Dynamical Parallel Applications on Distributed and High Performance Computing Systems

(Invited Paper)

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Abstract

This paper provides an extended overview of recent developments for exploiting distributed, Grid and High Performance Computing (HPC) resources with applications like Geoscientific Information Systems (GIS) based on the GISIG actmap-project. Focus is on frameworks for optimising the dynamical parallel use of computing resources for future cooperation and development concepts, integrating software and hardware architecture aspects. Using parallel processing and the method of event triggering from within Active Source can be used to exploit the vast computing power of distributed MultiCore parallel systems for a multitude of purposes like geoinformation processing, geophysical data analysis, information systems, and e-Science. An extended case study for an application InfoPoint demonstrates the algorithm here. As various obstacles showed up with implementing and minimising the complexity of the application-resource workflow, the creation of future Web and HPC services on top of HPC and Distributed Systems will be a solution for dedicated issues. The new extended framework of the Grid-GIS house is presented here, showing the case study for using these concepts for exploration purposes. For implementation testing distributed resources and the new multi-site supercomputer resources of HLRN-II (North-German Supercomputing Alliance) have been used.

Keywords

High Performance Computing; Distributed Systems; Grid-Computing; e-Science; Geoscientific Information Systems.

1. Introduction

The future of creating effective and efficient applications for dynamical visualisation and information systems is tightly linked with taking the advantage of parallel processing on MultiCore systems. Dynamical visualisation and advanced geoscientific information systems are prominent examples [1] at state of the art of development. Using Distributed Systems and High Performance Computing (HPC) resources therefore requires new concepts as integrating these resources, that in nearly all case do have an unique architecture and basic system configuration is a challenge for development and portability.

Extending the application spectrum, a new success story using InfoPoints (groups of active information objects) is presented implementing concepts of the Active Source framework for using distributed components and resources, suitable for Grid, Cloud, and HPC.

An extended implementation of the “Grid-GIS house” framework for building services on top of Distributed and HPC Systems for this purpose is presented here for the first time. Within the “Grid-GIS house” the state of the art in accounting and billing for has been considered for creating an integrated solution embracing all High End Computing (HEC) namely HPC and Cluster Computing as well as distributed and service oriented architectures with Grid Computing and Cloud Computing [2], [3]. At the state of the art of computing, hardware development today is getting near the physical limits and software development faces new challenges. This extended implementation is currently used for building interdisciplinary cooperations for the purpose of implementing geo-exploration systems based on parallel computing components. As the next generation of dynamical applications in the disciplines involved is as well strongly depending on backend software as on hardware components and high end networks this integrated modular framework has proven suitable.

In the last years strong interests emerged, regarding High End Computing like HPC and Distributed Computing, spanning industry as well as natural sciences [4], [5], [6]. HPC resources available with the North-German Supercomputing Alliance (HLRN) have been used for testing these developments. Software and hardware architecture are discussed as resources used in the future will have to be efficiently configured for the purpose of dynamic and interactive use.

Dynamical applications are characterised by the ability to present various information and context based on interaction in very flexible ways. The concept of Active Source and the

Object Graphics data type [7] based on source code, can be used to create and integrate such applications. An example is dynamical visualisation, being able to create complex dynamical charts and diagrams enriched with accompanying visual multimedia information, where the context can change the state of the view.

Dynamical applications are in many cases limited by the local resources as there can be large computational requirements for generating new dynamical views in a short time as for example with vertices calculation in Geoscientific Information Systems (GIS) or multimedia production on demand for Points of Interest (POI) data. Parallel programming can make use of distributed resources enabling thousands of parallel processes.

The combination of dynamical applications and parallel programming components lead to "Dynamical Parallel Applications" being able to use loosely coupled as well as embarrassingly parallel methods depending on the tasks.

Numerous applications and algorithms for handling dynamical visualisation and processing of scientific information could evolve even more flexibility and facilities if they could use existing computing power more directly, namely MPP (Massively Parallel Processing) and SMP (Symmetric Multi-Processing) resources. Large benefits can result from using many cores of large computing resources in parallel, within a shorter time interval, for quasi interactive use.

This paper presents the origins, problems and challenges (Section 2-4) as well as the status of the implementation (Section 5). A case study and a detailed InfoPoint example will illustrate this (Section 6-7). Issues on software and hardware resources used will be discussed, being essential for effective distributed applications in the future (Section 8). This leads to an evaluation and future work already begun with the extended service-oriented framework for Distributed and High Performance Computing (Section 9).

2. Origin and prior art

The idea of dynamical, distributed resource usage for geoscientific information was introduced with the concept of Active Source [7]. Over the years a Grid-GIS framework with many features had to be implemented within the GISIG actmap-project [8] including several programming libraries providing a suitable Application Programming Interface (API).

With computing resources evolving towards many cores [9], [10], [11], [12] the idea of using these systems more widely had been internationally presented and some major obstacles have been identified [13], [14]. For integration of HPC, Grid, and cluster resources these are:

- framework for the use of high end computing resources for dynamical visualisation and information systems,
- integrability of concepts (e.g. batch and scheduling),
- frameworks for the application of algorithms needed,
- interfaces for flexible and secure data and application transfer, interchange, and distribution,
- portability of implementations, extendability of existing methods, reusability of existing solutions.

Due to the limitations of "delivering" computing power from High Performance Computing, Grid Computing, and cluster computing resources interactively to a local application on some workstation, a framework is needed to integrate these resources. In absence of support for coupling these resources, in the past some features had to be last on the list to be addressed.

3. Problems addressed

As described in previous publications [13] GIS, Grid, and HPC are working on the GISIG implementation in order to overcome current obstacles, developing frameworks for the use of HPC and MultiCore computing resources, interfaces for data and application interchange, integrability, and portability.

This paper does proceed to implement and disseminate the proposed frameworks and interfaces for the purpose of demonstrating implementing ways for opening powerful High Performance Computing resources to specialised scientific applications and e-Science. It shows the first implementation results of case studies on a new HPC resource, using Massively Parallel Processing and Symmetric Multi-Processing components of the HLRN architecture with distributed resource locations.

Primary target disciplines are geoinformation processing, seismic processing for oil and gas, geophysical data analysis, computing expensive natural resource information systems, computational geology, hurricane tracking, dynamical cartography, and geostatistics.

4. Challenges identified

The most important challenges identified with these implementations on HPC resources have been grouped within this context in order to be briefly discussed.

