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A SYMMETRIC NEARLY PRESERVING GENERAL LINEAR METHOD FOR HAMILTONIAN PROBLEMS

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Abstract. This paper is concerned with the numerical solution of Hamiltonian problems, by means of nearly conservative multivalue numerical methods. In particular, the method we propose is symmetric, G-symplectic, diagonally implicit and generates bounded parasitic components over suitable time intervals. Numerical experiments on a selection of separable Hamiltonian problems are reported, also based on real data provided by Nasa Horizons System.

1. **Introduction.** The purpose of this paper is the analysis of the behaviour of nearly conservative multivalue numerical methods applied to a selection of Hamiltonian problems

$$\begin{aligned} \dot{p}(t) &= -\frac{\partial}{\partial q}\mathcal{H}(p(t), q(t)), \\ \dot{q}(t) &= \frac{\partial}{\partial p}\mathcal{H}(p(t), q(t)), \end{aligned} \tag{1}$$

of interest in Celestial Mechanics. The function $\mathcal{H} : \mathbb{R}^{2d} \to \mathbb{R}$ is the Hamiltonian of the system, while $p(t), q(t) \in \mathbb{R}^d$ respectively denote generalized momenta and coordinates associated to the mechanical system. The classical theory of numerical integrators for such problems is focused on the employ of symplectic Runge-Kutta (RK) methods [2, 15, 19, 21], which are meant to preserve, along the numerical solution, quadratic invariants possessed by the continuous problem (1). Modern numerical solvers for Hamiltonian problems are based on methods meant to guarantee a near conservation of invariants over suitably long time intervals [2, 3, 4, 6, 7, 8, 9, 14, 15].

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Following this recent path, the spirit of this paper is that of deriving diagonally implicit methods belonging to the family of General Linear Methods (GLMs, compare [1, 2, 10, 17] and references therein)

$$\begin{cases} Y_i^{[n]} = h\sum\limits_{j=1}^{s} a_{ij}F_j^{[n]} + \sum\limits_{j=1}^{r} u_{ij}y_j^{[n]}, & i = 1, 2, \dots, s, \\ y_i^{[n+1]} = h\sum\limits_{j=1}^{s} b_{ij}F_j^{[n]} + \sum\limits_{j=1}^{r} v_{ij}y_j^{[n]}, & i = 1, 2, \dots, r, \end{cases} \tag{2}$$

designed for the solution of the first order initial value problems

$$\begin{cases} y'(t) = f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \tag{3}$$

where $f : \mathbb{R}^d \to X$, being $(X, < \cdot, \cdot >)$ an inner product space. The formulation (2) is provided in correspondence of the uniform grid $\{t_0 + ih, i = 0, 1, \dots, N\}$, with $h = (T - t_0)/N$. The vector $y^{[n]} = [y_1^{[n]}, \dots, y_r^{[n]}]^{\intercal}$ denotes the vector of external approximations containing all the informations we decide to transfer from step n to step $n+1$, $Y_i^{[n]}$ provides an approximation to the solution of (3) in the internal point $t_n + c_ih \in [t_n, t_{n+1}]$, $i = 1, 2, \dots, s$, and $F_j = f(Y_j^{[n]})$. The methods we consider here are aimed to satisfy some specific properties needed to accurately approach Hamiltonian problems:

- G-symplecticity [2, 3, 4, 6, 7, 8, 9, 15], which ensures the conjugate-symplecticity of the underlying one-step method associated to the multivalue method (2). This means that a G-symplectic method has the same behavior of a symplectic one-step method after a global change of coordinates that is $O(h^p)$ close to the identity [12];
- symmetry of the numerical scheme [15], which is a suitable property providing the discrete counterpart of the reversibility of the exact flow, in case of reversible dynamical systems;
- boundedness of parasitic components over suitably long times [11, 15], which ensures that the parasitic components generated by the numerical method remain bounded over certain time intervals.

The above mentioned features are described in details in Section 2, where a method having such desired properties is also constructed. A selection of numerical experiments is reported in Section 3: some of them are based on real initial data taken from NASA Horizons System (`http://ssd.jpl.nasa.gov/?horizons`).

