Multiphysics Applications based on MpCCI Code Coupling Interface

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There is an increasing need for multidisciplinary simulations in various research and engineering fields. Fluid-structure interaction, magneto-hydro dynamics, thermal coupling, plasma computations or coupled manufacturing processes define only a subset of recent multi-physics activities. There is a common feeling in the community that in most cases not a single (proprietary) simulation system can provide all necessary features but that coupling the best codes of each discipline will enable more flexibility and simulation quality to the end user.

The MpCCI interface has been accepted as a ‘de-facto’ standard for simulation code coupling. MpCCI is developed at Fraunhofer Institute for Algorithms and Scientific Computing (SCAI) and will be distributed by CDAJ in Japan, Korea and China.

This article will describe recent MpCCI developments and some coupled applications.

1 MpCCI - The Standard for Simulation Code Coupling

1.1 Overview

MpCCI (Mesh-based parallel Code Coupling Interface) has been developed at the Fraunhofer Institute SCAI in order to provide an application independent interface for the coupling of different simulation codes. MpCCI is a software environment which enables the exchange of data between the meshes of two or more simulation codes in the coupling region. Since the meshes belonging to different simulation codes are not compatible in general, MpCCI performs an interpolation. In case of parallel codes MpCCI keeps track on the distribution of the domains onto different processes.

MpCCI allows the exchange of nearly any kind of data between the coupled codes; e.g. energy and momentum sources, material properties, mesh definitions, or global quantities. The intricate details of the data exchange are hidden behind the concise interface of MpCCI.

Most of the commercial CFD/FEM applications allow users to add additional features, physical models, or boundary conditions via a programming interface. Within these user routines access to internal data structures is possible, either through subroutine parameters and global variables, or via internal modules for reading and storing data. MpCCI uses these capabilities for code adaptation. A user-subroutine called after each iteration or time step works as a hook to MpCCI.

The current version of MpCCI 3.0.4 supports

- ABAQUS 6.5
- Ansys 7.1 to 9.0
- Fluent 6.1.22 to 6.2.16
- Permas 10
- StarCD 3.1.50 to 3.2.4
- RadTherm 7.1.1

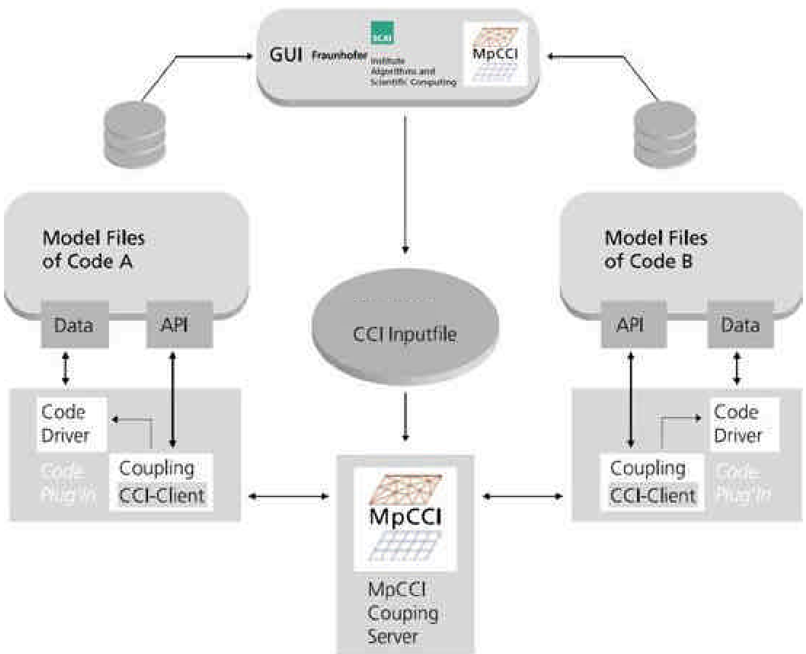
1.2 CDAJ – MpCCI Distribution partner in Far East

CD-adapco JAPAN (CDAJ) is a member of the CD adapco Group and does a wide business activity in Japanese and Chinese CAE fields. CDAJ does sales and technical supports for a variety of CAE software like the CFD codes, STAR-CD, the design optimization software, mode FRONTIER, the virtual engine/powertrain/vehicle simulation codes, GT-SUITE, the acoustic simulation codes, SYSNOISE and so on. The technical consulting and the system integration service are also done for various customers by using these software.

