Information Technology

High-Performance Computing and Networking

Report of the HPCN Simulation and Design Industrial Working Group

" HPCN enables us to improve the way we work"

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EXECUTIVE SUMMARY

This document reports the findings of the Industrial Working Group on the use of HPCN in Design and Simulation. This group, composed of senior representatives of user companies in a number of different industrial sectors, was to define common objectives of industry and actions leading to the exploitation of HPCN simulation in a wide variety of industrial sectors in the next 3 to 5 years

Simulation consists of predicting the behaviour of real physical systems in actual or hypothetical circumstances based on models of these systems. Simulation is widely used to support engineering design since it allows prediction of the performance of a product based on design data only, without the need to build a prototype. It thereby reduces the need for long and costly experimental tests. For example, the aerodynamic lift and drag of a plane can be estimated for different design options without any physical experiment, so that a more optimal design can be reached with fewer experimental tests. Other examples of use of simulation for design abound in most industrial sectors. Simulations are also being used to improve complex industrial processes in terms of efficiency, safety and security of service. For example, simulation is being used to predict the behaviour of an electrical power system. This may help define the most cost-effective set of plants to operate to satisfy customer demand, while taking appropriate measures to avoid electrical black-outs.

Simulations need to be accurate and often require massive amounts of computation. They have been pulling the state of the art in powerful computers and are now starting to benefit from the higher computational power offered by parallel processing. They also require complex computer programs to model the physical world and to harness the power of the fastest computers. While the first large simulation codes have been developed in universities in the 60's, powerful simulation codes for a number of disciplines are now available through licensed products, while others have been developed in-house by leading-edge user industries when they were felt to represent a critical competitive edge.

An important objective of manufacturing industry is to improve its competitiveness in international markets through better product design, more efficient process operation, reduction in time-to-market, or reduction in cost base. The adoption and exploitation of simulation techniques can help address many of these issues. Today, HPCN offers substantial advances in terms of performance and performance/cost ratio. A widespread adoption of HPCN simulation in industrial design and production, and its integration with existing practices are needed to fully exploit the benefits. There is also an important application potential in new sectors such as the optimisation of business processes.

The performance benefit of HPCN in simulation requires adaptation of existing software, as started e.g. in the HPCN EUROPORT actions. A wide deployment of the technology will also require R&D work to integrate simulation into current industrial practice, to extend the scope of existing applications to more complex problems and to multidisciplinary simulation, and to develop completely new industrial or commercial applications. The R&D actions should build on existing know-how and should help disseminate the benefits of simulation, for example by productisation of existing application codes and exploiting the human and computing resources of existing HPCN centres. These actions should follow guidelines ensuring industrial exploitation and efficient project operation. Finally, actions which increase the ease with which industry

and commerce can locate and exploit appropriate expertise in HPCN and simulation should be promoted.

An important aspect conditioning the acceptance of HPCN simulation in a wide variety of sectors and activities is the business case demonstrating that the investment in this new technology will be profitable. The business case will be better understood when more examples of successful exploitation are demonstrated, and the risks of investment in HPCN will be reduced when portability of software is better supported and when more application codes are offered for HPCN platforms.

The thrust of the proposed actions is to exploit the collective knowledge of applications and HPCN techniques to accelerate the deployment of simulation utilising HPCN as an integrated component of the design and business processes used by European industry. This will require continued emphasis on the development of HPCN applications with complementary initiatives to improve user environments. This balanced strategy will ensure that the full benefits of HPCN are realised with a corresponding impact on the quality of products and processes, and hence on competitiveness. An important component of the proposed actions is to broaden the exploitation of HPCN to planning, control, operational and manufacturing applications to achieve an extensive, widespread and sustainable impact with real business benefits. Accompanying measures aimed at increasing the level of interaction between the necessary actors to support the specific aims have been devised. The actions have been devised in a framework which places emphasis on focusing support to projects which have clear goals and require genuine collaboration between recognised experts in order to improve industrial practice within at most 3-5 years.

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1. Background and Introduction

1.1 Objectives

The Industrial Working Group on the use of HPCN in Design and Simulation was convened with the aim of establishing the objectives of industry regarding the use of HPCN simulation to improve their business, the obstacles to the exploitation of this technology, and proposed actions to ensure a wide adoption in all industrial sectors. This report of the findings of the group and the actions it proposes will directly contribute to the generation of a workprogramme for this area. The working group discussed a wide range of issues relating to the successful use of HPCN in this field. A constraint adopted by the working group was that the proposed actions should deliver results and business benefits within a timeframe of 3 to 5 years.

1.2 Scope of Discussion of Working Group

Current work areas in the field and future opportunities and challenges for industry have been discussed. Industrial perspectives include better performance and lower cost for applications in use today, better integration into the work practice of engineers, expanding current practice into new areas or new methods, and new applications.

The adoption of HPCN simulation in any industrial activity represents a change of technology, and there are always resistance factors to such changes. These barriers can be analysed with respect to the various ingredients needed for deployment, and to their sources of supply. Hardware platforms ranging from workstation clusters to massively parallel processors (MPP) were addressed. Basic software for parallel systems was discussed, and useful suggestions for this part of the programme were made. Last but not least, recommendations were made with respect to application software code and its support.

The group discussed different proposals including activities other than R&D, such as standards, training and awareness. These could all be included in the strategy of the focused cluster on HPCN.

An important component of the working group activities was to examine the business case relating to the use of HPCN in design and related activities, to examine factors that are likely to inhibit widespread rapid adoption in industry, and to devise actions to overcome these resistance factors. In a number of advanced user industries, powerful simulation codes are already exploited in the corporate R&D centres for industrial research, method development or direct service to business units. An important factor in those industries is the adoption of this practice by the business units and design departments for industrial production.

