Nationaal Lucht- en Ruimtevaartlaboratorium
National Aerospace Laboratory NLR

NLR TP 97113

Creating capabilities for effective and controllable scientific and engineering computations

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DOCUMENT CONTROL SHEET

	ORIGINATOR'S REF.		SECURITY CLASS.
	NLR 97113 U		**Unclassified**

ORIGINATOR
National Aerospace Laboratory NLR, Amsterdam, The Netherlands

TITLE
Creating capabilities for effective and controllable scientific and engineering computations

PRESENTED AT

AUTHORS	DATE	pp	ref
W. Loeve	**970214**	**18**	**9**

DESCRIPTORS
Computer networks
Computerized simulation
Configuration management
Data management
Information systems
Research facilities
Resource allocation
Software tools
Supercomputers
System effectiveness
Time sharing
User requirements

ABSTRACT

Computer simulation is part of engineering processes in many enterprises. Examples of simulation are computational fluid and solid mechanics that are used in engineering to determine characteristics of complicated products under development such as cars and airplanes. As such simulation is part of the chain of processes by which external customer requirements are translated into a product that satisfies the customer. Like for each process in the chain it is necessary that simulation is carried out in the right way first time, and that the enterprise focusses on reducing cost and time and increasing accuracy of simulation. Continuity, effectiveness and controllability of the application of simulation has to be safeguarded. In the present paper aspects of continuity, effectiveness and controllability of computer simulation are discussed on management level. Attention is paid to accessibility of geographically distributed high performance computing systems and to management and control of simulation related software, data and electronic documents. It is described that computers, software, data and electronic documents can be integrated in such a way that a simulation infrastructure is realized that can serve as a central nerve system for the enterprise for generating and sharing the use of simulation related data, software and electronic documents. It is argued that for this the infrastructure has to present itself to each user as one single computer that can be used on the basis of the look-and-feel principle. Continuity of simulation expertise in the organisation is the prime concern of Management. For this reason Management has to be involved in set up of the infrastructure and stimulating set up and application of procedures for management and control of all elements in the infrastruccture: computers, software, data and documents. Realization of the infrastructure requires involvement of IT professionals as well as of engineers that use the infrastructure for simulation.

Summary

Computer simulation is part of engineering processes in many enterprises. Examples of simulation are computational fluid and solid mechanics that are used in engineering to determine characteristics of complicated products under development such as cars and airplanes. As such simulation is part of the chain of processes by which external customer requirements are translated into a product that satisfies the customer. Like for each process in the chain it is necessary that simulation is carried out in the right way first time, and that the enterprise focusses on reducing cost and time and increasing accuracy of simulation. Continuity, effectiveness and controllability of the application of simulation has to be safeguarded.

In the present paper aspects of continuity, effectiveness and controllability of computer simulation are discussed on management level. Attention is paid to accessibility of geographically distributed high performance computing systems and to management and control of simulation related software, data and electronic documents. It is described that computers, software, data and electronic documents can be integrated in such a way that a simulation infrastructure is realized that can serve as a central nerve system for the enterprise for generating and sharing the use of simulation related data, software and electronic documents. It is argued that for this the infrastructure has to present itself to each user as one single computer that can be used on the basis of the look-and-feel principle.

Continuity of simulation expertise in the organisation is the prime concern of Management. For this reason Management has to be involved in set up of the infrastructure and stimulating set up and application of procedures for management and control of all elements in the infrastructure: computers, software, data and documents. Realization of the infrastructure requires involvement of IT professionals as well as of engineers that use the infrastructure for simulation.

