Finite Element Methods in Numerical Relativity

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- Variational problems and methods, Petrov-Galerkin methods, FE methods.
- Nonlinear approximation: Adaptive FE and fast elliptic solvers.
- Application to GR constraints: a priori & a posteriori estimates, adaptivity.
- Some examples with the Finite Element ToolKit (FEtk).
- Variational methods for constrained evolution.

Variational Problems.

Let $J: X \mapsto \mathbb{R}$, where X is a Banach space (complete normed vector space). J(u) is called stationary at $u \in X$ if:

$$\langle J'(u), v \rangle = 0, \ \forall v \in X.$$
⁽¹⁾

J' is the (Gateaux, or G-)derivative of J at u in the direction v,

$$\langle J'(u), v \rangle = \left. \frac{d}{d\epsilon} J(u+\epsilon v) \right|_{\epsilon=0}$$

At each point $u \in X$, $J'(u) \in X^*$ (space of bounded linear functionals on X). Stationarity (1) is e.g. a necessary condition for u to be a solution to:

Find
$$u \in X$$
 such that $J(u) \leq J(v), \forall v \in X$. (2)

However, the condition of stationarity is more general, since the functional J(u) may have only saddle points; (1) then includes the principle of stationary action in dynamics.

Variational Problems: A Nonlinear Example.

Let $X = W_0^{1,p}(\Omega)$, with $\Omega \subset \mathbb{R}^d$ a "smooth" bounded domain. Define:

$$J(u) = \frac{1}{2} \int_{\Omega} [\nabla u \cdot \nabla u - g(u)] \, dx, \quad \text{with } g(u) \in L^{1}(\Omega) \text{ when } u \in W^{1,p}(\Omega).$$

The notation here is $(1 \le p < \infty)$:

$$\|u\|_{W^{1,p}(\Omega)} = \left(\int_{\Omega} |u|^p + |\nabla u|^p \ dx\right)^{1/p},$$
$$W^{1,p}(\Omega) = \{u \in L^p(\Omega) : \|u\|_{W^{1,p}(\Omega)} < \infty \},$$
$$W^{1,p}_0(\Omega) = \{u \in W^{1,p}(\Omega) : \text{ trace } u = 0 \text{ on } \partial\Omega \}$$

The condition for stationarity of J(u) is:

Find
$$u \in W_0^{1,p}(\Omega)$$
 s.t. $\langle J'(u), v \rangle = \int_{\Omega} [\nabla u \cdot \nabla v - g'(u)v] dx = 0, \ \forall v \in W_0^{1,p}(\Omega),$

which (if a classical solution exists) is equivalent to determining u from:

$$-\nabla^2 u = g'(u) \text{ in } \Omega,$$

 $u = 0 \text{ on } \partial\Omega.$

Solving General Nonlinear Variational Problems.

Let X, Y be Banach spaces (possibly X = Y), and $F : X \mapsto Y^*$. Consider now:

Find $u \in X$ such that $F(u) = 0 \in Y^*$.

As a linear functional on Y, we can consider the general "variational" problem:

Find
$$u \in X$$
 such that $\langle F(u), v \rangle = 0, \ \forall v \in Y.$ (3)

If the nonlinear problem (3) is well-posed, one typically solves for u using a Newton iteration based on linearization with the *G*-derivative of $\langle F(u), v \rangle$:

$$\langle F'(u)w,v\rangle = \frac{d}{d\epsilon} \langle F(u+\epsilon w),v\rangle \Big|_{\epsilon=0}$$

Given an initial approximation $u^0 \approx u$, a (global, inexact) Newton iteration is:

(a) Find
$$w \in X$$
 such that: $\langle F'(u^k)w, v \rangle = -\langle F(u^k), v \rangle + r$, $\forall v \in Y$
(b) Set: $u^{k+1} = u^k + \lambda w$

One discretizes (a)-(b) at the "last moment", producing a matrix equation. Required Newton steps independent of discretization [Allgower et. al, 1986].

The Resulting Linear Problems when $X \neq Y$.

Solving the nonlinear problem (3) requires repeatedly solving a linear problem:

Find
$$u \in X$$
 such that $a(u, v) = f(v), \quad \forall v \in Y$, (4)

where for fixed $\bar{u} \in X$,

$$a(u,v) = \langle F'(\bar{u})u,v\rangle, \qquad f(v) = -\langle F(\bar{u}),v\rangle.$$

Assume the bilinear form $a(\cdot, \cdot)$ and linear functional $f(\cdot)$ satisfy four conditions:

$$\inf_{u \in X} \sup_{v \in Y} \frac{a(u, v)}{\|u\|_X \|v\|_Y} \ge m > 0, \qquad a(u, v) \le M \|u\|_X \|v\|_Y, \qquad f(v) \le L \|v\|_Y, \tag{5}$$

For each $0 \neq v \in Y$, there exists $u \in X$ s.t. $a(u, v) \neq 0$. (6)

It follows [Babuska-Aziz, 1972] that (4) is well-posed, and the *a priori* estimate:

$$\|u\|_X \le \frac{L}{m}$$

follows from

$$m \|u\|_X \le \sup_{v \in Y} \frac{a(u,v)}{\|v\|_Y} = \sup_{v \in Y} \frac{f(v)}{\|v\|_Y} \le L.$$

If some of the properties (5)-(6) are lost, or if the problem is nonlinear as in (3) itself, other *a priori* estimates may still be possible (case-by-case basis).

The Resulting Linear Problems when X = Y.

Consider again the linear problem, but now in special case of X = Y:

Find
$$u \in X$$
 such that $a(u, v) = f(v), \quad \forall v \in X,$ (7)

The following three conditions (with m > 0) are trivially equivalent to the three conditions (5) when X = Y (condition (6) is no longer needed):

$$a(u,u) \ge m \|u\|_X^2, \quad a(u,v) \le M \|u\|_X \|v\|_X, \quad f(v) \le L \|v\|_X.$$
 (8)

It follows [Lax-Milgram, 1957] that (7) is well-posed, and the *a priori* estimate:

$$\|u\|_X \le \frac{L}{m}$$

follows now simply from

$$m \|u\|_X^2 \le a(u, u) = f(u) \le L \|u\|_X.$$

Again, If some of the properties (8) are lost, or if the problem is nonlinear as in (3) itself, other *a priori* estimates may still be possible (case-by-case basis).

