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Algebraic data parallelism implementation in HPF

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1. Introduction

In parallel with the beginning of symbolical computations in 1973, the development of numerical methods began too. Over time computer algebra systems ran into difficulties with large scale engineering problems, special case is differential equations solution. The growing data amounts leaded to parallelization of computational problems. The usage of one computer machine for problem solution had grown into computations on several computers, that is data or computational processes parallelization. Well known system "Mathematica" [8] has powerful tools which can be used for algebraic data parallelization too. This system is the tool of choice at the frontiers of scientific research, in engineering analysis and modelling, in technical education and wherever quantitative methods are used. But this powerful system isn't independent language for parallelization [8]. In the issue no algebraic system was developed for formalized algebraic date parallelization yet. At this time there is only one specialized language for parallel programming and it is High Performance Fortran. That is why the HPF language was used for development of parallel computer algebra system.

The computer algebra system (CAS) PARAVIB is a HPF pre-processor for parallel analytical perturbation with very long polynomials, rational functions, trigonometric series and sparse matrices. PARAVIB consists of pre-processor and procedures library. Using pre-processor it is possible define analytical objects and to design new procedures that can be included into the PARAVIB library.

PARAVIB is the parallel version of CAS VIBRAN (VIBRotechnika and ANalitika) released in 1979 at Kaunas [1]. The system is in usage from the same year.

All variables and their degrees of expression in CAS are stored separately. Such storage allows analytical operations to be changed into operations with matrices.

Using parallel CAS PARAVIB algebraic data parallelism was implementated. The PARAVIB techniques were used in parallel numeric-symbolic analysis of the non-linear oscillation systems. Harmonic balance, small parameter and asymptotic methods are implemented for non-linear oscillation systems with multi-degree-of-freedom analysis. The Parallel Harmonic Balance Scheme presents the performance of PARAVIB (Fig. 1).

2. VIBRAN program processing, commands and procedures

In the CAS VIBRAN an combination of analytical and numerical calculations are implemented, the developed system performs only analytical calculations. All numerical

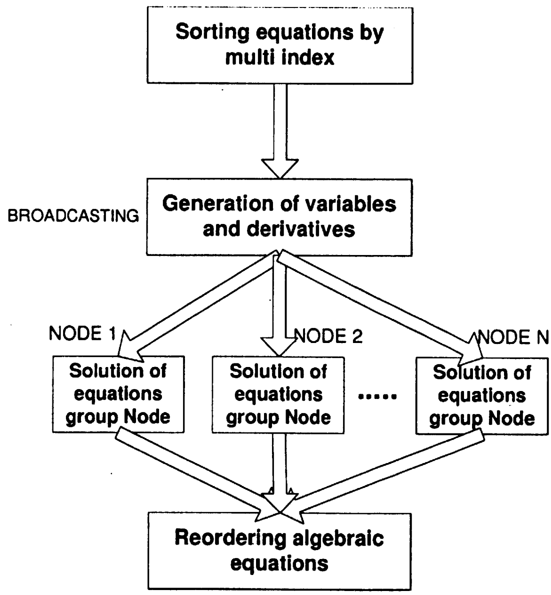

Fig. 1. Parallel harmonic balance scheme.

calculations are performed using programs written high level programming languages, concretely with FORTRAN programs [1].

The VIBRAN program consists of commands for analytical manipulations and FORTRAN operators. The program components are the main program and one or more subprograms.

In the VIBRAN program the FORTRAN commands, subroutines and other objects can coexist together with VIBRAN statements. The pre-processor skips them in compilation step.

Program in VIBRAN is processed in two steps. At the first step the analytical computations are executed and it results are inserted into disk. At the second step the subsystem of FORTRAN programs generation forms the subprogram for numerical computations.

The user can use standard VIBRAN commands or construct commands in FORTRAN and VIBRAN languages. In this case, user commands must have VIBRAN procedure format.

