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Integration of numerical tools for the combined thermal-hydraulics and structural analysis of Energy Amplifier components

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1 Introduction

The CRS4 R&D activity on the Energy Amplifier Demonstration Facility (EADF) [1] concerns the thermal fluid-dynamic and structural computational analysis in support to the design of some of the crucial components of the machine. We are currently studying the operating conditions of the spallation target [2-3] and the sub-critical core [4-5], including steady state, transient [31-32] and accidental conditions. The simulation activity also includes the analysis of multi-phase (liquid-gas systems with high void fractions) [6-7] and free surface Liquid Metal (LM) flows [8-9]. A parallel activity of benchmarking of numerical codes on LM experiments is in progress [10-12, 33-34], joined with a critical theoretical review of numerical models applied to LM flows [13-15].

The fluid-dynamic and structural numerical simulations are mainly performed with general-purpose commercial codes. The use of commercial codes presents many advantages: they allow the simulation of complex interacting physical phenomena, offer a wide selection of physical models and the possibility of implementing different or customised models through user routines. Moreover, they can be easily interfaced with CAD and mesh generators. On the other side, they have also some disadvantages: sophisticated models are often not well assessed or inaccurate, the numerical procedures are not always entirely documented, the most advanced research models are not implemented, the calculation efficiency is limited with respect to in-house codes.

The features and the reliability of many codes, with respect to the EADF project objectives, have been widely tested by the EA working group at CRS4 in the last two years.

In section 2 the main requirements of the simulation tools for the EADF activity at CRS4 are listed. A brief description of the codes is given in section 3, and their capabilities are evaluated in section 4. Finally, the assessed procedure adopted for the EADF calculations is presented in section 5.

2 Simulation tools requirements

The general requirements we considered important in the evaluation of the codes are the following:

<u>General requirements</u>:

- quality of documentation and technical support;
- interfacing capabilities with other codes: data import/export options and formats;
- possibility of implementing standard automatic procedures for parametric studies;
- license fees.

<u>CAD and meshing tools requirements</u>:

- full parametric CAD modelling;
- structured and unstructured meshing capabilities;
- parametric and geometry-related meshing.

<u>Structural analysis codes requirements</u>

– capability of performing both linear and non linear static, dynamic and thermal analysis.

Fluid-dynamic codes requirements:

– a wide selection of turbulence models;
– coupled fluid-solid thermal analysis;
– state-of-the-art models for multi-phase and free surface flows;
– possibility of easily inserting customised models through user subroutines;
– an exhaustive description of the physical models implemented in the code.

3 Description of simulation codes

3.1 Neutronics Codes

FLUKA

FLUKA [16] is a widely used Montecarlo code which is capable of transporting high energy particles (in our case 600 MeV protons) by taking into account not only electromagnetic interactions, but all kind of nuclear interactions induced by both primary and secondary generated particles (included neutrals) and gammas.

In our simulations, we are particularly interested in evaluating the heat deposited by the particle beam. Comparison with the experimental measurement have shown that the mean accuracy cannot be better than about 10 % when estimating the spatial density of deposited energy. We consider this level of accuracy acceptable for our studies.

FLUKA has no interfaces with other codes, so the models must be generated with its internal tools. Output data of heat generation can be directly read by fluid-dynamic codes, such as STAR-CD and CFX.

3.2 CAD/FEM Model Generation Tools

Numerical fluid-dynamic and structural analysis often requires the generation of complex geometries and meshes. Usually, fluid-dynamic and structural codes have a geometry and mesh generator integrated or associated with the solver. Mesh generators associated with structural codes are generally more advanced, and can be used for the CAD and meshing of both fluid-dynamic and structural models. We investigated the use of the tools that offered the most advanced CAD capabilities.

SDRC IDEAS MS 5

The IDEAS package [17] is a commercial CAD/meshing tool especially dedicated to structural calculations. The package presents the following main features:

– a CAD tool able to perform 2D and 3D parametric geometry modelling;
– a structured and unstructured mesh generator that supports triangular and quadrilateral shell elements as well as tetrahedrical and hexahedrical solid elements;

– a pre-processor dedicated to structural analysis;
– a post-processor for the visualisation and presentation of results.

