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ISSUES ON THE INTEGRATION OF CFD TO BUILDING SIMULATION TOOLS

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ABSTRACT

The simulation of a building behavior requires the concurrency of many physical phenomena: external flow, radiation, conduction through composite walls, internal fluid flow due to the HVAC system, infiltration and illumination, among other factors. Therefore, systemic simulation packages need to be fed with information obtained from specific software dealing with each phenomenon. Since the flow simulation (internal and external) is done through Computational Fluid Dynamics (CFD) techniques, which seems to be the most complex packages to be integrated, efforts in conflating CFD techniques with the whole building simulation (BS) package is of key interest in this area. This paper discusses aspects, considered crucial as viewed by the CFD side, for this integration and addresses an overview of the main characteristics of CFD techniques, pointing out that a careful approach must be exercised when conflating CFD tools with others systemic simulation tools.

INTRODUCTION

The so called CFD area comprises the techniques employed for the solution of fluid flows associated with heat and mass transfer, combustion, multiphase systems, radiation, etc. The development of usable CFD tools for application in engineering problems is far more complex than the development of the already complex numerical methods involved in CFD kernels. CFD is, therefore, by itself, a very rich area of research involving physics, numerical methods and computation. No suitable and successful packages, to be used in engineering applications, can be created if the three expertise involved are not treated with the same hierarchy. In the beginning of the 70s, CFD was used specifically for the solution of isolated problems requiring the knowledge of complex fluid flows associated or not with heat transfer. Aerodynamics was the leading area that has pushed the development of CFD techniques for compressible flows [1,2,3], while convection heat transfer was the major motivation for the solution of incompressible fluid flow problems [4, 5, 6], In those times any CFD solution would require the use of a supercomputer, keeping CFD away from realistic engineering problems. Integration of CFD with any other design technique would be unthinkable. Efforts in numerically calculating the isolated flow in rooms have been made since the sixties [7,8]. With the tremendous growth in the memory capacity and speed of computers, the application of CFD spread to all areas of engineering and physics. Using the new generation of desktop computers one can run any of the commercially CFD software available in the market for the solution of an engineering problem. As a consequence, the challenge nowadays is to integrate CFD to other design tools, being BS one of the areas in which strong efforts has been made in this direction [9,10,11]. This paper describes the current capabilities of the available CFD techniques, pointing out details of the methodologies and the major difficulties still precluding the full integration of CFD tools to systemic BS tools, like ESP-r[13], for example. Grid generation, discretization schemes, pressure-velocity coupling and turbulence calculation are some of the issues addressed in this paper.

LEVELS OF INTEGRATION IN BUILDING SIMULATION

The general problem of building simulation is depicted in Fig. 1, where the major heat and momentum transfer processes involved are identified. Other sub-systems, like internal wall room radiation and lighting, which also affects the indoor flow and temperature, can also be considered, as in [14]. Fig. 2, by its turn, classifies each phenomenon as sub-systems of the whole simulation system, showing the input variables. It is not mentioned but, of course, physical properties of fabrics and of the fluids must be known as input parameters.

When all these sub-systems are coupled together and solved simultaneously, one is faced with the highest level of integration for the transient simulation of a building, having the local velocity and temperature of each sub-system as the unknowns. Knowing velocities and temperatures (and its gradients), convection and diffusion fluxes can be calculated and all energy balances realized. The solution in this level would require, of course, that the time scale used attend the smallest time scale of the sub-systems. The coupling among the several sub-systems would be done through boundary conditions connecting each sub-system.

Clearly, in this level the systemic tool (the BS tool, for example,) would be a computer code to organize the solution of the sub-systems and to compute the bulk parameters required, like energy consumption, mass flow rates and so on. For each subsystem the appropriated tool would be used. For the determination of the flow and temperature fields CFD techniques would be required.

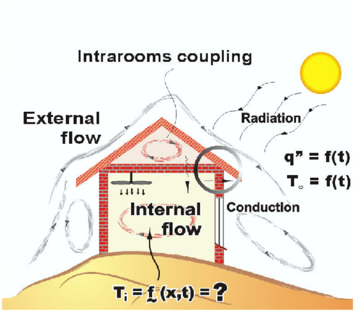

Fig. 1 – The building simulation problem

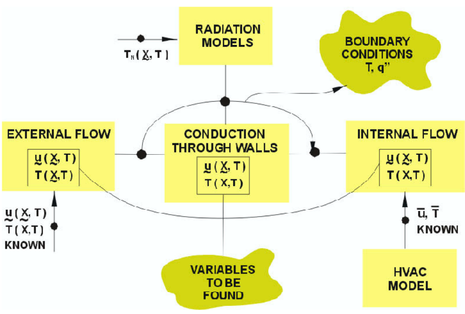

Fig. 2 – Main sub-models in a building simulation

This level of integration is not practical due to computer requirements and to the time scale of the different phenomena. An immediate lower level of integration would be to solve each sub-system in a fine discrete spatial and temporal level, integrating the results of each sub-system for the time scale used in the transient simulation. This is the level where much of the research efforts concentrate nowadays. In this level local heat flux (heat transfer coefficients) need to be known, a key question due to the existing difficulties for resolving the flow and temperature fields near walls for turbulent flows. Lower level would include lumping the domains using heat transfer coefficient from correlations (experimental+theoretical). All these discussed levels end up with the determination of the temperature with time, the variable needed for calculating the energy consumption of the whole system. It is a matter to be decided by the analyst in which level of integration the simulation need to be done.