Since last year, CDAJ started the distribution and the technical supports of MpCCI in Japan, Korea and China. The importance of the multi-physics simulations coupling between CFD and CSM is recently rising up because of the diversification of the analytical contents and the demand for the high accuracy. CDAJ's customers are various companies and universities in the automotive, electric, chemical, atomic energy, architecture, aerospace and heavy industries. In these industrial fields, the coupling simulations play important roles for solving problems of the complex multi-physics and MpCCI would be a powerful tool for these simulations.

1.3 MpCCI Architecture

MpCCI 3.0 enables a direct communication between the coupled codes by providing adapters for a growing number of commercial codes. These code-adapters make use of the already existing application programming interfaces (APIs) of the simulation tools. This technique allows for an easy installation of MpCCI at the end users site without changing the standard installation of the simulation codes.



The MpCCI 3.0 environment consists of several components:

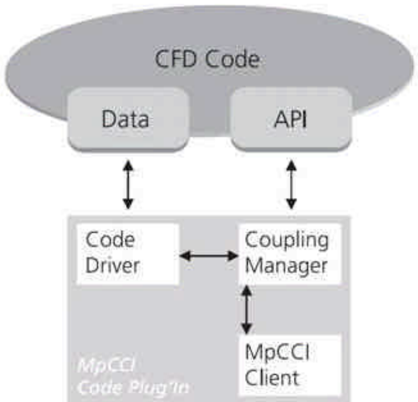
- MpCCI Code Adapter allow to adapt MpCCI to commercial codes through their standard code APIs without any changes in the source of the simulation code.
- The MpCCI-User-Interface provides a comfortable way to define the coupling setup and to start the simulation - independent of the codes involved in the coupled application.
- The MpCCI Coupling Server is the "heart" of the MpCCI system. Environment handling, communication between the codes, neighbourhood computation, and interpolation are part of this kernel.

MpCCI 3.0 uses different communication layers to establish interactions between each of its internal components:

- The MpCCI GUI scans the models files of the coupled codes by starting code specific scanner scripts on local or even remote file systems. The scan-information is then passed back to the MpCCI GUI.
- Perl scripts are used to start simulation tools local or remote; these scripts are invoked through rsh or ssh connections.
- The coupling communication between the codes (the code adapters) and the MpCCI coupling server uses TCP/IP protocols (sockets).
- The MpCCI Server uses the message passing layer MPI as its internal communication layer. This server internal usage of MPI does not interfere with any MPI entities potentially used in the codes.

This communication approach allows for a most general portability of the MpCCI system and for its application on distributed heterogeneous networks.

1.4 Code Adaptation



Within the MpCCI 3.0 system the code adapters establish a direct connection between the MpCCI Coupling Server and the codes themselves. They make use of the APIs of the commercial codes and thus (in most cases) need no modified versions of these codes. A code adapter is a library which will be linked to the code either statically or dynamically. Any code adapter consists of two modules - the Coupling Manager and the Code Driver. Additionally for each code there are code specfic scripts to scan the model input data, to start the codes and finally to stop the codes properly.

1.4.1 Standardised Quantities

One major advantage of having compatible code adapters for all codes supported by MpCCI is the standardisation of coupling parameters and procedures independent from the used code pairing. MpCCI provides unified quantity definitions for

- Globals: time, iteration, residuals
- Mass source and sink: production species

- Momentum sources: e.g. Lorentz forces
- Energy sources: e.g. joule heat
- Material properties: e.g. electrical conductivity
- Boundary condition values: e.g. temperature or pressure
- Boundary condition gradients: e.g. heat flux density
- Grid data: nodal positions or displacements
- And chemical components: e.g. for reaction kinetics

The current version of MpCCI needs consistent unit definitions for all quantities – better support for unit translation is planned for follow up versions. Based on these unified quantity definitions MpCCI provides a growing set of predefined coupling procedures.