Abbreviations

AQAP	Allied Quality Assurance Publication
CFD	Computational Fluid Dynamics
CSCW	Computer Supported Cooperative Work
ISNaS	Information System for flow Simulation based on the Navier-Stokes equations
ISO	International Organization for standardisation
IT	Information Technology
NICE	Netherlands Initiative for CFD in Engineering
SPINE	Software by which computers in a network are presented to the user as one single computer

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1 Introduction

Computer simulation is part of engineering processes in many enterprises. Examples of simulation are computational fluid and solid mechanics that are used in engineering to determine characteristics of complicated products under development such as cars and airplanes. As such simulation is part of the chain of processes by which external customer requirements are translated into a product that satisfies the customer. Like for each process in the chain it is necessary that simulation is carried out in the right way first time, and that the enterprise focusses on reducing cost and time and increasing accuracy of simulation. As a consequence continuity, effectiveness and controllability of the application of simulation has to be safeguarded.

Software for simulation is based on mathematical models of aspects to be simulated. Data generated by simulation has to be compared with data from other sources about the same aspects, to validate the simulation software for the specific use in the enterprise. It appears that software for simulation, data generated by simulations and from other sources and documents in which is described how to apply the simulation software, together is the information that represents much of the knowledge that is relevant for the continuation of the enterprise. For documents to be effective it is desirable to make them available in electronic form on the same systems as that are used as carrier of software and data. This in principle makes it possible to organize the documents in such a way that they can be accessed as help information in the context of current simulation activities.

The effectiveness of simulation to a large extent depends on the effectiveness of computing for simulation. In industry effective computing in simulation means:
- a variety of relevant physics for relevant geometries,
- resolution and accuracy sufficient for relevant results,
- graphical user interaction with the simulation tools.

These aspects determine the required computing power and type of computer system.

A prime concern of Management is to safeguard the continuity of knowledge in the enterprise as well as effectiveness in application of the knowledge. Continuity of knowledge about simulation means that it is necessary to facilitate that (successive generations of) specialists can share the use of software for simulation and data and electronic documents that are related to simulation. For many industry activities effective computing in simulation means that several disciplines that are involved in multi-disciplinary engineering can access software and can exchange simulation related data and documents easily. A local workstation or personal computer is needed to give engineers the opportunity to apply simulation. In cases of advanced simulation, effectiveness makes it undesirable that specialists are forced to or are allowed to restrict the speed or relevance of simulation to what is possible with a local workstation or personal computer. To avoid undesirable restrictions for simulation, in many cases a choice has to be made between installation of ever more powerful local systems or a combination of local and central compute power. This has to be done in such a way that the operation of the full enterprise technically and financially is optimized. This includes proper reasoning about both hidden and visible cost involved in operating computer systems and of the need that people at different locations share information.

Engineers that execute simulation have to be regarded as a supplier of information to the next process in the supplier/customer chain that is formed by all activities in the enterprise. The effectiveness of computing facilities for simulation shall be determined by the measure they contribute to producing better products at lower cost, in shorter time. By introducing the possibilities of information technology (IT), in practice effectiveness considerations often lead to the wish to make use of local workstations or personal computers as well as of central powerful compute servers.

Simulation also has to be controllable in order to safeguard correctness of simulation results and of correctness of the application of the results. This means that errors in simulation processes must be detectable and correctable. To be able to detect errors it is necessary that results of simulations can be compared with other information such as from simulations of comparable effects or situations. The enterprise shall be capable of building up simulation experience. This means it has to be possible to reconstruct what has been done in the past and to look at old results. Proper control of information and sharing of information between specialists in most cases leads to the need to make use of central information servers. All compute devices need to be connected via a network to allow information exchange between persons and access from the different locations of the persons.

Enterprise wide management and control of information and access to information requires support tools and discipline to use them. It is required that computing related information, support tools and computers in the network are integrated in a coherent infrastructure to facilitate application. The ideal is that the simulation infrastructure serves as central nerve system of the enterprise. This has to be so not only for supporting the various aspects of simulation but also for other information processing in the organisation. For the definition of the proper infrastructure it is necessary to draw up an IT plan that represents the short term vision as well as the long term vision on the role of IT in the enterprise. Drawing up the IT plan requires conceptual thinking about the infrastructure development and knowledge about possibilities that IT offers at short term as well as at long term. As a consequence it requires a contribution of IT professionals.

