Date	December 12, 2001	Memo Number	STI:01/10
Subject	**Sheldon's ANSYS Tips and Tricks: Flotran Enhancements at 6.0**		
Keywords	Flotran, SIMPLEN, COLG		

1. Introduction:

There have been several enhancements to Flotran at 6.0. These changes include more robust default settings, an additional advection scheme, a new coupling algorithm, and improvements to the ALE mesh morpher.

2. Robust Default Settings:

In Flotran incompressible thermal problems, the solution of the PRES (flow) and TEMP (energy) DOF often drive the solution. Prior to 6.0, the solver defaults were usually not satisfactory for two cases: use of tetrahedral meshes and conjugate heat transfer problems.

Tetrahedral meshes result in diagonally dominant matrices. Because of this ill-conditioning, the PCG iterative solver would solve the equations too 'easily' because of the loose solution tolerance (1e-7). The user often had to manually tighten the convergence criteria (FLDATA21). At 6.0, this convergence for PRES DOF using the PCG solver is 1e-12, which provides adequate accuracy for most problems.[1]

Conjugate heat transfer problems also result in ill-conditioned matrices because the conductivity of solid (e.g., aluminum) is often several orders of magnitude greater than that of the fluid (e.g., air). At 5.7 and prior, the TDMA solver was used for TEMP DOF. The TDMA solver is an approximate solver which does not have a convergence criterion. This was suitable for fluid-only problems, but not if solid elements were present, due to the ill-conditioning as noted above. At 6.0, the PGMR solver is now the default for TEMP DOF with a convergence accuracy of 1e-12, providing a tight enough criterion to solve models with both fluid and solid materials.

The SUPG approach is now the default method for the advection term discretization for the momentum, turbulence, and energy equations. Recall that for the general transport equation, we have transient, advection, diffusion, and source terms. The transient and advection terms can also be thought of as stemming from the full derivative of a variable ϕ with respect to time:

$$\frac{D}{Dt}\left(\rho C_\phi \phi\right) = \frac{d\rho C_\phi \phi}{dt} + \frac{d\rho C_\phi \phi}{dx}\frac{dx}{dt} = \frac{d\rho C_\phi \phi}{dt} + \frac{dv_x \rho C_\phi \phi}{dx}$$

The transient term is the first term (change with respect to time), and the advection term is the second (carried with fluid). Although MSU was the default at 5.7 and behaves much more smoothly, it is only first-order accurate. The SUPG method is second-order accurate; however, it may behave in an oscillatory manner, so, if that is the case, the author recommends running with MSU for a few iterations, then switching to SUPG.

3. New Features of 6.0:

There are three enhancements to Flotran at 6.0, which include a better ALE mesh morphing algorithm, an additional advection scheme, and a new coupling algorithm.

The ALE mesh morpher is now an elasticity-based. This simply means that, instead of morphing the mesh locally, the mesh morpher modifies elements adjacent to the ALE boundary conditions, producing less distortion and a much smoother internal mesh motion.

The COLG advection scheme (FLDATA33) is very similar to the SUPG approach.[2] However, the COLG method provides exact conservation for even coarse meshes (unlike SUPG, which is much more mesh-dependent). The COLG could be used for the energy equation in incompressible flow problems, if the SUPG method is not accurate enough for a given mesh density.

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[1] For users familiar with PCG solver usage in structural applications, please note that the structural PCG solver convergence tolerance (EQSLV) is the square root of the Flotran convergence criterion. In other words, the default PCG solver convergence tolerance is 1e-8 for structural problems but 1e-6 (sqrt(1e-12)) for CFD analyses.

[2] See Theory Manual, Section 7.2 "Derivation of Fluid Flow Matrices", for more details on advection schemes.

Flotran solves the nonlinear set of conservation equations (e.g., mass, momentum, energy) with a segregated solution algorithm, unlike most other ANSYS physics, which solve them in a coupled manner.[3] This means that each DOF is solved separately in each global iteration using a specific solver.

The segregated solution method is based on the work of Schnipke and Rice, called SIMPLEF. An enhanced algorithm called SIMPLEN has been added to Flotran at 6.0 (FLDATA37). The SIMPLEN algorithm improves convergence behavior for laminar problems with strong pressure-velocity coupling, although the author has found that it speeds up convergence for some other types of problems as well.

The SIMPLEN algorithm actually changes many default settings in Flotran, so the user should be aware of this when activating the new algorithm. The solver for the momentum and turbulence equations is usually TDMA, but because SIMPLEN relies on more accurate calculations of VX, VY, VZ, ENKE, and ENDS, the PBCGM solver is used instead. The relaxation factors are also adjusted since under-relaxation is not desired if the values are being solved for more accurately. Lastly, the advection scheme for turbulence equations are set to MSU instead of SUPG.

To illustrate an example where SIMPLEN improves the convergence behavior, the author used a simple valve model with one inlet and two outlets, as shown in the top right figure. The solution was run until the normalized rate of change of all DOF was below 1e-2.

With the default SIMPLEF method (including new solver and advection scheme defaults of 6.0), the solution converged in 63 global iterations, as shown in the middle right image. The total CPU time was 2256 seconds.

The solution was rerun with the SIMPLEN method and its default settings. The model converged in 37 iterations, taking 1462 CPU seconds.

Although the SIMPLEN method took longer per global iteration (39.5 vs. 35.8 seconds per iteration), because of changes to the default solvers, the overall solution time was much less since the convergence behavior was improved.

The author has found that not all models benefit from use of SIMPLEN, although most laminar flow problems or ones with strong pressure-velocity coupling benefit most from the enhanced algorithm.

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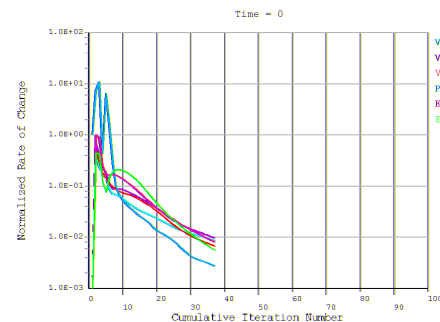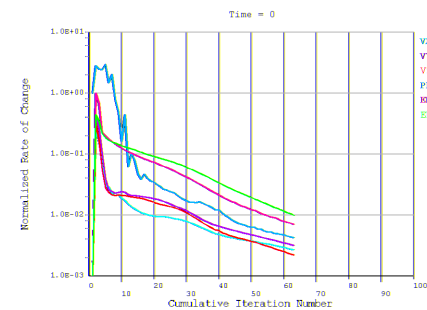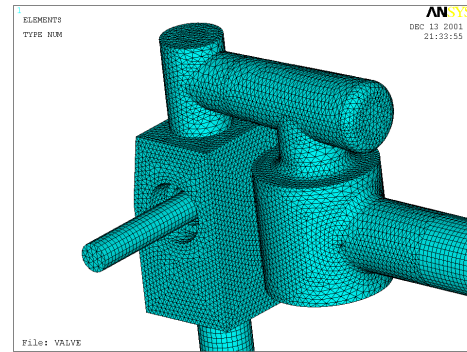
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[3] Either matrix- or load-vector coupling is used for most problems in ANSYS except for Flotran and sequential coupled problems, the latter of which utilize the PHYSICS environments and APDL.

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