International Tutorial INFOCOMP 2012

Decision Making and High End Computing

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Dr. rer. nat. Claus-Peter Rückemann[1,2,3]

[1] Leibniz Universität Hannover, Hannover, Germany
[2] Westfälische Wilhelms-Universität Münster (WWU), Münster, Germany
[3] North-German Supercomputing Alliance (HLRN), Germany

ruckema(at)uni-muenster.de

Contents

What is the tutorial about?

Directions:

- Is High End Computing a *solution* for decision making?
  No.
- Is decision making a *solution* to be used with High End Computing?
  No.
- Will the *goal* be computer-assisted decision making?
  No.

a) Decision making is the base for any process.
b) Decision making is process and result itself.

During the following discussion we will see (selected) aspects of decision making and what it can mean for High End Computing.

It is intended to have a live discussion and feedback on the consequences for various topics.

Aspects and Challenges

Focus:

Increasing the overall long-term efficiency of

- gathering and using information, knowledge and computing,
- scientific research,
- related application scenarios,
- respecting the interests of users and disciplines, services, and providers of resources.

Theory and Practice

Aspects:

- Learn from history and failures.
- Motivation.
- Processes.
- Techniques.
- Knowledge.
- Overview of High End Computing (HEC).
- Consequences for participated parties.
- Consequences for selected application scenarios.

Archaeology and History

Classical, medieval, modern, . . .

Heron of Alexandria: (greek antique, "Steam Ball")
$\Longrightarrow$ "entertainment" but **not used as technology**.

Isidore of Seville: (encyclopedic, broad documentation)
$\Longrightarrow$ end of medieval phase, **not further used**.

Polyhistor: (Martin Vogel, broad knowledge)
$\Longrightarrow$ broad base, **not further used**.

In percentage we nearly know nothing about the past.

- Ancient and historical objects are mostly lost.
- Ancient and historical documentation is mostly lost.
- Ancient and historical technology is not fully understood.
- Context of past applications is not available.

Way (not) to go: Delegation Principle

What others do: “Experts say: Best practice is for theory.”

Let us take a look on what a virtual, “effective” institution will do.

“N”ewtoneless
“U”niversity
“T”echnology
“S”ervice

NUTS set up, to ”accelerate and shorten” processes:

- **Executive chairing** in-house group,
- **Administrative expert** in-house group,
- **Technical delegation** somewhere group.

NUTS define **in-house** and nice to have:

- Good and best practice,
- Experiences,
- Knowledge (“present one”).

NUTS state the development idea:

- **Structures can be kept** when restructuring,
- **Quality** of Service **is definable**,
- **Hierarchy is on top** of expertise.

Way to go: Cultural and Technological Development (Motivation)

Knowledge base:

Knowledge transfer is essential.

Over generations of objects and subjects, this requires:

- Knowledge recognition (expertise).
- Knowledge documentation, for any aspect of nature and society (sciences, literature, technical descriptions, tools, cultural heritage, mythology, songs, media, ...).
- Long-term means.

Decision Making

Basics of Decision Making ("DM")

Decision making is the fundamental base for any process as well as decision making is a process and result itself.

Nevertheless it is very common

- … to have deficits in decision making processes.
- … to underestimate the value of knowledge creation.
- … to have opposition due to historical and social development.

Aware of!

- No decision is an influence to the "selection", too!
- To shorten planned decision making processes means significant interaction.

Introduction to Decision Making

What we can learn from others (references):

http://www.cartoonstock.com/directory/d/decision-making.asp
http://www.decision-making-solutions.com/management_cartoons.html
http://search.dilbert.com/comic/Decision%20Making

--- ABOVE EXAMPLES FOR DISCUSSION LEFT OUT HERE ---

About Decisions

Lemma 1:

- **It is easy to do any decision without expertise.**

Lemma 2:

- A decision (making process) should be **fast and perfectly correct**.

  In case a decision cannot be fast **and** perfect,
  it should be fast **or** perfect.

  In **no** case should a decision be slow and wrong.

Base for Decision

Essential relation:

Decision making! $\Longleftrightarrow$ **Selection making!**

Classics: Ask for Decision

. . . prominent YES or NO decision example:

(Y/N)?

Problem Analysis

Description:

- Performance analysis (current status / resulting status),
- Problem / target identification (e.g., deviations from performance standard, causes, change of distinctive feature),
- Problem / target description,
- Distinguishing marks between what has been effected by a cause and what has not,
- Deduction of causes from relevant changes found with the problem analysis (identification),
- Cause to a problem is most likely the one that exactly explains the sum of facts.

Example Decision Making Process

Description:

- Establishing the objectives,
- Classification of objectives,
- Place classified objectives in order of importance,
- Development of alternative actions,
- Evaluation of alternatives against all the objectives,
- The tentative decision is that alternative being is able to achieve all the objectives,
- Evaluation of the tentative decision for possible consequences,
- Take decisive actions, take additional actions (prevent adverse consequences from becoming problems)
- Start problem analysis and decision making process iteratively,
- Steps for decision model in order to determine an optimal production plan and reduce conflict potential.

Decision Planning Process

Description:

For best practice, introduce a decision planning process to important decisions in order to result in the following benefits:

1. **Establish independent goals.**
   That means a conscious and directed series of choices.
2. **Aim to a standard of measurement.**
   The measurement should provide information on the distance to the goal.
3. **Convert values to action.**
   The resulting information should be used to support the planning.
4. **Commit limited resources in an orderly way.**
   Planning and commitments for any kind of resources, e.g., staff, money, time.

Example Decision Making Phases

Phases:

Orientation stage: Starting with kick-off or warm-up, exchange with all parties.

Conflict stage: Dispute, arguments, working on common denominators and positions.

Emergence stage: Vague positions and opinions being discussed.

Reinforcement stage: Decision making and justification.

Selected Decision Making Techniques

Techniques:

Rational decision making: List the pro and contra (advantages and disadvantages) of each option. Contrast the costs and benefits of alternatives.

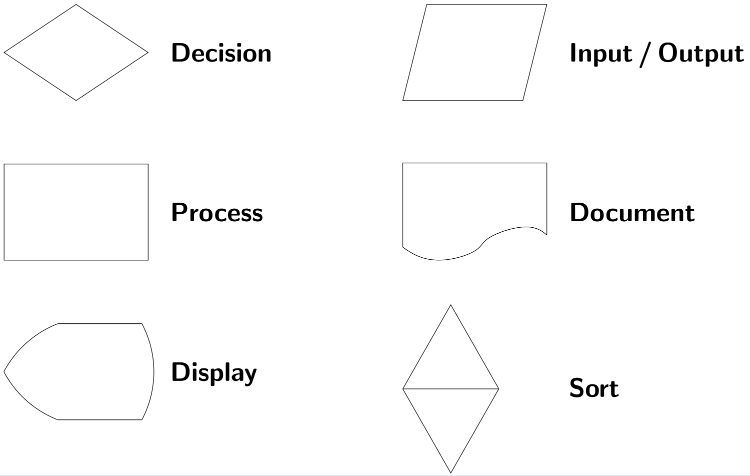
Elimination by aspects: Choosing alternatives by "mathematical psychology". Covert elimination process, comparing the available alternatives by aspects. Choose an aspect and eliminate the alternatives without the aspect. Repeat until one alternative remains.

Simple prioritisation: Choosing an alternative showing the highest probability-weighted utility from all alternatives, resulting from the decision analysis process.