- HPC resources and configuration,
- batch system and scheduling,
- accessing computing resources / Actmap Computing Resources Interface / Message Passing,
- distributing data,
- authorisation and system security,
- accounting jobs and processes.

The following sections briefly describe the basic approaches for the implemented solution before showing an overall case study of an information system using distributed resources.

5. Mastering complexity

As it has been shown, the problems we encounter with exploiting top-level backend resources are manyfold. Currently the systems available only provide access to local resources or there is only a batch implementation. In order to solve the problems with implementing a complex system, affords the integration of different technologies and methods:

- availability of Geoscientific Information System components at source level (actmap),
- support for event-driven dynamical applications (Active Source),
- access to High End Computing resources (SMP, MPP, MultiCore, Grid) and configuration,
- creation of loosely parallel coupling interfaces for interactive batch jobs,
- parallelisation of functional components and algorithms on High End Computing resources.

Emphasis has been put onto the integration of these topics. In practice experts from different disciplines, information sciences, geosciences, computer science, engineering, are engaged. The integration has been done by defining an open framework for this purpose, based und the Grid-GIS house.

6. Status of the implementation

For the work described here, various distributed and HPC resources of HLRN have been used. This is the derivative based on new complementary methods to the predecessor work handling Grid and Cluster Computing resources [15].

6.1. HPC resources and configuration

HLRN is the North-German Supercomputing Alliance. HLRN provides high-end High Performance Computing (HPC) resources jointly used and co-funded by the northern German states of Niedersachsen, Berlin, Bremen, Hamburg, Mecklenburg-Vorpommern, Schleswig-Holstein, and the Federal Government of Germany / German Research Society (DFG).

Those resources include HLRN-II [9], a system comprised of two identical computing and storage complexes, one located at the Leibniz Universität Hannover, Regionales Rechenzentrum für Niedersachsen (RRZN) and the other at the Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB). By connecting the two systems via the HLRN-Link dedicated fibre optic network (Cisco Catalyst switches), HLRN can operate and administer them as one system.

Each complex consists of MPP and SMP cluster components (SGI Altix ICE and XE) [16] installed in two phases. The first phase has been installed by Silicon Graphics Inc. in the year 2008.

The HLRN-II system (at 312 TFlop/s peak) operated with SLES is used by scientists for HPC applications from a wide range of disciplines, including Geosciences, Environmental Sciences, Climatology, Physics, CFD, Modeling and Simulation, Chemistry, Biology, and Engineering. All projects are supported by the HLRN service and competence network.

So while still in an early phase this resource installation, incorporating different computing components, gave the suitable context for individually configuring an implementation as described in the following sections. With the available HPC resources a number of software, application, and network components have been configured (Table 1) for integrating the framework and preparing a suitable software and hardware environment for the case study scenarios.

Component	*Software / Configuration*
Frameworks	GISIG, Actmap CRI, Grid-GIS
Operating System	S.u.S.E Linux / SLES
Batch system	Moab, Torque
Networks	MPI (InfiniBand), I/O (InfiniBand), service and administrative networks
Parallelisation	MPI, OpenMP, MPT, MPICH
Transfer / interchange	Secure Shell / keys, `pdsh`
Security	Sandboxing, Tcl, Tcl Plugin
Policies	`home`, `javascript`, `trusted`
Compilers	Intel Fortran, C, C++ suite, PGI, GNU
Libraries & Appl.	BLAS, LAPACK, NAG, ATLAS, CPMD, MOLPRO, FEOM, NAMD, Gaussian, FFT, TAU, NWChem, VMD, EnSight, ABAQUS, ANSYS, FLUENT, STAR-CD . . .
Parallelisation	SGI MPI / MPT, Intel MPI, OpenMP, MPICH, MVAPICH, SHMEM . . .

Table 1. HPC software components configured.

This is an excerpt of basic software components like applications, libraries and compilers, available for applications discussed in the context of this paper.

For security reasons a trusted computing interface using sandboxing has been configured as various security policies for integrating data and applications have been introduced and successfully tested.

This configuration allows very flexible transfer of data, secured execution of foreign Active Sources on demand, accounting as well as batch and interactive use of resources.

The basic trusted environment is independent from the computing architecture and can be used out of the box. The specific architecture dependent configuration part must be done accordingly to the purposes where it is neccessary for the service.

Primary targets might be key management, LDAP or firewall configuration. The components used for management of the components are shown in Table 2. Information on the current state of these resources can be found online [9].

Component	*Management / Configuration*
Additional Server	HOME, Data, Login, Batch, LDAP OSS, MDS, QFS, Repository
Mgmt. Altix ICE / XE	SGI Tempo / Scali Manage
Storage / Global FS	RAID 6, Storage Manager / Lustre
File Replication	NetVault Replicator (HLRN-Link)
Software Access	“Modules” (Compilers, Libs, Apps)
Monitoring	Nagios, Ganglia
Grid, Access, HA	Grid tools, Middleware, ...
Profiling / Debugging	Intel Threading & Tracing Tools, PCP, PerfSuite, TotalView, ddt, gdb
Configuration Mgmt.	Cfengine, CVS

Table 2. HPC management components configured.

6.2. Batch system and scheduling

The batch system, scheduling and resource management implemented on HLRN-II is based on Moab and Torque. With this system the PBS (Portable Batch System) resource specification language [17] [18] is used. Interactive use and calculation is highly dependent on features of the batch system used. Currently the end user application will have to do the job synchronisation. With a conventional system configuration the management of multi user operation is difficult. Both synchronising and multi user operation tend to work against interactive use.

6.3. Accessing computing resources

The Actmap Computing Resources Interface (CRI) is an actmap library containing procedures for handling computing resources. Examples for using High Performance Computing and Grid Computing resources include batch system interfaces and job handling.

Listing 1 shows a simplified source code part of the actmap call for loading the Actmap Computing Resources Interface (Tcl or TBC) into the application stack. This library can be extended and modified interactively on the fly or via scripting [19].

```
#BCMT-----------------------------------------------
###EN \gisigsnip{Load actlcri}
#ECMT-----------------------------------------------
if {"$behaviour_loadlib_actlcri" == "yes"} {
  catch {
    if {[info exists tcl_platform(isWrapped)]} {
      puts "actlcri.tbc␣library␣initialized␣..."
      source actlcri.tbc
      set status_in_actmap yes
    } else {
      puts "actlcri.tcl␣library␣initialized␣..."
      source [file join $ACTMAPHOME "actlcri.tcl"]
      set status_in_actmap yes
    } } }
```

Listing 1. Calling CRI.

