

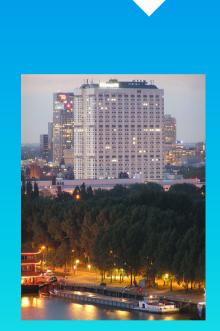
The Erasmus Computing Grid



Building a Super-Computer

for *Free*

Prof. U.D. Dr. Tobias A. Knoch



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A. Abuseiris, R. de Graaf, Michael Lesnussa

with

Biophysical Genomics and Erasmus Computing Grid, Cell Biology & Genetics, Erasmus MC

The Erasmus Computing Grid

The largest desktop grid for the biomedical research and care sectors with now ~13 Tera FLOPS and a potential ~50 Tera FLOPS and ~15,000 desktops, at two city wide institutions: the Hogeschool Rotterdam and the Erasmus Medical Center.



Research:

- ***** genomic and proteomic analysis
- epidemiology
- image analysis, e.g. Applied Molecular Imaging (AMI)

Education:

- ***** training of the coming grid generation of IT specialists
- developing new concepts for grid computing

Diagnostics:

- ✤ clinical image and data analysis
- ✤ operation planning and operation support

Industry:

brokerage of computing resources

Dedicated and Secured!

Erasmus Computing Grid

ECG Projects and Users

The projects and users currently run on the ECG are mainly basic research and application development in the biological and medical areas. Currently there are ~15 projects and ~10 users of the ECG with large expansion already in sight.

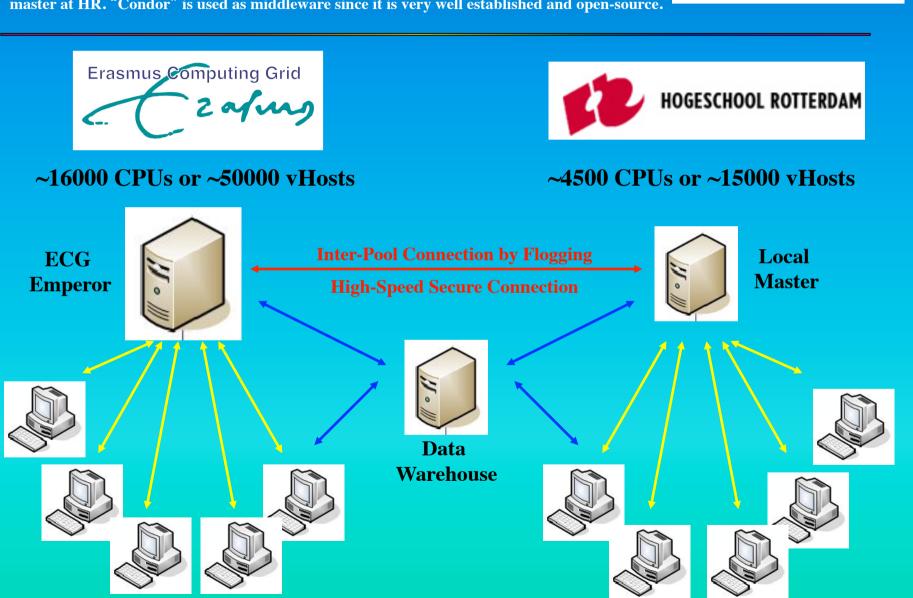


The ECG is one of the few grids on this level of complexity !

Image Analysis	->	Dept. Medical Informatics
DNA Sequence Correlation	->	Dept. Cell Biology & Genetics
Genome Duplication Analysis	->	Dept. Cell Biology & Genetics
Epidemiology studies	->	Dept. Public Health
CT Image Analysis	->	Dept. Internal Medicine
Structural Genome Simulations	->	Dept. Cell Biology & Genetics
Protein Motive Patterns	->	Dept. Urology
Mass Spektrometre Analysis	->	Center for Biomics
Chip & Sequencing Analysis	->	Center for Genomics
Genome Wide Association Studies	->	Dept. Internal Medicine
Protein Structure Prediction	->	Dept. Cell Biology & Genetics
Diffusion of Molecules	->	Dept. Pathology
Microscopic Image Analysis	->	Dept. Microscopy & Cell Biology

ECG Basic Grid Structure

The ECG consists of the computer pools of the Erasmus MC and the Hogeschool Rotterdam. The client computers are controlled by the general ECG Emperor of the grid at EMC and a local master at HR. "Condor" is used as middleware since it is very well established and open-source.