Satisficing: The examination of alternatives is stopped as soon as an acceptable alternative is found.

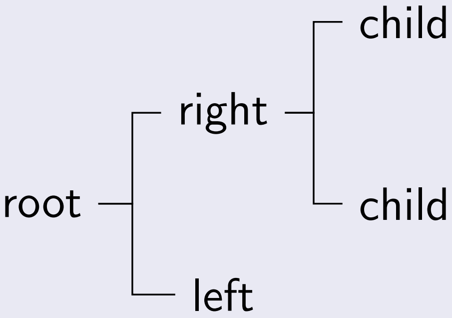
Visualising Flow Basics

Symbols



Trees and Forks

Trees and Forks



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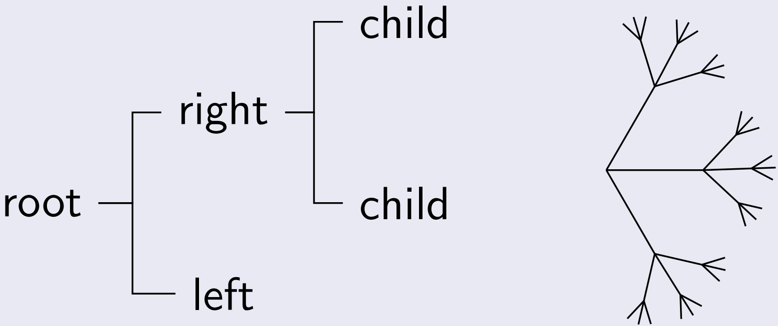

Areas of Automated Application

Commonly no tools with:

- Private,
- Evolution.

Prominent (support only) tools with:

- Environment,
- Catastrophy,
- Geostatistics,
- Military,
- Games,
- Exploration,
- Medicine,
- Traffic,
- Court,
- Contracts,
- Computer,
- Budget,
- Security,
- ...

Areas of Application

Examples for decision systems and support:

- **Environment:**
  - FLODIS: Sustainable Floodmanagement of the Oder river IS.
  - STEWARD: Support Technology for Environmental, Water and Agricultural Resource Decisions.
  - SDSS: Spatial Decision Support System.
  - LANDS: Land Analysis and Decision Support (system).
  - WEDSS: Whole Earth Decision Support System (international).
- **Catastrophy:**
  - WDSS: Warning Decision Support System (oceanography).
- **Geostatistics:**
  - MCDM: Multicriterion Decision Making.
- **Military:**
  - ADA: Applied Decision Analysis.
  - EOTDA: Electro-Optical Tactical Decision Aid.
- **Games:**
  - ...: For example, Chess, mathematical basics, defined alternatives.

Areas of Application and Why is Decision Support Imperfect

Why are there no systems for?:

- Natural sciences fundamentals,
- Informatics development,
- Basic algorithms,
- Geophysical data analysis,
- Computing architectures,
- Hardware systems development,
- ...

Add Forensics to the Decision

Invisible things can make a difference:

```




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Add Forensics to the Decision

Invisible things can make a difference:

```




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The invisible seen here:

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```

The translation is:

```
F
I
R
E
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```

Understanding Knowledge

Where knowledge is ...

Knowledge is created from a subjective combination of different attainments as there are intuition, experience, information, education, decision, power of persuasion and so on, which are selected, compared and balanced against each other, which are transformed and interpreted.

And the consequences ...

Authentic knowledge therefore does not exist, it always has to be enlived again. Knowledge must not be confused with information or data which can be stored. Knowledge cannot be stored nor can it simply exist, neither in the Internet, nor in computers, databases, programs or books.

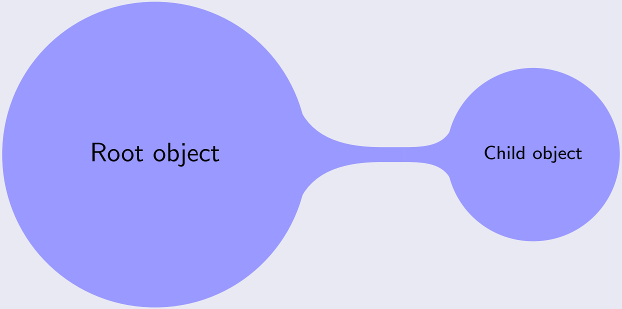
Knowledge and Application

Processes

- Knowledge base creation,
- Knowledge base transfer over generations,
- Documentation of requirements respective algorithms,
- Documentation of context respective architectures,
- Usage development within tender processes.

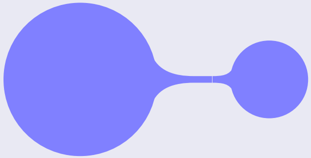
Objects and Relations

Objects and Relations



Object, Relations, and Quality (Mindmapping)

Quality of Relations



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Quality of Relations

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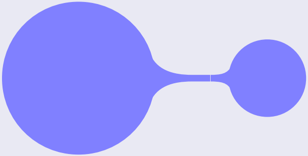
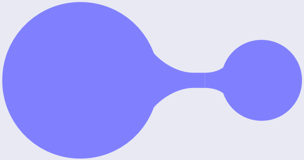
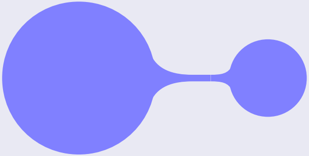
Quality of Relations





Quality of Objects



Object, Relations, and Quality (Mindmapping)

Quality of Relations

Quality of Objects

Knowledge: Prejudice and getting the right meaning

Wrong terms can be very persistent:

- Sunrise (earth is flat?),
- Sunset (from dusk till dawn?),
- Malaria (and prejudice is ahead of scientific results?).
- ...

Knowledge: Perception

Examples

- Depiction, traffic signs and their description different.
- Companies do try critical products in countries with reduced privacy perception.
- Overall personal security will mean insecurity for society.
- Color perception is different by society.

Description

- "*Standardisation*" and "*internationalisation*".
- Foreign word "*privacy*".
- Trend for *hidden security*.
- Words for new colors have been *added* to languages and perception.

Knowledge: Cultural Background

International and other differences

- Privacy perception,
- Different terminology,
- Legal regulations,
- Legal frameworks.

Knowledge: Language and Small Things

Even off-topic items can make a difference (not only in Harvard):

Small things can completely change the meaning without changing a word!

- Tweetie, Tom and Jerry do have different opinions.
- Tweetie, Tom, and Jerry do have different opinions.

Knowledge: Language and Small Things

Even off-topic items can make a difference (not only in Harvard):

Small things can completely change the meaning without changing a word!

- Tweetie, Tom and Jerry do have different opinions.
- Tweetie, Tom, and Jerry do have different opinions.

- Fishes, mammals and birds are three different kind of genus.
- Fishes, mammals, and birds are three different kind of genus.

Knowledge: Symbolisation and Language

Classical one: Who said this?

+

+

Knowledge: Symbolisation and Language

Classical one: Who said this?

 +  + 

Easier, English terms: Egg + Box + Girl.

Knowledge: Symbolisation and Language

Classical one: Who said this?


+

+


Easier, English terms: Egg + Box + Girl.

Hint: Try in different languages.

Selection on Structure, Content, Context, and Computing

Theory and practice

- Structural deficits.
- Content can be described and even signed to a certain extend.
- Context cannot be handled to a comparable extent. (Users can sign a PDF document, but what about signing it's context?)
- Long-term issues are mostly out of sight. (What will signature validity mean to archiving and reuse?)
- What does this in general mean to long-term knowledge-based processes?

Knowledge, Documentation, and Classification

Universal Decimal Classification (UDC)

The Universal Decimal Classification (UDC) is a general plan for the knowledge classification. UDC is a hierarchical decimal classification system that divides the main knowledge fields into 10 main categories (numbered from 0 to 9). Each field is in turn divided into 10 subfields, each subfield is inturn divided into 10 subsubfields, and so on. A more extensive classification code in general describes a more specific subject.

Faceted and multi-disciplinary context

"Facetted" and "multi-disciplinary" is synonym to the Universal Decimal Classification (UDC), `http://www.udcc.org`. UDC uses a "(...)" notation in order to indicate aspect. These descriptions are called facets. In multi-disciplinary object context a faceted classification does provide advantages over enumerative concepts.

The classification deployed for a universal documentation must be able to describe any object with any relation, structure, and level of detail. Objects include any media, textual documents, illustrations, photos, maps, videos, sound recordings, as well as realia, physical objects such as museum objects.

Documentation and Form

Form (UDC, excerpt, English)

