The Action-Grid project is funded by the European Commission under the FP7

European Commission’s Framework Programme 7: Virtual Physiological Human

- Centered on building models and simulations of the body linked with clinical data
- A long-term, challenging vision
- ACTION Grid: only project related to BMI and nano areas within its Call
- Challenge: expand the VPH scope with a “nano” perspective
Expanding the scope towards Converging Technologies

Nano  Bio

Info  Cogno

NBIC
The great philosopher Pangloss, 1st pioneer in Converging technologies!!

From Candide
(Voltaire, 1759)

"Master Pangloss taught the *metaphysico-theologo-cosmolonigology*. He could prove to admiration that there is no effect without a cause; and, that in this best of all possible worlds, the Baron's castle was the most magnificent of all castles, and My Lady the best of all possible baronesses".
Reflections on Biomedical Informatics: From Cybernetics to Genomic Medicine and Nanomedicine

Maojo and Kulikowski: Reflections on Biomedical Informatics: From Cybernetics to Genomic Medicine and Nanomedicine (First reference on Medline combining “Biomedical Informatics” and “Nanomedicine”)
Nanoinformatics: beginning (2007)

Workshop on Nanoinformatics Strategies
June 12-13, 2007, Westin Gateway Hotel, Arlington Virginia
Hosted by the National Nanomanufacturing Network

Agenda (talks & links)
Workshop Purpose
Participants

The Workshop on Nanoinformatics Strategies was supported by the National Science Foundation through a grant to the NSF Center for Hierarchical Manufacturing at the University of Massachusetts Amherst.
Workshop goals (Tuominen and Kim, 2007, before ACTION Grid)

- Identify nanoinformatics needs, challenges and priorities
- Discuss informatics activities currently underway that work to address needs in various research, development and education sectors (NCN, EHS, NNN, NIST, NCLT, nanomaterials and others)
- Share best practices on cutting edge techniques in data mining, visual analytics, Web 2.0 technologies, literature analysis, data standards, digital clearinghouses, web-based communication tools, and related topics, including those from the other fields (e.g., caBIG, bioinformatics, computer science and others).

- **Connection to bioinformatics, and other informatics areas**
  - Discuss interconnecting databases and mechanisms for defining the ontology of terms
  - Identify and prioritize strategies best suited for catalyzing nanotechnology research, development and education
ACTION Grid Objectives

Main objective

To establish a collaborative environment in Biomedical Informatics, Grid Computing and nanomedicine, among the following geographical areas:

- European Union
- Latin America
- Western Balkans
- North Africa
Action-Grid: a puzzle with many pieces (some of them not well defined)
The White Paper: scientific emphasis on Nanoinformatics (freely available at the ACTION Grid website, in large and summary versions)

- State of the Art of Nanoinformatics
- Analysis of areas:
  - Nanomedicine
  - Nanotechnology
  - Nanotoxicity
  - Public health issues
- Priorities
- Grand Challenges
- Conclusions

Proposal: Five Grand Nanoinformatics challenges (particularly from a pure informatics perspective)
1. Data, repositories & standards

- *To create a Nanoinformatics infrastructure* to collect, curate, annotate, organize and archive the available data
- *Design of extended web nano portals*, linking groups and information around the world to facilitate data sharing
- *To build repositories/databases of use cases, clinical trials experiments or databases* with nano-data, facilitating the reuse of the data—like Arrayexpress for genomic data.
- Creating *a repository of nano-related informatics tools*, which can be accessed and retrieved through specific nano infrastructures
2. Interoperability: semantic search and ontologies

- To intercommunicate different nanoportals, facilitating rapid exchanges and sharing of data and other resources
- Extended standards for interoperability in the nanoinformatics field.
- Development of a taxonomy of research tasks (rather than biomedical resources) in the BMI area
- Improved classification approaches, to create new hierarchies/taxonomies based on actual physical, chemical, clinical, toxic or spatial characteristics, added to pure ontological/semantic information
- Use of cloud-computing services and supercomputers to carry out complex computational tasks, such as simulating interactions between nanoparticles and cells of the human body, supporting research in the area of multiscale modelling.
- Communication with and between nanosensors and nanodevices located in the human body
- To establish standards in reporting/publishing results in nano-particle/nanotechnology research
Reporting open results from research projects