2. Industrial HPCN Simulation Objectives

2.1 General Objectives

The primary industrial objectives regarding HPCN simulation have to be seen in the context of the need for industry to maintain or improve competitiveness in increasingly open global markets. Industry is being faced with new requirements driven by customers, regulations and safety, which have resulted in a significant increase in product/process complexity, meaning more complex designs and systems, and an increasing number of design or operational options, together with the need to control operational costs. At the same time, it becomes increasingly important to introduce new products early on the market; a reduction of development times is critical to market success.

In the area of product/system design, the uptake of HPCN simulation promises to

- reduce product design time, allowing faster time to market.
- enable the design and efficient production of complex systems with better performance than today's systems, with reduced environmental impact, with lower maintenance level, and which are more reliable and safe.
- reduce design costs and risks
- reduce the need for long and costly experimental testing

Although HPCN simulation is being used today by design teams in a number of leading-edge industrial sectors such as aerospace, new advances in the performance and cost-performance ratio of HPCN platforms on the one hand and the availability of more powerful application codes in a variety of domains could allow a wide range of enterprises in all industrial sectors to exploit the above benefits.

The deployment of the technology and its use in the industrial design process is likely to proceed at an increasing pace over the coming years. The take-up will be facilitated if the barriers to entry are reduced and if the resulting advantages become more widely known. Key factors which will ensure adoption in industry include

- a reduction of the cost of simulation to levels that are competitive with alternative techniques when they exist. HPCN simulation will be seen as useful to industry only if its use brings direct and indirect economic returns. This point of view will be emphasised in section 4. of this report.

- a reduction of the turn-around time to levels compatible with current practice of design engineers, evaluated on a case by case basis e.g. a car wind tunnel test takes 2.5 days.

- increases in the scale, scope and accuracy of the problems which can be analysed with simulation. In practice this would be achieved through finer discretisation of the geometry, more complex models, the assessment of more options within the design space, the simulation of complete systems rather than system parts or the simulation of coupled physical phenomena.

- a full integration with other design, development and operational systems e.g. including mesh generation from CAD models.

- a complete and reliable set of user interaction systems, in particular for model building (pre-processing) and interpretation of results (post-processing)

Competitive pressures are also high in process industries, as exemplified by the contributions from the chemical and energy sectors. The deployment of HPCN simulation in these sectors should lead to comparable advantages in terms of improvement of output quality while controlling costs and environmental impact, and improving safety margins. In these sectors, simulation can be used for the optimisation of operation and control of existing processes, for helping decisions in long-term planning and for operator training. Finally, simulation is starting to find applications in the optimisation of business processes such as banking and distribution. It should be stressed that many members of the working party felt that the early adoption of HPCN in these fields was at least as likely as it is within the design process and would fuel growth in the HPCN user community by addressing a wider target audience.

2.2 Industrial HPCN Simulation Objectives: Examples by Sector

This section covers a number of examples of current or future uses of simulation in industry, and the objectives that could be reached within the timescale of 3 to 5 years. These examples are representative of a large number of industrial applications but do not intend to be exhaustive. The order of the contributions is not representative of priorities in terms of HPCN.

2.2.1 HPCN Objectives: Energy Exploration & Production

HPCN is used to process seismic data and recover an image of the substructure of the soil. This image is then used to simulate the extraction of gas/oil and to optimise production. This sector is traditionally a major user and early adopter of high-performance computers. Better models and finer meshes will provide better simulations which will in turn allow more optimal production. This may require large increases in computational power.

2.2.2 HPCN Objectives: Energy Generation & Distribution

The use of HPCN and customised CFD and other applications in the design/analysis of components and industrial processes (e.g. combustion, generation and removal of pollutants, explosion, cooling and condensation, core transients, thermal hydraulics, groundwater flow, chemical kinetics) within plant and storage (e.g. nuclear power stations, thermoelectric power stations, waste depositories). As well as the need to simulate the physical processes for safety purposes there is also the important requirement to optimise the design and identify how to operate plant at reduced margins for both economic and environmental benefits. Some of the phenomena and criteria involved in the design of fossil fuel plants, namely fluid dynamics, combustion, turbulence, are quite similar to those encountered in other industrial sectors such as the aerospace (see Section 2.2.5) and automotive (see Section 2.2.6). This may stimulate important synergies among different industrial sectors.

The use of HPCN and optimisation applications targeted at operational cost reductions e.g. in fuel purchase and usage, in plant maintenance and replacement (e.g. pipelines installation/replacement, fuel assembly exchange/rearrangement). Excellent potential for early adoption of HPCN is seen. The business case for adoption of HPCN may be influenced by organisational (e.g. internal accounting of fuel costs) and legislative issues.

The use of HPCN and simulation of power plants and electrical networks. In this field one objective is to create new designs which are both less expensive and safer. Simulation of existing plants allows for safer operation and increased availability. Simulation running faster than real-time can be used as decision support for operators in crisis situations. Simulation is also important for the training of operators, especially to situations which are costly, impractical or dangerous to experiment in practice. This includes critical situations of power networks or power plants, especially nuclear. For fossil fuel plants, simulation brings improvements in terms of operation efficiency and reduced toxic emissions. More accurate simulation may allow the operation of electrical power systems with reduced margins, thereby reducing future needs for investment in installed power. Accurate simulation of day-to-day operation leads to substantial energy savings while maintaining security of service. The opening of markets to third-party providers and the increase in cross-border transfers requires operation of the networks under conditions not envisaged during planning. Simulation of the multinational network is necessary to ensure security of operation under these conditions. For most of these applications, the requirements include simulation using larger and/or more accurate models, and the simulation of combined systems or combined physical phenomena.