```
(0.02)     Documents according to physical, external form
(0.03)     Documents according to method of production
(0.034)    Machine-readable documents
(0.04)     Documents according to stage of production
(0.05)     Documents for particular kinds of user
(0.06)     Documents according to level of presentation and availability
(0.07)     Supplementary matter issued with a document
(0.08)     Separately issued supplements or parts of documents
(01)       Bibliographies
(02)       Books in general
(03)       Reference works
(04)       Non-serial separates. Separata
(041)      Pamphlets. Brochures
(042)      Addresses. Lectures. Speeches
(043)      Theses. Dissertations
(044)      Personal documents. Correspondence. Letters. Circulars
(045)      Articles in serials, collections etc. Contributions
(046)      Newspaper articles
(047)      Reports. Notices. Bulletins
(048)      Bibliographic descriptions. Abstracts. Summaries. Surveys
(049)      Other non-serial separates
(05)       Serial publications. Periodicals
(06)       Documents relating to societies, associations, organizations
(07)       Documents for instruction, teaching, study, training
(08)       Collected and polygraphic works. Forms. Lists. Illustrations. Business publ.
(09)       Presentation in historical form. Legal and historical sources
(091)      Presentation in chronological, historical form. Historical presentation.
(092)      Biographical presentation
(093)      Historical sources
(094)      Legal sources. Legal documents
```

Documentation and Language

Languages, natural and artificial (UDC, excerpt, English)

```
=1      Indo-European languages of Europe
=11     Germanic languages
=12     Italic languages
=13     Romance languages
=14     Greek (Hellenic)
=15     Celtic languages
=16     Slavic languages
=17     Baltic languages
=2      Indo-Iranian, Nuristani (Kafiri) and dead Indo-European languages
=21     Indic languages
=29     Dead Indo-European languages (not listed elsewhere)
=3      Dead languages of unknown affiliation. Caucasian languages
=35     Caucasian languages
=4      Afro-Asiatic, Nilo-Saharan, Congo-Kordofanian, Khoisan languages
=5      Ural-Altaic, Palaeo-Siberian, Eskimo-Aleut, Dravidian and Sino-Tibetan
=521    Japanese
=531    Korean
=541    Ainu
=6      Austro-Asiatic languages. Austronesian languages
=7      Indo-Pacific (non-Austronesian) languages. Australian languages
=8      American indigenous languages
=81     Indigenous languages of Canada, USA and Northern-Central Mexico
=82     Indigenous languages of western North American Coast, Mexico and Yucatán
=84     Ge-Pano-Carib languages. Macro-Chibchan languages
=85     Andean languages. Equatorial languages
=86     Chaco languages. Patagonian and Fuegian languages
=88     Isolated, unclassified Central and South American indigenous languages
=9      Artificial languages
=92     Artificial languages for use among human beings. Int. aux. languages (interlanguages)
=93     Artificial languages used to instruct machines. Programming/computer languages
```

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Documentation and Computer Science

Computer Science and Technology (UDC, excerpt, English)

```
004.2        Computer architecture
004.3        Computer hardware
004.31       Processing units. Processing circuits
004.33       Memory units. Storage units
004.382.2    Supercomputers
004.4        Software
004.414      Definition phase of system and software engineering
004.414.2    Computer system analysis and design
004.414.3    Software requirements analysis
004.415      Development phase of system and software engineering
004.415.5    Software quality assurance
004.416      System and software maintenance
004.42       Computer programming
004.423      Syntax and semantics of programs
004.43       Computer languages
004.43.C     C programming language
004.43.C++   C++ programming language
004.43.FOR   FORTRAN programming language
004.431      Low level languages
004.432      High level languages
004.451      Operating systems
004.62       Data handling
004.7        Computer networks
004.71       Computer communication hardware
004.738.5    Internet
004.774      HTTP application. World Wide Web in the strict sense. Web resources / content
004.82       Knowledge representation
004.89       Artificial intelligence application systems. Intelligent knowledge-based systems
004.932      Image processing
004.94       Simulation
```

Creating Groups and References

UDC Operations

Standardised operations with UDC are, e.g.,

Operation	Symbol
Addition	"+"
Consecutive extension	"/"
Relation	":"
Subgrouping	"[]"
Non-UDC notation	"*"
Alphabetic extension	"A-Z"

besides place, time, nationality, language, form, and characteristics.

Examples

