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ROLE OF HIGH PERFORMANCE COMPUTING IN ENGINEERING DESIGN

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I. Introduction

Simultaneous developments of teraflop/petaflop supercomputers, advancednumerical algorithms, newerphysical and chemical models of flow physics in the recent years have revolutionized theengineering design throughout the world. These developments are playing a major role in advancing both basic and applied scientific/engineering researches in many fields including aerospace engineering, atmospheric science (modeling and simulation of monsoon, ocean modeling, thermosolutal convection, tropical cyclone early warning calculation etc.),nuclear sciences, astrophysics, biomedical research (drug discovery, predictive medicine, design of heart valve, stents etc.), design of domestic appliances, environmental engineering, mechanical, metallurgy and chemical engineering etc. The influences of High Performance Computing (HPC) in aerospace engineering in recent years are most dramatic. Presently, numerical methods are an essential part of the design process of air-frame and engines for all major aerospace companies in the world. While experimental testing will always remain an integral part of the design, numerical methods can decrease the dependence on the more expensive, time consuming experimental testing or rather using experimental work more effectively and economically. Advancement of computer architectures and numerical methods has saved the aircraft companies tens of millions of dollars over the past few decades. Improved turbo-machinery and reduced noise of present day aerospace engines is due to the improvement in the numerical methods from potential flows in 1970's to the current maturities of simulation methodologies to solve multi-scale and multi-physics problems. To have a focused discussion, the present article discusses the role of High Performance Computing systems in the development of various aerospace vehicles in the country.

II. Research activities on computational methods for aerospace design

The status of research activities (including the issues and achievements) on various numerical methods for the last few decades for aeropropulsive design of fighter aircraft, satellite launch vehicles and missiles in India are presented in Reference 1.

In America and Europe, different numerical algorithms were developed during 1960's and 1970's in the universities and national laboratories for solving fluid flow equations. These methods were applied to solve relatively simple geometries. In 1980's aerospace industries took major initiatives and number of industry standard Computational Fluid Dynamics (CFD) codes were developed to solve the flow field of the complete aerospace vehicle with all its geometrical complexities.

Aerospace industry is the major driver of the application of numerical methods in engineering problems in India. Numerical studies of fluid flow problems were initiated in IISc, IIT's, national laboratories and different universities in 1970's. Early works are mostly on integral equation methods (Jadavpur University and IIT, Kharagpur), Panel Methods (IIT, Kharagpur, Nation Aerospace Laboratory (NAL), Bangalore, Vikram Sarabhai Space Centre (VSSC), Thiruvananthapuram), Transonic Small perturbation equation methods, Method of Characteristics, Full potential equation methods (NAL and VSSC) etc. These results provided good understanding of flow physics in their range of applications.

The impact of numerical methods in aerospace vehicle design in Indiacould be observed after the organization of an international workshop in VSSC, Trivandrum in 1981 where number of international experts participated. A few indigenous Euler and Navier Stokes Codes were developed in VSSC for analyzing the flow field of strap-on separation from core vehicle, nozzle flow field with solid injection thrust vector control and stage separation flow field of multi stage launch vehicle.Although, these pioneering applications demonstrated the potential of numerical methods in solving complex problems in launch vehicle aerodynamics, but they did not become an integral part of the design process. No further follow-up actions were taken to improve the modeling, to validate, to make the codes user friendly. The code development activities ended with scientific papers that proclaimed, "Look, what can be done". One of the important numerical exercises that have gone into the design of launch vehicle in early years is the simulation of the effect of aerodynamics of heat shield separation test on ground [2]. The ground test results of heat shield separation were explained through numerical

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simulation and the safe separation of PSLV heat shield in vacuum was predicted. The designer had taken the numerical results on trust and gone ahead with the launch of PSLV vehicle without conducting any test of PSLV heat shield in a vacuum condition. Repeated success of PSLV heat shield separation is the testimony of correctness of the simulation approach.Recently, the work has been identified as high impact work for mission analysis in VSSC.