Pre-processor processes VIBRAN system commands to the call of corresponding FORTRAN subroutines. Subprograms in VIBRAN are called procedures. Procedure has the same format as FORTRAN subroutine, except that the VIBRAN procedure must have at least one parameter. Here is an example of program code with procedure utilization:

```
POLINOM A1, B
RACIONAL SUM
COMMON A1, B
ANAL (A1)
ANAL (B)
```

```
PRIN('A1', A1)
PRIN('A2', B)
DELS (SUM)
PRIN('SIGM', SUM)
STOP
END

PROCEDURE DELS(S)
POLINOM A, B
RACIONAL S, B1
COMMON A, B
POWR (S,A, 2)
POWR (B1, B, 2)
ADDA (S,B1)
RETURN
END
```

Here commands $ANAL(A1)$, $ANAL(B)$ in main program inputs from input steam polynomials $A1$ and B. Commands $PRIN('A1', A1)$, $PRIN('A2', B)$ prints their analytical values, command $DELS(SUM)$ calls the procedure, which calculates the sum of two polynomials each of them raised to the second power/polynomial squares. The polynomials A and B analytical values procedure gets through block $COMMON$ from the calling program. The result of addition the program gets through the parameter of procedure S [1].

An analytical expression occupies more space in memory then single number and the execution of analytical operation takes much more time than the execution of numerical one. So the usage of sparse matrices in analytical computation is considerably effective. Computer algebra system VIBRAN has special commands and operations for sparse matrices. Commands for operations with sparse matrices may be divided [1]:

1) service (element putting/getting in/from matrix, getting of the index of not null element);

2) input–output (writing/reading of the sparse matrices to/from the file, insertion and printing in/from files);

3) algebraic – (addition, multiplication of the sparse matrices, multiplication of the sparse matrix and vector or number);

4) usage of the operator (differentiation or integration either of the whole matrix, or it element, or line, or column.

3. Algebraic data parallelism implementation in HPF (High Performance Fortran)

HPF is the special language which direct purpose is the operations with matrices, which are easy parallelized (compare to objects and etc.). The parallelization of matrix structures can be done automatically.

The specific feature of CAS PARAVIB is the representation form of analytical expressions that are stored in matrix form. This feature distinct PARAVIB from other computer algebra systems. Sparse matrices technology is used for analytical operations with arrays. This technology enables effective parallel analytical perturbations. The PARAVIB system is designed for parallel numerical computational applications generation. Special PARAVIB procedure generates optimized HPF code from analytical expressions. This code can be used in the programs for parallel numerical analysis. The system picks out all repeating multiplications and stores them as an automatically generated vocabulary of additional arrays. The final expressions are generated using elements of this vocabulary and are stored in array with distributed memory. Here is an example of HPF code (parallel extensions):

```
POLINOM A(1000), B(3000)
RACIONAL C(10000)
!hpf distribute A ( block)
!hpf distribute B (cyclic)
!hpf distribute C (block) onto P
```

PARAVIB supports task parallelism, HPF local and serial routines, and FORTRAN 77 local procedures. The special EXTRINSIC attribute is used to explicitly state that the program unit, subprogram or interface program is coded/not coded in HPF [4].

$EXTRINSIC(HPF)$ attribute indicates that the program unit, subprogram, or interface body is HPF-conforming. Such a scoping unit is referred to as an HPF scoping unit.

$EXTRINSIC(HPF, LOCAL)$ indicates a program unit, subprogram or interface body that is targeted to a single processor, with many copies executing on different processors. Such procedure is referred to as a local procedure. The programming style in which many copies of the same program run on multiple is often referred to as single program, multiple data ($SPMD$).

$EXTRINSIC(HPF, SERIAL)$ indicates a program unit, subprogram or interface body that is targeted to a single processor,with only one instance of the program unit, subprogram, or interface procedure executing on only one processor. Such a procedure is referred to as a serial procedure. Serial procedures are useful for code written in other languages or current FORTRAN programs that you don't want to/cannot recompile. Here is an example of PARAVIB procedure definition [5]:

```
EXTRINSIC(HPF,local) PROCEDURE DELS (S)
```

For programme code parallelization high qualification specialists and a lots of time are needed. At this moment HPF is the only special programming language for algebraic data parallelization, which can be done automatically.