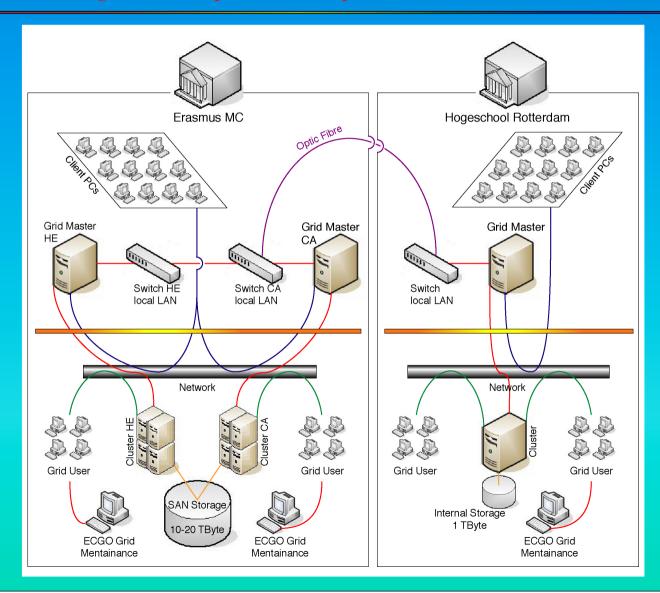
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ECG - Infrastructure

The new infrastructure of the ECG will consist of a dedicated architecture respecting client, user and management security and efficiency in respect to the fact that the ECG is one of the largest grids in the world with the highest possible degree of complexity.



The new ECG infrastructure guaranties the exploitation of the capabilities to the maximum !



MediGRID and Services@MediGRID

MediGRID and Services@MediGRID operate the national biomedial research and care cluster-grid within the national German D-Grid initiative and integrate various disciplines, institutions, and states throughout Germany.



Module Coordination:

coordination of the distributed office

Module Resource Integration:

***** sharing of the integrated resources

Module Middleware:

✤ grid technical virtualization

Module Ontology Tools:

ontology development for grid user projects

Module BioMedical Informatics:

user projects in biomedical research

Module Clinical Imaging:

✤ user projects in clinical imaging

Module Clinical Research:

user projects in general clinical research

Module e-Science:

general research on e-grid science

Services@MediGRID:

services towards MediGRID

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Large-Scale Resource Sharing in IT:

The *Inverse* Tragedy of the Commons



The grid phenomenon and its implications are similar complicated to the ecology/climate/ environmental challenge!

The Tragedy of the Commons:

=> A resource belonging to all and being on limited demand is overexploited / destroyed by the users due to responsibility diffusion!

<= transforms into =>

:The Inverse Tragedy of the Commons

A Resource belonging to all and being in affluent availability on limited demand is <= underexploited by potential users due to responsibility diffusion !!!!!

Similarity: Renewable Energy Resources The grid challenge lies in the e-Social embedding of grid phenomenons:

- Micro-Social: the sharing attitude and socialization of the individual.
- Macro-Social: the organization culture of the embedding institution.

Autopoietic Social Sub-Systems:

The Grid Challenge of Integration



The social systems theory by Niklas Luhmann (1927-1998) based on the autopoietic concept of Humberto Maturana and Francisco Varela (1946-2001) is so far the most advanced social systems theory existing to describe the complexity of grid implementation.

The Social Sub-Systems Involved:

- Religion
- ✤ Education
- ✤ Science => currently grid involves only considerably => SCIENCE
- Art
- ***** Economy
- ✤ Jurisdiction
- Policy

:The Autopeitic Tragedy of Social Sub-Systems

The subsystems have their own code of communication and are separated from each other in a way blocking in principle a consistent integration although they form a society with all their contradictions !!!!!

The e-Social challenge lies in the integration of sub-systems towards a working grid society:

- Micro-Sub-Systems: the sub-system stickiness of individuals.
- Macro-Sub-Systems: the integration of institutionalized sub-systems via soft interfaces.