2. **Symmetry and G-symplecticity of General Linear Methods.** Poincare's theorem (see [15]) guarantees the symplecticity of the flow generated by Hamiltonian systems. The discrete counterpart, only in the case of quadratic Hamiltonians, is the property of symplecticity, which is prerogative of one-step methods: this property assures that quadratic invariants of the mechanical systems are also preserved along the numerical solution. Runge-Kutta methods

$$\begin{cases} Y_i = y_n + h\sum\limits_{j=1}^{s} a_{ij}f(Y_j), & i = 1, 2, \dots, s, \\ y_{n+1} = y_n + h\sum\limits_{i=1}^{s} b_i f(Y_i), \end{cases}$$

are symplectic, by definition, if the matrix $A = (a_{ij})_{i,j=1}^s$ and the vector $b = (b_i)_{i=1}^s$ satisfy the algebraic constraint [2, 15, 19, 21]

$$M = \operatorname{diag}(b)A + A^{\mathsf{T}}\operatorname{diag}(b) - bb^{\mathsf{T}} = 0, \tag{4}$$

where $\operatorname{diag}(x)$ denotes the diagonal matrix having the vector x on the diagonal.

One-step methods are the only candidates for symplecticity (compare [15, 23] for linear multistep methods and [5, 14, 18] for irreducible multivalue methods). This is due to the fact the multistep and multivalue methods generate parasitic components in the numerical solution which destroy the overall long-time accuracy (see [11, 15]). Hence, if one aims to derive non-symplectic methods which are capable of nearly preserving invariants over the numerical solution, the parasitic behaviour of such methods has to be taken under control over long time intervals [11].

As announced in the introduction of the paper, let us recall the desired property we impose to derive a multivalue method able to accurately preserve the symplectic structure of the flow also along the numerical solution.

- *G-symplecticity.* As mentioned, the multivalue nature of GLMs does not allow them to be symplectic, unless they reduce to RK methods. However, a near-conservation property achievable by multivalue methods has been provided and analyzed by the recent literature, defined as follows. If $y^{\mathsf{T}}Ey$ is a quadratic first integral of the differential problem $y' = f(y)$, where E is a symmetric matrix, G-symplecticity assures that

$${y^{[n+1]}}^{\mathsf{T}}(G \otimes E)y^{[n+1]} = {y^{[n]}}^{\mathsf{T}}(G \otimes E)y^{[n]}, \tag{5}$$

(compare [12]), being $G \in \mathbb{R}^{r\times r}$ a symmetric matrix. This conservation property is equivalent to the following algebraic conditions on the coefficients [2, 15]

$$G = V^{\mathsf{T}}GV, \qquad DU = B^{\mathsf{T}}GV, \qquad DA + A^{\mathsf{T}}D = B^{\mathsf{T}}GB. \tag{6}$$

Hence, a G-symplectic multivalue method does not preserve quadratic first integrals, but a related quadratic form (5). The relation can be clarified by power series arguments: indeed, the first terms of the expansion in powers of h of the quadratic form ${y^{[n]}}^{\mathsf{T}}(G\otimes E)y^{[n]}$ is $y^{\mathsf{T}}Ey$ (compare [12]). Thus, the more h is small, the more the two forms are close each other. For larger stepsizes, it is important to control the parasitic components as long as possible in order to achieve an accurate near conservation of the quadratic first integrals of the problem.

- *Symmetry.* The numerical counterpart of reversibility of mechanical systems is the property of symmetry of a numerical method, which assures the coincidence between a numerical method and its adjoint. In the case of GLMs, the notion of symmetry can be given as follows [15].

Definition 2.1. Let $L \in \mathbb{R}^{r\times r}$ be an involution matrix and $P \in \mathbb{R}^{s\times s}$ a permutation matrix. A GLM (2) is symmetric if

$$P^{-1}AP = UV^{-1}B - A,\ UL = PUV^{-1},\ BP = LB,\ VL = LV^{-1}. \tag{7}$$

Symmetric methods provide a reversible numerical flow, which is a desired property when we integrate reversible mechanical systems, but also provide an important constructive advantage in the derivation of methods. This is due to the fact that symmetric methods have even order of convergence [15], hence we only need to impose order conditions related to trees of odd order.