Example: Nonlinear Potential Equation.

From our earlier example, if

$$J(u) = \frac{1}{2} \int_{\Omega} [\nabla u \cdot \nabla u - g(u)] \, dx,$$

the condition for stationarity of J(u) is:

Find $u \in W_0^{1,p}(\Omega)$ such that $\langle F(u), v \rangle = 0, \ \forall v \in W_0^{1,p}(\Omega),$

where

$$\langle F(u), v \rangle = \langle J'(u), v \rangle = \int_{\Omega} [\nabla u \cdot \nabla v - g'(u)v] dx.$$

To build a Newton iteration, we only need the additional derivative:

$$\langle F'(u)w,v\rangle = \left.\frac{d}{d\epsilon}\langle F(u+\epsilon w),v\rangle\right|_{\epsilon=0} = \int_{\Omega} \left[\nabla w\cdot\nabla v - g''(u)wv\right] dx.$$

Well-posedness of the linearized problem in a Newton iteration:

Find
$$w \in W^{1,p}(\Omega)$$
 such that $\langle F'(u)w, v \rangle = -\langle F(u), v \rangle$, $\forall v \in W^{1,p}(\Omega)$,

is assured by establishing coercivity and boundedness properties on F' and F.

Discretizing Nonlinear Variational Problems.

A Petrov-Galerkin (PG) method looks for an approximation $u_h \approx u$ satisfying the variational problem (3) in subspaces:

Find $u_h \in X_h \subseteq X$ such that $\langle F(u_h), v_h \rangle = 0$, $\forall v_h \in Y_h \subseteq Y$.

A Galerkin method is the special case of Y = X and $Y_h = X_h$.

Consider now the case $\dim(X_h) = \dim(Y_h) = n < \infty$.

If span{ ϕ_1, \ldots, ϕ_n } = $X_h \subseteq X$ and span{ ψ_1, \ldots, ψ_n } = $Y_h \subseteq Y$ for bases { ϕ_j }, { ψ_j }, the problem is then to determine the appropriate coefficients in the expansion:

$$u_h = \sum_{j=1}^n \alpha_j \phi_j.$$

The variational problem gives n (nonlinear) equations for the n coefficients:

Find
$$u_h = \sum_{j=1}^n \alpha_j \phi_j$$
 such that $\langle F(u_h), \psi_i \rangle = 0, \ i = 1, \dots, n.$

Petrov-Galerkin Approximation Error $(X \neq Y)$.

To analyze the error, consider a linear problem and its PG approximation:

Find
$$u \in X$$
 s.t. $a(u, v) = f(v), \forall v \in Y,$ (9)

Find
$$u_h \in X_h \subseteq X$$
 s.t. $a(u_h, v_h) = f(v_h), \quad \forall v_h \in Y_h \subseteq Y,$ (10)

where the following are assumed to hold for [X, Y] (AND ALSO $[X_h, Y_h]!$):

$$\inf_{u \in X} \sup_{v \in Y} \frac{a(u, v)}{\|u\|_X \|v\|_Y} \ge m > 0, \qquad a(u, v) \le M \|u\|_X \|v\|_Y, \qquad f(v) \le L \|v\|_Y.$$
(11)

The following *a priori* error estimate [Babuska;Brezzi] for PG approximation:

$$||u - u_h||_X \le \left(1 + \frac{M}{m}\right) \inf_{w_h \in X_h} ||u - w_h||_X,$$

follows from $a(u - u_h, v_h) = 0$, $a(u - w_h, v_h) = a(u_h - w_h, v_h)$, $\forall v_h \in Y_h$, from $m \|u_h - w_h\|_X \le \sup_{v \in Y_h} \frac{a(u_h - w_h, v)}{\|v\|_Y} = \sup_{v \in Y_h} \frac{a(u - w_h, v)}{\|v\|_Y} \le M \|u - w_h\|_X$,

and from the triangle inequality

$$||u - u_h||_X \le ||u - w_h||_X + ||u_h - w_h||_X \le \left(1 + \frac{M}{m}\right) ||u - w_h||_X.$$

If some of the properties (11) are lost, or if the problem is nonlinear, a priori estimates for PG methods may still be possible (case-by-case basis).

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Galerkin Approximation Error (X = Y).

To analyze the error, consider a linear problem and its Galerkin approximation:

Find
$$u \in X$$
 s.t. $a(u, v) = f(v), \forall v \in X,$ (12)

Find
$$u_h \in X_h \subseteq X$$
 s.t. $a(u_h, v_h) = f(v_h), \quad \forall v_h \in X_h \subseteq X,$ (13)

where again

$$a(u,u) \ge m \|u\|_X^2, \quad a(u,v) \le M \|u\|_X \|v\|_X, \quad f(v) \le L \|v\|_X.$$
 (14)

The following *a priori* error estimate [Cea's Lemma] for the Galerkin approximation:

$$\|u-u_h\|_X \le \left(\frac{M}{m}\right) \inf_{w_h \in X_h} \|u-w_h\|_X,$$

follows again from $a(u - u_h, v_h) = 0$, $\forall v_h \in X_h$, but now simply from

$$m\|u-u_h\|_X^2 \le a(u-u_h, u-u_h) = a(u-u_h, u-w_h) \le \|u-u_h\|_X \|u-w_h\|_X.$$

If some of the properties (14) are lost, or if the problem is nonlinear, *a priori* estimates for Galerkin methods may still be possible (case-by-case basis).

Finite Element Methods.

For a PG approximation $u_h = \sum_{j=1}^n \alpha_j \phi_j$, an $n \times n$ matrix equation is produced:

$$AX = B,$$

where

$$A_{ij} = a(\phi_j, \psi_i), \qquad X_i = \alpha_i, \qquad B_i = f(\psi_i).$$

Regarding this linear system, for practical reasons one hopes that:

- The cost of storing the matrix A is as close to optimal O(n) as possible;
- The cost of inverting the matrix A is as close to optimal O(n) as possible.

