FENET - MULTI-PHYSICS ANALYSIS (MPA) THEME: A REVIEW OF COMMERCIAL MPA CAPABILITY IN 2005

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SUMMARY
As a part of the FENET Multi-physics analysis (MPA) theme a regular web based survey of the emergence of commercial MPA capability has been carried out. This contribution presents the results of the most recent survey and assessment of the multi-physics capability of the major commercial computer aided engineering (CAE) analysis software technologies is presented. The capability of commercial tools has developed considerably over the last 3 years, both with regard to specialist products and the combination of phenomena specific tools through specialist interfacing software, typically based upon the MpCCI technology. MPA based simulation is very compute intensive and so the challenges associated with achieving scalable parallel implementation are raised.

1: INTRODUCTION

One of the key themes of the FENET [1] network is in multi-physics (MP) analysis. When the network began the concept of multi-physics analysis was largely unfamiliar to the engineering analysis community. However, over the last 4 years all that has changed – there has been a significant research effort in developing capabilities to couple a variety of physical phenomena solvers in addressing complex problems. Moreover, many engineering analysis tools and software technologies have been developed and embedded in the period since the network was inaugurated. Periodically, the coordinators of the MPA theme provided a survey of the multi-physics capability and capacity of commercial tools. The objective of this contribution is to provide an overview of the multi-physics capability in commercial engineering analysis software as at April 2005, as the FENET project draws to a close.

As part of the assessment, it seemed appropriate to take a take stock and consider:

- Clarity on what is meant by multi-physics.
- The progress at the commercial level over the last three years
- The role for high performance computing clusters in MP analysis
- What developments there have there been in user environments

2: MULTI-PHYSICS SIMULATION

Multi-physics may be defined as closely coupled interactions amongst the separate component of continuum physics phenomena. However most CAE analysis software tools have been developed in the context of a single of related discipline group such as:

- Computational Fluid Dynamics (CFD), i.e. fluid flow, heat transfer and combustion
- Computational Structural Mechanics (CSM), i.e. structures, dynamics, contact and heat transfer
- Computational Electro Magnetics (CEM)
- Computational Aero Acoustics (CAA), i.e. acoustics coupled with fluid flow

Until recently, unless their interactions were natural, as in the case of thermo-mechanics or thermo-fluid, the interaction between any other phenomenon has largely been ignored or greatly simplified.

One of the reasons that such interactions have been ignored is due to the distinctive approaches used in solver strategies by the various phenomena specific software, for example:

- CFD typically uses Finite Volume (FV) techniques with segregated iterative solvers
- CSM uses Finite Element (FE) techniques with direct solvers or at least the structure to employ direct solvers.
- CAA & CEM uses either FE/FV techniques

The distinctive features of the above solvers, combined with their consequent heritage software structure, have made all but the loosest coupling between phenomena very difficult.

When physical phenomena are coupled this means that information from one has to be transformed and included in the simulation of another, predominantly either through changing boundary conditions or through the provision of a source term (e.g. a body force). Hence, in all types of MP analysis, it is essential that data for volume source and boundary conditions from one phenomenon to another is mapped or filtered in such a way that there is no loss in accuracy. In addition, if mesh movement is required then the mesh and geometries must deform compatibly.

3: CLASSIFYING MULTI-PHYSICS

Most CAE software vendors claim multi-physics capabilities, but in reality, what most of them offer at the present time, is multi-disciplinarity, i.e. data generated by one code is used as input into another, either as boundary data or as a volume source, where the data transfer is one way. This is distinguishable from full multi-physics analysis, which involves the two-way exchange of information, which could involve implicit convergence within a time-step (e.g. thermo-mechanical). There is also an additional level of sophistication with regard to multi-physics, i.e. closely coupled multi-physics. This type of analysis adds a further level of complexity since both time and space accurate exchange of data is required. Hence, the type of problem under consideration will influence the level of coupling that is required for MP analysis, as detailed below.