Available interfaces with other codes include the following import data formats: ABAQUS, ANSYS, IDEAS universal file, IGES, NASTRAN bulk data, NASTRAN output2, CATIA. The following export data formatsare avaliable: ABAQUS, ANSYS, IDEAS universal file, IGES, NASTRAN bulk data, CATIA.

The technical support from SDRC is efficient, but the level of assistance is sometimes inadequate for an advanced use of the meshing tools. Only on-line documentation exists, whose quality is good.

<u>MSC/PATRAN v8.0</u>

The PATRAN [18] package provides a CAD environment, including pre- and post-processing tools. No parametric modelling is possible.

The mesh generator supports tetrahedral, hexahedral and p-type elements. It also provides access to meshed models from other CAD systems. Available interfaces include the following import data formats: NASTRAN bulk data, NASTRAN output2, IGES, CATIA, EUCLID3, PRO/ENGINEER, Unigraphics, PATRAN Neutral. The following export data formats are avaliable: PATRAN Neutral, IGES, NASTRAN bulk data.

The PATRAN post-processor offers a wide range of features for the visualisation of the results.

The assistance support from MSC is generally efficient, but the level of assistance is sometimes inadequate for an advanced use of the software.

<u>Control Data ICEM-CFD</u>

The ICEM-CFD [19] package is a commercial tool dedicated to the generation of computational meshes for CFD simulations. It is structured in different modules of which we tested the following ones:

– a CAD for the generation of the model geometry (DDN package);
– a structured and unstructured mesh generator (PCUBE and HEXA packages);
– a post-processor package to visualise the generated mesh and to perform some type of operations, such as smoothing, evaluation of mesh quality, etc. (LEO package).

The import/export capabilities include interfaces with CATIA, ICEM Surf, PRO/ENGINEER, IDEAS, Unigraphics. It is also possible to export data in IGES format.

Both the documentation and the technical support from Control Data are very poor and inadequate.

3.3 Structural Analysis Codes

<u>MSC/NASTRAN v70.5</u>

NASTRAN [20] is a commercial finite element code for structural analysis. Its distinctive characteristic is the reliability for linear and non linear static, dynamic and thermal analysis. It is closely linked to the pre- and post-processor of PATRAN, in an integrated environment for modelling and analysis. User and program documentation are well written and easily accessible. A good level of technical support is available in Italy.

CASTEM 2000

CASTEM 2000 [21] is a FEM simulation code for the structural analysis, integrating the functions of construction and pre-processing of the model, calculation and post-processing of the results.

The main fields of applicability of CASTEM 2000 are: linear elastic static and dynamic analysis, heat transfer and thermal analysis, mechanical non-linear analysis.

With respect to other codes, where the solution procedures are fixed, the peculiarity of CASTEM 2000 is the possibility of combining a set of independent solution modules to obtain a customised solution procedure.

The only interfacing format of CASTEM 2000 with other simulation codes is the AVS format. There is no assistance service, but a great quantity of documentation provided by CASTEM developers is available.

3.4 Thermal-Fluid-Dynamic Simulation Codes

As said above, we carefully considered the use of commercial codes for CFD analysis. Although a great number of codes exists on the market, we took into account only the ones we considered the most developed and well assessed, namely STAR-CD, CFX and FLUENT. These codes are by far the most diffused on the market and companies developing them are strongly expanding and heavily investing in code development, in order to reasonably include state-of-the-art modelling into their products. We have been extensively using STAR-CD and CFX, but we only recently acquired FLUENT, which we will evaluate only in the future.

All these codes have a pressure-based formulation for the solution of the fluid-dynamic equations and a module for the coupled solution of the conduction equation in the solids. They offer a wide selection of physical models for the simulation of complex flows, like reacting flows, multiphase and free surface flows, flows with moving meshes and others. The most assessed turbulence models are available in all the three codes.