Roughly speaking, finite element (FE) methods are computational techniques that allow management of two issues related to PG approximation:

- 1. Control of the approximation error: $E(u u_h) = ||u u_h||_X$,
- 2. Space/time complexity of storing and solving the *n* equations: AX = B.

Locally Supported FE Bases and Simplex Subdivision.

FE methods use piecewise polynomial spaces (controls $E(u - u_h)$) with local support (generates sparse matrices A), defined on *elements* such as simplices.



Error-estimate-driven adaptive finite element methods often based on simplex subdivision. (Above: 2/4/8-section and conformity.)

Assembling FE Systems Using An Atlas of Charts.

An interesting feature of FE methods is that one typically uses coordinate transformations to assemble the matrix problem AX = B.

For example, if our variational problem a(u, v) = f(v) involves

$$a(u,v) = \int_{\Omega} [\nabla u \cdot \nabla v + cuv] \, dx, \qquad f(v) = \int_{\Omega} fv \, dx,$$

and if the domain $\Omega \subset \mathbb{R}^d$ is disjointly covered by conforming elements T_k ,

$$\bar{\Omega} = \bigcup_{k=1}^{m} T_k, \qquad \emptyset = \bigcap_{k=1}^{m} \operatorname{int}(T_k),$$

then

$$A_{ij} = a(\phi_j, \psi_i) = \int_{\Omega} [\nabla \phi_j \cdot \nabla \psi_i + c\phi_j \psi_i] \, dx = \sum_{k=1}^m \int_{T_k} [\nabla \phi_j \cdot \nabla \psi_i + c\phi_j \psi_i] \, dx,$$

$$B_i = f(\psi_i) = \int_{\Omega} f\psi_i \, dx = \sum_{k=1}^{\infty} \int_{T_k} f\psi_i \, dx.$$

Implementation involves performing the integral on each element T_k by first doing a coordinate transformation to a model of \mathbb{R}^d (the *reference element*), doing the integral there using transformation jacobians, and then mapping the result back to the element T_k using coordinate transformations again.

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Nonlinear Approximation using Adaptive Methods.

Adaptive FE alorithms: build approximation spaces adaptively, meeting target quality using spaces having minimal dimension. This is *nonlinear approximation*.

A priori estimates (generally non-computable) establish convergence; these asymptotic statements not useful for driving adaptivity.

A posteriori error estimates (by definition computable) are critical for driving adaptivity in nonlinear approximation schemes.

FE codes such as PLTMG (2D) and FEtk (3D; described below) equi-distribute error over simplices using subdivision driven by *a posteriori* error estimates:

- 1. Construct problem (build mesh, define PDE coefficients, etc)
- 2. While $(E(u u_h)$ is "large") do:
 - 1. Find $u_h \in X_h$ such that $\langle F(u_h), v_h \rangle = 0, \forall v_h \in Y_h$
 - 2. Estimate $E(u u_h)$ over each element, set $Q1 = Q2 = \phi$.
 - 3. Place simplices with large error in "refinement" Q1
 - 4. Bisect simplices in Q1 (removing from Q1), placing nonconforming simplices created in temporary Q2.
 - 5. Q1 is now empty; set Q1 = Q2, $Q2 = \phi$.
 - 6. If Q1 is not empty, goto (d).
- 7. end while

A posteriori error estimation for driving h-adaptivity.

Idea: estimate $E(u - u_h)$ and use information to improve u_h . Some standard options with a well-developed literature:

- 1. Nonlinear (strong) residual error estimation [Babuska, Verfurth,...].
- 2. Linearized global dual problem error estimation [Johnson, Estep,...].

Residual estimation: given Banach spaces X, Y, and $X_h \subset X$, $Y_h \subset Y$, consider

$$F(u) = 0, \quad F \in C^1(X, Y^*), \quad F_h(u_h) = 0, \quad F_h \in C^0(X_h, Y_h^*).$$

The nonlinear residual $F(u_h)$ can be used to estimate $||u - u_h||_X$:

$$\left[\frac{1}{2}\|DF(u)\|_{\mathcal{L}(X,Y^*)}^{-1}\right] \cdot \|F(u_h)\|_{Y^*} \le \|u-u_h\|_X \le \left[2\|DF(u)^{-1}\|_{\mathcal{L}(Y^*,X)}\right] \cdot \|F(u_h)\|_{Y^*}.$$

Theorem 1. (E.g., [H1]) (Residual-based) The galerkin solution u_h satisfies

$$E(u-u_h) = \|u-u_h\|_X \le C\left(\sum_{s\in\mathcal{S}}\eta_s^p\right)^{1/p}, \quad (p \text{ depends on choice of } X \text{ and } Y)$$

where η_s is a computable element-wise error "indicator" and C is a "constant". Outline of Proof: A few inequalities and a quasi-interpolation argument. \Box

Duality-based a posteriori error estimation.

Assume $F: X \mapsto Y$, X and Y Banach spaces, and $F \in C^1$, s.t.

$$F(u+h) = F(u) + \left\{ \int_0^1 DF(u+\xi h)d\xi \right\} h.$$

Taking $h = u_h - u$, F(u) = 0, and u_h a Galerkin approximation to u, gives

$$F(u_h) = F(u+h) = F(u+[u_h - u]) = F(u) + \mathcal{A}(u_h - u) = -\mathcal{A}(u - u_h),$$

where

$$\mathcal{A} = \int_0^1 DF(u+\xi h)d\xi.$$

We wish to estimate linear functionals $E(u - u_h) = \langle u - u_h, \psi \rangle$ of the error $u - u_h$. **Theorem 2. (E.g., [H1])** (Duality-based) If ϕ_h is a Galerkin approximation to the solution of the dual problem: $\mathcal{A}^T \phi = \psi$, then

$$E(u-u_h) = -\langle F(u_h), \phi - \phi_h \rangle.$$

Outline of Proof:

$$E(u - u_h) = \langle u - u_h, \psi \rangle = \langle u - u_h, \mathcal{A}^T \phi \rangle = \langle \mathcal{A}(u - u_h), \phi - \phi_h \rangle = -\langle F(u_h), \phi - \phi_h \rangle$$

Solving the resulting nonlinear discrete equations.