However, not only the coupled problem (in its different level, as commented) for simulating the transient behavior is of interest. Each flow can be solved separately answering different, but not less important, building engineering questions, like the flow and temperature behavior around and inside buildings.

Therefore, one can define three major classes of problems in which CFD can be helpful in understanding building behavior:

1. The transient simulation, in its different levels, as described above. In this class it is included the level where the heat transfer coefficient need to be known accurately.
2. Calculation of the bulk flow around buildings; and
3. Calculation of the bulk internal flow.

In the second category one is interested in calculating the flow with the main purpose of determining the ventilation characteristics and the potentiality for infiltration through windows and leakages. Location of the building, its shape and windows position can be analyzed efficiently. For example, the flow pattern around a block of buildings may be also of interest for calculating regional city climate. Since the ventilation characteristics can be determined with the aid of the mean flow, no fine grids are required and the crucial problem, to be addressed later, of calculating transport properties at the walls, is avoided. The potentiality for infiltration can be calculated through the determination of the pressure coefficient and this coefficient depends mainly on the shape of the body, and not on the viscous flow, thus not requiring accurate boundary layer calculation. There are several papers published in this issue [12,15,16], demonstrating that CFD techniques are extremely useful for this type of calculation. Of course, this is not an integration, as previously defined, of CFD techniques to building simulation software.

In the third class of problems one encounters the very important issue of flow distribution inside rooms caused, principally, by HVAC system and infiltration. The feeling of comfort due to the movement of cold/hot air in the room is one of the most important parameter in the location of the HVAC air outlets and heaters. The current capabilities of CFD software can do a very good job in predicting the temperature field inside very complex building geometries [17,18], again not requiring accurate boundary layer calculation. Recall that this approach does not allow precise calculation of heat fluxes, precluding a good estimation of energy consumption of the HVAC system.

It is in the first class of problems that resides the difficulty in integrating CFD and BS tools, since the heat transfer through the walls (or the convection heat transfer coefficient) is required as boundary condition. Its determination in internal and external walls requires the knowledge of the temperature gradient, which is time dependent and need to be determined along the simulation time, in general, monthly or yearly. It also changes according to the geometry and the flow, requiring, therefore, its local determination. An accurate determination of the convection heat transfer coefficient, along with supportable CPU time and easiness in using the simulation package is the challenging task for those developing new tools for conflating CFD to BS packages.

The next section defines the problem of determining the heat transfer coefficient and its consequences in the numerical methodologies. The remaining of the paper is dedicated to describe the features of CFD techniques that are important in the integration of this type of tool to other simulation tools. As mentioned, emphasis is given on the difficulty of accurately predicting the convection heat transfer coefficient

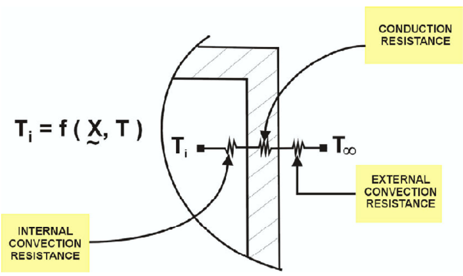

Fig. 3 – Global heat transfer coefficient

HEAT TRANSFER COEFFICIENT (h)

Fig. 3 depicts the problem of determining the heat transfer coefficient (h) to be used in a BS simulation tool. As is well known the h coefficient is a definition, used to simplify engineering calculations. To calculate this coefficient, it is necessary to determine the real physical effect, represented by the heat transfer flux. As will be pointed latter, to correctly predict the temperature gradient is crucial. There are several physical issues in determining the convection heat transfer coefficient for application in building simulation:

a) The different time scales of the whole phenomenon;

b) The flow regime inside rooms, natural/forced convection, laminar/turbulent flow; and

c) Being the flow turbulent, the physical model to correctly predicting the flow.

In other words, the absence of a reliable physical model to describe the complex internal and external flow is a obstacle for the accurate calculation of the heat transfer coefficient. Added to this, one has the numerical difficulties in calculating very resolved flows near walls.

