Influence of time step length and sub-iteration number on the convergence behavior and numerical accuracy for transient CFD

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ABSTRACT

The aim of this investigation is to study the time step length and the sub-iteration number, which can be optimized, for the integration of the Reynolds averaged Navier-Stokes equations to improve the accuracy of numerical models. Two cases have been chosen as test examples. It has been concluded that a smaller time step with a few outer-loop iterations is better than a too large time step with more outer-loop iterations.

1. INTRODUCTION

Fluid flow phenomena can be classified into unsteady and steady problems. To simulate the unsteady problem, a time step is applied to integrate the Reynolds averaged Navier-Stokes equations. For steady problems, a time step can be taken as a relaxation to increase the robustness of the solver.

Obtaining accurate results at the lowest CPU cost is always the expectation of computational fluid dynamics (CFD) engineers. The proper selection of the time step length and the number of sub-iterations within one time step, also called outer-loop iterations, is an important factor that affects the speed of convergence and the numerical accuracy.

It is well known that taking a large time step for the numerical simulation can save CPU time for transient cases, but at a cost of numerical accuracy. The computation can even diverge if the time step is too large for cases with complex geometries or cases with high Reynolds number. Increasing the outer-loop iteration number can be a remedy for the losses of numerical accuracy resulting from the time step increase. However, large sub-iteration numbers result in much longer CPU time. There is a trade-off between the time step length and outer-loop iteration numbers, in terms of the convergence speed and numerical accuracy.

The aim of this investigation is to study the influence of the time step length and the sub-iteration number for the integration of the Reynolds averaged Navier-Stokes equations, to improve the accuracy and efficiency of the numerical simulation of transient flow phenomena.

For a transient case, if accurate information during the whole transient process is expected from the numerical results, every time step must be converged to obtain sufficient accuracy for the whole process. The time step can be calculated from the CFL (Courant-Friedrichs-Lewy) number[1-2], also called Courant number:

$$CFL = \frac{u\Delta t}{\Delta L}$$

Where u is the characteristic speed, Δt is the time step, ΔL is the size of the control volume. Theoretical study has shown that, to get a stable simulation the largest CFL (or Courant) number anywhere in the flow field must strictly obey[1-2]:

$$CFL < CFL_{critical}$$

To optimize the time step, the optimization of CFL number is essential, which is both algorithm and problem dependent. Typical allowable values of CFL $_{critical}$ for simple, perfect gas, viscous flow with implicit time integration range from 0.1 to 1.2[1-2].

For a transient case, if the information only at a certain time instant is needed, the results at other time instants do not necessarily have to be fully converged, provided that the final result is converged. If the iteration is stable, larger CFL number can be used, say 1 to 100, which is case dependent. As the complexity of the flow conditions, geometry, and physical model increase, the maximum allowable CFL may be reduced.

Two classes of transient flow were considered in this study: buoyancy-related turbulent flow and forced turbulent flow. All the cases are computed on a PC with an 1800MHz Athlon processor.

2. BUOYANCY DRIVEN FLOW

For mixed convection flow that buoyancy effect is related, the experiment of ventilated fire in enclosures by the Lawrence Livermore National Laboratory (LLNL)[3] is taken as an example.

Cox and Kumar[4], Lockwood and Malalasekera[5], Yan[6] simplify the wall heat conduction into one-dimensional problem and take the thermal penetration depth as a known value, satisfactory temperature profile was obtained for the fluid domain.

In this paper, a compromised approach, which takes the exterior wall heat transfer coefficient and the ambient air temperature as the input data, is applied for the modeling. The computation domain is extended to the exterior surface of the solid wall to compare with the physical case. Thermal radiation was modeled by the P1 model, which is built in CFX5. Heat conduction, convection and thermal radiation is integrated together in the numerical modeling.

For this case, only the flow field and temperature field at 20 minutes (1200s) after the start of the fire is of our interest, and the quantitative comparison of temperature field is made at this time instant.

Figure 1 is a view of the geometry of LLNL fire case.

The ventilation airflow rate is 0.5m^3/s. A constant heat source of 400 kW is taken to represent the heat generated from the fire after its ignition. For the computation of the LLNL test case, the total element number is 170,000. Unstructured mesh is applied, the mesh size ranges from 0.018m to 0.3m. Shear Stress Transport model (SST) built in CFX-5 is used for turbulence modeling. Second-order high resolution differencing scheme is employed for the spatial discretization.