Each iteration of these types of adaptive algorithm requires:

- 1. Solve discrete nonlinear problem (e.g. via Global Inexact Newton).
- 2. Estimate the error in each simplex.
- 3. Locally adapt the mesh; go back to 1.

Solution of Newton linearization systems completely dominate space and time complexity of overall adaptive algorithm (everything else has linear complexity).

Fundamental Problems:

- Our algorithms need to have (nearly) linear space and time complexity on a sequential computer. (Linear in number of discrete degrees of freedom.)
- Our algorithms need to scale (nearly) linearly with the number of processors on a parallel computer.
- MG *does not* have linear space or time complexity on locally adapted meshes.

Our Solutions: Fast linear elliptic solvers based on:

- BPX-type [Bramble-Pasciak-Xu] and stabilized HB [Bank;Vassilevski-Wang] methods for locally adapted FE spaces [AH].
- De-coupling algorithms for scalability on parallel computers [BH].





Application to the Constraints in GR.

To discuss the GR constraints, we need some notation.

Let \mathcal{M} be a Riemannian *d*-manifold with boundary submanifold $\partial \mathcal{M}$, split into two disjoint submanifolds satisfying:

$$\partial_0 \mathcal{M} \cup \partial_1 \mathcal{M} = \partial \mathcal{M}, \qquad \partial_0 \mathcal{M} \cap \partial_1 \mathcal{M} = \emptyset. \qquad (\overline{\partial_0 \mathcal{M}} \cap \overline{\partial_1 \mathcal{M}} = \emptyset)$$

Assume that \mathcal{M} is endowed with a metric $\hat{\gamma}_{ab}$ inducing a boundary metric $\hat{\sigma}_{ab}$. The differential structure on \mathcal{M} is denoted as follows. Covariant differentian w.r.t. $\hat{\gamma}_{ab}$ is denoted:

$$\hat{D}_{b}V^{a} = V^{a}_{;b} = V^{a}_{,b} + \hat{\Gamma}^{a}_{bc}V^{c},$$

with

$$V^{a}_{,b} = \frac{\partial V^{a}}{\partial x^{b}}, \qquad \Gamma^{a}_{bc} = \frac{1}{2}\hat{\gamma}^{ad} \left(\frac{\partial \hat{\gamma}_{db}}{\partial x^{c}} + \frac{\partial \hat{\gamma}_{dc}}{\partial x^{b}} - \frac{\partial \hat{\gamma}_{bc}}{\partial x^{d}}\right). \qquad (\Gamma^{a}_{bc} = \Gamma^{a}_{cb}).$$

The Lichnerovich operator is denoted:

$$(\hat{L}W)^{ab} = \hat{D}^{a}W^{b} + \hat{D}^{b}W^{a} - \frac{2}{3}\hat{\gamma}^{ab}\hat{D}_{c}W^{c}.$$

The Momentum Constraint as a Variational Problem. Let $X = W_{0,D}^{1,2}(\mathcal{M})$, $(\hat{E}V)^{ab} = \frac{1}{2} \left(\hat{D}^b V^a + \hat{D}^a V^b \right)$, and $J_{\mathrm{M}}(W^a) = \int \left(\frac{1}{2} C^a_{\ b} W^b - Z^a \right) W_a \ ds + \int \left(\frac{2}{2} \phi^6 \hat{D}^a \mathrm{tr} K + 8\pi \hat{j}^a \right) W_a \ dx$

$$+\frac{1}{2}\int_{\mathcal{M}} \left(2(\hat{E}W)^{ab}(\hat{E}W)_{ab} - \frac{2}{3}\hat{D}_{a}W^{a}\hat{D}_{b}W^{b}\right) dx.$$

The condition for stationarity is:

Find
$$W^a \in \overline{W}^a + W^{1,2}_{0,D}(\mathcal{M})$$
 s.t. $\langle J'_{\mathcal{M}}(W^a), V^a \rangle = 0, \quad \forall \ V^a \in W^{1,2}_{0,D}(\mathcal{M}),$

where

$$\begin{aligned} \langle J'_{M}(W^{a}), V^{a} \rangle &= \int_{\partial_{1}\mathcal{M}} (C^{a}_{\ b}W^{b} - Z^{a}) V_{a} \ ds + \int_{\mathcal{M}} \left(\frac{2}{3} \phi^{6} \hat{D}^{a} \mathrm{tr}K + 8\pi \hat{j}^{a} \right) V_{a} \ dx \\ &+ \int_{\mathcal{M}} \left(2(\hat{E}W)^{ab} (\hat{E}V)_{ab} - \frac{2}{3} \hat{D}_{a} W^{a} \hat{D}_{b} V^{b} \right) \ dx = 0. \end{aligned}$$

This gives the momentum constraint:

$$\hat{D}_b(\hat{L}W)^{ab} = \frac{2}{3}\phi^6 \hat{D}^a \operatorname{tr} K + 8\pi \hat{j}^a \text{ in } \mathcal{M},$$
$$(\hat{L}W)^{ab} \hat{n}_b + C^a_{\ b}W^b = Z^a \text{ on } \partial_1 \mathcal{M},$$
$$W^a = F^a \text{ on } \partial_0 \mathcal{M}.$$

Momentum Constraint: Well-posedness and Estimates. Assumption 1. [HB1] M is a connected compact Riemannian 3-manifold with Lipschitz-continuous boundary ∂M .

$$K^{ab} \in W^{1,6/5}(\mathcal{M}), \quad \phi \in L^{\infty}(\mathcal{M}),$$

$$\hat{j}^{a} \in H^{-1}(\mathcal{M}), \quad C^{a}_{\ b} \in L^{2}(\partial_{1}\mathcal{M}), \quad Z^{a} \in L^{4/3}(\partial_{1}\mathcal{M}), \quad F^{a} \in H^{1/2}(\partial_{0}\mathcal{M}),$$
$$\int_{\partial_{1}\mathcal{M}} C^{a}_{\ b}V^{b}V_{a} \ dx \geq \sigma \|V^{a}\|^{2}_{L^{2}(\partial_{1}\mathcal{M})}, \quad \forall \ V^{a} \in L^{4}(\partial_{1}\mathcal{M}), \quad \sigma > 0.$$