TIME SCALE OF THE SUB-SYSTEMS

The two main transient physical processes involved in the whole problem are the heat flux through the walls and through the thermal boundary layer in natural and/or forced convection. Therefore, to analyze the time scales lets consider the transient conduction in a slab and the transient diffusion/convection in the boundary layer inside the room. The governing equation for the 1D heat conduction through a slab is given by

$$\frac{1}{\alpha}\cdot\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \tag{1}$$

Following [19], the scale analysis gives the order of magnitude for the penetration of the heat flux in the wall as

$$t \sim \frac{L^2}{\alpha} \tag{2}$$

For example for a wall with thermal diffusivity $\alpha \sim 10^{(-5)}$ m^2/s and $L \sim 10^{(-1)}$ m, the time for the heat to penetrate through the wall is of the order of 10^3 seconds, or is of the order of hours. For the transient flow inside the room consider air being heated by a change of ΔT Celsius in the wall. Again, following [19] one finds the order of the magnitude of the time required for reaching the steady state natural convection flow as

$$t \sim \left(\frac{\nu H}{g\beta\Delta T\alpha}\right)^{\frac{1}{2}} \tag{3}$$

Considering a typical room filled with air at a typical temperature, one finds that the time for reaching steady state is of the order of 10^1 seconds. This means that the time scale ratio of the two phenomena is of the order of 10^2. Numerically this implies that the natural/convection flow and the conduction in the wall need to be calculated in different time levels.

WHY FINITE VOLUME CFD METHODS?

The literature review shows that almost all methodologies in building simulation uses finite volume techniques for the CFD calculation. Although all numerical methods can be viewed as derived from the Weighted Residual Method, differing, therefore, only in the weighting function used in the integration procedure, the conservative methodologies, like finite-volume, are preferred due to its conservative properties even for coarse grids. It is clear that for refined grids all consistent methods should give the same answer. However, at the engineering and practical level very, very refined grids can not be used and conservation should be preserved for any grid size. There are two big reasons for requiring conservation at discrete level for any grid size. First, one wants to solve the partial differential equations satisfying conservation at point level, why not have, as intermediate step, a method that satisfies conservation at finite level? Doing this one is "on the road" for the solution one is seeking for. Second, the finite volume procedure of obtaining the approximate equations also produces linear systems with positive coefficients and diagonal dominance. This is helpful since even with non-robust solvers the solution can be obtained. If robust solvers are used, stability characteristics are enhanced.

MAJOR ISSUES IN THE INTEGRATION OF CFD AND BS TOOLS

The proper integration of all sub-models described in Fig. 2 requires that all models run with the same level of hierarchy and accuracy and with the same level of stability. Building simulation tools should be design for being used by engineers and architects, and therefore, ideally, it should hide the complexity and expertise of each specific area of the sub-models. In this respect CFD poses major problems for this integration, since it is a tool that deals with very complex systems of non-linear partial differential equations, and no mathematical proof is available to guarantee stability, accuracy and convergence. There are several questions that need to be addressed by the analyst when using CFD techniques. These key questions still preclude the full integration of CFD with other techniques, not only BS, if a specified level of accuracy is required. These questions and alternatives for minimizing them, by adequately managing the CFD method are described in the next section. The guidelines which follow are useful when using a commercial CFD package, as well as when the CFD tool is being developed specifically to be incorporate in a BS package.

TIME. Despite the tremendous growth in the capacity and speed of computers, the time consumed by CFD techniques, when compared to other engineering tools involved in the simulation, is significantly higher. This poses serious difficulties in the integration since time consuming needs to be similar in each sub-model. The setting up of the problem, by setting fluids, materials, and boundary conditions are a cumbersome activity in a CFD simulation. The get the geometry from a CAD system, to choose the proper grid topology and generate it is also a high consuming task that involves directly the user. Inside the numerical kernel, the time consuming for solving the linear systems takes around 70% of the whole CFD simulation time. To reduce these figures are essential. Time for setting up the problem and create the geometrical model for grid generation can be faced with the development of good interfaces. In the other hand, reducing the solver CPU time requires strong research activities in the CFD area.

STABILITY AND CONVERGENCE. The requirement for convergence of a numerical method is consistency and stability. Consistency is the characteristic of the algorithm to reduce the numerical operator to its differential operator when the discretization (in time and space), tends to zero. This means, the truncation error must tend to zero when the grid is refined. Stability is the characteristic of obtaining the exact solution of the approximate linear system of the algebraic equations. If the algorithm exhibits consistency and stability it converges, that is, you obtain the solution of the approximate equations and it tends to the solution of the partial differential equations when the grid is refined. Stability is one of the weakest points in all CFD methods, mainly due to coupling difficulties of the mass and momentum conservation equations. This issue will be addressed latter.

