Project No. FP7 – 212348

NFFA
Nanoscience Foundries and Fine Analysis

D2.2
NFFA Science Programme

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Deliverable D2.2: Draft of NFFA in-house scientific programme

1. INTRODUCTION

1.1. Purpose of the document

The purpose of this document is to show the need for a NFFA centre to have an internal and user science programme and to describe a framework of the NFFA in-house science programme. It is not intended to give full details on what science programme each NFFA centre should have, but rather an outline and direction. The detailed science programme will be decided according to the full analysis of which analytical large scale facilities will be actually connected to NFFA centres.

1.2. Application Area

The targets of this document are the members of the NFFA Project, the EC Project Officers, and the general public.

1.3. References

Description of Work (DoW). See at web site:
http://nffa.tasc.infm.it/pmwiki/pmwiki.php?n=NFFA.AnnexI-DoW
ESFRI Roadmap Update 2008:
ftp://ftp.cordis.europa.eu/pub/esfri/docs/esfri_roadmap_update_2008.pdf
GENNESYS:
http://www.mf.mpg.de/mpg/websiteMetallforschung/english/veroeffentlichungen/GENNESYS/index.html
Productive Nanosystems roadmap: http://www.foresight.org/roadmaps/PRINS:
http://www.prins-online.eu/

1.3.1. Objective of Work Package 2

To identify an in-house science programme in NFFA centres, which includes scientific activities carried out by NFFA centre internal staffs and by users of NFFA centres.

1.3.2. Description of work broken down into tasks

The following task was defined in WP2:

T2.2) Definition of a science programme for NFFA-RI, which will be composed of two synergic activities: the in-house research projects under the responsibility of NFFA-RI staff and associated scientists and the users' scientific projects.

1.4 Abstract

Visits had been made in 2008 by the task leader to the Centre for Functional Nanomaterials in Brookhaven National laboratory, US, and the Centre for Nanophase Materials Sciences in Oak Ridge National Laboratory, US. Visits to the Molecular Foundry in Lawrence Berkeley National Laboratory, US, and to the Sandia National Laboratory, US, were also made by other members of the NFFA consortium. By examining the existing nanoscience centres in the US and other similar centres in Europe, including all the partner's institutions as well as the Karlsruhe Institute of Technology (Germany), MyFAB (Sweden), Inspire (Ireland), IINL (Spain-Portugal), it is evident that a NFFA centre needs its own internal science programme in addition to user proposals. A good internal science programme is a means to train NFFA centre staffs to high level scientific competence which will better support the user access and programmes.

The general mission of NFFA is to provide an advanced platform for developing the new frontiers of nanoscience by making the best use of the most advanced characterisation probes and matter-shaping tools that are available and under further development at radiation sources. The role of NFFA in European science is therefore to host innovative research as well as being a key resource for research led by others (users). The general guideline is to seek as much as possible synergy between NFFA internal science programmes specialised in the different centres or based on whole infrastructure programmes and external user proposals. Each NFFA centre will contribute to the general NFFA mission, taking into account the needs of the local scientific environment. However, each NFFA centre can play its own strength and establish unique capabilities. The key to realise the goal is to have an appropriate management structure and procedure in place. In general, the NFFA infrastructure will address the users to the most appropriate centre for carrying out their proposal, but all centres should be capable to satisfy the needs of state-of-the-art support to nanoscience projects.

The NFFA centres, being closely connected with nearby analytical large scale facilities (ALSF), which are powerful tools for the characterisation and the understanding of materials and processes at the atomic level, are intended to be basic science centres. Nevertheless, due to the converging character of nanoscience and nanotechnology, which are bridging different disciplines and heterogeneous application fields, the NFFA science centres will also carry out application oriented research and development, including prototyping and technological proofs of principle whenever of scientific/technological development merit.
Therefore, in defining a science centre, the scientific programme is a fundamental building block to qualify the scientific profile of the infrastructure itself.

2. STRUCTURE OF NFFA SCIENCE PROGRAMME

2.1. Background

A NFFA centre is a user facility, like the analytical large-scale facilities (ALSF) with which it is co-located. Supporting users in their nanoscience and nanotechnology research is the paramount goal of the NFFA centres. Most of the users' demands require participation of internal staffs that can provide professional advice and help. The experience of the DOE nanoscience centres in the US, all connected with ALSF, has further demonstrated the need of an internal research activity.

