psi^{cd}\partial_c\partial_d\psi_{ab} &= -\nabla_{(a}H_{b)} + \gamma_0[t_{(a}C_{b)} - \frac{1}{2}\psi_{ab}t^c C_c] + ... \\ \psi_{ab}\nabla_c\nabla^c x^b &= H_a(x,\psi) \end{aligned}$$

The constraint equations

$$C_a := H_a + \frac{1}{2}\psi^{ab}(\partial_b\psi_{ac} + \partial_c\psi_{ab} - \partial_a\psi_{bc}) = 0$$

- the constraints are used to derive the BSSN system form the Einstein equation,
- constraints are necessary to distinguish physical solutions from all solutions.

Numerical Solution of Systems with Differential Constraints

For the robustness of the numerical method it is important that

- *a well-posed IBVP be specified for the system with differential constraints, ideally in a manner suitable for computations;*

  Well-posed constraint-preserving boundary conditions, methods of analysis for IBVP.

- *techniques be developed for the numerical treatment of the constraint equations.*

  Technique of constrained evolution, constraint projection, constraint-preserving boundary conditions, constraint damping, constraint-free methods.

Methods for Formulating Well-Posed IBVPs for Systems with Differential Constraints

The Model System

Let $A : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^n)$, $A^* = -A$ and $B : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^k)$.

$$\begin{aligned} \partial_t u &= Au + F \\ Bu &= g \end{aligned}$$

The key assumption $BA = NB$, $N^* = -N$. Then the evolution of $p := Bu - g$ obeys:

$$\partial_t p = \partial_t(Bu - g) \quad = \quad BAu + BF - \partial_t g = NBu + BF - \partial_t g = Np + \mathcal{F}$$

If $BF - \partial_t g = \mathcal{F} = 0$, then the system is said to *preserve the constraints*. Two options are then available

- Constrained Evolution: solve both the evolution and constraint equations;
- Free Evolution: solve the evolution equations, constraint equations are only monitored.

The problem is well-posed in a unbounded domain. Existence is guaranteed (locally in time), if the initial data satisfies the constraint equations.

In a bounded domain, well-posedness of the IBVP is contingent to the existence of well-posed constraint-preserving boundary conditions.

Example 1. The Maxwell's Equations

$$
\begin{aligned}
\partial_t u &= \mathbf{curl}\, v \\
\partial_t v &= -\mathbf{curl}\, u \\
p := \mathbf{div}\, u &= 0 \\
q := \mathbf{div}\, v &= 0
\end{aligned}
$$

Propagation of the constraints: (use $\mathbf{div}\ \mathbf{curl} = 0$)

$$
\begin{aligned}
\partial_t p &= 0 \\
\partial_t q &= 0
\end{aligned}
$$

Solve the free evolution problem, e.g., use $\mathbf{div}$-free elements.

Well-posedness on an IBVP is automatic since propagation of the constraints is static: *boundary data does not disturb constraints quantities.*

Example 2. The linearized BSSN system

$$
\begin{aligned}
\partial_t \varphi &= -\frac{1}{6}\kappa, \\
\partial_t \kappa &= -6\Delta\varphi, \\
\partial_t \tilde{\gamma}_{ij} &= -2A_{ij}, \\
\partial_t A_{ij} &= -\frac{1}{2}\Delta\tilde{\gamma}_{ij} + \nabla_{(i}\Gamma_{j)} - 8\nabla_i\nabla_j\varphi, \\
\partial_t \Gamma_i &= -\frac{4}{3}\nabla_i\kappa.
\end{aligned}
$$

Subject to the constraint equations

$$
H := \mathbf{div}\,\Gamma - 8\Delta\varphi = 0, \quad M_i := (\mathbf{div_r} A)_i - \frac{2}{3}\nabla_i\kappa = 0, \quad C_i := \Gamma_i - (\mathbf{div_r}\tilde{\gamma})_i = 0
$$

Evolution of constraints:

$$
\partial_t H = 0, \qquad \partial_t C_i = -2M_i, \qquad \partial_t M_i = -\tfrac{1}{2}\Delta C_i + \tfrac{1}{2}\nabla_i H.
$$

Systems are reducible to a FOSH system, possesses a well posed energy (Gundlach and Martin-Garcia (2004), Alekseenko (2005)). *Constraint compatible boundary conditions are essential for the well-posedness.*

