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EMBEDDED BLOCK PARALLEL METHODS FOR INITIAL CAUCHY PROBLEM NUMERICAL SOLUTION

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Abstract

This article is devoted to the design and analysis of the efficiency of parallel algorithms for embedded forms based on implicit block methods. The developed algorithms are implemented on parallel systems with distributed memory and the topology of the hypercube. The estimations of the runtime and exchanges, total overhead of parallelism, speedup and efficiency of parallel solutions are defined.

Keywords: implicit block method, parallel algorithms, numerical solution

Introduction

Simulation of real economic, technological and other processes described by systems of ordinary differential equations (SODE) of high dimensionality is a wide class of tasks, which require the use of high performance computers. It is confirmed by the famous list of problems "*Grand Challenges*" where these tasks occupy one of the leading places [1].

The study of numerical methods for solving Cauchy problems for first order SODE with known initial conditions based on finite-difference schemes showed that the properties of respective parallel algorithms are largely determined by the type of underlying numerical scheme. The least complicated methods are explicit ones; however, these schemes have certain drawbacks (in particular conditional stability), which restrict their application. In this connection, implicit schemes are of great importance. Despite their high computational complexity such schemes have no alternative among one-step methods in solving stiff dynamic problems [2].

Let us consider a Cauchy problem numerical solution associated with first order SODE with known initial conditions:

$$\begin{cases} \dfrac{d\bar{y}(x)}{dx} = \bar{f}(x, \bar{y}(x)), \\ \bar{y}(x_0) = \bar{y}_0, \end{cases} \tag{1}$$

where F (the right side of the system) is in general a nonlinear function describing the mapping $F = \bar{f} : R \times R^m \to R^m$.

Block multipoint methods for solving the initial value problem

Block multipoint methods for solving Cauchy problem are of particular importance, because they agree well with parallel computer systems architecture and do not require calculations in intermediate points, so the counting becomes more efficient. Such methods are very stable; they are initially parallel as they can be used to find solutions for several points of an integration grid simultaneously.

Let the set of points of a uniform grid $\Omega_h : \{ x_j \}, j = \overline{1, M}$ be divided into *N* blocks. Each block contains *k* points, and $N \le M$. The total number of points for all units is: $M = k \times N$. Within the block all the points are equidistant from each other:

$$x_{n,i} = x_{n,o} + ih, i = \overline{1, k}, \tag{2}$$

where i is the number of points in a block $i = \overline{1,k}$; n is the number of a block $n = \overline{1,N}$; $x_{n,i}$ is a point with number i belonging to the block n; $x_{n,0}$ is the starting point of the n^{th} block; $x_{n,k}$ is the end point of the n^{th} block.

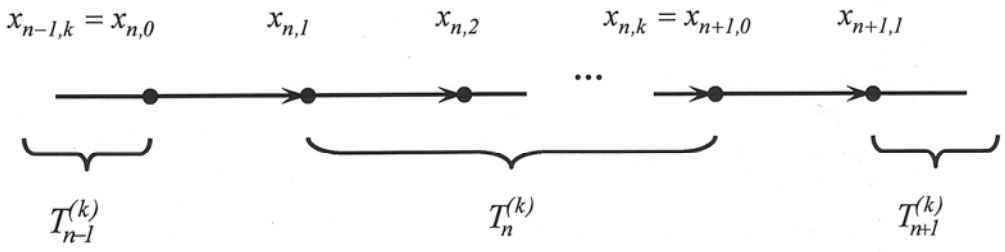

Figure 1. Scheme of partitioning into blocks for one-step k-point method

A set of points of the n^{th} block of k points is designated as $T_n^{(k)}$. In this case $x_{n,k} = x_{n+1,0}$. Let $y_{n,0}$ be an approximate value of the Cauchy problem solution at the starting point of the processed block $x_{n,0}$.

The equations of one-step block difference methods applied to the ODE for the block of k points can be written as:

$$y_{n,i} = y_{n,0} + ih\left[b_i F_{n,0} + \sum_{j=1}^{k} a_{i,j} F_{n,j} \right]; i = \overline{1,k}; n = \overline{1,N}. \tag{3}$$

Taylor series expansion for functions of defect shows that one-step k-point block method has the highest order of approximation, which equals $k+1$; therefore, the local error in the nodes of the block is of the order $O(h^{k+2})$ [3-5]. Block parallel methods are implicit, so in order to calculate the approximate values of the Cauchy problem solution we need to solve a system of nonlinear equations. One way of obtaining the solution is the method of simple functional iteration:

$$\begin{cases} y_{n,i,0} = y_{n,0} + ihF_{n,0},\ i = \overline{1,k},\ n = 1,2,...,N, \\ y_{n,i,l+1} = y_{n,0} + ih(b_i F_{n,0} + \sum_{j=1}^{k} a_{i,j} F_{n,j,l}),\quad l = \overline{0,L-1}, \end{cases} \tag{4}$$

where $F_{n,i} = f\left(x_{n,i}, y_{n,i}\right)$, n is the block number, $n = 1,2,...N$; i is the point number, $i = \overline{1,k}$; l is the number of current iteration, $l = \overline{0,L-1}$; L is the maximum number of non-zero iterations.