Grid Psychology Erasmus Computing Grid **From Individual to Cultural Risk Management** Grid implementation and social spread is carried first by individuals as with any meme introduced into society: in the focus of the transformation of society to e-Society stands - as always - the balance between potential risk and opportunity. linking grid psychology with autopoietic social sub-systems **The Risk Psycholgy Matrix:** :The Autopoietic Link Individual Security Perception & Risk Acceptance **Genetics & Deep Psychology (C.G. Jung)** Knowledge-Based Security & Risk Acceptance **Education & Science** Incidental Security Reaction Behaviour **Economics & Realities** Legal and Political Security Scenarios **Jurisdiction & Politics** Religious & Cultural Security Archetypi **Religion, Art & Culture**

The grid challenge lies in a unified concept addressing the psychology of grid:

- Micro-Risk-Management: the micro-risk in the perception the individual and its emotional well-being.
- Macro-Risk-Management: the macro-risks in the procedural and institutionalization in organizations.

Security of the ECG

One of the major issues concerning grids is to create a security level sufficient for all involved parties as we did for the ECG. The technology, culture and even the psychology of security have been and are treated very seriously by the ECG and are to the highest achievable level guarantying the integrity and privacy of the system and data !

Erasmus Computing Grid

Security Technology

- ✤ system hardening
- ✤ firewalling
- encrypted network communications
- intrusion detection monitoring
- ✤ logging of session
- ***** auditing and testing of applications
- virus/trojan checking of in-/output
- authentication

Security Culture

- trained employees
- ✤ secure programming
- ✤ change management system
- ✤ constant check of procedure
- constant test and training of employees
- ***** transparent management structure
- ✤ transparent infra structure
- ✤ NAN and ISO certification

The highest security level guarantying privacy is just good enough for us. & We still would like to have it better.

e-Human "Grid" Ecology

Overcoming of the "Dare-To-Share" Attitude



The success of grid is based on a sustainable grid ecology within the e-Society, i.e. the e-Human Ecology of Grid reaches a equilibrated space within the integration of grid psychology with autopoietic e-Social sub-systems. Human Ecology first evolved in Chicago in the 1920's in the area of city development by Robert Park (1864-1944) and Ernest Burgess (1886-1966).

The Definition of e-Human "Grid" Ecology:

"Under c-Human "Grid" Ecology we understand the complete science of the relationships of grid to the surrounding environment to which we can count all conditions of existence in the widest sense."¹

¹ Haeckel, E., Generelle Morphology der Organismen, Berlin, Band 2, Allgemeine Entwicklungsgeschichte, p. 286, 1866.

² Haeckel, E., Natürliche Schöpfungsgeschichte, 9. Auflage, Berlin, p. 793, 1898

(e-Human "Grid" Ecology "is) ...the relationship between grid and all other e-Social systems." ²

The solutions of the grid challenge on the operational layer are addressed by:

• Micro-Operationality: the participative integration of fundamental IT application of major individual users complying with the psychology of grid in an e-Human Ecology manner.

Macro-Operationality: the set-up of an open and sustainable management structure complying to all the autopoietic e-Social sub-systems in an e-Human Ecology manner.

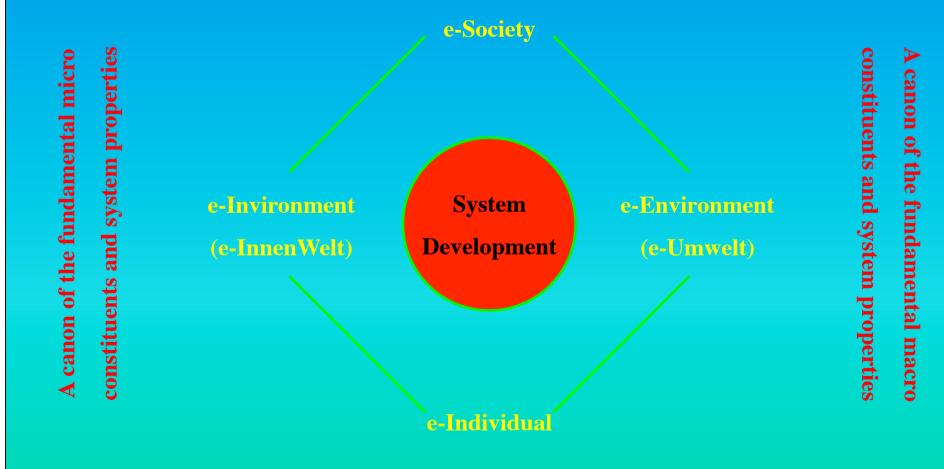
The Curriculum of e-Human Ecology

Curricula of the canon and grammar of e-Human Ecology need to contain the further developed classic contents of the human ecology rectangle as well as the knowledge and understanding of the special aspects of e-Life and a-Life.

nderstanding of the special aspects of e-Life and a-Life.