 $\hat{\gamma}_{ab} \in \{W^{k,p}(\mathcal{M}) \mid \text{Imbedding, Compactness, Trace, } \dots \text{ Theorems hold for } \mathcal{M} \dots\}$ **Theorem 3. [HB1]** Let Assumption 1 hold. there exists a unique solution $W^a \in \overline{W}^a + W^{1,2}_{0,D}(\mathcal{M})$ to the momentum constraint. Moreover,

 $U^a = W^a - \overline{W}^a \in W^{1,2}_{0,D}(\mathcal{M})$ satisfies:

$$||U^{a}||_{W^{1,2}(\mathcal{M})} \leq ||U^{a}||_{L^{2}(\mathcal{M})} + \frac{L}{\alpha}.$$

If $meas(\partial_0 \mathcal{M}) > 0$ and m is the ellipticity constant, then $||U^a||_{W^{1,2}(\mathcal{M})} \leq L/m$.

Outline of Proof: Korn + Gårding + Riesz-Schauder theory. \Box

Regularity of solutions: If $\hat{j}^a \in L^p$, $6/5 \le p \le +\infty$, and boundary smoothness and non-intersection, one has $W^a \in W^{2,p}(\mathcal{M})$ or $W^a \in W^{1,\infty}(\mathcal{M})$.

Momentum Constraint: A Priori Error Estimates.

Galerkin approximation of the momentum constraint:

Find
$$u_h \in V_h \subset V$$
 s.t. $a(u_h, v) = a(u, v) = f(v), \quad \forall v \in V_h \subset V.$

Natural approximation subspace quality assumption $(V \subset H \equiv H^* \subset V^*)$:

$$||u - u_h||_H \le a_n ||u - u_h||_V$$
, if $a(u - u_h, v) = 0$, $\forall v \in V_h^n \subset V$,

where $\lim_{n\to\infty} a_n = 0$.

Theorem 4. [H1] For n sufficiently large, there exists a unique approximation u_h satisfying the momentum constraint for which the following quasi-optimal a priori error bounds hold where C is independent of n:

$$||u - u_h||_V \le C \inf_{v \in V_h^n} ||u - v||_V,$$

$$||u - u_h||_H \le Ca_n \inf_{v \in V_h^n} ||u - v||_V.$$

If $K \leq 0$ in the Gårding inequality then the above holds for all n.

Outline of Proof: Use of a technical tool due to Schatz circa 1973. \Box

The Hamiltonian Constraint as a Variational Problem. Let $X = W_{0,D}^{1,p}(\mathcal{M})$, and

$$J_{\rm H}(\phi) = \int_{\partial_1 \mathcal{M}} \left(\frac{1}{2}c\phi - z\right)\phi \, ds + \int_{\mathcal{M}} g(\phi) \, dx + \frac{1}{2} \int_{\mathcal{M}} \hat{D}_a \phi \hat{D}^a \phi \, dx,$$

where $g(\phi) = \frac{1}{16}\hat{R}\phi^2 + \frac{1}{72}(\text{tr}K)^2\phi^6 + \frac{1}{48}(\hat{A}_{ab} + (\hat{L}W)_{ab})^2\phi^{-6} + \pi\hat{\rho}\phi^{-2}$.

The condition for stationarity is:

Find
$$\phi \in \mathcal{K} \subseteq \overline{\phi} + W^{1,p}_{0,D}(\mathcal{M})$$
 s.t. $\langle J'_{\mathrm{H}}(\phi), \psi \rangle = 0, \quad \forall \ \psi \in W^{1,p}_{0,D}(\mathcal{M}),$

where

$$\langle J'_{\rm H}(\phi),\psi\rangle = \int_{\mathcal{M}} \hat{D}_a \phi \hat{D}^a \psi \ dx + \int_{\mathcal{M}} g'(\phi)\psi \ dx + \int_{\partial_1 \mathcal{M}} (c\phi - z)\psi \ ds,$$

and where $g'(\phi) = \frac{1}{8}\hat{R}\phi + \frac{1}{12}(\mathrm{tr}K)^2\phi^5 - \frac{1}{8}(\hat{A}_{ab} + (\hat{L}W)_{ab})^2\phi^{-7} - 2\pi\hat{\rho}\phi^{-3}$.

This gives the Hamiltonian constraint:

$$\hat{D}_a \hat{D}^a \phi = g'(\phi) \text{ in } \mathcal{M},$$
$$\hat{n}_a \hat{D}^a \phi + c\phi = z \text{ on } \partial_1 \mathcal{M},$$
$$\phi = f \text{ on } \partial_0 \mathcal{M}.$$

Hamiltonian Constraint: Well-posedness and Estimates.

There are many results for the Hamiltonian constraint on compact manifolds without boundary, going back to the early 1970's [O'Murchadha-York, 1973].

The case of weak solutions, on manifolds with boundary, remains mostly open.

The Hamiltonian constraint is a Sobolev critical exponent problem:

 $-\Delta u = u^p + f(x, u), \text{ on } \mathcal{M},$ $u > 0, \text{ on } \mathcal{M},$ $u = 0, \text{ on } \partial \mathcal{M}.$

The limiting case p = (d+2)/(d-2) in the Sobolev embedding $H^1(\mathcal{M}) \subset L^{p+1}(\mathcal{M})$ is not compact. (When d = 3, we have p = 5.)

Loss of compactness results in the energy $J_{\rm H}(\phi)$ failing the Palais-Smale condition: There exists sequences which are not relatively compact.

Pohozaev's non-existence result: If \mathcal{M} is star-shaped and $f(x, u) \equiv 0$, then there is no positive solution to the problem above.

To complicate matters for us, the Isometry-based boundary conditions on holes requires negativity assumption c < 0.

Hamiltonian Constraint: Some Existing Results.