Potentially, the calculations for block multipoint methods contain two sources of internal parallelism:

- parallelism across the system (limited by SODEdimension, m);
- parallelism across the block (limited by the number of points in the block, k).

In contrast to explicit methods of solving SODE, the implementation of alternative approaches to *a posteriori* local error estimation based on block methods is associated with the following:

1) There are no relevant coherent analogs, therefore it is necessary to develop and justify a method of estimating the local error.

2) Varying the integration step is only possible after all the values in k nodes of the current n^{th} block had been calculated.

3) In case if truncation error estimation is not satisfactory and it is necessary to change the step of integration, almost all the calculations for the points of the block will be in vain.

Parallel realizations of embedded one-step block multipoint methods for solving the IVP

The idea of embedded forms proposed for the estimation of truncation error of ordinary differential equations numerical solution by means of Runge-Kutta methods can be used in one-step block multipoint methods based on two different approaches:

1) a combination of independent formulas of different orders of accuracy;

2) a combination of selected formulas of different orders of accuracy.

The first approach is the use of two different independent block methods of adjacent orders of accuracy $r(\hat{r}), \hat{r} = r \pm 1$ on the same integration grid: Ω_h. In this case the first approach determines the solution approximation based on k-point one-step method, and the second approach involves $\hat{k}$-point one-step method. The second approximate solution in the respective nodes of the blocks $T_{n,i}^{(k)}$ and $T_{n,j}^{(\hat{k})}$ of the grid Ω_h is used to estimate the *a posteriori* local error:

$$\begin{cases} y_{n,i} = y_{n,0} + ih\left[b_i f(x_{n,0}; y_{n,0}) + \sum_{j=1}^{k} a_{i,j} f(x_{n,j}; y_{n,j}) \right]; i = \overline{1,k}; n = \overline{1,N}, \\ \hat{y}_{n,i} = \hat{y}_{n,0} + ih\left[\hat{b}_i f(x_{n,0}; \hat{y}_{n,0}) + \sum_{j=1}^{\hat{k}} \hat{a}_{i,j} f(x_{n,j}; \hat{y}_{n,j}) \right]; i = \overline{1,\hat{k}}; n = \overline{1,\hat{N}}. \end{cases}$$

Suppose the block method of lower order of accuracy is the basic one; that is: $\hat{k} = k + 1$. The local error of the approximate solution (for one-step *k*-point method) in the i^{th} node of the block for a single equation is defined according to the following formula: $y(x_{n,i}) - y_{n,i}^{r} = O(h^{k+2}); i = \overline{1,k}$. For *(k +1)*-point method in the same node it is equal to: $y(x_{n,i}) - y_{n,i}^{\hat{r}} = O(h^{k+3}); i = \overline{1,\hat{k}}.$

From these relations it follows that the estimation of the local error of a formula of lower order of accuracy (*k*-point method) can be approximately calculated as follows: $y_{n,i}^{r} - y_{n,i}^{\hat{r}}; i = \overline{1,k}.$ This approach to evaluating the local error is more effective than Runge rule, as it is rather simple and reduces computational efforts. For example, in order to apply the rule of step duplication we need to solve three systems of nonlinear algebraic equations of k dimension, and for the application of the embedded method we should solve two systems: one of the same dimension and the other of $(k+1)$ dimension.

The second approach to the development of block embedded methods involves the idea of a sequentially increasing order of accuracy [2-3]. It is aimed at reducing computational efforts through a combination of selected formulas of different orders. Let the solution of Cauchy prob-

lem for ODE at a certain interval of integration be performed using k-point one-step block method. The following quantity can be taken as an estimate of the local error in each node of the current n^{th} block:

$$d_{n,i} = \hat{y}_{n,i} - y_{n,i} = y_{n,i,l'} - y_{n,i,l''}, i = \overline{1,k}, l' = l'' \pm 1,$$

where $y_{n,i,l'}$ and $y_{n,i,l''}$ are the l'^{th} and l''^{th} approximations obtained by solving (3) using iterative method (4).

