

3D CFD PROBLEM SOLUTION USING PARALLEL COMPUTATIONS BY MEANS OF GDT PACKAGE

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Abstract. Nowadays numerical simulation of complicated CFD problems by means of parallel computation is widely used all over the world. There are many CFD codes which can work on multiprocessor systems. The GasDynamicsTool[®] (GDT) package developed by the GDT Software Group is one of them. It is meant for the numerical simulation of gas-dynamics processes in a wide range of initial and boundary conditions. Fluid jets, inner and outer problems of aerodynamics, ballistics, combustion and detonation, fluid-structure interaction - these are just a few of the phenomena that can be simulated with the help of the GDT package. GDT can work on different software and hardware platforms. The package is based on a modified large particle method and uses a uniform cubic grid. Parallelization is provided by means of computation domain division into a number of subdomains. The number of subdomains equals the number of cluster nodes. On every time step each node calculates the results in every grid cell of its subdomain, and after that the subdomain boundary cells results exchange between the nodes takes place. As a result of such an approach the GDT has a high computation speed and good scalability characteristics. For example, one time step computation for 960 million 3D cell domain on 16-node cluster of ICAD RAS lasts 39 seconds. The package is capable of computing up to 30 million 3D cells for each gigabyte of the working memory. GDT Software Group actively uses its developments to solve complicated CFD problems. Present work devotes to description of a parallel version of the GDT package features and capabilities and to applying experienced approaches to three-dimensional problems of CFD. Several simulation examples are presented. Particular attention is devoted to complicated geometry and import from CAD/CAE systems as well as complicated 3D flows visualization.

1 INTRODUCTION

3D CFD problem simulation is of an exclusive importance for different branches of human activity. Traditional applications are aircraft and rocket design. However CFD problem solution is also necessary, when estimating accident consequence in chemical plants, analyzing the cause and estimating consequences of explosions in industry and guaranteeing different explosive work safety. The variety of existing problems due to the multiplicity of initial and boundary conditions and the requirement that their solutions is without essential simplification, lead to the necessity of development of universal application programs based on numerical integration of the equation system of gas dynamics.

One of the most significant and crucial aspects of building such programs is also the problem of computation parallelization and distribution. Recently, due to the progressing development of multi-processor technologies the problem of parallelization has become yet more topical.

This article is related to development and practical applications of a parallel version of the GDT software package, developed to simulate gas-dynamics processes in a wide range of initial and boundary conditions. It provides for high performance parallel computing, works on different software and hardware platforms and supports 64-bit CPUs AMD OpteronTM, Intel Itanium2TM, IBM Power 4+TM.

2 PACKAGE FEATURES AND CAPABILITIES

The mathematical model used in the package is based on a total system of nonlinear nonsteady equations of mechanics of continua. There have been several submodels¹ implemented that allow using the package in the exploration of specific physicochemical processes:

- Euler model (allows to simulate 3D ideal gas flows);
- Navier-Stokes model (allows to simulate 3D chemically reactive multiphase flows of viscous gas using Arrhenius kinetics);
- High-explosives model (allows to simulate 3D high-explosives detonation using Euler equations);
- LDE/FAE model (allows to simulate 3D two-phase flows with solid and gas phase chemical reactions).

For the computational equation integration the package provides an explicit two-step scheme of a modified large-scale particle method which allows finding a solution for the whole denumerable domain using a single algorithm without any preliminary extraction of distinctive features. The program uses a uniform grid consisting of cubic meshes, which is one of the reasons of its efficient production: the computation of one time step in a 1000000 3D cell domain on the computer with Intel Centrino 1GHz takes 1 second.

The efficient multi-platform technology of dynamic parallelization relies on the use of novel approaches to computation synchronization management². Parallelization is provided by means of computation domain division into a number of subdomains. The number of subdomains equals the number of cluster nodes. On every time step each node calculates the results in every grid cell of its subdomain, and after that the subdomain boundary cells results

exchange between the nodes takes place.

