

Generating Symmetric Composition Methods through Memetic Algorithms

Y.G. Petalas¹, Ch. Tsitouras², G.S. Androulakis³ and M.N. Vrahatis^{1,4}

¹Computational Intelligence Laboratory (CI Lab), Department of Mathematics,
University of Patras Artificial Intelligence Research Center (UPAIRC),
University of Patras, GR-26110 Patras, Greece

² Department of Applied Sciences, TEI of Chalkis, GR-34400 Psahna, Greece

³ Department of Business Administration, University of Patras, GR-26110 Patras, Greece

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Abstract: A new method for generating symmetric composition methods is presented which is based on the minimization of the truncation error terms. To properly tackle this minimization task, Memetic Algorithms are used which are population based search algorithms for global optimization. The possible solutions attained by the population of Memetic Algorithms are coefficients of the symmetric composition methods which are evolved in order to minimize and through this to vanish their truncation errors to a certain order. We produce a sixth order method of this type with eleven stages. Numerical test justifies the effort.

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1 Introduction

Composition methods [3, 4, 9, 10] are used to solve Hamiltonian problems:

$$\frac{dp}{dt} = -\frac{dH(p, q)}{dq}, \quad \frac{dq}{dt} = \frac{dH(p, q)}{dp},$$

where the Hamiltonian $H(p_1, p_2, \dots, p_d, q_1, q_2, \dots, q_d)$ represents the total energy; q 's are the position coordinates and p 's the momenta for $i = 1, 2, \dots, d$, with d the number of degrees of freedom [3, p.4]. So let Φ_h be a basic method and $\gamma_1, \gamma_2, \dots, \gamma_s$ real numbers. Then the method

$$\Psi_h = \Phi_{\gamma_s h} \circ \Phi_{\gamma_{s-1} h} \circ \dots \circ \Phi_{\gamma_1 h}, \quad (1)$$

is said to be its corresponding *composition method* [3, p.39]. The method (1) is actually formed by applying consequently the basic method Φ_h , with step sizes $\gamma_1 h, \gamma_2 h, \dots, \gamma_s h$. The main purpose

⁴Corresponding author: e-mail: vrahatis@math.upatras.gr, Phone: +30 2610 997374, Fax: +30 2610 992965

of this contribution is to evaluate γ 's in order to achieve higher order method based in a low order one. Evolutionary and Memetic algorithms are among the choices for accomplishing this task.

Recently, in [7], Evolutionary Algorithms (EAs) [2] have been proposed to generate Runge-Kutta methods with as small as possible local truncation error. We have applied EAs because they are very effective when the objective function has many local optima (as in our case) and can be applied in situations where the objective function is not differentiable or/and discontinuous. Alternatively, in this contribution, we propose Memetic Algorithms (MAs) for the generation of composition methods using a similar approach as in [7]. MAs are metaheuristic search algorithms for global optimization. They are hybrid methods using EAs and local search methods. They have the ability to reach for the optimum solutions very effectively and efficiently.

The rest of the paper is organized as follows. In Section 2 the algebraic system for the coefficients of symmetric composition of symmetric methods is presented. In Section 3 MAs are described. The proposed method is exhibited in Section 4 while in Section 5 some preliminary results from the application of the proposed method are shown.

2 Symmetric Composition of Symmetric Methods (SCSM)

In the case of a separable Hamiltonian system $H = H(p, q) = T(p) + V(q)$, $T(p) = \frac{1}{2}p^\top p$. Then the general form of an s -stages symplectic integrator is given by [5, 9],

$$q_{i+1} = q_0 + c_i h \frac{\partial T}{\partial p}(p_0), \quad p_{i+1} = p_0 - d_i h \frac{\partial V}{\partial p}(q_0), \quad i = 1, 2, \dots, s-1,$$

with q_0 and p_0 the initial values at $t = t_0$, and q_s and p_s the numerical solution at $t_0 + h$. The transformation from q_0, p_0 to q_s, p_s is symplectic.

Yoshida in [10], suggested that $s = 2r + 1$ and then set $d_{2r+2} = 0$, $d_1 = d_{2r+1} = \gamma_r$, $d_2 = d_{2r} = \gamma_{r-1}, \dots, d_r = d_{r+2} = w_1$, $d_{r+1} = \gamma_0 = 1 - 2 \sum_{i=1}^r \gamma_i$ and $c_1 = c_{2r+2} = \frac{1}{2} \gamma_r$, $c_2 = c_{2r+1} = \frac{1}{2} (\gamma_r + \gamma_{r-1}), \dots, c_{r+1} = c_{r+2} = \frac{1}{2} (\gamma_1 + \gamma_0)$. Actually this is a symmetric composition method, consisting of r repetitions of Leap Frog method using the proper step $\gamma_i h$. Under these assumptions the equations of even order vanish and the equations of condition to be solved for achieving sixth order are three. One equation of fourth order, namely $\sum_{k=0}^{s-1} \gamma_k^3 = 0$. Another two equations for sixth order, namely $\sum_{k=0}^{s-1} \gamma_k^3 = 0$ and $\sum_{k=0}^{s-1} \gamma_k^3 (\gamma_k/2 + \sum_{l=0}^{k-1} \gamma_l)^2 = 0$ [3, p.143]. The equation $\sum_{k=0}^{s-1} \gamma_k = 1$ needed for getting second order of accuracy is already satisfied from the initial choice of γ 's. As a consequence p is an even number only.

