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Line Integral Methods: an ICNAAM Story, and Beyond

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Abstract. In recent years, the class of *Line Integral Methods* has been devised for efficiently solving *conservative problems*, namely, problems with invariants of motion. Their main instance is given by *Hamiltonian Boundary Value Methods (HBVMs)*, a class of energy-conserving Runge-Kutta methods for Hamiltonian problems. It turns out that the efficient derivation of such methods relies on a local Fourier expansion of the vector field along a suitable orthonormal basis. However, this procedure can be also regarded as a spectral expansion, which can be adapted to a number of differential problems. The foundation of the theory and relevant paths of investigation underlying this class of methods have been developed during the past editions of the ICNAAM Conference series.

INTRODUCTION

The numerical solution of Hamiltonian problems is a very active field of investigation, due to the fact that Hamiltonian problems are not generic as dynamical systems, so that perturbations introduced by a numerical method may destroy their properties. A canonical Hamiltonian problem has the form

$$\dot{y} = J\nabla H(y) \equiv f(y), \qquad y(0) = y_0 \in \mathbb{R}^{2m}, \tag{1}$$

with $J = \begin{pmatrix} & I_m \\ -I_m & \end{pmatrix}$ a skew-symmetric and orthogonal matrix (hereafter, I_r will denote the identity matrix of dimension r. When not specified, its dimension can be deduced from the context), and $H : \mathbb{R}^{2m} \to R$ its Hamiltonian function, or Hamiltonian. In the sequel, we shall use either one or the other notation, for the vector field in (1), depending on the needs. The main property of the dynamical system induced by (1) is the symplecticity of its map, which can be characterized as $\Phi_t'(y_0)^\top J\Phi_t'(y_0) = J$, with $y(t) = \Phi_t(y_0)$ the flow associated with (1). *Symplectic methods* are then derived by imposing that the discrete map induced by a corresponding method be symplectic as well. Such methods have been studied for a long time (see, e.g., the monographs [1, 2, 3] and references therein). Another relevant property is the conservation of the Hamiltonian, since, for the solution trajectory of (1),

$$\frac{\mathrm{d}}{\mathrm{d}t}H(y) = \nabla H(y)^\top \dot{y} = \nabla H(y)^\top J\nabla H(y) = 0,$$

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due to the skew-symmetry of J. At a continuous level, the conservation of H derives from the symplecticity of the map. However, in general, symplectic methods do not conserve the Hamiltonian: they only approximately conserve it. The conservation of the Hamiltonian, in turn, is a relevant feature: as matter of fact, when modelling isolated mechanical system, it has the physical meaning of the total energy of the system. For this reason, it is often referred to as the *energy*. Methods able to conserve the energy are, therefore, named *energy-conserving*. Approaches for deriving such methods can be found, e.g., in [4, 5, 6].

Our approach for deriving energy-conserving methods is based on the use of a discrete counterpart of the line integral of a vector field. The collaborative atmosphere of the ICNAAM Conference series has inspired fruitful discussions which have considerably speeded up the development of the bulk of the theory, as we will testify hereafter.

The idea is that of reformulating the conservation of the Hamiltonian as the vanishing of a suitable *line integral*. In fact, at a continuous level, one has

$$H(y(t)) = H(y_0) + \int_0^t \nabla H(y(\tau))^\top \dot{y}(\tau)\,\mathrm{d}\tau = H(y_0) + \int_0^t \nabla H(y(\tau))^\top J \nabla H(y(\tau))\,\mathrm{d}\tau = 0, \tag{2}$$

due to the fact that y satisfies (1) and J is skew-symmetric. The function $y(t)$ is the unique function satisfying such a conservation property for all $t \geq 0$, since the integrand in (2) vanishes. However, if we look for a discrete time dynamics, ruled by a *timestep* $h > 0$, then there are infinitely many paths $\sigma : \mathbb{R} \to \mathbb{R}^{2m}$ such that $\sigma(0) = y_0$ and

$$H(\sigma(h)) - H(y_0) = H(\sigma(h)) - H(\sigma(0)) = h \int_0^1 \nabla H(\sigma(c))^\top \dot{\sigma}(c)\,\mathrm{d}c = 0, \tag{3}$$

without requiring that the integrand in (3) be identically zero. A given *line integral method* is then characterized by a specific path σ such that (since we shall speak about one-step methods, it is enough defining their first step):

$$\sigma(0) = y_0, \qquad \sigma(h) =: y_1 \approx y(y), \qquad H(y_1) - H(y_0) = h \int_0^1 \nabla H(\sigma(c))^\top \dot{\sigma}(c)\,\mathrm{d}c = 0. \tag{4}$$

This kind of approach has been tackled in [7, 8, 9], which are proceedings and a special issue of the ICNAAM 2007 and ICNAAM 2008 Conferences, and generalized in [11, 12, 13], which are the proceedings and a special issue of the ICNAAM 2009 Conference, where *Hamiltonian Boundary Value Methods (HBVMs)* have been presented (the methods where also presented a few weeks in advance at the MCALV65 Conference [10], too). The same special issue contains the paper [14], inspired by the presentation of HBVMs at the conference. Developments of the line integral approach were presented at all the subsequent editions of the ICNAAM Conference: in particular, at the 2015 edition an advance copy of the monograph [15] was made available.

