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Exploiting New Features of COMSOL Version 4 on Conjugate Heat Transfer Problems

Abstract Users of COMSOL Multiphysics at version 3.5a and earlier have enjoyed many features that have provided not only a good user experience at the graphical user interface (GUI), but also the capability to solve many classes of problems in a consistent manner with the physics being simulated. With the new release version 4.0 and later (4+) of COMSOL, the user is provided a dramatic new interface from which to interact, and many new features "under the hood" for solving problems more efficiently and with even greater accuracy and consistency than before. This paper will explore several of these new version 4+ features for the conjugate heat transfer class of problems. Our environment is challenging in that we demand high-quality solutions for nuclear-reactor systems and the models tend to become large and difficult to solve. Areas investigated include turbulence modeling, distributed parallel processing, solver scaling, and OpenGL graphics issues in a Linux computing environment.

Keywords conjugate heat transfer, parallel processing, solver settings, Linux, COMSOL

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1 Introduction

The COMSOL application area for this paper is the High Flux Isotope Reactor (HFIR) of Oak Ridge National Laboratory (ORNL) which we have introduced in earlier COMSOL conferences[1–5]. The present research emphasis at HFIR is to investigate all aspects of the transition from a highly-enriched uranium (HEU) fuel to a low-enriched uranium (LEU) fuel. The foundation for this research has been laid with direct comparison between the present design and safety basis codes[6, 7] using both version 3.4 and 3.5a of COMSOL. New details of this work are the subject of additional papers in this conference.

When transitioning from v3.5a to v4+ of COMSOL, we naturally have adapted to the dramatic new graphical user interface (GUI), or COMSOL desktop as it has come to be called. The focus of this paper is not on the GUI, but rather, upon several improvements that have been made to the underlying physics, solution techniques, and hardware interfaces that we typically utilize. All of these changes will directly effect the problem class of conjugate heat transfer and coupled structural mechanics analysis.

2 Low Reynolds Number Extension to $k-\varepsilon$ Turbulence Model

Our current focus is on conjugate heat transfer in the fuel plate regions of HFIR. The flow region of interest is fully turbulent with Reynolds number defined and computed based on inlet fluid conditions and channel width:

$$\begin{aligned} Re \equiv \frac{\rho u D}{\mu} &= \rho(p = 468 \text{ psia}, T = 140\ ^\circ\text{F}) \\ &\times 15\ \frac{\text{m}}{\text{s}} \times\ 0.050 \text{ inches} \\ &\div\ \mu(p = 468 \text{ psia}, T = 140\ ^\circ\text{F}) \\ &\approx 4 \times 10^4 \end{aligned}$$

Most importantly, the rigors of our nuclear regulatory environment requires thorough knowledge of the solution up to and through the wall condition. With the introduction of the new CFD module of COMSOL-4.0a, a new turbulence model has been included which is called "Low Reynolds

Number $k-\varepsilon$ Turbulence Model." Hereafter in this paper, this model will referred to as the "Low Reynolds number extension." The COMSOL manuals refer to the phrase "low Reynolds number" as the region close to the wall where the viscous effects from laminar flow dominate and the turbulent flow effects are essentially not present. This new model "provides equations for resolving regions of slow flow (close to the walls) far better. ... It should be used in models where the effects of walls are important. This is particularly relevant for applications in non-isothermal flow where the heat flux at solid-liquid interfaces is important to the final solution." Therefore, the new COMSOL Low-Reynolds number extension to the turbulence models is of strong importance to our work.

A simple 2D problem, depicted by Figure 1, is used to demonstrate the new improvements in the turbulence modeling of COMSOL 4.0a in a similar manner to a HFIR fuel plate. The central area is a water coolant channel $= 0.050$ inches wide. Coupled to each side of the coolant channel is a half-width aluminum-6061 plate. Only the first 2.0 inches of the channel are modeled, thus providing for ample length to obtain full development of the turbulent profile. Since $\frac{L}{D} \approx 20$ is considered adequate for full development in channel flows, the present design of $\frac{L}{D} \approx 40$ should be more than adequate to be fully developed. A uniform volumetric heat source $(\dot{q}''')$ is applied to the solid material at a rate of $\dot{q}''' = 10^{10} \frac{W}{m^3}$. The boundary conditions are shown in Figure 1 typical of a HFIR heat transfer condition. The mixture of units is representative of both the flexibility of the COMSOL input and the reality of the systems analysis of a research nuclear reactor.