Let us assume the following designations:

1) $y_{n,i}^{[v]}, i = \overline{1,k}$ is the value of the numerical solution in the i^{th} node $x_{n,i}$ of the n^{th} block calculated with local error $O(h^v)$;

2) $F_{n,i}^{[v]} = f\left(x_{n,i}, y_{n,i}^{[v]}\right)$ is the reference to the right side of the original differential equation calculated at the point $\left(x_{n,i}, y_{n,i}^{[v]}\right)$.

Let the approximate value of $y_{n,0}$ solution at the initial point of the n^{th} block be calculated with some local error – $O(h^v)$ providing sufficient accuracy for the giving task. The reference to the right side of the original differential equation can be calculated with the same error $F_{n,0}^{[v]}$. If we perform calculations for zero iteration using the first formula of the iterative method, we obtain $ó_{n,i,0}^{[2]} = ó_{n,0}^{[v]} + ihF_{n,i,0}^{[v]}, i = \overline{1,k},$ as the local error of Euler formula is of the order $O(h^2)$. Each subsequent calculation according to the second formula (4) gives a higher order of accuracy for the method of simple iterations:

$$l = 0: \; y_{n,i,1}^{[3]} = y_{n,0}^{[v]} + ih \cdot \left(b_i F_{n,0}^{[v]} + \sum_{j=1}^{k} a_{i,j} F_{n,j,0}^{[2]} \right), i = \overline{1,k},$$

$$l = 1: \; y_{n,i,2}^{[4]} = y_{n,0}^{[v]} + ih \cdot \left(b_i F_{n,0}^{[v]} + \sum_{j=1}^{k} a_{i,j} F_{n,j,1}^{[3]} \right), i = \overline{1,k},$$

$$F_{n,j,0}^{[v]} = f(x_{n,j}, y_{n,j,0}^{[v]}), j = \overline{1,k}.$$

This process can not be continued indefinitely, if $l = k - 1$ we will obtain the results which correspond to the ultimate local accuracies of approximate formulas (4). Since the difference schemes corresponding to block one-step k-point methods approximate differential equation (1) of the order $O(h^{k+1})$, further iteration gives no result:

$$l = k - 1: y_{n,i,k}^{[k+2]} = y_{n,0}^{[v]} + ih \cdot \left(b_i F_{n,0}^{[v]} + \sum_{j=1}^{k} a_{i,j} F_{n,j,k-1}^{[k+1]} \right), i = \overline{1,k}.$$

So, in order to estimate the local error we can chose two arbitrary successive approximations of the solution (accuracy must be taken into account). In the above described embedded block k-point method all the extra computational efforts (aimed at local error estimation) are confined to additional iteration (within limiting values) in the process of solving the systems of nonlinear algebraic equations of k dimension. The formulas for the n^{th} block of embedded multipoint method №2 are:

$$\begin{cases} y_{n,i,0} = y_{n,0} + ihF_{n,0},\ i = \overline{1,k}, \\ y_{n,i,l+1} = y_{n,0} + ih(b_i F_{n,0} + \sum_{j=1}^{k} a_{i,j} F_{n,j,l}),\quad l = \overline{0,l'-1}, \\ \hat{y}_{n,i,l'} = y_{n,0} + ih(b_i F_{n,0} + \sum_{j=1}^{k} a_{i,j} F_{n,j,l'}),\quad l' = l, l'' = l+1. \end{cases}$$

Let us compare two different embedded block methods (Figure 2). When a system of nonlinear algebraic equations is being solved convergence rate of the iterative process depends on the properties of a particular system, and, consequently, on the coefficients of the block method itself. That is why our comparison will be for the maximum possible number of iterations. Theoretical analysis and the experiment lead to the following conclusion:

1) In both sequential and parallel implementations the first embedded block algorithm requires more time than the second one: $T_1^1 > T_1^2$ and $T_p^1 > T_p^2$. And for parallel algorithms this difference is greater.

2) Speedup and efficiency coefficients of the first embedded block method are smaller than respective coefficients of the second method for different values of problem, method and parallel system parameters: $S^1 < S^2$, $E^1 < E^2$.

It should be mentioned that the complexity of the right side of the ODE is an important factor influencing the quality of parallelism. As a result, with the same values of communication constants and parameters that define a unique block method, speedup and efficiency are reduced almost by 2 times during the transition from the dominant to trivial right sides. The influence of communication constants is traditional for the given methods and exchange operations.

The increase in the number of points in a block leads to the increase of speedup rate $\uparrow k \Rightarrow \uparrow S$ and the decrease of efficiency ratio $\uparrow k \Rightarrow \downarrow E$. This dependence is explained by the fact that the number of points in a block is associated with the number of the processors used.