Related use of line integral methods may be found in, e.g., [16, 17, 18, 19, 20, 21, 22, 23, 24]. Here, our main concern will be the approach defined in [25], from which one sees that HBVMs can be regarded as an expansion of the vector field along a suitable orthonormal basis, which we choose as the Legendre polynomial basis $\{P_j\}_{j\geq 0}$:

$$P_j \in \Pi_j, \qquad \int_0^1 P_i(x) P_j(x)\,\mathrm{d}x = \delta_{ij}, \qquad i, j = 0, 1, \ldots, \tag{5}$$

having set, as is usual, Π_j the vector space of polynomials of degree j, and δ_{ij} the Kronecker symbol. Let us then consider the expansion of the vector field in (1), on the interval $[0, h]$, along the Legendre basis:

$$\dot{y}(ch) = \sum_{j\geq 0} P_j(c)\gamma_j(y), \qquad c \in [0, 1], \qquad y(0) = y_0, \qquad \gamma_j(y) = \int_0^1 P_j(\tau) f(y(\tau h))\,\mathrm{d}\tau. \tag{6}$$

Integrating both sides of the first equation in (6), one obtains the solution in term of the unknown Fourier coefficients,

$$y(ch) = y_0 + h\sum_{j\geq 0}\int_0^c P_j(x)\,\mathrm{d}x\,\gamma_j(y), \qquad c\in[0,1].$$

To get a polynomial approximation, it is sufficient truncating the above series to a finite sum:

$$\dot\sigma(ch) = \sum_{j=0}^{s-1} P_j(c)\gamma_j(\sigma), \qquad c\in[0,1], \qquad \sigma(0)=y_0, \tag{7}$$

with $\gamma_j(\sigma)$ defined according to (6) upon formally replacing y by σ, and

$$\sigma(ch) = y_0 + h\sum_{j=0}^{s-1}\int_0^c P_j(x)\,\mathrm{d}x\,\gamma_j(\sigma), \qquad c\in[0,1]. \tag{8}$$

The equation (8) has been named *Master Functional Equation* in [13]. The polynomial path σ arising from (7)-(8) defines an energy-conserving line-integral method. In fact, by considering that $\sigma(0)=y_0$ and setting

$$y_1 =: \sigma(h) = y_0 + h\int_0^1 \dot\sigma(ch)\,\mathrm{d}c,$$

one has, by taking into account that $f = J\nabla H$, and considering (7):

$$H(y_1)-H(y_0) = H(\sigma(h))-H(\sigma(0)) = h\int_0^1 \nabla H(\sigma(ch))^\top\dot\sigma(ch)\,\mathrm{d}c = h\sum_{j=0}^{s-1}\gamma_j(\sigma)^\top J\gamma_j(\sigma) = 0,$$

since J is skew-symmetric. Moreover, it can be shown that $y_1 - y(h) = O(h^{2s+1})$, i.e., we have defined an order $2s$ approximation procedure [13]. The polynomial path σ defines a *HBVM*(∞, s) method (the meaning of the first argument will be clear after formula (9)). However, it is not yet a ready-to-use numerical method, since the integrals defining the Fourier coefficients $\gamma_j(\sigma)$, $j=0,\dots,s-1$, need to be computed or suitably approximated. However, HBVM(∞, s) methods can be regarded as *continuous-stage Runge-Kutta methods*, as it has been shown in [26, 27]. Conversely, if we consider the Gauss-Legendre quadrature rule of order $2k$, with abscissae and weights (c_i, b_i), $i=1,\dots,k$, we obtain

$$\gamma_j(\sigma) = \int_0^1 P_j(c)f(\sigma(ch))\,\mathrm{d}c \approx \sum_{i=1}^k b_iP_j(c_i)f(\sigma(c_ih)) =: \hat\gamma_j, \qquad j=0,\dots,s-1. \tag{9}$$

