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# Large-Scale Computation at PSI Scientific Achievements and Future Requirements

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# Large-Scale Computation at PSI Scientific Achievements and Future Requirements

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## 1. Introduction Summary and Outlook

Computational modeling and simulation are among the disciplines that have seen the most dramatic growth in capabilities in the 20th Century. Within the past two decades, scientific computing has become an important contributor to all scientific research programs, even far beyond those of technical i.e. engineering science. Computational modeling and simulation are particularly indispensable for solving research problems that are unsolvable by traditional theoretical and experimental approaches, hazardous to study, or time consuming or expensive to solve by traditional means. Many such research areas are found in PSI's research portfolio, however it appears that the significance/impact was not recognised at PSI until recently [4].
The ASCI program, [2] in the USA, has given the high-performance computing (HPC) community and the HPC industry a large impulse. It has, however, put heavy emphasis on the use of commodity-off-the-shelf components. This has led to a tendency to use only standard products, which in turn favors the largest vendors of these products. The ASCI program (hardware oriented), accompanied previously by the Grand Challenges and now by the Scientific Discovery through Advanced Computing (SciDAC) [3] program, have brought the USA into a unique leadership position. With the advent of the Earth Simulator in March 2002 [5], this leadership was partially taken away; however, the Earth Simulator and its associated research is based on a small segment and are still not comparable with the US effort. With the IBM Blue Gene system and, very recently with the first petaflop system (Road Runner), the US is leading again the top 500 fastest super computers (`www.top500.org`).
Advances in computing technologies (including hardware and software) during the past decade have set the stage for a major step forward in modeling and simulation. We have now arrived at a situation where we have a number of otherwise unsolvable problems, where simulations are as complex as the systems under study. In 2008 the HPC community entered the *petascale* area with the heterogeneous Opteron/Cell machine, called *Road Runner* built by IBM for the Los Alamos national Laboratory `http://www.lanl.gov/roadrunner`. We are on the brink of a time where the availability of many hundreds of thousands of cores will open up new challenging possibilities in physics, algorithms (numerical mathematics) and computer science. However, to deliver on this promise, it is not enough to provide "peak" performance in terms of peta-flops, the maximum theoretical speed a computer can attain. Most important, this must be translated into a corresponding increase in the capabilities of scientific codes. This is a daunting problem that can only be solved by increasing investment in

- hardware
- the accompanying system software that enables the reliable use of high-end computers and
- scientific competence i.e.the mathematical (parallel) algorithms that are the basis of the codes, and education.

In the case of Switzerland there is the *The Swiss National Strategic Plan for High Performance Computing and Networking: SNSP-HPCN* [1] white paper which is discussing this complex and providing a plan to prevent Switzerland from quote: "falling even further behind [6]".

| Cluster | Nodes | Cores | Storage [TB] | Users |
|---|---|---|---|---|
| Merlin | $24+2$ | 104 | 3 (NFS) + 10 (GPFS) | HPC PSI |
| LCMEG | 16 | 64 | 88 (GPFS) | MEG |
| LCLTH | 12 | 48 | 8 (NFS) | LTH |
| LCLEV | 13 | 68 | 2 (NFS) | CRL |
| LCCFD | 4 | 16 | 0.5(NFS) | LTH+LRS |
| LCLRS | 4 | 16 | AFS | LRS |
| LCTH | 6 | 24 | AFS | Theory |
| FELSIM | 8 | 64 | 6 (GPFS) | XFEL/GFA |
| Marvin | 16 | 16 | | SLS/TOMCAT |
| CmsTier3 | $8+6+7$ | 168 | 105TB (Phase A) | CMS/LHC |
| Total | | 588 | 13.5(NFS) 209(GPFS) | |

TABLE 1.1. Summary of the PSI LINUX Clusters.

In this report, scientific results which are made possible by PSI's HORIZON engagement [4] will be summarised and PSI's future high-performance computing requirements will be evaluated. The data collected shows the current situation and a 5 year extrapolation of the users needs w.r.t. HPC resources are made. In consequence this report can serve as a basis for future strategic decisions with respect to a *non-existing* HPC road-map for PSI.

1.1. **HPC Capabilities at PSI.** PSI's institutional "HPC area" started hardware-wise approximately in 1999 with the assembly of a 32-processor LINUX cluster called *Merlin*. Merlin was upgraded several times, lastly in 2007. The Merlin cluster at PSI is used for small scale parallel jobs and data post processing has a an availability of 97% and is the only general purpose computing system at PSI. Several dedicated small scale clusters such as the FELSIM (Free Electron Laser SIMulations) followed the Merlin scheme. The resources are listed in Table 1.1. We also note that many of the clusters are used to analyse data from experiments at PSI or CERN (LHC). At the moment it is understood that dedicated clusters are most efficient, hence it does not make sense to use machines like the Cray at CSCS. This is the reason why none of the data analysis problems will be further discussed in this report.

1.2. **PSI's Involvement in the CSCS Horizon Machine.** The scientific rationale for PSI's engagement in the existing HPC capability machine at CSCS, named hereafter as Horizon, is a matter of record in [4]. The intellectual and financial involvement of the procurement (including a machine update in 2007) result in a PSI share of 25 % of the available computing resources. Figure 1.1 is shows the usage of our share over the course of time. Figure 1.1 clearly demonstrates the (over) usage of available computing resources by PSI scientist. We can also infer from Figure 1.1 that we actually get more computing cycles than we have paid for. The reason is the *fair share* policy that is implemented on the Horizon machine. This policy allows us to get cycles, with a low priority, even when our bi-monthly share is used.

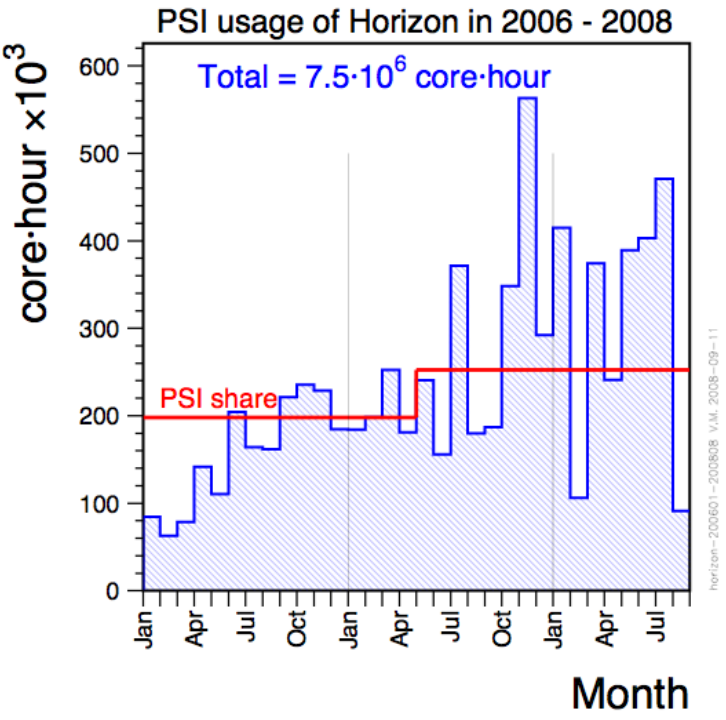


FIGURE 1.1. Usage of PSI share

1.3. **Summary and Conclusions.** The collected data in this report, are in more detail elaborated in the Sections 2 to 10. Five important observations can be drawn from the analysis of the scientific output and the survey of future requirements of main PSI HPC users:

(1) High Performance Computing is a main pillar in many important PSI research areas
(2) there is a lack in the order of **10** times the current computing resources (measured in available core-hours per year)
(3) there is a trend to use in the order of **600** processors per average production run
(4) the disk and tape storage growth is dramatic
(5) small HPC cluster located at PSI are important and in line with the SNSP-HPCN [1] proposal.

Table 1.2 summarizes the resource requirements **projected 5 years into the future**. Consequently, without a substantial increase in computing resources for PSI, several first-class research projects will become increasingly dependent again on foreign computing resources, and in doing so, will risk losing leadership in their fields.
On the more conceptional agenda, in the HPC community, it is clear that we are moving into an area in which many drastic new paradigms will arise; many-core architectures, heterogeneous systems, fault-tolerant systems and fault-tolerant algorithms. This is a very important observation, because at PSI many of the HPC users are developing their own

| Section | Cores | Memory [GB] | Disk [TB] | Tape [TB] | CORE [h×10$^3$] |
|---|---|---|---|---|---|
| 10 | 128 | 8 | 1 | 1 | 500 |
| 8 | 512 | 1024 | 10 | 1 | 2000 |
| 7 | 64 | 16 | 10 | 1 | 25 |
| 6 a) | 2048 | 512 | 5 | 5 | 5000 |
| 6 b) | 2048 | 512 | 10 | 10 | 5000 |
| 9 | 96 | 1750 | | | 960 |
| 4 | 256 | 512 | 10 | 1 | 460 |
| 3 a) | 512 | 512 | 10 | 1 | 1000 |
| 3 b) | 500 | 500 | 10 | 1 | 2000 |
| 3 c) | 1024 | 2 | 10 | 1 | 2000 |
| 3 d) | 512 | 512 | 0.5 | 0.5 | 250 |
| 2 a) | 512 | 1024 | 10 | 100 | 250 |
| 2 b) | 32 | 64 | 10 | 100 | 150 |
| 5 | 256 | 40 | 2 | | 300 |
| **Total per year** | | | $\sim$ 98 | $\sim$ 250 | 19895 |
| **Average per prod. run** | $\sim$ 600 | $\sim$ 500 | | | |

TABLE 1.2. Summary of the future requirements by PSI HPC users, projected 5 years into the future. In this table "Cores" and "Memory" is per average production run, "Disk", "Tape" and "CORE" requirements are on a yearly base.

parallel algorithms and programs and are dependent on the availability of state-of-the-art HPC infrastructure.
At PSI, within a time horizon of 5 years, on the order of 20 million core hours per year will be needed, production runs are crossing the 600 core barrier using approximately 500 GByte of memory per job. Disk requirements are on the order of 100 TByte per year and 250 TByte will be stored on persistent tape.
The Horizon project, as a joint PSI-CSCS venture, can be assessed as an excellent value for money for PSI users. This framework of partnership with a big national HPC center, where PSI has a special meta-user status, would be very desirable in the future PSI HPC strategy. On this basis, we strongly recommend discussing the possibility of a new joint venture with CSCS as an effective means of fulfilling the most demanding requests mentioned above.
Given the role of HPC at PSI we believe it is imperative to define a HPC strategy for PSI in order to secure the needed resources, which potentially go beyond cpu-cyles, and hence to efficiently use the third pillar of science - high performance computing.

In Chapter 2 to 10 details of the scientific achievements in the period 2006 to 2008 are summarised by individual groups of PSI. The future requirements w.r.t. HPC resources are very briefly described. On page 29 you will find a glossary of computational science expressions/acronyms.

## References

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## 2. Material Science & Simulation

Project Leaders: Peter Derlet, Helena Van Swygenhoven
Project Collaborators:
PSI Group: ASQ/NUM

2.1. **Outline of scientific work on Horizon (2006, 2007 & 2008).** Classical molecular dynamics simulations (using moldyPSI) and ab initio calculations (using the commercial density function theory package VASP) were performed in 2007 on Horizon. This work was concerned mainly with the study of the fundamental aspects of material strength and interatomic bonding within bulk nanocrystalline metals. The work involves three PhD Students, one Post-doc and one PSI staff scientist and is funded by the SNF, KTI, FP-6 EU, and UKEA Culham.
As part of its synergy between simulation and experiment, the MSS group performs large scale molecular dynamics (MD) simulations to investigate the mechanical properties of pure metallic bulk nanocrystalline (nc) materials, where plasticity is studied in relation to grain boundary (GB) structure and GB network structure. The molecular dynamics code, moldyPSI, used by the group has been developed in house and uses the Message Passing Interface (MPI) to attain efficient parallelisation through spatial decomposition. The code provides on-the-fly atomic structure analysis for easy visualization of complex atomic scale processes that lead to the bulk simulated plasticity. A variety of projects also investigate fundamental material modeling issues with the view of developing new and innovative atomistic simulation techniques.

2.2. **Papers Published due to computer work done on Horizon.** This is a summary on papers published, submitted or talks given in the period from 2006 to 2008 due to results obtained from simulations on Horizon [1, 11, 4, 3, 10, 5, 9, 8, 7, 6, 2, 12].

2.3. **Estimate of required CPU resources for 2008.**

2.3.1. *Classical Molecular dynamics.* At present our large scale atomistic simulations deal with atom numbers that are typically below 10 million. Currently we are concerned with being able to run long simulations enabling us to slow down the strain rates (which are typically higher than done in experiments). Thus for 2008 our computational requirements are influenced on extending the time scale rather than the spatial scale, although we will perform some shorter simulations for larger systems 40 million atoms.
A typical production run will involve between 128 to 256 cores per job and can involve up to several hundred job submissions (depending on how many hours per job are requested). For a number of past runs, a twelve hour job per day using up to 128-256 cores would allow us to complete a production run in the timeframe of approximately one to two months. This would constitute up to 265*12*30 92Kh per month.