2.2.3 HPCN Objectives: Electronics Industry

Simulation is used for the design of electronic systems to verify electronic and logic operation of ASIC and circuit board designs, thermal behaviour and electronic interference problems. It currently takes about 10 hours to simulate ASICS with 50,000 gates on a typical workstation. For the design of ASICS with 200,000 to 300,000 gates, the use of parallel computing will be needed. Cadence, as an example, is a major software supplier to European companies in this field, and they already provide a means to distribute simulation on a small number of workstations. If HPCN (workstation clusters in the first instance) were successfully applied to this area (i.e. to deliver higher quality products and reduced time to market) then the results would impact a large number of users i.e. designers. Rising clock speeds in electronic devices increases electromagnetic interference. It will be important to consider these effects when designing new products, which will require the integration of CAD tools with electromagnetic modelling.

The use of HPCN in electromagnetic modelling for the design of components such as klistron power tubes, gyrotrons and antennae. All of these components are custom built. HPCN is expected to cut design, development and testing timescales and costs, and reduce business risk in bidding for contracts by allowing achievable performance to be predicted. At present, the analysis of a radiation pattern for an antenna takes 4 hours of Cray YMP time for one single frequency. Many applications are currently out of reach due to computational complexity, and hence cost.

The use of HPCN and full-wave analysis in complex 3-D geometrical configurations e.g. of high frequency high power microwave and integrated circuit systems will be essential to optimise the performance of the coupled system.

2.2.4 HPCN Objectives: Chemical and Pharmaceutical Industry

The use of HPCN in process engineering and CFD applications (preference for use of third party applications, many sourced in Europe) for chemical plant design in order to improve product quality, make savings in materials and energy, and increase safety. This covers modelling, dynamic, steady state simulation and optimisation of sub-components up to whole chemical plants. State of the art applications include Speadup (European) and

AspenPlus (US). A minimum of one order of magnitude in cost-performance is needed over traditional computing systems to meet requirements. European CFD codes used/wanted include FLOW3D, FLUENT, PHOENIX, POLYFLOW. In-house developments are also expected to take place from a recognition that industrial HPCN objectives will not be entirely solved by these applications alone as they are limited in their capabilities particularly for complex 3-D geometries.

The use of HPCN and planning/scheduling applications using mixed integer nonlinear programming and other techniques to tackle combinatorial optimisation problems such as those encountered in the operation of plant and production scheduling. This field is seen as most promising for initial penetration of HPCN as the companies have control over the software used and financial support for the work and equipment is available as there are clear business benefits to be accrued within 2 to 3 years.

The use of HPCN to optimise the properties of materials (e.g. polymers) used in other industrial processes (e.g. injection moulding) and to ensure that these materials meet the requirements of new legislation (e.g. that the material is biodegradable). This is a field in which rapid responses to market trends are required in order to maintain competitiveness, and business funding is available. Such studies are often undertaken in collaboration with suppliers or customers and as such offers the potential for technology diffusion, possibly to SME's.

The use of HPCN and molecular dynamics/quantum chemistry applications using a variety of techniques (e.g. ab initio and semi-empirical) for design of, and research into, improvements in materials and new drugs. Simulation offers a unique lever to the design and development of chemical products (i.e. other experimental techniques do not, in isolation, meet business goals). In some companies this activity will account for roughly half of the production cycle requirement. There is a strong requirement for use of third party applications, many sourced from United States. European codes used/wanted include GAMESS-UK, GROMOS, ADF, TURBOMOLE. The European codes do not cover all requirements to fulfil design objectives. US. codes used/wanted include DMOL, SYBYL, from Biosym, Tripos. In-house applications are the exception and are not desirable because of the need to support them, although some initial parallel implementations have been tackled in this way. European codes are developed in collaboration with University departments which have an established reputation in the appropriate field. Existing projects within EUROPORT (addressing GAMES-UK, TURBOMOLE, GROMOS, MINDO92, VAMP, ADF) are viewed positively and seen as a mechanism for HPCN champions to demonstrate the capabilities to their management. Although improvements in molecular modelling are important for the design of new products there remain long delays for some products due to certification procedures which extend the time to market.

In this industry, the use of symmetric multiprocessors and workstation clusters is seen as an incremental strategy to HPCN which is adequate until a business case for an MPP system can be shown. In the meantime, there is a strong interest in evaluation of different MPP systems in HPCN centres .

2.2.5 HPCN Objectives: Aerospace Industry

The use of HPCN and CFD, structural analysis, impact analysis and related applications for design of all aspects of aircraft (particularly engines, airframe and their interaction).

The design process aims to optimise the conflicting engineering constraints of aerodynamic efficiency, weight, stress and vibration (defining lifetime and maintenance periods), noise, emission levels, and manufacturing costs. Getting the right product at the right cost requires all of the relevant objectives and constraints to be taken into account simultaneously. This can be supported by integrated or coupled simulations. Such analyses will reduce design times and development costs, and increase the likelihood to reach the right design at the first time.

Specialised requirements in this sector (but common to requirements in other sectors) include combustion, chemical kinetics, fatigue, crashworthiness, Monte Carlo techniques for modelling atmospheric re-entrance. Combustion, which is also important in other sectors such as energy and automotive, is an obvious candidate for HPCN due to the computational requirements of the problem. This is common to other coupled problems where different time constants of physical phenomena, here chemical reaction and fluid flow, require large numbers of time steps in the simulation.

The CFD codes used tend to be in-house with use of 3rd party codes particularly in the related fields of stress, vibration and impact analysis (NASTRAN, DYNA-3D, ABAQUS from the US. and SAMCEF, PERMAS from Europe). Pre-processing costs have motivated use of unstructured techniques though these are not fully into production use. HPCN could impact both turnaround time and quality of modelling leading to business benefits such as design risk reduction, and reduction of product development time and cost. Unstructured viscous flow solvers are seen as an important development area where MPP is required to make advances over inviscid techniques. Direct Numerical Solution and Large Eddy Simulation techniques are seen as important research topics that will improve and simplify turbulence and transition models used in industry.

