Chapter 8

Conclusions

Context of the work and overview

In the short and medium term, parallel computers will be essential tools for computational fluid dynamics and heat transfer. This is a challenging situation: On one hand, there is a huge computing power available to scientists. But on the other hand, to exploit parallel computers is a difficult task. The most efficient conventional algorithms are sequential and the affordable parallel computers (clusters of PCs) tend to be loosely coupled systems, i.e., high computing power compared with its network performance. The capability to use these new hardware tools to make substantial advances in the numerical simulations depends on the reformulation of existent parallel algorithms and on the design of totally new formulations to overcome the difficulties of the available hardware (e.g., high latency). The know-how acquired in this process would allow the adaptation of the algorithms to future computer architectures.

As an example, for the case of parabolic flows, an efficient parallel solver for loosely coupled systems has already been implemented (section 4.7). Next goal would be to obtain the same level of efficiency for all the flow types.

For the case of incompressible flows, the solution of the pressure correction (or similar) equations is the bottleneck of the algorithm (sections 1.2 and 2.7). The main goal of this work has been to advance in the solution of this problem rather than to implement a complete parallel CFD code. To do so, multigrid algorithm has been chosen as it is one of the best options for sequential computers. However, as discussed in section 5.1.1, it is difficult to implement on loosely coupled systems.

A review and implementation of different sequential multigrid algorithms (segregated and coupled ACM, section 3) has been carried out. ACM has been used to solve the pressure correction equation in a direct numerical simulation of a natural convection flow in a closed cavity (section 3.3.3). In this context, it has been shown that it is a better option than a band LU solver.

Different alternatives for latency-tolerant parallel multigrid have been examined (section 5). The analysis of the DDV cycle, proposed by Brandt and Diskin, revealed that the use of a direct solver for the coarsest level and the overlapping areas are important aspects. The conclusion was not so clear respect to the suppression of the pre-smoothing iterations. The cycle was extended to two-dimensional domain decompositions.

The main ideas of the DDV algorithm have been extrapolated to the ACM context (section 7). The main motivation to do so, in spite of the better performance of DDV and other classic MG approaches, has been to provide an easy path for the parallelization of DPC for the case of non-parabolic flows. The new algorithm developed has been called DDACM. From a numerical point of view, it is similar to the existent sequential solver in DPC, so it is expected to behave well with the existent applications.

The need to find a very efficient method to solve the coarsest level in DDACM led to the development of a variant of Schur complement for small, constant matrices (section 6). The opposite point of view is also possible: DDACM could be considered as a way to extend the use of Schur complement to larger problems that otherwise would need a huge amount of RAM memory (or the use of conventional approaches instead of the implementation proposed here).

Main contributions of the work

1. Development of a fast version of the Schur complement algorithm, adequate for loosely coupled parallel computers. It has been designed for the cases where a relatively small and constant pentadiagonal matrix is to be used to solve for a large number of right-hand-side vectors. After a pre-processing stage, the algorithm can be used for the fast solution of linear equation sets. Areas of application (considering the order of magnitude of the RAM memory of computers currently available) can be the pressure correction equations of incompressible flows, solved with relatively small meshes (i.e., $\approx 10^5$ control volumes), or the coarsest equation of a parallel algebraic multigrid algorithm, such as DDACM.

2. Development of the Domain-Decomposed Additive Correction Multigrid (DDACM) algorithm, an algebraic MG equivalent to the DDV. It can be considered as a combination of a parallel ACM algorithm with BILU as smoother and the previously discussed Schur complement direct solver. Another possible point of view could be to consider DDACM as a method to extend the proposed version of the Schur complement algorithm (very efficient but limited by the available RAM memory) to larger meshes. Its main features are:

    - It can be used as a black-box linear solver (like for instance Krylov subspace algorithms), allowing a clear separation of discretization and solution stages, important from the software engineering point of view.
    - It has a high numerical efficiency: the number of iterations does not increase significantly with the number of processors.
    - In the essential points, it is equivalent to ACM with an ILU smoother, so it is expected to behave well with a variety of flow problems.
    - It is tolerant to high latency networks as it does not rely on the iterative solution of coarse levels with a low number of nodes and requires less halo update operations than conventional multigrid algorithms. For the case of the largest problem considered (with 1.3×10^6 unknowns), DDACM provided a speedup of ≈ 14 with 16 processors on the JFF cluster of PCs with a conventional 100 Mbits/s network.

An important aspect of DDACM is that its essential idea, the combination of a fast direct algorithm with a multilevel solver, can be implemented using other techniques, and not necessarily BILU, Schur complement and ACM correction equations. Additionally, it can be tuned for different parallel architectures. The implementation proposed in this work can be easily changed to suit different parallel architectures. Compared with the JFF cluster used for the benchmarks:

- If network latency (respect to the floating point performance of each processor) decreases, the number of levels can be increased and other cycles with better convergence ratio (that need more halo updates) can be used.

