

CACTUS CFD TOOLKIT: COMBINATION OF AERODYNAMIC SOLVER WITH ADVANCED COMPUTING TECHNOLOGIES

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ABSTRACT

Cactus[1] is a general-purpose, modular PSE(Problem Solving Environment) designed for scientists and engineers. Since 1995, the base framework has been developed and mainly applied for large scale astrophysics simulations[2]. From those researches, Cactus proved to be a valuable tool for scientific and engineering applications that are tightly coupled, have regular space decomposition, and huge memory and processor time requirements. Currently, Cactus is under the progress of being applied to various studies including CFD(Computational Fluid Dynamics)[3], quantum relativity, chemical reaction and EHD(Electro-Hydro-Dynamics). Especially for CFD simulations, aerodynamicists at 'Seoul National University', 'KISTI Supercomputing Center' and 'KAIST' have been collaborating to make a compressible CFD toolkit working on the Cactus framework. Present paper introduces the current status of a CFD toolkit on the Cactus.

INTRODUCTION

Accuracy and efficiency are two key issues to CFD(Computational Fluid Dynamics) researches. Inaccurate solution will bring about the wrong resultant, while inefficiency will result in the failure of manufacturing within demanded time. Researchers usually increase mesh size, conduct turbulent analysis, increase the order of spatial accuracy and tune turbulent parameters for specific applications in order to get an accurate solution. But, all these techniques except parameter tuning are inevitably the enemy to efficiency. On the other hand, faster and inaccurate solution requires increasing safety factor to satisfy the safety standard and it increases manufacturing cost.

Apparently, parallel and Grid computing can be the answer to this conflict. More computing power guarantees faster solution. Besides, a group of moderate processors is far cheaper than single processor with the same capacity in total. The only difficulty is that progress of computer technology enforces application scientists to have additional knowledge on computing techniques. For example, researchers have to include MPI library[4] on their application program for parallelization. And they need to be well aware of many additional softwares like Globus[5] to conduct Grid computing.

In this aspect, the authors have been searching for a convenient computing environment and adopted Cactus framework as a base PSE(Problem Solving Environment). On the basis of Cactus framework, the authors added some of computational modules for CFD simulation and improved Cactus architecture. And, a compressible flow solver is implemented to the Cactus framework. Up

to now, developed CFD toolkit can be applied to the single-block mesh system with body-fitted coordinate.

DEVELOPMENT OF CFD TOOLKIT

Cactus Framework

Cactus is mainly composed of a central core (flesh), application modules (thorns), the computational supports (drivers) and the plugins to different softwares. Among the components, flesh arranges application thorns, drivers and linkable softwares and interacts with all the others. Thorns are the modules that are applicable to specific researches. Driver supports the Grid service, parallel processing including automatic domain partitioning or communication across inter-processor boundary. Finally, users can link Globus, PETSc and other softwares to the existing Cactus framework.

Cactus has the following advantages. Firstly, users do not have to learn a new programming language and convert their application solver to a specific language since Cactus supports multiple languages including Fortran and C. Secondly, Cactus runs on a wide range of architectures and operating systems. And, Cactus automatically performs parallel programming, so users do not need to have additional knowledge of parallel processing. Additionally, as Cactus supports object-oriented environment, researchers can work with collaborators on the same code and avoid having your programs fragmented. Finally, users can make use of the latest software technologies, like the fastest way of transmitting simulated data and the optimal visualization technique, by adopting associated modules from supported Cactus thorns.

Governing Equations And Numerical Techniques

The three dimensional compressible Navier-Stokes equations are adopted. The full Navier-Stokes equations can be written in general curvilinear coordinates $(\mathbf{x}, \mathbf{h}, \mathbf{z})$ as follows:

$$\frac{\partial \hat{Q}}{\partial t} + \frac{\partial \hat{E}}{\partial \mathbf{x}} + \frac{\partial \hat{F}}{\partial \mathbf{h}} + \frac{\partial \hat{G}}{\partial \mathbf{z}} = \frac{1}{\text{Re}} \left(\frac{\partial \hat{E}_v}{\partial \mathbf{x}} + \frac{\partial \hat{F}_v}{\partial \mathbf{h}} + \frac{\partial \hat{G}_v}{\partial \mathbf{z}} \right) \quad (1)$$

where \hat{Q} is the conservative variable vector, \hat{E} , \hat{F} , \hat{G} are the inviscid flux vectors and \hat{E}_v , \hat{F}_v , \hat{G}_v are the viscous flux vectors

As a spatial discretization, AUSMPW+ (modified Advection Upstream Splitting Method based on Pressure Weight functions)[6] scheme is applied. As an implicit time integration method, LU-SGS (Lower-Upper Symmetric Gauss-Seidel) scheme[7] is used. The viscous flux Jacobian is neglected in the implicit part since it does not influence the accuracy of a solution. Time step is determined by local time stepping. And, for the accurate representation of turbulent flowfield, 2-equation $K-\omega$ SST model[8] is adopted.

Porting CFD Code Into Cactus Framework

The authors have been trying to improve current Cactus framework by adding some modules. To support curvilinear coordinate system, a mesh reader and a transformation module are newly developed. Additionally, for the various types of application solvers, current data structure has been reconfigured to include FVM (Finite Volume Method) as well as existing FDM (Finite Difference Method). As for boundary conditions, the functions of existing Cactus boundary condition are

properly applied for specific applications. But boundary condition will be generalized more and located as separate CFD functions.