In practice conflicts arise between short term interests to finish specific limited simulation activities as quick as possible, and the long term interest of organisations to maintain control over a collection of activities that are distributed in time and place. This is why Management in consultation with the engineers that apply the simulation tools has to be involved in the definition of the computing infrastructure for simulation by IT specialists. Management and engineers also together have to design management and control procedures for simulation related information, compute systems and support tools. The resulting inter disciplinary cooperation has to be made possible by proper quality management procedures. This means the set up of project plans for realization of the IT infrastructure, appointment of responsible people for the different aspects, checking progress of activities against project plans and experiences and definition and control of possibly required corrective actions.

2 The Proper IT Infrastructure for Simulation

For application of simulation in many cases high performance compute servers are required to realise the performance that is needed for relevant results. CFD is an example for which computing power often is a bottle neck. The most powerful computers however are installed in research organisations such as universities and institutes. Only large companies are in the position to operate top of the line computers in house. This is clear from the TOP500 list in which the 500 most powerful computers in the world are listed [1]. In the list dated November 18, 1996 it can be seen that in the Netherlands only Shell Company, three university computing centres and NLR operate computers that are on the TOP500 list. In many cases it appears that only a relatively limited number of people make use of available high performance computing power.

The importance of high performance computing is recognized by governments. Many stimulation programs are being launched and have been launched in the past. It is considered to be of national interest to make high performance computing available to all enterprises that can improve the effectiveness of their operations by application of high performance computing. This requires removing technical and organisational barriers that limit the applicability of high performance computing.

One of the restrictions that make high performance computing outside the reach of many organisations is cost involved. There are various causes for this:

- the total need for high performance computing is limited and as a result in-house high performance computing facilities are out of reach financially,
- the total need for high performance computing justifies in-house computing facilities but all money is spent on a distributed collection of computing devices,
- cost for commercial software are too high and in-house software development is out of the question,
- cost for familiarization with software are too high because of the research character of the software,
- remote access to the required high performance computing is difficult to organise.

  Even in cases that the cost considerations mentioned above are not applicable many other causes may limit the possibilities to make use of high performance computing in simulation. Frequently occurring causes are:

- Software heterogeneity. Programs come from different sources (e.g., public domain, commercial, developed in-house), and hence usually lack uniformity with respect to user interface and data interface. Incidental use is practically impossible because of time required to familiarize.

- Hardware heterogeneity. Programs run on different heterogenous computers in the network. As a result the problems can be:
    - finding out on which computer a specific program may run in a network,
    - remote login and remote execution, facing the user with aspects such as authentication and accounting,
    - operation of different operating systems or variants of the "same" operating system, commonly with a variety of possibly incompatible utilities,
    - exchange of files between computers,
    - incompatible data formats due to different byte ordering and representation of real numbers in different computers,
- Users get faced with organizing, managing, and finding a way through an amount of on-line information that is much larger than that on a single computer.
- Software is realized by researchers and has no proper error handling facilities which makes application practically impossible,
- Software is realized by researchers and is not designed for maintenance, so error removal and adaptation to new needs is practically impossible by other people than the originator of the software.

Many of the technical and organizational shortcomings mentioned above can be removed in a proper computing infrastructure. Information (data, documents and software) shall be made available on-line. Information shall be managed and controlled in such a way that reconstruction of old information remains possible and that the information can be exchanged between specialists in the same way as if they all make use of one computer. Further it has to be safeguarded that in industry only software is used of which architecture and construction principles are applied that safeguard maintainability, testability and continuity of the software. Proper error handling also is a prerequisite for software to be applicable in industry [ref. 2]. Accessibility of the software has to be such that the user does not have to be skilled in areas such as mathematics, numerical algorithms, computer programming, computer operating systems and computer network tools. Finally the software has to be integrated in the infrastructure in such a way that the user is assisted in organizing, re-using and integrating a continuously growing amount of software, data and supporting help information.

Summarizing the requirements for effective and controllable computing in simulation, the infrastructure shall present itself to each user as one single computer. This virtual computer shall have tools for information management and control, initiating computing and analysing results on the basis of look-and-feel. Only by making high performance computing a natural part of desktop workstation applications, the use of high performance computing in engineering will spread according to the need for competitive enterprise operation.

