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Unified Formulation of Galerkin and Runge-Kutta time discretization methods

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based on joint work with

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Error Control

Problem: prove a posteriori estimates for the time dependent problem:

$$u' + A(u) = 0 \,.$$

The general problem: let U an approximation to u obtained by a numerical scheme. We would like to show

$$\|u - U\| \leq \eta(U)$$

such that

- the estimator $\eta(U)$ is a computable quantity which depends on the approximate solution U and the data of the problem;
- $\eta(U)$ decreases with optimal order for the lowest possible regularity permitted by our problem;

Our approach to error control: Reconstruction operators

- High order time-discrete schemes: Akrivis, M. and Nochetto: 2004 -08,...
- Space-discrete: M. and Nochetto 2003, Karakatsani and M. 2007, Georgoulis and Lakkis 2008...
- Fully discrete schemes: Lakkis and M. 2006, Demlow, Lakkis and M. 2009, Kyza 2009...

Given U, find an appropriate Reconstruction $\hat{U}$ - (continuous object)

and estimate

$$u - \hat{U} \quad \text{and} \quad \hat{U} - U$$

Previous use of time reconstructions for backward Euler : Nochetto Savare Verdi 2000, Picasso 98, ...

An example: Time discerization with Backward Euler

Let $0 = t_0 < t_1 < \cdots < t_N = T$ be a partition of $[0, T]$,
$I_n := (t_n, t_{n+1}]$, and $k_n := t_{n+1} - t_n$.

$$\frac{1}{k_n}(U^{n+1} - U^n) + AU^{n+1} = f_k^{n+1}\,.$$

Here

(BE): $f_k^{n+1} = f(t_{n+1})$

(dG0): $f_k^{n+1} = \frac{1}{k_n}\int_{I_n} f(s)ds$

One can considered the approximations to be piecewise constant in time. I.e. define U as the piecewise constant function and the projection $\Pi_0 f$ of f:

$$U|_{I_n} \in \mathbb{P}_0(I_n), \quad U|_{I_n} = U^{n+1}, \qquad \Pi_0 f = f_k^{n+1}$$

Backward Euler reconstruction

[a]

- Let $\hat{U}(t)$ be the piecewise linear (in time) interpolant of U^n.
- Then in each $I_n : \hat{U}'(t) = \frac{1}{k_n}(U^{n+1} - U^n)$

New way of writing the scheme

$$\hat{U}'(t) + A\hat{U}(t) = \Pi_0 f + A[\hat{U}(t) - U(t)], \qquad t \in I_n\,.$$

Then

- $\hat{U}(t) - U(t) = \hat{U}(t) - U^{n+1} = \ell_0^n(t)(U^n - U^{n+1})$

where $\hat{U}(t) = \ell_0^n(t)U^n + \ell_1^n(t)U^{n+1}$

[a] R. H. Nochetto, G. Savaré, and C. Verdi, Comm. Pure Appl. Math. **53** (2000) 525–589

Error equation

- Let $\hat{e} = u - \hat{U}(t)$

then

$$\hat{e}'(t) + A\,\hat{e}(t) = (f - \Pi_0 f) - A\,[\hat{U}(t) - U(t)], \qquad t \in I_n\,.$$

Finally

$$\max_{0 \le t \le T} |\hat{e}|^2 + \int_0^T \|\hat{e}\|^2 dt \le \ \alpha \Big(\sum_{n=0}^{N-1} k_n \|A^{1/2}(U^{n+1} - U^n)\|^2 + \int_0^T \|f - \Pi_0 f\|_\star^2 . \Big)$$

Semigroup approach : estimates via Duhamel's principle.

We shall use Duhamel's principle in the above error equation. Let $E_A(t)$ be the solution operator of the homogeneous equation

$$u'(t) + Au(t) = 0, \quad u(0) = w,$$

i.e., $u(t) = E_A(t)w$. It is well known that the family of operators $E_A(t)$ has several nice properties, in particular it is a semigroup of contractions on H with generator the operator A. Duhamel's principle states ($f = 0$)

$$\hat{e}(t) = \int_0^t E_A(t-s)\Big[A\,[U(t) - \hat{U}(t)]\Big]\,ds\,.$$

Time discretization methods

To define the methods it will be convenient to work with a general nonlinear problem:

$$\begin{cases} u'(t) + F(t, u(t)) = 0, & 0 < t < T, \\ u(0) = u^0, \end{cases}$$

where $F(\cdot, t) : D(A) \to H$ in general a (possibly) nonlinear operator.