1.4.2 Grid Morphing

In fluid-structure-interaction (FSI) a major requirement to the fluid codes is an efficient support for changing fluid domain boundaries. As not all CFD codes provide an automatic mesh deformation tool MpCCI has an internal mesh morphing tool which may support the code adapter of such CFD codes. The MpCCI Grid Morpher is an external program running as an additional process besides the application. The grid-morpher fully supports parallel runs of e.g. StarCD.

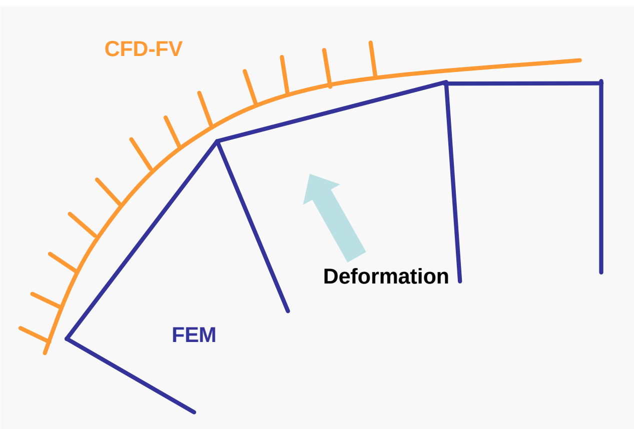
Through various control parameters the user may control how and which regions of the CFD mesh shall be morphed. The grid-morpher does not change the mesh topology – it does not provide a remshing of the CFD domain.

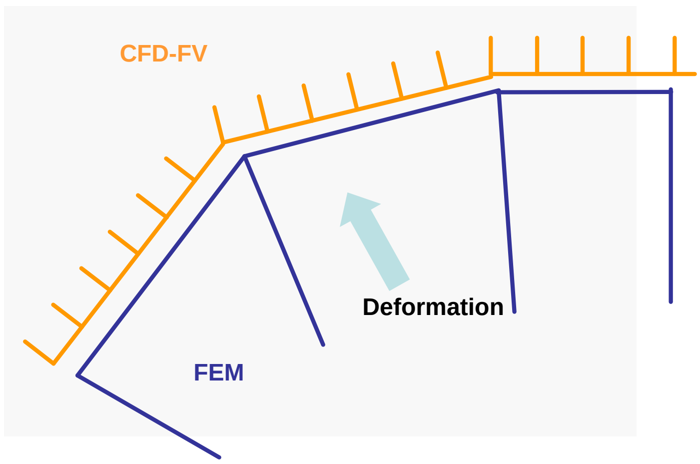
1.4.3 Displacement vs. absolute nodal positions

A typical application of fluid-structure interaction is the computation of stresses and deformations of structures:

- The CFD code calculates pressure distribution over the coupling surface;
- the FEM code claculates stresses and as a reaction the structural deformation on the coupling surface;
- MpCCI has to interpolate deformation values from FEM discretisation to CFD discretisation.
- CFD has to adjust its mesh model to the new surface definition

Model accuracy may differ on both sides - CFD and FEM. Usually the granularity of CFD meshes is finer than that of the FEM side (compare left figure).





There are two ways on how to transport the latest positions of the structural surface from FEM to CFD:

- by absolute nodal coordinates or
- by presenting relative or absolute displacements

Working with absolute nodal coordinates however has a general drawback: this method does not preserve the shape of the initial CFD model but - after a few coupling steps - adjusts the CFD shape to that of the FEM model. Based on the most recent positions of the structural nodes MpCCI interpolates the new positions of the CFD nodes. This interpolation does not take into account the previous (and potentially more accurate) geometric definition of the CFD model (compare right figure).

Using displacements instead of absolute positions solves this problem. In this case the calculation of the new CFD nodal positions will be based on the previous CFD positions and the relative displacements as being interpolated from the structural displacements.

1.5 Coupling of incompatible Model Discretisations

The heart of the MpCCI engine is the neighbourhood computation and quantities interpolation part. If the meshes are positioned in the same reference system, these meshes will be prepared for the coupling. The method for associating meshes and the physical quantities to be transferred need to be chosen. The association method determines which entities are associated. There are three different association methods available:

- Point Element (PE): A node of one mesh is associated with the element of the other mesh containing the node. The location of the node is given by the local coordinates.
- Element Element (EE): Elements of one mesh are associated with all intersecting elements of the other. The intersection figure is used as associative link. It is used for element based data.