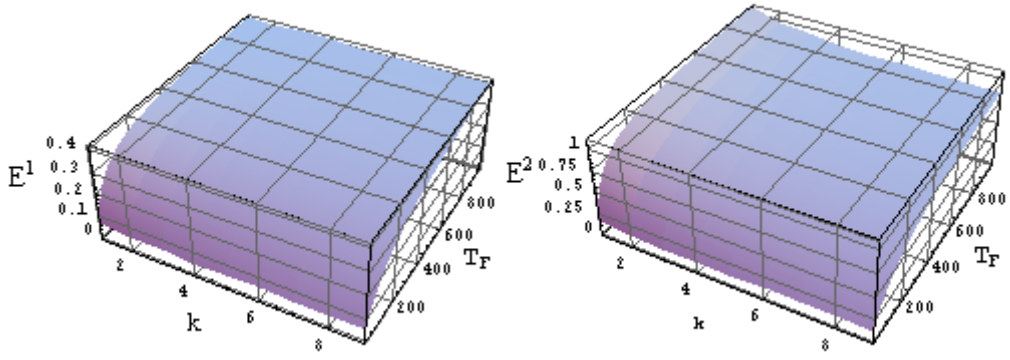

Figure 2. Efficiency of two embedded block one-step methods depending on the number of points in a unit and complexity of the right side of ODE

Summarizing the results obtained we come to the conclusion that the second method has obvious advantages as compared to the first one. The developed computational schemes of parallel block methods for a single differential equation can be generalized to a system of differential equations. And then it will be possible to use system parallelism. In the future we are planning to

carry out a comparative analysis with fully implicit methods (like Runge-Kutta), which have the same field of application, namely stiff problems.

Conclusion

In this paper, which is the continuation of previously published works [6-10], we have analyzed the use of parallel methods for Cauchy problem numerical solution. The paper does not include the results for hybrid, multi-step and multi-stage Runge-Kutta methods and multistep Adams-Bachfort and Adams-Moulton methods.

References:

1. Grand Challenges: High performance computing and communications // A report by the Committee on Physical, Mathematical and Engineering Science, NSF/CISE, 1800 G. Street NW, Washington, DC 20550, 2001.
2. Хайрер Э. Решение обыкновенных дифференциальных уравнений. Нежесткие задачи: пер. с англ / Э.Хайрер, С.Нёрсетт, Г.Ваннер. – М.: Мир, 1990. – 512 с.
3. Крылов В.И. Вычислительные методы / В.И. Крылов, В.В. Бобков, П.И. Монастырский. – М.: Наука, 1976. – Т. I.– 303с.
4. Фельдман Л.П. Параллельные алгоритмы моделирования динамических систем, описываемых обыкновенными дифференциальными уравнениями / Л.П. Фельдман // Электронное моделирование. – 2004. – Т. 26. – №1. – С.19-30.
5. Feldman L.P., Dmitrieva O.A., Gerber S. Abbildung der blockartigen Algorithmen auf Parallelrechnerarchitekture. In: Tavangarian,D., Grützner,R. (Hrsg.): Tagungs-band 15. ASIM-Symposium Simulationstechnik in Rostock, September 2002, SCS-Europe BVBA, Ghent/Belgium 2002, S.359-364.
6. Feldman L.P. Implementierung und Effizienzanalyse von parallelen blockartigen Simulationsalgorithmen für dynamische Systeme mit konzentrierten Parametern. In: Möller, D.P.F. (Hrsg.): Tagungsband 14. ASIM-Symposium Simulationstechnik in Hamburg, September, 2000, SCS-Europe BVBA, Ghent/Belgium 2000, S. 241-246.
7. Фельдман Л.П., Назарова И.А. Параллельные алгоритмы численного решения задачи Коши для систем обыкновенных дифференциальных уравнений / Л.П.Фельдман, И.А. Назарова // Математическое моделирование. – 2006. – Т.18. – № 9. – С. 17-31.
8. Фельдман Л.П., Назарова И.А. Эффективность параллельных алгоритмов оценки локальной апостериорной погрешности для численного решения задачи Коши / Л.П.Фельдман, И.А.Назарова // Электронное моделирование. – 2007. – Т. 29. – № 3. - С.11-25
8. Фельдман Л.П. Многопроцессорная реализация неявных многоточечных методов решения жестких задач / Л.П. Фельдман, И.А. Назарова // материалы VII Международной конференции по неравновесным процессам в соплах и струях (NPNJ'2008).– М.: Вузовская книга, 2008. – С. 255–257.
9. Назарова И.А. Анализ масштабируемости параллельных алгоритмов численного решения задачи Коши / И.А. Назарова // Наукові праці Донецького національного технічного університету. Серія: Інформатика, кібернетика та обчислювальна техніка. – 2009. Вип. 10(153). - С. 21-26.

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