```
(0.02/.08)                Special auxiliary subdivision for document form
=1/=8                     Natural languages
=1/=2                     Indo-European languages
=9/=93                    Artificial languages
59+636                    Zoology and animal breeding
(7):(4)                   Europe referring to America
311:[622+669](485)        statistics of mining and metallurgy in Sweden
004.382.2:[902+550.8] CPR Supercomputers ref. to archaeology and geosciences, CPR author
```

Obstacles

Obstacles reducing success and efficiency with the processes

- Time consumption (e.g., staff, project timelines),
- Documentation (e.g., low percentage of reusability),
- Classification (e.g., limited views),
- Tools (e.g., changing repeatedly),
- "Standards" (e.g., changing repeatedly),
- ...
- Different perception of goals, strategies, and completeness.

Complementary

Structure

- Must be able to contain and refer to any content.

Full text and keywords

- Groups, regular expressions, search functions, ...

Soundex

- Algorithm for calculating codes from text strings, representing phonetic properties.
- Originally only used for names, in Englisch.
- The original algorithm mainly encodes consonants.
- Goal is to encode homophones with the same representation, minor spelling differences do result in the same representation.
- Various modifications for any language, topics, any kind of words, support for many programming environments.

Helpers – What you always need

Staff and resources

- **Quantity of Staff and Resources depends.**
- **Quality of Data (QoD) can optimise requirements for staff and resources.**

Examples for Multi-Disciplinary Use

Multi-disciplinary status

- Medical Informatics,
- Geoinformatics,
- Legal Informatics,
- Geoforensics,
- Archaeology and Digital Archaeology,
- Medical Geology,
- Digital Forensics,
-
- ...

Archaeology

Content

- Overall information is widely distributed.
- Sometimes very difficult and a long lasting challenge not only to create information but even to get access to a few suitable information sources.
- Digital and realia objects.
- All participating disciplines, services, and resources have to be prepared for challenges as big data, critical data, accessibility, longevity, and usability.

. . . digital and long-term issues

- Even best practice cannot preserve realia and data context.
- Context is often destroyed.
- Long-term issues.
- Currently neither a standard being used for one discipline nor an international standard.
- . . .

Archaeology

Goal

- Need integrated knowledge base for archaeological and natural sciences.
- Necessary to collect data from central data centers or registers. Examples archaeological and geophysical data:
  - North American Database of Archaeological Geophysics (NADAG).
  - Center for Advanced Spatial Technologies (CAST).
  - Archaeology Data Service (ADS).
  - Records as with Center of Digital Antiquity.
  - Records as with the Digital Archaeological Record (tDAR).
- An integrated "Collaboration house" framework is designed to consider all aspects and to handle any kind of object.

Medicine

... digital and long-term issues

- Documentation.
- Natural sciences data integration?
- Catalogs (International Classification / Catalog of Diseases, ICD).
- Classification (Universal Decimal Classification, UDC).
- Data security.
- Privacy.
- Anonymity.
- ...

Libraries

. . . digital and long-term issues

- Documentation.
- Catalogues.
- Classification (Universal Decimal Classification, UDC). Today about 150000 libraries are using UDC classification and implementing information systems herewith.
- Referencing.
- Search.
- Licensing.

High End Computing

Basics and prerequisites

- Real goals. Define the goals, different views.
- Need for basic understanding and knowledge base for HEC.
- Prominent HEC and collaboration aspects decision making processes are necessary for.
- Separate the topics (disciplines, resources, ...).
- Gather the real requirements for the analysis.
- Up-to-date resource policies in theory and practice.
- Interesting fields of application are processes within disciplines.
- Future deployment of integration and classification with components of complex systems.

Decisions and Computing

Components (all areas, no sort order):

- Architecture,
- Operating System,
- Applications,
- Programming languages,
- Tools,
- System modeling,
- Vendors,
- Strategy,
- Targets,
- Staff,
- Operation,
- Services,
- System management,
- Complex licensing,
- Policies,
- Governance,
- . . .

Decisions and High End Computing

Components (all areas, no sort order):

- Components (all areas) with strong focus on
- Applicability, efficiency,
- Architecture applicability,
- Operating System applicability,
- Efficient applications,
- Programming languages,
- Tools,
- System modeling,
- Vendors,
- Strategy,
- Targets,
- Staff,
- Operation,
- Services,
- System management,
- Complex licensing,
- Policies,
- Governance,
- ...

High Performance Computing / Advanced Scientific Computing

Overview

- Requirements
  - Fast CPU.
  - Parallel processing.
  - Large memory.
  - Fast I/O.
- Hardware / resources
- System / software / configuration
- Applications
- Examples?

- High Performance Computing. Base, parallel developments are integrated for HPC.
- Cluster computing, optimised utilisation of heterogeneous resources (Condor).
- Cloud and Grid Computing (e.g., Globus Toolkit, UNICORE).

- Cloud and Grid islands: Different companies – different technology and terms.

Architecture and Security

Architecture and Security

- Hardware / Computing.
  - MPP (Massively Parallel Processing). — MPP compute nodes
  - SMP (Symmetric Multi-Processing). — SMP compute nodes
- System software.
  - Operating systems. — Login server, admin server
  - Cluster management. — Management server
  - Storage management. — Storage server
  - File management. — File server
- Networks.
  - InifiniBand for I/O.
  - InifiniBand for Message Passing Interface (MPI).
  - NumaLink.
  - Service networks.
- Parallel filesystems (GPFS, Lustre, . . .). — MDS server, OSS server
- Batch system, scheduling, load balancing. (Moab, Torque, . . .). — Batch server
- Accounting . . .
- Data handling, archive / backup. — Archive / backup server
- Optional Grid, Cloud services level.

Best Practice Recommendations

Common ones

- Use abstraction,
- Use standards,
- Use high-level,
- Use modularisation,
- Use process and workflow modeling,
- Consider legal regulations,
- Define policies,
- Iterate processes,
- Implement an independent auditing,
- (consult other best practice, if available),
- . . .

Isolated Approaches

Isolated Approaches in computing:

- Internationalisation,
- Transliteration,
- Syntax unification,
- Semantics,
- ...

Isolated Approaches in programming:

- High level languages,
- Object-oriented paradigms,
- Literate programming,
- Standardisation,
- ...

Intermediate Status

Anyhow, on the current base today:

Has someone seen an implementation that has been done perfect?

Information Technology

Selection processes need to be made for:

- Purpose and usage,
- Budget,
- Components,
- Content and data security,
- Science, research, and staff,
- Policies,
- Access,
- Security,
- Operation and staff,
- ...

Selection Process

For which purpose do we need a selection process regarding:

- Resources,
- Information Mining and Management,
- Broadband networks,
- Fibre channel networks,
- Mobile Services,
- ...

Cloud and Grid Islands

Terms, brands, names (historical excerpt)

- Sun:
  - Cluster Grids
  - Enterprise Grids
  - Global Grids
- HP:
  - Utility Computing
- IBM:
  - Autonomic Computing, resources, dynamic VO
  - Grid + provisioning via Cloud Computing (SaaS, DaaS, AaaS ...)
- ...

Standard security personnel

Security engineer:

- disciplines: working security, factory security, IT, ...
- *employee of the company*,
- *exclusively honorary function*,
- *shall not be a disciplinary superior*,
- *supports the professional and technical experts* by keeping an eye on security devices and possible threats, perils,
- can *in no case* take the function of a specialist for the security in the disciplines handled.

Filesystems

Categories of filesystems:

Filesystem type	*Examples*
Distributed	NFS, AFS, NCP, CIFS/SMB, XtreemFS, Ceph, Btrfs, HDFS
Shared	SAN, CXFS, GFS, Polyserve, StorNext, QFS
Parallel	GPFS, Lustre, PVFS, IBRIX, OneFS, PanFS, NFS/pNFS

User Management in High End Computing

Basic issues:

- Administration, Authentication, Authorisation, Accounting.
- Full management tool set should be available.
- With individually customised user management the overall system does not get simpler but it can get much more complex!
- Different requirements and conventions in Supercomputing and Grid / Cloud computing.

Present and future concepts of user management:

- Currently no standardised components and no modularisation and separation of data and implementation.
- Currently invasive customisation necessary.
- Future vendor support for standardised interfaces.
- Future centralised and decentralised components and interfaces.

User Management in High End Computing

Available components and status (selection)

- Lightweight Directory Access Protocol (LDAP): Inflexible structure in complex environments.
- Dynamic Host Configuration Protocol (DHCP): For nodes, invasive, can reduce availability.
- Pluggable Authentication Module (PAM): For nodes, invasive.
- Preboot Execution Environment (PXE): For nodes.
- Network File System (NFS): For nodes.
- Batch system and scheduler: Should by itself support the user management and monitoring.
- Shell scripts: In distributed environment error prone.
- Radius / Eduroam: Small number of attributes for diversity of user groups (e.g., no separation of user, employee, consultant)
- Moonshot: Not for productive use, very invasive, special ssh
- Shibboleth: Attributes available but invasive to complex infrastructures and policies special PAM ECP, NSSWITCH, etc., reduced data security level (unqualified, trust-based due to sshd).

User Support for Advanced Scientific Computing in High End Computing

Distributed and bundled implementations:

- Singular, standalone system,
- Cooperation, distributed,
- Alliance, distributed,
- Other.

Benefits (excerpt)

- Support for all disciplines, 365/7/24 via several means of communication.
- Support can be provided for efficient use of resources (HW, SW, compiler, libraries, MPI / OpenMP / others, I/O systems, batch systems, etc.).
- Provisioning and support of SW (commercial and freely available).
- Programming and algorithm support.
- Feedback for the overall community (not only for the providers!).
- Archiving and backup.

Do not promise this if you do not have an excessive and long-term support base!
Support base: quantity and quality, staff, consultants, . . .

Governance and IT-Governance

Information Technology Governance

- IT-Governance is a subset discipline of Corporate Governance focused on IT systems and their performance and risk management.
- http://en.wikipedia.org/wiki/Governance
- http://en.wikipedia.org/wiki/Information_technology_governance

Legal aspects and effects on software development, IT-Governance

Legal aspects and IT-governance

- Rising interest in IT-Governance is partly due to compliance initiatives, as well as the acknowledgment that information technology systems, operation, and projects (e.g., networks, computing, cloud) can be hard to control and can heavily affect the overall performance of institutions and organisations.
- Compliance initiatives:
  - Basel II, Europe.
  - Sarbanes-Oxley Act (SOX), USA.

IT and Information Security, ISO/IEC 27000, 27001, 27002

ISO and IEC

- http://en.wikipedia.org/wiki/ISO/IEC_27000
- http://en.wikipedia.org/wiki/ISO/IEC_27001
- http://en.wikipedia.org/wiki/ISO/IEC_27002
- ...

Legal Issues with High End Computing

Challenges with:

- International collaboration,
- Frameworks and standards,
- Services provisioning,
- License models,
- Software Licenses (core numbers, floating, etc.),
- Not hardware, not software (firmware),
- Third parties,
- Operation,
- Maintenance,
- Non-deniability,
- Security,
- ...

Security

Aspects

- Infrastructure security (power on/off security),
- Information technology security (power on/off security),
- Data security,
- Privacy,
- ...

Categories:

- Scientific security research, encryption, in-silico security,
- Low level security (end user application, end user devices and algorithms),
- Day to day / trivial services and support issues,
- ...

Operating System Protection

Operating System Protection Profile (OSPP)

- Local auditing,
- Crypto-communication,
- Access control,
- Communication packet filtering,
- Security management.

((Practical/theoretical security.))

Data and Content Security

Issues:

- Research – Industry,
- Homomorphic application environments,
- Policies,
- Encryption,
- Signatures,
- Privacy,
- Anti-privacy,
- Plagiarism prevention and detection,
- ...

Content and Plagiarism in Information Science and Technology

Categories:

- Plagiarism prevention.
- Plagiarism detection.

Principal, legal, and technical issues:

- Authors/student work before copyright signed in review.
- Databases of third parties, reliability issues.
- Introduction into databases of third parties.
- Problem with double blind / blind review.
- Removal of references and / or citations.
- Self-plagiarism only for a small extend.
- Graphics cannot be checked.
- Sources checked with and without permission of authors?
- Sources might even not be published by authors.
- Too heterogeneous conditions in practice.
- Very time intensive process for authors, reviewers, editors, and publishers.
- Restrictions due to workflow, widely used procedures and structures.
- ...

Documentation

Aspects

- Trivial documentation,
- Technical and applications' documentation,
- Scientific documentation,
- Structure,
- Classification,
- Re-use.

License Models and Patents

Long-term problems?

- Public Domain,
- Freeware,
- GPL (and derivatives),
- Charityware (vim),
- Postcardware,
- Giftware,
- . . .
- Open Access model, Open Access publishing,
- . . .
- Open Source is trademark but this does not mean products labeled with Open Source are provided without limitations of any kind.
- Bilsky Case.
- Patent Absurdity.

Modeling and applications

Unified Modeling Language (UML)

The Unified Modeling Language (UML) can be used for various purposes with information sciences, software development, and even independent from information sciences, e.g. in economics and business context:

- "business model"
- classes
- messages, objects in their timing sequence
  - coarse overview
  - dynamic
  - parallel processes
  - distributed systems

UML Diagrams

UML Diagrams

- Use-case diagram
- Class diagram
- Package diagram
- Interaction diagram
- State diagram
- Activity diagram
- Implementation diagram

Use-case Diagram, Class Diagram, Package Diagram

Use-case diagram

Diagram: Use-Case

Phase: Requirements, predefinition, application design – building, delivery

Operational area: business processes, common

Use-case Diagram, Class Diagram, Package Diagram

Use-case diagram

Diagram: Use-Case

Phase: Requirements, predefinition, application design – building, delivery

Operational area: business processes, common

Class diagram

Diagram: class diagram

Phase: predefinition, application design – building

Operational area: anywhere, the class diagram is the most important UML diagram.

Use-case Diagram, Class Diagram, Package Diagram

Use-case diagram

Diagram: Use-Case
Phase: Requirements, predefinition, application design – building, delivery
Operational area: business processes, common

Class diagram

Diagram: class diagram
Phase: predefinition, application design – building
Operational area: anywhere, the class diagram is the most important UML diagram.

Package diagram

Diagram: package diagram
Phase: application design – building
Operational area: overall orientation purposes, which classes in which modules. partitioning into sub-projects, libraries, translation units.

Interaction Diagram and State Diagram

Interaction diagram

Diagram: interaction diagram

Phase: Requirements, predefinition, application design – building, delivery

Operational area: shows the message flow an therefore the cooperation of objects in timing sequence.

Special interaction diagrams are:

- Sequence diagram: timing call structure with few classes.
- Collaboration diagram: timing call structure with few messages.

Interaction Diagram and State Diagram

Interaction diagram

Diagram: interaction diagram

Phase: Requirements, predefinition, application design – building, delivery

Operational area: shows the message flow an therefore the cooperation of objects in timing sequence.

Special interaction diagrams are:

- Sequence diagram: timing call structure with few classes.
- Collaboration diagram: timing call structure with few messages.

State diagram

Diagram: state diagram

Phase: Requirements, predefinition, application design – building, delivery

Operational area: presentation of dynamical behaviour

Activity diagram and Implementation Diagram

Activity diagram

Diagram: activity diagram

Phase: predefinition, application design – building

Operational area: various purposes.

Activity diagram and Implementation Diagram

Activity diagram

Diagram: activity diagram

Phase: predefinition, application design – building

Operational area: various purposes.

Implementation diagram

Diagram: Implementation diagram

Phase: predefinition, application design – building, delivery

Operational area: especially for presentation of distributed applications and components; in general: presentation of implementation aspects (translations units, executable programs, hardware structure)

Special implementation diagrams are:

- component diagram: coherence of software.
- deployment diagram: hardware structure.

View: Disciplines

– View: Disciplines –

Requirements

Needs and requirements from disciplines classically are in contrast with how resources and services are managed and operated.

Building services on this base typically polarises interests of participated groups.

From this point of view, most building processes regarding computing environments reveal a very small grade of efficiency.

Disciplines Involvement with High End Computing

Disciplines involvement goals, examples:

- Long-term knowledge creation (results, data, algorithms, computing instructions, etc.).
- Structure of knowledge.
- Reasoning (society and needs).
- Perception (grow with needs).
- Redundancy and availability.
- Formats, portability.
- System architectures.
- Batch-queue configuration.
- Workarounds and science / technology balance.

What does this mean for knowledge resources and transfer?

Infonomics / Information Management

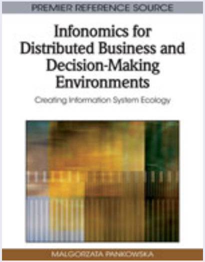
References:

- Infonomics for Distributed Business and Decision-Making Environments
  http://www.igi-global.com/reference/details.asp?ID=34799
- Infonomics Society
  http://www.infonomics-society.org
- Infonomics Internet- and database recherche
  http://www.infoseeking.de
- AIIM Infonomics
  http://www.aiim.org/infonomics/
- Infonomics.nl
  http://www.infonomics.nl
- Infonomics.at
  http://www.infonomics.at
- Infonomics.com.au
  http://www.infonomics.com.au

Infonomics for Distributed Business and Decision-Making Environments

References

C.-P. Rückemann: *Accounting and Billing in Computing Environments*,
in: Infonomics for Distributed Business and Decision-Making Environments:
Creating Information System Ecology, M. Pankowska (ed.),
Business Science Reference, IGI Global, Hershey, Pennsylvania, USA, 2009, ISBN: 978-1-60566-890-1 (hardcover), 421 pages.



http://www.igi-global.com/reference/details.asp?ID=34799

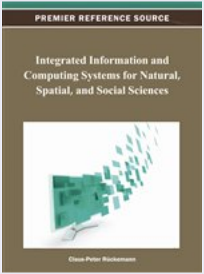
Integrated Information and Computing Systems

References

C.-P. Rückemann (ed.): *Integrated Information and Computing Systems for Natural, Spatial, and Social Sciences*, 21 chapters, IGI Global, Hershey, Pennsylvania, USA, 2012, Premier Reference Source, DOI: 10.4018/978-1-4666-2190-9, ISBN-13: 978-1-4666-2190-9 (hardcover), EISBN: 978-1-4666-2191-6 (e-book).

Topics:

- Integrated Systems, Information, Communication, and Computation