3.1 Levels of physical coupling

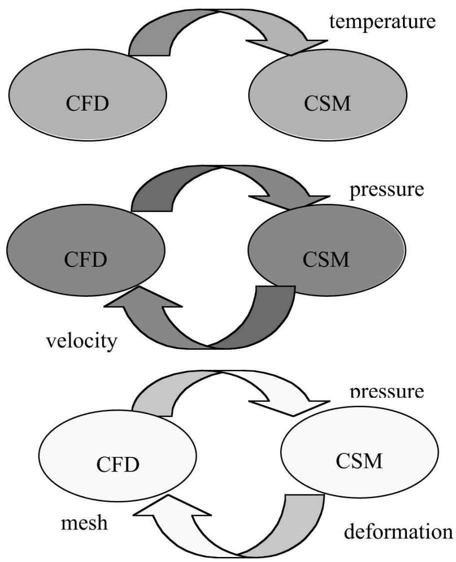

Figure 1: Levels of Coupling

From the above summary it is clear that for MP analysis it is convenient to consider three possible levels of coupling between phenomena specific software:

- Low level of coupling

  One way, where phenomenon A imposes boundary conditions or a volume source on phenomenon B, but the effect of phenomenon B on A is ignored. This is usually achieved by simple file between codes. Low-level coupling is essentially multi-disciplinary, e.g. an electric field loading a thermal calculation

- Medium level of coupling

  Two-way coupling both to and from phenomenon A to phenomenon B, which is more complex, requires mesh compatibility and imposes time step constraints.

- High level of coupling

  Again, this involves two way coupling , but in such a way as to be both time and space accurate; this is very challenging in every respect, e.g. dynamic fluid structure interaction.

Multi-physics solver approach
There are two main solution strategies for MP analysis:

- Directly Coupled Solution, i.e. a monolithic scheme, where all the variables are solved for in one integrated scheme.
- Staggered Solution, which may be either explicit or implicit, where groups of variables , usually associated with a specific phenomenon, are solved for in a suite of schemes.

4: OTHER REQUIREMENTS FOR MULTI-PHYSICS SIMULATION

CAE analysis technology has developed conservatively over the last decade – its users wish to protect their own investment over many years. Thus, in the context of commercial CAE analysis codes, then multi-physics simulation generally involves building upon established technologies and so typically involves the coupling of separate phenomena specific codes. Hence, it is essential to have phenomena specific solver software that can accept boundary data, volume source data and modifications to property data from other codes. For those cases where there is not a common database good filters are required to exchange boundary and volume source data from one solver module to another.

On a practical level, it is often necessary to have very good filters for mapping numerical information from one solver to another even when the meshes for each code are entirely compatible. Wherever possible the opening and closing of data files should be avoided i.e. a common database is desirable so that numerical information may be read directly by one solver from another. This is made more complex, because multi-physics solver strategy needs to accommodate, either a direct or an iterative schemes, employing either an Eulerian or a Lagrangian spatial discretization formulation or some kind of mixture used within the phenomena specific code components.

CAE phenomena specific software products are frequently scaleable parallel. Unfortunately, however, this does not guarantee that the coupling strategy based on such codes is compatible with scalable parallelism. Ironically, of course, the computational challenge of multi-physics simulation is just the situation in which parallel scalability is desirable for such large complex problems.

The problem here is essentially as follows:- the challenge is to ensure that the parallel mapping minimises the movement of data between the processors for the solution of each of the components. It is natural to put each component solver on a separate processor or processor group. Unfortunately, this maximises the movement of data around system and may compromise scalability, such that alternative strategies must be employed.

5: MULTI-PHYSICS COUPLING ISSUES

5.1 Code interoperability

In an ideal world, all solvers would be written in one software environment with a common numerical approach with regard to discretisation, meshing, solver strategy, and parallelisation strategy, where the data would be held in one common database. However, this is not practical if one wishes to use separate well-established commercial codes for each phenomena. Hence, a filter structure is needed to enable phenomena specific codes to exchange information directly from each other's database without opening closing files, which effectively requires interoperability of separate codes.

Coupling software currently available derives from tools originally developed for parallelisation, especially PVM (Parallel Virtual Machine)[2], MPI (Message Passing Interface) [3] and specifically MpCCI (Mesh-based parallel Code Coupling Interface) [4]. However, the challenge that remains is the parallel scalability of interoperable codes, as each code may run in parallel but their coupling may severely compromise scalability. Currently, MpCCI is frequently used to couple existing software for MP analysis, so it is discussed below.

