# Inhoudelijke programmabeschrijving

Programmatitel NPSC: Netherlands Platform for Scientific Computing

# Probleemstelling

Scientific Computing (SC) is the computer simulation discipline based on mathematical modelling and numerical mathematics. SC supplements theory and replaces expensive, impractical, or impossible laboratory experiments. SC is rapidly gaining importance due to improvements in algorithms, chip design and increasingly widespread use of mathematical models. Internationally, SC is playing a major role in national research agendas because of its wide-ranging impact on the development of the sciences and technology and hence for economy, industry and society at large. Three USA reports urge to invest, viz. the '04 SCaLeS (Science-Based Case for Large-Scale Simulation) report, the '05 PITAC (President's Information Technology Advisory Committee) report—which calls SC the most important technology development for the 21<sup>st</sup> century—and the '06 NSF report 'Simulation-Based Engineering Science' (see <a href="http://www.npsc.nl">http://www.npsc.nl</a> for supplementary material).

## Doelstelling

Scientific leadership and development in SC is as important for the Netherlands as it is for the USA. The NWO Research Council for Physical Sciences underlined this in 2000 with the research program 'Computational Science'. We propose a strong follow-up focusing on numerical simulation. Advanced numerical algorithms lie at the very heart of the computational science approach and future progress of computational science will strongly depend on future progress within numerical mathematics. For NL this is critical because research capacity is low. For example, Germany currently has at least 50 chairs in numerical mathematics compared to only 5 in our country. We will initiate NPSC, a platform with mission *Fostering Advanced Use of Scientific Computing*. The ambition is creating a national platform for groups across all sciences, laboratories, industries and companies dependent on numerical simulation. NPSC builds on a core of expert and user groups which annually meet within the 'Werkgemeenschap Numerieke Wiskunde', further extended with new user groups, in particular from SMEs. The response confirms the urgency of SC for NL. Involved in this proposal now are groups from 10 SMEs, active in engineering, medical applications or software consultancy, 6 large companies (ABN AMRO, Boal, 3 Philips divisions, Shell), 8 laboratories (GTI's, CWI, FOM, NIOZ), Erasmus Medical Center, and 7 universities.

### Beoogde resultaten

Maintaining leadership in SC in areas where NL excels and increasing development in other areas, requires continual focus on novel algorithm research driven by challenging applications and guided by user interaction. To achieve this, we propose two main NPSC activities (i) a multidisciplinary, comprehensive research programme and (ii) a service-providing research-outreach office.

(i) The research programme. Frontier research in SC is mostly driven by applications giving rise to partial differential equations and matrix problems. In consultation with user groups from various disciplines as represented by the above mentioned organizations, expert groups from numerical partial differential equations and matrix problems have selected a number of challenging research projects which combined will constitute the research programme (a preliminary text has been put on <a href="http://www.npsc.nl">http://www.npsc.nl</a>). Individual projects will last 4 years within an overall proposed 8-year Smart Mix window to relieve the labour-market and to allow recruitment of excellent junior researchers (55 PhDs and postdocs). The selected projects are classified into six main application areas:

(1) Science. Grid computing as an enabling tool for scientific computing.

(2) Engineering and Design. Hydrocarbon exploration. Electronic devices in optics. Electronic circuits in chips. Magnetohydrodynamics in liquid propulsion. Materials science in the alloy industry.
(3) Complex Flows. Turbulence modelling. Extreme water waves in connection with off-shore/coastal protection and ships. Hydrodynamics of bubble columns. Solvers for CFD packages in industry.
(4) Bio(techno)logy and Health. Damaging of human tissues exposed to electromagnetic systems. Patient-specific simulation for improved stroke prediction. Hybrid (bio)chemical modelling.

(5) Sustainable World (climate, energy, ecology). New approaches to climate and weather modelling. Coupling phytoplankton and climate models. Simulating the next generation of off-shore wind farms.
(6) Finance and Business. Computational finance and option pricing.

This programme spans the entire spectrum: fundamental—applied—developmental. Designing novel algorithms will be the focal point on the fundamental side, whereas on the developmental side groups will deal with numerical software design and implementing and prototyping new applications.