It has been demonstrated to be possible to realize high performance computing in simulation with top of the line computers in a way that fulfils the requirements. The demonstration is given in the project that is financially supported by the Netherlands government via the Foundation HPCN. The project called Netherlands Initiative for CFD in Engineering (NICE) aims at development of the NICE simulation environment in which is made available to industry: commercial CFD software and software developed by institutes and universities in The Netherlands. The most powerful computer that is available in the NICE project is a NEC SX-4 supercomputer. This computer is the third powerful supercomputer that has been procured in the Netherlands by the National Aerospace Laboratory NLR.

Since computers were introduced in NLR in the late fifties this institute has applied a centralized IT approach. The main reasons were described in 1976 [ref 3]. They were economy of scale and the need to be able to procure the computing power that is required for the most demanding applications. In addition in-house software development for CFD by industry and in industry was performed by IT professionals centralized in an IT Division. In this development much attention was paid always to quality management. This resulted for instance in an ISO 9001 and AQAP-110 certificate for development of simulation software. It also resulted in development of architecture and construction principles for CFD software that allow control of software development according to industry needs [ref 2]. Finally it resulted in development of a software tool called SPINE that makes it possible that a software environment for simulation on a distributed high performance computer network presents itself as one computer to users [ref 4]. The first application of this software was the realization of ISNaS, a software environment for CFD [ref. 5].

All computers used in the NICE environment run vendor-supplied UNIX. The software environment of NICE is based on SPINE, a product developed by NEC and NLR. SPINE contains [ref. 4]:

- A user shell that supports presentation integration in that it provides uniformity with respect to the presentation and manipulation of files and the invocation and execution of programs,
- a tool for managing the versions of the source code of a software product,
- a tool for managing data files in a CSCW environment,
- a tool for managing on-line documents,
- a tool that supports automatic localising software in a network,
- a tool that provides a basis for organizing and applying conversion programs.

In SPINE communication with applications is realized with specific so called drivers for data exchange and with so called scripts for application runs. It is very easy to integrate new applications into existing SPINE infrastructures. All functions in a SPINE infrastructure are available through a graphical user interface. SPINE controls multiple windows in combination with multi-tasking. This makes it possible to execute operations while others are running. SPINE is portable. SPINE is the proper framework to provide contextual help to users. SPINE also has proved to be applicable to integrate remote workstations in the NICE IT infrastructure to give access not only to NLR's NEC SX-4 vector computers and CFD software, but also to compute power and software in other organisations that contribute to the NICE project. The application of the NICE environment via remote access is supported by Internet.

3 Development of an IT Infrastructure Requires Management Involvement

The prime concern of Management is continuity of the enterprise. Software, data and documents that are related to simulation represent knowledge. This knowledge has to be conserved in such a way that it is applicable by successive generations of specialists. Consequently information (data, documents and software) shall be managed and controlled in such a way that reconstruction of old information remains possible and that the information can be exchanged between specialists. Because of the discipline that is required for this it is recommendable for Management to nominate a system manager for this.

Another concern of Management is to make sure that expertise is used for core business. Management's interests may be to see to it that engineers only are spending time on generating simulation results and not on adapting software. This in many cases nowadays means that in-house development of tools such as for simulation is discouraged in industry in favour of obtaining appropriate software from outside. Use of commercially available software is preferred by Management. In some cases specific software is required. This offers opportunities for R&D organisations to play the role of supplier of advanced simulation software to industry because these very often have the application knowledge and experimental infrastructure for support of the validation of the software.

Implementing knowledge from research in software can be an appropriate way to transfer knowledge from R&D to industry. Management of the R&D organisation however has to make sure that software developed in R&D environments meets proper operational requirements such as proper error reporting, maintainability and applicability for engineers. Introduction of proper quality management in the production of software as a consequence is the challenge for Management and experts together in R&D organisations. It is described in [ref. 2] that development of simulation software that has to be used in industry needs a contribution of experts that know the aspects to be simulated, mathematicians and IT specialists. Management has to organize the cooperation of the various experts involved on the basis of decomposition of the total task and proper control mechanisms [ref. 6]. It seams that this challenge best can be met in parts of R&D organisations that are forced to compete for funding from contracts.