MpCCI is a coupling tool that enables the exchange of data between the meshes of two or more simulation codes in the coupling region. In general the meshes belonging to different simulation codes are not compatible, hence MpCCI performs an interpolation. In three-dimensional analysis, the most popular type of coupling is surface coupling and other types of coupling are also supported, for example volume coupling in 3D and line coupling for simulation codes computing in 2D. In case of parallel codes, MpCCI keeps track of the distribution of the domains onto different processors.

MpCCI emerged from an European Union project to develop public domain Open Source tools for code interoperability in a parallel context. At the 6th MpCCI User Forum held at Schloss Birlinghoven in February 2005 a number of MpCCI facilitated code couplings were shown:

ABAQUS [6]+ FLUENT [7] for DFSI
STAR-CD [8]+ MSC-NASTRAN [9] for DFSI
Computational aero-acoustics (CFD + acoustics)

Although MpCCI potentially facilitates genuine coupling across the board the initial experiences have not been trouble free.

5.2 PRE and POST processing

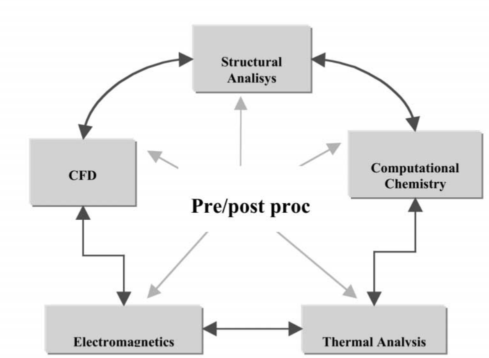

Figure 2: Multi-user Environment

In the multi-disciplinary environment a number of different numerical simulation software tools may be used, see Figure 2 , hence there is a need to for such environments to be able to read and write data in a number of different formats. A range of tools now provide such facilities, such as FEMGV[10] , FEMap [11], ANSYS [12], MSC-PATRAN [13], amongst others.

6: SOFTWARE TECHNOLOGIES

6.1 Sector specific "multi-physics" software

There are a number of industry sectors, notably in manufacturing, where the key features to be simulated involve some measure of multi-physics phenomena. From a web survey a number of sector specific MP software tools were identified within a set of activity groups:

Shape Castings

- PROCAST [14]
- MAGMASOFT [10]

Forming and Forging

- DEFORM [16]
- SUPERFORGE [9]
- FORGE3 [17]

Polymer Processing

- C-Mold [17]
- Moldflow[18]

Joining Processes

- SYSWELD (Welding software) [14]

Electronic Cooling

- Flotherm [20], which in the last year or so has acquired some additions to this software which enable loosely coupled solid mechanics analysis.

In general, with the exceptions noted, there has been little change for the above products functionality over the last 3 years of this survey.

6.2 Industry consolidation

Over the past three years additional physics capabilities have been bought to a number of existing software tools through industry consolidation. Examples include ANSYS [12] acquiring CFX [21] and AUTODYN [22] (through acquisition of Century Dynamics) and ESI [19] acquiring CFD-ACE and PROCAST[14]

6.3 Commercial CAE technologies

A web survey of tools claiming multi-physics capabilities was carried out and the key results are summarised below:

• ANSYS/Multi-physics [12]
ANSYS provides both direct and sequential methods as identified above, to couple multiple physics together:

At least two iterations, one for each physics module, in sequence, are needed to achieve a coupled response. The question remains of how close is the coupling and under what circumstances does it matter? There are also examples of MpCCI[4] interfacing of ANSYS[12] with CFX [21]for DFSI

Available physics include

- Structural
- Thermal
- CFD (now CFX [21])
- Acoustic
- Electromagnetic

Couplings include

- Thermo-mechanical
- Thermo-fluid
- Piezo-thermal-structural-electric
- Fluid structure interaction (employing MpCCI)