Noation We consider piecewise polynomial functions in arbitrary partitions $0 = t^0 < t^1 < \cdots < t^N = T$ of $[0, T]$, and let

$$J_n := (t^{n-1}, t^n]$$

and

$$k_n := t^n - t^{n-1}.$$

p.w. polynomial spaces

$$\mathscr{V}_q^{\mathsf{d}}, \qquad \text{and} \qquad \mathscr{H}_q^{\mathsf{d}} \quad q \in \mathbb{N}_0,$$

the space of possibly discontinuous functions at the nodes t^n that are piecewise polynomials of degree at most q in time in each subinterval J_n, i.e., $\mathscr{V}_q^{\mathsf{d}}$ consists of functions $g : [0,T] \to D(A)$ (or H) of the form

$$g|_{J_n}(t) = \sum_{j=0}^{q} t^j w_j, \quad w_j \in D(A) \quad (\text{or } H),$$

without continuity requirements at the nodes t^n; the elements of $\mathscr{V}_q^{\mathsf{d}}$ are taken continuous to the left at the nodes t^n.

$\mathscr{V}_q(J_n)$ consist of the restrictions to J_n of the elements of $\mathscr{V}_q^{\mathsf{d}}$.

$$\mathscr{V}_q^{\mathsf{c}} \qquad \text{and} \qquad \mathscr{H}_q^{\mathsf{c}}$$

consist of the continuous elements of $\mathscr{V}_q^{\mathsf{d}}$ and $\mathscr{H}_q^{\mathsf{d}}$, respectively.

The general discretization method.

Π_ℓ will be a projection operator to piecewise polynomials of degree ℓ,

$$\Pi_\ell : C^0([0,T];H) \to \oplus_{n=1}^N \mathscr{H}_\ell(J_n)$$

$$\widetilde{\Pi} : \mathscr{H}_\ell(J_n) \to \mathscr{H}_\ell(J_n)$$

is an operator mapping polynomials of degree ℓ to polynomials of degree ℓ.

We seek $U \in \mathscr{V}_q^{\mathsf{c}}$ satisfying the initial condition $U(0) = u^0$ as well as the pointwise equation

$$U'(t) + \Pi_{q-1} F(t, \widetilde{\Pi} U(t)) = 0 \quad \forall t \in J_n.$$

relation to Continuous Galerkin method (cG)

Recall that the continuous Galerkin method is : We seek $U \in \mathscr{V}_q^{\mathsf{c}}$ such that

$$\int_{J_n} \Big[\langle U', v \rangle + \langle F(t, U(t)), v \rangle \Big] \, dt = 0 \quad \forall v \in \mathscr{V}_{q-1}(J_n),$$

The Galerkin formulation of our schemes is

$$\int_{J_n} \Big[\langle U', v \rangle + \langle \Pi_{q-1} F(t, \widetilde{\Pi} U(t)), v \rangle \Big] \, dt = 0 \quad \forall v \in \mathscr{V}_{q-1}(J_n),$$

for $n = 1, \dots, N$.

i.e., $\Pi_{q-1} := P_{q-1}$, with P_ℓ denoting the (local) L^2 orthogonal projection operator onto $\mathscr{H}_\ell(J_n)$, for each n,

$$\int_{J_n} \langle P_\ell w, v \rangle \, ds = \int_{J_n} \langle w, v \rangle \, ds \quad \forall v \in \mathscr{H}_\ell(J_n).$$

The pointwise formulation of cG is

$$U'(t) + P_{q-1} F(t, U(t)) = 0 \quad \forall t \in J_n.$$

One step methods = cG + numer. integration The continuous Galerkin method is indeed the simplest method described in the above form with $\Pi_{q-1} = P_{q-1}, \widetilde{\Pi} = I$.

One thus may view the class of methods (1) as a sort of numerical integration applied to the continuous Galerkin method.

We will see that this formulation covers all important implicit single-step time stepping methods. In particular

- the cG method with $\Pi_{q-1} := P_{q-1}$, and $\widetilde{\Pi} = I$,
- the RK collocation methods with $\Pi_{q-1} := I_{q-1}$, with I_{q-1} denoting the interpolation operator at the collocation points, and $\widetilde{\Pi} = I$,
- all other interpolatory RK methods with $\Pi_{q-1} := I_{q-1}$, and appropriate $\widetilde{\Pi}$
- the dG method with $\Pi_{q-1} := P_{q-1}$ and $\widetilde{\Pi} = I_{q-1}$, where I_{q-1} is the interpolation operator at the Radau points.