- Collaboration, Frameworks, and Legal Aspects
- Advanced Cognition, Intelligent Systems, and Security Management
- High End Computing, Storage, and Services
- Supercomputing, High Performance Computing, Computing Systems, Energy Efficiency, and Cloud
- Communication, Computation, Advanced Scientific Computing
- Advanced Applications, Modelling and Simulation in Natural Sciences, Geosciences, Medicine
- Big Data Exploration, Visualisation, Education, and Social Media
- Spatial Sciences, Social Sciences, Teaching, Learning, and Digital Media



http://www.igi-global.com/book/integrated-information-computing-systems-natural/67413
http://dx.doi.org/10.4018/978-1-4666-2190-9

View: Services and Developers

– View: Services and Developers –

Provided

In almost all cases the percentage of re-used knowledge over system generations is very small, leading to perpetuous "re-invention" and "re-discussion" for every cycle.

The suggested rate of re-use is below 10 percent.

Compute Portfolio

Services differ by physics and intention, especially:

- **Latencies and bandwidth:** Low segment: Latency 100 μs to several milliseconds (distributed), latency 1–2 μs (local), bandwidth 1.5–4 GB/s (local),
- **Distributed data transfer:** Data transfer for supercomputing is essential with any big (volume) data, physics provide limitation to economical distributed solution.
- **Distributed memory usage:** Shared memory usage for supercomputing is essential with shared memory algorithms, physics provide limitation to economical distributed solution.

HPC IO

High Performance Computing I/O Compute Resource (HPC Center)

- minimal entry level per job (logical AND):
- publicly funded research, no production jobs or industry users
- will be validated that the minimal access requirements are fulfilled and reasonable
- 512 nodes
- 4096 Cores (e.g., Intel)
- maximum: about double nodes and cores
- 3 GB memory usage per core
- already parallelized MPI read/write into 1-1000 files
- extensive and already optimised MPI I/O communication from mostly all cores used (max 1-2 TB per second overall)
- runtime per job 12 hours
- job must be batch system based
- environment fixed, depending on installation
- ssh access only
- programming, compilation, installation by user

HPC

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- publicly funded research, no production jobs or industry users
- will be validated that the minimal access requirements are fulfilled and reasonable
- 512 nodes
- 4096 Cores (e.g., Intel)
- maximum: about double nodes and cores
- 3 GB memory usage per core
- already parallelized MPI read/write into 1-100 files
- extensive MPI compute communication from mostly all cores used
- runtime per job 36 hours
- job must be batch system based
- environment fixed, depending on installation
- ssh access only
- programming, compilation, installation by user

HPC SMP and Shared Memory

High Performance Computing SMP Resource (HPC Center)

- minimal entry level per job (logical AND):
- publicly funded research, no production jobs or industry users
- will be validated that the minimal access requirements are fulfilled and reasonable
- 32 nodes
- 32x8 Cores (e.g., Intel)
- maximum: 2-3 jobs/tasks in parallel
- 512 GB memory usage per job
- OpenMP communication
- runtime per job 12 hours
- job must be batch system based
- environment fixed, depending on installation
- ssh access only
- programming, compilation, installation by user

Cloud and Grid

Cloud / Grid (Provider, Computing Center)

- minimal entry level per job:
- 1-64 nodes
- *n* (Intel or other) cores depending on architecture and provider
- small to medium sized memory usage per core
- small I/O (Giga-Bytes not TeraBytes overall)
- hundreds of cores
- loosely coupled, parallel jobs, task-parallel, moderate MPI parallel
- further services/anything else per-pay that scientific HPC Centers might not provide
- efficiency requirements depend on provider and customer agreements
- middleware and access depending on provider

View: Providers

– View: Providers –

Requirements

- Economical environment.
- Efficient operation.
- Sustainable investment.
- Defined policies.
- ...

High End Systems

More than a tool? Always think of knowledge:

- Content.
- Context.

Facets besides Knowledge

A knowledge base has to be multi-disciplinary and facetted:

- Disciplines,
- Services,
- Providers.

Architecture

Which architecture?

- Standalone / workstation,
- Cluster,
- Grid,
- Cloud,
- High Performance Computing (HPC),
- Other.

Provisioning

How do you provision services or resources?

- Institute,
- Alliance,
- Hosting,
- Housing,
- Other.

Type

Which type?

- Research
- Industry
- Mix
- Other

State

Which kind of usage?

- Interactive
- Batch
- Hybrid
- Other

Usage

How can the architecture be used efficiently?

- MPP (Massively Parallel Processing),
- SMP (Shared-Memory Parallel),
- Other.

Programming

Which model?

- Low Level: MPI (Message Passing Interface),
- Low Level: OpenMP,
- High Level: PGAS (Partitioned Global Address Space),
- Virtualisation: PVM (Parallel Virtual Machine),
- Other.

Productivity

How do you gather information about productivity?

- Profiling,
- Benchmarking,
- Polling,
- Quality of ... "measurements",
- Other.

How do YOU gather knowledge?

. . . and are there differences?

- In general.
- Within disciplines.
- With High End Computing.

High End Computing Requirements Study and Disciplines

How to build long-term knowledge transfer?

- Requirements studies with user groups,
- Documentation of tender processes,
- Documentation of operation and service,
- ...

Disciplines: Natural sciences, spatial sciences, archaeology, geosciences, etc.

- Disciplinary,
- Inter-disciplinary,
- Multi-disciplinary,
- ...

Tender Process – How Requirements are Currently "Considered"

Multi-step cycle of 4-7 years:

Requirements:

- **Users / disciplines**
  $\Longrightarrow$ request users / disciplines for comments.
- **Infrastructure**
  $\Longrightarrow$ participate infrastructure planners, architects, administration, etc.
- **Legal regulations (non-discrimination / environment / procedures)**
  $\Longrightarrow$ participate lawyers.
- **Technical developments**
  $\Longrightarrow$ information from developers and industry.
- **Future planning**
  $\Longrightarrow$ participate hierarchy.
- ...

This should be drastically improved by PARTICIPATING experience and knowledge, practically experienced auditing, on-topic users, developers, and industry ...

Comparison of High End Systems

Can High End Systems be compared seriously? Remember:

- Every HEC / Supercomputing system is unique in it's overall hardware, software stack, and configuration.
- Development cyle is about 5 years.
- Most tests for the bleading edge components have to be done on final, entire systems.

Extraordinary With Singular Aspects: The Greatest, Biggest, Greenest

Top500
: Top500 list with the "fastest" supercomputers in the world.
`http://www.top500.org`.
Only standard-benchmark: High Performance Linpack (HPL).

Green500
: "Ecological" list going for performance in relation to energy consumption.
`http://www.green500.org`.
Only energy, and only in operation.

...

Complex Systems

Supercomputing Resources – Examples

For the further dialog within the tutorial, the tutorial discusses some selected historical and up-to-date High Performance Computing systems and hardware and components used with Advanced Scientific Computing.

- Cray2
- JUMP
- BSC
- HLRB
- Shenzhen
- Jaguar
- Tianhe
- SuperMUC
- Sequoia
- and others ...

--- ABOVE EXAMPLES FOR DISCUSSION LEFT OUT HERE ---

Application Scenarios in Research and Education

– Application Scenarios –

Application scenarios and decision making support

The following case studies show simplified, practical application scenarios for

- separating essential knowledge
  (e.g., knowledge resources, structure)
- creating knowledge based components
  (e.g., Active Source)
- supporting increased decision potential
  (e.g., UDC classification)
- integrating high end resources
  (e.g., compute and storage)

Hardware Trace

View: Content and context

One view: *(classification)*

- Type: Poster,
- Format: Image,
- Content: Supercomputing system,
- Context: Type and size of resources,
- System: North-German Supercomputing Alliance (HLRN),
- Secondary information: PDF/image information (author, subject),
- Originary sources: long-term, LX Hardware Trace, created: 2008,

Another view: *(classification)*

- Content: Number of cores, compute nodes, disks, hardware architecture, massively parallel system, communication properties.
- Context: Supercomputing system,
- Usage and application: Geosciences, earth sciences, physics, . . .
- System: HLRN-II, North-German Supercomputing Alliance (HLRN),

Integrated Systems

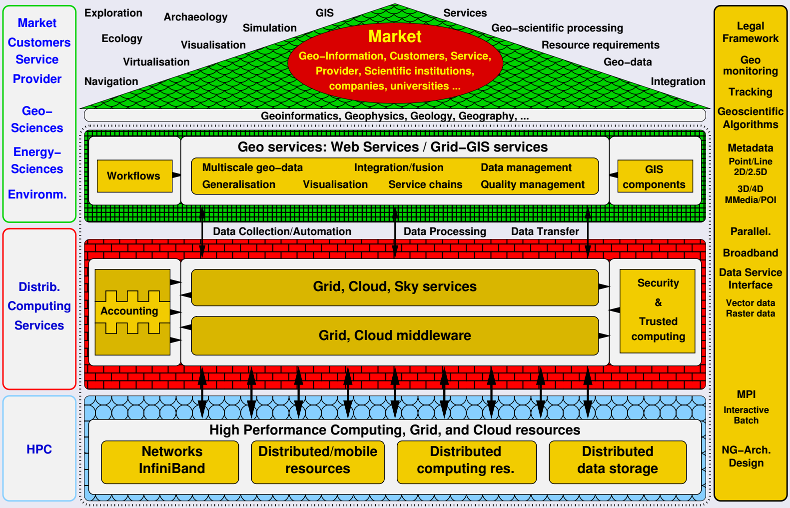
Frameworks supporting integration of:

- Information *(e.g., knowledge resources)*,
- Computation *(e.g., advanced scientific computing)*,
- Collaboration *(e.g., collaboration frameworks)*.

- Disciplines *(e.g., knowledge, collaboration, interfaces)*,
- Services *(e.g., policies, interfaces)*,
- Resources *(e.g., management, architecture, policies)*.

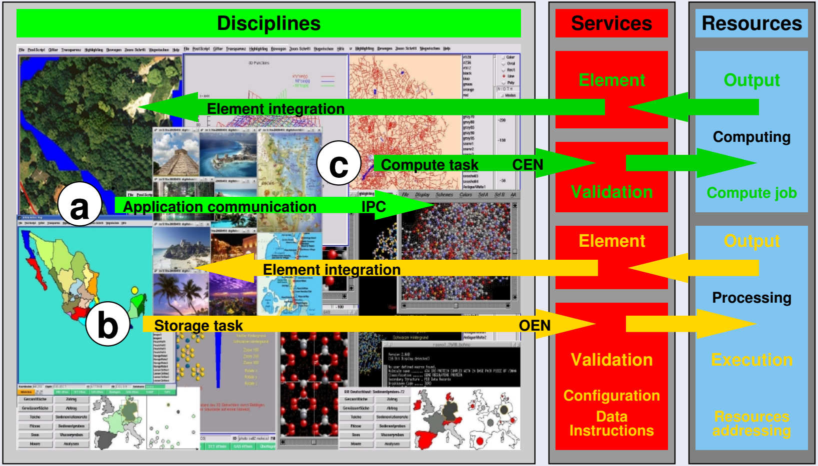
Information, computing, and collaboration

Collaboration house framework, integrating information and scientific computing



Implementation of the Different Dynamical Tasks

Integrated systems and resources for advanced scientific computing (GEXI)



Envelope Components

Using the following concepts, we can, mostly for any system, implement:

- Application communication via IPC.
- Application triggering on events.
- Storage object requests based on envelopes.
- Compute requests based on envelopes.

Used for demonstration and studies with Integrated Systems:

- Active Source Information System components for
- Flexible implementation,
- Maximum transparency,
- Separate knowledge (Structure, UDC, CEN OEN),
- Allowing OO-support (object, element) on application level,
- Multi-system support.

Application communication

Application communication with framework-internal and external applications (IPC)