The material properties input into COMSOL are specific for the HFIR and are analyzed nonlinearly in full detail as a function of temperature and pressure where applicable (water).

Note that this model definition is similar, but not completely accurate of, a HFIR geometry. For example, the actual HFIR fuel plate is 24.0 inches in length, with an unfueled entrance and exit length of 2.0 inches. Further, the material within the plate is uranium-based and distributed in a designed manner and then clad with aluminum. These HFIR-specific details are not necessary for this demonstration, but are certainly to be included in the final design and safety analyses.

Both v3.5a and v4.0a are compared in several simulated cases with identical mesh design. With sufficient mesh refinement near the wall, it was realized that exact wall offset mesh matching was not necessary. Therefore, in creating the mesh an "extremely fine" free mesh is used initially which is altered from the default to provide a minimum of 16 elements in thin regions. Then a boundary layer mesh is imposed on the wall with a COMSOL parameter set of 15 elements (number of boundary layers), a 1.2 boundary layer stretching factor, and a unit thickness adjustment factor. For the single case of a "Low Re, fine mesh", the boundary layer mesh in the coolant is mirrored on the adjacent solid plate side of the wall condition. A graphical view of the mesh at the flow exit is given in Figure 2.

In v3.5a of COMSOL, the wall offset must be specified in either dimensional or non-dimensional form. The recommended range of validity for the COMSOL v3.5a models is $30 < y^+ < 100$. This range is exceeded by specifying $y^+ = 10$ and then $y^+ = 6$ in order to compare to the v4.0a temperature profiles. The "wall function" choice of wall condition in v4.0a (non-Low Reynolds extension or non-Low-Re) is the nearest equivalency to the v3.5a setup, with the exception that the wall offset is not configurable, but rather, computed automatically. Two additional cases, a coarse and fine mesh, are examined with the new v4.0a Low-Re extension. The distinction between the coarse and fine mesh is in the solid mesh at the boundary (mentioned previously).

The resulting steady-state velocity distribution at the 2D exit plane is shown in Figure 3. The major difference between the six cases investigated are the extension of the velocity profile from the wall offset region to the wall where the velocity is zero due to the no-slip condition imposed. Minor differences in the velocity are apparent along other portions of the profile which can be examined using the electronic copy of this paper.

Of primary interest with respect to the new Low-Re extension to the turbulence modeling is the temperature distribution as shown by Figure 4. The previous wall function approaches used in v3.5a and v4.0a (non-Low Re) result in a "jump condition" between the coolant temperature adjacent to the wall, and the wall surface temperature of the solid. Recall that this condition was imposed in v3.5a and earlier by conserving the heat flux as a boundary condition between two separate subdomains of the COMSOL model. Alternatively, the Low-Re extension resolves the laminar sublayer and provides for a complete temperature distribution throughout the solution domain. Therefore, instead of two variables to track as in v3.5a (T_s and T_f), only the single variable T is required in the Low-Re extension of v4.0a. Right at the wall, where the heat flux is conserved on either side, the gradient of the temperature is defined by the ratio of the thermal conductivity of each material (solid and fluid-turbulent).

In addition to the completeness of the temperature distribution (the temperature is continuous through the fluid-solid interface and no "jump condition" exists as in the purely wall function formulation that existed in version 3.5a of the code) we also find significant difference in the magnitude of the temperature in the solid region. Indeed, the v3.5a $y^+ = 30$ profile in the solid region is a minimum of 30 K higher than the other cases investigated in this problem which is the recommended lower bound for y^+. Yet we find that $y^+ = 10$ under v3.5a will yield approximately the same solid temperature profile as the v4.0a "wall function" model for this problem. In order for a v3.5a solution to be comparable to this v4.0a Low-Re model solution, $y^+ = 6$ is required. And finally, a COMSOL v4.0a user might be advised that additional mesh may also be required in the solid region in order to arrive at the intended accuracy of the model.

3 Distributed Parallel Processing

In order for the computer-code analysis of HFIR components and systems to be accepted by the DOE sponsors, they must meet certain quality assurance (QA) requirements. The method by which we satisfy these requirements has been presented earlier[2]. One of the verification problems included in this work concerned the performance of COMSOL in a shared-memory parallel processing environment. This same problem was attempted at v4.0-beta2, in which not all features were fully available. Therefore, a very similar 3D representative problem was executed instead. We hope to repeat this verification case with v4.0a now that all the features are available.