4. An example of algebraic data parallelism implementation in nonlinear oscillation systems analysis

Simulations by means of numerical methods are powerful tools for investigations in mechanics but they do have drawbacks, e.g., finite precision, errors generated when evaluating expressions. A broader understanding of mechanical phenomena can be gained by means of analytical methods. Computerized symbolic manipulation is a very attractive means to reliably perform analytic calculations with even complex formulas and expressions. But often, a semi-analytical approach, combining the features of analytical and numerical computations, is the most desirable synthesis. This allows the analytic work to be pushed further before numerical computations start.

Computer algebra techniques were applied to analyze nonlinear oscillation systems with several degrees of freedom. For this purpose mechanical system is divided into the linear and nonlinear parts. The linear part of the system can be formalized without difficulties as usual.

For numeric-symbolic computation of the nonlinear oscillation systems with several degrees of freedom computer algebra system PARAVIB was used.

As was mentioned above, PARAVIB has a special procedure for optimized HPF code generation from obtained analytical expressions, which can be directly used in the programs for numerical analysis. These steps are presented in Fig. 1.

The proposed method provides smaller expressions for analytical computation and allows to analyze systems with greater order. After good known perturbations the equations of motion can be rewritten in the matrix form:

$$[A]\{\ddot{q}\} + [B]\{\dot{q}\} + [C]\{q\} = \{H(q, \dot{q}, t)\} + \{f(t)\}.$$

Marking:

$q_i, \dot{q}_i, t$ – generalized coordinates of system and time;

$[A], [B], [C]$ – matrices of coefficients of the linear part of system; $f(t)$ – periodic function;

$H(q, \dot{q}, t)$ – nonlinear part of system, calculated by spec. program;

s – number of degrees of freedom;

$f(t)$ – generalized force, nonlinear (polynomial and periodical or Fourier expansion) and linear parts.

Solution of the above mentioned system can be expressed using harmonic balance method in the form:

$$\{q\} = \{D_0\} + \{D_1\}\cos(wt) + \{D_2\}\sin(wt) + \dots$$

Marking:

$\{D_i\}$ – the unknown vectors that can be found from the nonlinear algebraic equations.

Following harmonic balance method these equations for the first three vectors coefficients are:

$$\begin{vmatrix} C & 0 & 0 \\ 0 & C - Aw^2 & Bw \\ 0 & -Bw & C - Aw^2 \end{vmatrix} * \begin{vmatrix} D_0 \\ D_1 \\ D_2 \end{vmatrix} + \begin{vmatrix} f_0 \\ f_1 \\ f_2 \end{vmatrix} + \begin{vmatrix} H_0(D_0, D_1, D_2) \\ H_1(D_0, D_1, D_2) \\ H_2(D_0, D_1, D_2) \end{vmatrix} = 0$$

or in matrix form:

$$[U]\{D\} + \{f(D)\} = \{Q\}.$$

Marking:

f_i – coefficients of function $f(t)$ Fourier expansion.

Analogously equations for other harmonics could be found by PARAVIB program. The expressions of H_i and theirs required derivatives are expressed in closed form using computer algebra techniques with HPF code generation procedure. The programs structure is shown in Fig. 1.

5. Conclusions

The parallel extension of computer algebdra system VIBRAN is presented. PARAVIB was developed for generation of parallel symbolic processing programs. Special algebraic part of CAS VIBRAN for parallelization corresponds to the High Performance Fortran standards. Thus the system can run on all computer systems, which has HPF.

High Performance Fortran is the special language which direct purpose is the operations with matrices, which are easy parallelized (compare to objects and etc.). The parallelization of matrix structures can be done automatically. Sparse matrices technology is used for analytical operations with arrays. This technology enables effective parallel analytical perturbations.

