New Automatic Code Radiation Earth with Parallel Computing

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New perspective opportunities of mathematical modelling of atmospheric radiation of the Earth are connected with elaboration of software tools for the wide region of applications using supercomputers with parallel architecture. The availability of such tools enables to carry out precise calculations, numerical experiments, imitation modeling, verification of approximate techniques and fast algorithms of updated solutions of scientific and development as well as applied problems along with to improve the related radiation block for general circulation models of the atmosphere, forecasting problem, climate, photochemical kinetics, dynamics of ozone in the atmosphere, transboundary pollution transfer in air basins.

The algorithms of parallel calculations are given by according to physical models:

- multispectral;
- optical and geophysical weather (using specified coefficients);
- in accordance with the relevant sources.

The complex of mathematical models and methods represents the open developed system of mathematical simulation. The resources of its adapting to conditions of concrete objects and on different high capacity computing systems are stipulated.

Usage Perl scripts [1], wrapping in itself calls of Fortran-programs in the multitask environment, provides portability of applications. We wrap Fortran programs up in a bit of Perl and make its interface more modern and simple.

The purpose of development – to provide the greatest possible portability of the "inherited" complex of programs and to provide transparent operation in the distributed network environment. The program complex should without considerable alterations work on a cluster of workstations and - or the massively parallel processor (MMP).

The parallelism is implemented in the system of mass calculations of a major set of boundary value problems of the theory of carry of radiation in a wide range of a spectrum of lengths of waves for sets " of optical weather ", states of a spreading surface, sources of radiation.

The outcomes of single calculations are stored in archives of solutions and will be utillized in further for calculation of various functionals in interests of concrete target applications. The program for calculation of "single" variant is implemented on the Fortran77. It is essential, that during the scores of variant and at record in archive of solutions the operators of direct access Fortran will be utillized.

The implementation of control function and network interaction by the "inherited" complex of programs is yielded with the help of scripts, written on the description language, Perl.

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We use:

1. An isolated script;
2. Pipeline;
3. Wrapper;
4. Compiled extensions.

The operating system Linux (RedHat 6.2.-7.3.) will be used, that provides a complete set of regular tools, including compilers from the programming languages C (gcc), Fortran 77 (g77 [2]), Perl 5.6.

For the main program, some subroutines from the software package APGRAF and software package DINAMF (dynamic memory allocation through COMMON bloks) the wrappers on the language C with usage cfortran.h are written. cfortran.h is an easy-to-use powerful bridge between C and FORTRAN. It provides a completely transparent, machine independent interface between C and FORTRAN routines and global data, i.e. structures and COMMON blocks [3]. cfortran.h works by using the C pre-processor to create 'wrapper' functions to call appropriate routines. These c-wrappers are for interaction Fortran of programs with programs on the language Perl DATA Language [4] (object-oriented extension of the language Perl for manipulation major multivariate data sets and maps) with PDL::PP [5] – Perl module (Generate PDL routines from concise description).

At build-up of a control system of the complex we guess, that there are at least two workstations or two account'a on one.

On a main workstation are available:

• Workplace for the operator of preparation of packages initial data for mass calculations;
• Monitor for management of mass calculations;
• Complete archive of solutions both program of the package of processing and manipulation with archives.

On others and – or of same workstation are available account's and disk spaces, in which the monitor controlling a chain of single calculations within the framework of a set of packages of the initial data.

The monitor is realized with the help Parallel::Pvm – Perl extensions for the Parallel Virtual Machine Message Passing System [6].

The set of packages of the initial data is made out as a macro library of the initial data and job definition for start of single variants. The set of packages of the initial data is transferred on a free workstation on FTP either in hand-held, or in the automatic mode.

The automatic move mode is organized with the help of the unit on the language Perl, implemented on base auto_ftp.pl [7]. The module takes away files with the packed jobs definitions from the particular directory on the main workstation and transfers in the given directory on the workstation-calculator.

The file with the jobs definitions can contain inside itself Structure of directories, files of the initial data and control script file on the language Perl. The jobs are started automatically (or become in queue of the tasks) in accordance with arrival of initial data files in the directory on the workstation-calculator on FTP or SFTP.

After the termination of calculations the filled designed archive gets on FTP on a main workstation by the monitor of this workstation. If a main workstation and workstation-calculator have the same hardware platform, the archives are transferred in the binary format. If the hardware platforms different, the archive beforehand is translated in ASCII format, and then is transferred. On a main workstation the unpacking, converting and assembly of designed archives of variants and association them in complete archive of solutions on frequency for after treatment is yielded. The monitor of the main workstation batchly scans files of protocols of operations of workstations for a closing -up and presence of failures. This elementary variant batch-processing can utillize transfer and with the help of the protected protocols SSH and SFTP, depending on that what access is allowed on the computer complex.

Such approach requires, however, continuous operation of the monitor, or several copies of the monitor on the main workstation and monitors on all used workstations calculators. The service ability of the program complex NACRE was checked on the test problems on the following computers: IBM PC Pentium II, III, IV c by different versions of an operating system RedHat Linux. On domestic multiprocessor computer complexes MBC-100 and series MBC-1000.

Thus, the multisequencing of calculations on physical analogs is reached(achieved) with the help of start of the jobs(definitions) on several calculators or / or several processors of one calculator.

On a main workstation the unpacking, converting and assembly of designed archives of variants and association them in complete archive of solutions on frequency for aftertreatment is yielded.

The complex of handlers APGRAF allows to carry out all necessary manipulations with archives of solutions (junction and squeezing of archives, sampling from archives, etc.). APGRAF allows to shape various chains of processing and works as in the independent mode as the package Fortran of programs, and as the library of programs accessible in frameworks Perl Data Language.

In this case programming of operations on processing and visualization happens on the language Perl to usage accessible of PDL of external libraries (for example, PGPLOT [8]) and multivariate data structures, particular resources PDL.

Acknowledgement

References

1. Using and Porting GNU Fortran. James Craig Burley. Last updated 2002-04-29 for version GCC-3.2 http://gcc.gnu.org/onlinedocs/g77.ps.gz
2. *T.Jenness and S.Cozens,* Extending and Embedding Perl (Manning Publications Co., 2002).
3. http://www-zeus.desy.de/~burow/cfortran/cfortran.html
4. http://search.cpan.org/aujthor/KGB/PDL-2.3.2/
5. http://pdl.sourceforge.net/PDLdocs/PP.html
6. http://theoryx5.uwinnipeg.ca/CPAN/data/Parallel-Pvm/Pvm.html
7. Joshua Curtis, auto_ftp.pl v. 0.4. http://www.curtisonline.net/software/
8. http://www.aao.gov.au/local/www/kgb/pgplot/