The Meta Strategy for the Well-Posed IBVP

$$\begin{aligned} \partial_t u &= Au + F \\ Bu &= g \end{aligned}$$

Consider propagation of the constraints. We assume that $BA = NB$, $N^* = -N$ (or that $\exists B$, $B > 0$, such that $(BN)^* = -BN$). Then $p := Bu - g$ obeys:

$$\partial_t p = Np + \mathcal{F}$$

To construct the constraint-preserving boundary conditions:

- find the BCs that imply $p = \text{const.}$ ($\textit{ideally also minimize reflections at the artificial boundary}$);
- replace p with its definition, obtain ($\textit{higher order differential}$) BCs for u;
- study the well-posedness of the resulting IBVP using either the energy methods or the Kreiss technique of pseudo-differential reduction.

Example 1. 1D Wave Equation

$$\partial_t^2 u = \partial_x^2 u, \qquad x \in [x_0, x_1]$$

$$C = \partial_x u = 0$$

Notice that C obeys $\partial_t^2 C = \partial_x^2 C$. Consider

$C|_{x_0} = 0$,

$\partial_x u|_{x_0} = 0$

This is a constraint preserving Neumann boundary condition.

In 3D it is possible to find a combination of homogeneous Neumann and Dirichlet BCs that are constraint-preserving. Inhomogenous Neumann and Dirichlet BCs require integration of a PDE system restricted to the boundary.

Example 2. 1D Wave Equation

$$\partial_t^2 u = \partial_x^2 u, \qquad x \in [x_0, x_1]$$
$$C = \partial_x u = 0$$

Notice that C obeys $\partial_t^2 C = \partial_x^2 C$. Consider

$(\partial_t C - \partial_x C)|_{x_0} = 0$,

$\partial_t \partial_x u - \partial_x^2 u = 0$,

Use the evolution equation to replace $\partial_x^2 u = \partial_t^2 u$:

$\partial_t^2 \partial_x u - \partial_t^2 u = 0$.

Or $\partial_t(\partial_t u - \partial_x u) = 0$.

Therefore, set
$(\partial_t u - \partial_x u)|_{x_0} = \partial_t u(x_0, 0) - \partial_x u(x_0, 0)$

In 3D the "trading of the second normal derivatives" step will introduce tangential derivatives in the BCs. The energy proofs are not obvious. However, the Kreiss techniques of pseudo differential reduction proved to be very effective to rule out the bad cases.

An alternative Meta Strategy for the Well-Posed IBVP

Notice that the problem

$$\partial_t^2 u = \partial_x^2 u, \quad x \in [x_0, x_1]$$
$$C = \partial_x u = 0$$

does not need any boundary conditions. Instead, one can reduce it to

$$\begin{aligned} \partial_t^2 u &= 0 \\ C = \partial_x u &= 0 \end{aligned}$$

and integrate from any compatible initial data. Notice that in the new system, $\partial_t C = 0$.

This suggests *An Alternative Meta Strategy for the Well-Posed IBVP:*

- reduce to a system that evolves constraint quantities statically, find boundary conditions that are "essential" for the system;
- *use the essential boundary conditions in the original system, complement with the data that enforces the constraint and makes the problem well-posed.*
- try to prove the well-posedness of the IBVP using the energy methods or the Kreiss techniques of pseudo-differential reduction.

Example 4. The 3D Wave Equation

Vector wave equation ($u_i \in \mathbb{R}^3$) in a polyhedral domain Ω (Friedrich and Nagy 99, Sarbach and Reula 05, Alekseenko 07)

$$\begin{aligned} \partial_t^2 u_i &= \Delta u_i \\ C &:= \mathbf{div}\, u = 0 \qquad\qquad (\partial_t^2 C = \Delta C) \end{aligned}$$

Use the relationship to Maxwell's equations, $\Delta u_i = -\mathbf{curl}\ \mathbf{curl}\ u_i + \nabla_i \mathbf{div}\, u$,

$$\begin{aligned} \partial_t^2 u_i &= -\mathbf{curl}\ \mathbf{curl}\ u_i \\ C &:= \mathbf{div}\, u = 0 \qquad\qquad (\partial_t^2 C = 0) \end{aligned}$$