NFFA must represent a facility oriented at a substantial advance in the quality of research in nanoscience by providing, on the same footing, excellent infrastructure service and advanced science programmes to be carried out by internal as well as associated staff. Both aspects are needed in order to pursue the NFFA mission. Consequently the NFFA centres will be attractive for scientists to become staff members, with full access to the advanced laboratory infrastructure as well as continuous benchmarking with top European users.
By conducting internal research with high calibre scientists, the NFFA centres can become international focus points in nanoscience research and nanotechnology development, which will consequently attract more users to come to the centres to work with the internal staffs on high impact research.

2.2. Thematic areas

The science programme in NFFA centres should focus on key thematic areas of current and future nanoscience research and nanotechnology development:

- *Fundamental nanoscale phenomena and processes*. Discovery and development of fundamental knowledge pertaining to new phenomena in physical, biological and engineering sciences that occur at the nanoscale. Elucidation of scientific and engineering principles related to nanoscale structures, processes and mechanisms

- *Nanomaterials*. Research aimed at the discovery of novel nanoscale and nanostructured materials and at a comprehensive understanding of the properties of nanomaterials (ranging across length scales, and including interface interactions). R&D leading to the ability to design and synthesise, in a controlled manner, nanostructured materials with targeted properties.

- *Nanoscale devices and systems*. R&D that applies the principles of nanoscale science and engineering to create novel, or to improve existing, devices and systems, including the incorporation of nanoscale or nanostructured materials to achieve improved performance or new functionality. Though the devices or systems may not be restricted to nanoscale, the enabling science and technology must be at the nanoscale.

- *Instrumentation research* including next generation techniques and technical solutions for extending the direct benefits of fine analysis to complex nano-synthesis or real environments.

- *Common metrology and standards* needed to advance nanotechnology research and commercialisation, by means of round robin activities to compare protocols for metrology and for synthesis of nanostructured materials

- *Nanomanufacturing*. R&D aimed at enabling scaled-up reliable and cost effective manufacturing of nanoscale materials, structures, devices and systems

- *Environment, health and safety*. Research primarily directed at understanding the environmental, health and safety impacts of nanotechnology development and corresponding risk assessment, risk management and methods for risk mitigation

- *Atomic precision*. In addition, atomic precision is being pursued as a possible new paradigm for exploiting quantum effects to produce functional systems. This is beyond the current definition of nano-science methods and techniques. NFFA will provide the most adequate environment for developing atomic-precision metrology and fabrication.

- *Development of the data repository* that for a science centre may become the relevant and most effective instrument to make nanoscience outcome promptly available to the widest share of stakeholders.

A key difference of NFFA with respect to other European initiatives like the *Partnership for Structural Biology* or the *Partnership for Soft Matter Science* of Grenoble is that the latters have been stimulated by well established users' communities of the radiation source based methods of fine analysis seeking better complementary infrastructure for their research.

In the case of NFFA the need of integrating radiation based methods comes largely from nanoscience programmes that up to now use only marginally these methods of fine analysis, knowing that these are now understood to be of key importance for a fast progress of this field of research.

These concepts have been developed in several foresight exercises including GENNESYS that anticipate the idea of "strategic access" to the analytical large scale facilities for supporting nanoscience/nanotechnology development, the National Nanotechnology Plan of the U.S. and the Productive Nanosystems Roadmap.

2.3. Structures

The NFFA science programme must address the main challenges of nanoscience in particular by identifying the methodological and instrumental platform that will support advanced research to meet them. Users will have special needs of design, simulation, synthesis, and characterisation that must find adequate support in the NFFA centre. Users may also be actually attracted by the NFFA internal research programme and participate to it. The choice of the best-suited analytical facilities to be connected to NFFA is crucial in order to provide the best selection of fine analysis means coupled with the NFFA. Figure 1 gives an overview of the interplay of external and internal programmes and the associated LSFs (large scale facilities).

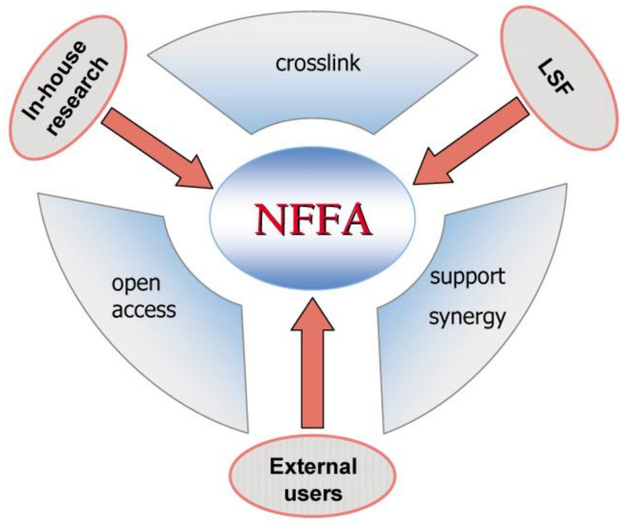


Fig.1 Structure of the interplay of external and internal programmes and large scale facilities (LSFs)