USER EXPERTISE. The main goal of the engineers is to have available a user-friendly software that can give correct answers in a short time. This is also, of course, the objective of software developers. In the case of CFD tools, in spite of the strong effort for developing user-friendly packages, their efficient use still requires an expert user. This represents a significant difficulty in integrating CFD to other tools. In principle, all tools, software and hardware, should only require from the user the full knowledge of the physical problem under consideration and how to use the tool. If it is required from the user deep knowledge of the methodology and excessive interaction in specialized levels, it reveals that the methodology is not "ready", requiring improvements to bring it to a level in which a professional, knowing the physics of the phenomenon and reasonable knowledge of the methodology, could use it. It is the author opinion that this is the stage of the CFD techniques nowadays. They still require too much expertise of the user. The answer for this problem is not only to create beautiful interfaces and color visualizations of the velocity and temperature fields. The problem is in fact deeply related to the mathematics of non-linear partial differential equations modeling the flow of fluids. It would be nice to be possible to choose a time step and a spatial discretization that would give us the solution with a known level of accuracy set by the user. It would be also wonderful to choose the coupling procedure that would guarantee the stability of the solution. Nowadays none of the above can be done in commercial or academic software. Instead, the CFD user runs several times his(her) problem until he(she) "feels" and gain intimacy with the problem. This "getting-used-to-the-problem" procedure involves changing time steps and size of the grid, generating new grids, changing iterations loops dealing with the non-linearities and coupling, may be altering interpolation functions, and so on. Of course, to do this with knowledge, it is required to be a CFD expert. The CFD community is aware of this difficulty and a lot of research activities are nowadays devoted in eliminating such uncertainties inherent to the methodology, with the objective of allowing CFD software to be used by a larger number of professionals and be more easily integrated to other tools.

PHYSICAL MODELING. Finally, the absence of a physical modeling able to describe the diversity of flow regimes seems to be the most serious barrier to overcome. There is a lot to be don in turbulence modeling and physical properties determination, including thermal conductivity, porosity and permeability of porous structures.

BASIC STEPS OF A CFD CALCULATION

The coming section discusses the basic steps of a CFD methodology, focusing in what need to be done in order to by-pass the drawback just mentioned.

GRID GENERATION. Grid generation, although not always recognized as this, is the most time consuming part of the procedure and the most cumbersome for the user. Putting real geometries into CAD systems to feed a grid generator is painful and time consuming. Generally, the geometry is complex and requires to be subdivided by blocks for generating the grid for each block. In building simulation this is the case, since the building contains many rooms interconnected to each other, being almost impossible to generate a single grid for all domain, unless an unstructured grid is laid out, with no preoccupation about the quality of the grid close to the walls. If no compromise exists in calculating heat transfer coefficients, the quality of the grid can be relaxed and could be introduced as a hidden procedure through a graphical interface that selects the type of the grid and the number of cells. Many simulations encountered in the literature for flows inside the whole building are interested only in the bulk flow [15,16] and, therefore, can be solved with a grid without too much concern about its refinement close to the walls.

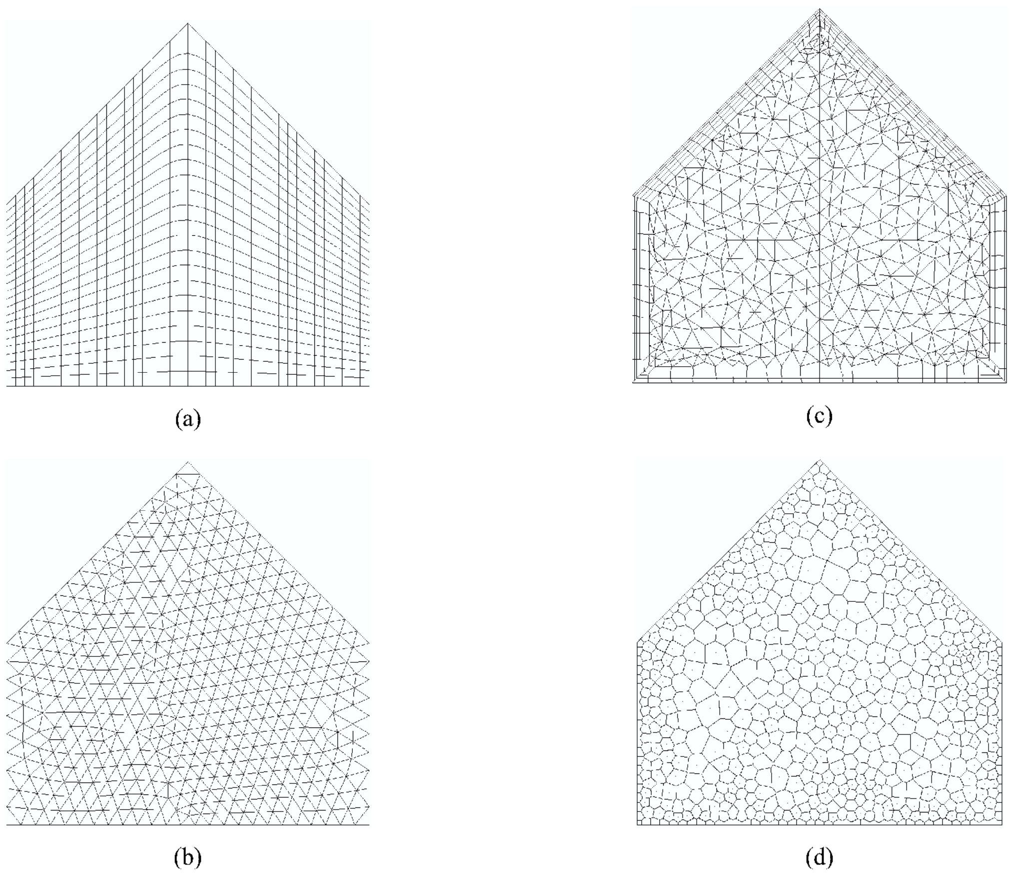

Fig 4 – Types of domain discretization

Otherwise, if heat transfer fluxes are needed, a careful grid construction, observing the physics of the flow, need to be generated. Each wall may have a different type of flow due to the presence of heaters, HVAC outlets or windows, requiring different discretization for each one. Nowadays Cartesian, general curvilinear, unstructured, mixed and Voronoi grids can be used. These grids are shown in Figs. 4.