3 Memetic Algorithms

Memetic Algorithms (MAs) are metaheuristic-search algorithms used for global optimization tasks. Their name comes from the word "meme" that was first introduced by Dawkins in [1] and represents a unit of cultural evolution that can exhibit refinement. MAs were also inspired from models of adaptation in natural systems that combine evolutionary adaptation of individuals with individual learning within a lifetime. MAs include a stage of individual optimization or learning, usually in the form of a local search, as part of their search operation [6]. MAs are hybrid algorithms that combine evolutionary and local search algorithms.

As stated in Törn and Žilinskas [8], every proposed algorithm for global optimization faces the challenge to find the best (a good) trade off between *exploration* and *exploitation*. Good exploration will provide the algorithm the ability to visit the whole search space and good exploitation to investigate with accuracy a specific part of this space. Thus, MAs try to efficiently balance this trade off. They use evolutionary algorithms to achieve exploration of the search space and local search methods to exploit smaller regions.

In MAs context, Local Search is embedded in the basic steps of an EA. An abstract description of a MA is shown below.

```

Begin
  Population Initialization
  Repeat
    Select a set  $S_{rec} \subseteq population$ 
    Recombination on  $S_{rec}$ 
    Select a set  $S_{mut} \subseteq population$ 
    Mutation on  $S_{mut}$ 
    Select a set  $S_{loc} \subseteq population$ 
    LocalSearch on  $S_{loc}$ 
    Evaluation
    Selection
  Until stopping criterion is satisfied
  Return best solution
End
    
```

First the population is initialized. Afterwards, some or all the individuals of the population are selected and the operations of recombination and mutation are taken place. Then Local Search is applied to individuals according to some criterion. All the individuals are evaluated and some of them are selected and survive to the next generation. These steps are repeated until a stopping criterion is met.

4 The Proposed Approach

The population of MAs are coefficients of SCSM. The individuals of the population will evolve according to the MAs steps.

- Step 1. Split the SCSM vector coefficients into two parts, free coefficients and calculated directly coefficients. The individuals of the population will consist of the free variables.
- Step 2. Initialize the MA.
- Step 3. Apply the MA operators (recombination, mutation)
- Step 4. Choose some individuals to apply local search.
- Step 5. Evaluate the population and select the population for the next generation. Evaluation of each individual happens using the principal truncation error terms. If the termination criterion is not satisfied go to Step 3.

We applied the above described method to the set of equations listed in Section 2. We chose $r = 5$, so the method we have obtained shares $s = 11$ stages. Simultaneously we minimized $max(|\gamma_i|)$, $i = 1, 2, \dots, 5$. Observe that $\gamma_i = \gamma_{11-i}$ for $i = 1, \dots, 5$ and $\gamma_0 = 1 - 2 \sum_{k=1}^5 \gamma_k$. The coefficients we found are given below:

$$\gamma_1 = 0.21131358389813, \gamma_2 = 0.18690875502428, \gamma_3 = 0.1771240508769,$$

$$\gamma_4 = -0.44339384791537, \gamma_5 = 0.11594616405181.$$

5 Experimental Results and Conclusions

We choose the Kepler problem in order to perform our tests. Its potential is $V(q) = -1/\|q\|$. As initial conditions we have $p^1 = 0$, $p^2 = \sqrt{(1+e)/(1-e)}$, $q^1 = 1-e$, $q^2 = 0$. The eccentricity is chosen to be $e = 1/2$. The solution is then 2π periodic and the problem was run in the interval $[0, 6\pi]$. The end-point errors were measured in the absolute maximum norm of \mathbb{R}^4 . The new method was compared with the best of the seven stages methods of Yoshida [3, p.142]. Both methods used the same number of function evaluations. So the results given in Table– 1 correspond to the same computational cost for both methods. It is worthy noticing here that our method which is

Table 1: Accurate digits over the Kepler problem.

stages→	1540	2310	3080	3850	4620	5390	6160
Yoshida	3.7	4.7	5.5	6.1	6.5	6.9	7.3
NEW	4.6	5.7	6.5	7.1	7.5	8.0	8.3

$\frac{11}{7} - 1 = 57\%$ more expensive than Yoshida’s method, is clearly more efficient.

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