Let $|\alpha| < 1$, u_n - normal and u_A - tangential components of u_i on the boundary $\partial\Omega$

$$\begin{aligned} \partial_t u_A + \partial_n u_A - \partial_A u_n &= \alpha(\partial_t u_A - \partial_n u_A + \partial_A u_n) + g_A \\ \partial_t u_n + \partial_n u_n &= -\alpha(\partial_t u_t - \partial_n u_n) + g \end{aligned}$$

Implies that $\partial_t C + \partial_n C = \alpha(\partial_t C - \partial_n C)$

This problem is well-posed in the generalized sense (Alekseenko 07), see also (Reula and Sarbach, 2005) and (Kreiss etal., 2007, `arXiv:0707.44188v2.`*)*

Methods for Solving Numerically the Systems with Differential Constraints

Solving the Constrained Evolution Problems Numerically

Let $A : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^n)$, $A^* = -A$ and $B : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^k)$,

$$\begin{aligned} \partial_t u &= Au + F \\ Bu &= g \end{aligned}$$

Prescribe the constraint satisfying initial data and constraint-preserving boundary data.

Constraint equations are still violated in the numerical simulations due to the discretization errors!

Methods to maintain the constraint equations:

- Include the constraint equations into the solution.
- Make periodical projections to the constraint manifold
- Add terms to the evolution equations that damp the small constraint violations
- Use sophisticated discretization techniques, e.g., constraint-free elements.

Incorporating the Constraint Equations into Evolution

Let $A : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^n)$, $A^* = -A$ and $B : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^k)$. Consider

$$\begin{aligned} \partial_t u &= Au + F && (1) \\ Bu &= g && (2) \end{aligned}$$

Include the constraint equations into the evolution. For example, introduce

$$\begin{aligned} \partial_t u &= Au - B^* p + F \\ \partial_t p &= Bu - g - \lambda^2 p \end{aligned}$$

Can check that (we assume that $BA = NB$, $N^* = -N$:)

$$\partial_t^2 p = Np - BB^* p - \lambda^2 \partial_t p - \partial_t g$$

The energy estimate

$$\partial_t [\|\partial_t p\|^2 + \|B^* p\|^2] = -\lambda^2 \|\partial_t p\|^2 - \int_\Omega \partial_t g \partial_t p$$

Enforcing the Constraint Equations by a projection

Let $A : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^n)$, $A^* = -A$ and $B : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^k)$. Consider

$$\begin{aligned} \partial_t u &= Au + F \\ Bu &= g \end{aligned}$$

Keep both the evolution and constraint equations are under control by solve the evolution equations and periodically project u back on the constraint manifold, e.g. by computing

$$\tilde{u} = \{w : \mathcal{L} = \|w - u\|^2 + \lambda(Bw - g) \to \min\}$$

Disadvantages: the projection may be expensive.

Using the Constraint Damping

Let $A : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^n)$, $A^* = -A$ and $B : C^\infty(\Omega, \mathbb{R}^n) \to C^\infty(\Omega, \mathbb{R}^k)$. Consider

$$\begin{aligned} \partial_t u &= Au + F \\ Bu &= g \end{aligned}$$

Introduce terms in evolution equations (not necessarily all of them) that *a) are proportional to the constraint quantities, b) do not disturb the symmetric hyperbolicity of the system and c) force the small constraint violations to decay exponentially in time.* The recipe is non-unique. Essentially, we are looking for an algebraic operator $\Lambda : \mathbb{R}^k \to \mathbb{R}^n$ such that

$$\partial_t u = Au - \Lambda(Bu - g) + F$$

has the desired properties.

One of the requirements is that $B\Lambda(Bu - g)$ does not produce higher order terms, so Λ has to be rather sparse and imply equation of the form

$$\partial_t p = -LL^* p - \mu^2 p$$

Example 1. The Scalar Wave Equation

$$\partial_t^2 \psi - \Delta \psi = 0$$

Introduce $\pi = \partial_t \psi$, $\varphi_i = \nabla_i \psi$, decompose into the FOSH system (Holst etal, 2004)

$$\begin{aligned} \partial_t \psi &= \pi \\ \partial_t \pi &= \mathbf{div}\, \varphi \\ \partial_t \varphi_i &= \nabla_i \pi \end{aligned}$$