As a result of such approach GDT has an outstanding computation speed and good scalability characteristics. For example, one time step computation for the 960 million 3D cells domain on 16-node cluster of ICAD RAS lasts 39 seconds. A high processor utilization factor has been achieved. Thus, for a double-processor PC this factor reaches a figure of 0.96 – 0.98.

This technology has been implemented on the Windows and Unix platforms (Linux, Solaris) in an SMP version. Implementation on the Unix platform conforms to the POSIX standard requirements, which makes the technology usable on diverse computer platforms. In the Unix version there has also been realized for cluster approach, which makes it possible to use all the accessible cluster nodes as well as all the processors available on each node.

The package has got an intuitive and friendly graphical user interface (GUI) and a multifunctional visualization system. The code allows calculating about 30 million cells for each Gb of OS. The computation for one step takes approximately 30 seconds on a Dual ATHLON 1800+ CPU.

Nowadays package can be effectively realized for clusters with hybrid architecture. All the modules are available for the following four OS: Win32, Linux, Solaris, Mac OS. The package is implemented on the platforms UltraSPARC и x86 (Solaris).

This approach makes it possible to handle objects with dynamically changing properties, among other things diverse geometry objects, periodical sources of energy, variable boundary conditions, etc. Solution of this kind of problems has traditionally presented difficulty regarding inter-processor data exchange.

The important development stage of numerical program is the maximum use of graphical possibilities of modern PC to visualize a considered process. In described package screen output of fields of all gas-dynamics parameters was designed, scalar values being presented with the help of scale or various color gradations, vector values are presented by segments directed along velocity vector, segment length is proportional to vector modulus. There is gas-dynamic parameter record in given points of calculated domain with the following visualization of graphical dependencies of these parameters on time, forces and moment acting on solid bodies in calculated domain. There is a storage mechanism for subsequent process stage information that provides the possibility to produce video clips illustrating flow process development in time. The best advantage of designed product is its applicability for PC that makes affordable the conduction of gasdynamic calculations to the wide range of users without special background in gasdynamics.

GDT package can be applied for scientific and engineering investigations of gas-dynamic processes in many branches of science, engineering and technology, for example in ecology, machine buildings air-space industry and metallurgy; in physical chemical investigations of combustion processes; in study of interior, intermediate, exterior ballistics and explosion, detonation and combustion physics, shock wave action on constructions; when simulating processes similar to oil gas industry plant and pipeline functioning.

GDT package has wide range of possibilities of various problem solutions³. As the program possesses powerful interface allowing even unprepared user to formulate and realize setting, debugging and solving the most complicated technical and scientific problems fast

and effectively. We present the most frequent used program possibilities and characteristic service interface possibilities. The program allows to:

- investigate gas-dynamic flow processes taking into account viscosity, thermal and mass diffusion;
- study gas-dynamic processes taking into account catalysis and adsorption;
- investigate gas-dynamic processes related with chemical reactions including combustion;
- study detonation processes in condensed and gaseous HE;
- take into account heat transfer in solid thermal conductive bodies;
- perform gas-dynamic calculation for two-dimensional plane and axial symmetric and three-dimensional flow;
- investigate non-steady processes in the wide range of initial and boundary conditions;
- study subsonic and supersonic flow regimes;
- investigate gas and body system evolution of arbitrary geometrical configuration;
- calculate stationary processes in stagnate flow regimes;
- perform calculation with arbitrary number of initial areas with different values of gas-dynamic parameters;
- perform calculation in presence of any number of arbitrarily shaped bodies in flow;
- preserve given initial flow configuration with the possibility of its further application;
- store and look up calculation results;
- present values of all gas-dynamic parameters in any cell of calculation domain during calculation;
- change modeling problem configuration fast;
- change color scale structure and value intervals of considered parameters operationally;
- use specific types of boundary condition inside the calculation domain;
- resume calculation stopped earlier;
- produce gas-dynamic parameter diagram;
- store and present the change of parameters in time and any cell of the domain;
- output results in standard video- and graphical formats.