At the beginning, only serial computers are used with very less memory and grid generations around complex geometries were very tedious. Several thousands of simulation in 10 to 30 million grids for any practical configuration design was computationally prohibitive. Hence, the use of numerical methods was restricted to analyzing some isolated flow phenomena and not contributing significantly in the design process. The major impact of numerical methods in launch vehicle aerodynamics could be seen with the advent of Cartesian based three dimensional Navier Stokes PARAS code [3] in VSSC in mid 90's. The code enabled the use of numerical techniques for analyzing practical configurations as the grid generation efforts were highly simplified. The code was parallelized in multi-node cluster configurations using Message Passing Interface (MPI), so that quick results could be obtained as per designer's requirement. Sufficient user friendliness was incorporated to allow the use of this code by any aerospace designer. This code was used extensively to study various flow fields of launch vehicles, fighter aircrafts and missile geometries in the country.

In late 1980's, Aeronautical Development Agency (ADA) took a major initiative to unite all the CFD researchers in the country towards analyzing the Light Combat Aircraft (LCA) configurations. Number of research projects was given to all CFD research centers and were continuously guided and reviewed by designers and senior aerospace faculties. Due to this focused interaction between the designer and CFD researcher led to the development of number of indigenous 3D Euler and Navier Stokes codes for addressing various aspects of LCA design.The numerical results obtained consequent upon this effort contributed very significantly in LCA aerodynamic design right from the initial design phase. National Aeronautical Laboratory, Bangalore developed indigenous industry standard Euler and Navier stokes codes for aerodynamic characterization of their in-house aviation projects HANSA and SARAS and also to support different missile and launch vehicle programs in the country.

In 1990, initiative of Dr. APJ Abdul Kalam, the then Director, Defence Research and Develoment laboratory (DRDL), has resulted in successful applications of numerical methods in missile design. Algorithmic research in upwind methods and grid free methods by Prof S M Deshpande and his students at Indian Institute of Science in Bangalore were used in developing indigenous three dimensional Euler codes for solving various complex missile aerodynamic problems. Development of industry standard 3D grid free method Q-LSKUM [4] has facilitated the solution of many complex problems like characterization of control surface deflection, store separation of missiles from fighter aircraft, separation of petal separation at hypersonic Mach number in significant atmosphere etc. which are not easily amenable to available commercial codes.

An integrated separation dynamics suite [5] has been developed to carry out the store separation dynamics of air to air missilesmissilefrom fighter aircraft at various free stream condition. The suite consists of a preprocessor(to generate the chimera cloud of nodes and their connectivity), grid-free kinetic upwind Euler solver with aerodynamic damping (to obtain the aerodynamic forces and moments) and a 6-DOF trajectory solver (to predict the trajectory including tip-off dynamics). This suite was validated with the wind tunnel tests of a generic store separating from a wing pylon. The store separation suite is used to simulate the release of inboard and outboard missiles from the fighter aircraft at various flow conditions and safe separation of the missiles from the fighter aircraft is predicted. Numbers of release flight of the missile from the fighter aircraft were carried out without wind tunnel tests and the results matched with pre flight prediction. The results gave so much confidence to the test pilots that they insists for CFD results before testing the missiles in any new flight conditions.

State-of-the-art 3D RANS solver CERANS [6] was developed indigenously in DRD. Different advanced numerical schemes, physical modeling were incorporated to make the code very robust. Extensive validations were carried out to find its range of application and error band. The developed RANS code is routinely applied for characterization of various missile configurations in complete M - α carpet and to generate important design inputs for many complex missile aerodynamic problems. Lack of user friendliness is one the major impediments for this advanced code to be used by other aerospace designers. Development and applications of different indigenous CFD codes in aerospace industry is presented in Ref. 7.

III. Status of supercomputer in India and Abroad

Problems of high-speed computing and high memory that hindered the growth of numerical methods applications in engineering design in the yester years do not exist anymore. Teraflop/petaflop computing can be bought, built or hired. Most of the indigenous CFD codes are parallelized in multi-node configurations using open source parallel environment. These codes are scalable and portable to any kind of operating environment and producing the data for complex configurations. The status of computing platforms[8] in the world and in our country is presented in Tables 1 and 2 and a wide gap in the capacity is observed. The power of fastest computer in the world is 93 PetaflopatNational Supercomputing Center in Wuxi, China compared to 0.9 PetaflopofSahasraT (SERC - Cray XC40) computerat Indian Institute of Science, Bangalore. There is an urgent need to bridge the two orders of magnitude gap in the computing power to meet the designer's need of total characterization of aerospace vehicles through numerical simulation.