This library (`actlcri`) can hold functions and procedures and even platform specific parts in a portable way. It can be used by calling the source code library as well as the byte code library generated with a compiler like TclPro. From an application, calling Actmap CRI can be done as follows. For various applications, byte code (TBC) [7] has been considered for any part of applications and data.

With CRI being part of Active Source, parallel processing interfaces for Message Passing e.g. using InfiniBand, can be used, for example MPI (Message Passing Interface) and OpenMP. Listing 2 and Listing 3 show an MPI and an OpenMP job script used with Actmap CRI.

```
#!/bin/bash
#PBS -N myjob
#PBS -j oe
#PBS -l walltime=00:10:00
#PBS -l nodes=8:ppn=4
#PBS -l feature=ice
#PBS -l partition=hannover
#PBS -l naccesspolicy=singlejob
module load mpt
cd $PBS_O_WORKDIR
np=$(cat $PBS_NODEFILE | wc -l)

mpiexec_mpt -np $np ./dyna.out 2>&1
```

Listing 2. Active Source MPI (SGI MPT) script.

```
#!/bin/bash
#PBS -N myjob
#PBS -j oe
#PBS -A myproject
#PBS -l walltime=00:10:00
#PBS -l nodes=1:ppn=4
#PBS -l feature=xe
#PBS -l naccesspolicy=singlejob
cd $PBS_O_WORKDIR
export OMP_NUM_THREADS=4

./dyna.out 2>&1
```

Listing 3. Active Source OpenMP script.

Scripts of this type will on demand — this means using event binding — be sent to the batch system for processing. The sources can be semi-automatically generated, can be called from a set of files or can be embedded into an actmap component, depending on the field of application.

6.4. Distributing data

Within event triggered jobs, MPI and batch means can be used for distributing and collecting data and job output. For distributing files automatically within the system e.g. `dsh`, `pdsh`, C3 tools, Secure Shell (`ssh` and `scp`) are used. Interactive communication is supported by the appropriate Secure Shell key configuration. It must be part of the system configuration to correctly employ authorisation keys and `crontab` or `at` features.

6.5. Authorisation and system security

Authorisation for accessing data and information associated with the calculation currently affords to have one instance of the application present on one of the servers of the HPC resource, e.g. login or batch. A dedicated network using secure keys can be configured for the purpose of interactive application access in order to simplify communication and data transfer between the nodes. As for system security reasons large installations will tend to be restricted to dedicated users with this scenario. For execution of dynamic sources the trusted computing interface has been configured as `policy trusted`.

6.6. Accounting jobs and processes

The implemented framework is incorporated in an integrated solution for monitoring, accounting, billing supporting the geoinformation market. An outlook has been given for Geographic Grid Computing at the International Conference on Grid Services Engineering and Management (GSEM). Especially for the extended use of GIS and computing resources, the Grid-GIS framework, the “Grid-GIS house” has been created [13] and is used within the D-Grid [20], [21] and with Condor. The Active Source components used here, are part of this framework, on top of the Grid services, Grid middleware, and the HPC and Grid resources.

7. Case study

The selected case study overview shows different high level GIS views implemented with dynamical cartography (Active Map) in order to enable geocognostic insights. With this solution, processing, data storage, and information retrieval is done by using distributed resources. Handling is triggered from within the application by events via the Active Source framework. In oder to concentrate on the views we omit features previously demonstrated, such as active elements handling and visualisation, multimedia objects and raster and vector layering.

With a suitable interface, distributed computing resources can be used for creating any part of the application or data. So data collection and automation, data processing, and data transfer can be handled via existing means.

For example parallel processing of satellite data or satellite photos can be triggered from within the Active Map. The precalculation of views (Listing 4) can be automated from the application, processing several hundred views at a time using dedicated compute nodes for each calculation.

```
convert -scale 2400x1200 inview01.jpg outview01.jpg
convert -scale 2400x1200 inview02.jpg outview02.jpg
convert -scale 2400x1200 inview03.jpg outview03.jpg
...
```

Listing 4. Precalculation of satellite data.

An event binding command is shown in Listing 5. These bindings can bind events to selective objects of a category. The number of objects handled in object source is only limited by the system and hardware used. This way it is possible to provide any part of the application with support of distributed computing and storage resources, e.g. for simple cases via HTTP or HTTPS. The functional part can be a procedure, another component or an executable.

```
$w bind precalc_bio <Button-1> {exec precalc_bio.sh}
```

Listing 5. Binding of precalculation script.

For the following examples all the components are linked by the GISIG Active Source framework using event programming and the most computing intensive operations are done in the background on HPC compute resources.

Figure 1 shows part of an active satellite worldmap calculated on a HPC compute node as described. The respective action for calculating the view is linked into the Active Source data via an event bind call (Tcl) to the batch script. The batch script using scripting and MPI is executed by the batch system (Moab / Torque) to run on the compute nodes of the specified MPP component.

The result is transferred back to an application working directory from where the results calculated on the compute nodes are loaded into the active map (Tcl canvas) in order to build the desired view. Any objects of these views do get unique identification keys and may be automatically equipped with logical identification strings.

From within this interactive view one might want to switch to an active ocean / depth or plate tectonics view in a next step as in Figure 2 and end up in showing a vegetation / biology view as in Figure 3.

Once calculated all the maps exist at the same time, they can be regarded “precalculated”. Active Source uses a layer concept meaning any number of objects can be grouped in separate layers with all layers representing a stack of layers. It can be defined for the specific Active Source application if all of the calculated views do reside in memory, stacked in layers inside of the application as described or if they shall be removed in favour of releasing memory.

In the first case no data has to be recalculated, any views precalculated this way can be accessed interactively. It can be easily switched between the views by predefined events. The standard ways for doing so are key bindings to rotate views and mouse events to bring the next or a defined view to the front.