This eventually defines a k-stage Runge-Kutta method, called *HBVM*(k, s), with Butcher tableau

$$\begin{array}{c|c} \mathbf{c} & \mathcal{I}_s\mathcal{P}_s^\top\Omega \\ \hline & \mathbf{b}^\top \end{array},$$

where:

$$\mathbf{c} = \begin{pmatrix} c_1\\ \vdots\\ c_k\end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1\\ \vdots\\ b_k\end{pmatrix}, \quad \Omega = \mathrm{diag}(\mathbf{b}), \quad \text{and} \quad \mathcal{P}_s = \Big(\ P_{j-1}(c_i)\ \Big), \mathcal{I}_s = \Big(\ \int_0^{c_i} P_{j-1}(x)\,\mathrm{d}x\ \Big) \in \mathbb{R}^{k\times s}.$$

Moreover, by setting $\hat{\boldsymbol{\gamma}} = (\hat{\gamma}_j)$ the vector, of block dimension s, with the approximate Fourier coefficients (9), it can be shown that the stage vector Y, of block dimension k, can be written, by setting $\mathbf{e} \in \mathbb{R}^k$ the vector with all unit entries, as $Y = \mathbf{e} \otimes y_0 + h\mathcal{I}_s \otimes I\hat{\boldsymbol{\gamma}}$. This, in turn, leads to a discrete problem, in terms of the approximate Fourier coefficients $\hat{\boldsymbol{\gamma}}$ only, in the form

$$\hat{\boldsymbol{\gamma}} = \mathcal{P}_s^\top \Omega \otimes I f(\mathbf{e} \otimes y_0 + h\mathcal{I}_s \otimes I\,\hat{\boldsymbol{\gamma}}). \tag{10}$$

As is shown in [28], this problem can be effectively solved by using a Newton-type iteration, derived from the so called *blended iteration* defined in [29, 30]. It is worth noting that the (block) dimension of the discrete problem (10) is s, *independently* of k. This, in turn, allows the use of large values of k, so that the approximate Fourier coefficients (9) can be evaluated exactly (in case of a polynomial Hamiltonian), or with an accuracy up to round-off errors. In such a case, the Hamiltonian error can be shown to be $O(h^{2k+1})$ [25]. Moreover, this also allows using HBVMs as *spectral methods in time*, by selecting a degree s of the polynomial approximation σ large enough such that it is indistinguishable from the solution y, within the used finite precision arithmetic [32]. This approach turns out to be extremely effective for numerically solving multi-frequency highly-oscillatory problems [31, 33] and Hamiltonian PDEs [34, 35, 36]. With this interpretation, the approach resulting into HBVMs can be extended to virtually any kind of differential problems, as we are going to sketch in the sequel.

GENERALIZATIONS

We now reformulate the previous approach in an equivalent way, in order to generalize it to different kinds of problems [37], confirming that HBVM(∞, s) can be regarded as spectral methods in time (see, e.g., [38] for an introduction to spectral methods). Let us then consider a polynomial approximation $\sigma \in \Pi_s$ to (1), where now we allow the problem to be a general IVP, and expand its derivative (having degree $s-1$), along the Legendre basis (5), thus obtaining:

$$\dot{\sigma}(ch) = \sum_{j=0}^{s-1} P_j(c)\gamma_j, \qquad \sigma(ch) = y_0 + h\sum_{j=0}^{s-1}\int_0^c P_j(x)\,\mathrm{d}x\,\gamma_j, \qquad c \in [0,1], \tag{11}$$

for suitable coefficients γ_j, $j = 0, \ldots, s-1$, to be determined. For this purpose, we impose the residual function, $r(ch) := \dot{\sigma}(ch) - f(\sigma(ch))$, be orthogonal to Π_{s-1}:

$$0 = \int_0^1 P_j(c)r(ch)\,\mathrm{d}c = \int_0^1 P_j(c)\left[\dot{\sigma}(ch) - f(\sigma(ch))\right]\,\mathrm{d}c, \qquad j = 0, \ldots, s-1.$$

One then obtains, by taking into account (11),

$$\gamma_j = \int_0^1 P_j(c) f(\sigma(ch))\,\mathrm{d}c, \qquad j = 0, \ldots, s-1, \tag{12}$$

i.e., the same expressions providing $\gamma_j(\sigma)$ as in (7)-(8), and (6).