IV. National Supercomputing Mission.

Department of Electronics and Information Technology (DEITY) and Department of Science and Technology (DST) have jointly initiated National Supercomputing Mission (NSM) to make India a world leader in High Performance Computing (HPC) and to enhance the computing capability in solving grand challenge problems in national and global relevance. The goal of the mission is toempower the scientists and researchers with state-of-the-art compute facilities for their cutting edge research in their respective domain. The scope of the mission include (1) Setting up supercomputing centers of different sizes and scales matching with the demands of HPC user applications in the country (2) Supercomputing applications development through partnership (3) Creating a national grid by interconnecting various HPC systems over NKN (4) Creating cloud infrastructure for HPC user community (5) HPC manpower development and (6) Initiating R&D for next genarationExascale HPC.

Four different expert groups are created on (1) Infrastructure, (2) R&D, (3) Application development and (4) Human resources to address various development aspects of the mission. The task of expert group on application is to expand scientific and engineering application frontiers. Identification of the applications keeping in mind the requirements of end users in extramural application domains, investigation on key application breakthroughs, quantifying their societal, environmental and economical impacts and performing a gap analysis between current situation and our required targets are some of the major activities of the expert group. The group was also asked to identify key scalable algorithms, libraries targeted towards selected hardware platforms that can be used in identified applications. Seven different subgroups namely (1) Drug development platform (2) Predictive and personalized medicine (3) Materials and Computational chemistry (4) Climate, weather and disaster prediction and (5) CFD for engineering applications (6) Astronomy and Computational Physics and (7) Geophysics and Oil exploration are formed in the application group. Since, CFD applications encompasses many areas involving fluid flows, the research and application problems are being categorized into different areas such as aerospace engineering, nuclear reactor, automotive sector, civil structure design, naval application, power sector, mechanical, chemical and metallurgical processes, algorithmic research, etc. The expected outcome of the mission is one/ two order of qualitative & quantitative improvement in R&D/ higher education in science, technology &engineering disciplines,solid Foundations for supercomputing ecosystem and conducive environment for scientific breakthroughs.

V. Conversion of indigenous CFD codes from MPI to CUDA for GPGPU platforms

General Purpose Graphics Processing Units (GPGPUs) provide a low cost solution to high performance computing. GPU is especially designed for problems that are composed of data-parallel computations, that is, same operation is performed on a large set of data elements (SPMD) in parallel. As same program is executed on each data element, the need for complex control statements in the program is low. In Data-parallel processing, each processing thread works on a data element in parallel and application programs, which operate on large data sets can exploit data-parallel programming model to speed up the computations. This is also referred to as SIMT (Single Instruction Multiple Threads) architecture.

In 2006, NVIDIA introduced Compute Unified Device Architecture (CUDA), a general purpose parallel computing architecture with a new parallel programming model along with an instruction set architecture, whichtakes advantage of the parallel compute engine in NVIDIA GPUs to solve many complex computational problems in a more efficient way than on a CPU. The general CUDA programming model is shown schematically in Fig. 1.CUDA is enhanced with a software environment that allows developers to program in C/C++ as a high-level programming language. Other languages or application programming interfaces are also supported such as CUDA FORTRAN, OpenCL and DirectCompute.

The application programs for multi-core programs cannot be seamlessly and transparently scaled to exploit the increasing number of processors / cores. The main design objective of CUDA parallel programming model is to overcome this challenge, while offering a low learning curve for programmers, who are familiar with standard programming languages such as C. The GPGPU, which executes CUDA threads, is a physically separate device that operates as a coprocessor to the host running the main C program. That means, the rest of the C program executes on CPU in parallel, when the kernel is launched and executed on a GPU. Master-slave software architecture has been employed to convert a well validated indigenous three-dimensional grid-free inviscid flow solvers and finite volume viscous flow solvers to CUDA to run in GPGPU computing platforms[9]. Convergence histories and aerodynamic forces obtained from GPGPU computing are compared with that of sequential computing results and a close match between the two is obtained. Results show significant improvement (~16 X) in the performance.