(ii) The research-outreach office. Such an office is a new concept. It will be the de facto national contact point for all user groups dependent on numerical simulation. It will provide services, organize and promote concerted knowledge transfer in numerical simulation. This is crucial, because new algorithms, even when spectacularly outperforming old ones, take a long time to permeate production software, one reason being lack of expert knowledge by users. Also, development work on algorithms is fragmented over application fields with insufficient exchange between disciplines. Service will primarily take the form of *high-level help-desk projects*, through which junior and senior staff will commit substantial time to ensure the incorporation of advanced technology in user applications. Such projects may concern algorithms needed for specific applications, sophisticated numerical software, etc. High-level user-tailored software development is a major instrument for knowledge transfer within SC. Comprehensive support of this sort will also create ideal conditions to timely signal spin-off opportunities. Within the budget a total of 20 postdoc-years is allocated for this service over the proposed 8 Smart Mix years. In addition to help-desk projects, the office will organize *theme years* on specific topics and a *traineeship program* for talented master students.

#### Toetsing aan criteria

- Focus and mass. NPSC joins forces. Building on the existing 'Werkgemeenschap Numerieke Wiskunde', NPSC joins all academic numerical research groups in the country with leading and new groups from the listed application areas, while focusing on strategically chosen subjects.

- *Track record.* All senior researchers involved are highly experienced in SC. The citation report 'Results of the bibliometric study on Dutch mathematics research 1993-2002', CWTS, Leiden University, Draft version Nov. '04, issued by NWO, shows a high impact of past Dutch applied and numerical mathematics. A comparison of impact to the worldwide field average '88 - '97 shows that the scores are the best among disciplines, and considerably higher than all others mentioned.

- Added value. The potential of simulation is evident. Any scientific, technical, societal, industrial, financial, medical, etc. problem that lends itself to mathematical modelling can be dealt with. In many situations simulation is the only option. National excellence in simulation will be more and more crucial for competitive societies being industry-oriented as well as knowledge-oriented. NPSC will contribute to such excellence, both through its research programme and outreach office. NPSC pays special attention to the SC potential for SMEs.

### Implementatieplan

- Administration. NPSC will be administered by CWI, a renowned institute. The outreach office will also be located at CWI. Its director will appoint a scientific and a managerial NPSC director who will install a consortium board for advice and monitoring. The scientific NPSC director will be in charge.

- *Duration*. Allocated research projects will last 4 years within an 8-year Smart Mix window. For the outreach-office, funding is requested for the full 8 years, in size mainly for the anticipated help-desk projects amounting to an estimated number of 20 postdoc-years.

- *Permanent staff.* About 4.6 fte (4 years) professor level and 21 fte (4 years) senior level for the research program, including staff from universities, laboratories and companies Some permanent staff involvement will also be needed for research-outreach.

- *Monitoring*. The NPSC directors will install and utilize schemes for auditing progress of projects, for monitoring activities, for reporting results, for consulting the advisory consortium board, etc.

- Interaction. In addition to theme year activities, all researchers involved in the research programme will meet regularly in workshops, project meetings, etc. to discuss progress and exchange results. All NPSC events will be public. An active website and newsletter will be organized for PR.

- *Knowledge transfer.* NPSC will build a unique SC platform for researchers from universities, laboratories, industry, the financial sector, the medical sector, etc. So doing, NPSC will contribute significantly to knowledge transfer. For a significant amount of the research programme this is warranted by appointing project leaders from the application areas. By running a research-outreach office further excellent perspectives for knowledge transfer will be solicited and created.

- Scientific innovation. Except for the grid computing project, all projects involve participation of expert and user groups. By exploiting the expertise of senior researchers from the universities and the combination of expert and user groups, scientific innovation in the application areas is ensured, especially for new groups from SMEs.

- Competence build-up. The 55 junior positions within the research programme and an estimated 20 postdoc years for the anticipated help-desk projects will result in a significant competence build-up, both at the universities, the laboratories and the companies involved. Training and education in SC is of major importance for technological development based on computer simulation.

- Career assistance. An active career-assistance policy will be developed for all junior NPSC researchers. A focal point will be employment within the Netherlands. In this connection the participation of SMEs is expected to be highly beneficial for junior NPSC researchers.