To compare the performances of different combination of time step length and sub-iteration number, four cases have been setup as shown in table-1. Temperature data along the east rake and west rake are extracted from each case. The east rake is a vertical line that extends up to the ceiling vertically from a point, which is situated in the mid-way between the fire source and the wall that has no gas exit. The west rake is a vertical line that extends up to the ceiling vertically from a point, which is situated in the mid-way between the fire source and the wall that has a gas exit.

In calculation case FIRE1, we choose a time step of 5 seconds, and an outer loop iteration of 5, the computation just diverged before 1200 seconds is reached. This is because the time step is too large and the residuals are accumulated. In calculation case FIRE2, we decrease the time step to 0.5 seconds, and we additionally reduce the outer loop iteration to 3, computation is converged and numerical results can be obtained.

To improve the numerical accuracy and to save CPU time, a non-constant time step is applied in the cases FIRE3 and FIRE4. This means, smaller time step is applied in the initial stage, as shown in table 2, because the development of flow field and temperature field is fast.

Figure 2 shows the iso-surface of the temperature in the room. It reveals that within about 30% of the region in the room, the air temperature is above 230˚C.

Figures 3-4 give a comparison of temperature distribution in vertical direction along east rake and west rake. Numerical simulation was conducted with a time step of 0.1-0.5s. An outer-loop iteration number of 3 and 1 are taken for Case FIRE3 and FIRE4, respectively. It can be judged visually that both cases can get good results, with case FIRE3 more accurate than FIRE4. This shows that smaller time-step can avoid diverge, and three outer-loop iterations in case FIRE3 can improve the numerical accuracy.

3. FORCED FLOW

For the forced flow, the well-known vortex shedding downstream of a square cylinder[7], is taken as an example. Physical time simulated in this study is 500 seconds. To obtain the accurate transient result, the whole transient process must be accurately modeled. The standard k-ε model is taken for the modeling of small-scale turbulence. The shedding frequency, the amplitude of the lift force coefficient and the averaged drag force coefficient are taken as the comparison criteria.

Figure 5 is the grid layout of the whole computation domain. Fine mesh is employed in the region near the wall of the square cylinder, and mesh is coarser in the region far from the wall. The total element number is 23680 with the grid size ranging from 0.015m to 0.8m. Only two elements are taken in the third direction. The yplus value near the square cylinder surface is between 0 and 45. The square cylinder measures 1m×1m×1m, uniform inflow of 0.3m/s is placed 10m upstream of the cylinder. The outlet is located 20m downstream of the square cylinder. To eliminate the effect from the boundary conditions, the computation domain is extended 10m above and below the cylinder. Reynolds number based on the cylinder size is about 22,000.

Table-3 gives an overview of the computation plan and the CPU costs.

The computation case VS1 takes a time step of 0.5s with a sub-iteration number of 3. Computation started from a uniform-velocity initial condition. Steady vortex shedding frequency develops 300 seconds later. Figures 6a and 6b show the development of the drag and lift force coefficients obtained in case VS1.

In computational case VS2, the time step length is increased to 1s, at a sub-iteration number of 3, the vortex shedding remains. Figures 7a and 7b show the transient flow field at one time instant, which are computed using a time step of 1s, a sub-iteration number of 3 (case VS2).

The vortex shedding frequency is represented by the non-dimensional Strouhal number, which is one of the validation criteria for the vortex shedding case.

$$St=fL/U_0$$

Where f is shedding frequency, L is square cylinder size, and U_0 is the upstream airflow velocity.

The numerical result obtained from case VS1 is St=0.135. Amplitude of lift force coefficient C_L is 1.18. Averaged drag coefficient C_D is 1.85. These values agree fairly well with the experiments (Igarashi, 1987: St=0.139, C_D=2.24, C_L=1.2), except that the drag coefficient has larger discrepancies.