In the new COMSOL v4+, distributed parallel processing (DPP) capability is available for the `MUMPS` direct solver. The family of iterative solvers are not yet compatible with distributed parallel processing in COMSOL v4.0a and earlier. Therefore, an appropriately-sized problem must be scoped in order for DPP solutions to be obtained.

Our Linux cluster is maintained to comply with ORNL security requirements using the Red Hat Enterprise Linux (RHEL) v5.3 operating system which of course includes the necessary MPI libraries to allow for the distributed parallel mode between each cluster node and shared-memory mode within each node of the cluster. We have 8 compute nodes and a single control node in the cluster. Each node is made up of dual amd64 processors with 4 cores each. Therefore, we have a total of 64 compute cores and 8 control cores in the cluster. Note that on a per-node basis, shared memory parallel processing is utilized by COMSOL. Since 64 GB of memory is available on each compute node (8 GB on the control node), a fairly large problem may be solved. We expect soon to double the number of compute nodes with the same 64 GB base size of the shared memory which seems to be an appropriate size. We also intend to increase our communication speed between nodes through installation of an infiniband system. We have found (as a rule of thumb) that a segregated iterative solver in v3.5a will fully utilize $\approx$ 40 GB of shared memory for a fully-coupled fluid-solid non-isothermal conjugate heat transfer problem of $\approx$ 6 million degrees of freedom (DOF). We have not yet determined the rule of thumb limits for v4.0a.

The DPP verification problem investigated here is 3D Navier Stokes with coupled heat transfer through a turbulent wall boundary. The problem evaluates all material properties in the typical non-linear manner including hydrogen as the flowing fluid for added compressibility. The geometry is a simple pipe. The mesh is sufficiently refined with a free-mesh texahedral elements and added boundary-layer meshing to adequately capture the boundary layer. The resulting problem yields a total of 180206 DOF. The reference solution on a single node and single core uses $\approx$ 8667 cpu-seconds, and $\approx$ 10.6 GB of memory.

A script was written to process the reference solution through all 64 possible configurations of DPP possibilities on our cluster and results were saved to individual log files containing the iteration output produced by COMSOL. From this information a set of compute speed-up and memory utilization data were generated and plotted as “carpet plots” in Figures 5 and 6 respectively. Examining the speed-up plot, one can find the expected increase in speed-up with increasing number of nodes and cores (processors/node). Along the line for a single node, one can verify a purely shared-memory speed-up to be consistent with previous findings [2] for v3.5a. Note that for increasing nodes, COMSOL v4+ suffers from the classic overhead losses experienced by all codes of the DPP type. Based on Figure 5 alone, one might speculate that the speed-up of COMSOL v4+ might be approaching a plauteau near the cluster maximum of 64. Indeed, a fluctuation in speed-up is evident at about 6 nodes and 8 cores suggesting a “sweet spot” in efficiency. In order to be certain, we must test on a larger number of nodes. Nevertheless, a significant speed-up of $\approx$ 5.7 can certainly be achieved with COMSOL v4+ on this cluster.

The companion memory utilization shows decreasing memory requirements per node as the number of nodes is increased. As one might expect the level of memory requirements also increases with increasing number of cores. The memory reduction for the complete cluster suggests on the order of a factor of 3 might be expected for this cluster on a problem of this class. Therefore, it is expected that a direct solution of conjugate heat transfer problem that requires about 192 GB (3×64 GB) on a single node might be solvable on this cluster using DPP.

4 Solver Scaling

It has been the experience of the authors that the solver in COMSOL version 3.5a and earlier has benefited tremendously by the use of manual scaling in the advanced tab of the solver settings. Typically for conjugate heat transfer problems the values used for the scaling are a nominal maximum expected value of each state variable in the set. For example, the 2D problem discussed in Section 2 might use the following scaling settings in version 3.5a:

$$\{u\ 20\ v\ 20\ p\ 1.0e5\ log(k)\ 10\ log(d)\ 10\ T_s\ 400\ T_f\ 400\}$$

The new Version 4+ still offers manual scaling as an option. However, there has obviously been some improvements in the automatic scaling setting, and in addition, a new option of “parent” scaling is available.

