GEOMETRIC INTEGRATION
BY PLAYING WITH MATRICES

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Dedicated to the 70\textsuperscript{th} birthday of Gerhard Wanner

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1 - Overview

- Geometric Integration
- some history
- geometric Runge-Kutta methods
- matrix formulation of the methods
- generalized W-transform
- energy-conservation (and some generalizations)
- symplecticity
- both of them, too . . .
- concluding remarks
2 - Conservative problems

We shall deal with problems in the form

\[ y'(t) = f(y(t)), \quad y(0) = y_0 \in \mathbb{R}^m, \]

for which there exists \( L: \mathbb{R}^m \rightarrow \mathbb{R}^\nu \)

such that

\[ L(y(t)) = L(y_0), \quad t \geq 0. \]

That is, the dynamical system admits \( \nu \) constants of motion.
The numerical solution of conservative problems is an active field of investigation:

- the numerical methods induce a corresponding discrete vector field;
- it is desirable that the latter is able to reproduce geometrical properties of the continuous one.

Because of this reason, it has become customary to refer this field of investigation to as geometric integration.
Conceptually, geometric integration:

- can be led back to the early work of G. Dahlquist on differential equations, about 50 years ago,
- his aim being to reproduce the asymptotic stability of equilibria for the trajectories produced by the numerical methods,
- thus resulting in the well-known linear stability analysis of the methods.
5 - Hamiltonian Problems

In particular, we shall deal with the numerical solution of Hamiltonian problems, which are encountered in many real-life applications, ranging from the nano-scale of molecular dynamics, to the macro-scale of celestial mechanics:

\[ y' = J \nabla H(y), \quad y(0) = y_0 \in \mathbb{R}^{2m}, \quad J = \begin{pmatrix} I_m & I_m \\ -I_m & I_m \end{pmatrix}, \]

where \( J^T = -J = J^{-1} \). The scalar function \( H(y) \) is the Hamiltonian of the problem and its value is constant during the motion, namely

\[ H(y(t)) \equiv H(y_0), \quad \forall t \geq 0, \]

since

\[ \frac{d}{dt} H(y(t)) = \nabla H(y(t))^T y'(t) = \nabla H(y(t))^T J \nabla H(y(t)) = 0. \]
6 - Energy conservation

Often, the Hamiltonian $H$ is also called the energy, since for isolated mechanical systems it has the physical meaning of total energy.

Consequently, energy conservation is an important feature in the simulation of such problems.

“Usual” numerical methods often exhibit a drift in the energy.

This, in turn, hinders the possibility of performing correct long-term simulations.
7 - Symplecticity of the map

The continuous map associated with the Hamiltonian problem,

$$\phi_t : \mathbf{y}_0 \rightarrow \mathbf{y}(t),$$

can be proved to be symplectic. That is, by setting $\phi'_t$ the Jacobian of $\phi_t$, then

$$\left(\phi'_t\right)^T J(\phi'_t) = J.$$

The conservation of the Hamiltonian can be proved to derive from the symplecticity of the map, via an infinite number of infinitesimal contact transformations (see, e.g., [1]).

A rough idea about symplectic methods can be found in early work of Gröbner [2]. Symplectic Runge–Kutta methods have been then studied by Feng Kang [3], Sanz-Serna [4], and Suris [5].

Such methods are obtained by imposing that the discrete map, associated with a given numerical method, is symplectic, as is the continuous one.
Symplectic methods usually perform much better than standard ones.

Since for the continuous map symplecticity implies energy-conservation, then one expects that something similar happens for the discrete map as well.

As a matter of fact, under suitable assumptions, it can be proved that, when a symplectic method is used with a constant step-size $h$, then the numerical solution satisfies a perturbed Hamiltonian problem [6],

$$\tilde{y}' = J \nabla \tilde{H}_h(\tilde{y}), \quad \tilde{y}(0) = y_0 \in \mathbb{R}^{2m}.$$ 

10 - Energy conservation

The previous result then provides a quasi-conservation property of the Hamiltonian over “exponentially long times”. (See also the comprehensive monograph [7]).

Even though this is an interesting feature, nonetheless, it constitutes a somewhat weak stability result since, in general,

- it doesn’t extend to infinite intervals,
- cannot avoid severe restrictions on the stepsize,

as a classical stability analysis would require.

Moreover, if the stepsize $h$ is not small enough, sometimes the perturbed Hamiltonian could not well approximate the exact one.