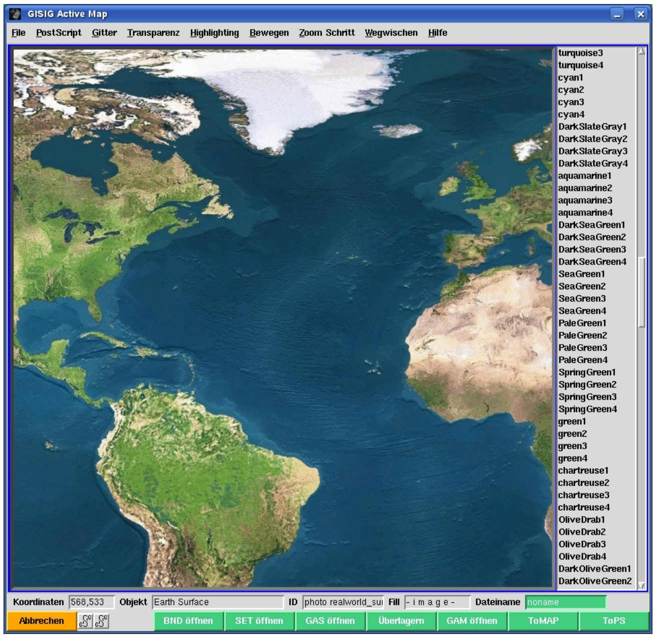

Figure 1. Precalculated topography view.

Any operation on the data suitable for interactive and batch mode can be done from within the Active Source framework. With this capability batch jobs can be created, e.g. for dynamically adding synthetic data and raytraced elements in interactive mode. Using parallelised applications like parallel POV-Ray from within these jobs, distributed computing resources can be used most effectively.

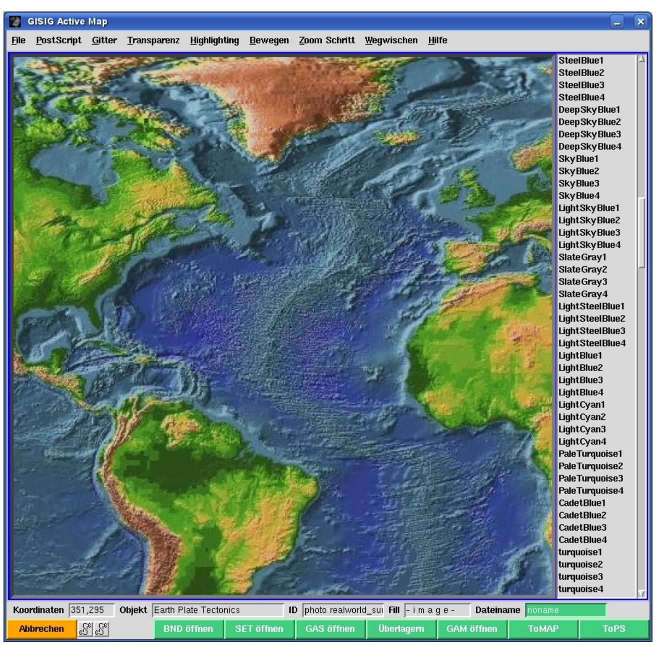

Figure 2. Precalculated plate tectonics view.

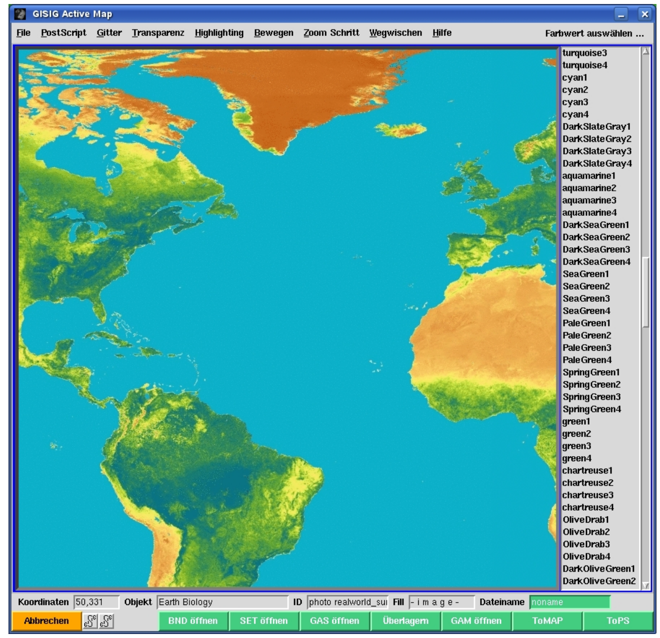

Figure 3. Precalculated biology view.

This can e.g. be encouraged in order to enhance geocognostic views by generating hundreds of data sets for points of interest. Ongoing from Figure 3, decision may fall to viewing the pollution distribution within a city in a distinct area as in Figure 4. One will select an “active spot” on the map that is linked with an appropriate detailed active city map. Most flexible geocognostic views can be created this way using the local and background computing resources at any time in the process of user interaction. GISIG Active Maps can consist of vector and raster layers as well as of multimedia components and events. Problems of dynamical cartography and geocognostic views with millions of data points having to be connected with live, interactive data being very computing intensive can be solved.

The example (Figure 4) shows a dynamical event-driven city map containing environmental and infrastructure data that is delivered from distributed sources. Now if one wants to take a look at pollution values of the largest lake within this city, as in Figure 5, a right click onto that object will display the results. Any interactive and batch events may be defined. A defined key bound will toggle a legend. Further zooming can be done to any extent, e.g. to resolve elementary objects within views. This demonstrates cartography combined with aerial data (vegetation and topography), and vector data (infrastructure and surfaces of water) all linked by events, and extensible by event triggered computing.

The selected part shown, is a highly zoomed area of the previously presented map, here in different thematical geocognostic context. Arbitrary detailed satellite maps and supporting data may be calculated on the HPC resources using the described algorithm.

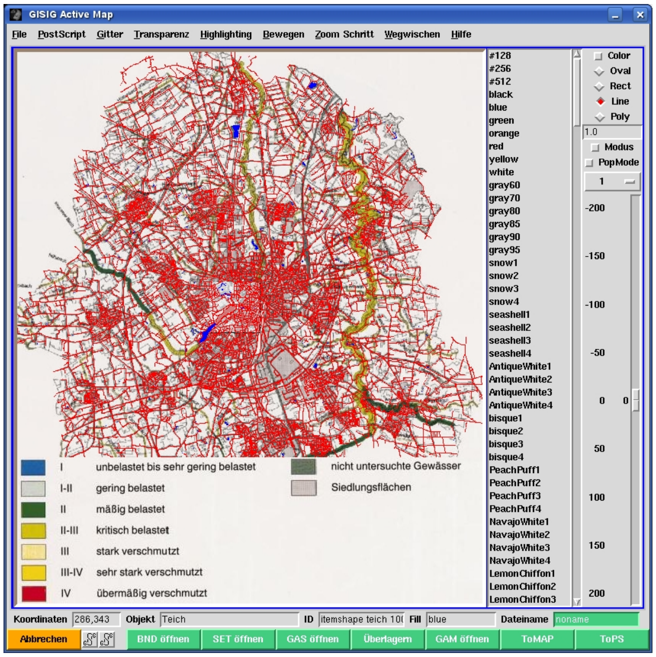

Figure 4. City, vector / raster layers, events.