The model problem discussed in Section 2 was evaluated for various scaling settings for both versions 3.5a and 4.0a with the results shown in Table 1. Version 3.5a has consistently shown significant improvements as shown below for the manually-scaled case. However, in version 4.0a, the same level of improvement in convergence rate has not been verified. Indeed, the automatic scaling shows essentially the same performance as the manually controlled scaling. The new parent scaling in version 4.0a showed a slightly lower convergence rate for this problem. The state variable definitions changed in version 4.0a, so there may be some further improvements we could achieve in manual scaling.

version	type	iteration
v3.5a	manual	45
v3.5a	auto	70
v4.0a	manual	66
v4.0a	auto	68
v4.0a	parent	75

Table 1 Scaling Performance Comparison for COMSOL

5 Retaining OpenGL Capability in the Linux Environment

The new version 4+ of COMSOL made significant improvements in the GUI. Among these improvements, the developers took advantage of the generally improved graphics standard brought about by both the open- and closed-source communities (OpenGL and DirectX respectively). We found several of our Linux workstations/servers were not able to run with COMSOL 4+ unless the "software" option was chosen for the graphics perferences. Since this reduced level of performance was not desirable, COMSOL technical support was contacted and asked about the minimum level of the OpenGL standard necessary to achieve compliance for COMSOL 4+ on the Linux platform; and the answer was ... OpenGL v1.5 and higher.

As we studied the Nvidia graphics hardware on our Linux systems, we discovered that only a single graphics card, which was our newest Nvidia card, was meeting this standard. All of our Linux systems were using the distributed Nvidia driver packages of the latest stable releases of either Debian or Ubuntu. We deleted these standard packages and decided to install the latest drivers available directly from Nvidia for each of the graphics cards. Even though the diversion from the standard packaging system is not desirable, these updated drivers installed cleanly and worked great. Indeed, all of our Linux systems now meet the new OpenGL requirements for COMSOL 4.0a, and we did not need to purchase any new additional hardware.

6 Conclusions

We have found many powerful improvements thus far in our upgrade path while learning the new features of COMSOL 4+. We expect the Low-Reynolds number extension of the turbulence models to yield more realistic results for our conjugate heat transfer problems. Our problems are large and time consuming to solve, so we look forward to taking advantage of the new distributed parallel processing capability available in version 4.0a. The previously-used manual scaling in version 3.5a appears to be unnecessary in version 4.0a. The OpenGL graphical rendering capability of COMSOL could be achieved by either deploying the latest hardware or by upgrading key software drivers. This avoids the lower-performing "software" graphics option which is the alternative without modern OpenGL compliance. We look forward to finding other new and improved features of this latest version in COMSOL.

7 Graphical Results

Figures 1 through 6 inclusive, which have been referenced earlier, are inserted below. Each figure is inserted such that the reader may verify details by examination of the electronic copy (.pdf format) included with the conference proceedings.

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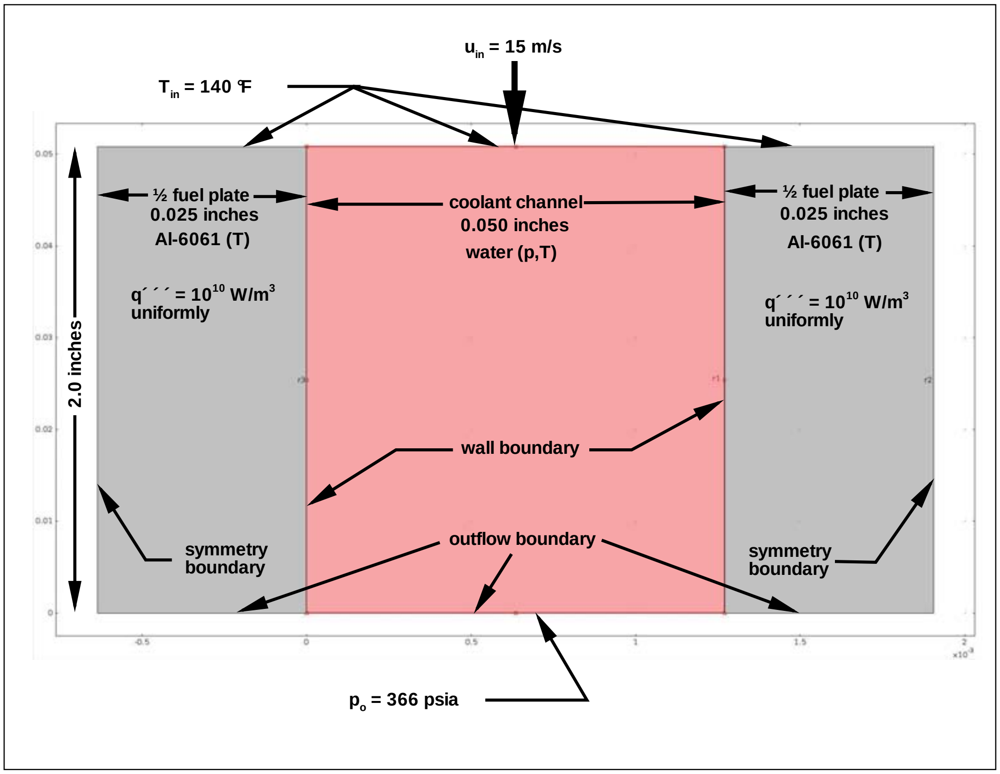