As an example, consider the problem defined by the Hamiltonian:

$$H(q, p) = p^2 + (\beta q)^2 + \alpha(q + p)^{2n}.$$ 

The corresponding dynamical system has exactly one (marginally stable) equilibrium at the origin.
12 - An example

Let us fix the following parameters [8]:

\[ \beta = 10, \quad \alpha = 1, \quad n = 4, \]

and suppose we are interested in approximating the level curves of
the Hamiltonian passing from the points:

\[ (q_0, p_0) = (i, -i), \quad i = 1, \ldots, 8. \]

This could be done by integrating the trajectories starting at such
initial points, for the corresponding Hamiltonian system.

[8] L. B., F. Iavernaro, D. Trigiante. A note on the efficient implementation of
13 - Level curves
14 - 2-stage Gauss method, $h = 10^{-3}$
15 - 2-stage Gauss method, $h = 10^{-3}$
A way to get rid of this problem is then that of directly looking for energy-conserving methods, able to exactly satisfy the conservation property of the Hamiltonian along the numerical trajectory.

The very first attempts to face this problem were based on projection techniques coupled with standard non-conservative numerical methods.

However, it is well-known that this approach suffers from many drawbacks, in that this is usually not enough to correctly reproduce the long-term dynamics, as is shown, e.g., in [9]

A completely new approach is represented by discrete gradient methods.

They are based upon the definition of a discrete counterpart of the gradient operator, so that energy conservation of the numerical solution is guaranteed at each step and for any choice of the integration step-size [10,11].


A different approach is based on the concept of time finite element methods [12], where one finds local Galerkin approximations on each subinterval of a given mesh of size $h$ for the given ODE-IVPs.

This, in turn, has led to the definition of energy-conserving Runge–Kutta methods [13,14], when replacing the involved integrals with suitable quadrature formulae.

A partially related approach is given by discrete line integral methods [15,16,17].

In such a case, the key idea is to exploit the relation between the method itself and the discrete line integral, i.e., the discrete counterpart of the line integral in conservative vector fields.


The use of discrete line integrals allows, in turn, exact conservation for polynomial Hamiltonians of arbitrarily high-degree.

This resulted in the class of methods later named Hamiltonian Boundary Value Methods (HBVMs), which have been developed in a series of papers (e.g., [18–22]).

Another approach, strictly related to the latter one, is given by the Averaged Vector Field method [23, 24] and its generalizations [25], which have been mainly analysed in the framework of B-series [26] (i.e., methods admitting a Taylor expansion with respect to the step-size).

The basic idea HBVMs rely on is very simple. Indeed, one has that energy conservation follows as well from the vanishing of the line integral

\[ H(y(t)) - H(y_0) = \int_0^t \nabla H(y(s))^T y'(s) ds = 0, \]

which is due to the fact that

\[ y'(s) = J \nabla H(y(s)) \quad \text{and} \quad J^T = -J. \]
However, one can derive conservation at $t = h$ along any suitable path $\sigma(\cdot)$ joining

$$y_0 = \sigma(0) \quad \text{to} \quad y_1 \equiv \sigma(h),$$

such that

$$H(y_1) - H(y_0) \equiv H(\sigma(h)) - H(\sigma(0))$$

$$= \int_{0}^{h} \nabla H(\sigma(s))^T \sigma'(s) ds$$

$$= h \int_{0}^{1} \nabla H(\sigma(\tau h))^T \sigma'(\tau h) d\tau = 0.$$
24 - Polynomial path

We choose $\sigma$ to be a polynomial of degree $s$, and expand its derivative along a suitable polynomial basis $\{P_j\}_{j \geq 0}$:

$$
\sigma'(ch) = \sum_{j=0}^{s-1} \gamma_j P_j(c), \quad c \in [0, 1].
$$

By imposing the condition $\sigma(0) = y_0$, one obtains, formally,

$$
\sigma(ch) = y_0 + h \sum_{j=0}^{s-1} \gamma_j \int_0^c P_j(\tau) d\tau, \quad c \in [0, 1].
$$
In particular, we choose, as polynomial basis, the Legendre polynomials, which are shifted on the interval \([0, 1]\), and scaled such that they are orthonormal:

\[
\int_0^1 P_i(c)P_j(c)\,dc = \delta_{ij}, \quad \forall i, j \geq 0.
\]
26 - Energy conservation