Brezis-Nirenberg (1983) showed the critical exponent problem p = (d+2)/(d-2) was solvable in $H_0^1(\mathcal{M})$. (d = 3 was most difficult case.)

They showed low-order terms allow local version of PS-condition; similar idea exploited for Yamabe and related problems in geometry (Schoen, 1984; Brezis, 1986; Schoen-Yau, 1988, Struwe, 1984,1986; other examples.)

Using other techniques (strong maximum principles and sub/super-solutions), Isenberg characterized (strong) CMC data into twelve classes: 3 Yamabe classes times 4 combinations of zero/nonzero trK and $[A^{ab} + (\hat{L}W)^{ab}]$.

Recent work of Arnold-Tarfulea gives existence for case of isometry boundary conditions on bounded domains when critical exponent term not present.

Weak solutions in the manifold with boundary case with critical exponent: there are 48 separate situations; Isenberg's 12 classes times 4 BC permutations. Some cases have been extended to weak solutions; one result is: **Theorem 5.** [HB1] If conditions similar to Assumption 1 hold, and if $W^a \in W^{1,\infty}(\mathcal{M})$, then there exists a unique weak solution ϕ to the Hamiltonian constraint, with $\phi \in H^1(\mathcal{M}) \cap L^{\infty}(\mathcal{M})$, and $0 < \alpha < \phi < \beta < +\infty$, a.e. in $\overline{\mathcal{M}}$.

Outline of Proof: Variational methods using weak convergence techniques. \Box

Hamiltonian Constraint: A Priori Error Estimates.

Galerkin approximation of the Hamiltonian constraint:

Find
$$u_h \in V_h \subset V$$
 s.t. $a(u_h, v) + \langle b(u_h), v \rangle = f(v), \quad \forall v \in V_h \subset V.$

Natural approximation subspace quality assumption $(V \subset H \equiv H^* \subset V^*)$:

$$||u - u_h||_H \le a_n ||u - u_h||_V$$
, if $a(u - u_h, v) + \langle b(u) - b(u_h), v \rangle = 0$, $\forall v \in V_h^n \subset V$,

where $\lim_{n\to\infty} a_n = 0$. Discrete *a priori* bnds imply a Lipschitz cond:

$$\langle b(u) - b(u_h), u - v \rangle \leq K ||u - u_h||_V ||u - v||_V.$$

Theorem 6. [H1] A Galerkin approximation u_h to the Hamiltonian constraint satisfies the quasi-optimal error bounds where C is independent of n:

$$||u - u_h||_V \le C \inf_{v \in V_h^n} ||u - v||_V,$$

$$||u - u_h||_H \le Ca_n \inf_{v \in V_h^n} ||u - v||_V.$$

Outline of Proof: Fairly involved analysis of particular nonlinearity class on best approximation problem. \Box

Other Numerical Solutions of the GR Constraints.

Cook: Nonlinear (FAS) MG (Hamiltonian), Spectral methods (Hamiltonian+momentum), Non-adaptive (un-published adaptive).

Matzner group: Gummel-like iteration (Hamiltonian+momentum). French group: Pseudo-spectral (Hamiltonian+momentum). Thornburg: Multi-patch (Hamiltonian). Brandt/Brugmann: Gauss-Seidel for two holes (Hamiltonian).

Pfeiffer et al.: (Hamiltonian+momentum) Newton's method + MG (multigrid).

Arnold/Mukherjee: (Hamiltonian only) Adaptive FE + Newton + MG.

Many other related works appear in the literature.

We focus primarily on finite element methods, due to:

- 1. Representation of complex domain shapes and boundaries.
- 2. Discretization of general nonlinearities and bndry conds.
- 3. Well-suited for general coupled nonlinear elliptic systems.
- 4. General nonlinear (adaptive) approximation theory framework.
- 5. Ideal setting for building optimal multilevel solvers.

Some examples using FEtk (Finite Element ToolKit).

FEtk (MALOC + MC + SG) is a general FE ToolKit for geometric PDE.

Developed collaboratively over a number of years, it has the following structure:



Application-specific codes such as APBS and GPDE are built on top of FEtk.

Unusual features of MC (Manifold Code).

MC, the finite element kernel of FEtk, allows for the adaptive treatment of nonlinear elliptic systems of tensor equations on 2- and 3-manifolds.

MC implements a variant of the solve-estimate-refine iteration described earlier, and has the following features:

- Abstraction of the elliptic system: PDE defined only through the nonlinear weak form $\langle F(u), v \rangle$ over the domain manifold, along with the associated bilinear linearization form $\langle DF(u)w, v \rangle$.
- Abstraction of the domain manifold: Domain specified via polyhedral representation of topology, with set of user-interpreted coordinate labels (possibly consisting of multiple charts).
- *Dimension-independence*: The same code paths are taken for both 2D and 3D problems, by employing the simplex as the fundamental topological object.

These abstractions are inherited by application codes built on top of FEtk.

The RInged VERtex datastructure in MC.

The fundamental topology datastructure in MC is the RIVER (RInged VERtex) datastructure:



Examples using FEtk.

Generating an initial "coarse" simplex mesh is surprisingly difficult.

The following idea for two-holes is due to D. Bernstein [HB2].

Step 1: 2D Delaunay.



Step 2: Axis rotation to 3D tetrahedral tori.

Holes can be filled for e.g. neutron star models.





Schwarzschild example: solution on the coarse mesh.



Schwarzschild example: refinements on hole surface.



Schwarzschild example: an adapted solution.



Brill-wave example: adaptive solution from afar.



Brill-wave example: adaptive solution near hole.



Brill-wave example: non-symmetry around hole.



Brill-wave example: isosurfaces around hole.











Binary hole example: subdomain adaptivity.





Binary hole example: two subdomain solutions.





Variational Methods for Constrained Evolution.

Constrained (hyperbolic or parabolic) evolution systems have the form:

$$\partial_t u = B(u), \quad t \in (0, T], \tag{15}$$

$$0 = C(u), \quad \forall t, \tag{16}$$

with $B(u): X \mapsto X^*$, $C(u): X \mapsto Y$, $u(t) \in X \ \forall t$, and $u(0) = u_0 \in X$ given.