3 GRAPHICAL USER INTERFACE

The GUI provides for numerous service capabilities (see fig. 1). Among those:

- output in a standard video- and graphic layout (displaying scalar quantities and their gradients by means of the color scale or the shades of gray; vector quantities with the help of scaled vectors; animation of any parameter; construction of time dependence graphs);
- color scale management and management of output parameter limits;
- epure construction for gas-dynamic parameters;
- finding of integral forces and moments, affecting the solids.

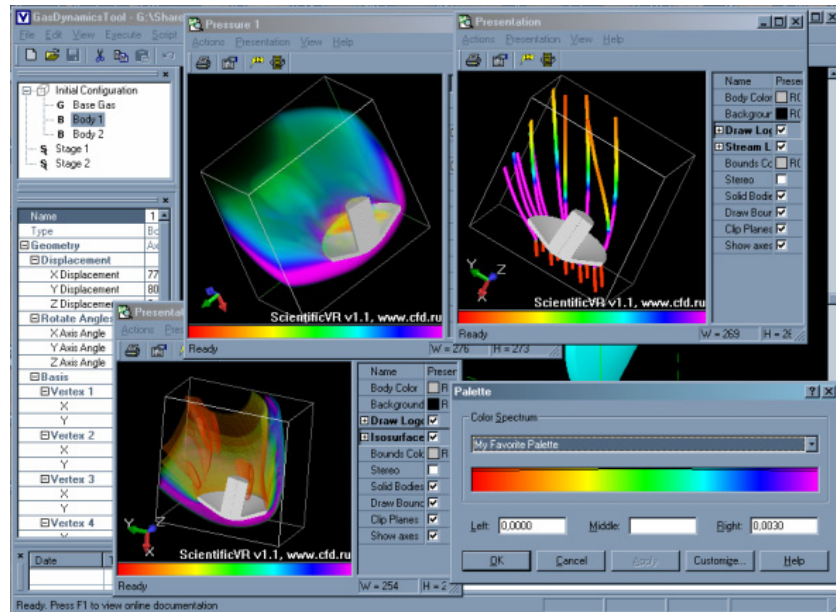


Figure 1: Graphical user interface

4 GEOMETRY AND CAD/CAE COMPATIBILITY

Simulating three-dimensional processes of gas dynamics the problems occurred in initial configuration input and complex shape objects geometry⁴. Solving these problems with the GDT package, one is able to go on two ways: for relatively simple shapes it has plug-in preprocessor permitted to input such primitives as ellipse, box, cone, planar figure, solid of revolution and they combinations; another way is import from CAD system (see fig. 2).



Figure 2: Three-chamber muzzle brake geometry, imported by GDT using CAD graphical format.

5 VISUALIZATION SYSTEM

Data obtained from computation are visualized by means of ScientificVR[®] (SVR) visualization system developed by the GDT Software Group⁵.

As part of the parallel version of the GDT package, it is featuring “on-the-fly” dynamic visualization of data obtained from nodes of distributed computing systems, and is based on a modified variant of visualization on a visualization node (see fig. 3).

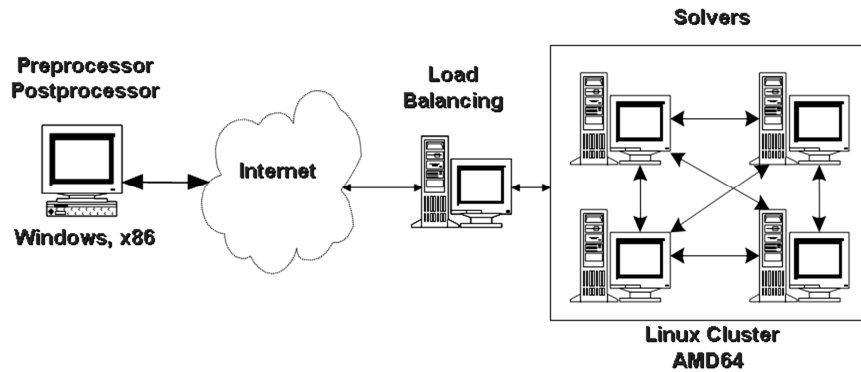


Figure 3: Functioning pattern of the hybrid technology

The most significant features of the visualization system are the following: “on-the-fly” extra large data visualization, plug-in architecture, semitransparent voxel graphics and full color 3-d stereoscopic presentations.