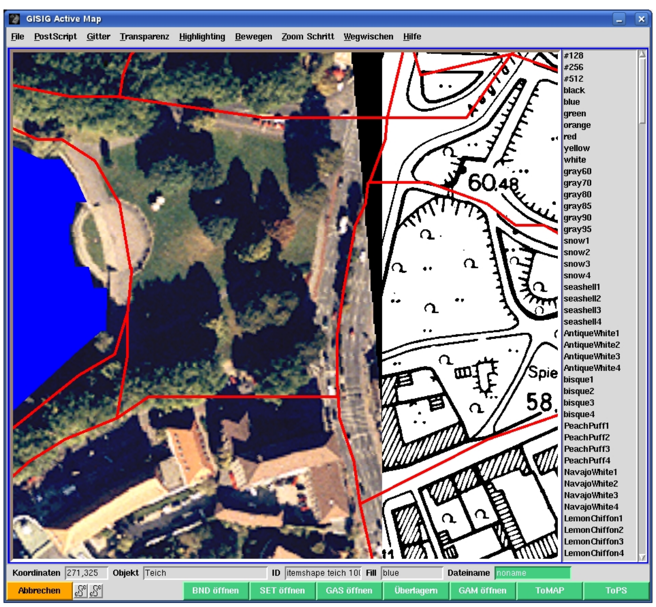

Figure 5. Detail, combined geocognostic view: map data, aerial data, and vector data.

Used from via a login node the solution with HPC compute nodes does show less latency than for previous solutions with distributed Grid resources. The login nodes used, are configured for interactive use of the batch system so there is no queue wait-time and much less time necessary for scheduling and re-scheduling. That way, avoiding a standard batch system configuration and a high job load, interactive applications are possible, reducing the wait times from about 12 up to 24 hours down to 1 to 10 minutes for medium expensive computation events. For less consumptive computation events the overall wait times are in the range of seconds.

e-Science applications like dynamical cartography and visualisation can use distributed resources in combination with Inter-Process Communication (IPC) and remote control within the application in a standard way as the parts calculated externally have been delivered back and loaded into the application. Any part can be reloaded or removed from memory separately so that memory usage is minimised.

8. InfoPoints using distributed resources

Using auto-events, dynamical cartography, and geocognostic aspects, views and applications using distributed compute and storage resources can be created very flexibly.

As with the concept presented resources available from Distributed Systems, High Performance Computing, Grid and Cloud services, and available networks can be used. The main components are:

- interactive dynamical applications (frontend),
- distributed resources, compute and storage, configured for interactive and batch use,
- parallel applications and components (backend), as available on the resources,
- a framework with interfaces for using parallel applications interactively.

Besides the traditional visualisation a lot of disciplines like exploration, archaeology, medicine, epidemology and for example various applications within the tourism industry can profit from the e-Science components. These e-Science components can be used for Geoscientific Information Systems for dynamical InfoPoints and multimedia, Points of Interest based on Active Source (Active POI), dynamical mapping, and dynamical applications.

8.1. InfoPoints and dynamical cartography

Figure 6 shows an interactive Map of México. The yellow circle is an event sensitive Active Source object containing a collection of references for particular objects in the application. This type of object has been named InfoPoint. InfoPoints can use any type of start and stop routines triggered by events. Figure 7 shows a defined assortment of information, a view set, fetched and presented by triggering an event on the InfoPoint.

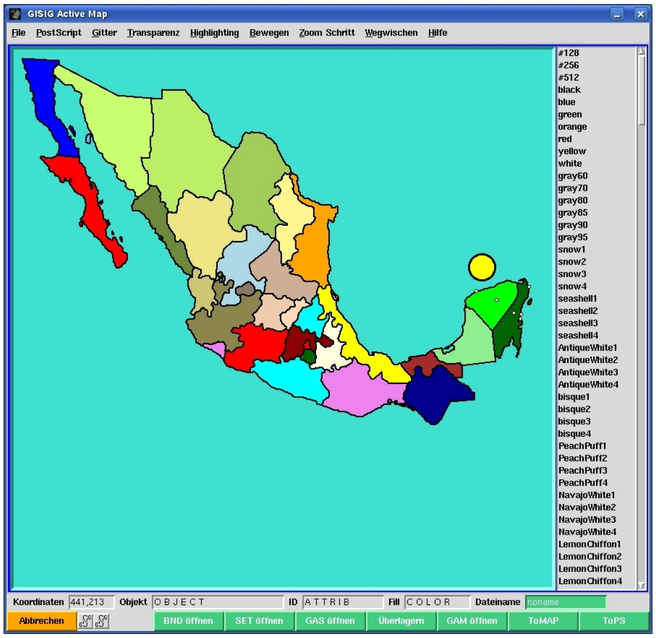

Figure 6. Interactive México with InfoPoint Yucatán.

Figure 7. Sample view set of InfoPoint Yucatán.

The information has been referenced from within the World Wide Web in this case. InfoPoints can depend on the cognitive context within the application as this is a basic feature of Active Source: Creating an application data set it is for example possible to define the Level of Detail (LoD) for zoom levels and how the application handles different kinds of objects like Points of Interest (PoI) or resolution of photos in the focus area of the pointing device.

8.2. Inside InfoPoints

The following passages show all the minimal components necessary for a fully functional InfoPoint. The example for this case study is mainly based on the Active Source framework. Triggered program execution ("Geoevents") of applications is shown with event bindings, start and stop routines for the data.

8.3. InfoPoints bindings and creation

Listing 6 shows the creation of the canvas for the InfoPoint and loading of the Active Source via bindings.

```
#
# actmap example -- (c) Claus-Peter R\"uckemann,␣2008,␣
 2009
#

#
# Active map of Mexico
#

erasePict
$w configure -background turquoise

pack forget .scale .drawmode .tagborderwidth \
  .poly .line .rect .oval .setcolor
pack forget .popupmode .optmen_zoom

openSource    mexico.gas
removeGrid

##EOF:
```

Listing 6. Example InfoPoint Binding Data.