Erasmus Computing Grid

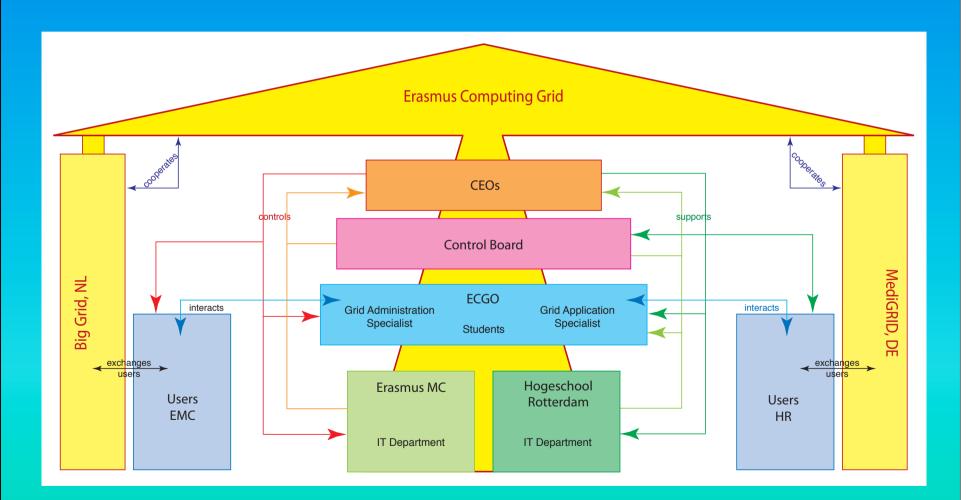
The classic human ecology triangle is transformed into the *human ecology rectangle*, to complete the circle for creation and dependencies for a curriculum canon and grammar!



ECG - Management

To guaranty the integrity and efficiency of the ECG, a dedicated management structure has been put in place with corresponding checks and balances. The organization is made such, that also collaborations with other grids as e.g. the Dutch Big-Grid, the German nationwide MediGRID / D-Grid, or other European Grids as EGEE, EDGES can be exploited most efficiently.

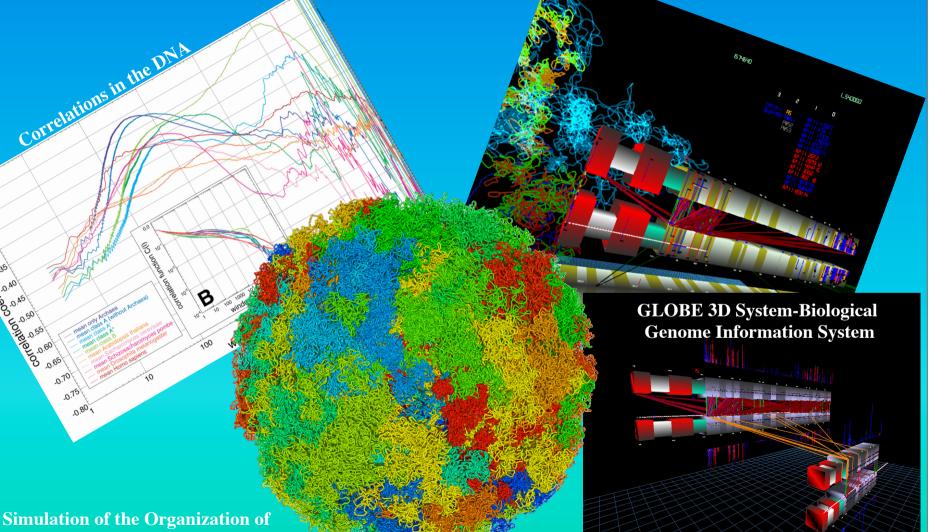




The Happy End - Profits Sharing the Commons

Both the Erasmus Computing Grid and the MediGRID/Services@MediGRID examples show that the IT challenges mankind faces in the biomedical research and care sectors can be successfully approached by exploitation of the commons by e-Human "grid" Ecology means.





an entire Human Cell Nucleus

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The Erasmus Computing Grid

Building a Super-Computer for Free

Knoch, T. A., Abuseiris, A., de Graaf, R., Lesnussa, M. & Grosveld, F. G.