In case VS3, the time step length is increased to 2s, the sub-iteration number remains unchanged. Even though the computation stated from the result of case VS1, the vortex shedding dies down gradually. In case VS4, the time step length is the same as case VS2, the sub-iteration number is increased to 6, and the computation started from the well-developed vortex shedding result of case VS1, the vortex shedding wake also disappears gradually, as shown in figure 8a and 8b. This means, increasing the sub-iteration number cannot serve as a remedy of the accuracy loss resulted from the increase of time step, though case VS4 and case VS2 takes the same CPU time.

Based on the numerical test on the above-mentioned cases, it can be concluded that smaller time step with a few outer-loop iterations is favorable to large time step that combines with more outer-loop iterations. The time step choosing should take CFL as a reference, which is case dependent.

4. CONCLUSION

Appropriate time step is given by the CFL condition. In the view of convergence, a small time step is always favorable to a large one. A large time step with more outer-loop iterations is not suggested because of its poor convergence performance, while a smaller time step with a few outer-loop iterations is recommended.

5. REFERENCES

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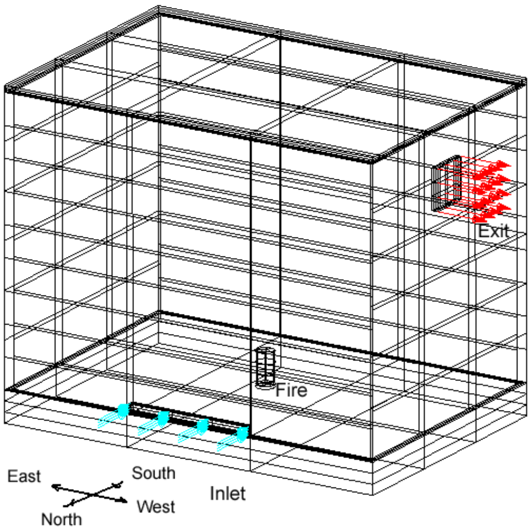

Figure 1: Schematic of the test room(LLNL, 1984)