Here, X and Y suitable Banach spaces with norms $\|\cdot\|_X$ and $\|\cdot\|_Y$.

If $C(u) \in C^1(X, Y)$, a classical result is that the subset of X satisfying the constraint (16) is a differentiable manifold \mathcal{M} :

$$\mathcal{M} = \{ u \in X : C(u) = 0 \}.$$
(17)

For many systems such as Einstein, (16) is redundant in that if $u(0) \in \mathcal{M}$, then any solution u of (15) also satisfies $u(t) \in \mathcal{M}$, for all t > 0.

Numerical approximations to (15) *do not* preserve (16), even to good approximation, due to overdetermined nature of system.

If (16) is linear, one can attempt to build bases for approximation subspaces of X which satisfy (16); approximations to (15) using this basis will satisfy (16).

Linear constraints in Maxwell & incompressible NS have been handled this way.

Variational Approach to One-Step Projection Methods.

When (16) nonlinear, the only options appear to be:

- 1. Tolerate violation of (16), producing non-physical numerical solutions;
- 2. Modify standard numerical evolution techniques for (15) to produce approximations satisfying (16) to high precision.

Variational approach to option 2: characterize solution to (15)-(16) as the solution to a constrained minimization problem: Find $u(t): (0,T] \mapsto X$ such that

$$J(u) \leq J(v), \quad \forall v(t) : (0,T] \mapsto X,$$
(18)

$$0 = C(u), \quad \forall t. \tag{19}$$

E.g., $J(u) = \int_0^T \|\partial_t u - B(u)\|_{X^*} dt$, spacetime norm of the residual.

To avoid discretizing all of spacetime at once, one can semi-discretize in time using a one-step method, and then simply solve (18)-(19) at each discrete time step: Find $u \in X$ such that

$$J(u) \leq J(v), \quad \forall v \in X, \tag{20}$$

$$0 = C(u), \tag{21}$$

for some suitable objective functional $J(u): X \mapsto \mathbb{R}$.

Constrained Optimality and Lagrange Functionals. Given $u^{(k)} \approx u(t_k)$, one-step methods determine $u^{(k+1)} = \bar{u} \approx u(t_{k+1})$ by solving:

$$D(\bar{u}, u^{(k)}) = 0.$$
(22)

E.g., explicit Euler uses $D(u^{(k+1)}, u^{(k)}) = u^{(k+1)} - u^{(k)} - hB(u^{(k)}) = 0.$

Once $\bar{u} \approx u(t_{k+1})$ is computed, generally with $\bar{u} \notin \mathcal{M}$, we can define:

 $J(v) = d(\bar{u}, v)$, using any convenient positive metric $d: X \times X \mapsto \mathbb{R}$.

The unconstrained minimizer of J(v) is just \bar{u} , but solving the constrained problem (20)–(21) "projects" \bar{u} back onto \mathcal{M} , giving $u^{(k+1)} \in \mathcal{M}$.

A necessary condition for the solution to (20)-(21) is stationarity w.r.t. $T_u\mathcal{M}$:

$$\langle J'(u), v \rangle = 0, \quad \forall v \in T_u \mathcal{M} \subseteq X.$$
 (23)

A standard result is that one can avoid identifying entire tangent bundle $T\mathcal{M} = \bigcup_{u \in \mathcal{M}} T_u \mathcal{M}$, since (23) holds iff

$$\langle J'(u), v \rangle + \langle \lambda, C'(u)v \rangle = 0, \quad \forall v \in X,$$
(24)

for a fixed bounded linear Lagrange functional λ on Y.

The Final Step-And-Project Method: Block Systems.

We can view this as the condition for stationarity w.r.t. both u and λ of:

$$L(u,\lambda) = J(u) + \langle \lambda, C(u) \rangle.$$
(25)

Stationarity condition is: Find $\{u, \lambda\} \in X \times Y^*$ such that $\forall \{v, \gamma\} \in X \times Y^*$:

$$\langle J'(u), v \rangle + \langle \lambda, C'(u)v \rangle = 0, \qquad (26)$$

$$\langle \gamma, C(u) \rangle = 0. \tag{27}$$

The complete step-and-project algorithm is then:

- 1. Given $u^{(k)} \approx u(t_k)$, with $u^{(k)} \in \mathcal{M}$, determine $\bar{u} \approx u(t_{k+1})$ using any standard one-step method (typically, $\bar{u} \notin \mathcal{M}$);
- 2. Use \bar{u} to formulate and solve the coupled system (26)-(27) for $u = u^{(k+1)} \approx u(t_{k+1})$ and λ , with now $u^{(k+1)} \in \mathcal{M}$.

The system (26)-(27) can be solved coupled or using e.g. Uzawa's algorithm.

These types of step-and-project methods have been carefully studied in the ODE (and mechanics) literature over the last fifteen years (Jay, Leimkuhler, Leimkuhler-Reich, Leimkuhler-Skeel, Hairer-Lubich-Wanner, many others.)

True (Variational) Projection Methods Preserve Order.

One can show that the projection step does not deteriorate various properties of the underlying one-step method, such as time discretization order.

If \bar{u} has (discrete time) approximation order $\mathcal{O}(h^p)$ as an approximation to $u(t_{k+1})$ with respect to the metric $d(\cdot, \cdot)$, or in other words if

$$d(u(t_{k+1}),\bar{u}) = Qh^p, \tag{28}$$

for some constant Q, then since $u(t_{k+1}) \in \mathcal{M}$, this is an upper bound on $d(\bar{u}, \mathcal{M})$. Solving the constrained minimization problem for the projection $u^{(k+1)} \approx u(t_{k+1})$ guarantees that:

$$d(\bar{u}, u^{(k+1)}) \le d(\bar{u}, v), \quad \forall v \in \mathcal{M}.$$
(29)

Order preservation is then a simple consequence of the triangle inequality:

$$d(u(t_{k+1}), u^{(k+1)}) \le d(u(t_{k+1}), \bar{u}) + d(\bar{u}, u^{(k+1)}) \le 2d(u(t_{k+1}), \bar{u}) = 2Qh^p.$$
(30)

Note that if the constrained minimization problem (26)-(27) is *not* solved to determine $u^{(k+1)}$, then in general there is no control over error (29) introduced by "projection", and convergence order (and other properties) of the underlying one-step method is destroyed.