Fig. 1 Representative conjugate heat transfer problem definition.

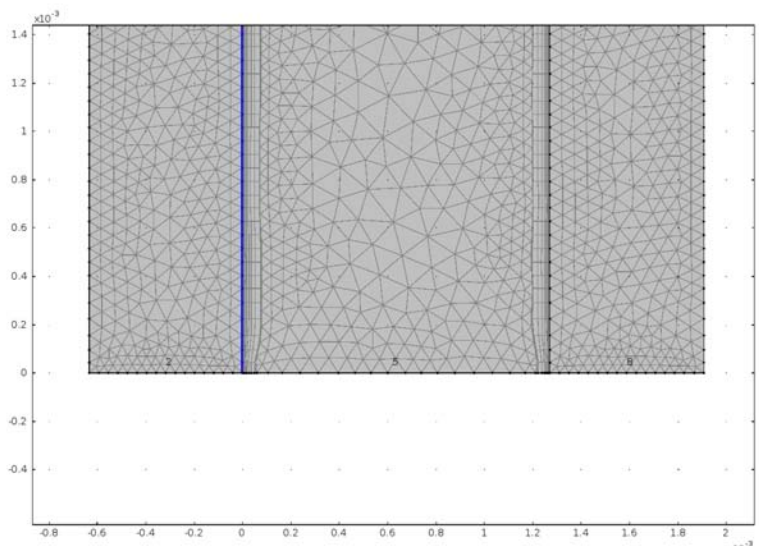

Fig. 2 Mesh design used in the model problem for COMSOL turbulence model comparison.