```
catch {
 send {rasmol #1} "$what"
}
```

- Self-descriptive Tcl syntax.
- Inter-Process Communication send starting molecular graphics visualisation.
- Catching messages for further analysis by the components.

Application triggering and components

Application triggering, linking to application components

```
text 450.0 535.0 -tags {itemtext relictrotatex} -fill
 yellow -text "Rotate␣x" -justify center
...
$w bind relictrotatex <Button-1> {sendAllRasMol {rotate x
 10}}
$w bind relictballsandsticks <Button-1> {sendAllRasMol {
 spacefill 100}}
$w bind relictwhitebg <Button-1> {sendAllRasMol {set
 background white}}
$w bind relictzoom100 <Button-1> {sendAllRasMol {zoom
 100}}
```

Storage object requests

Generic Object Envelopes (OEN)

```
<ObjectEnvelope><!-- ObjectEnvelope (OEN)-->
<Object>
<Filename>GIS_Case_Study_20090804.jpg</Filename>
<Md5sum>...</Md5sum>
<Sha1sum>...</Sha1sum>
<DateCreated>2010-08-01:221114</DateCreated>
<DateModified>2010-08-01:222029</DateModified>
<ID>...</ID><CertificateID>...</CertificateID>
<Signature>...</Signature>
<Content><ContentData>...</ContentData></Content>
</Object>
</ObjectEnvelope>
```

- OEN containing element structures, handling and embedding data / information.
- End-user public client application, implementation via browser plugin / services.
- Instructions embedded in envelopes, content-stream and content-reference.
- Respect any meta-data for objects, handle different object formats, staying transparent, portable, keep original documents unmodified, supports signed object elements and PKI, usable with sources and binaries like Active Source.

Compute requests

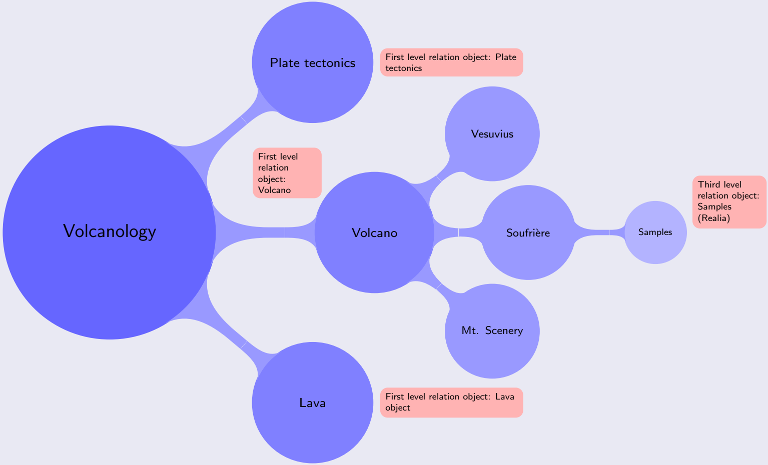
Generic Compute Envelope (CEN)