All physical quantities are assigned to an interpolation type characterizing the data transfer. There are two types of data transfer schemes:

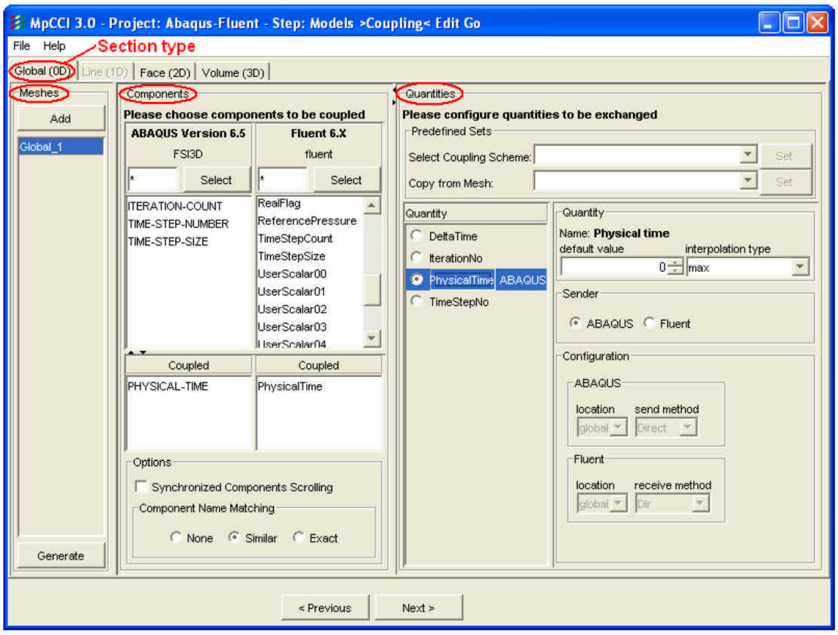
- ‘Flux’: The data is treated as a flux, which means that it is transferred in a conservative way.
- ‘Field’: The data is treated as field data, where the transfer is not bound to be conservative.

1.6 User Interface

MpCCI has been designed as a neutral interface between various commercial and inhouse simulation codes. While the user interfaces of the coupled codes differ, MpCCI itself provides a unique and code-independent way to specify all coupling relevant parameters. The MPCCI GUI allows to set-up and start the coupled application on a computing network.

The GUI guides the application engineers through a number of basic configuration steps towards a coupled simulation run:

- The user has to select the codes and to specify the corresponding input files containing the model data.



- The next step is to select those element groups in each of the coupled codes which define a coupling region where the coupling interaction takes place; any number of independent coupling regions can be specified during MpCCI setup.
- For each of these coupled components the quantities to be transferred have to be specified; quantities may be physical values like pressure or temperature.
- Additional coupling parameters like neighborhood search configuration, mesh quality checks, or output parameters can be set.
- Finally the job can be started on a network of computing resources. The MpCCI server has to be launched first. Then the coupled codes will be activated, either in command or in interactive mode.

2 Future Developments

2.1 *Code adaptation*

MpCCI intends to be the standard for simulation code coupling. An ongoing effort therefore is to extend the list of code adapters for MpCCI. Within the next year the following codes will be supported:

- MSC.Nastran and MSC.Marc,
- ANSYS/CFX,
- and the EMAG-code Flux.

The adaptation of inhouse codes will be enabled by some kind of API (‘adapter’ programmer interface) which allows to create and to customise code adapters by end users themselves.

To allow for a better post-processing support Fraunhofer SCAI is in cooperation with CEI to realise FSI related features in the EnSight visualisation tool. The midterm goal is to have an easy way to merge FEM outputs (from e.g. Abaqus) and CFD results (from e.g. StarCD) in one single view. The CFD pressure distribution as well as the FEM stress or deformation values will then be presented in a single window (or in two sysnchronised windows) to the user.

2.2 *MpCCI Features*

For the MpCCI engine itself there are several items planned for the next year.