The use of HPCN and electromagnetics applications is seen as an area with crucial business importance. As a result, many application codes are developed in-house. In the aerospace sector, the cost and difficulty of experimental techniques has fuelled a great deal of interest in MPP use (and led to some notable MPP deployments). The challenge of designing electrically large, geometrically complex bodies composed of different materials yields modelling requirements that outstrip available computer resources and have forced use of out of core solver techniques. This trend is expected to continue into the foreseeable future, and will be joined by a movement towards unstructured techniques to reduce preprocessing overheads (as with CFD).

The use of HPCN in Computational Material Dynamics applications are also required for modelling of manufacturing processes such as casting, metal forming and plastic forming to improve yield, integrity and optimise production techniques. Again, further improvements are foreseen by the development of multidisciplinary applications supporting multiple materials and physical processes.

The use of HPCN with other specialist applications such as acoustic modelling (for identification and removal of sources of noise), thermal modelling and crack propagation.

As discussed more generally in Section 2.3.2, there are strong requirements for the improvement of all components of a complete computer aided engineering system, including advances in mesh generation and visualisation.

In this industry, the use of workstation clusters is seen as an incremental strategy to HPCN which is adequate until a business case for an MPP system can be shown. In the meantime, there is a strong interest in evaluation of different MPP systems in HPCN centres .

2.2.6 HPCN Objectives: Automotive Industry

The use of HPCN and a wide variety of engineering applications to provide a fast, robust and reliable alternative to, and complement for, experimental testing during product design and development. The reduction of product design and development timescales and costs whilst improving product quality is the major objective.

Simulation using HPCN has not yet become fully integrated within the design and development process and in many disciplines there are major challenges to achieve the required improvements in modelling accuracy, numerical techniques and computational performance before it will be financially and technically viable. As a result companies in this sector are in a process of ``technology watching" to assess the correct time to introduce and integrate HPCN simulation in each component of the overall design process. A wide use of simulation in product development could increase design efficiency (time/costs) by up to 30%. Simulation is used for both short term design and longer term development problems. In all cases the pre- and post-processing stages are equally as important as the simulation itself, and there are a large (and increasing) number of test cases to be assessed.

The use of HPCN and applications (e.g. FIRE and STAR-CD) coupling nonlinear systems such as CFD, reaction kinetics, mixture preparation and emission mechanisms are needed for piston engine design. This is required to meet future emission legislation and reduce fuel consumption and noise. The main barrier to the introduction of these techniques within the design process is achieving dynamic analysis on realistic moving engine geometries (e.g. manifolds, cylinder heads) over a wide range of engine loads within acceptable computing costs. It is estimated that each test case should not require more than 0.5 days on a large MPP system. A significant step towards integrating this capability within the design process is achievable within 3 years, based on results from previous projects.

The use of HPCN and similar coupled applications are required for the design of heating/cooling systems and passenger cabins.

The use of HPCN in finite element analysis and computational material dynamics applications (e.g. Nastran, Abaqus, Pamcrash, Pamstamp) are required for crash analysis, assessment of fatigue and the improvement of modelling of manufacturing processes such as stamping, casting, hardening and friction welding to improve yield, product integrity and optimise production techniques.

The use of HPCN and electromagnetic modelling to meet EM interference legislation.

The use of HPCN for microscopic traffic system simulation. Developments in this field are required to meet economic and ecological demands on transportation systems through evaluation of plans for a traffic management infrastructure before the year 2000. Providers of equipment to this market will require access to such applications of HPCN, as will transport service companies and government.

The use of HPCN for optimisation of entire vehicle system dynamics.

The use of HPCN in design, development and production of new materials such as alloys and ceramics.

The pressure for cost and timescale reductions in product design and development is forcing the common use of CAD (and in the future CAE) tools between major manufacturers and component suppliers (possibly SME's). There is hence a tendency for technological change to percolate through the supply chain.

2.3 General Requirements for Improved Use of HPCN in Simulation and Design

2.3.1 Building on existing know-how in application codes

Existing applications embody a vast amount of know-how from the points of view of mathematical models of physical phenomena, of algorithms for the efficient and accurate solution of these models, and of user-interfaces to the design engineers. This know-how should be built upon by integrating existing application codes into the overall strategy as has been started with the EUROPORT actions. Advances in the implementation of algorithms on HPCN platforms and advances in the implementation of complex models are addressed in this section, whereas the interfaces are covered in Section 2.3.2. There are doubts that simple "porting" of existing application codes would suffice to fully benefit from the performance of MPP architectures. It is the case that some major applications will, at least in part, have to be rewritten for MPP's. Since this may be a formidable task for complete application codes, a first step may be to define the parts of these codes used in the most common application examples and to rewrite only those parts. End-user industry is prepared to stimulate porting of application codes by Independent Software Vendors (ISV) but will generally not enter into complex arrangements that would involve long term commitment.

Extension of the scope of simulation packages through the coupling of systems from different disciplines is an important objective in different industrial sectors. This could be done at a number of different levels of integration from allowing the simulations to work within a common design environment through to true integrated multi-disciplinary applications allowing concurrent design with respect to all the required engineering disciplines simultaneously.

The development of new applications is envisaged in a number of industrial design and planning disciplines. These applications will exploit fundamentally new approaches to simulation and problem solving (e.g. genetic algorithms for solution of non-linear optimisation problems and Large Eddy Simulation techniques for calculation of turbulent flow). These applications will complement existing techniques rather than replace them. The advancement of the state-of-the-art in solving large non-linear optimisation problems would have an extensive and widespread impact across both the industrial sectors discussed here and also within many commercial sectors. Genetic algorithms, which are inherently parallel, can build upon existing problem solving techniques, and which may address both multi-objective optimisation and covering problems are seen as a particularly important emerging field in HPCN.

Finally, a wide deployment of simulation codes will be greatly facilitated by improving their integration in the environment of design or operation engineers. This requires improvements in the pre-processing and post-processing packages, as well as in user interfaces. These topics are discussed in more detail in the following section.