Engineers are interested in performing tasks with minimal interference from the environment in what they consider the most economic way. In practice this means that engineers will argue that they need a workstation for performing simulation. In case the workstation has insufficient performance for the required simulation the first idea of most engineers is to claim a more powerful workstation or a cluster of workstations. Management has to decide what to do in such cases. Direct cost and hidden cost of distribution of ever more workstation power has to be compared with total cost of a combination of workstations with limited capacity that are linked to compute servers and central information management servers.

In case extreme powerful compute servers are only required incidently it has to be decided by Management if the servers have to be installed in-house or if use shall be made of external facilities. The considerations have to be based on proper IT plans. As has been suggested in the preceding chapter this requires a contribution of IT experts. Management has to organise this. As has been mentioned above, the most powerful compute servers in many countries are installed in universities and R&D institutes. It is a national interest that owners of these computer servers give appropriate access to these systems to industries that need this. So far remote application of compute servers was psychologically and operationally difficult. It is much easier since remote compute servers can be integrated with local workstations as if the combination is one computer. Of course security measures are required. Also for this measures can be taken. The contribution of Management is indispensable to realize what is possible technically.

For support of management decisions various tools are available. One of the tools is accounting of computing and networking. It will be surprising how much workstations really cost and what the limitations are in handling growth of simulation problems. In [refs. 1,7] the price/performance of current workstations and supercomputers is compared for the list price component of the cost. At the time NLR decided to purchase a supercomputer the price/performance of this system was better than that of workstations [ref. 7]. Ease of use of modern supercomputers is described for CFD applications in [ref. 8]. All this has lead to the decision by NLR Management to procure the third supercomputer. NLR Management stimulates the use of the powerful central compute servers by accounting the use of all compute servers including workstations and by not accounting the use of the network.

The IT infrastructure of enterprises shall be open in the sense that it is easy to replace components. This concerns hardware as well as software. Management shall see to it that in view of this the proper standards are applied. In-house development of software shall be minimized in view of development and maintenance cost. Because of this Management supports the IT development team of SPINE to make maximum use is of commercial off-the-shelf software and public domain software in satisfying user requirements in presenting a computer network to the user as if it is one single computer.

At NLR Management and specialists cooperate in defining for what applications and for what group of users the computer network and the information in it shall be presented as one single shared computer. Examples of results of this type of decisions are the generation with SPINE of a computer supported cooperative work environment for CFD [ref. 5] and for control engineering and simulation of multi-body systems [ref. 9].

Two other examples of joint decisions of Management and specialists in the development of SPINE are:

- Access to the computing resources and information available from SPINE-generated environments shall be manageable according to existing policies in organizations. In view of this security and authorization in the SPINE-generated environments shall be left to the underlying UNIX network. Consequently, access to computers and information is controlled by the standard UNIX protection mechanisms (login passwords, file protection modes, ".rhost" files).
- SPINE and the SPINE-generated environments shall be supportive for the application of quality management, according to the ISO 9001 industry standard, to the development of information systems. In view of this SPINE provides facilities for the execution of quality assurance procedures.

Three types of specialists have to be involved in realizing the IT infrastructure for simulation in engineering: engineers that use simulation, IT experts that actually build the infrastructure and management representatives that control the development. The cooperation has to be such that the people involved act as members of a multi-disciplinary team.

4 Concluding Remarks

The IT infrastructure for simulation of an enterprise can serve as a central nerve system of the enterprise for sharing information (data, software and electronic documents) and for conservation of knowledge that is present in information. This can be realized with commercially available and public domain software tools in such a way that several computers in a network are presented to users as one single computer.

Management representatives, IT specialists and users of information have to cooperate in the realization of the IT infrastructure of the enterprise.

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