The first order system has a constraint $C_i = \varphi_i - \nabla_i \psi$ that is evolving statically,

$$\partial_t C_i = \partial_t(\varphi_i - \nabla_i \psi) = \partial_t \varphi_i - \nabla_i \partial_t \psi = \partial_t \varphi_i - \nabla_i \pi = 0.$$

or

$$\partial_t C_i = 0$$

Example 1. The Scalar Wave Equation

Introduce the modified system:

$$\begin{aligned}\partial_t\psi &= \pi \\ \partial_t\pi &= \mathbf{div}\,\varphi \\ \partial_t\varphi_i &= \nabla_i\pi - \mu^2(\varphi_i - \nabla_i\psi)\end{aligned}$$

The new system is still symmetric hyperbolic:

$$\begin{aligned}\partial_t\psi &= \pi \\ \partial_t(\pi - \mu^2\psi) &= \mathbf{div}\,\varphi + \mu^2(\pi - \mu^2\psi) + \mu^4\psi \\ \partial_t\varphi_i &= \nabla_i(\pi - \mu^2\psi) - \mu^2\varphi_i\end{aligned}$$

and it implies

$$\partial_t C_i = -\mu^2 C_i$$

Example 2. The Vector Wave Equation

Consider the vector wave equation ($u_i \in \mathbb{R}^3$)

$$\begin{aligned} \partial_t^2 u_i &= \Delta u_i \\ C &:= \mathbf{div}\, u = 0 \qquad\qquad (\partial_t^2 C = \Delta C) \end{aligned}$$

Want to solve first order in time, second order in space. Introduce $\pi_i = \partial_t u$. Use $\Delta u_i = -\mathbf{curl}\,\mathbf{curl}\ u_i + \nabla_i \mathbf{div}\, u$, rewrite the evolution equation as

$$\begin{aligned} \partial_t u_i &= \pi_i \\ \partial_t \pi_i &= -\mathbf{curl}\,\mathbf{curl}\ u_i + \nabla_i \mathbf{div}\, u \end{aligned}$$

Introduce $\varphi_i = \mathbf{curl}\, u_i$, $C = \mathbf{div}\, u$, reduce to the FOSH system

$$\begin{aligned} \partial_t u_i &= \pi_i \\ \partial_t \pi_i &= -\mathbf{curl}\ \varphi_i + \nabla_i C \\ \partial_t \varphi_i &= \mathbf{curl}\, \pi_i \\ \partial_t C &= \mathbf{div}\, \pi \end{aligned}$$

Want to enforce $C = 0$ by adding damping terms to the last equation.

Example 2. The Vector Wave Equation

Introduce the modified system:

$$\begin{aligned} \partial_t u_i &= \pi_i \\ \partial_t \pi_i &= -\mathbf{curl}\, \varphi_i + \nabla_i C \\ \partial_t \varphi_i &= \mathbf{curl}\, \pi_i \\ \partial_t C &= \mathbf{div}\, \pi - \mu^2 C \end{aligned}$$

Verify that C now obeys

$$\partial_t^2 C = \delta C - \mu^2 \partial_t C \qquad \Rightarrow \qquad \partial_t [\|\partial_t C\|^2 + \|\nabla_i C\|^2] = -\mu^2 \|\partial_t C\|^2$$

Finally, go back to first order in time second order in space

$$\begin{aligned} \partial_t u_i &= \pi_i \\ \partial_t \pi_i &= -\mathbf{curl}\ \mathbf{curl}\ u_i + \nabla_i \mathbf{div}\, u - \mu^2 \int_0^t \mathbf{e}^{-\mu^2 (t-\tau)} \mathbf{div}\, u(\tau) d\tau \end{aligned}$$

Conclusion

- *We did not talk about the techniques for proving the well-posedness of IBVP for evolution systems with differential constraints. Numerical relativity spurred development of new techniques based on the pseudo-differential reduction and the energy methods (Kreiss and Lorenz, 89; Gustafsson, Kreiss and Oliger 95; Sarbach and Reula 2005, Kreiss and Winicour, 2006; Rinne, 2006; Kreiss, Reula, Sarbach and Winicour, 2007).*

- *A work is underway to implement techniques of constraint-damping, constraint preserving boundary conditions for a model problem for Einstein equations in first order in time second order in space form using the DG method.*

- *It is interesting to apply these techniques to other problems in numerical relativity, such as gauge driving*