- **Unit translation**: there is a strong need to allow for different unit systems in the coupled codes. The MpCCI GUI will support the specification of units for each code and help to define the transformation rules between them.
- **Handling of geometric incompatibilities**: besides different unit systems the coupled models may also differ in their coordinate systems and in the accuracy of geometric modelling: e.g. in CFD small parts like welding points will not be modelled – but in FEM these parts are important. MpCCI will provide tools for an automatic coordinate system adjustment and some new interpolation and extrapolation algorithms to map values between non-conforming regions.
- **Fast remeshing support inside MpCCI**: if there is a remeshing of the coupled surfaces during simulation the current version of MpCCI needs to do a complete recalculation of mesh neighbourhoods. Future versions will improve these neighbourhood calculations by more sophisticated algorithms.
- **Coupling algorithms and synchronisation**: A major question for each coupled application is: *When should the quantities be exchanged*? Due to the differences in the physical phenomena there may be different time scales in the coupled models. Future MpCCI versions will provide a common and easy description for the physical problem (transient/steady) and timescales and the appropriate coupling procedure based on the physical problems.
- **Shutdown and restart facilities**: The restart capability of MpCCI and the coupled codes have to be synchronised in a proper way.

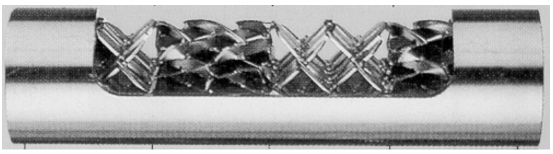
3 Application Areas

3.1 Fluid-Structure with Deformable Structures

Typical FSI example are defined by the dynamic effects over a deformable structure which is located in a fluid or air stream. Flexible flaps or valves may deform due to the normal and viscous fluid forces of the moving fluid or air stream. Or the structure might deform due to external loads – and the fluid domain has to follow these deformations.

In the following few examples will highlight different aspects of FSI with deformable structures.

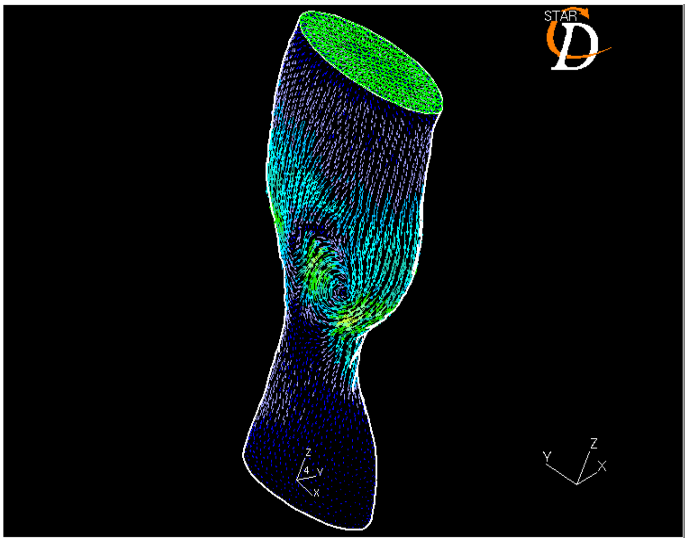
3.1.1 Static Mixers



Static or dynamic mixers as used in the chemical industry deform due to high pressure loads. Such a mixer is the Sulzer SMX as shown in figure on right. It is designed for the mixing of liquids of high viscosity where the flow is laminar. The complex structures of the blades generate layers which drive the process of mixing. Special versions of the mixer are designed for applications (e.g. polymer melt blending) featuring a pressure drop across the structure of the mixer of up to 100 bar or higher. The mechanical forces and stresses in the structure caused by the flow are given by the pressure drop of each of the blades. The resulting total force is transferred from the mixer structure to the outer pipe e.g. at one end of the mixer.

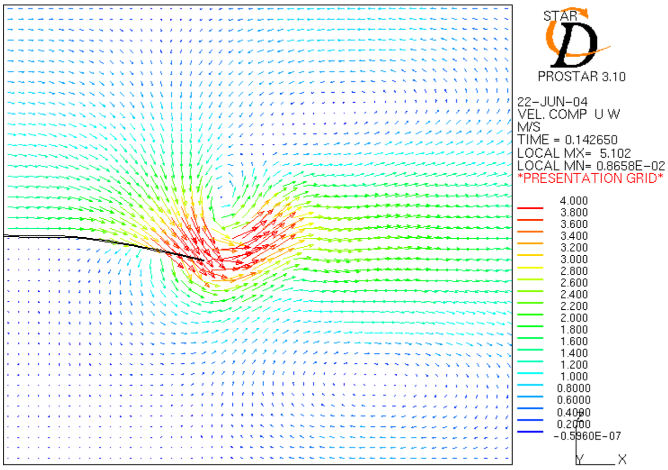
This application was done with a coupled StarCD-Permas environment at Sulzer Innotec in Switzerland [wintergerste2005].