- If RAM memory available increases, the number of levels can be decreased, using the direct solver for larger meshes.

Appendix A

Lewis Fry Richardson

Probably, the first person who imagined the use of parallel computing for numerical solution of partial differential equations was Lewis Fry Richardson. This was in 1922, before the first sequential computers. In his pioneering work, “Weather Prediction by Numerical Process”, Richardson envisioned 64.000 mathematicians working in a great hall to forecast the weather, using finite difference approximations of the governing PDEs. Outside he also imagined playing fields, houses, mountains and lakes, for Richardson belived that “those who compute the weather should breathe of it freely”. He wrote:

> “After so much hard reasoning, may one play with a fantasy? Imagine a large hall like a theatre... The walls of this chamber are painted to form a map of the globe. The ceiling represents the north polar regions, England in the gallery, the tropics in the upper circle, Australia on the dress circle and the antartic in the pit. A myriad of computers are at work upon the weather of the part of the map where each sits, but each computer attends only to one equation or part of an equation...Numerous little “night signs” display the instantaneous values so that neighbouring computers can read them. Each number is thus displayed in three adjacent zones so as to maintain communication to the North and South on the map. From the floor of the pit a tall pillar rises to half the height of the hall. It carries a large pulpit on its top. In this sits the man in charge of the whole theatre...One of his duties is to maintain a uniform speed of progress in all parts of the globe. In this respect he is like the conductor of an orchestra in which the instruments are slide-rules and calculating machines. But instead of waving a baton he turns a beam of rosy light upon those who are behindhand.”
>
> Lewis Fry Richardson, 1922 (from [195])

The famous verses about turbulence pictured as a cascade of vortices are also from his 1922 publication:

Big whorls have little whorls
Which feed on their velocity;
And little whorls have lesser whorls,
And so on to viscosity
(in the molecular sense).

Remarkably, he also studied the problem of the length of a coast as a function of the side of the polygonal line used to measure it, anticipating the concept of fractal dimension.

Appendix B

JFF Cluster at CTTC

The Beowulf cluster at CTTC is called JFF, in memorial of Joan Francesc Fernandez, computer science professor of the Universitat Politecnica de Catalunya. It is a 16 nodes cluster, to be soon upgraded to 24 nodes, with two 100 Mbit/s networks. One of them, provided with a switch, is used for MPI and the other, with a HUB, is to be used for NFS.

Specifications of the nodes

Main board	ASUS K7M (AMD-751 chipset)
Processor	AMD K7 (Athlon)
Cache Memory	128 kbytes L1 cache plus 512 kbytes outside the processor
Maximum RAM memory	768 Mbytes
Installed RAM Memory	15 "thin" nodes with 256 Mbytes; 1 "fat" node with 768 Mbytes
Swap area	8 areas of 128 Mbytes per processor
Hard disk	8 Gbytes

Specifications of the network

Network boards	Two 100 Mbits/s boards per node (3COM Etherlink fast PCI cyclone)
Switch	24 ports 100 Mbits/s (3COM Superstack II switch 3300)
Hub	24 ports 100 Mbits/s (3COM Superstack II Baseline Dual Speed hub)

Software

Operating System	Linux
Distribution	Debian 2.1
Kernel	2.2.13
MPI	LAM

Appendix C

Acronyms

ACM	Additive Correction Multigrid
AMG	Algebraic Multigrid
BACM	Blockwise Additive Correction Multigrid
BILU	Block Incomplete (approximate) Lower-Upper factorization
CFD	Computational Fluid Dynamics
CS	Correction Scheme (MG equations)
CGA	Coarse grid Galerkin aproximation
CTTC	Centre Tecnologic de Transferencia de calor
CPU	Central Processing Unit
DNS	Direct Numerical Simulation
DPC	biblioteca per al Desenvolupament de Programes aplicats a la resolució de problemes Combinats de transfèrencia de calor i massa
DDV	Domain-decomposed V cycle
DDACM	Domain-decomposed ACM
FAS	Full Approximation Storage (MG algorithm)
FCV	Finite Control Volume (discretization method)
FMG	Full Multigrid
GS	Gauss-Seidel
ILU	Incomplete (approximate) Lower-Upper factorization
JFF	Joan Francesc Fernandez cluster (Appendix B)
LU	Lower-Upper factorization
MG	multigrid
MSIP	Modified Strongly Implicit
MPI	Message Passing Interface
NFS	Network File System
PCFD	Parallel Computational Fluid Dynamics
PDE	Partial Derivative Equation
RGBS	Red-Black Gauss-Seidel
SAM	Schwarz Alternating Method
TDMA	Tri-Diagonal Matrix Algorithm

Appendix D

Main publications done in the context of this work

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14. J.Castro, L.Leal, M.Soria, A.Oliva, Calculation of enhanced water vapour absorption in falling films of LiBr aqueous solutions using the domain decomposition method, Proc. of the Fifth European Computational Fluid Dynamics Conference, Barcelona 2000
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