2.3.2. *Ab initio calculations.* Ab intio calculations are performed using VASP which has been farmed out in batches of 32 core processors with each job requesting up to twelve hours CPU time. For a production simulation up to several tens of jobs are needed giving 32*12*10 3.8Kh per complete simulation. A number of such simulations will be needed in 2008. Although a small part of our computational requirements, it will increase

over the next years due to the beginning of PhD project performing entirely ab initio calculations. Thus we could easily use up to 20-30Kh per month. The current 32 process limitation arises because of bad scaling with the standard implementation of VASP. This year we intend to work (possibly with CSCS) to improve the situation in order to increase the number of core per job.

**CPU time requirements**

With the above in mind, 2008 would require up to 100-150 KCPUh per month. Maximum number of cores would be 256-512(for the larger samples).

**Memory requirements**

For all our molecular dynamics simulations, memory requirements per core have until now been satisfied, we do not expect the need for greater memory requirements for our standard MD runs. Some of our work which involves using a commercial linear solver has requirements that exceed the current core memory, but problems have been avoided by appropriate choice of simulation. As cores become more powerful more atoms per core can be simulated and then memory requirements will go up. For our ab initio calculations, we have yet to experience memory problems.

The Table 2.1 summarizes the resource requirements projected 5 years into the future.

| Problem | Cores | Memory [GB] | Disk [TB] | Tape [TB] | Core [h$\times 10^3$] |
|---|---|---|---|---|---|
| a) Classical MD | 256-512 | 1024 | 10 | 100 | 250 |
| b) Ab initio calculations | 32 | 64 | 10 | 100 | 150 |

TABLE 2.1. Summary of the future requirements by Material Science & Simulation group. Cores and Memory are per average production run. Disk, Tape and Core-hour requirements are on a yearly base.

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# 3. Beam Dynamics Calculation on PSI's Existing and Future Accelerators

Project Leaders: Andreas Adelmann, Sven Reiche
Project Collaborators: ETHZ, IBM-Rüschlikon
PSI Group: GFA / PSI-XFEL

3.1. **Bunch Compressor Chicanes.** In bunch compressor chicanes it is possible that synchrotron radiation emitted by trailing particles overtakes and interacts with particles ahead. Consequently, beam dynamics depends not only on external fields but also strongly on the internal electromagnetic forces. In computer simulations this leads to a scaling of the computational effort with $N^2$. To calculate the force acting on a particle the electromagnetic potentials have to be integrated at the retarded positions of all other particles. This way distributions of a few 100 particles can be tracked on a single CPU. On the other hand, for a proper sampling of a realistic charge distribution orders of magnitude more particles are required. Hence, the use of parallel computers is inevitable. Simulations were performed on Horizon to confirm the results by simplified simulations of bunch compressors designed for the CLIC project. Currently, an effort is on going to simulate and understand measurements of CSR effects performed at CTF2. Additionally, a detailed study of the impact of transverse em-fields in bunch compressor chicanes was started. One Ph.D student is working on a 3-d coherent synchrotron radiation code in the PSI-XFEL context.

3.2. **Start to End Simulations of the PSI -FEL.** The type of simulation needed to obtain a detailed quantitative picture of the physics in such a machine depends heavily on state-of-the-art numerical methods and high-performance computing.
Up to the undulator we are required by our challenging machine parameters to perform high resolution 3D particle tracking studies which includes $\mathcal{O}(10^9)$ particles with meshes up to the same orders of magnitude.
In time-dependent free-electron laser simulations the radiation field is represented by discretized wavefronts at each wavelength, which in the case of the PSI X-ray FEL corresponds to about 500.000 wavefronts. A single wavefront requires about 100 kByte of memory to store in memory. However, the FEL algorithm is progressing sequentially through the wavefronts and does not hold in memory no more than 2000 wavefronts at any time. Specific problems in FEL dynamics (HGHG Cascading, strong frequency chirp FEL pulses, HHG seeds) might require to extend the algorithm on the cost to hold more wavefronts in memory at the same time, though it is very unlikely that it will exceed 100.000 wavefronts, distributed over several nodes. In addition some spontaneous background simulation are required which have no significant memory demand but favors a large number of nodes for parallel computation. One Ph.D student is working on a 3-d finite element time domain Maxwell solver for large accelerator structures, a PSI FoKo proposal was accepted in October 2008 for the *Multi Objective Optimisation of the 250 MeV Injector*, the fist part of the PSI-XFEL.

3.3. **Simulations Supporting the High Power Upgrade Program.** Space charge effects play an important role in high intensity cyclotrons, as the most important collective effects. For high intensity cyclotrons with small turn separation, single bunch space charge

effects are not the only contribution. The interaction of radially neighboring bunches is also present but its effects have not yet been investigated in greater detail. In 2008, or the first time, a new PIC based self-consistent numerical simulation model is presented, which covers neighboring bunch effects and is implemented in a three-dimensional object-oriented parallel code OPAL-CYCL , a flavor of the OPAL framework. A invited oral paper was presented [8] and a longer publication is in preparation [7]. The required level of accuracy in the simulation is $\mathcal{O}(10^{-4})$ and can only be achieved by the use of state of the art numerical methods together with high performance computing.

3.4. **Papers Published due to simulations done on Horizon.** This is a summary on papers published, submitted or talks given in the period from 2006 to 2008 due to results obtained from simulations on Horizon [3, 9, 5, 4, 1, 2, 10, 6].
The Table 3.1 summarizes the resource requirements projected 5 years into the future.

| Problem | Cores | Memory [GB] | Disk [TB] | Tape [TB] | Core [h$\times 10^3$] |
|---|---|---|---|---|---|
| a) High Power Upgrade | 512 | 512 | 10 | 1 | 1000 |
| b) XFEL Bunch Compressor | 500 | 500 | 10 | 1 | 2000 |
| c) XFEL Particle Tracking | 1024 | 2 | 10 | 1 | 2000 |
| d) FEL Simulation | 512 | 512 | .5 | 0.5 | 250 |

TABLE 3.1. Summary of the future requirements by GFA/ABE & the PSI-XFEL project. Cores and Memory are per average production run. Disk, Tape and Core-hour requirements are on a yearly base.