2.3.2 General advances needed in Pre-processing, Post-processing and Modelling

In order to fully benefit from the performance improvements of simulation codes, it is necessary to match these improvements with advances in other components of the complete computer aided engineering chain, notably the mesh generation (pre-processing) and visualisation (post-processing) packages.

Pre- and post-processing were recognised as critical for all areas of simulation in engineering design. An important aspect of pre-processing in product design is the generation of a mesh covering the geometry of complex parts being designed. The main bottleneck in post-processing is efficient visualisation, i.e. the reduction of large amounts of data into forms which can help engineers make design decisions. An example of successful integration of pre-processing and post-processing with a simulation code was achieved in ESPRIT HPCN Project IDENTIFY.

Pre-processing

The generation of meshes for simulation is recognised as a serious bottleneck that is costly, limits the benefits of MPP and consumes the time of trained design staff. The use of appropriately designed meshes is essential for controlling the accuracy and timeliness of simulation runs. The integration of CAD modelling and simulation via mesh generation remains a major challenge in which standardisation may play a major role.

As an example, the generation of a multi-block mesh, an advanced type of geometrical model, can take up to 6 months, and subsequent editing (following analysis of the initial results of a simulation run) is also a significant overhead due to the size and complexity of models representing the 3-D geometry and materials. These issues have led to a trend towards automatic mesh generation, and there have been significant recent advances in algorithms (e.g. the coupling of advancing front techniques with Delauney triangulation) which has reduced mesh generation times to a few minutes on workstations. Possible use of MPP's has also led to interest in solving more problems of increasing complexity (e.g. viscous flow for which an order of magnitude more cells will be required) which further compounds the pre- and post-processing problems.

Some mesh quality issues have been tackled at the research level and require consolidation. Nevertheless improvements in the robustness of algorithms are required. These include accuracy control, handling overlaps and holes (created by bringing together different CAD models) and optimising the quality of the mesh to make maximum effective use of HPCN systems. For example, when the time evolution of a system is computed at regular intervals, a good quality mesh optimises the number of time steps needed for a given accuracy of the results. An important element is the further development of generators of unstructured meshes and of solvers adapted to these.

Currently an engineering design may have to be meshed more than once, each mesh being tailored to the requirements of the simulation being performed. The goal should be to devise intelligent meshing algorithms that exploit knowledge (e.g. of mathematical models used, the geometry of the object, the likely behaviour during simulation) to optimise the mesh. These points are seen as particularly important to avoid wasting cycles on expensive MPP systems. Visualisation could play a major role in identifying and rectifying flaws in simulation models.

Certain engineering design studies (e.g. engine design) will require further advances to realise mesh adaptation algorithms to allow modelling of moving walls (e.g. pistons) and analysis of transient phenomena. These algorithms will have to be fully integrated with the simulation code itself, and hence will have to run on MPP systems.

The development and maintenance of complex mesh generators are costly operations which are increasingly difficult for a user industry to support in-house. Vendors have appreciated the importance of this area to levering the use of HPCN in design and have developed state of the art mesh generators. Such developments, along with in-house developments of end-users or from Universities, could form the basis for an action leading to a commercially supported system..

Post-processing

Postprocessing is an important area due to the volumes of data representing many physical variables at many different points produced over long sequences of timesteps during the simulation. HPCN visualisation techniques will be required for users to assess this data in terms of the transient behaviour of the designs simulated. Current data analysis take time and is costly. An interactive visualisation tool is needed which would allow dynamic control of the simulation and instant assessment of results. Fast simulation and high I/O bandwidths to the engineers graphics workstation are prerequisites for achieving this objective.

User environment

It is generally recognised that much better HCI's are required and that ``applications generators" are needed as the trend towards multi-disciplinary and concurrent design continue. Progress in pre-processing and post-processing would contribute to improving the user environment. Intelligent interfaces could assist the engineer in the specification of simulation code control parameters on the basis of the application, assist with data reduction in presentation of results and optimisation of design parameters.

Modelling

The simulation of industrial processes and the simulation of the dynamics of complete systems involves, beyond the simulation of the behaviour of individual components, the modelling of the interactions among large numbers of coupled individual components. Traditionally, interactions are studied with simplified models for the individual components. This requires substantial effort of model tuning, and limits the scope of the simulations. The larger computational power offered by HPCN would allow models closer to the design models to be used. This may reduce the effort of model build-up and will allow simulations to be extended beyond normal operational conditions. This is important to predict the behaviour of critical systems such as nuclear power plants or electrical networks in abnormal conditions.

2.3.3 General Parallel Software Requirements

From the point of view of the user of simulation applications, standard environments ensuring portability should be used as much as possible. Requirements for these environments include widespread availability (on workstation networks through to MPP's), platform specific implementations and robust behaviour. Public domain implementations of message passing systems were seen as catalytic in encouraging use of parallel systems but may not be suitable for production usage.

An important aspect of the provision of versions of existing applications on HPCN systems is that the user interface must be preserved and the exploitation of parallelism must be completely transparent (automatic configuration)

Scalability of system performance when the number of processors is increased is also important.

The application programmer should be abstracted from levels of detail of the parallel implementation through the provision of appropriate libraries and programming interfaces. Libraries of mathematical functions optimised for parallel machines, when available, should be used as much as possible. These libraries should provide robust interfaces and high performance. Their use frees the application programmer from implementation issues related to pre-conditioning, out-of-core implementation or concurrent execution.

2.3.4 Building on existing know-how in HPCN

There are now a large number of organisations which have invaluable expertise in HPCN within Europe. These can be broadly classified as HPCN centres within universities or government laboratories, vendors of HPCN systems, software consultancies and groups within companies who have adopted, or are planning to adopt, HPCN technology. There is a general requirement to expand the size of the industrial and commercial base of knowledge in HPCN by supporting access to HPCN centres (or vendors) where advice and guidance is readily available. An important requirement is to identify where specific skills and resources are available as has been initiated by the EC Parallel Centres Initiative. The dossier of these skills and resources should cover all aspects of HPCN in design and should not just be limited to HPCN tools and techniques or HPCN facilities but should also incorporate know-how in new simulation and modelling techniques. This will allow industry to find the most appropriate organisation to approach based on their specific needs, and this will encourage ``training by doing" as discussed in section 2.3.5.