RK and collocation methods

For $q \in \mathbb{N}$, a $q-$stage RK method is described by the constants a_{ij}, b_i, τ_i, $i, j = 1, \ldots, q$, arranged in a Butcher tableau,

$$
\begin{array}{ccc|c}
a_{11} & \ldots & a_{1q} & \tau_1 \\
\vdots & & \vdots & \vdots \\
a_{q1} & \ldots & a_{qq} & \tau_q \\
\hline
b_1 & \ldots & b_q &
\end{array}
.
$$

Given an approximation U^{n-1} to $u(t^{n-1})$, the n-th step of the RK method is

$$
\begin{cases}
U^{n,i} = U^{n-1} - k_n \sum_{j=1}^{q} a_{ij} F(t^{n,j}, U^{n,j}), \quad i = 1, \ldots, q, \\
U^n = U^{n-1} - k_n \sum_{i=1}^{q} b_i F(t^{n,i}, U^{n,i});
\end{cases}
$$

here $U^{n,i}$ are the intermediate stages, which are approximations to $u(t^{n,i})$.

Collocation Methods

It is well known that the collocation method: find $U \in \mathscr{V}_q^{\mathrm{c}}$ such that

$$U'(t^{n,i}) + F\Big(t^{n,i}, U(t^{n,i})\Big) = 0, \quad i = 1, \dots, q,$$

for $n = 1, \dots, N$, is equivalent to the RK method with

$$a_{ij} := \int_0^{\tau_i} L_j(\tau) d\tau, \quad b_i := \int_0^1 L_i(\tau) d\tau, \quad i, j = 1, \dots, q,$$

with $L_1, \dots, L_q$ the Lagrange polynomials of degree $q-1$ associated with the nodes $\tau_1, \dots, \tau_q$, in the sense that $U(t^{n,i}) = U^{n,i}$, $i = 1, \dots, q$, and $U(t^n) = U^n$;.

Then, since U' and $I_{q-1}F$ are polynomials of degree $q-1$ in each interval J_n, is written as

$$U'(t) + I_{q-1}F(t, U(t)) = 0 \quad \forall t \in J_n,$$

with I_{q-1} denoting the (local) interpolation operator onto $\mathscr{H}_{q-1}(J_n)$ at the points $t^{n,i}, i = 1, \dots, q,$

$$I_{q-1}v \in \mathscr{H}_{q-1}(J_n): \quad (I_{q-1}v)(t^{n,i}) = v(t^{n,i}), \quad i = 1, \dots, q.$$

RKC = cG + Numer. Integration

$$U'(t) + I_{q-1}F(t,U(t)) = 0 \quad \forall t \in J_n,$$

Thus the RK Collocation (RK-C) class is a subclass of the general methods with $\Pi_{q-1} = I_{q-1}$ and $\widetilde{\Pi} = I$.

Note the relation to cG:

$$\int_{J_n} \left[\langle U', v \rangle + \langle I_{q-1}F(t,U(t)), v \rangle \right] dt = 0 \quad \forall v \in \mathscr{V}_{q-1}(J_n),$$

Interpolatory RK and perturbed collocation methods

It is known, that a $q-$stage RK method with pairwise different $\tau_1,\dots,\tau_q$ is equivalent to a collocation method with the same nodes, if and only if its stage order is at least q.

Nørsett and Wanner 1981:

$\widetilde{\Pi}:\mathscr{H}_q(J_n)\to\mathscr{H}_q(J_n)$, by

$$\widetilde{\Pi}v(t)=v(t)+\sum_{j=1}^{q}N_j\Big(\frac{t-t^{n-1}}{k_n}\Big)v^{(j)}(t^{n-1})k_n^j,\quad t\in J_n\,.$$

Here N_j are given polynomials of degree q.

Each interpolatory RK method with pairwise different $\tau_1,\dots,\tau_q$ is equivalent to a perturbed collocation method of the form: find $U\in\mathscr{V}_q^{\mathsf{c}}$ such that

$$U'(t^{n,i})+F\Big(t^{n,i},\Big(\widetilde{\Pi}U\Big)(t^{n,i})\Big)=0,\quad i=1,\dots,q,$$