A proposal for reporting open results from Biomedical Research projects, reported at the Science Careers Bog, from the Science journal.
3. Extending the European VPH programme and US initiatives

- BMI researchers have created a large number of *models and simulation tools which could be reused* or adapted to nanomedicine.
- To create a hypothetical, “*extended nanotype*” —including a large catalog of nanoparticles and biological targets, their interactions, potential nanotoxicities and relations to different diagnostic and therapeutic uses
- To *simulate “in silico” the effects, reactions or toxicity* of new compounds or materials before the “in vivo” studies. Multilevel simulations might predict effects of nanoparticles
- Theoretical studies of the *interactions between nanoparticles with the most common components of human cells*
4. Translational nanoinformatics

- Nanoinformatics might imply a continuum of BMI, but new insights are needed for *data and knowledge integration at the nano level* as well as basic research.
- The nature of nanomaterials and the *unknown effect of many nanoparticles* must be addressed prior to semantic or ontological analyses.
- **Medical imaging.** A key issue for nanomedicine is to create new contrast agents to target specific organs, functions, or cell types.
- We still lack a *unified theory of biomedical information* in an area like BMI. The analysis of differences between bits and quantum bits—a measure of information at the quantum level—, their appearance in nature and the diversity of meanings of the term “information”, might lead to new insights and research in this fundamental area.
5. Linking nanoinformation to EHRs

- **To link nanomedicine-related data to patient EHRs.** New standards will be needed for storing data or augmenting clinical vocabularies and terminologies —like SNOMED— or for exchanging electronic medical information —like HL7— and how they can incorporate nano-related information, terminologies and procedures.

- Questions related to **patient safety** and possible secondary effects related to the use of nanoparticles need to be addressed.

- The creation of large databases that would store nano-related information can be complemented by **new approaches to building EHRs.** It will require a collaborative effort from a number of researchers.

- New diagnostic and therapeutic methods based on new nanomaterials can enhance recent proposals for “personalized medicine” —currently mostly being built based on “–omics” advances. New models of EHRs, including nano information, must be **developed for use by medical professionals.**
The Action-Grid project is funded by the European Commission under the 7th framework project.

New industrial areas of development. New informatics techniques may allow new companies and academic settings to work on nanotechnology and nanomedical research, without the large budget resources that are usually necessary for traditional research in the area.

Enormous financial importance, with exponential growth in terms of investment and revenues. Large expectations for new job opportunities.

European groups can be funded by the US NIH and NSF and vice versa, facilitating collaborative research and exchange. International collaboration should foster interactions.

The EC has dealt with nano-related issues in directorates covering Nanotechnology and Health issues, but not in areas like ICT for Health. Opportunities for new programmes might arise, linking directorates and people working in the involved areas.

New synergy between established disciplines like Biomedical Informatics and Nanomedicine, leading to a new subdiscipline or area which could be called Nanoinformatics.

New academic programmes can be created or classical programmes — e.g., BMI or medicine — can be expanded. New working groups in societies like IMIA, EFMI or AMIA can address nano-related issues.

Nanotechnology and nanomedicine have important associated issues, like nanotoxicity — both animal and environmental —, and also ethical, cultural, media, entertainment, philosophical and even religious aspects.

There are challenges for linking BMI and Nanoinformatics objectives, methods and tools that can be shared, exchanged and reused. Examples include databases, informatics tools, ontologies (biomedical and nano), services, etc.
World-Wide Scope of ACTION-Grid: challenges for future international collaborations

The Action-Grid project is funded by the European Commission under the FP7
Action-Grid: a finally (hopefully) coherent global, scientific vision

The Action-Grid project is funded by the European Commission under the FP7

Victor Maojo
Medline: 5 (+1) papers retrieved with the term “Nanoinformatics”

   PMID: 20113825
   Related citations

   PMID: 19811635
   Free PMC Article
   Related citations

   PMID: 19745461
   Related citations

   PMID: 19745412
   Related citations

   PMID: 18993444
   Related citations

The Action-Grid project is funded by the European Commission under the FP7
The Action-Grid project is funded by the European Commission under the FP7
And the sixth one is coming...