This dynamical application can be created by loading the Active Source data with the `actmap` framework (Listing 7).

```
/home/cpr/gisig/actmap_sb.sfc mexico.bnd
```

Listing 7. Example creating the dynamical application.

8.4. InfoPoints Active Source

The following Active Source code (Listing 8) shows a tiny excerpt of the Active Source for the interactive Map of México containing some main functional parts for the InfoPoint Yucatán (as shown in Figure 6).

```
#BCMT--------------------------------------------------
###EN \gisigsnip{Object Data: Country Mexico}
###EN Minimal Active Source example with InfoPoint:
###EN Yucatan (Cancun, Chichen Itza, Tulum).
#ECMT--------------------------------------------------
proc create_country_mexico {} {
global w
#  Yucatan
$w create polygon 9.691339i 4.547244i 9.667717i \
  4.541732i 9.644094i 4.535433i 9.620472i 4.523622i \
  9.596850i 4.511811i 9.573228i 4.506299i 9.531496i \
  4.500000i 9.507874i 4.518110i 9.484252i 4.529921i \
  9.460630i 4.541732i 9.437008i 4.547244i 9.413386i \
  4.553543i 9.384252i 4.559055i 9.354331i 4.565354i \
  9.330709i 4.588976i 9.307087i 4.612598i 9.283465i \
  4.624409i 9.259843i 4.636220i 9.236220i 4.641732i \
  9.212598i 4.641732i 9.188976i 4.648031i 9.165354i \
  4.653543i 9.141732i 4.659843i 9.118110i 4.665354i \
```

```
  9.094488i 4.671654i 9.070866i 4.677165i 9.047244i \
  4.688976i 9.023622i 4.695276i 9.000000i 4.707087i \
  8.976378i 4.712598i 8.952756i 4.724409i 8.929134i \
  4.730709i 8.905512i 4.736220i 8.881890i 4.748031i \
  8.858268i 4.766142i 8.834646i 4.783465i 8.811024i \
  4.801575i 8.787402i 4.813386i 8.763780i 4.830709i \
  8.751969i 4.854331i 8.740157i 4.877953i 8.734646i \
  4.901575i 8.728346i 4.925197i 8.746457i 4.937008i \
  8.751969i 4.966929i 8.751969i 4.978740i 8.763780i \
  5.007874i 8.763780i 5.019685i 8.787402i 5.025984i \
  8.805512i 5.031496i 8.817323i 5.049606i 8.846457i \
  5.055118i 8.876378i 5.055118i 9.248031i 5.468504i \
  9.673228i 4.896063i 9.744094i 4.748031i 9.720472i \
  4.553543i \
 -outline #000000 -width 2 -fill green -tags {itemshape province_yucatan}
}

proc create_country_mexico_bind {} {
global w
$w bind province_yucatan <Button-1> {showName "Province␣Yucatan"}
$w bind province_quintana_roo <Button-1> {showName "Province␣Quintana␣Roo"}
}

proc create_country_mexico_sites {} {
global w
global text_site_name_cancun
global text_site_name_chichen_itza
global text_site_name_tulum
set text_site_name_cancun         "Cancún"
set text_site_name_chichen_itza   "Chichén␣Itzá"
set text_site_name_tulum          "Tulum"

$w create oval 8.80i 4.00i 9.30i 4.50i \
  -fill yellow -width 3 \
  -tags {itemshape site legend_infopoint}
$w bind legend_infopoint <Button-1> \
  {showName "Legend␣InfoPoint"}
$w bind legend_infopoint <Shift-Button-3> \
  {exec browedit$t_suff}

$w create oval 9.93i 4.60i 9.98i 4.65i \
  -fill white -width 1 \
  -tags {itemshape site cancun}
$w bind cancun <Button-1> \
  {showName "$text_site_name_cancun"}
$w bind cancun <Shift-Button-3> \
  {exec browedit$t_suff}

$w create oval 9.30i 4.85i 9.36i 4.90i \
  -fill white -width 1 \
  -tags {itemshape site chichen_itza}
$w bind chichen_itza <Button-1> \
  {showName "$text_site_name_chichen_itza"}
$w bind chichen_itza <Shift-Button-3> \
  {exec browedit$t_suff}

$w create oval 9.76i 5.20i 9.82i 5.26i \
  -fill white -width 1 \
  -tags {itemshape site tulum}
$w bind tulum <Button-1> \
  {showName "$text_site_name_tulum"}
$w bind tulum <Shift-Button-3> \
  {exec browedit$t_suff}
}

proc create_country_mexico_autoevents {} {
global w
$w bind legend_infopoint <Any-Enter> {set killatleave [exec ./mexico_legend_infopoint_viewall.sh $op_parallel ] }
$w bind legend_infopoint <Any-Leave> {exec ./mexico_legend_infopoint_kaxv.sh }

$w bind cancun <Any-Enter> {set killatleave [exec $appl_image_viewer -geometry +800+400 ./mexico_site_name_cancun.jpg $op_parallel ] }
$w bind cancun <Any-Leave> {exec kill -9 $killatleave }

$w bind chichen_itza <Any-Enter> {set killatleave [exec $appl_image_viewer -geometry +800+100 ./mexico_site_name_chichen_itza.jpg $op_parallel ] }
$w bind chichen_itza <Any-Leave> {exec kill -9 $killatleave }

$w bind tulum <Any-Enter> {set killatleave [exec $appl_image_viewer -geometry +800+400 ./mexico_site_name_tulum.jpg $op_parallel ] }
$w bind tulum <Any-Leave> {exec kill -9 $killatleave }
}

proc create_country_mexico_application_ballons {} {
global w
global is1
gisig:set_balloon $is1.country "Notation␣of␣State␣and␣Site"
gisig:set_balloon $is1.color "Symbolic␣Color␣od␣State␣and␣Site"
}

create_country_mexico
create_country_mexico_bind
create_country_mexico_sites
create_country_mexico_autoevents
create_country_mexico_application_ballons

scaleAllCanvas 0.8
##EOF
```

Listing 8. Example InfoPoint Active Source data.