By imposing the vanishing of the line integral to obtain energy conservation, one has

\[ 0 = \int_0^1 \nabla H(\sigma(\tau h))^T \sum_{j=0}^{s-1} \gamma_j P_j(\tau) \, d\tau = \sum_{j=0}^{s-1} \left( \int_0^1 \nabla H(\sigma(\tau h)) P_j(\tau) \, d\tau \right)^T \gamma_j. \]

In view of the skew-symmetry of matrix \( J \), this holds true by choosing the (vector) coefficients \( \gamma_j \) as

\[ \gamma_j = J \int_0^1 \nabla H(\sigma(\tau h)) P_j(\tau) \, d\tau, \quad j = 0, \ldots, s - 1. \]
With this choice, the nonlinear system defining the unknown coefficients $\gamma_j$ becomes, by setting $f(\cdot) = J \nabla H(\cdot)$,

$$\gamma_j = \int_0^1 P_j(\tau) f \left( y_0 + h \sum_{i=0}^{s-1} \gamma_i \int_0^\tau P_i(c) dc \right) d\tau,$$

$$j = 0, \ldots, s - 1.$$

By considering that $P_0(\tau) \equiv 1$, the new approximation is then given by

$$y_1 \equiv \sigma(h) = y_0 + h\gamma_0.$$

We stress, however, that the previous formulae do not represent an operative method unless the integrals are approximated by means of a suitable quadrature formula.
For this purpose, let us consider the interpolation quadrature formula defined at the abscissae

\[ 0 \leq c_1 < \cdots < c_k \leq 1, \]

and the corresponding weights \( \{b_i\} \). The final shape of a HBVM method, denoted by \( \text{HBVM}(k,s) \), is then given by

\[
\gamma_j = \sum_{\ell=1}^{k} b_\ell P_j(c_\ell) f \left( y_0 + h \sum_{i=0}^{s-1} \gamma_i \int_{0}^{c_\ell} P_j(c) \, dc \right),
\]

\[ j = 0, \ldots, s - 1, \]

which is a system of \( s \) nonlinear vector algebraic equations in the unknowns \( \{\gamma_j\} \), for any value of \( k \).
29 - Runge-Kutta formulation

Substituting the obtained expression of $\gamma_j$ into

$$\sigma(ch) = y_0 + h \sum_{j=0}^{s-1} \gamma_j \int_0^c P_j(\tau) \, d\tau, \quad c \in [0, 1],$$

and setting

$$Y_i = \sigma(c_i h), \quad i = 1, \ldots, k,$$

one then obtains:

$$Y_i = y_0 + h \sum_{j=0}^{s-1} \int_0^{c_i} P_j(s) \, ds \sum_{\ell=1}^k b_{\ell} P_j(c_\ell) f(Y_\ell), \quad i = 1, \ldots, k,$$

with the new approximation given by

$$y_1 = y_0 + h \sum_{i=1}^s b_i f(Y_i).$$
Evidently, the previous equations represent the following \( k \)-stage Runge-Kutta method,

\[
\begin{array}{c|c}
  c_1 & A \equiv \left( b_j \sum_{\ell=0}^{s-1} P_{\ell}(c_j) \int_{c_i}^{c_i} P_{\ell}(x)dx \right)_{i,j=1,\ldots,k} \\
  \vdots \\
  c_k \\
  \hline
  b_1 & \ldots & b_k
\end{array}
\]

defining the Runge-Kutta shape of a HBVM(\( k, s \)) method.
Assume to place the nodes at the \( k \) Gauss-Legendre points in \([0, 1]\). Then, for all \( k \geq s \), HBVM\((k, s)\):

- has order \( 2s \),
- the quadrature is exact for all polynomial Hamiltonians of degree no larger than
  \[
  \nu \leq \frac{2k}{s},
  \]
- for general (suitably regular) Hamiltonians, the energy error is
  \[
  O(h^{2k+1}),
  \]
  thus implying a practical conservation, provided that \( k \) is large enough, also in the non-polynomial case.
We can easily express the Butcher matrix of an HBVM\((k, s)\) by introducing the following matrices:

\[
\begin{align*}
\mathcal{P}_s &= \begin{pmatrix}
P_0(c_1) & \cdots & P_{s-1}(c_1) \\
\vdots & \ddots & \vdots \\
P_0(c_k) & \cdots & P_{s-1}(c_k)
\end{pmatrix}, \\
\mathcal{I}_s &= \begin{pmatrix}
\int_0^{c_1} P_0(x)\,dx & \cdots & \int_0^{c_1} P_{s-1}(x)\,dx \\
\vdots & \ddots & \vdots \\
\int_0^{c_k} P_0(x)\,dx & \cdots & \int_0^{c_k} P_{s-1}(x)\,dx
\end{pmatrix} \in \mathbb{R}^{k \times s}
\end{align*}
\]
They are related as follows,

\[ \mathcal{I}_s = \mathcal{P}_{s+1} \hat{\mathbf{X}}_s, \]

via the structure matrix:

\[ \hat{\mathbf{X}}_s = \begin{pmatrix} \frac{1}{2} & -\xi_1 \\ \xi_1 & 0 & \ddots \\ & \ddots & \ddots & -\xi_{s-1} \\ & & \xi_{s-1} & 0 \\ \xi_s & & & \xi_s \end{pmatrix} \equiv \begin{pmatrix} X_s \\ 0 \ldots 0 \xi_s \end{pmatrix} \in \mathbb{R}^{s+1 \times s}, \]

with \[ \xi_i = (2\sqrt{4i^2 - 1})^{-1}, \quad i = 1, \ldots, s. \]
34 - Matrix form

By also introducing the diagonal matrix with the quadrature weights,

$$\Omega = \begin{pmatrix} b_1 & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ b_k \end{pmatrix} \in \mathbb{R}^{k \times k},$$

we finally obtain

$$A = \mathcal{I}_s \mathcal{P}_s^T \mathcal{Y} \equiv \mathcal{P}_{s+1} \hat{X}_s \mathcal{P}_s^T \Omega \in \mathbb{R}^{k \times k},$$

whose rank is $s$. 
In general, $k \geq s$. In the case $k = s$, one obtains due to the fact that $P_s(c_i) = 0$, $i = 1, \ldots, s$,

$$P_{s+1} = \begin{pmatrix} P_s & 0 \end{pmatrix}, \quad P_s^{-1} = P_s^T\Omega,$$

so that we obtain the s-stage Gauss method,

$$A = P_s X_s P_s^{-1}.$$

In this sense, for $k \geq s$,

$$A = P_{s+1}\hat{X}_s P_s^T\Omega$$

can be regarded as a generalized W-transform [27].

From the previous result, it follows that, for all $k \geq s$, HBVM($k, s$) share the same spectrum.

Indeed, the matrix

$$A = P_{s+1} \hat{X}_s P_s^T \Omega \in \mathbb{R}^{k \times k}$$

has constant rank $s$, so that it has a $(k - s)$-fold 0 eigenvalue. The remaining ones can be easily seen to coincide with the $s$ eigenvalues of $X_s$ (i.e., those of the Butcher matrix of the $s$-stage Gauss method) [28].

The low-rank structure of the Butcher matrix of HBVM\((k, s)\), allows to make their implementation more efficient. Indeed, by setting \( Y \) the block vector of dimension \( k \) with the stages of the method, one has to solve

\[
Y = 1 \otimes y_0 + h(I_s \, P_s^T \Omega) \otimes I \, f(Y),
\]

where \( f(Y) \equiv J \nabla H(Y) \) is a block vector. By setting

\[
\gamma = P_s^T \Omega \otimes I \, f(Y)
\]

the block vector of dimension \( s \) with the coefficients of the polynomial \( \sigma \), one has

\[
Y = 1 \otimes y_0 + hI_s \otimes I \gamma,
\]

and, then,

\[
\gamma = P_s^T \Omega \otimes I \, f(1 \otimes y_0 + hI_s \otimes I \gamma).
\]
Let us consider again the problems defined by the Hamiltonian:

\[ H(q, p) = p^2 + (\beta q)^2 + \alpha(q + p)^{2n}, \]

with parameters

\[ \beta = 10, \quad \alpha = 1, \quad n = 4, \]

and initial points:

\[ (q_0, p_0) = (i, -i), \quad i = 1, \ldots, 8. \]

We use the HBVM(k,s) method with \( s = 2 \) and \( k \geq s \), so that the method has order 4, with the same stepsize \( h = 10^{-3} \) as before.
By placing the $k$ abscissae $c_1, \ldots, c_k$ for the quadrature at the Gauss-Legendre points in $[0,1]$, we have that the error in the Hamiltonian is:

- $O(h^{2k+1})$ for $k = 2, 3, \ldots, 7$;
- in particular, for $k = 2$ we recover the 2-stage Gauss method;
- 0, for $k \geq 8$, due to the fact that the Hamiltonian is a polynomial of degree 8.
HBVM(3,2) method, $h = 10^{-3}$
HBVM(3,2) method, $h = 10^{-3}$
42 - HBVM(8,2) method, $h = 10^{-3}$
43 - HBVM(8,2) method, $h = 10^{-3}$
It is worth mentioning that the basic idea on which HBVMs rely, can be extended to cope with any conservative problems.