Cartesian grids are not well suited since building geometries have complex geometries and this type of grid does not allow precise application of boundary conditions. Structured general curvilinear grids, in spite of its ability to conform complex geometries, are not able to generate a single block grid for complex building geometries. In this case multi-block generation is recommended. An alternative to the multi-block generations is to use unstructured grids of tetrahedral or hexahedral shapes, as shown in Fig. 4(b) for a 2D situation. This grid is casy to generate but introduces severe difficulties near the wall, where boundary conditions, and specially turbulence wall laws, need to be applied. This region requires a grid as regular as possible and normal to the wall, to correctly represent the stress parallel to the wall and to adequately locate the nodes obeying the y+ requirements. An alternative, already available in the commercial software is to laid-down a prismatic grid near the wall and then fill the domain with an unstructured grid, as shown in Fig. 4(c). Fig. 4(d) shows another type of discretization which is unstructured but is locally orthogonal, called Voronoi discretization. The grid construction is such that the line joining two grid points is normal do the control volume surface, facilitating the calculation of fluxes at the interfaces. Voronoi grids can also be generated such that the volumes closed to the walls follow a structured grid, as shown in Fig. 4(c) for general triangular meshes.

DISCRETIZATION ALGORITHMS. The discretization procedure is the transformation of the partial differential equation into a system of algebraic linear equations. In fluid flow with heat transfer calculations this amounts in obtaining a set of linear systems, each one representing one of the conservation equations. The usual procedure for obtaining the approximate equations using finite volume techniques can be found in several books [20,21,22], and amounts in integrating the conservation equation, in its conservative form, in time and over the finite volume, or realizing a balance of the property in the finite volume. The conservation equation for a general scalar ϕ can be written as

$$\frac{\partial}{\partial t}(\ \phi)+\frac{\partial}{\partial x}\left(u\phi - {}^{\phi}\frac{\partial\phi}{\partial x}\right)+$$
$$\frac{\partial}{\partial y}\left(v\phi - {}^{\phi}\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(w\phi - {}^{\phi}\frac{\partial\phi}{\partial z}\right)=S^{\phi} \quad (4)$$

where for ϕ equal to 1, u, v, w and T, the mass, momentum and energy conservation equations are recovered. Additional equations are constructed to account for turbulence. In the k-ε model, for example, two extra partial differential equations are needed, for k and ε. In the calculation of pollutants dispersion, the general scalar variable represents the concentration of the species. The integration of Eq.(4) in time and over the control volume shown in Fig. 5, taking, for illustration purposes, only the advective and diffusive terms in the x-direction, gives

$$\ldots\left[\ u\phi\,\big|_e - u\phi\,\big|_w\right]\ y+\ldots=$$
$$\left(\ {}^{\phi}\frac{\partial\phi}{\partial x}\Big|_e - {}^{\phi}\frac{\partial\phi}{\partial y}\Big|_w\right)\ y+\ldots \quad (5)$$

As can be seen by the above equation, fluxes (advective and diffusive) are the natural information to be given at the finite volumes interfaces. Since the variable ϕ is not known at the interface an interpolation function must be used. The interpolation function is a key choice of the numerical technique. It tries to represent the behavior of the exact solution between grid points. If the interpolation function is the exact solution of the partial differential equation, the resulting numerical equations give the exact solution, independent of the number of volumes used for the discretization. Take for example, the transient flow in a slab discretized using a central differencing scheme in space and forward differencing in time. For the steady state regime, the numerical solution is identical to the analytical solution, independently of the number of control volumes.