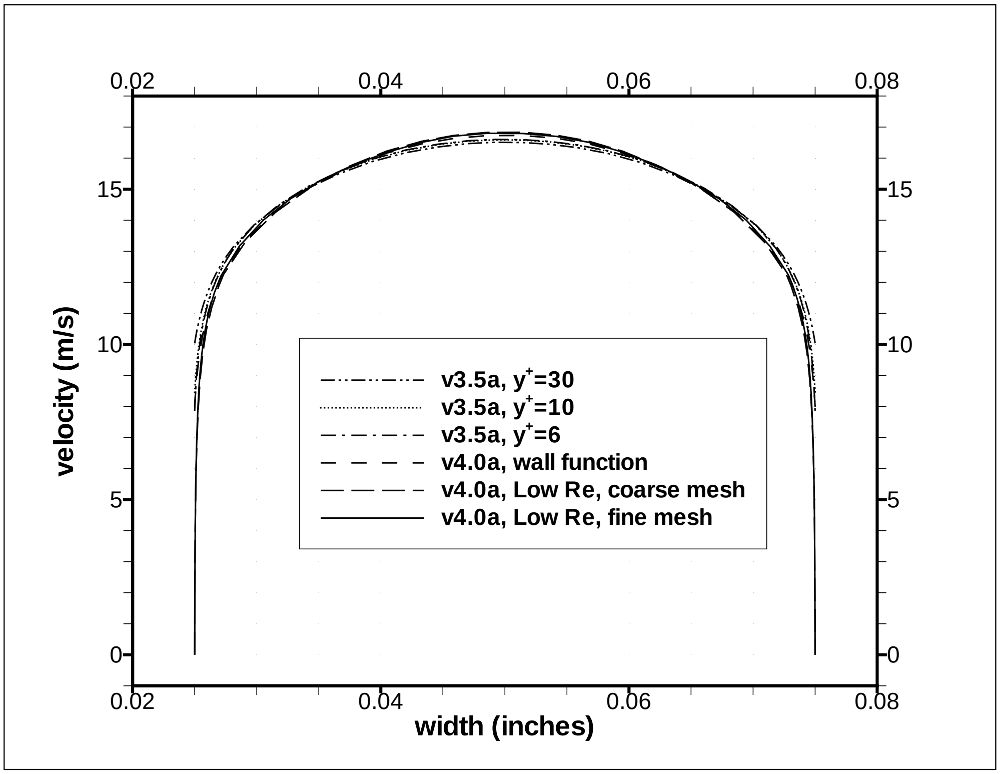

Fig. 3 Velocity comparison between COMSOL versions v3.5a and v4.0a with turbulence model sensitivity on a representative conjugate heat transfer problem.

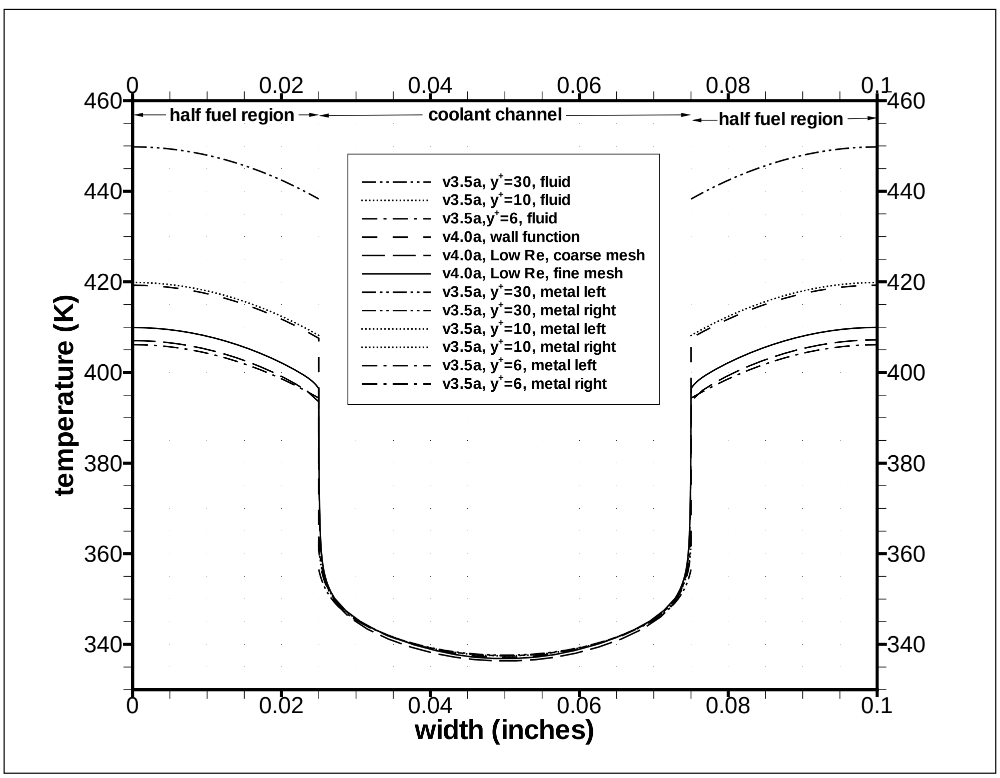

Fig. 4 Temperature comparison between COMSOL versions v3.5a and v4.0a with turbulence model sensitivity on a representative conjugate heat transfer problem.