Indeed, let us suppose that a general ODE-IVPs,

$$y' = f(y), \quad y(0) = y_0,$$

has $\nu$ (independent) smooth invariants:

$$L(y(t)) = L(y_0) \in \mathbb{R}^\nu, \quad t \geq 0.$$
The basic idea is now that of modifying the form of the polynomial $\sigma(\cdot)$ as follows:

$$
\sigma'(ch) = \sum_{j=0}^{s-1} \gamma_j P_j(c) + \phi_0 \alpha, \quad c \in [0, 1],
$$

with

$$
\alpha \in \mathbb{R}^\nu,
$$

and, in general,

$$
\phi_j = \int_0^1 P_j(\tau) J_L^T (\sigma(\tau h)) d\tau, \quad j \geq 0,
$$

being $J_L(\cdot)$ the Jacobian matrix of $L(\cdot)$. 
By imposing, as usual, the conservation through a line integral, one then obtains:

\[ 0 = L(\sigma(h)) - L(\sigma(0)) = h \int_0^1 J_L(\sigma(\tau h))\sigma'(\tau h))d\tau \]

\[ = h \left( \sum_{j=0}^{s-1} \phi_j^T \gamma_j + \phi_0^T \phi_0 \alpha \right). \]

Which is satisfied provided that

\[ \alpha = - \sum_{j=0}^{s-1} \phi_j^T \gamma_j. \]

\[ \text{spd "matrix"} \]
By suitably discretizing the involved integrals, one obtains the class of methods, which has been named Line Integral Methods (LIMs).

\[
\text{Line Integral Methods (LIMs)}
\]

\[
\text{LIM}(\underbrace{\phi_j \text{ quadrature}}, \underbrace{\gamma_j \text{ quadrature}}, \underbrace{k}, \underbrace{s}, \underbrace{\text{degree of } \sigma})
\]

In particular:

- LIM(0,k,s) coincide with HBVM(k,s);
- LIM(0,s,s) coincide with s-stage Gauss methods.
Fully conservative variants of both:

- HBVM($k,s$) methods, i.e., LIM($k,k,s$), and
- $s$-stage Gauss-Legendre methods, i.e., LIM($k,s,s$),

are reported in [29].


Also presented at ICNAAM 2011.
A noticeable extension of symplectic Gauss-Legendre methods has been recently devised in [30], starting from the Runge-Kutta formulation of HBVMs, which have been called Symplectic low-rank Runge-Kutta methods.

They can be quite straightforwardly obtained from the matrix form of HBVM(k,s).

\[
\begin{array}{c|c}
   c_1 & A \equiv P_{s+1} \hat{X}_s P_s^T \Omega \\
   \vdots \\
   c_k & b_1 \ldots b_k \\
\end{array}
\]

Involved matrices

\[ \mathcal{P}_s = \begin{pmatrix} P_0(c_1) & \ldots & P_{s-1}(c_1) \\ \vdots & \ddots & \vdots \\ P_0(c_k) & \ldots & P_{s-1}(c_k) \end{pmatrix} \in \mathbb{R}^{k \times s}, \]

\[ \hat{\mathcal{X}}_s = \begin{pmatrix} 1 & -\xi_1 \\ \xi_1 & 0 & \ddots \\ \ddots & \ddots & -\xi_{s-1} \\ -\xi_{s-1} & 0 & \ddots \\ \xi_{s-1} & 0 & \ddots & -\xi_s \end{pmatrix} = \begin{pmatrix} X_s \\ 0 & \ldots & 0 & \xi_s \end{pmatrix} \in \mathbb{R}^{s+1 \times s}, \]

\[ \Omega = \text{diag}(b_1, \ldots, b_k). \]
By using the criterion for symplecticity stated in [31] on the HBVM(k,s) method, one has, by setting $b = \Omega 1$:

$$\Omega A + A^T \Omega - bb^T = \xi_s \left( v_s v_{s-1}^T + v_{s-1} v_s^T \right),$$

with

$$v_r = \left( b_1 P_r(c_1) \ldots b_k P_r(c_k) \right)^T, \quad r = s - 1, s,$$

so that the method is not symplectic.