In press in *Methods of Information in Medicine*
Research topics at the UPM group

Nanoinformatics: a challenging research context, where former experiences can be applied

Novel idea (Nanoinformatics), a (possible) new discipline linked to Biomedical Informatics and Nanomedicine, with almost no previous publications at all

Amazing number of related problems to Biomedical Informatics, from an informatics perspective, with deep differences but also similarities
Challenges for Medical Informatics /Bioinformatics interactions
(Maojo and Kulikowski, JAMIA, Nov. 2003)
Our approach to clinical and -omics (heterogeneous) database integration
### Mapping schema

<table>
<thead>
<tr>
<th>Physical DB</th>
<th>Physical schema</th>
<th>Mapping relations in XML</th>
<th>Virtual schema</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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</table>

#### Table 1
- Attribute 1.1
- ... Attribute 1.M

#### Table 2
- Attribute 2.1
- ... Attribute 2.M

#### Table N
- Attribute N.1
- ... Attribute N.M

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#### Domain ontology

- Concept 1
- Concept 2
- Concept 3
- Concept K

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- Rel. 1
- Rel. 2
- Rel. 3
- Rel. L

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Victor Maojo
Homogenization model
Mapping tools
Clinical and Genomic database integration
Expanding to integration of structured and non-structured sources (ONTOFUSION)
Results
Applications: integration of structured and non-structured sources (ONTOFUSION)

- Unified Model
  - 257 concepts.
  - 106 hierarchical relationships
  - 425 “ad-hoc” relationships
Automatic Extraction of Resources’ Information from the literature (like PubMed & PMC)

Public Open Source BioMedical Informatics Resources Inventory
The Analysis process

Structure
(dive in sections the input paper)

Analysis
(lexical and morphological features and stemming)

Name and functionality

Classification
(extract the category)
How to build the Resource Knowledge Base
Towards a bioinformatics resourceome

**BIRI: A new method for the automatic discovery and indexing of bioinformatics references from the literature, designed to create a repository of resources**
Expanding the work on text mining to other Bioinformatics topics
Expanding research directions towards nano issues (UPM)

- Creating an inventory of nanobiomedical resources (towards a “Nano Resourceome”)
- Text mining methods for extracting information from the literature and link them to augmented electronic health records (EHRs)
- A new approach for building nano-taxonomies based on quantitative and graphical information of nanoparticles
- Linking heterogeneous databases, including biomedical and nano-related information
An Inventory of Nanoresources (primarily reported at KES 2008)

• Currently being developed at our group

• Provides detailed information on different nanoparticles/nanodevices/nanomaterials/tools
  – Morphology
  – Drug-delivery- related information
  – Nanotoxicology information
  – Informatics Tools
  – Relevant Publications

• All the information is automatically extracted from the literature using methods and tools borrowed from BMI
The Toxicity Searcher

- A literature retrieval system linking nanoparticles/nanomaterials to different anatomical locations
- Useful to retrieve papers dealing with drug delivery and nanotoxicity
- An application that relates ontologies from the BMI and Nanoinformatics fields
Research approach

- To create a system to retrieve documents about nanoparticles, their medical application, functionality and toxicity

- To build a literature retrieval search engine
- To create a system to generate and manage documental indexes
- To create a service to access information
Patient-based Biomedical Literature Retrieval

• Open source browser extension, a plug-in to connect nano-related information from to medical records

• EHR locally parsed using NLP techniques to identify relevant MeSH terms

• Automatic queries are generated regarding:
  – Pathology
  – EHR MeSH Terms
  – MeSH Qualifiers
  – Information about nanoparticles and secondary effects
BIOINFORSALUD 2009

BIOINFORSALUD 2009 is the International Symposium on Research in Grid/Nano/Bio/Medical Informatics.

It will be held on Monday 16th of March 2009 in the Palacio de Congresos de la Castellana - Madrid

The symposium registration is FREE and it will be done in the site of the conference (online registration is NOT available).

A Nanoinformatics conference held in Madrid in 2009, part of ACTION Grid