We are also investigating the use of our research code KARALIS, which, in spite of a limited selection of physical models (compared with commercial codes), offers the advantage of a better accuracy and performance, and the implementation of more advanced models and numerical schemes. Applications of this code are very refined simulations of parts of the EADF where a high accuracy is required.

ADAPCO STAR-CD 3050A

Peculiarities of STAR-CD [22] version 3050A, related to our applications, are:

- capability of handling complex geometries using unstructured meshes of hexahedrons, prisms and other polyhedrons, unmatched meshes and partial boundaries;
- an efficient mesh generator and an highly interactive pre-processor;
- a wide range of import-export formats for the interfacing with other CAD and mesh generators (including PATRAN, NASTRAN, ICEM, IDEAS, PRO-ENGINEER, IGES and ANSYS);
- a wide range of two-layer models for turbulence treatment near solid walls and a low Reynolds κ-ε model;
- a good post processor, completely integrated with the mesh generator and pre-processor module.

AEA CFX 4.2

CFX version 4.2 [23] is a structured multi-block code. With respect to an unstructured code like STAR-CD, it is less capable of handling complex geometries, although the possibility of using non-conform blocks reduces this disadvantage. The code is modular, in the sense that meshing tool, pre-processor, solver and post processor are different packages integrated through interface files. Meshes from other CAD/mesh generators can be imported through an interface program (CFX-Meshimport), supporting PATRAN, IDEAS and ASTEC formats. The main peculiarities of CFX, related to our applications, are:

– low Reynolds κ-ε and κ-ω models, Reynolds stress and Reynolds flux turbulence models;
– a wide selection of two-phase flow models, among which a model for free surface flows.

KARALIS

KARALIS [24-25] is the CFD parallel multi-block code under development by the Fluid-dynamics and Combustion Area of CRS4. The code solves the fully compressible Navier-Stokes equations where all couplings between dynamics and thermal-dynamics are allowed.

This formulation, typical of compressible flows, shows efficiency even for incompressible flows as well as for flows of incompressible fluids, once equipped with a preconditioner. Merkle's preconditioner [35] has been implemented because it can be easily formulated for arbitrary equations of state given by both analytical expressions and tabular form.

It uses a fully-coupled explicit time-marching algorithm (as opposite to both CFX and STAR-CD which make use of segregated algorithms), namely a multi-stage Runge-Kutta method in conjunction with multi-grid acceleration. The turbulence models implemented are: the algebraic Baldwin-Lomax [36], the 1-equation Spalart-Allmaras [37], and the low Reynolds 2-equation κ-ω model by Wilcox [36].

KARALIS can import multi-block structured meshes generated with the CFX pre-processor and makes regular use of the TECPLOT post-processing system.

3.5 Post-Processing Tools

Although all codes offer good post processing features, we considered also the option of using a fully dedicated tool in order to have a uniform format in the visualisation of results from different sources.

TECPLOT

TECPLOT [26] is a post-processing code for the visualisation of CFD simulation results. Its general features are: animations, 3D surfaces and volumes, streamlines and vectors representations, mesh plots, 2D and 3D finite element data, contour plots, data extraction, creation and transformation, scatter plots, XY plots, batch processing/macro language, presentation-quality output.

The main peculiarities of this code, related to our applications, are:

– ease of use;
– high data manipulation capabilities;
– possibility of saving style sheets which can be used with different input files.

4 Evaluation of simulation tools

In the following we will briefly review the main reasons behind the choice of the simulation tools we use in the project. The problems related to the code interfacing are considered in detail. A more complete critical review on the physical models and codes accuracy and reliability can be found, for example, in references [8-12, 24, 25, 27, 28].