However, by setting \( \xi_s = 0 \), one obtains that the following method, denoted by \( \text{SLIRK}(k,s) \), is trivially symplectic:

\[
\begin{align*}
\begin{array}{c|c}
  \mathbf{c}_1 & \mathbf{b}_1 \\
  \vdots & \vdots \\
  \mathbf{c}_k & \mathbf{b}_k \\
\end{array}
\end{align*}
\]

\[ A \equiv \mathcal{P}_s X_s \mathcal{P}_s^T \Omega \]

The rank of \( A \) is obviously \( s \), for all \( k \geq s \).
SLIRK\((k,s)\) inherit many properties of the underlying \(s\)-stage Gauss method, which is obtained when \(k = s\) and the abscissae are placed at the Gauss-Legendre nodes in \([0,1]\):

- it is symmetric and symplectic;
- it has order \(2s\);
- the Hamiltonian error is of the same order.

It cannot improve over such method.
54 - $\text{SLIRK}(8,2), \ h = 10^{-3}$

[Graph showing a time series with logarithmic y-axis labeled 'Hamiltonian Error' and linear x-axis labeled 't']
55 - SLIRK(8,2), $h = 10^{-3}$
Let consider a separable Hamiltonian problem with additive noise,

\begin{align*}
dq &= pdt, \quad q(0) = q_0, \\
dp &= -V'(q)dt + \sigma dW, \quad p(0) = p_0,
\end{align*}

with the Hamiltonian

\[ H(q, p) = \frac{1}{2}p^2 + V(q), \]

and \( W(t) \) a Wiener process satisfying

\[ \langle W(t)W(s) \rangle = \min(t, s). \]
57 - SLIRK\((k,s)\) for stochastic Hamiltonian problems

The solution of the above problem is formally given by

\[
q(t) = q_0 + \int_0^t p(\tau)\,d\tau,
\]

\[
p(t) = p_0 - \int_0^t V'(q(\tau))\,d\tau + \int_0^t \sigma\,dW(\tau).
\]

In such a case, the use of a higher value of \(k\) allows a better approximation of the involved stochastic integral, and better statistical results are reported in [32], w.r.t. the underlying \(s\)-stage Gauss method.

---

Is it possible, for a numerical method, to have both the symplecticness of the map and the energy-conservation property?

Attempts to incorporate both symplecticity and energy conservation into the numerical method will clash with two non-existence results.

The first [33] refers to non-integrable systems, that is systems that do not admit other independent first integrals different from the Hamiltonian function itself:

If [the method] is symplectic, and conserved $H$ exactly, then it is the time advance map for the exact Hamiltonian system up to a reparametrization of time.

The second negative result [34] refers to B-series symplectic methods applied to general (not necessarily non-integrable) Hamiltonian systems:

The only symplectic method (as B-series) that conserves the Hamiltonian for arbitrary $H(y)$ is the exact flow of the differential equation.

Nevertheless...

The impossibility for a constant time stepping algorithm to be at the same time symplectic and energy-conserving has led to research into methods which could inherit both features in a weaker sense.

This delicate aspect has been thoroughly faced in [35] where the authors prove the existence of symplectic-energy-momentum preserving integrators by using time-adaptive steps.

Here time-step adaption is used to impose energy conservation (see also [36]).


By following a different route, in [37,38,39] a new class of methods, named

**Energy and QUadratic Invariants Preserving (EQUIP)** methods,

has been defined. Their straightforward formulation can be easily sketched by using the framework of matrices.