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## 4. Radiation Metrology

Project Leaders: S. Mayer
Project Collaborators:
PSI Group: LOG/ASI
In the Radiation Metrology Section besides the routine work, computational dosimetry is performed for the characterization of dosemeters (energy response, angular dependency,...) and irradiation facilities by using MCNPX Monte Carlo simulations. Moreover, as far as metrology is concerned, the appropriate assessment of uncertainties by modern methods (i.e. simulations) may be considered as the backbone of quality assurance.
The last scientific work on Horizon was done in the course of an international intercomparison of approaches to uncertainty assessment in computational dosimetry within a work package of CONRAD (EU Coordinated Network for Radiation Dosimetry).
Our past simulations required 128 cores, for 12 hours over a period of 2 months per year. For the next year, these requirements will remain unchanged, giving a total CPU time of 128x12x30x2 = 92Kh per year. This will apply to the first year only.
After that we will extend out computational requirements further as we are planning on adding a PhD candidate/post-doctoral fellow to our section, focusing on Monte Carlo simulations of neutron dosimetry.
Hence, for years 2-5, our projected requirements are 256 cores, for 12 hours per day for 5 months every year, leading to a total annual CPU requirement of 256x12x30x5 = 460 Kh per year."

4.1. **Papers Published due to computer work done on Horizon.** This is a summary on papers published, submitted or talks given in the period from 2006 to 2008 due to results obtained from simulations on Horizon [1, 2]

The Table 4.1 summarizes the resource requirements projected 5 years into the future.

| Problem | Cores | Memory [GB] | Disk [TB] | Tape [TB] | Core [h$\times 10^3$] |
|---|---|---|---|---|---|
| MCNPX | 256 | 512 | 10 | 1 | 460 |

Table 4.1. Summary of the future requirements by the Radiation Metrology section. Cores and Memory are per average production run. Disk, Tape and Core-hour requirements are on a yearly base.

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## 5. Hadron Transport, Activation and Shielding

Project Leaders: S. Teichmann, D. Kiselev, M. Wohlmuther, L. Zanini
PSI Group: GFA

5.1. **Outline of scientific work on Horizon, 2007.** MCNPX is a Monte Carlo particle transport code developed at Los Alamos National Laboratory. Over the past 10 years it has become one of the standard transport codes for the purpose of hadron transport in an energy range of several tenths of m(illi)eV up to several GeV (2-3) in complex geometries. MCNPX can be used in two modes. The first (and older one) is the so called fixed source mode. This means that the user specifies a source of particles in a well defined phase-space volume - generally the particles possess a designated energy, or some distribution of energy, and are started at a specific point (volume) within an user defined geometry. In accelerator applications one is faced with these fixed source problems. The second possible mode of operation is to calculate Eigenvalues for a system containing fissionable material. Generally these are problems related to reactor applications (s. sec. 10). At PSI both modes are used by several groups, spread out over the institute.
In the accelerator part of PSI, MCNPX is used for the calculation of a large variety of problems. One of them is the calculation of shielding for the accelerator facilities, which by definition is a problem which needs a lot of computation time and power. The few particles which are able to penetrate a biological shield have to be tracked without creating a bias. The quantities of interest in such calculations are dose rates (and therefore particle fluxes) behind the biological shield, which are supposed to be very low. For instance the forward shielding of the Ultracold Neutron Source (UCN) has been evaluated with MCNPX; a presentation was given at the ICRS-11 this year [12]. Another example of a (time-consuming) shielding application is the calculation of an access labyrinth for the PROSCAN facility [6].
Moreover, the targets of UCN and the existing neutron source SINQ have been evaluated and improved [7]. A talk on these calculations was given at [3]. The new solid spallation target which is going to be operated from 2009 onwards has been fully optimized with MCNPX on HORIZON, as accurate and fast results were needed. A publication of the results is under preparation. Besides the improvement of the SINQ solid target we are working continuously on the characterization of beam lines at SINQ. In the last year the ICON facility was fully characterized using MCNPX and McStas [2]. These calculations would not have been possible without HORIZON, as high statistics in a very limited volume of a large facility were needed.
Another topic that we are now able to tackle with MCNPX operated on HORIZON, is the direct calculation of residual nuclei distributions of components which are going to be disposed. It is a requirement of the authorities that those components are characterized as accurately as possible. With the advent of HORIZON and the development of an improved method for the calculation of residuals from impurities and trace elements of a material we are now able to compute activities with an, up to now, impossible accuracy [1]. First publications of these results can be found in [11, 5, 4].
HORIZON was also extensively used for calculations on the disposal of the currently built spallation neutron source UCN, see [8] and [9]. Further, we are able to predict dose rates with MCNPX coupled to a build-up and decay program. This is important for the

planning of work procedures if a component has to be taken out from the radiation area for repair or replacement. In addition the thickness of the shielding (for the protection of the personnel or for transportation of the component) can be estimated and prepared in advance. Such a dose rate mapping was done for the third vacuum chamber of the PIREX beam line before it was removed [10]. A similar dose rate mapping is planned for the region around Target E. Due to its complexity it will require large computer resources.

5.2. **Papers Published due to computer work done on Horizon.** This is a summary on papers published, submitted or talks given in the period from 2006 to 2008 due to results obtained from simulations on Horizon [1] – [12]

The Table 5.1 summarizes the resource requirements projected 5 years into the future.

| Problem | Cores | Memory [GB] | Disk [TB] | Tape [TB] | Core [h$\times 10^3$] |
|---|---|---|---|---|---|
| MCNPX | 256 | 40 | 1-2 | 0 | 300 |

TABLE 5.1. Summary of the future requirements by the Hadron Transport, Activation and Shielding group. Cores and Memory are per average production run. Disk, Tape and Core-hour requirements are on a yearly base.

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# 6. HORIZON usage by LES

Project Leaders: Sergey Churakov, Georg Kosakowski and Wilfried Pfingsten
Project Collaborators: Helmholtz Centre for Environmental Research (UFZ), ETHZ Geotherm-Project
PSI Group: LES
HORIZON is used by LES for (1) atomistic simulations of mineral fluid interfaces and (2) macroscopic reactive transport simulations of deep geological waste disposals:
Atomistic simulations:

- Diffusive ion transport in compacted clays
- Structure of water-clay interface at edge sites
- Structure of crystalline cement phases

Reactive transport

- Finite element transport code RockFlow / GeoSys
- Random walk transport code MCOTAC

## 6.1. **Atomistic simulations.**

6.1.1. *Diffusive ion transport in compacted clays.* Classical molecular dynamics and Monte Carlo simulations are used to simulate the spatial distributions and diffusion coefficients of cations (Na+, Cs+ ) and water in the swelling clays as function of temperature, water content and ionic concentrations. The results of the simulations are used for the interpretation of the macroscopic diffusion experiments in compacted clays.

6.1.2. *Structure of water-clay interfaces.* The uptake of radionuclides by clay minerals takes place by two basic mechanisms: (a) cation exchange and (b) pH dependent sorption on the edge sites of clay particles. The water  clay interface was modelled by ab initio molecular dynamics simulation. The results of the simulation provided the surface concentration of the sorption sites and their proton affinities. This information has been incorporated in the surface complexation models which are used for the predictive modelling of the macroscopic radionuclide transport.