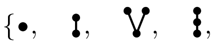
- *Control of parasitism.* Due to their multivalue nature, GLMs introduce parasitic components in the numerical solution, which have to be controlled in order to achieve a long-term near conservation of the invariants. Rigorous bounds on parasitic solution components have recently been obtained in [11], where the authors have proved that, for carefully constructed methods, the error in the parasitic components typically grows like $h^{p+4}exp(h^2Lt)$, where p is the order of the method, and L depends on the problem and on the coefficients of the method.

A basic property of boundedness for the parasitic components of multivalue methods is achieved by annihilating the so-called growth parameters [11, 15]

$$\mu_j = \xi_j^{-1} v_j^* B U v_j, \tag{8}$$

where ξ_j are the eigenvalues of the matrix V such that $\xi_j \neq 1$, v_j and v_j^* are the right and left eigenvectors, respectively ($Vv_j = \xi_j v_j$ and $v_j^* V = \xi_j v_j^*$) satisfying $v_j^* v_j = 1$. Examples of methods with zero-growth parameters, in the context of multivalue methods, have been provided in [3, 8, 9].

2.1. **A method with minimal error constant.** We now aim to derive an example of G-symplectic and symmetric GLM (2) of order 4, with zero growth parameters (8). Some coefficients of the method will be chosen in order to minimize the error constant, which can be easily provided by means of B-series arguments [2, 16]. We recall that, in correspondence to the set of rooted trees

$T = \{$  $, \ldots\}$,

a B-series $B(a, y)$ for (3) is defined as a formal series

$$B(a, y(x_1)) = a(\emptyset) y(x_0) + \sum_{\rho(t)\geq 1} \frac{h^{\rho(t)}}{\sigma(t)} a(t) F(t)(y(x_0)), \tag{9}$$

where the functions ρ, σ, F and a are defined as in [16]:

- $\rho(t)$ is the order of $t \in T$, i.e. the number of vertices of t;
- $\sigma(t)$ is the symmetry of $t \in T$, i.e. the cardinality of the symmetry group of t;
- $F(t)$ is the elementary differential of f corresponding to $t \in T$;
- $a(t)$ is the coefficient of the series corresponding to the tree $t \in T$.

The approximation of the solution given by a GLM is a B-series [2] which can be expressed, after one step, in the form

$$\begin{cases} \eta(t) &= A\eta D(t) + U\xi(t), \\ \hat{\xi}(t) &= B\eta D(t) + V\xi(t), \end{cases} \tag{10}$$

and the method (2) has order p if $\hat{\xi}(t) = E\xi(t)$ for any $t \in T$, with $\rho(t) \leq p$ (compare [2], also for the definition of $E\xi(t)$ which is here omitted for brevity). For a method of order p, it is easy to extract the leading term of the error

$$\sum_{\rho(t)=p+1} \frac{h^{\rho(t)}}{\sigma(t)} \hat{\xi}(t) F(t)(y(x_0)) = h^{p+1} \sum_{\rho(t)=p+1} \frac{1}{\sigma(t)} (B\eta D(t) + V\xi(t)) F(t)(y(x_0)), \tag{11}$$

which we will next aim to minimize.

First of all, we aim to derive a GLM (2) depending on three internal stages (i.e. $s = 3$) and two input values (i.e. $r = 2$). By imposing zero-stability [2, 17], consistency [2, 17], G-symplecticity (6), symmetry (7) and zero growth parameters