Projection Methods: A Simple Example.

Scalar field in curved spacetime:

 $\nabla^{\mu}\nabla_{\mu}\psi = 0.$

Splitting background spacetime metric 3 + 1 as usual:

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

allows for a "pathological" symmetric-hyperbolic representation of the system:

$$\partial_t \psi - N^k \partial_k \psi = -N\Pi,\tag{31}$$

$$\partial_t \Pi - N^k \partial_k \Pi + N g^{ki} \partial_k \Phi_i = N J^i \Phi_i + N K \Pi, \tag{32}$$

$$\partial_t \Phi_i - N^k \partial_k \Phi_i + N \partial_i \Pi - \gamma_2 N \partial_i \psi = -\Pi \partial_i N + \Phi_j \partial_i N^j - \gamma_2 N \Phi_i.$$
(33)

 $(\Phi_i \text{ is spatial gradient } \partial_i \psi, \Pi \text{ is time derivative of } \psi$. *K* and *J*^{*i*} known functions, depend only on background geometry.)

System suffers from serious bulk and boundary generated constraint violations; good model of constraint violating problems in the Einstein equations.

Equation (33) produces the bulk constraint violations.

Projection Methods: Lagrangian for the Example.

System is symmetric-hyperbolic with symmetrizer (up to scalar multiple):

$$ds^2 = S_{\alpha\beta}du^{\alpha}du^{\beta} = \Lambda^2 d\psi^2 - 2\gamma_2 d\psi \, d\Pi + d\Pi^2 + g^{ij}d\Phi_i d\Phi_j \qquad . \tag{34}$$

(Λ is an arbitrary constant.)

Solutions of system are also solutions to the original scalar wave equation iff the constraints are satisfied: $0 = c^A \equiv \{C_i\}$, where

$$\mathcal{C}_i = \partial_i \psi - \Phi_i, \tag{35}$$

A projection method can be produced by defining the Lagrangian (density):

$$\mathcal{L} = g^{1/2} \left[S_{\alpha\beta} (u^{\alpha} - \bar{u}^{\alpha}) (u^{\beta} - \bar{u}^{\beta}) + \lambda_A c^A \right] = g^{1/2} \left[\Lambda^2 (\psi - \bar{\psi})^2 - 2\gamma_2 (\psi - \bar{\psi}) (\Pi - \bar{\Pi}) + (\Pi - \bar{\Pi})^2 + g^{ij} (\Phi_i - \bar{\Phi}_i) (\Phi_j - \bar{\Phi}_j) + \lambda^i (\partial_i \psi - \Phi_i) \right],$$
(36)

using the symmetrizer $S_{\alpha\beta}$ of the hyperbolic evolution system.

Projection Methods: Condition for Stationarity.

Condition for sationarity is simply:

$$\nabla^i \nabla_i \psi - (\Lambda^2 - \gamma_2^2) \psi = \nabla^i \bar{\Phi}_i - (\Lambda^2 - \gamma_2^2) \bar{\psi}, \qquad (37)$$

$$\Pi = \bar{\Pi} + \gamma_2(\psi - \bar{\psi}), \qquad (38)$$

$$\Phi_i = \partial_i \psi, \tag{39}$$

 $(\nabla_i \text{ is spatial covariant derivative compatible with spatial metric <math>g_{ij}$.)



Left Figure: Constraint violations of the standard system ($\gamma_2 = 0$): constraint pres. BCs and no constraint projection.

Center Figure: Constraint violations of pathological system ($\gamma_2 = -1/M$): constraint pres. BCs and no constraint projection.

Right Figure: Constraint violations of pathological system ($\gamma_2 = -1/M$): constraint pres. BCs and constraint projection ($\Lambda = \sqrt{2}/M$ every $\Delta T = 2M$).

Projection Methods: Insight from the Simple Example.

- Constraint preserving boundary conditions alone can not control the growth of constraints in a system with bulk constraint violations.
- Constraint projection without constraint preserving boundary conditions does not produce numerically convergent step-and-project methods.
- Cost of constraint projection may not be significant even when it constraint projection equations are elliptic.
- Naive constraint projection (using an indefinite metric in the construction of the objective functional J) does not preserve order, and emperically does not appear to give stable evolutions.
- The boundary conditions used in the elliptic constraint projection step must be compatible with those used in evolution steps to produce stable/convergent methods.
- Optimal constraint projection does not depend sensitively on the free parameter Λ in the symmetrizer metric. (Convergence rate depends on Λ).

Relevant Manuscripts and Collaborators.

• Estimates, adaptive methods, and PUM methods for geometric PDE.

- [H1] MH, Adaptive numerical treatment of elliptic systems on manifolds. Advances in Computational Mathematics, 15 (2001), pp. 139–191.
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- [AH] B. Aksoylu and MH, Local refinement and multilevel preconditioning: Optimality of the BPX Preconditioner and Stabilizing hierarchical basis methods. (To appear in SIAM J. Numer. Anal.)
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 - Weak solutions of the Einstein constraint equations.
 - [HB1] MH and D. Bernstein, Weak solutions to the Einstein constraint equations on manifolds with boundary. (Preprint)
 - [HB2] MH and D. Bernstein, Adaptive finite element solution of the Einstein constraint equations in general relativity, (Preprint)

Summary.

- Crash course on variational PDE and finite element methods.
- Adaptive FE algorithms for nonlinear approximation [H1,H2,BH].
- Fast elliptic solvers for locally adapted discretizations [AH,ABH].
- The GR constraints as variational problems; well-posedness [HB1].
- A priori and a posteriori error estimates for GR constraints [H1].
- Examples using FEtk [H1,H2,BH,HB2].
- Projection methods for constrained evolution [HLOPSK].
- FEtk software framework (ANSI-C) is downloadable from:

 $MALOC, SG, MC \hookrightarrow http://www.FEtk.ORG$

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