Implicit Differential and Differential Algebraic Equations (IDE/DAEs)

In such a case, one considers problems in the form

$$F(\dot{y}(ch), y(ch)) = 0, \qquad c \in [0,1], \qquad y(0) = y_0 \in \mathbb{R}^m, \qquad F : \mathbb{R}^{m\times m} \to \mathbb{R}^m.$$

We can look for a polynomial approximation $\sigma \in \Pi_s$ in the form (11), whose coefficients γ_j, $j = 0, \ldots, s-1$, are obtained by imposing the residual, $r(ch) := F(\dot\sigma(ch), \sigma(ch))$, be orthogonal to Π_{s-1}:

$$0 = \int_0^1 P_j(c) F(\dot\sigma(ch), \sigma(ch))\, \mathrm{d}c, \qquad j = 0, \ldots, s-1.$$

Solving such equations then provides the unknown coefficients γ_j, $j = 0, \ldots, s-1$. An important simplification is obtained in the case of linearly implicit differential equations, i.e., equations in the form:

$$M\dot y(ch) = f(y(ch)), \qquad c \in [0,1], \qquad y(0) = y_0 \in \mathbb{R}^m, \qquad M \in \mathbb{R}^{m\times m},$$

with M possibly singular. Also in this case, by looking for a polynomial approximation in the form (11), and requiring the residual function $r(ch) := M\dot\sigma(ch) - f(\sigma(ch))$ be orthogonal to Π_{s-1}, one arrives at the set of equations

$$M\gamma_j = \int_0^1 P_j(c) f(\sigma(ch))\, \mathrm{d}c, \qquad j = 0, \ldots, s-1,$$

which can be effectively solved by extending the approach in [28] as was done in [39] for the blended iteration. A thorough analysis of the IDE/DAE case is still lacking.

Delay Differential Equations (DDEs)

We consider equations in the form

$$\dot y(t) = f(y(t), y(t-\tau)), \quad t \ge 0, \qquad y(t) = \phi(t), \quad t \in [-\tau, 0], \qquad \tau > 0, \qquad \phi : [-\tau, 0] \to \mathbb{R}^m,$$

with τ fixed and ϕ a known function. In such a case, by using a timestep $h = \tau/K$, for a given integer K, and setting

$$\sigma_n(ch) = y_{n-1} + h \sum_{j=0}^{s-1} \int_0^c P_j(x)\, \mathrm{d}x\, \gamma_j^n, \qquad c \in [0,1],$$

the approximation over the interval $[t_{n-1}, t_n] \equiv [(n-1)h, nh]$, and $y_{n-1} := \sigma_{n-1}(h)$, by imposing the residual $r(ch) := \dot\sigma_n(ch) - f(\sigma_n(ch), \sigma_{n-K}(ch))$ be orthogonal to Π_{s-1}, one arrives at the set of equations

$$\gamma_j^n = \int_0^1 P_j(c) f(\sigma_n(ch), \sigma_{n-K}(ch))\, \mathrm{d}c, \qquad j = 0, \ldots, s-1,$$

where it is assumed, by induction, that σ_{n-K} is known. This approach has been fully investigated in [40], and it has been used to solve a Covid-19 model presented at the ICNAAM 2020 Conference [41].

Fractional Differential Equations (FDEs)

In such a case, for a given $\alpha \in (0, 1]$, we consider the Caputo FDE [42]

$$D^\alpha y(ch) \equiv \frac{1}{\Gamma(1-\alpha)} \int_0^{ch} (ch - x)^{-\alpha} \dot y(x)\, \mathrm{d}x = f(y(ch)), \qquad c \in [0,1], \qquad y(0) = y_0 \in \mathbb{R}^m.$$

As was presented at the ICNAAM 2018 Conference [43], if we look for a polynomial approximation $\dot\sigma$ to the *derivative* of the solution as in (11), one then obtains a *quasi-polynomial* approximation to the solution in the form:

$$\sigma(ch) = y_0 + h^\alpha \sum_{j=0}^{s-1} \gamma_j I^\alpha P_j(c) \equiv y_0 + h^\alpha \sum_{j=0}^{s-1} \gamma_j \frac{1}{\Gamma(\alpha)} \int_0^c (c-x)^{\alpha-1} P_j(x)\, \mathrm{d}x, \tag{13}$$

with $I^\alpha P_j(c)$ the corresponding Riemann-Liouville integrals (see [44] for a stable algorithm for their computation). As done before, by imposing the residual $r(ch) := D^\alpha\sigma(ch) - f(\sigma(ch))$ be orthogonal to Π_{s-1}, one formally arrives at the set of equations (12), but with σ given by (13). As is shown in [43, 44], this approach proves to be very promising.

CONCLUSIONS AND FUTURE DEVELOPMENTS

In this note, we have recalled how the numerical solution of several differential problems can be studied within a single framework. The analysis of this approach has been completely carried out only in the IVP and DDE case, and needs to be done for IDE/DAEs and FDEs. Further, for FDEs, a multi-step approach, extending the global one sketched above, is also under investigation.

We would like to emphasize once again that the genesis of such an approach is tightly connected with the ICNAAM Conference series, chaired by Theodore Simos, whom we wish to sincerely thank.

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