The source contains a minimal example with the active objects for the province Yucatán in México. The full data set contains all provinces as shown in Figure 6. The functional parts depicted in the source are the procedures for:

- `create_country_mexico`:
  The cartographic mapping data (polygon data in this example only) including attribute and tag data.
- `create_country_mexico_bind`:
  The event bindings for the provinces. Active Source functions are called, displaying province names.
- `create_country_mexico_sites`:
  Selected site names on the map and the active objects for site objects including the InfoPoint object. The classification of the InfoPoint is done using the tag `legend_infopoint`. Any internal or external actions like context dependent scripting can be triggered by single objects or groups of objects.
- `create_country_mexico_autoevents`:
  Some autoevents with the event definitions for the objects (Enter and Leave events in this example).
- `create_country_mexico_application_ballons`:
  Information for this data used within the Active Source application.
- Call section: The call section contains function calls for creating the components for the Active Source application at the start of the application, in this case the above procedures and scaling at startup.

Any number of groups of objects can be build. This excerpt only contains Cancun, Chichen Itza and Tulum. A more complex for this example data set will group data within topics, any category can be distinguished into subcategories in order to calculate specific views and multimedia information, for example for the category `site` used here:

- `city` (México City, Valladolid, Mérida, Playa del Carmen),
- `island` (Isla Mujeres, Isla Cozumel),
- `archaeological` (Cobá, Mayapan, Ek Balam, Aktumal, Templo Maya de Ixchel, Tumba de Caracol),
- `geological` (Chicxulub, Actun Chen, Sac Actun, Ik Kil),
- `marine` (Xel Há, Holbox, Palancar).

Objects can belong to more than one category or subcategory as for example some categories or all of these as well as single objects can be classified `touristic`.

The data, as contained in the procedures here (mapping data, events, autoevents, objects, bindings and so on) can be put into a database for handling huge data collections.

8.5. Start an InfoPoint

Listing 9 shows the start routine data (as shown in Figure 7). For simplicity various images are loaded in several application instances (`xv`) on the X Window System. Various other API calls like Web-Get `fetchWget` for fetching distributed objects via HTTP requests can be used and defined.

```
xv -geometry +1280+0   -expand 0.8 mexico_site_name_cancun_map.jpg &
xv -geometry +1280+263 -expand 0.97 mexico_site_name_cancun_map_hotels.jpg &

xv -geometry +980+0    -expand 0.5 mexico_site_name_cancun.jpg &
xv -geometry +980+228  -expand 0.61 mexico_site_name_cancun_hotel.jpg &
xv -geometry +980+450  -expand 0.60 mexico_site_name_cancun_mall.jpg &
xv -geometry +980+620  -expand 0.55 mexico_site_name_cancun_night.jpg &

xv -geometry +740+0    -expand 0.4 mexico_site_name_chichen_itza.jpg &
xv -geometry +740+220  -expand 0.8 mexico_site_name_cenote.jpg &
xv -geometry +740+420  -expand 0.6 mexico_site_name_tulum_temple.jpg &
#xv -geometry +740+500  -expand 0.3 mexico_site_name_tulum.jpg &
xv -geometry +740+629  -expand 0.6 mexico_site_name_palm.jpg &
```

Listing 9. Example InfoPoint event start routine data.

8.6. Stop an InfoPoint

Listing 10 shows the stop routine data. For simplicity all instances of the applications started with the start routine are removed via system calls.

```
killall -9 --user cpr --exact xv
```

Listing 10. Example InfoPoint event stop routine data.

Using Active Source applications any forget or delete modes as well as using Inter Process Communication (IPC) are possible.

9. Software and hardware resources used

For using High Performance Computing (HPC) and Grid Computing resources (ZIVGrid, ZIVcluster, ZIVsmp, HLRN) for Distributed Computing with Geoscientific Information Systems (GIS) it is has been shown [13], [1], [2] to be necessary carrying out an integration and configuration regarding software and hardware components.

For the HPC resources it is an ongoing research and development goal to optimise the single-system-properties with the software and hardware installation used for the case studies discussed within this paper. Several software / hardware configurations have been tested with the complex multi-cluster-multi-site installation of HLRN-II in order to ensure that the resulting system will be seen as one single system for system administration and various user applications.

9.1. Integrating SW and HW resource components

As the HLRN consists of two complexes located at two sites one goal is, to enable operation and use of all resources as one single system. The integration of the different SMP and MPP systems into this concept is an essential part, so accessing these resources via applications will be managed with an uniform interface. On the other hand it shall be possible to use the redundancies of the complexes to increase availability and minimise overall maintenance downtimes as with the system architecture it has been taken care that each complex can be down for full maintenance separately. The most important aspects of the single-system-properties in this context regard:

- Joint user and job management for one uniform user space, regarding an uniform addressing, use, and administration.
- System-spanning home directories including mirroring and replication, reducing the need for explicit data transfer and data synchronisation.
- Joint job and data scheduling with automated data transfer (data staging).
- Storage integration, integration of SAN capabilities, Data-Grid.
- MPI communication for very large applications using MPI-2 in user space in order to use resources of the spatially distributed complexes.

For the complexity involved with this, the following sections focus on the architecture and the hardware and software components and applications that had to be configured with the installation.

Currently application use cases have been internationally presented for this installation from application view only. The example use cases and most important results on hardware and software configuration are referenced in a separate section. This paper concentrates on the hardware and software components that had to be configured for creating a suitable integrated HPC resource base.

9.2. Architecture and phases

Table 3 gives a compact overview of the most important hardware resources of the HLRN-II system available for applications within the main installation phases. For the specific areas of application from the usage spectrum, the complexes consist of suitable SMP and MPP components. Separate InfiniBand networks for fast MPI and IO are available. The system complexes at the sites Hannover and Berlin are extended in two phases, with identical components and configuration. The hardware configuration details left out here due to legal issues will be provided in phase 2 of the installation process.

As with computing at the top edge of maximum performance and minimum of obstacles the story is not all about software only. There is a number of limits reducing efficiency that are immanently appearent with the architecture, in theses cases ordered by priority for use with the examples presented here:

- latencies of network and batch system limiting the response times for interactive use,
- throughput / IO limiting the streaming facilities with model calculation on the compute nodes and data servers,
- scalability of existing algorithms for computational problem solving,
- memory limiting efficient high-resolution simulation,
- storage capability limiting chain job restart and checkpointing,
- number of CPUs (cores) limiting the number of loosely coupled highly parallel compute events,
- availability of resources due to competitive jobs for different user applications,
- non-certified components limiting flexibility with application porting and configuration.