3.1.2 Biomechanical Applications (JAERI)



Computational biomechanics of vascular system, diseases, and thrombosis has been often concerned with the local hemodynamics conditions of blood flow that are computed by various of CFD (Computational Fluid Dynamics) methods, since it is well known that unusual hemodynamics condition may cause an abnormal biological response. Meanwhile, since pulse blood flow in arteries causes wall stresses to oscillate and non-uniform, biologists become recently more and more interesting in computational analyses of arterial wall stresses by CSD (Computational Structure Dynamics) methods to predict patient disease risks, like plaque rupture endothelial injury, etc., or to help plan surgery operation. Herein wall elasticity has to be taken into account which is neglected on many situations as the secondary importance feature generally. Consequently, it is necessary to analyze hemodynamics conditions of blood flow by CFD and stress distribution on arterial wall by CSD simultaneously from view of clinical request [guo2002]. In the figure the velocity distribution on carotid artery is shown.

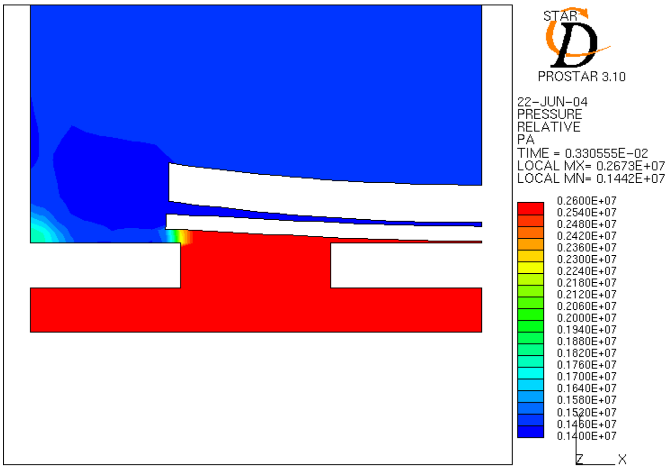
3.1.3 Piezo Elements



In the electric industries, the piezoelectric actuators are used as pump, speaker and fan. The piezoelectric device oscillates by alternately changing axial strains caused by A.C. voltage loading. In order to analyze such phenomena, only the piezoelectric/structural analyses have been used usually. In these cases, one of the key components, the fluid force, is simplified as an easy damping model. However MpCCI enables the coupling analysis between CSM and CFD now and the more realistic behavior can be solved by defining the exact fluid forces on the device [moriyama2005].

3.1.4 Compressor Valves

Another example is the valve in the compressor used in the various fields. These valves are opened by the gas compressed by the piston motion and exhaust the gas (see figure, pressure field around the valve). This is solved as FSI case because the valve is deformed by the pressure force of the compressed gas. The analysis results of the pressure and deformation of valve are compared with the experimental data. The coupling analysis via MpCCI is going to be useful for the design of the compressor [moriyama2005].



3.1.5 Tire Hydroplaning Simulation

Tire hydroplaning simulations are of high interest for automotive and tire companies. Together with NUMECA S.A. and the two tyre companies Pirelli and Michelin MSC Netherlands realised a solution for multi-physics tyre simulation. The relevant design variables for tyres under hydroplaning conditions are, among others, the pressure distribution on the ground, the stresses in the reinforcing cords in the tyre and the contact patch of the tyre on the ground. Tyre modelling then is a complex non-linear process that has to take into account the contact between the tyre and the ground (including friction), the interaction with the water and the strongly non-linear behaviour of the tyre itself, due to its large elastic deformations. For this application the codes MSC.Marc and Numeca's FINE/Hexa CFD code were coupled through MpCCI interface [vosbeek2005].