The web page shows a good deal of multi-disciplinary analysis, but more restricted fully multi-physics analysis. For example, multi-physics contact, where the current and resultant Joule heating in a switch contact is modelled as the switch is actuated. The mechanical, thermal and current flow are modelled using direct-coupled field elements. This is a good example of natural solver 'fit'

• ABAQUS [6]
Traditionally Abaqus has been very strong on non-linear solid mechanics analysis, but has recently announced technical collaboration with FLUENT[23] for DFSI using MpCCI. Examples of coupled problems include:

- Thermo - mechanical either sequentially or fully coupled, the web page gives a fully coupled example MP analysis of a disc brake.
- Thermo - electrical
- Pore fluid flow - mechanics
- Stress with mass diffusion , sequentially coupled
- Piezoelectric (linear only)
- Acoustic - mechanical (linear only)

It is useful to note here, that besides the FSI feature facilitated by MpCCI, all the couplings above involve either solver structural with a potential solver or two potential solvers.

• ADINA [24]
ADINA is a well established software toolkit for thermal-fluid-structural problems, using a variety of coupling levels. The example on the web is for a fuel system, exemplifying large structural motion and fluid flow. The software includes various turbulence models, incompressible oand slightly or fully compressible flow solvers. Different meshes are employed for the distinct computational domains e.g. different meshes for fluid & structure sub-domains. It is not clear either to what extent the software can effectively exploit parallel cluster technology and what is provided in the way of a user environment.

• ALGOR [25]
The Professional Multiphysics core package includes analysis capabilities for:

- Static stress
- Mechanical Event Simulation (MES)
- Linear and nonlinear material models
- Linear dynamics
- Steady-state and transient heat transfer
- Steady and unsteady fluid flow, and
- Electrostatics

The software simultaneously replicates the dynamic flexing behaviour of a component or mechanism to predict stresses that may result from motion or from the interaction of the part with other independent objects. One of the web examples is for the thermo-mechanical analysis of diesel engine cylinder head.

• AUTODYN [22]
Previously owned by Century Dynamics Ltd, Horsham, UK but recently acquired by ANSYS [12]. AUTODYN employs a mixed FV (velocity), FE (displacement) and DEM formulation in any mixture for fluid structure interaction. The software's focus is on extreme impact events, such as collapse and explosions. It is fully 3D and parallel.

• CFD – ACE [14]
Rather a solver environment than a solver, using PVM [1] as the means of interoperability. Coupled simulation for a variety of phenomena is claimed:

- Fluid flow
- Thermal
- Chemical
- Biological
- Electrical
- Mechanical phenomena.

• LS-DYNA [26]
LS-DYNA is well known as a dynamic explicit structural analysis software technology, however, it also has capabilities for multi-physics analysis. There are two examples of fluid

–structure interaction on their website, showing fluid flow between two glasses. Amongst a range of other examples on the web there is an unusually example of human-clothing interaction of a brassiere, exemplifying dynamic non-linear FE analysis of contact interaction with the body, showing large displacements. This example shows stresses in the bra cups and straps. In the same area of application are airbags and seatbelts in cars. It is unclear from the example whether the human tissue had been modelled and if so whether it was modelled using solid mechanics or whether it had been modelled as non-Newtonian fluid, which in view of the nature of human tissue may be more accurate.

• FEMLAB [27]

This software uses FE methods in both 2D and 3D and was originally built upon MATLAB [28], although it now has its own kernel solver technology. It has a clear and easy to use user environment and is increasingly widely used in undergraduate teaching.

- Capabilities include:
- Heat transfer
- Solid mechanics
- Electro-magnetics

Fluid Flow (Navier Stokes, incompressible, 2-equation turbulence model)

Most of the early work on multi-physics using FEMLAB essentially involved the coupling of potential solvers. However, there is now an example on their website showing fluid-structure interaction where the viscous forces and the system's pressure impose forces on the surface of a structure. The resulting deformation in the soft structure is not small and therefore the fluid regime changes dynamically, showing that the structure is coupled back to the fluid dynamics. The web illustration shows the velocity field and deformation at steady state.