(8), we obtain the GLM

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{ccc|cc} \frac{1}{2}\alpha & 0 & 0 & 1 & u_{32} \\ \alpha & \frac{1}{2}\beta & 0 & 1 & u_{32} \\ \alpha & \beta & \frac{1}{2}\alpha & 1 & u_{32} \\ \hline b_{13} & b_{12} & b_{13} & 1 & 2u_{32} \\ b_{23} & -2b_{23} & b_{23} & 0 & -1 \end{array}\right] \tag{12}$$

where $\alpha = b_{13} + b_{23}u_{32}$ and $\beta = b_{12} - 2b_{23}u_{32}$. In order to achieve order 4, due to symmetry (compare [15]), we only need to impose conditions of order 3, obtaining

$$\left[\begin{array}{c|c} A & U \\ \hline B & V \end{array}\right] = \left[\begin{array}{ccc|cc} \frac{1}{6}\gamma & 0 & 0 & 1 & u_{32} \\ \frac{1}{3}\gamma & -\frac{1}{6}\delta & 0 & 1 & u_{32} \\ \frac{1}{3}\gamma & \frac{1}{6}\delta & \frac{1}{6}\gamma & 1 & u_{32} \\ \hline \frac{1}{6}\varphi & -\frac{1}{4} - \frac{2\sqrt[3]{2}}{3} - \frac{\sqrt[3]{4}}{3} & \frac{1}{6}\varphi & 1 & \frac{1}{12} \\ b_{23} & -2b_{23} & b_{23} & 0 & -1 \end{array}\right], \tag{13}$$

where $\gamma = 2 + \frac{\sqrt[3]{4}}{2} + \sqrt[3]{2}$, $\delta = \left(1 + \sqrt[3]{2}\right)^2$, $\varphi = \frac{15}{4} + 2\sqrt[3]{2} + \sqrt[3]{4}$. Finally, we consider the quantities $\hat{\xi}(t)$ appearing in (11) for $t \in T, \rho(t) = 5$ and we minimize the sum of their absolute values by employing the `Mathematica` intrinsic routine `Minimize`. We perform a constrained minimization process depending on the following constraints

$$0 < u_{32} < \frac{1}{4} \qquad 0 < b_{23} \leq 1,$$

and achieve $u_{32} = \frac{1}{8}$ and $b_{23} = \frac{1}{2}$. These values lead to the following coefficient matrices

$$A = \begin{bmatrix} \frac{1}{6}\left(2 + \frac{1}{\sqrt[3]{2}} + \sqrt[3]{2}\right) & 0 & 0 \\ \frac{1}{3}\left(2 + \frac{1}{\sqrt[3]{2}} + \sqrt[3]{2}\right) & -\frac{1}{6}\left(1 + \sqrt[3]{2}\right)^2 & 0 \\ \frac{1}{3}\left(2 + \frac{1}{\sqrt[3]{2}} + \sqrt[3]{2}\right) & -\frac{1}{3}\left(1 + \sqrt[3]{2}\right)^2 & \frac{1}{6}\left(2 + \frac{1}{\sqrt[3]{2}} + \sqrt[3]{2}\right) \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{1}{6}\left(\frac{29}{8} + 2\sqrt[3]{2} + 2^{2/3}\right) & \frac{1}{24}\left(-5 - 16\sqrt[3]{2} - 8\ 2^{2/3}\right) & \frac{1}{6}\left(\frac{29}{8} + 2\sqrt[3]{2} + 2^{2/3}\right) \\ \frac{1}{2} & -1 & \frac{1}{2} \end{bmatrix},$$

$$U = \begin{bmatrix} 1 & \frac{1}{8} \\ 1 & \frac{1}{8} \\ 1 & \frac{1}{8} \end{bmatrix}, \qquad V = \begin{bmatrix} 1 & \frac{1}{4} \\ 0 & -1 \end{bmatrix}.$$

We also observe that, for such method, $\hat{\xi}(t)$ is zero for all trees of order 5 except $[[[[\tau]]]]$ (compare [2]), whose value is approximately equal to 0.17.

3. **Numerical experiments.** We now present the numerical evidence originated by comparing the GLM derived in Section 2.1 with the partitioned RK method of order 4 and depending on 12 internal stages derived in [22], which gives rise to an overall explicit scheme in case of separable Hamiltonians. The tests have been performed on a node with CPU Intel Xeon 6 core X5690 3,46GHz, of the E4 multi-GPU cluster of Department of Mathematics (University of Salerno).