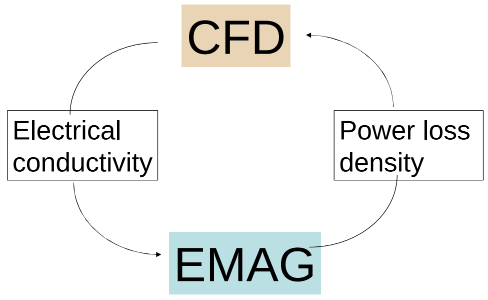
3.2 Thermal Management in Automotive Systems

Calculation of underhood component temperatures of passenger cars requires the combination of even three different disciplines: structural analysis, fluid dynamics and radiation. For the simulation of thermal conduction and convective heat transfer a coupled fluid-structure environment is needed. With regard to the whole car geometry also radiation plays an important role in the overall heat management calculation. In areas with relevant fluid flows (e.g. engine compartment, gear box or exhaust system) convective heat transfer and radiation need to be calculated in a coupled environment. DaimlerChrysler starts to use a fully coupled 3-code environment based on StarCD, Permas and Posrad (radiation code from CD adapco) to solve thermal management applications [maihöfer2004] [weidmann2005].

3.3 Thermo-Electrical Coupling

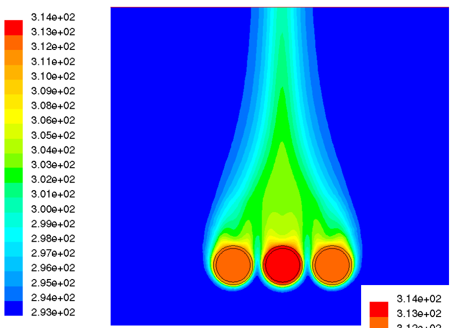
The prediction of heating and cooling processes is of eminent importance in the development of electrical devices. The flow of the alternating current induces heating due to losses by Ohms' law and the usual mechanism for cooling is free convection. The increasing tendency of miniaturization requires to fully utilizing the thermal potential of the materials involved. Heat dissipating surfaces are, however, reduced in a way that can result in temperatures which may destroy the complete device or parts of it [zolfaghari2005].

The free convection is simulated by the CFD Software (e.g StarCD). The electromagnetic quantities, governed by the Maxwell equations, are calculated using Finite Element Code ANSYS. It calculates Joulean heat in the conducting cables and sends it to the flow simulator as an energy source term. The conductivity depends on temperatures; it is, therefore, being calculated within CFD by means of a user defined function. The complete data transfer between the flow and the electromagnetic simulation is done by MpCCI .



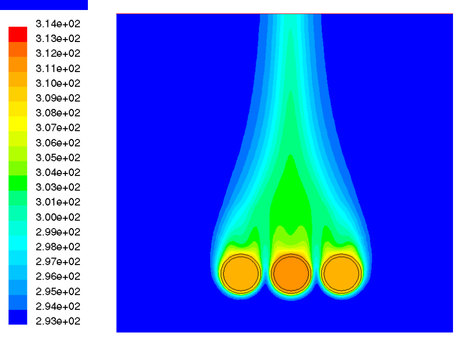
The CFD simulation leads to a stationary solution, ANSYS operates in frequency domain. The power loss density can be derived from the harmonic solution and the exchange of data between the two simulations codes is performed as soon as new results (power loss densities and conductivities) are available.

The cables are insulated by a non-conducting PVC layer. Skin and proximity effects lead to a non-uniform distribution of the current density resulting in a non-uniform temperature field. Skin- and proximity effects which are taken into account in the coupled simulation actually play an important role. If one neglects such effects and assumes a constant power loss density the heating behaves substantially different. The figure shows results from a simulation based on a constant power loss density. It is obvious, that the heating of the middle phase is definitely underestimated.



Non-uniform power loss density (coupled solution

Constant power loss density



4 Conclusion

MpCCI 3.0 provides a lot of new features for the coupling of simulation codes. Together with MpCCI code adapters now a complete toolbox for multidisciplinary simulation is ready for use with standard commercial simulation codes. Various solutions demonstrate the applicability of this concept and the valuable outcome for the end users. A growing number of commercial codes is supported by MpCCI code adapters.

5 Literature

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