The NFFA science programme will be the basis of negotiation with the analytical facilities for agreeing on strategic access issues to the radiation sources. In fact double peer-review of the users' proposals should be avoided. This is an important point to be addressed by WP4 and the results of it will feed back into the evolution of the NFFA science programme.

NFFA will cover the main fields of nanoscience and fine analysis. This implies that a complete offer of complementary tools at the radiation sources will be included. In turn this means that the characteristics of specific sources (low energy X-rays, Hard X-rays, nanobeams, Ultra-short pulses, neutrons) will be guidance for the choice of where to establish the NFFA centres. Clearly the locations offering a multiplicity of state of the art fine analysis methods as well as specific outstanding facilities in the neighbourhood will have advantages in the competition for selection.

Interrelationship of the NFFA centres: The NFFA is a European distributed facility according to ESFRI definition. It is identified by its science programme and its unique access portal. The individual NFFA centres will develop strong synergy with the local analytical facility that may go beyond the international access programme in establishing possible local partnerships. Each centre should play its own strength and develop its own distinctive science programme. This may imply that one or more centres may focus on biology, whilst others may e.g. focus on nano-materials, photonics science, or energy research.

For sake of example, the synchrotron light source in the UK (Diamond) has strong emphasis on bioscience. In this case, a potential NFFA nanocentre in the UK might focus on the nano-bio science area. Since, nevertheless, nano-bioscience will be carried out also at other NFFA centres (according to the concept of a European distributed facility*), such centre may play a reference and coordination role in the specific domain, both for the users' projects and for the institutional programme.

A mechanism will be established to integrate and distribute the expertise and facility developments obtained in different NFFA centres. The NFFA centres will also develop and operate a data repository. The structure and interrelationship for the NFFA nanoscience centre cluster is shown in Fig.2. The NFFA central management will provide the coordinating role, to make sure users' needs are met in one NFFA centre or another. The centres themselves must have an appropriate management structure.

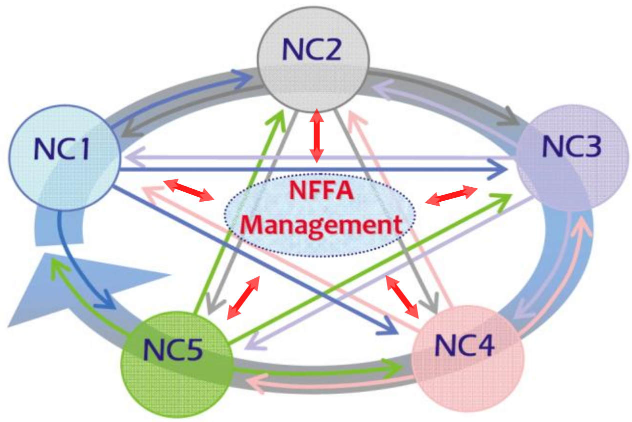


Fig.2 The interrelationship of NFFA Nanocentres (NCs) follows the concept of the distributed infrastructure

* The concept of "distributed infrastructure" has been defined by ESFRI as follows: "A European Distributed Infrastructure, as recognised by ESFRI, is a singular Research Infrastructure, having a unique Name and legal status, Management Structure (director or board of directors), Strategy and Development Plan, Access point for users, Annual Report and Fiscal address although its research facilities are distributed in multiple sites".