6.1.3. *Structure of crystalline cement phases.* Cement is used in the multi-barrier systems of the radioactive waste repositories. The basic structural elements of cement are the so called CSH phases: amorphous hydrous calcium silicates. The thermodynamic and mechanical properties of these phases are described on the basis of their crystalline analogues (Xonotlite, Tobermorite, etc.). Due to a high complexity and highly disordered character the structure of crystalline phases is poorly understood. Ab initio simulations have been used to identify the state of the water and the structure of defects in the crystalline cement phases. The results obtained support the thermodynamic modelling and structure understanding of the amorphous cement materials.

## 6.2. **Reactive transport.**

6.2.1. *Finite element transport code RockFlow / GeoSys.* Together with the Helmholtz Centre for Environmental Research Leipzig (UFZ) we are developing a parallel version of the general purpose flow- and transport code RockFlow / GeoSys that is coupled to the Gibbs Energy Minimization program GEMIPM2K (PSI version: `http://gems.web.psi.ch`) for geochemical equilibrium modelling. A first version of this code will be available in 2/2008. This coupled code will enable us to run large-scale 2D/3D applications for reactive transport with a complex geochemistry. One application will be related to the GEOTHERM project (Geothermal reservoir processes: research towards the creation and sustainable use of enhanced geothermal system. `http://www.cces.ethz.ch/projects/nature/GEOTHERM`) which will start in November 2008. The scalability of the code on the CRAY-XT3 machine at CSCS was reported in DEISA Digest 2008.

6.2.2. *Random walk transport code MCOTAC.* Reactive transport calculations will be performed to investigate complex geochemical interfaces such as cement-bentonite-clay, cement-sand-clay, etc. and to understand the long-term evolution of a repository near-field. In addition, radionuclide transport including competitive sorption processes will be calculated for a transient geochemical repository environment in 1D and in 2D. Because of the complexity of these geochemical systems, increased use of parallel computing is necessary to achieve modelling results in reasonable times.

This is a summary on papers published, submitted or talks given in the period from 2006 to 2008 due to results obtained from simulations on Horizon
[1, 2, 3, 5, 6, 7, 8, 11, 12, 9, 4, 10].

The Table 6.1 summarizes the resource requirements projected 5 years into the future.

| Problem | Cores | Memory [GB] | Disk [TB] | Tape [TB] | Core [h$\times 10^3$] |
|---|---|---|---|---|---|
| a) Molecular modelling | 2048 | 512 | 5 | 5 | 5000 |
| b) Transport modelling | 2048 | 512 | 10 | 10 | 5000 |

TABLE 6.1. Summary of the future requirements by LES. Cores and Memory are per average production run. Disk, Tape and Core-hour requirements are on a yearly base.

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## 7. Intrinsic defects and impurities in semiconductors

Project Leader: Ulrike Grossner
PSI Group: TEM/PIF
Program name: VASP

7.1. **State of research in the field.** In principle, all electronic devices today are based on one or the other semiconducting material, mainly Si, but also SiC, GaAs, GaN, or ZnO. For using these materials in reliably working components, their intrinsic defects, such as point defects like vacancies or extended defects like threading edge dislocations, need to be understood and the role of impurities needs to be clarified. For several decades, Density Functional Theory (DFT) has been used to get an microscopic insight into structural, electrical and optical properties of semiconductors. A comprehensive picture of the numerical concepts and a detailed derivation of the DFT can be found in numerous publications, such as [3, 4, 5, 2]. Within DFT, many-body system like a semiconductor crystal are simulated using the Born-Oppenheimer approximation [1], where the electronic and nuclear degrees of freedom are separated. The problem of a system of interacting electrons has been mapped onto a system of non-interacting electrons moving in an effective potential using a local density approximation. Simultaneously, the many-body problem of the ground state is traced back to a set of single-particle equations. Since the effective potential itself depends on the density, the underlying equations have to be solved simultaneously (self consistency problem). This problem is treated by the application of an iteration cycle for these equations.

7.2. **Status of Research at PSI.** At the Proton Irradiation Facility (PIF) of the PSI, electronic devices are tested on their radiation hardness. Most of the devices tested consist of semiconducting materials, like Si. In an ongoing project, also new materials, such as SiC, GaN, and ZnO will be tested on their radiation hardness. A special focus is given to devices, like p-n diodes or optoelectronic devices, such as in quantum well laser diodes. Here, the challenge is the microscopic understanding of the defects as created by proton irradiation. In general, the impact of protons on an material leads to an transfer of energy enough for the creation of point and extended defects. Typical examples are carbon vacancies in SiC or threading edge dislocations in GaN. In parallel to the experimental investigation with state-of-the-art electrical characterization subsequently to the proton irradiation, such defects shall also be studied by ab-initio calculations.
The Vienna Ab-initio Simulation Package (VASP, `http://cms.mpi.univie.ac.at/vasp/vasp/vasp.html`) is a package for performing ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set. The approach implemented in VASP is based on a finite-temperature local-density approximation (with the free energy as variational quantity) and an exact evaluation of the instantaneous electronic ground state at each MD-step using efficient matrix diagonalization schemes and an efficient Pulay mixing. The interaction between ions and electrons is described using ultrasoft Vanderbilt pseudopotentials (US-PP) or the projector augmented wave method (PAW). Both techniques allow a considerable reduction of the necessary number of plane-waves per atom for transition metals and first row elements.

7.3. **Role of HPC for the Research.** For the simulation of defects in semiconductors, large super-cells of the respective host crystal need to be considered to guarantee that the defects do not artificially interact via the electron density. Therefore, cell sizes should exceed at least 128 atoms for point defects with localized wave functions, whereas defects with more de-localized electron states require a cell size of at least 256 atoms. For a proper treatment of atoms like Ga and Zn, whose 3d-electrons are resonant in energy with the nitrogen 1-s and oxygen 2-p orbitals, respectively, the 3d electrons need to be treated as valence electrons contributing to the electron density. Therefore, the calculations require a higher number of basis sets leading to a higher numerical effort. VASP runs equally well on super-scalar processors, vector computers and parallel computers. The computer resources for PSI include a running version of VASP at a Cray computer as well as a Linux cluster.

7.4. **Requested HPC Resources for the Project.** The Table 7.1 summarizes the resource requirements projected 5 years into the future.

| Problem | Cores | Memory [GB] | Disk [TB] | Tape [TB] | Core [h$\times 10^3$] |
|---|---|---|---|---|---|
| VASP | 64 | 16 | 10 | 1 | 25 |

TABLE 7.1. Summary of the future requirements by TEM/PIF. Cores and Memory are per average production run. Disk, Tape and Core-hour requirements are on a yearly base.