2.3.5 Training

Industrial Staff

The needs for training to HPCN technology are different for the staff who are or who will use simulation applications and for staff who will develop or tailor such software codes.

End-users of HPCN simulation applications must be trained on the use of HPCN simulation and on the evaluation and selection of these systems. Given the importance of the evaluation of HPCN systems, especially in the support of industrial investment in HPCN, system evaluation appears as an appealing training mechanism. This could take the form of activities related to benchmarking of an existing parallel application and would encourage broader familiarity with parallel systems. If no application exists, short application feasibility projects could be conducted to assess the suitability of parallel systems. This might act as a catalyst for further work on HPCN in industry. It is envisaged that these training activities could be supported by experts from HPCN centres or SME's with expertise in the field working directly alongside the industrial participant.

End-users should not need extensive training in the details of parallel algorithms.

Training is required for software developers (a small number compared to the potential end-user community) within industry and emphasis must be placed on ensuring that it is relevant to the direct activities of those being trained i.e. ``on the job" training or ``training by doing".

Academic Training

Training of young graduates, through the introduction of HPCN in University curricula, is already underway. The integration of these graduates will ensure that HPCN know-how gradually permeates industry. As in other fields, it is important to ensure that university graduates are exposed to the needs of industry. This could be done by industrial placement, or by working on industrial problems in HPCN centers.

3. HPCN BUSINESS CASE

3.1 Summary

In the previous section, the need for the availability of application software tailored for HPCN was discussed together with the need for integration of these codes within other enterprise systems. In this section, the economic elements affecting the decision to invest in HPCN simulation and to deploy it in business operation are analysed.

There is an overall business aim to achieve better results with reduced costs, i.e. to develop better quality products (increased safety, lower capital and operational costs) at lower design and development costs and timescales and with reduced risk. A major goal is the replacement of costly design and development processes. For each process there is a threshold point that must be reached before simulation is accepted into the design process. This threshold may be low as alternative techniques are expensive or untractable (e.g. electromagnetics), or high as alternative techniques are widely used, trusted and accepted (e.g. car body aerodynamics).

The adoption of HPCN simulation represents a change of technology which may take different facets. It may consist of replacing simulations running on conventional computing systems or a change from experimental tests to computer tests. This change may require re-training, capital investment, and reorganisation of other activities to put into place. These changes always involve resistance factors There is then a threshold where the expected benefits outweigh the perceived start-up costs and risks. The HPCN programme should help to push a variety of simulation topic areas over this threshold of acceptance. Barriers include a lack of applications software (third party and in-house), and a lack of information to support the internal business case and develop a new computing strategy. Use of HPCN systems in centers to build up production usage and the business case might, for example, be one component of a strategy to overcome these barriers.

3.2 Discussion of Issues

To date, HPCN (and specifically MPP systems) have only been adopted for a small number of specific types of very demanding applications (e.g. computational electromagnetics, computational molecular dynamics and specialised forms of computational fluid dynamics) which have been parallelised to a high degree, and for concurrent batch processing of serial applications. A general characteristic of these types of applications is that they are crucial for the competitiveness of the user companies and that alternative design and development techniques either do not exist, or do not represent cost-effective substitutes to simulation. A majority of these application areas had already been precursor users of vector supercomputers in the 70's and 80's.

It can be argued that only a limited number of engineers are concerned with the leading-edge applications already using HPC. Other design areas potentially affecting many more users should be targeted to expand the HPCN end-user community. Applications of simulation to operation and control of industrial processes and to the commercial sector may also improve the productivity in a large number of jobs. The challenge for any workprogramme in this area is to contribute towards the expansion of the business case for the adoption of HPCN to a wider range of activities and industrial sectors.

The deployment of HPCN simulation in industrial practice represents a change of technology, which can take different facets. For leading-edge applications, MPP solutions will be competing with upgrades of vector supercomputer systems. For a large number of applications where some form of computer simulation is already used, parallel implementations would replace implementations on workstations. Finally, there are a large number of domains where simulation will increasingly replace or complement experimental testing.

An important element in the evaluation of the business case in each one of those situations is the availability of application software codes or the cost and risk associated with the adaptation or development of appropriate versions of such codes. The combined effect of platform change and software adaptation are discussed in more detail below.

For design applications which are already running efficiently on vector supercomputers, the migration to MPP technology is seen as strategically important, but with a risk of interference with the on-going design practice. On the one hand, an upgrade to a more powerful vector machine may represent a high cost option but has an immediate, quantifiable impact on the turnaround of the design applications. On the other hand, the migration of the design applications to a new MPP platform takes time and achievable performance levels are either not known or are perceived to be risky. As a result there is a perceived risk of being left ``high and dry" without a stable, working solution to the design problem if the MPP route is taken.

For applications which are currently being run on workstations, the transition to parallel technology may be perceived as a more limited risk option if the workstation cluster path is considered. Indeed, if the parallel implementation experiment fails, the resource can be used as a set of workstations in the traditional way. It turns out that, for MPP systems based on commodity components, the boundary between MPP and workstation cluster is diminishing, as both can be used either as one large system allocated to a single task or as a collection of individual processors running separate tasks. However, the perception remains different and for this reason, workstation clusters may currently be preferred by company management.