```
<ComputeEnvelope><!-- ComputeEnvelope (CEN)-->
<Instruction><Filename>Processing_Batch_GIS612.pbs</Filename>
<Sha512sum>...</Sha512sum>
<DateCreated>2010-08-01:201057</DateCreated>
<DateModified>2010-08-01:211804</DateModified>
<CertificateID>...</CertificateID><Signature>...</Signature>
<Content><DataReference>https://doi...</DataReference></Content>
<Script><Pbs><Shell>#!/bin/bash</Shell>
<JobName>#PBS -N myjob</JobName>
<Oe>#PBS -j oe</Oe>
<Walltime>#PBS -l walltime=00:10:00</Walltime>
<NodesPpn>#PBS -l nodes=8:ppn=4</NodesPpn>
<Feature>#PBS -l feature=ice</Feature>
<Partition>#PBS -l partition=hannover</Partition>
<Accesspolicy>#PBS -l naccesspolicy=singlejob</Accesspolicy>
<Module>module load mpt</Module>
<Cd>cd $PBS_O_WORKDIR</Cd>
<Np>np=$(cat $PBS_NODEFILE | wc -l)</Np>
<Exec>mpiexec_mpt -np $np ./dyna.out 2>&1</Exec>
</Pbs></Script></Instruction></ComputeEnvelope>
```

- Compute requests for resources handled via CEN interfaces, self-descriptive, environment preconfigured, references parallel processed on various architectures.

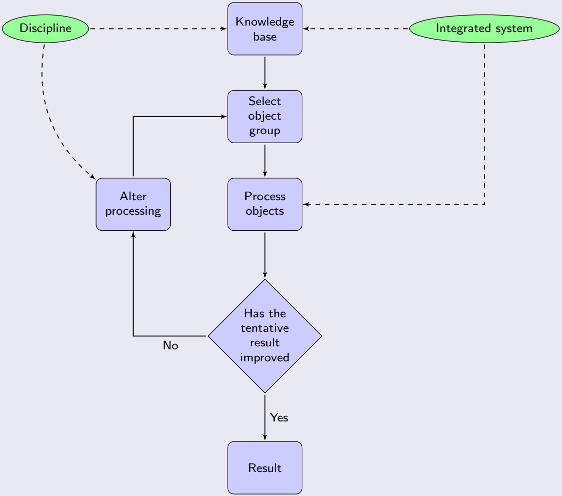
Knowledge Resources: Objects and Relations, Classification

Example: Search objects and realia references in volcanology dimension



Knowledge Resources: Workflows

Example: Simple workflow with knowledge base



Summary and Lessons Learned

– Summary –

Decision Making

Effective decision making does mean selection based on knowledge!

Decision Making and High End Computing

Process fundamentals:

- Knowledge and experience are more important than hierarchy.

Decision Making and High End Computing

Process fundamentals:

- Knowledge and experience are more important than hierarchy.
- Find the essential information.

Decision Making and High End Computing

Process fundamentals:

- Knowledge and experience are more important than hierarchy.
- Find the essential information.
- Rational problem analysis and decision planning.

Decision Making and High End Computing

Process fundamentals:

- Knowledge and experience are more important than hierarchy.
- Find the essential information.
- Rational problem analysis and decision planning.
- Add forensics to all possible information.

Decision Making and High End Computing

Process fundamentals:

- Knowledge and experience are more important than hierarchy.
- Find the essential information.
- Rational problem analysis and decision planning.
- Add forensics to all possible information.
- The decision making process needs to define the focus.

Decision Making and High End Computing

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- The decision making process needs to define goals.

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Process fundamentals:

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- The decision making process needs to define goals.
- There should be only one final instance for selection processes.

Decision Making and High End Computing

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- Rational problem analysis and decision planning.
- Add forensics to all possible information.
- The decision making process needs to define the focus.
- The decision making process needs to define goals.
- There should be only one final instance for selection processes.
- Multiple views for a process must be allowed and supported.

Decision Making and High End Computing

Process fundamentals:

- Knowledge and experience are more important than hierarchy.
- Find the essential information.
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- Best practice should be used in order to support the process.

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- Acknowledge that for some party prestige and presentation might be an aspect with any system.

Decision Subjects

Decision on:

- User (scientific and industry) requirements,
- Content,
- Context,
- Operation lifecycle,
- Staff and operation,
- Services,
- Architecture (specification, networks),
- Policies,
- Goals (of the system/service),
- Dissemination,
- (Funding).

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- Mid- and long-term: Context.

HEC on these topics at this years' conference

Presentation: Using UDC with computing and information systems

- **Monday, 2012-10-22, 15:45 – 17:30**

  INFOCOMP 3–Session, Discussion on:
  Enabling Dynamical Use of Integrated Systems and Scientific Supercomputing Resources for Archaeological Information Systems.

  Program: `http://www.iaria.org/conferences2012/ProgramINFOCOMP12.html`

International Panel INFOCOMP 2012

- **Monday, 2012-10-22, 17:30 – 19:00**

  International Panel on Future High End Systems:
  Chances and Challenges for Intelligent Applications and Infrastructures.

  Program: `http://www.iaria.org/conferences2012/ProgramINFOCOMP12.html`

Networking

Thank you for your attention!

Wish you an inspiring conference and a pleasant stay in Venice!