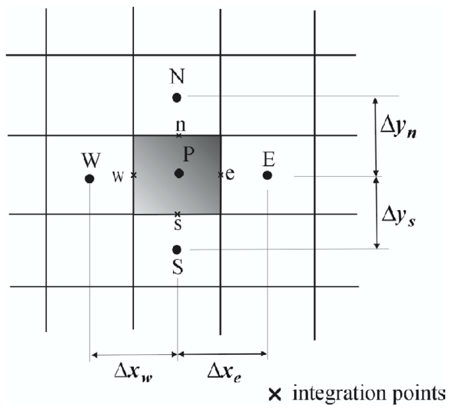

Fig. 5 – Cartesian control volume

Therefore, the interpolation function is responsible for the truncation error embodied in the numerical solution. The truncation error is the most important one, since it vanishes, as the grid is refined. The interpolation function also influences the stability of the numerical scheme. If an upwind scheme (UDS) is used, the solution may suffer from numerical diffusion, smearing all gradients in the domain. This is highly undesirable when one is interested in calculating quantities that involve gradients, like heat fluxes. Upwind schemes, in the other hand, stabilize the solution, avoiding oscillations and possible divergence. Avoiding divergence is essential if one wants to integrate the CFD tool and have it employed by non-expert users. High order schemes, like central differencing schemes (CDS), in the other hand, due to its non-dissipative nature [21] may introduce undesirable numerical oscillations, a numerical pathology which makes the solution to present over and undershoots. In this case gradients are better calculated than using UDS, but the value of the function can be severely affected. If the magnitude of the temperature is sought, the numerical answer may be far from the expected value. The commercial packages offer several choices for the users to select a interpolation function. As accuracy and stability is demanded, computer time also increases, normally in a non-linear fashion. After choosing an interpolation function, the ϕ values and its derivatives at the control volume interfaces are substituted in Eq. (5) resulting in an approximate equation of the type

$$A_P\phi_P = A_e\phi_E + A_w\phi_W + A_n\phi_N + A_s\phi_S + B \qquad (6)$$

where the central coefficient is given by

$$A_P = \sum A_{nb} - S_P\ V + \frac{V}{t} \qquad (7)$$

where S_P comes from the linearization of the source term [20] by

$$S = S_P\phi + S_C \qquad (8)$$

Having SP negative the matrix will be diagonal dominant, an important feature of the finite volume methods. One should always try to maintain this characteristic.

Eq. (6) can be written as

$$\left[A^{\phi}\right]\left[\phi\right] = \left[B^{\phi}\right] \qquad (9)$$

where the entries of the matrix A depends on ϕ, due to the non-linear character of the conservation equations. An equation similar to Eq. (6) is written for each variable resulting in a set of linear algebraic equations to be solved.

An excellent alternative for developing CFD codes with generality is to use the Control Volume Finite Element approach. In this technique several important features are reunited:

a) The scheme is conservative, as in any other finite volume method. Therefore, all properties of conservative scheme are assured.

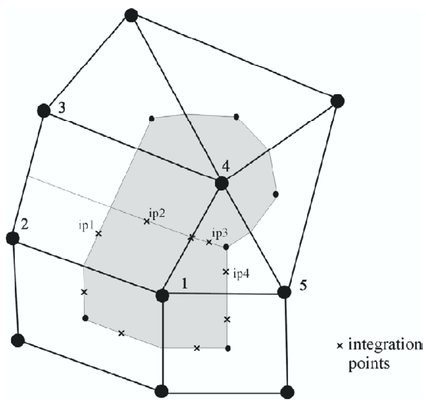

Fig. 6 - Control Volume Finite Element Approach

b) Grid generality is attained, since unstructured grids that can be mixed with structured ones. Prismatic and tetrahedral grids can be put together without cumbersome codes, and
c) The conservation equations are constructed using the element-by-element assembly, very popular in finite element methods. This characteristic renders to the method the possibility of using the most advances computational strategies, like C++ object oriented programming, helping the integration to other tools and the construction graphical user interfaces and visualization.

Fig. 6 shows a control volume mixing quadrilateral and triangular grids (hexas and tetras in 3D), depicting the integration points. At the integration points the values and the derivatives of the dependent variables are interpolated. Comparing Figs. 5 and 6 one sees that in the usual finite volume method one has only four integration points, against eight in the CVFEM approach. Recall that the number of integration points is related to the accuracy of the numerical scheme. Integrating Eq.(4) and using appropriated interpolation functions one obtains a similar equation to Eq. (6), given by

$$\begin{aligned} A^{uu}u + A^{uv}v + A^{pu}P &= B^u \\ A^{uv}u + A^{vu}v + A^{pv}P &= B^v \qquad (10) \\ A^{pu}u + A^{pv}v + A^{pp}P &= B^p \end{aligned}$$

where, in this case, interpolation function involving u v and p where used [35]. To introduce u, v and P in the interpolation function allows create a strong coupling between these variables, permitting coupled solvers to be used. As stated before, the stability of the iteration procedure is a strongly desired characteristic of the methodology for integration.

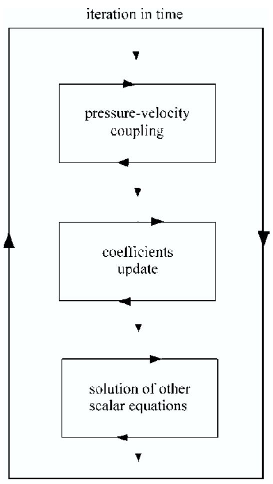

Fig. 7 – Iteration levels

BASIC ITERATIVE LOOPS OF A CFD METHOD. The iterative loops of a CFD calculation are strongly dependent of the approach used for treating the coupling between the conservation equations. The most important coupling to deal with is the pressure-velocity coupling, that is, how the pressure field drives the flow such that mass conservation is satisfied. Since the majority of the commercial CFD codes employ a segregated procedure, that is, each linear system are solved independently, the iterative loops for this approach will be discussed. In this case iterations are necessary for taking into account the coupling between the variables and the non-linearity of the partial differential equations, expressed by the matrices coefficients that depend on the variables. Solving each equation separately and if the flow is incompressible, a pressure-velocity coupling is required. The most known pressure-velocity coupling method are the SIMPLE[20] and SIMPLEC[23] methods.