FLUKA

The use of FLUKA is a necessary step for the analysis in which a high energy beam particle interacts with the matter. The FLUKA mesh cannot be the same employed in CFD analysis, since it must be adapted to the collection of statistics from the Montecarlo calculation whose requirements are very different. Output data of heat generation can be extracted in table format on user grids and are put into files that are generally directly read by fluid-dynamic codes or manually interpolated. Therefore, when undergoing complex parametric studies, heavily time-consuming manual operations are needed.

CAD/FEM Model Generation Tools

Concerning geometry modelling and mesh generation, IDEAS has been preferred to PATRAN and ICEM for its good capabilities in generating parametric geometries. Moreover, a very efficient set of geometry-related structured and unstructured meshing tools, supporting a wide range of finite elements shapes, is available.

IDEAS graphic interface makes the entire operation of building and modifying a full meshed model very user-friendly. The mesh generated on a model is strictly related to the geometry. Any modification of the geometric parameters produces an automatic re-generation of the mesh on the modified geometry. This operation is not fully automatic when performed on triangular or tetrahedral unstructured meshes: in this case, some manual refinement may be requested. The automatic re-meshing operation is not possible if the topology of the geometry on the meshed model is modified: in this case, the mesh definition will be deleted and the model has to be re-meshed. The pre-processing features, such as applying constraints, loads and boundary conditions are also very efficient. IDEAS is well interfaced with other simulation codes, like NASTRAN, STAR-CD and CFX.

The CAD and meshing capabilities of PATRAN are not suitable for our purposes, showing the limitations of this product of not being a real CAD tool, but essentially a pre- and post-processor for the NASTRAN solver.

On the other side, whereas IDEAS was conceived as a CAD/meshing tool dedicated to structural analysis, ICEM is a grid generator developed for fluid-dynamic applications. However, the lack of available documentation and support service and the poor parametric capabilities of ICEM, makes IDEAS a more suitable tool for our applications. See also Ref. [29-30] for details.

Structural Analysis Codes

We decided to use NASTRAN as the reference code for the structural analysis within the EADF project due to its good reliability for large scale linear static, dynamic and thermal analysis. However, it should be noted that the non-linear capabilities of the code are limited with respect to other competitors available on the market (e.g. SPECTRUM, ANSYS, ABAQUS or CASTEM 2000). Moreover, the related documentation is not so developed as it is for the linear structural analysis. Depending on the type of analysis to be made, this might be a serious limitation, and its impact on the future work has to be carefully assessed.

CASTEM 2000, in spite of a good range of analysis capabilities, has been estimated unsuitable for a massive computation activity, and its utilisation is foreseen only in future analysis to perform extremely refined and accurate investigations on very specific problems.

Fluid-Dynamic Analysis Codes

The capability of handling many kind of meshes, the ease of interfacing with other codes, and the efficiency of the pre- and post-processing tools make STAR-CD the most suitable code for the massive computational activity of CRS4 on the EADF project. However, two-phase and free surface models are less developed with respect, for example, to CFX. Moreover, no Reynolds stress and Reynolds flux turbulence models are implemented. Some problems were found in the upgrading of the STAR-CD version: in particular, different results were obtained for a simulation performed with the same model but with different STAR-CD versions. No satisfactory explanation for this behaviour was provided by the assistance. The french assistance showed to be very inadequate for our needings. On the contrary, a very good support was provided by the english team.

CFX v4.2 was found to be more efficient than STAR-CD for two-phase and free surface flows. Reynolds stress and Reynolds flux models are implemented, although no two-layer models for the near-wall turbulence treatment are provided. Pre and post processors are less efficient than in STAR-CD. The technical support from the italian supplier was inadequate for our purposes. It was found that the user manual description of some numerical models does not correspond to the real procedure implemented in the code.

Up to now, KARALIS has not been extensively used in the EADF project, so an evaluation of the code is still premature.

Post-Processing Tools

Every commercial code evaluated has an internal tool for the displaying of the results (with the exception of NASTRAN, whose dedicated post-processor is PATRAN). This is very useful for a quick and simple visualisation of results, but it can be limiting when a more complex analysis is required.