Using implemented algebraic data parallelism techniques new parallel symbolic algorithms can be provided. Algebraic data parallelism realization in CAS PARAVIB was presented using nonlinear oscillation systems analysis.

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Algebrinių duomenų lygiagretumo realizavimas HPF'e (High Performance Fortran)

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Kartu su simboliniais skaičiavimais, lygiagrečiai buvo vystomi ir skaitiniai metodai. Laikui bėgant kompiuterinės algebros sistemos turėjo apdoroti vis didesnius duomenų kiekius, tai yra buvo susidurta su aukštos skalės operacijų problemomis. Šiuos klausimus bandoma spręsti pasitelkus lygiagretųjį programavimą. Tačiau kol kas dar nėra sukurtos formalizuotų algebrinių duomenų lygiagretinimui skirtos kompiuterinės algebros sistemos. Gerai žinoma sistema „Matematika" turi priemonių skirtų lygiagretinimui, tačiau tai tik priemonių rinkinys, o ne atskira kalba. HPF šiuo metu yra vienintelė tokia kalba skirta lygiagrečiajam programavimui. Todėl kompiuterinės algebros sistemos VIBRAN praplėtimas buvo kuriamas naudojantis šia priemone. HPF yra specialiai pritaikyta programavimo kalba darbui su matricomis, todėl lygiagretinimas atliekamas automatiškai ir šiam darbui nereikia nei aukštos kvalifikacijos specialistų, nei daug laiko sąnaudų.

Lygiagreti kompiuterinės algebros sistema PARAVIB'as yra HPF priešprocesorius skirtas analitinių išraiškų, tokių kaip labai ilgi polinomai, racionalinės funkcijos, trigonometrinės eilutės bei išretintos matricos, analitinėms lygiagretinimo operacijoms.

Šią sistemą sudaro HPF priešprocesorius ir procedūrų bibliotekos. Algebrinė sistema atlieka duomenų\procesų lygiagretinimą, palaiko HPF paprogrames ir FORTRANO 77 procedūras. PARAVIB'as yra lygiagreti kompiuterinė algebros sistemos VIBRAN versija (VIBRotechnika and ANalitika).

PARAVIB'e analitinės išraiškos, kintamieji ir jų laipsniai saugomi atskirai. Toks saugojimo būdas leidžia analitinius skaičiavimus pakeisti matricinėmis operacijomis.

Išretintų matricų technologija yra taikoma analitinėse operacijose su masyvais. Naudojantis šia technologija atliekami efektyvūs lygiagretieji skaičiavimai. PARAVIB'e yra speciali procedūra skirta optimizuoto HPF programinio kodo generavimui iš analitinių išraiškų. Šis kodas vėliau gali būti panaudotas lygiagrečiuose skaitmenininiuose skaičiavimuose. Kita galinga priemonė HPF kodo generavimui yra pasikartojančių skaičiavimų išrinkimas ir saugojimas tam tikrame žodyne. Galutinės išraiškos yra generuojamos panaudojant šį žodyną ir išsaugomos masyve su paskirstyta atmintimi.

Nors kompiuterizuotos simbolinės operacijos yra labai patraukli priemonė analitinių skaičiavimų su kompleksinėmis ir ilgomis formulėmis atlikimui, tačiau dažnai analitinių ir skaitmeninių skaičiavimų kombinacija yra geresnis būdas aukštos skalės operacijų atlikimui. Tokia kombinacija leidžia atlikti analitinius veiksmus pirma skaitmeninių.

Pateiktas kompiuterinės algebros sistemos VIBRAN specialus praplėtimas PARAVIB'as skirtas lygiagrečių simbolinių programų kūrimui. PARAVIB'as atitinka HPF standartus, tokiu būdu sistema gali dirbti kiekvienoje kompiuterinėje sistemoje, kuri turi HPF bei atlikti algebrinių duomenų lygiagretinimą. Šią technologiją galima taikyti naujų lygiagrečių simbolinių algoritmų kūrime. Algebrinių duomenų lygiagretinimas buvo pritaikytas netiesinių svyravimo sistemų analizėje.