6 MAIN APPLICATION FIELDS

6.1 Aerospace engineering

The GDT package can be used for the numerical simulation of hypersonic, supersonic and subsonic flows around aircrafts, space shuttles and landing modules; modeling of rocket start-up, jet-launcher interaction and booster separation processes, etc.

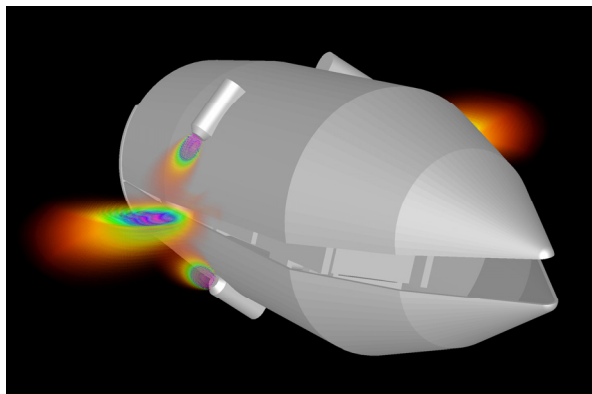


Figure 4: Cowl opening. Density distribution. Voxel graphics

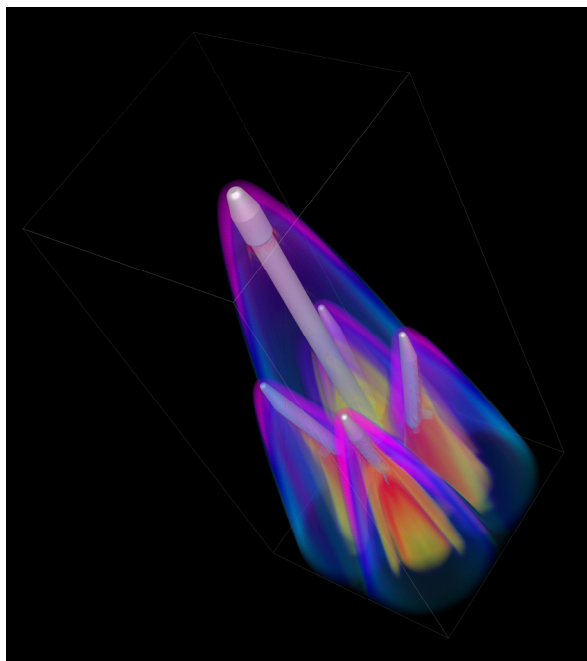


Figure 5: Booster separation process. Density distribution.
Voxel graphics in isosurface realization

6.2 Processes of combustion and detonation, as well as shock wave generation, transmission and fluid-structure interaction

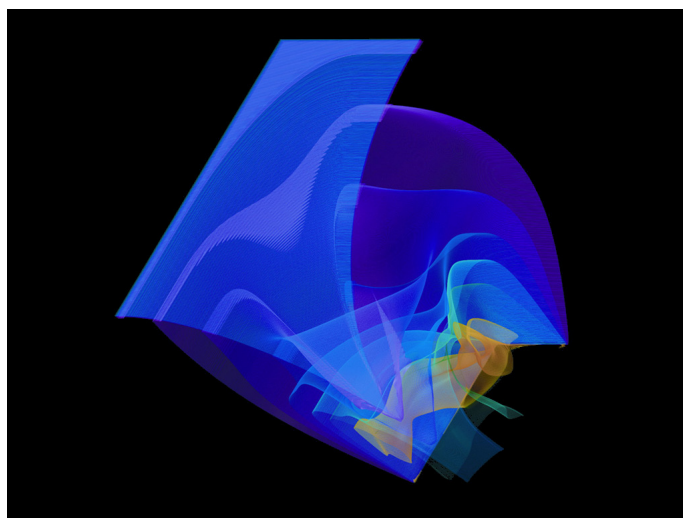


Figure 6: Shock wave diffraction on a 3D edge. Density distribution.
Voxel graphics in isosurface realization

6.3 Counter-terrorism

Using the GDT one can estimate high-explosive, thermobaric, fuel-air detonation impact

on people and constructional elements. These data can be used to analyze the safety level of nuclear plants, stadiums, supermarkets in case of terrorist acts.