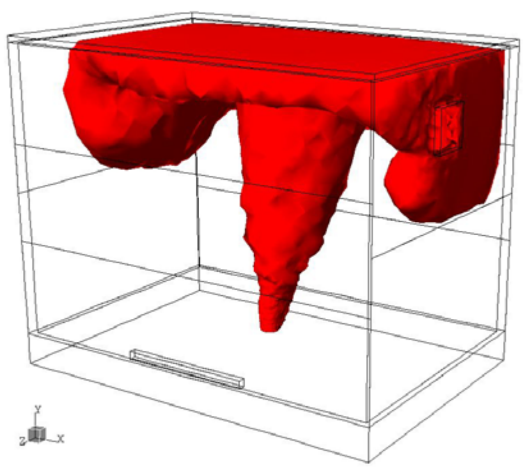

Figure 2: Iso-surface of gas temperature at 230˚C

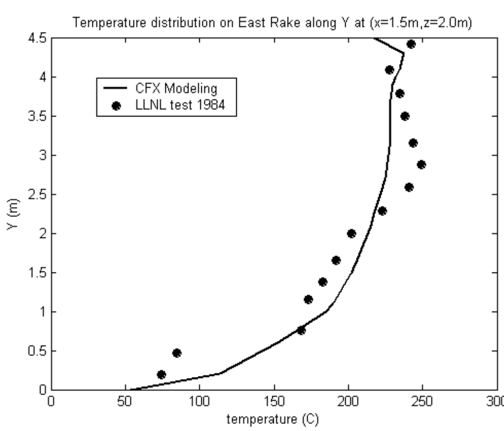

Figure 3a: East rake of FIRE3

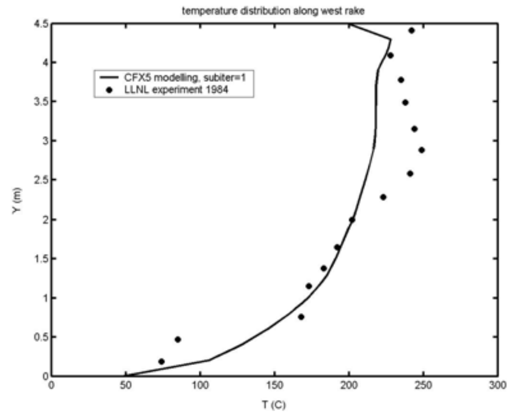

Figure 3b: East rake of FIRE4

Figure 3: Comparison of the temperature on east rake of case FIRE3 and FIRE4

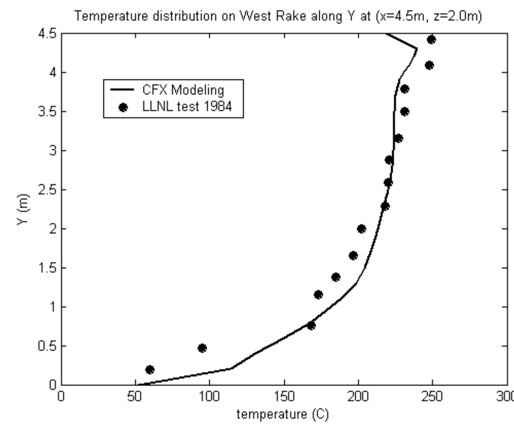

Figure 4a: West rake of FIRE3

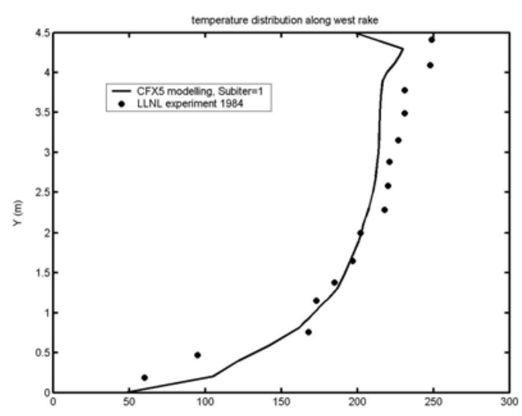

Figure 4b: West rake of FIRE4

Figure 4: Comparison of the temperature on west rake of case FIRE3 and

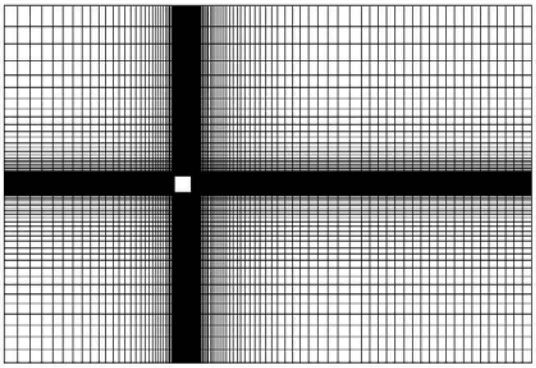

Figure 5: Grid layout

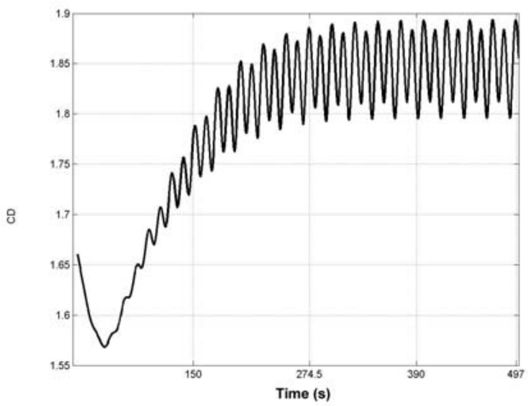

Figure 6a: Drag force coefficient C_D

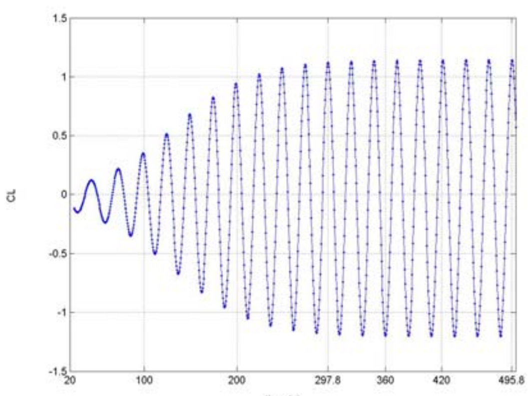

Figure 6b: Lift force coefficient C_L

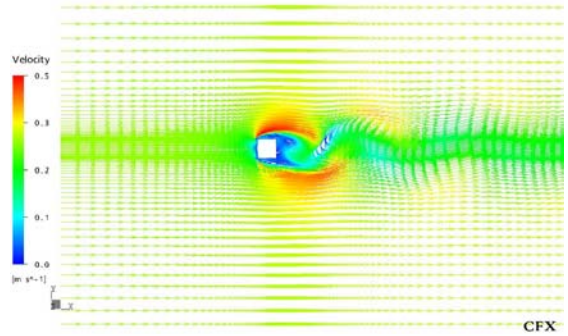

Figure 7a: Velocity vectors of vortex shedding captured in case VS2

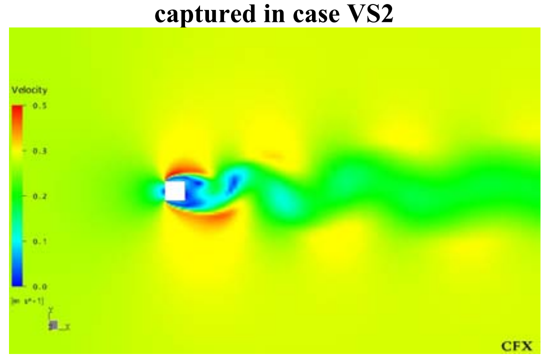

Figure 7b: Velocity contours of vortex shedding captured in case VS2

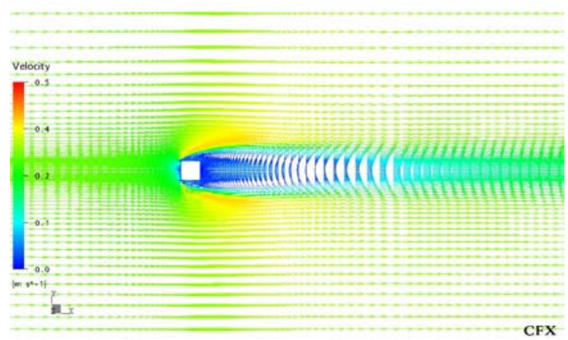

Figure 8a: Velocity vectors: Vortex shedding disappears in case VS4