---


Let consider the $W$-transform of the Butcher matrix of the $s$-stage Gauss method:

$$A = \mathcal{P}_s X_s \mathcal{P}_s^T \Omega,$$

which satisfies the conservation property for quadratic invariants, i.e.,

$$\Omega A + A^T \Omega - bb^T = \Omega \mathcal{P}_s (X_s + X_s^T) \mathcal{P}_s^T \Omega - bb^T = 0,$$

due to the fact that

$$X_s + X_s^T = e_1 e_1^T$$

and

$$\Omega(\mathcal{P}_s e_1) = \Omega 1 = b.$$
The above property continues to hold, provided that we replace matrix $X_s$ by

$$X_s(\alpha) = X_s + \alpha W,$$

with $W^T = -W$, due to the fact that

$$X_s(\alpha) + X_s(\alpha)^T = X_s + X_s^T + \alpha (W + W^T) = X_s + X_s^T.$$

The free parameter $\alpha$ can be chosen in order to get, at each integration step, energy-conservation.
In particular, by setting

\[
X_s(\alpha) = \begin{pmatrix}
\frac{1}{2} & -\xi_1 \\
\xi_1 & 0 & \ddots \\
& \ddots & \ddots & - (\xi_i + \alpha) \\
& & \ddots & \ddots \\
& & & \ddots & -(\xi_{s-1} + \alpha) \\
& & & & \xi_{s-1}
\end{pmatrix},
\]

it can be proved that \( \alpha = O(h^{2(s-i)}) \), so that the order \( 2s \) of the original Gauss method is retained by its EQUIP variant [40].

65 - EQUIP variant of the 2-stage Gauss method

As an example, for $s = 2$, one obtains,

$$X_2(\alpha) = \begin{pmatrix} \frac{1}{2} & -\left(\xi_1 + \alpha\right) \\ (\xi_1 + \alpha) & 0 \end{pmatrix},$$

from which one obtains the fourth-order EQUIP variant:

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\frac{1}{4}$</th>
<th>$\frac{1}{4}$</th>
<th>$-\frac{\sqrt{3}}{6}$</th>
<th>$-\alpha$</th>
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<td>$\frac{1}{4}$</td>
<td>$\frac{1}{4}$</td>
<td>$\frac{\sqrt{3}}{6}$</td>
<td>$+\alpha$</td>
</tr>
</tbody>
</table>

When $\alpha = 0$ one retrieves the original 2-stage Gauss method.
In such case, we have the following two sixth-order EQUIP variants:

- **First variant:**

\[
X_3(\alpha) = \begin{pmatrix}
\frac{1}{2} & -(\xi_1 + \alpha) & 0 \\
(\xi_1 + \alpha) & 0 & -\xi_2 \\
0 & \xi_2 & 0
\end{pmatrix},
\]

with \( \alpha = O(h^4); \)

- **Second variant:**

\[
X_3(\alpha) = \begin{pmatrix}
\frac{1}{2} & -\xi_1 & 0 \\
\xi_1 & 0 & -(\xi_2 + \alpha) \\
0 & (\xi_2 + \alpha) & 0
\end{pmatrix},
\]

with \( \alpha = O(h^2); \)
When $\alpha = 0$ one retrieves the 3-stage Gauss method.
68 - Second sixth-order EQUIP variant

\[
\begin{array}{c|cccc}
\frac{1}{2} - \sqrt{\frac{15}{10}} & \frac{5}{36} & \frac{2}{9} - \sqrt{\frac{15}{15}} - \alpha \frac{2}{3} & \frac{5}{36} - \sqrt{\frac{15}{30}} + \alpha \frac{2}{3} \\
\frac{1}{2} & \frac{5}{36} + \sqrt{\frac{15}{24}} + \alpha \frac{5}{12} & \frac{2}{9} & \frac{5}{36} - \sqrt{\frac{15}{24}} - \alpha \frac{5}{12} \\
\frac{1}{2} + \sqrt{\frac{15}{10}} & \frac{5}{36} + \sqrt{\frac{15}{30}} - \alpha \frac{2}{3} & \frac{2}{9} + \sqrt{\frac{15}{15}} + \alpha \frac{2}{3} & \frac{5}{36} \\
\hline
\frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
\]

Also in this case, when \( \alpha = 0 \) one retrieves the 3-stage Gauss method.
69 - EQUIP(2), $h = 10^{-3}$
70 - EQUIP(2), $h = 10^{-3}$
Matrix formulation of Runge-Kutta methods constitutes a powerful framework for Geometric Integration;

Energy-conserving HBVM(k,s) Runge-Kutta methods can be efficiently analyzed in this framework, as well as their efficient implementation;

The larger class of Line Integral Methods can be obtained as a straightforward generalization;

Low-rank symplectic Runge-Kutta methods are also easily derived within this framework;

Energy and QUadratic Invariants Preserving methods can be derived, thus providing a further direction of investigation.
Hippocrates platanus
Happy birthday, Gerhard!