7.5. **Impact of HPC on R&D Plans for the Future.** By investigating the formation energies of intrinsic and extrinsic defects in semiconductors and their influence on the electrical and optical properties of the host crystal, the stability of electronic devices in harsh environments can be understood and estimated. This knowledge will allow the identification of failure mechanisms in existing devices as well as the suggestion of alternative materials for well-defined applications, as for example dosimetry and space applications.

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## 8. LRS/NES - Materials Science, Chemistry

Project Leaders: Marcella Iannuzzi, Matthias Krack
Project Collaborators: CEA, JRC-ITU Karlsruhe, Imperial College London, SCK-CEN
PSI Group: NES seed action (LRS)

8.1. **Horizon usage 2007/2008 (CSCS).** In the first stage of the project, we focused on the assessment of atomistic models for $UO_2$ taking into account a few pre-existing empirical force fields. The models have been tested by evaluating the stability of the crystallographic structure at various temperatures and external pressures. Three different empirical force fields have been employed and compared: Two based on standard fixed charge distributions and one based on a shell model approach, which can explicitly include polarization effects. The validation procedure has taken into account structural properties at equilibrium as well as deformation and failure processes under external load. In particular, we have simulated the failure of the lattice under tension, leading to the formation of fractures along the (111) crystallographic plane. Moreover, since we are interested in diffusion processes and microstructure rearrangements, we have started some calculations to reproduce the most probable migration events in stoichiometric $UO_2$. The ions mobility has been analyzed in bulk and in presence of a $\Sigma 5$ grain boundary. Molecular dynamics (MD) simulations have been carried out at different temperatures ranging from 300 K up to 3000 K, and the set-up of disorder in the oxygen sublattice above 2600 K has been reproduced in agreement with previous studies. As expected, we observe, that in the vicinity of the grain boundary, the mobility of the oxygen atoms and the occurrence of distortion are enhanced. Geometry optimizations and molecular dynamics (MD) simulations at 300 K have been carried out also for a few defective structures containing Frenkel pairs or Schottky defects. By starting from different initial configurations, and after the equilibration of the system, the formation energy of the defect has been computed and the local rearrangement of the structure has been characterized. A paper draft is in preparation to account on these first results obtained by classical MD simulations of $UO_2$, where we focus on the different behaviors induced by the specific choice of the force field.
Parallel to the classical MD simulations, we started to setup the electronic structure calculations based on Kohn-Sham density functional theory (DFT).Firstly, we generated small- and large-core pseudopotentials for uranium including scalar-relativistic effects. In the next step, various Gaussian basis sets were optimized for these pseudopotentials. Structure optimization of small molecules containing uranium in all possible oxidation states were carried out using a plane waves code to assess the accuracy and transferability of the new basis sets and pseudopotentials.

8.2. **New Proposal.** Uranium dioxide ($UO_2$) is the main component of the currently employed nuclear fuels. An in-depth knowledge about the fuel material and its behaviour under various conditions is crucial to ensure the safe operation of nuclear power plants. However experiments with hot materials are difficult and very costly. Alternatively, computer simulations can be employed nowadays to investigate the nanostructure and the structural dynamics of fuel materials like $UO_2$. In the proposed project we plan to investigate $UO_2$ using an electronic structure method based on density functional theory

(DFT). Finite temperature molecular dynamics (MD) simulations will be performed at DFT level to deliver insights from first principles into the structural and dynamical behaviour of pristine and defective $UO_2$ at the atomic level. The program package CP2K [2, 1] (`http://cp2k.berlios.de`) which is developed in our group will be employed for the study. CP2K has already proven to run on parallel supercomputers with high efficiency. The proposed activity will be performed in the framework of the EU FP-7 project F-BRIDGE.
The Table 8.1 summarizes the resource requirements projected 5 years into the future.

| Problem | Cores | Memory [GB] | Disk [TB] | Tape [TB] | Core [h$\times 10^3$] |
|---|---|---|---|---|---|
| CP2K (DFT) | 512 | 1024 | 10 | 1 | 2000 |

TABLE 8.1. Summary of the future requirements by LRS/NES - Materials Science, Chemistry group. Cores and Memory are per average production run. Disk, Tape and Core-hour requirements are on a yearly base.

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# 9. High Temperature Materials

Project Leaders: Maria Samaras
Project Collaborators: Anne-Christine Uldry, Ning Gao, Botond Bako, Roberto Iglesias
PSI Group: Laboratory for Nuclear Materials / NES

9.1. **Outline of scientific work on Horizon, 2007.** Materials modelling, whether structural or fuels, is finding a firm place in many experimental programs internationally as a next step in materials development. This is due to the advances that modelling can bring to understanding materials issues as well as the reduction in program costs. Fission researchers are faced with the scientific challenge to determine the long term damage evolution of materials under service exposure in advanced reactors which entails a broad range of phenomena such as creep, swelling, fracture, fatigue rates, cracking, corrosion, the correlation between nano- and micro-structural features, effects of radiation damage, hardening and embrittlement, irradiation induced precipitation which lead to phase instabilities, void swelling, high temperature He embrittlement and irradiation creep. Such a broad spectrum of issues indicate the necessity to understand the related physical phenomena on a range of scales from the microscopic level of single defect damage effects all the way up to macroscopic effects. To overcome lengthy and expensive trial-and-error experiments, the modelling of materials behaviour under irradiation at high temperature, fluence and mechanical load is a promising tool, bringing new insights into the fundamental understanding of basic mechanisms [11, 20, 10, 21]. It has a predictive aspect of materials behaviour, probes beyond currently possible experimental approaches and allows the set-up of better tuned experiments. In the distant future, it is envisaged that development of tailor-made alloys, ceramics and fuels with optimized composition would be possible as an outcome of accurate materials modelling.