These methods replaced the mass conservation equation by an equation for pressure. Considering a transient incompressible flow, the simplest iterative loops of a procedure, according to Fig. 7, are:

a) The iteration loop in time
b) The pressure-velocity coupling loop
c) The loop for updating the coefficients
d) Loops for updating other scalar variables.

It is possible to save considerable CPU time if these iterations loops are conveniently used. For example, if the variables do not change too much in time, or if the time step is small, compared with the time scale of the problem, it is possible to linearize the equations, using in each time level all coefficients calculated with the variables from the previous time level. The pressure velocity coupling, by its turn, involves the solution of three linear systems, normally solved iteratively. During the solutions of these linear systems, keeping the coefficients frozen, it is not wise to iterate too tightly in the linear system solver, since the coefficients are from a wrong solution. If for every u, v and p calculation, the coefficients for u, v and pressure are updated, this identifies a procedure where the pressure-velocity coupling and non-linearities are taken into account simultaneously. Choosing to have different loops for u-v-p coupling and non-linearities, we may freeze the coefficients for a number of iterations, allowing the solution to find its way in solving the pressure-velocity coupling. Scalar like temperature, turbulent quantities, species conservation, etc., requires similar analysis, defining when such quantities are going to enter the iterative procedure. Some scalar variables may be kept frozen for a number of iterations, while others need to update each iteration. For buoyancy flows, for example, since the driving force of the flow is the temperature difference, it is known [26] that the coupling between temperature and velocity is important. In this case temperature need to be solved in the same hierarchy as velocity, as opposed to forced convection flows, where temperature may be kept frozen, being activated only when fluid physical properties need to be updated. This velocity-temperature coupling is seldom considered in CFD packages. The above discussion demonstrates how difficulty is to have default parameters that always work in a CFD package, with no need of relying on the expertise of the user for the success of the calculation.

COUPLED VERSUS SEGREGATED SOLVERS. One of the major causes of slow convergence and proneness to divergence of CFD codes is the quality of the coupling procedure for pressure and velocity. It is widely reported in the literature that the use of segregated approaches employing SIMPLE-like pressure velocity-coupling methods does not confer robustness to the whole numerical method. When solving in a segregated manner, each variable needs to have an evolution equation in order to be advanced during the iteration procedure. It is natural that the evolution equations for u and v be the x and y momentum equations.

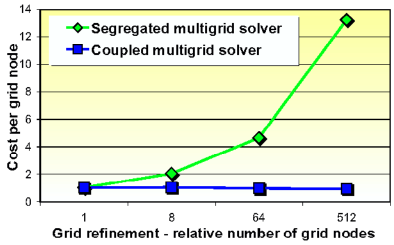

Fig.8-Coupled solver x Segregated solver

As a consequence, pressure does not possesses an evolution equation, since it is not present in the mass conservation equation. This poor link between pressure and mass conservation introduces serious difficulties in the solution, especially for the segregated ones. The alternative is to solve u-v and p in a coupled fashion. A description of a collection of methods for this purpose is described in [27]. A more attractive approach is to create the coupling between mass and momentum equations through the interpolation function and then solving velocity and pressure simultaneously

Fig.8 shows the cost per grid node of a commercial software when the solution is obtained using a segregated and coupled approaches with the linear system solved using a multigrid method. It can be seen that the effort does not increases as the grid is refined for the coupled solver, opposed to the exponential growth of the cost when the segregated solver is used. Fig. 9 shows, for the same package, the cost per node in the solver of the linear system as the grid is refined. Again it can be seen that the multigrid is highly superior when compared with a line and conjugate gradient solver. These results show that coupled solvers with efficient methods for the solution of the linear systems are needed if one wants to integrate CFD packages to other simulation tools. Recall that strong convergence characteristics and small computer time are the two main requisites to be obeyed by a good CFD package.

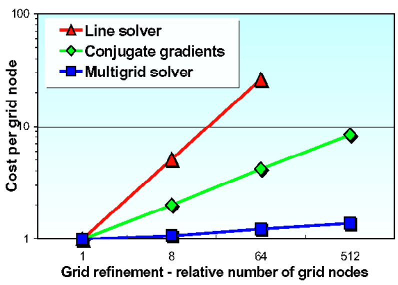

Fig. 9 – Solver comparison

PARALLEL PROCESSING. Parallel computation is another strategy in use to decrease the CPU time in the simulation of large problems. With the increase in the use of cluster of PCs, it will become reasonable for professional to have four or eight machines running in parallel. Parallel features are already available with a speedup near to the optimum, i.e., the speedup is almost equal to the number of processors. Certainly, this is a feature that will become a default in any competitive CFD package.