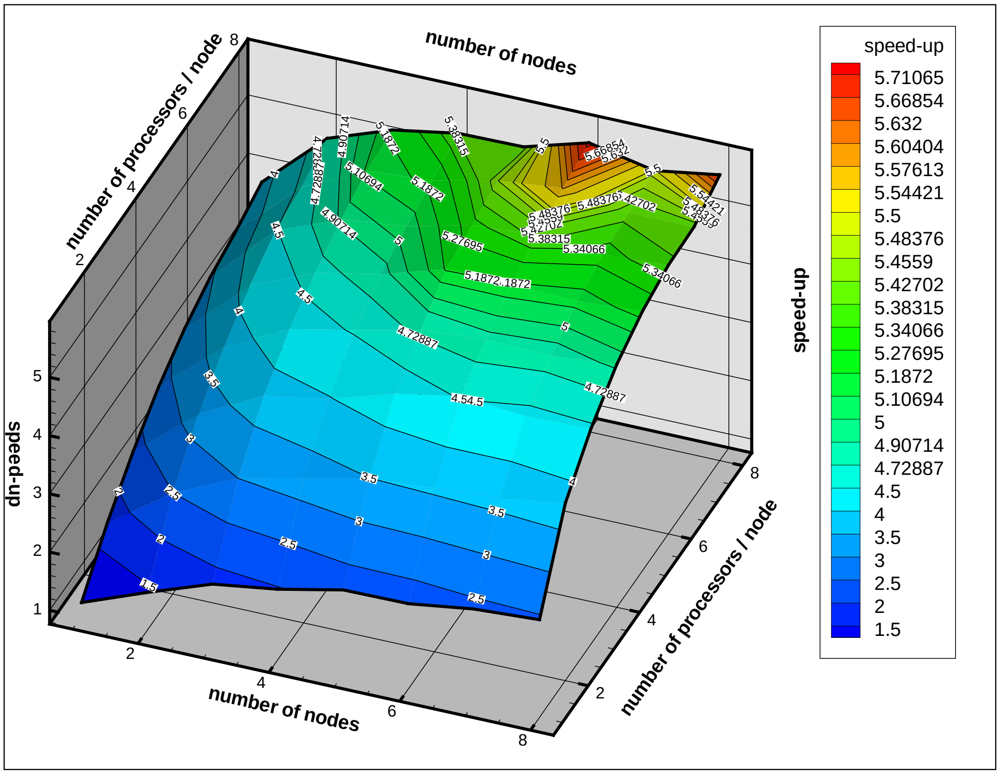

Fig. 5 Distributed parallel processing speedup using COMSOL v4.0-beta2 on a representative 3D conjugate heat transfer problem.

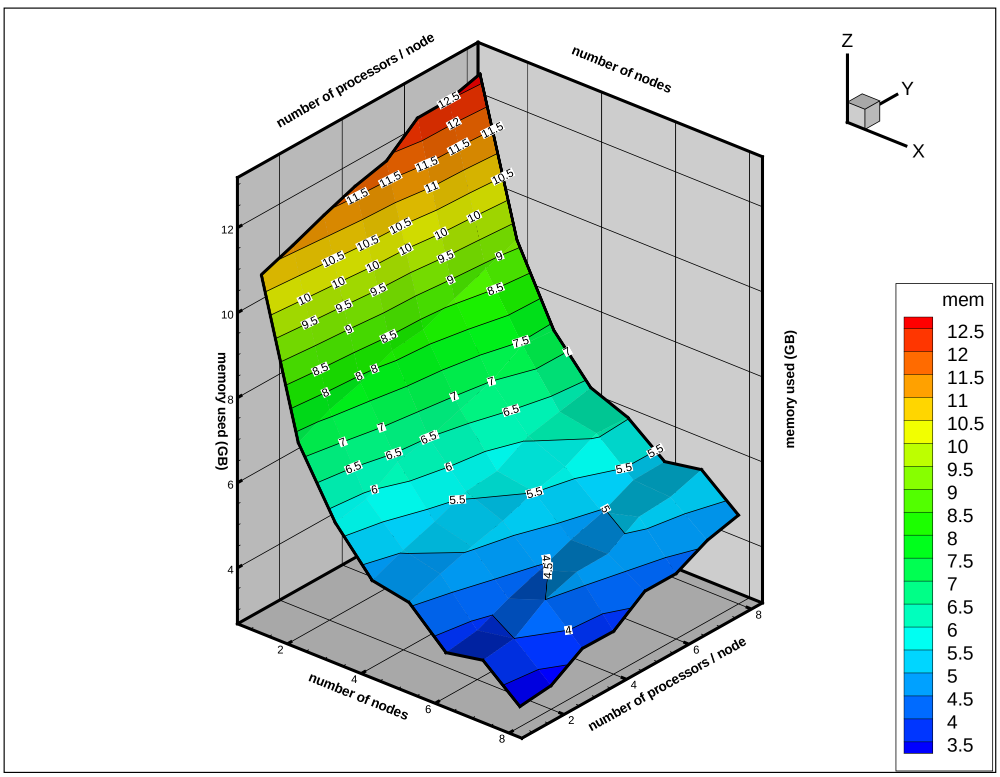

Fig. 6 Distributed parallel processing memory utilization using COMSOL v4.0-beta2 on a representative 3D conjugate heat transfer problem.