First of all, let us consider the following second order system describing the evolution of N particles under the effects of the reciprocal gravitational attraction

$$m_i \ddot{q}_i = \sum_{i=1, i\neq j}^{N} \frac{G m_i m_j (q_j - q_i)}{\|(q_j - q_i)\|^3},$$

where m_i and q_i are respectively the mass and the position vector of the i-th body and G is the gravitational constant. Such system, provided a set of starting values, is known as the N-body problem and it has applications in many fields [15, 20]. The N-body problem can be rewritten as a first-order system and it results to be Hamiltonian with Hamiltonian function

$$\mathcal{H}(p, q) = \frac{1}{2} \sum_{i=1}^{n} \frac{1}{m_i} p_i^{\intercal} p_i - G \sum_{i=1}^{n} \sum_{j=1}^{i-1} \frac{m_i m_j}{\|q_i - q_j\|}. \tag{14}$$

We consider the N-body problem applied to the motion of two subsets of planets of the solar system. Our computations are based on the employ of real initial data, taken from NASA Horizons System

`http://ssd.jpl.nasa.gov/?horizons`

The results, reported in Figs. 1, 2, 3 and 4 show the orbits generated by both the GLM and the partioned RK methods: we can observe that also our GLM preserves the symplecticity of the phase space.

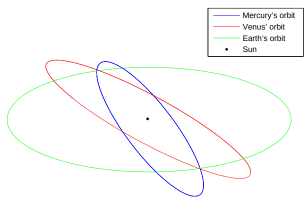


FIGURE 1. Mercury, Venus and Earth orbits generated by the GLM constructed in Section 2.1, with $h = 100$

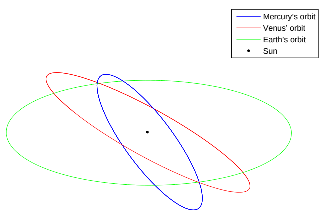


FIGURE 2. Mercury, Venus and Earth orbits generated by the symplectic partitioned RK method [22], with $h = 100$

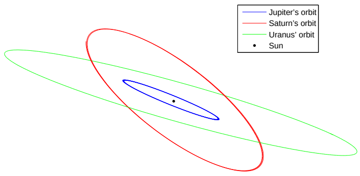


FIGURE 3. Jupiter, Saturn and Uranus orbits generated by GLM constructed in Section 2.1, with $h = 100$

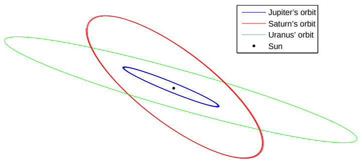


FIGURE 4. Jupiter, Saturn and Uranus orbits generated by the symplectic partitioned RK method [22], with $h = 100$

We next consider the following classical Hamiltonian problems of interest in Celestial Mechanics:

- the Kepler problem [15]

$$\begin{cases} \dot{p_1}(t) = -\dfrac{q_1(t)}{(q_1^2(t)+q_2^2(t))^{\frac{3}{2}}}, \quad \dot{p_2}(t) = -\dfrac{q_2(t)}{(q_1^2(t)+q_2^2(t))^{\frac{3}{2}}}, \\ \dot{q_i}(t) = p_i(t), \quad i = 1,2, \\ p_1(0) = 0, \quad p_2(0) = \sqrt{\frac{1+e}{1-e}}, \quad q_1(0) = 1-e, \quad q_2(0) = 0, \end{cases} \tag{15}$$

  where the value of the eccentricity $e \in [0,1[$ is fixed to $\frac{1}{2}$. The Hamiltonian of this problem is

$$\mathcal{H}(p(t), q(t)) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}};$$

- the Hènon-Heiles Problem [15]

$$\begin{cases} \dot{p_1}(t) = -q_1(t)(1 + 2q_2(t)), \quad t \in [0, 50] \\ \dot{p_2}(t) = -(q_2(t) + q_1^2(t) - q_2^2(t)), \\ \dot{q_i}(t) = p_i(t), \quad i = 1,2, \\ p_1(0) = \sqrt{0.3185}, \quad p_2(0) = q_1(0) = q_2(0) = 0, \end{cases} \tag{16}$$

  with Hamiltonian

$$H(p(t), q(t)) = \frac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3}q_2^3.$$

The observed Hamiltonian deviations are reported in Figs. 5, 6, 8 and 9, while the observed deviations in the angular momentum for the Kepler problem are presented in Figs. 7 and 10. We observe that our GLM, with a lower computational cost, is able to reproduce analogous conservation properties of a symplectic integrator, as it can be advised from Table 1.