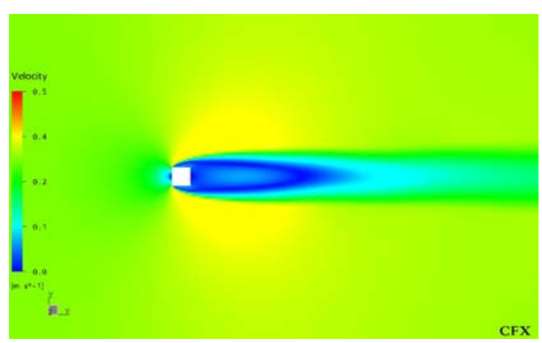

Figure 8b: Velocity contours: Vortex shedding disappears in case VS4

Table-1: Numerical study of ventilated fires

Case #	Time step (s)	Maximum CFL	Sub-iterations	Total number of time steps	CPU time
FIRE1	5.0	66	5	240	diverge
FIRE2	0.5	6.6	5	2400	140 hours
FIRE3	0.1~0.5	1.3 ~ 6.6	3	3140	120 hours
FIRE4	0.1~0.5	1.3 ~ 6.6	1	3140	42 hours

Table-2: Time step length and iteration number for cases FIRE3 and FIRE4

Physical time	Time step length	Total number of time steps	Sub-iteration number		Total number of Iterations	
			FIRE3	FIRE4	FIRE3	FIRE4
0-60s	0.1s	600	3	1	1800	600
60-120s	0.2s	300	3	1	900	300
120-180s	0.3s	200	3	1	600	200
180-1200s	0.5s	2040	3	1	6120	2040
Total time step number		3140	Total iteration number		9420	3140

Table-3: Numerical test of vortex shedding case on an Athlon 1900MHz PC

Case #	Time step	Maximum CFL	Sub-iterations	Total number of iterations	CPU time/result
VS1	0.5s	10	3	3000	9 hours/shedding
VS2	1.0s	20	3	1500	4.5hour/shedding
VS3	2.0s	40	3	750	2.2 hours/steady
VS4	2.0s	40	6	1500	4.4 hours/steady