NFFA as methodological and instrumental platform: The advancement of nanoscience and the exploratory work on atomic precision manufacturing will take full advantage of the availability, within the NFFA portfolio of methods, of the following list of state of the art probes, available at the analytical facilities:

- X-ray micro beams and nanobeams for structural analysis (medium high energy synchrotron, high energy FELs)
- Coherent X-ray beams for coherent imaging (medium high energy synchrotrons, medium-high energy FELs)

- Small Angle Scattering of x-rays and neutrons with time microsecond time resolution (medium energy synchrotrons, high energy synchrotrons, spallation neutron sources, neutron reactors)

- Element specific XAS-EXAFS and resonant techniques (medium energy synchrotrons, FEL, high energy synchrotrons)

- Femtosecond dynamics (all range FELs, high power lasers)

- Picosecond-nanosecond dynamics (synchrotrons)

- High resolution (energy, momentum, time, spin) photoemission and photoelectron spectromicroscopy (low-medium energy synchrotrons, low-medium energy FELs, neutrons)

- High resolution collective dynamics (neutron sources, medium-high energy synchrotrons)

- Radiation based synthesis (synchrotrons, FELs)

Associated with these probes at LSFs, the NFFA centres will provide

- In situ sample characterisation with atomic precision/resolution (TEM, STM, AFM, coupled scanning probes and radiation beams)

- In situ nanofabrication and patterning of nanostructures and microstructures

- In situ synthesis of materials, template growth, combinatorial material libraries

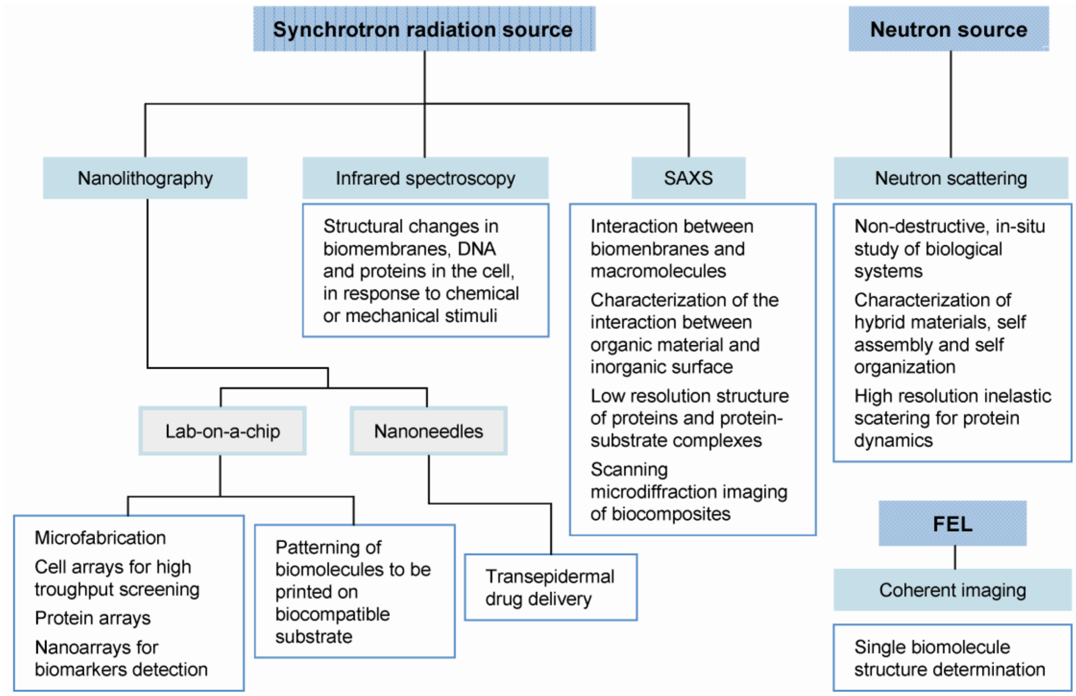
- In situ micro/nano-sample manipulation (optical trapping methods, micro-fluidics)

- Full state-of-the-art synthesis and characterisation with nanoscience methods and with atomic precision methods