9.1.1. *Ab initio calculations on Fe-Cr.* The Fe-Cr system represents the fundamental building block of structural materials design due to its superior properties of increased strength and hardness, low oxidation rate, corrosion resistance and retention of strength at high temperatures. The aim of this work last is to understand how the magnetic structure of the Fe-Cr alloy changes with Cr content as a result of its anisotropic behaviour in order to determine optimal Cr concentrations in these alloys for use under extreme conditions. These issues are being investigated by first principle calculations within the Density Function Theory framework, devoted to find equilibrium configurations and energies of the alloy, examine the effect of Cr and vacancies on the heterogeneous magnetic structure, as well as investigate the orbital and spin moments of Fe and Cr. The results will have an impact on a broad spectrum of materials users and developers who use Fe-Cr as their basis matrix such as fission, fusion, aeronautical, space and magnetic storage and device technologists.
Ab initio simulations have been run on a number of Fe-Cr systems, ranging from a pure bcc Fe unit cell to 64 atom supercells with one to eight Cr atoms acting as substitutional impurities for Fe atoms and/or one and two vacancies using the WIEN2k computational commercial package executed first on Horizon (Cray XT3) and subsequently on Blanc (IBMP5) supercomputers. Results obtained include equilibrium energies and volumes, the total and local magnetic moments of both species after internal structural relaxation,

preliminary XAS and XMCD spectra, the band structures and the electronic densities. Some of these results have already been compared on a one to one basis with XMCD experimental performed within our group, giving good agreement [5].
This is a summary on papers published, submitted or talks given in the period from 2007 to 2008 due to results obtained from simulations on Horizon [16, 14, 13, 3, 2, 1]; there are a couple of papers in preparation [15, 17]. Partial funding from FP7 project GetMat [12]; accepted for funding from SNF [18].

## 9.2. **Outline of scientific work on for the future.**

9.2.1. *Ab initio calculations on Fe-C.* Similar work as that performed in Fe-Cr is now also being performed on Fe-C using combinations of Wien2K and VASP in order to study steels. The expected effect of including carbon is the production of a lattice distortion manifesting itself as a change in magnetism, which justifies a separate study of the FeC system to help in the understanding of ferritic/austenitic steels.

9.2.2. *GB MD simulations.* A large number of materials of technological use are composed of polycrystals. Grain boundaries (GBs) play an important role in crystalline materials as they control many of the materials physical and chemical properties. At high temperature and during irradiation, GBs act as sinks or sources for interstitials and vacancies. In nuclear applications, diffusion of such defects in GBs is of great interest. Understanding how atoms move to and within GBs enables the study of voids and/or bubble nucleation at GBs, whose fast accumulation leads to cracks and is important in comprehending the creep lifetime expectancy of metals. To investigate the role of the GB, the following investigations are currently underway:

9.2.3. *Simulations to study He mobility in and near GBs to understand bubble nucleation.* (in collaboration with P. Derlet and H. Van Swygenhoven (NUM)) [19] The mechanical properties of materials alter under exposure to extreme conditions such as those present in the nuclear environments of fission and fusion reactors. In such environments, one of the main gaseous byproducts is helium, whose presence and further production is known to decrease ductility, fatigue life and weldability, reduce creep and stress rupture properties of materials as well as promote swelling. These effects lead to the drastic modification of the materials mechanical properties with possible consequences of crack, fatigue and embrittlement even at low concentrations. Helium precipitates into voids to form helium bubbles. At high temperatures the clustering of such bubbles in Grain Boundaries (GBs) results in embrittlement even in intrinsically ductile materials. It is possible to investigate such voids and GB bubbles by studying the mobility of helium near and in GBs using MD simulations.

9.2.4. *Simulations of irradiation of nanocrystalline Fe system.* A better understanding of irradiation requires an understanding at the microscopic level of single defect damage. Modelling of their microstructure is undertaken using Molecular Dynamics (MD) computer simulations of the displacement cascade evolution during the initial stages of radiation damage. The abundance, combination in clusters, mobility and absorption by sinks of uncombined Frenkel pairs define the changes seen in mechanical properties of irradiated materials. To address the absorption of these defects at sinks such as grain

boundaries (GBs), the samples simulated in this work are on bcc nanocrystalline (nc) iron samples. Nc materials should have increased radiation resistance due to the large number of sink sources present in the samples, with significant reductions in defect production compared to their coarser grain counterparts. The aim of this project is study displacement cascade using MD simulations and various potentials.

9.2.5. *Simulations of irradiation of SiC (CP2K).* [19]

9.2.6. *Dislocation Dynamics.* The inclusion of ODS (oxide dispersion strengthening) particles in materials is performed in order to improve the properties of materials used under extreme conditions. Studying the dislocation-dispersoid interactions has been found to be one of the key factors in obtaining the critical resolve shear stress of the material [7, 9, 8, 6, 4, 5]. Although none of these presentations/papers were done using Horizon, it is envisaged that in the future ParaDis, a parallel dislocation Dynamics code will be used within HT-MAT modelling and therefore references performed with serial code have been included to show the capacity of research using this code. ParaDis will enable larger scale simulations and the study of phenomena such as creep and dislocation-dislocation interactions. Unfortunately due to a bug found in this code, it is currently not in use. If the bug in the ParaDis code is fixed, then simulations would also be conducted on Horizon.
The Table 9.1 summarizes the resource requirements projected 5 years into the future.

| Problem | Cores | Memory [GB] | Disk [TB] | Tape [TB] | Core [h$\times 10^3$] |
|---|---|---|---|---|---|
| VASP | 96 | 1750 | | | 960 |

TABLE 9.1. Summary of the future requirements by the Fe-Cr System group. Cores and Memory are per average production run. Disk, Tape and Core-hour requirements are on a yearly base.

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# 10. REACTOR PHYSICS

Project Leaders: M.A. Zimmermann, H. Ferroukhi, M.F. Murphy
Project Collaborators: E. Kolbe, A. Vasiliev, G. Perret, P. Grimm
PSI Groups: NES/LRS, STARS/ANSR and PROTEUS

10.1. **Outline of scientific work on Merlin/Horizon.** The Monte Carlo radiation transport code MCNPX, in combination with modern continuous energy neutron cross section libraries, has been applied at the LRS within the STARS/ANSR-projects for a range of tasks: (1) Criticality safety evaluations of light water reactor high-density storage racks and transport casks, (2) Modeling of the fast neutron fluence on a reactor pressure vessel and internals, (3) Benchmark calculations of the fuel inventory in combination with the Monteburns system of codes (which links MCNPX with the decay and depletion code ORIGEN2).
In the PROTEUS group MCNPX is mainly used to: (1) compare measurements performed in the zero-power research reactor PROTEUS with MCNPX predictions, (2) predict critical core loading in various configurations, and (3) investigate core designs for future experiments. Examples of recent measurements analysed with MCNPX are the axial and radial distributions of fission and $^{238}$U capture rates in the fuel rods of Westinghouse SVEA-96+ and SVEA-96 Optima2 boiling water reactor assemblies. MCNPX has been qualified against experimental data and has also been used as a reference to qualify deterministic neutronic calculations.

10.2. **Papers published based on computer work done in the last 2 years.** This is a summary of the papers published within the STARS/ANSR-projects and by the PROTEUS group in the period from 2007 to 2008 based on the results obtained from simulations on Merlin and Horizon [5, 4, 8, 6, 3, 1, 7, 2, 12, 10, 11, 9, 13].