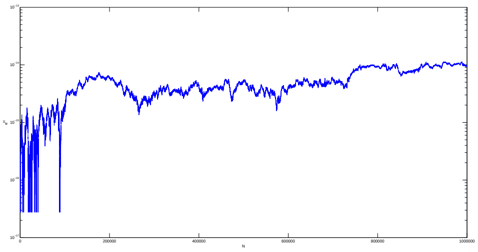


FIGURE 5. Hamiltonian deviation for the partitioned RK method of order 4 in [22] to (16) over one million step points

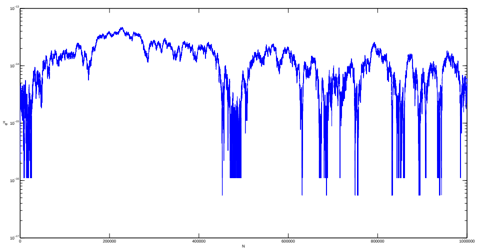


FIGURE 6. Hamiltonian deviation for the partitioned RK method of order 4 in [22] to (15) over one million step points

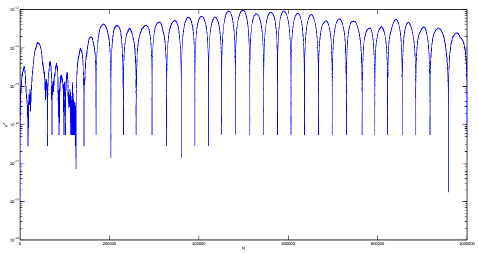


FIGURE 7. Angular momentum deviation for the partitioned RK method of order 4 in [22] to (15) over one million step points

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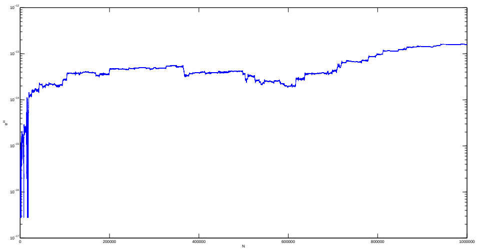

FIGURE 8. Hamiltonian deviation for the GLM derived in Section 2.1 to (16) over one million step points

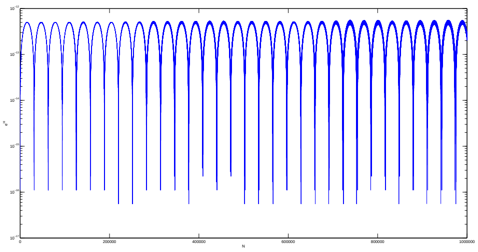

FIGURE 9. Hamiltonian deviation for the GLM derived in Section 2.1 to (15) over one million step points

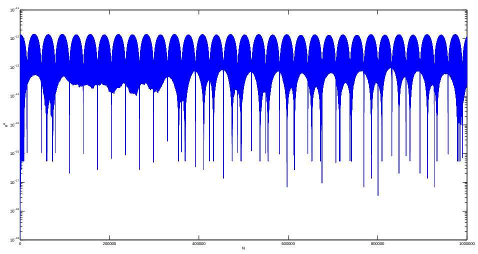

FIGURE 10. Angular momentum deviation for the GLM derived in Section 2.1 to (16) over one million step points

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Table 1. Comparison of the Hamiltonian (dev) and angular momentum deviations ($adev$) for the GLM derived in Section 2.1 and the partitioned RK method (PRK, [22]) applied to (15), (16)

	PRK	GLM
Kepler problem	$dev = 4.70e-14$ $fe = 12000000$	$dev = 5.61e-13$ $fe = 11162232$
Kepler problem	$adev = 9.56e-14$ $fe = 12000000$	$adev = 1.44e-12$ $fe = 11162232$
Hènon-Heiles problem	$dev = 1.13e-14$ $fe = 12000000$	$dev = 1.65e-13$ $fe = 9637008$

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