The procedure of 3-D turbulent flow analyses is as follows. At pre-processing level, mesh reading is conducted. At initial step, the initialization of flow conditions and transformation to curvilinear coordinate are carried out. Then, time scale is determined at pre-evolution step by local time stepping method. And, at evolution level, flux calculation by spatial discretization, time integration and the application of boundary conditions are conducted iteratively. After iterative computational step is finished, resultant data are visualized and analyzed. For the compressible CFD research, an arrangement named ‘CFDComp’ is generated and each component in analysis process is made as a separate thorn inside the arrangement. Figure 1 shows the structure of overall compressible CFD toolkit and the scheduling of 3-D turbulent flow analysis. Here, each thorn is configured by CCL (Cactus Configuration Language) scripts and, analysis subroutine is stored inside the src/ directory by modifying parameters and functions into Cactus format.

NUMERICAL RESULTS

Developed flow solver has been applied to the aerodynamic problems as presented in Ref. 3. And recently, authors improved the existing solver for the simulation of an aircraft. Model geometry is a Smart-UAV configuration which is under development in KARI (Korea Aerospace Research Institute). Original geometry and simplified mesh system are depicted in figure 2. The mesh system is a single-block, O-type mesh with mesh points of $183 \times 58 \times 21$. As for flow conditions, conventional UAV flies at incompressible flow regime. But, a compressible flow condition is given for the simulation by a compressible CFD toolkit. The result at figure 3 shows the pressure contour at Mach number of 0.84 and angle of attack of 3.06 degrees. Even though no experimental data is present at this flight speed, the pressure distribution is physically reasonable.

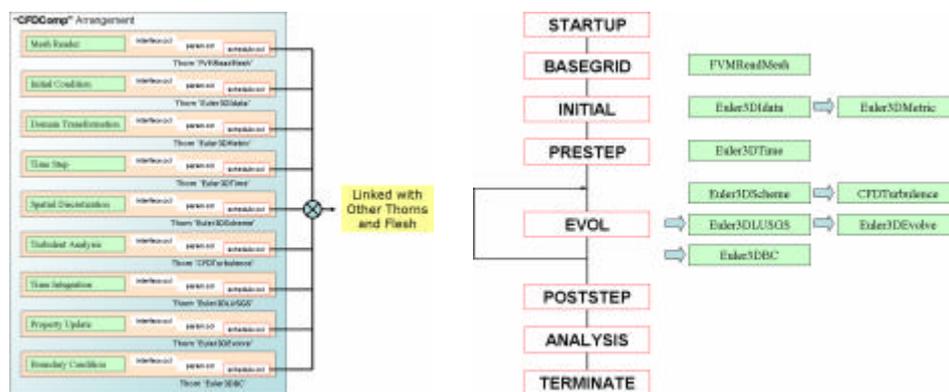


Figure 1. Structure of Compressible CFD Toolkit and Scheduling Bins

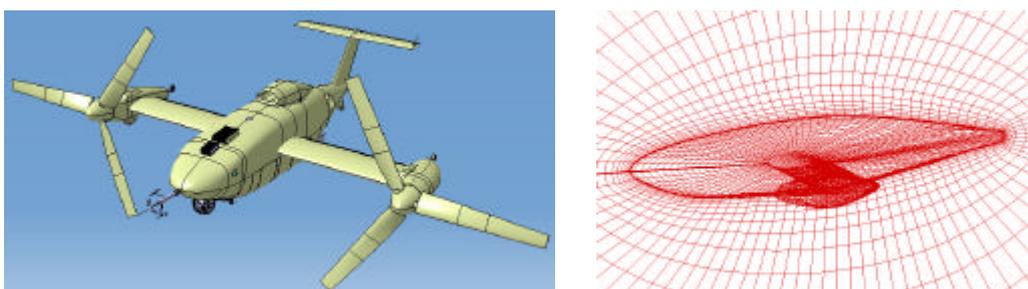


Figure 2. Original Geometry and Simplified Configuration

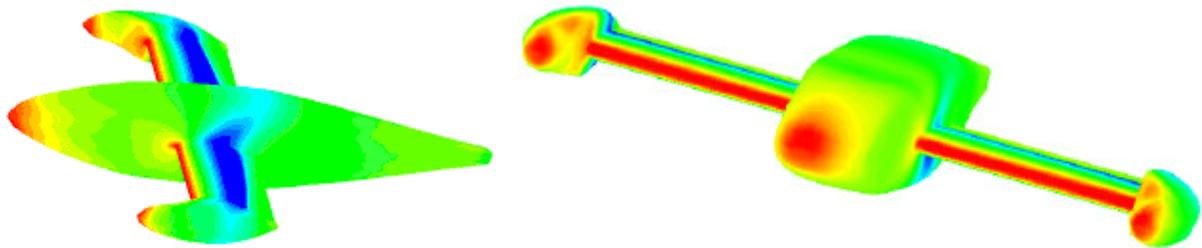


Figure 3. Surface Pressure Contour of Compressible Analysis

CONCLUSION

A compressible CFD solver is ported on Cactus framework and flow analysis around a simplified aircraft is conducted. Developed computing environment currently supports the flow analysis of a single-blocked system, with various advanced computational conveniences including automatic parallelization and efficient numerical algorithms. Using the developed toolkits, various CFD applications have been successfully simulated and they show the possibility of Cactus framework as a problem solving environment for general and complex CFD analyses.

CONCLUSION

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