The choice of the tools for the numerical analysis has been strongly influenced by their compatibility with other codes. Some problems in translating data were encountered. A brief description of the interfacing capabilities is given.

- IDEAS to STAR-CD translator is able to easily export the grids and the boundary conditions in IDEAS universal file format; no problems have been reported.
- IDEAS to CFX: the grid and the boundary conditions are exported in universal file format. We have been reported a problem of compatibility in CFX translator (Meshimport): it was not updated with the new IDEAS universal file format; the assistance service sent a patch file to solve this problem.
- IDEAS to NASTRAN and PATRAN: the grid and the boundary conditions can be exported in NASTRAN bulk data format. No problems have been reported.
- PATRAN to IDEAS: no problems have been reported in importing data in NASTRAN bulk data format.
- PATRAN to NASTRAN: no problems have been reported in exporting data in NASTRAN bulk data format.

– NASTRAN to PATRAN: the results of NASTRAN calculations are given in NASTRAN output2 format, directly readable by PATRAN for the post-processing; no problems have been reported.
– STAR-CD to NASTRAN: no problems have been reported in exporting data in NASTRAN bulk data format.
– CFX to NASTRAN: no problems have been reported in exporting data in NASTRAN bulk data format.

5 Calculation strategy and integration of numerical tools

The scheme of the assessed calculation strategy is illustrated in Fig. 1.

FLUKA is employed to calculate the heat source distribution from the interaction of high energy particles, as in the case of the beam target. The heat source distribution coming from the neutronic analysis is imported in STAR-CD and CFX to be used as input data for the fluid-dynamic calculation. It consists of a simple ASCII file tabulated on a FLUKA user grid, which must be interpreted by CFD codes FORTRAN user routines.

The mesh is created with IDEAS. Boundary layers near the solid walls are meshed with structured grids, being easier to handle and more suitable for the application of the turbulent near-wall algorithms. Mixed structured and unstructured grids are used for the internal regions. The three-dimensional grids for the fluid-dynamic analysis are exported from IDEAS to STAR-CD and CFX. While STAR-CD supports both structured and unstructured grids, CFX supports structured grids only.

IDEAS is not able to create the boundary conditions for the fluid-dynamic analysis, but the CFX translator (Meshimport) allows IDEAS to apply boundary conditions and to define solid or porous regions of the models, identifying groups of different regions of nodes and elements (2D and 3D). In the models generated for STAR-CD, different materials properties are assigned to the main parts of the model (i.e. solids, fluids, boundary layers), allowing the identification of the different mesh blocks and the pre-processing operations in STAR-CD. The grids and the boundary conditions for the structural analysis (e.g. loads and constraints) are exported from IDEAS in NASTRAN bulk data format to be pre-processed in PATRAN.

The fluid-dynamic analysis is performed with STAR-CD or CFX, depending on the nature of the considered problem. In some cases both the codes are used for the same calculations, in order to compare the results for different models. The results are usually visualised with the internal post-processor of STAR-CD and CFX or using TECPLOT.

The temperature maps to be used as input data for the structural analysis are exported from STAR-CD and CFX in NASTRAN bulk data format. The temperature field and the pressure distribution coming from the fluid-dynamic analysis are assigned to the nodes of the mesh as load input data for the NASTRAN structural calculation. The grid used in the fluid-dynamic simulation is also adopted for the structural analysis. If a refined grid is required, PATRAN pre-processing tools can be employed to apply the temperature field on a new IDEAS grid, and then to export the temperature loads in NASTRAN bulk data format. The results from NASTRAN are post-processed with PATRAN and TECPLOT

Non-linear (plastic range) analysis are planned to be performed with NASTRAN and CASTEM 2000.

6 Conclusions

The reliability and the integration of many commercial different simulation tools has been tested by the EA working group at CRS4 in the last two years, leading to the definition of the most suitable simulation tools for the scopes of our analysis and of an assessed procedure for the calculation process.