• MSC- Suite of Programmes [13]

The major change is that this software suite has been coupled with STAR-CD [8] for DFSI through MpCCI [4]. The MP example on the web is for an Air Launched Cruise Missile, which is subject to engulfing fuel fire at a temperature of 1273 K. The FE model was created using MSC-Patran and MSC-PATRAN-Thermal was used for radiant heating. The external software employed was from Sandia [29] i.e. Coyote for thermo-chemical-fire, Pronto for dynamic analysis, Jaq for structural analysis and Toro for electro-magnetic analysis. EXODUS [29] PCL was employed for the interface. Again this is definitely a multi-disciplinary example but it is open to question as to whether it is a genuine closely coupled multi-physics analysis.

• PHYSICA+[30]

The origin of this software toolkit is the University of Greenwich, London, but as from 2004 it has been licensed through PHYSICA Ltd, Croydon. It primarily employs Finite Volume Unstructured Mesh (FV-UM) methods and its focus is on closely coupled problems. The web examples demonstrate:

- Navier Stokes flows (turbulence, free surfaces)
- Heat transfer (phase change, reactions)

- Solid mechanics (non-linear)
- Electro-magnetics

This software targets closely coupled multi-physics simulation, especially in the context of process manufacturing e.g. casting, forming, welding and it has implemented in parallel from outset. The core solver technology interfaces with a number of software products including ANSYS[12], FEMGV[10], NASTRAN[13], etc. Examples on the web include DFSI for AGARD 445.6 wing and extrusion through U-shaped die including parallel results

• STAR-CCM [8] and COMET[31]
COMET [31] was originally developed at the TU Hamburg, Germany, but bought out by CD-Adapco in September 2002 and withdrawn from market. Subsequently, it was re-engineered and reappeared as STAR-CCM+ late in 2004. It is based upon FV-UM approach and is essentially 3D. It claims to include

- Fluid flow
- Heat transfer and combustion
- Solid mechanics including fluid-structure interaction
- Vertex based polyhedral mesh based solver technology facilitating closely coupled simulation
- Operation in parallel

Currently there are limited examples multi-physics applications on web page although it appears to have the necessary framework for full MPA.

7: EXPLOITING PARALLEL CLUSTER TECHNOLOGY

What is clear from the above survey is that the established CAE products are facilitating closely coupled multi-physics simulation whether through coupling of existing codes or through the acquisition and incorporation of specialist multi-physics tools. The benefit of MpCCI[4] and other filter technologies is that they enable interaction at the code database level of separate codes. This is essential if otherwise separate codes are to be effectively coupled for multi-physics simulation. However, the drawback here is that all of the data exchange must go via filter and this may well form a compute bottleneck with respect to scalability on parallel clusters. A number of bespoke multi-physics simulation technologies which claim parallel scalability have clearly attempted to address the issue of ensuring minimising data exchange between processors whilst at the same time retaining an even load balance across the parallel system. There are more lessons to be learnt here by the established CAE products if they are to be effectively scaled in parallel when coupled to others in multi-physics simulation.

CONCLUSIONS

Consolidation is a major driver for enabling multi-disciplinary and multi-physics simulation. There has been some genuine progress in multi-physics simulation over the last few of years, but maybe not as much as might be expected superficially. The main reason for this is that coupling of codes to achieve reliable multi-physics simulation is an extremely difficult task, requiring knowledge and expertise over a range of disciplines, and the ability to work with a variety of software architectures.

PVM [2] and especially MPI [3] through its use in MpCCI [4] play their role in enabling code interoperability, as the first and necessary stage of coupling and most commercial tools demonstrate some coupling capability. Hence in the last few months we have seen the demonstration of ANSYS coupled to CFX and ABAQUS coupled to FLUENT in delivering fully coupled dynamic fluid structure interaction calculations. This development may well herald a significant advance in enabling rather more general multi-physics simulation across the full physics spectrum over the next year or two.

There are two remaining key issues to address:

- One is the effective exploitation of cluster based computer technologies in delivering scalable parallel multi-physics simulation by coupled separate codes in MPA
- The education of users to exploit technologies which house very complex physics 'cocktails'. Friendly user environments cannot replace the need to understand the physics and the interactions involved in delivering simulations which can be safely used in system design and assessment.

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