VI. Conversion of numerical methods from analysis tool to design tool

Though numerical methods have matured very significantly for solving many complex problems in aerospace design, it is still used as an analysis tool. Graduation of theses computational methods from an analysis tool to design tool is a very challenging process. A five-phase approach has been suggested in the literature [10]. After the development of the demonstrator code, efficient pre processor and post processor should be added to produce user friendly, well-understood and maintainable software. In the next phase, it should enter application research, where the code developer needs to work closely with design engineer and project manager. When the computational and experimental data do not match, questions whether the assumptions made in the formulation are adequate to explain the flow physics and what additional algorithmic research, geometric preprocessing, physical modeling are required should be asked. Bypass of this stage by taking the code and placing directly with the designer must be avoided. Designer may not understand underlying theoretical models, algorithm and other numerical issues and may not use the code effectively. When the application expert, code developers and project managers have together learned the capabilities, limitations and proper applications of the code, important stand-alone design decision can be taken without supporting experimental comparison and computational codes can occupy proper position in the design tool box.

VII. Conclusions

The role of supercomputers and computational methods in engineering design is described. Aerospace design is taken as a test case and the status of the numerical methods in simulating complex flow fields is described. Although, number of computational codes with advanced numerical schemes and physical modeling are developed indigenously in various aerospace laboratories and academic institutions in the country, they are mostly used to analyse some isolated aerodynamic problems. It is perceived that considerable interaction between the designers, the code developers and the project managers is required to make these computational codes a key tool in the design activities. Although significant progress is made in the country in computer power and memory, there exists two order of magnitude gap of computer power between India and other developed countries. Recent initiatives of National Supercomputing Mission (NSM) to improve the computing power and computing ecosystems in the country are expected to reduce the gap of computing power. The number of high performance computing researchers in the country should increase significantly to handle the growing need of solution of different kind of problems involving fluid flow including atmospheric sciences, naval sciences, biomedical research, mechanical, metallurgical and chemical processes.Various natural disasters like tsunami in Bay of Bengal and Indian Ocean, wildfire in Russia, cloudburst in Lehetc are amenable to numerical simulation through HPC. Efforts should be intensified to simulate such natural calamities to provide important information to the disaster management authorities for better planning for the reduction of their impact.

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Table 1: Major computing Platforms in the world

World rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)
1	National Supercomputing Center in Wuxi, China	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9
2	National Super Computer Center in Guangzhou, China	Tianhe-2 (MilkyWay-2) - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P ,NUDT	3,120,000	33,862.7	54,902.4
3	Swiss National Supercomputing Centre (CSCS), Switzerland	Piz Daint - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries inter-connect , NVIDIA Tesla P100 Cray Inc.	361,760	19,590.0	25,326.3
4	Japan Agency for Marine-Earth Science and Technology Japan	Gyoukou - ZettaScaler-2.2 HPC system, Xeon D-1571 16C 1.3GHz, Infiniband EDR, PEZY-SC2 700Mhz ExaScaler	19,860,000	19,135.8	28,192.0
5	DOE/SC/Oak Ridge National Laboratory, United States	Titan - Cray XK7, Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x,Cray Inc.	560,640	17,590.0	27,112.5

Table 2: Major computing Platforms in the world

World Rank	Site	Name	Rmax (TFlop/s)	Rpeak (TFlop/s)
165	Indian Institute of Science	SahasraT (SERC - Cray XC40)	901.5	1244.2
260	Indian Institute of Tropical Meteorology	Aaditya (iDataPlex DX360M4)	719.2	790.7
355	Tata Institute of Fundamental Research	TIFR - Cray XC30	558.8	730.7
391	Indian Institute of Technology Delhi	HP Apollo 6000 Xl230/250	524.4	1,170.1