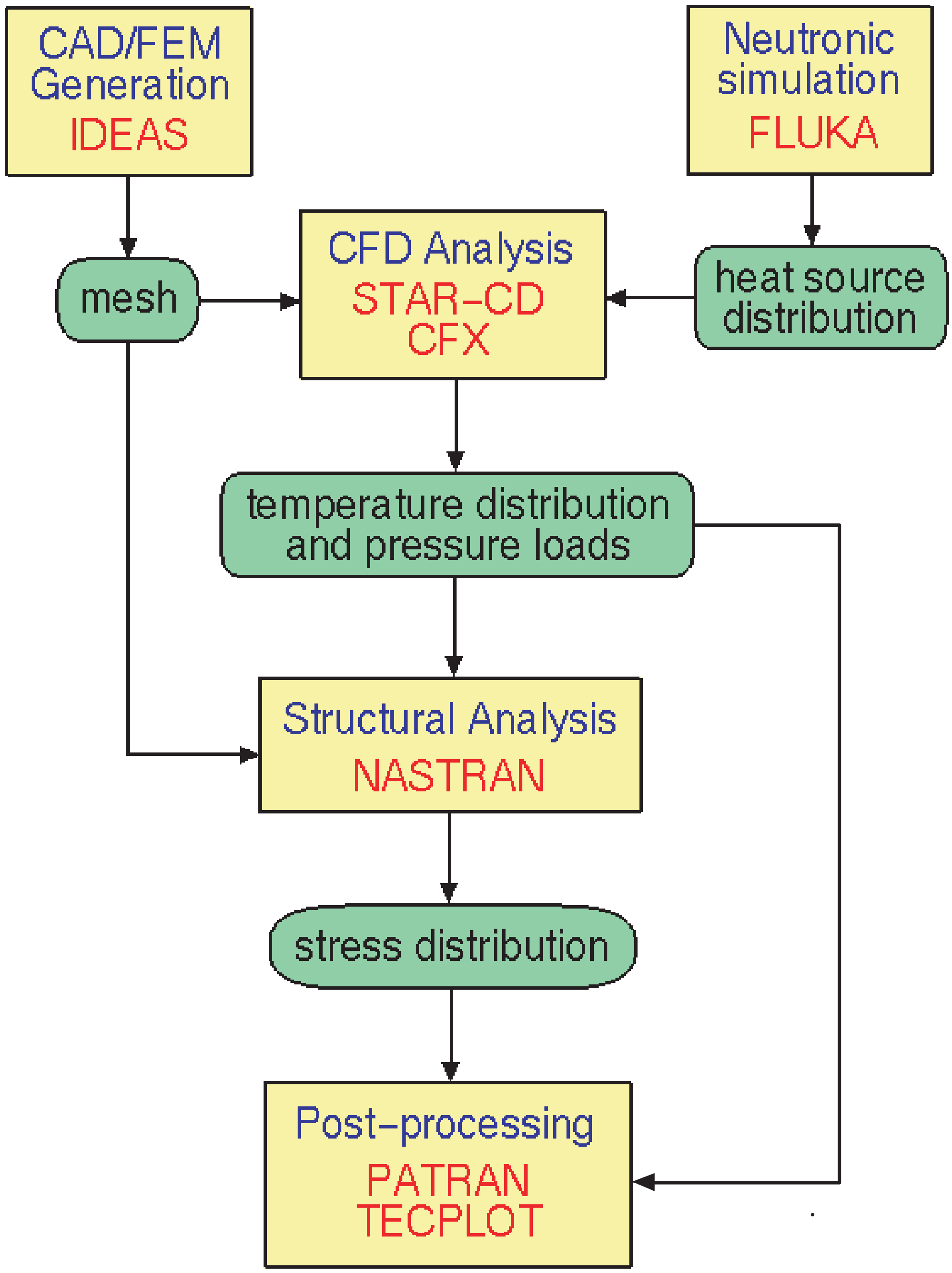

Fig. 1 – Flow-chart of the numerical calculation strategy.

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