It has already been stated that the deployment of HPCN platforms crucially depends on the availability of simulation applications targeted for these platforms. Leading-edge users of HPCN simulation have been developing a number of such codes in-house during the past decades. The business case for the continued development of in-house software within large European companies is under pressure despite the strategic need for innovative applications that deliver competitive advantage over third party application offerings. As a result there appears to be a general trend and willingness to directly, or via spin-off companies, sell and support this software. The main inhibiting factor is a ``chicken & egg" situation of the cost of commercialisation without an established market to guarantee return on investment. The commercialisation and support of such codes by these companies or by third party software vendors should be facilitated. The arrival of the new technology of parallel computing is viewed as an opportunity for Europe to productise such innovative applications developments and re-capture market share and control from US. software vendors. The migration of applications from expensive supercomputers to more affordable systems would increase the market for the applications. This would also help to encourage commercialisation through development of a wider user community.

One of the points of discussion concerned the deployment of HPCN technology from the research centers of large companies to their business units. The business case for initial acquisition of an HPCN system must be argumented with a 3 year return on investment period, the depreciation period for such systems, and use must relate strongly to the activities of business units to be justifiable. The profitability is usually argumented on the basis of services provided by the design process developers to the business units. This is achieved using a mixture of corporate and business unit funding. The aim of the design process developers is to use this mechanism to lever widespread adoption of HPCN by the REAL end-user community within their business units in the long term.

3.3 Involvement of SME's

The role of SME's in HPCN simulation can be seen from two points of view, namely as users of simulation and as developers of simulation applications.

SME's developing advanced products are being pressed to adopt higher levels of technology by the competitive situation or by the need to ensure compatibility with integrators. For these organisations, the barriers to the uptake of HPCN simulation, e.g. in investment and risks may weigh even higher than for larger companies. As a consequence, solutions based on workstation clusters, which are seen as lower risk, will generally be preferred. Producer/Supplier links may be exploited to catalyse HPCN usage by SME's. This would require targeting specific design topics where this link exists.

The productisation, commercialisation and support of simulation applications are often performed by SME's. As mentioned earlier, the new parallel computing technologies may give a window of opportunities for such organisations to launch new applications on the market. targeting the commercial marketplace are likely to have more targets and give faster results than those in Science and Engineering.

4. Topics and Rationale

This section describes a number of topics for a programme on HPCN simulation, and justifies their importance. Specific actions related to these topics are described in Section 4.

4.1 HPCN Applications for Design

The work already supported by the EC, to develop and exploit existing know-how in HPCN simulation, can be usefully expanded and continued. Further investment in this topic will help to maximise the potential customer base for European third party applications. Emphasis should be placed on bringing benefits of HPCN to a large number of end-users of applications or related services, or identifying compelling cases for use of HPCN leading to rapid deployment. European Universities or large companies should be encouraged to bring in-house applications to market, preferably through European independent software vendors. Third party application suppliers should be encouraged to support emerging industrial needs. The result will be to continue to increase confidence in HPCN and hence a two year timescale should be adopted.

4.2 Multi-disciplinary Design

This topic represents one of the most significant challenges facing European industry today. The design of competitive new products and materials relies on the integration of expertise from different scientific and technological disciplines. HPCN will play a vital role in integrating the effects of different engineering constraints and objectives in product design. In some areas, practical steps forward are possible that will have a direct impact on design capabilities in a 2-3 year timescale. Other areas will not lead to short term results, but there is an urgent need to catalyse the exchange of information.

4.3 Improved Pre-processing

The generation of meshes for complex geometries currently represents a serious bottleneck and introduces long delays in the use of simulation for design. The turn-around time and productivity will be significantly improved by consolidation and dissemination of recent advances in this area, with efforts to improve robustness and integration of systems. Improved pre-processing will have a significant impact on the efficiency, ease of use, and hence uptake, of HPCN. HPCN simulation applications need to be integrated with these pre-processing techniques to ensure the transparency and efficiency of use of HPCN systems. Progress in this area would also assist in the improvement of customer-supplier links and hence assist in the diffusion of HPCN to SME's in the long term.

4.4 Improved post-processing

Visualisation of results of simulation will become increasingly important as HPCN becomes adopted within the design process. The advancements that HPCN will allow in the design process will be limited by the ability to rapidly assess results and interactively control applications running on HPCN systems. Actions are required which improve productivity of analysis tasks despite increasing volumes of data. It is of vital importance that HPCN computing strategies are mature and reflect the need for designers to quickly access and assess the data relevant to their needs.

4.5 Application of HPCN Simulation in planning, operation and control of industrial processes and infrastructure

There are many applications of simulation which do not directly fit into the traditional model of designing materials or products. These applications require attention because they potentially offer enormous business benefits through improved management and planning of large scale systems which represent, or will require, significant financial investment. The continued operation and development of these systems is critical to economic development and underpins the successful operation of many other important businesses and industries.

4.6 Use of HPCN for Optimisation of Business Processes

The trend towards exploiting HPCN in design has helped to motivate interest in the use of HPCN for optimisation in related business and technical fields. Business modelling and optimisation is one of the key issues in many areas today. In the service sectors of banking and insurance, key applications include optimal portfolio selection, asset liability management and trading. More generally, simulation and optimisation models can provide an integrated view of the enterprise activity for strategic planning purposes.

In many cases the barriers towards HPCN deployment in these areas are lower, often because the business case is more compelling or there are fewer complex technical issues to be resolved. The impact of HPCN use in this area could be significant. Deployment for such applications could spearhead and support wider use of HPCN in design. There are additional benefits to be accrued by improving generic optimisation techniques which exploit HPCN in order to apply them to both business and design problems.

4.7 Reducing human barriers to adoption of HPCN

The development and demonstration of HPCN applications is clearly an important aspect in encouraging the uptake of the technology. The number of people involved in this activity is still relatively small, and the activities are quite focused and specific. There is a strong requirement to complement the existing activities by expanding the knowledge of HPCN technology and the awareness of its benefits and risks. This will lead to more confidence within businesses as to their ability to deploy HPCN systems and more consideration that HPCN solutions might be viable. The target audience are methods developers, rather than end-users. End-users should benefit through functional and performance improvements within the design process.