10.3. **Estimate of required HPC resources for the future.** In the near future it is planned to extend the criticality safety evaluations described above by: (1) including burn-up credit, (2) performing sensitivity studies and uncertainty analysis for the assessed spent fuel systems. With respect to fluence modeling extensions towards reactor dosimetry and activation analysis are aimed for. Finally, a general extension of the MCNPX code usage is expected in order to obtain reference calculations of core neutronic characteristics at steady-state conditions to be used for the validation of deterministic solutions.
The upcoming upgrade of the PROTEUS facility will also entail a rising demand for detailed MCNPX simulations of the reactor including the various test zones that will be set up to perform the LIFE@PROTEUS experimental program.
All of these enterprises are expected to increase the needed HPC resources by a factor of 3 to 5. The estimated future requirements are summarized in Table 1 below.

## References

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| Problem | Cores | Memory [GB] | Disk [TB] | Tape [TB] | Core [h×$10^3$] |
|---|---|---|---|---|---|
| MCNPX | 128 | 8 | 1 | 1 | 500 |

TABLE 10.1. Summary of the future requirements by the STARS/ANSR and PROTEUS groups at NES/LRS. Cores and Memory are per average production run. Disk, Tape and Core-hour requirements are on a yearly base.


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# Glossary

This section contains the explanation of some often-used terms that either are not explained in the text or, by contrast, are described extensively and for which a short description may be convenient.

**Architecture**: The internal structure of a computer system or a chip that determines its operational functionality and performance.

**Architectural class:** Classification of computer systems according to its architecture: e.g., distributed memory MIMD computer, symmetric multi processor (SMP), etc. See this glossary and section architecture for the description of the various classes.
**ASCI:** Accelerated Strategic Computer Initiative. A massive funding project in the USA concerning research and production of high-performance systems. The main motivation is said to be the management of the USA nuclear stockpile by computational modeling instead of actual testing. ASCI has greatly influenced the development of high-performance systems in a single direction: clusters of SMP systems.
**Beowulf cluster:** Cluster of PCs or workstations with a private network to connect them. Initially the name was used for do-it-yourself collections of PCs mostly connected by Ethernet and running Linux to have a cheap alternative for "integrated" parallel machines. Presently, the definition is wider including high-speed switched networks, fast RISC-based processors and complete vendor-preconfigured rack-mounted systems with either Linux or Windows as an operating system.
**Cache — data, instruction:** Small, fast memory close to the CPU that can hold a part of the data or instructions to be processed. The primary or level 1 caches are virtually always located on the same chip as the CPU and are divided in a cache for instructions and one for data. A secondary or level 2 cache is mostly located off-chip and holds both data and instructions. Caches are put into the system to hide the large latency that occurs when data have to be fetched from memory. By loading data and or instructions into the caches that are likely to be needed, this latency can be significantly reduced.
**Capability computing:** A type of large-scale computing in which one wants to accommodate very large and time consuming computing tasks. This requires that parallel machines or clusters are managed with the highest priority for this type of computing possibly with the consequence that the computing resources in the system are not always used with the greatest efficiency.
**Capacity computing:** A type of large-scale computing in which one wants to use the system (cluster) with the highest possible throughput capacity using the machine resources as efficient as possible. This may have adverse effects on the performance of individual computing tasks while optimising the overall usage of the system.
**ccNUMA:** Cache Coherent Non-Uniform Memory Access. Machines that support this type of memory access have a physically distributed memory but logically it is shared. Because of the physical difference of the location of the data items, a data request may take a varying amount of time depending on the location of the data. As both the memory parts and the caches in such systems are distributed a mechanism is necessary to keep the data consistent system-wide. There are various techniques to enforce this (directory

memory, snoopy bus protocol). When one of these techniques is implemented the system is said to be cache coherent.
**Clock cycle:** Fundamental time unit of a computer. Every operation executed by the computer takes at least one and possibly multiple cycles. Typically, the clock cycle is now in the order of one to a few nanoseconds.
**Clock frequency:** Reciproke of the clock cycle: the number of cycles per second expressed in Hertz (Hz). Typical clock frequencies nowadays are 400 MHz–1 GHz.
**Communication latency:** Time overhead occurring when a message is sent over a communication network from one processor to another. Typically the latencies are in the order of a few $\mu s$ for specially designed networks, like Infiniband or Myrinet, to about 100 $\mu s$ for (Gbit) Ethernet.
**Core & multi-core** A multi-core CPU (or chip-level multiprocessor, CMP) combines two or more independent cores into a single package composed of a single integrated circuit (IC), called a die, or more dies packaged together. A dual-core processor contains two cores, and a quad-core processor contains four cores. A multi-core microprocessor implements multiprocessing in a single physical package. A processor with all cores on a single die is called a monolithic processor.
**Distributed Memory (DM):** Architectural class of machines in which the memory of the system is distributed over the nodes in the system. Access to the data in the system has to be done via an interconnection network that connects the nodes and may be either explicit via message passing or implicit (either using HPF or automatically in a ccNUMA system).
**Grid — 2-D, 3-D:** A network structure where the nodes are connected in a 2-D or 3-D grid layout. In virtually all cases the end points of the grid are again connected to the starting points thus forming a 2-D or 3-D torus.
**Message passing:** Style of parallel programming for distributed memory systems in which non-local data that is required explicitly must be transported to the processor(s) that need(s) it by appropriate send and receive messages.
**MPI:** A message passing library, Message Passing Interface, that implements the message passing style of programming. Presently MPI is the de facto standard for this kind of programming.
**OpenMP:** A shared memory parallel programming model in which shared memory systems and SMPs can be operated in parallel. The parallelisation is controlled by comment directives (in Fortran) or pragmas (in C and C++), so that the same programs also can be run unmodified on serial machines.
**RISC:** Reduced Instruction Set Computer. A CPU with its instruction set that is simpler in comparison with the earlier Complex Instruction Set Computers (CISCs) The instruction set was reduced to simple instructions that ideally should execute in one cycle.
**Shared Memory (SM):** Memory configuration of a computer in which all processors have direct access to all the memory in the system. Because of technological limitations on shared bandwidth generally not more than about 16 processors share a common memory.
**SMP:** Symmetric Multi-Processing. This term is often used for compute nodes with shared memory that are part of a larger system and where this collection of nodes forms the total system. The nodes may be organised as a ccNUMA system or as a distributed

memory system of which the nodes can be programmed using OpenMP while inter-node communication should be done by message passing.

**Torus:** Structure that results when the end points of a grid are wrapped around to connect to the starting points of that grid. This configuration is often used in the interconnection networks of parallel machines either with a 2-D grid or with 3-D grid.


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