For a given RK method, the polynomials N_j needed in the construction of $\widetilde{\Pi}$ can be explicitly constructed. It then follows, since U' and $I_{q-1}F$ are polynomials of degree $q-1$ in each interval J_n, is written as

$$U'(t) + I_{q-1}F(t, \widetilde{\Pi}U(t)) = 0 \quad \forall t \in J_n,$$

Thus : $\Pi_{q-1} = I_{q-1}$ and $\widetilde{\Pi}$

The dG method

The time discrete dG(q) approximation V to the solution u is defined as follows: we seek $V \in \mathscr{V}_{q-1}^{\mathsf{d}}$ such that $V(0) = u(0)$, and

$$\int_{J_n} \Big[\langle V', v \rangle + \langle F(t,V), v \rangle \Big]\, dt + \langle V^{n-1+} - V^{n-1}, v^{n-1+} \rangle = 0 \quad \forall v \in \mathscr{V}_{q-1}(J_n),$$

$n = 1, \dots, N.$

The approximations in the unified formulation are continuous piecewise polynomials; in contrast, the dG approximations may be discontinuous.

We need to associate discontinuous piecewise polynomials to continuous ones. To this end, we let $0 < \tau_1 < \cdots < \tau_q = 1$ be the abscissae of the Radau quadrature formula in the interval $[0,1]$; this formula integrates exactly polynomials of degree at most $2q-2$. These points are transformed to the Radau nodes in the interval J_n as $t^{n,i} := t^{n-1} + \tau_i k_n$, $i = 1, \dots, q$.

dG Reconstruction

We introduce an invertible linear operator $\tilde{I}_q : \mathscr{V}_{q-1}^{\mathsf{d}} \to \mathscr{V}_q^{\mathsf{c}}$ as follows: To every $v \in \mathscr{V}_{q-1}^{\mathsf{d}}$ we associate an element $\tilde{v} := \tilde{I}_q v \in \mathscr{V}_q^{\mathsf{c}}$ defined by locally interpolating at the Radau nodes and at t^{n-1} in each subinterval J_n, i.e., $\tilde{v}|_{J_n} \in \mathscr{V}_q(J_n)$ is such that

$$\begin{cases} \tilde{v}(t^{n-1}) = v(t^{n-1}), \\ \tilde{v}(t^{n,i}) = v(t^{n,i}), \quad i = 1, \dots, q. \end{cases}$$

We will call $\tilde{v}$ a reconstruction of v (M. and Nochetto 2008)

Using the exactness of the Radau integration rule, we easily obtain

$$\int_{J_n} \langle \tilde{v} - v, w' \rangle \, dt = 0 \quad \forall v, w \in \mathscr{V}_{q-1}(J_n),$$

i.e.,

$$\int_{J_n} \langle \tilde{v}', w \rangle \, dt = \int_{J_n} \langle v', w \rangle \, dt + \langle v^{n-1+} - v^{n-1}, w^{n-1+} \rangle \quad \forall v, w \in \mathscr{V}_{q-1}(J_n);$$

Conversely, if $\tilde{v} \in \mathscr{V}_q^{\mathsf{c}}$ is given and I_{q-1} is the interpolation operator at the Radau nodes $t^{n,i}$, i.e., $(I_{q-1}\varphi)(t^{n,i}) = \varphi(t^{n,i})$, $i = 1,\dots,q$, we can recover v locally via interpolation, i.e., $v = I_{q-1}\tilde{v}$ in J_n; furthermore, $v(0) = \tilde{v}(0)$. Thus, $I_{q-1} = \tilde{I}_q^{-1}$.

Using the dG reconstruction $\widetilde{V} \in \mathscr{V}_q^{\mathsf{c}}$ of $V \in \mathscr{V}_{q-1}^{\mathsf{d}}$,

$$\int_{J_n} \Big[\langle \widetilde{V}', v \rangle + \langle F(t,V), v \rangle \Big] \, dt = 0 \quad \forall v \in \mathscr{V}_{q-1}(J_n),$$

$n = 1,\dots,N$. Therefore

$$\int_{J_n} \Big[\langle \widetilde{V}', v \rangle + \langle F(t, I_{q-1}\widetilde{V}), v \rangle \Big] \, dt = 0 \quad \forall v \in \mathscr{V}_{q-1}(J_n),$$

Pointwise formulation

$$\widetilde{V}'(t) + P_{q-1}F\Big(t, (I_{q-1}\widetilde{V})(t)\Big) = 0 \quad \forall t \in J_n.$$

Here $\Pi_{q-1} = P_{q-1}$ and $\widetilde{\Pi} = I_{q-1}$, with I_{q-1}

We denote by $U = \widetilde{V}$ the continous in time approximation associated to the dG method:

$$U'(t) + P_{q-1}F\Big(t, (I_{q-1}U)(t)\Big) = 0 \quad \forall t \in J_n,$$

where $P_{q-1}$and I_{q-1} as above.