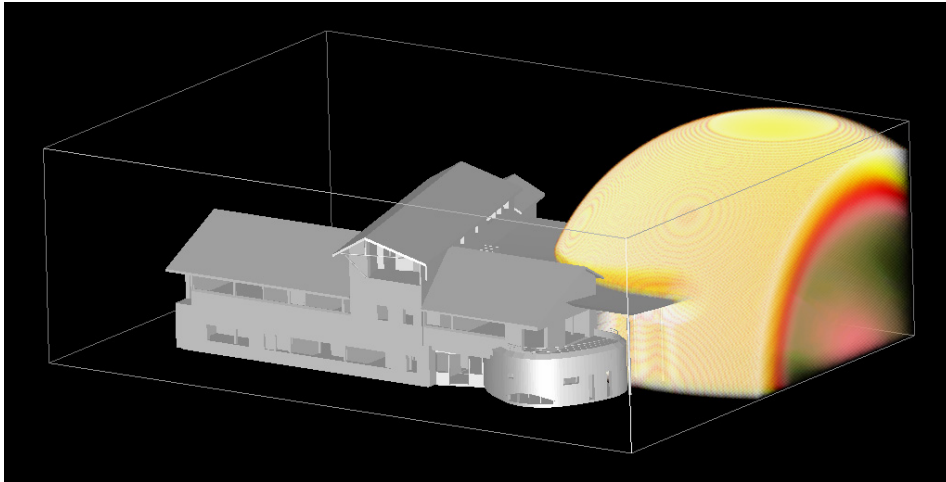


Figure 7: Acetylene tank explosion near a building. Density distribution.
Voxel graphics in isosurface realization

6.4 Defense technologies

The package can be used for the numerical simulation of functioning of missiles, MLRS, artillery systems, small-arms systems, etc.

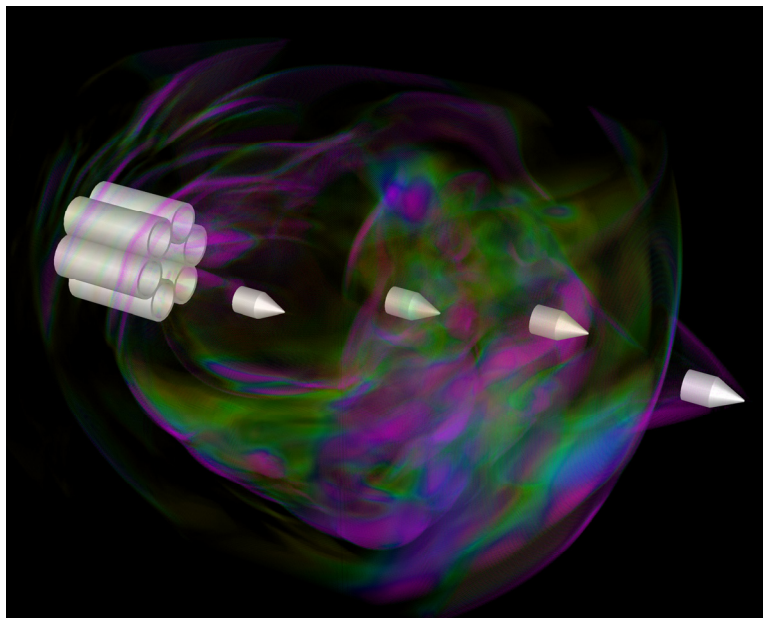


Figure 8: High speed gun operation. Shock wave pattern. Voxel graphics

7 CONCLUSIONS

- The parallel version of the GDT package with good scalability characteristics providing fast, high-quality simulation of gas dynamics processes in a wide range of initial and boundary conditions has been developed.
- Fluid jets, inner and outer problems of aerodynamics, ballistics, combustion and detonation, fluid-structure interaction are just a few of the phenomena that can be simulated with the help of the GDT package described.

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