4.8 Parallel Software to Support Applications

The scale and scope of HPCN application development is rapidly increasing. A crucial requirement of end-users is that application codes can run on HW systems from a variety of vendors. This is best fulfilled by ensuring that portable application programming interfaces are proposed and adhered to. Unfortunately, the applications programming interface available on most systems is not well matched to the needs of developers. It is critical that this situation is improved and that developments in standardisation and libraries are encouraged and exploited in order that the investment in application development is used to best effect. Since actions leading to this objective do not fall directly within the remit of this group, they are proposed under Section 7 as requirements from the area of basic systems and tools.

5. Recommended Actions

5.1 R&D Tasks

5.1.1 HPCN Simulation applications for Design

- Porting and re-engineering of existing simulation applications

- Improvement of capabilities of existing (preferably parallel) simulation applications.

- Development of completely new applications in emerging, critical application areas.

- Multidisciplinary design. Activities may range from coupling and integration of simulation packages to the proof of use of HPCN for new applications to simulate multiple, complex and dynamic phenomena relevant to design of materials and products

- Use of HPCN for optimisation of design of complete systems

5.1.2 User Environment

- Improved integration of CAD and simulation (including standardisation issues)

- Development of automatic, robust mesh generation packages for HPCN simulation. Capabilities required include control and optimisation of solver parameters such as numerical accuracy, timestep and other parameters, integration to simulation packages, integrated domain decomposition, possibly parallel application generation.

- Intelligent data reduction techniques for interactive visualisation and simulation control.

5.1.3 HPCN simulation applications to planning/operation/control

This topic area concerns primarily industrial and commercial processes, and infrastructure. It covers long-term planning leading to decisions in investments, short-term planning for operation of existing processes, and real-time control. R&D tasks in this area are similar to those for design applications.

- Porting and re-engineering of existing simulation applications

- Improvement of capabilities of simulation of applications

- Development of completely new applications in emerging, critical application areas.

- Development of simulation systems and pre-processing systems which can directly exploit design models

- Development of new HPCN applications to simulate complex and dynamic phenomena in manufacturing processes

- Development of HPCN applications in simulation and optimisation of complex business processes such as those occurring in banking and insurance as well as in complex industrial organisations.

5.1.4 Tools for numerically intensive applications

- New numerical libraries to support latest iterative, direct solvers and pre-conditioners. Out of core solvers as required.

Other topics of a more general nature are included in Section: 7: input to other groups

5.2 Accompanying measures

The objective of these measures is to bring the exploitation of the potential in HPCN simulation to a wide set of business sectors and activities

- Best practice: the aim is to facilitate the deployment in new sectors. For example, the programme could support additional costs of deploying HPCN in industrial areas where simulation would be newly introduced. These actions would include an Evaluation of the technical and economic impact of HPCN simulation in industrial practice and dissemination of information helping develop the business case of HPCN simulation in other sectors

- Facilitating the commercialisation and support of simulation codes developed in-house or in academic centers, where these respond to important industrial needs.

- Training of industrial engineers to the use of HPCN simulation, especially in order to increase the awareness of the potential of HPCN simulation and to promote its use in new industrial sectors.

- Training of simulation application developers in industry to efficient exploitation of HPCN. This could be done efficiently through joint projects with HPCN competence centers.

- Enrichment of university curricula with HPCN material, and familiarisation of advanced students with industrial problems through graduate industrial placement.

- Setup of industrially led Networks of Excellence on specific topics such as multidisciplinary design in industrially important areas.

- Set up and dissemination of a dossier of skills and facilities in centres of expertise in HPCN and applications

5.3 Overall considerations

In order to ensure that R&D projects supported by the programme respond to the needs of industry and that their results directly and widely benefit industrial practice, it is proposed to require

-Strong role of industrial users in the projects, preferably as coordinators.

- Consortium structure and commitment to make the results widely used.

- Work up to deployment in industrial practice.

- Limited duration projects (2 years, maximum 3 years).

- Limited consortium sizes (for example, 1 user, 1 Application SW specialist, 1 HPCN specialist, possibly 1 HW supplier or a numerical specialist).

- Use of parallel software techniques and algorithms ensuring portability/scalability

- Industrial evaluation of system performances and dissemination of the aspects leading to the appreciation of benefits and limitations of HPC

APPENDIX. INPUT TO OTHER WORKING GROUPS

The major contributions of the working group to topics covered by the work of other groups include those on software environments and on subjects for longer term research.

A. Parallel Software to support Applications

Rationale

The scale and scope of HPCN application development is rapidly increasing. Unfortunately, the applications programming interface available on most systems is not well matched to the needs of developers. Parallel compilers are unlikely to meet all the needs for widespread availability or support the development of new irregular and dynamic applications. Message passing systems are widely available but do not, in isolation, meet the objective of application developers to improve the functionality and performance of applications. Parallel input/output is at a primitive stage of development. It is critical that this situation is improved and that developments in standardisation and libraries are encouraged and exploited in order that the investment in application development is used to best effect.

Proposed actions

- Development/adoption of libraries to support generic application parallelisation techniques and I/O, with emphasis on support for new computational techniques (unstructured, adaptive, unbalanced regular)

- Encouragement for use of standards e.g. MPI, HPF

- HPCN program configuration standards

B. Topics of work with longer term impact

A number of areas of engineering design involve the combination of complex physical phenomena. For example, combustion may involve the combination of multiphase flow, multiple chemical reactions, complex moving geometries and the designer may be interested in resulting aspects such as efficiency, toxic emissions, temperatures, noise, etc. As it is not possible today or in the near future to tackle the full complexity of such problems, more advanced work is needed, combining the expertise of the various physical/chemical domains involved, together with expertise in numerical algorithms and parallel computing. Such work should also take into account the requirements of a number of industrial sectors concerned.

Other topics for longer term work include turbulence, interaction between flow, mechanical structure, vibration and noise, and ab-initio molecular modelling.