TURBULENCE. So far we have spoken about numerical difficulties that hinders the full integration of CFD to other simulation tools. However, the difficult in modeling the real physics of the airflow inside the building is the most challenging problem. For room the nature of the flow is very diverse, due to the different driving forces that are encountered in building simulation, like HVAC and heaters, combined with existence of windows and air infiltration. Room airflows exhibit fully turbulent flows close to HVAC outlets, mixed flow regimes, if heaters are present, re-circulation regions and even laminar flows. The effects of turbulence inside rooms are well-known, since it promotes mixing and influences the comfort conditions [28]. Turbulent flows are unsteady, irregular, 3D and composed of many different scales in time and space. The last five decades of efforts from the fluid mechanics community, although good progress was made, did not result in a closed method that applies to the different flow regimes. Besides the difficulty in modeling the physics of the turbulence, the existing turbulence models require special treatment near the wall, then associating physical with numerical difficulties, the later ones already discussed in this paper. There are few levels of complexity being considered for the solution of turbulent flows. Direct Numerical Simulation (DNS), Large Eddy Simulation (LES), RANS (Reynolds Averaged Navier-Stokes Equations). DNS proposes to solve the momentum equations considering the time and space scales of turbulence in the simulation. This represents and enormous computing task since time steps and grids would be extremely small. For example, for Reynolds number equal to 10^7, it would require $7x10^7$ grid cells, representing an effort of 10^{16} times the required for a RANS simulation [29]. LES, by its turn solves the large scales and models the small scales. Filters are required to select the small scales to be modeled. It is more general than RANS but requires finer resolution near the wall. It may be applied for airflows near HVAC outlets, since it is better suited for jet flows than for boundary-layer flows. It is still required a model for the small scales. RANS simulation is the most widely used among the engineers, since average quantities are usually of interest. The averaging procedure gives rise to the Reynolds stress tensor that requires modeling. In this class of methods one encounter the well known k-ε, k-ω, Low-Re k-ε, Low-Re k-ω. The discussion of turbulence models is outside the scope of this work. The interested readers are referred to a recent work comparing several turbulent models for engineering applications [30]. The literature shows that the existing tools that integrate CFD to BS tools rely mostly on recommended empirical and experimental correlations for the heat transfer coefficients that feeds the model. Examples of experimental correlations for isolated walls as well as walls integrated in a room can be fond in [31,32] among others. It was found in [31] that the available correlations for isolated surfaces have large discrepancies when compared to each other. Comparing these correlations for real size enclosures they also show differences. A strong statement is that since many dynamic simulation packages uses correlations for isolated surfaces, care should be exercise by the analyst when using such correlations. These differences may put in danger the full results of the simulation in terms of energy consumption of the building.

PERSPECTIVES AND CONCLUSIONS

The discussion presented demonstrated that good progress has been made in integrating CFD techniques to BS tools. It was also identified that for attaining efficient integration and to spread the use of simulation methodologies among the different professionals involved in building behavior analysis, it is required improvements in the modeling of the physics and in the CFD numerical kernels. In the side of the physics, turbulence modeling is the challenging task. As state, in spite of the tremendous efforts devoted for the developing of new models, none of them can fulfill the engineering needs. In the case of building simulation, the different internal flow regime precludes the use of a single turbulence model in the simulation. The k-ε, even with the known difficulties is the most widely used. New models, like k-ω and SST shows good promises, at least for the tests conducted for industrial flows. DNS, that would bring generality, is yet not practical. Another tendency observed recently in the development of numerical tools is that excessive generality should be avoided. This approach would greatly help the development of more robust and confident tools. For example CFD tools can be specialized for analyzing the problems of classes 2 and 3 mentioned before. Calculation of flows around and inside buildings is a routine nowadays, but it is required customized software for these classes of problems.

In the numerical side, methodologies did not follow the growth and speed of the computers. Like in turbulence modeling, although good progress was made, most of the numerical stability and convergence problems still remain. The reason is because one is faced with a very complex coupled non-linear system of equations. The difficulties for solving this system of equations are enormous, and require a joint effort among fluid dynamicists, applied mathematicians and computer scientists. If a close look at the CFD literature is given, one sees that very little contribution from applied mathematicians are embodied in the available CFD software. The fault is a lack of interaction between engineers and applied mathematicians. On the contrary, enormous contribution from computer science is embodied in the packages, as can be seen by the powerful graphical interfaces. New programming strategies are also under way, where oriented object programming is offering the possibilities of constructing software with easier improvements and reusability. These programming facilities do not take part yet of commercial tools.

Since building simulations tools are to be used by engineers, architects and other professionals, training in the physics and numerical aspects involved is essential. Therefore, teaching software with expert graphical user interfaces should be developed [34] for training purposes. Students also should have contact with such methodologies and training programs.

Finally, it is important to say that the tool to be used in any engineering problem depends on the quality of the answer you want. Depending on the level of accuracy, you may be satisfied with a "reasonable" solution obtained in a coarse grid. This decision, however, can only be made based on the expertise and knowledge of the user.

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