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Abstract

Today advances in scientific research as well as clinical diagnostics and treatment are inevitably connected with information solutions concerning computation power and information storage. The needs for information technology are enormous and are in many cases the limiting factor for new scientific results or clinical diagnostics and treatment. At the Hogeschool Rotterdam and the Erasmus MC there is a massive need for computation power on a scale of 10,000 to 15,000 computers equivalent to ~20 to ~30 Tflops (10^{12} floating point operations per second) for a variety of work areas ranging from e.g. MRI and CT scan and microscopic image anlysis to DNA sequence analysis, protein and other structural simulations and analysis. Both institutions have already 13,000 computers, i.e. ~18 Tflops of computer power, available!

To make the needed computer power accessible, we started to build the Erasmus Computing Grid (ECG), which is connecting local computers in each institution via central management systems. The system guaranties security and any privacy rules through the used software as well as through our set-up and a NAN and ISO certification process being under way. Similar systems run already world-wide on entire institutions including secured environments like government institutions or banks. Currently, the ECG has a computational power of \sim 5 Tflops and is one of or already the largest desktop grid in the world. At the Hogeschool Rotterdam meanwhile all computers were included in the ECG. Currently, 10 departments with \sim 15 projects at the Erasmus MC depend on using the ECG and are preparing or prepared their analysis programs or are already in production state. The Erasmus Computing Grid office and an advisory and control board were set-up.

To sustain the ECG now further infrastructure measures have to be taken. Central hardware and specialist personal needs to be put in place for capacity, security and usability reasons for the application at Erasmus MC. This is also necessary in respect to NAN and ISO certification towards diagnostic and commercial ECG use, for which there is great need and potential. Beyond the link to the Dutch BigGrid Initiative and the German MediGRID should be prepared for and realized due to the great interest for cooperation. There is also big political interest from the government to relieve the pressure on computational needs in The Netherlands and to strengthen the Dutch position in the field of high performance computing. In both fields the ECG should be brought into a leading position by establishing the Erasmus MC a centre of excellence for high-performance computing in the medical field in respect to Europe and world-wide.

Consequently, we successfully started to build a super-computer at the Hogeschool Rotterdam and Erasmus MC with great opportunities for scientific research, clinical diagnostics and research as well as student training. This will put both institutions in the position to play a major world-wide role in high-performance computing. This will open entire new possibilities for both institutions in terms of recognition and new funding possibilities and is of major importance for The Netherlands and the EU.

Corresponding author email contact: TA.Knoch@taknoch.org

Keywords:

Genome, genomics, genome organization, genome architecture, structural sequencing, architectural sequencing, systems genomics, coevolution, holistic genetics, genome mechanics, genome statistical mechanics, genomic uncertainty principle, genome function, genetics, gene regulation, replication, transcription, repair, homologous recombination, simultaneous co-transfection, cell division, mitosis, metaphase, interphase, cell nucleus, nuclear structure, nuclear organization, chromatin density distribution, nuclear morphology, chromosome territories, subchromosomal domains, chromatin loop aggregates, chromatin rosettes, chromatin loops, chromatin fibre, chromatin density, persistence length, spatial distance measurement, histones, H1.0, H2A, H2B, H3, H4, mH2A1.2, DNA sequence, complete sequenced genomes, molecular transport, obstructed diffusion, anomalous diffusion, percolation, long-range correlations, fractal analysis, scaling analysis, exact yard-stick dimension, box-counting dimension, lacunarity dimension, local nuclear dimension, nuclear diffuseness, parallel super computing, grid computing, volunteer computing, Brownian Dynamics, Monte Carlo, fluorescence in situ hybridization, chromatin cross-linking, chromosome conformation capture (3C), selective high-resolution highthroughput chromosome interaction capture (T2C), confocal laser scanning microscopy, fluorescence correlation spectroscopy, super resolution microscopy, spatial precision distance microscopy, auto-fluorescent proteins, CFP, GFP, YFP, DsRed, fusion protein, in vivo labelling, information browser, visual data base access, holistic viewing system, integrative data management, extreme visualization, three-dimensional virtual environment, virtual paper tool.

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