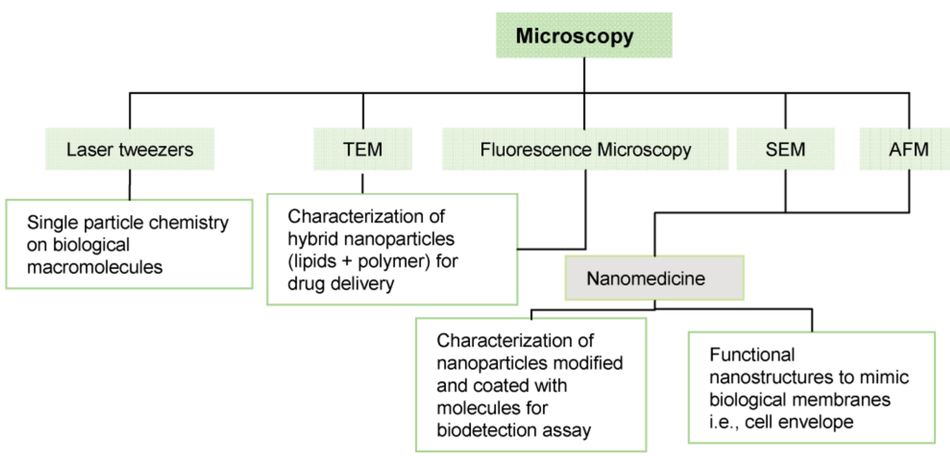
- Atomic precision metrology

Within this framework it will be possible to match the general scope of NFFA with specific “site dependent” capabilities that take also into account that the NFFA centres will be funded by national governments for the construction phase and therefore will have to provide services that are perceived as a priority by those “local” scientific communities that will be first neighbours of each Centre. The common platform of NFFA Centres will guarantee that such requirements are fulfilled, as well as the overall science remit of NFFA.

As an example of one chapter of the NFFA science programme, possible developments of the nano-bio activities are summarised in the following diagram:



The nano-bio applications will take advantage of fine analysis tools that will be available in the dedicated laboratories at the facility, as in example, microscopy tools:



3. APPLICATION DOMAINS

Research in nanoscale phenomena is of central concern to ensure the competitiveness of Europe, as it is evident form national and European roadmaps of science and technology development. The role of NFFA is to support nano science at the fundamental level as well as at the level of development of synthesis protocols, nano-systems, and advanced characterisation.

There are several suggested themes for the NFFA science programme, as described in Section 3.2, fitting into the general application domains identified by FP7:

- Information technology
- Renewable and clean energy sources
- Environment protection and sustainable development
- Healthcare

Internal as well as user scientific proposals will be generally aligned with the above application domains, which will enable the centres to be in good position to apply for regional/national/international funding. This should be considered in NFFA Workpackage 4.

4. FUNDING MECHANISMS

It is assumed that the European funding to support the NFFA centres will mainly support operation and user access programmes. To qualify for European funds the NFFA Research Infrastructure and each of its centres will have to demonstrate a sizable user base. In order to attract users to the NFFA facilities, the equipment base, the level of scientific expertise and the internal science programme will all play a part. The internal science programme and its achievements can be a showcase to the user community, demonstrating the capability of an NFFA centre and proving that accessing an NFFA centre can really make a great impact on their research.

Nanoscience research has to be seen in connection with nanotechnology development and commercial applications. Current criteria for funding include the economic impact of the proposed research. Some questions have to answered such as “who will benefit from the research?”, “How will they benefit from this research?”, “What will be done to ensure that they benefit from this research?”.

The quality and level of funding of NFFA from national agencies will equally imply some priorities that will have to be met by the science programme.

5. CONCLUSIONS

The following key points are derived from the NFFA in-house science programme study:

- High impact research conducted by NFFA scientific staff will establish the facility as a reference for European nanoscience research and nanotechnology development. Each individual NFFA centre will also be perceived in its national relevance as a national centre of excellence. Providing open access to state-of-the-art instrumentation will benefit existing users of the ALSF but most importantly will attract new users. The building of scientific communities and interest groups around the NFFA facilities and the ALSFs will enhance cooperation among research groups and will benefit the international competitiveness of the European research communities.

- It is important to have an appropriate management structure and procedures in an NFFA centre to ensure the science programme, whether by internal staff or external users, is properly defined and executed.

- The in-house science programme will qualify NFFA as a main actor on the European scene of nanoscience. The availability of state-of-the-art instrumentation and the synergy between theory, synthesis, characterisation, access to ALSFs will make NFFA staff positions attractive for ambitious scientists who, in turn, will provide also the best quality support to the NFFA users

- Any science project conducted at a NFFA centre whether internally or by user's access will depend on its funding mechanisms. The Open Access protocol will depend on EC support programmes for users, via I3 or other specific Research Infrastructure actions. National funding for the operation of NFFA centres will be needed and these will possibly be in forma of an annually allocated dowry or project based. Annually allocated budget allows a NFFA centre to have more freedom to decide what type of science programme it wants to run, while project based funding will put more pressure on a NFFA centre to have high impact scientific research programmes.

- NFFA will be an Open Access facility. It is envisaged that the user science programmes will be peer reviewed by independent scientific panels. Advisory and scientific committees, including representatives of the funding bodies, will monitor the science and technology performance of NFFA and of each of its centres.

- The number of NFFA centres should be sufficient to guarantee its scientific mission, which is fundamentally different from what could be provided by networking some users-support actions at the ALSFs.