As a detailed description for a hardware solution is out of scope of this paper, the most important aspects for the applications handled are latencies and throughput. Fast dedicated networks for example using InfiniBand fabrics can help to reduce the bottlenecks and latencies for highly parallel as well as for dynamical and interactive applications. For example with event triggered "dynamically" changing visualisation controlled from within an interactive information system, large computation tasks as well as large visualisation IO (several hundred megabytes per second per task) can result. This will even increase in the near future. As far as separate physical networks dedicated for MPI and IO are available, applications will profit.

10. Evaluation and lessons learned

The current work of implementing and configuring software components and the case study shows use of computing resources with the Active Source framework, spatial event handling, and cognitive dynamical application.

With this solution it is possible to build sets of interactive, extensible, portable, and reusable applications with interdisciplinary background based on the computing power of MultiCore and HPC Systems.

In the last years many "flavours" of High End Computing have been evaluated. Summing up the experiences of the longterm project regarding this aspect, applications on the following architectures and paradigms have been successfully implemented and tested:

- Distributed and High Performance Computing (DHPC) on MPP, SMP, and vector computers,
- Grid Computing and Distributed Computing,
- Cluster Computing,
- Mobile, Utility, Tool, and Ubiquitous Computing.

With the current plans, the next topic on the agenda will be the Cloud Computing top service level – XaaS (Application as a Service, AaaS; Software as a Service / Security as a Service, SaaS) based on the base levels (Infrastructure as a Service, IaaS; Platform as a Service, PaaS; Desktop as a Service, DaaS).

The InfoPoint concept has been demonstrated, working for various disciplines, visualising and extending various features of cartography and e-Science under cognostic aspects. These applications may also use resources interactively but any short latencies are difficult to achieve with most current computing installations.

For optimising the use of resources the software configuration will have to be coordinated with the hardware configuration in order to build an efficient system architecture. Although the Active Source framework can integrate various concepts, it is highly dependent on the system configuration. The most obvious obstacles limiting efficiency and ease of use are the current state of HPC environments and the missing standardisation and modularisation of system components like for the batch system and scheduling. As in the HPC world every installation comes with an unique configuration, this is a crucial point. So always not only take a look on the software side but on the hardware, too.

11. Future work

The topics in focus for the next years can be grouped in three sections: technical aspect, collaboration work, and work within the participating disciplines.

11.1. Technical aspects

The basic algorithms have been implemented and tested for enabling distributed and HPC systems for dynamical use.

HLRN-II Overview	*Phase 1 (2nd Quarter 2008)*	*Phase 2 (from 2009 on)*	*Total*
Complex H/B each, MPP	MPP 1: SGI Altix ICE 8200EX (ICE+)	MPP 2: SGI Carlsbad 2	
Number of nodes (blades)	320 (Colfax-S w/ Seaburg)	960	1280
Number of sockets / cores	640 (Quad-Core) / 2560	[details provided in phase 2]	
Processor	Intel Xeon Harpertown, 3 GHz / 80 W	[Intel Next Generation Xeon]	
Memory & network	5.1 TByte (2 GByte/core, IB 4×DDR)	29.3 TByte (IB 2×Dual DDR)	34.4 TByte
System peak performance	30.7 TFlop/s	≈100 TFlop/s	≈130 TFlop/s
Complex H/B each, SMP	SMP 1: SGI Altix XE 1300	SMP 2: SGI UltraViolet	
Number of nodes	47 CN (+2 HN, XE250)	136	183
Number of sockets / cores	94 (Quad-Core) / 376	[details provided in phase 2]	
Processor	Intel Xeon Harpertown, 3 GHz / 80 W	[Intel Next Generation Xeon]	
Memory & network	2.8 TByte (8 GByte/core, IB 4×DDR)	8.7 TByte (NumaLink 5)	11.5 TByte
System peak performance	4.2 TFlop/s	≈22 TFlop/s	≈26 TFlop/s
Complex H+B overall	***Phase 1***	***Phase 2***	***Total***
Storage capacity (gross)	1.15 PByte (RAID-Array)	1.15 PByte (RAID-Array)	2.3 PByte
IO bandwidth	14 GByte/s	14 GByte/s	28 GByte/s
Number of cores (CN)	5824	19360	25184
Memory	16 TByte	76 TByte	92 TByte
System peak performance	70 TFlop/s	≈242 TFlop/s	≈312 TFlop/s

Table 3. HPC hardware resources in test situation, HLRN-II complexes Hannover (H) and Berlin (B).

The necessary configuration of systems and resources has to be standardised for practicing a uniform setup and in order to minimise invasive overhead. In the future it cannot be the user having the need to trigger most of the configuration of complex system components on every system an application should be run, there will have to be suitable interfaces.

There will have to be standard interfaces for parallelisation in the future. For both distributed and High Performance Computing, monitoring and accounting is necessary in order to handle interactive use.

The application of the frameworks presented for high level research and development consortium has already begun and will accelerate to develop standardised means of communication, like Web Services for HPC services for dedicated issues.

Currently the collaboration partners prepare to integrate the methods presented here for using distributed resources developed into components of open and commercial geoscientific information systems for productive use.

11.2. Collaboration work

Based the current organisational structure for combining work of the different interest groups, the block diagram in Figure 8 illustrates the future directions of integrating and co-developing large collaborative target frameworks and applications for service-oriented Distributed and High Performance Computing on management level. It shows the dependencies of

- market and services (green colour, shingle and cross pattern),
- computing services (red colour, brick pattern),
- HPC and distributed resources (blue colour, gravelly pattern),
- and resources to be provisioned or developed (yellow colour).

The collaboration partners in the fields of HPC, services, geosciences and exploration, do regard the modular three level framework structure essential for future development of an integrated solution.

As presented during the DigitalWorld conference 2009 in Cancún, México and with the Leadership in Research consortium, the proposed Computing Industry Alliance has been regarded to be a suitable umbrella organisation for Distributed and High Performance Computing and geoexploration sciences. The framework described is an example currently building the base for creating efficient interdisciplinary industry research cooperations for implementing the next generation of dynamical applications on Distributed and High Performance Computing resources based on the "Grid-GIS house" [13]. Interests to force this development exist not only in the Gulf of México region but as well in Russia and Saudi Arabia.

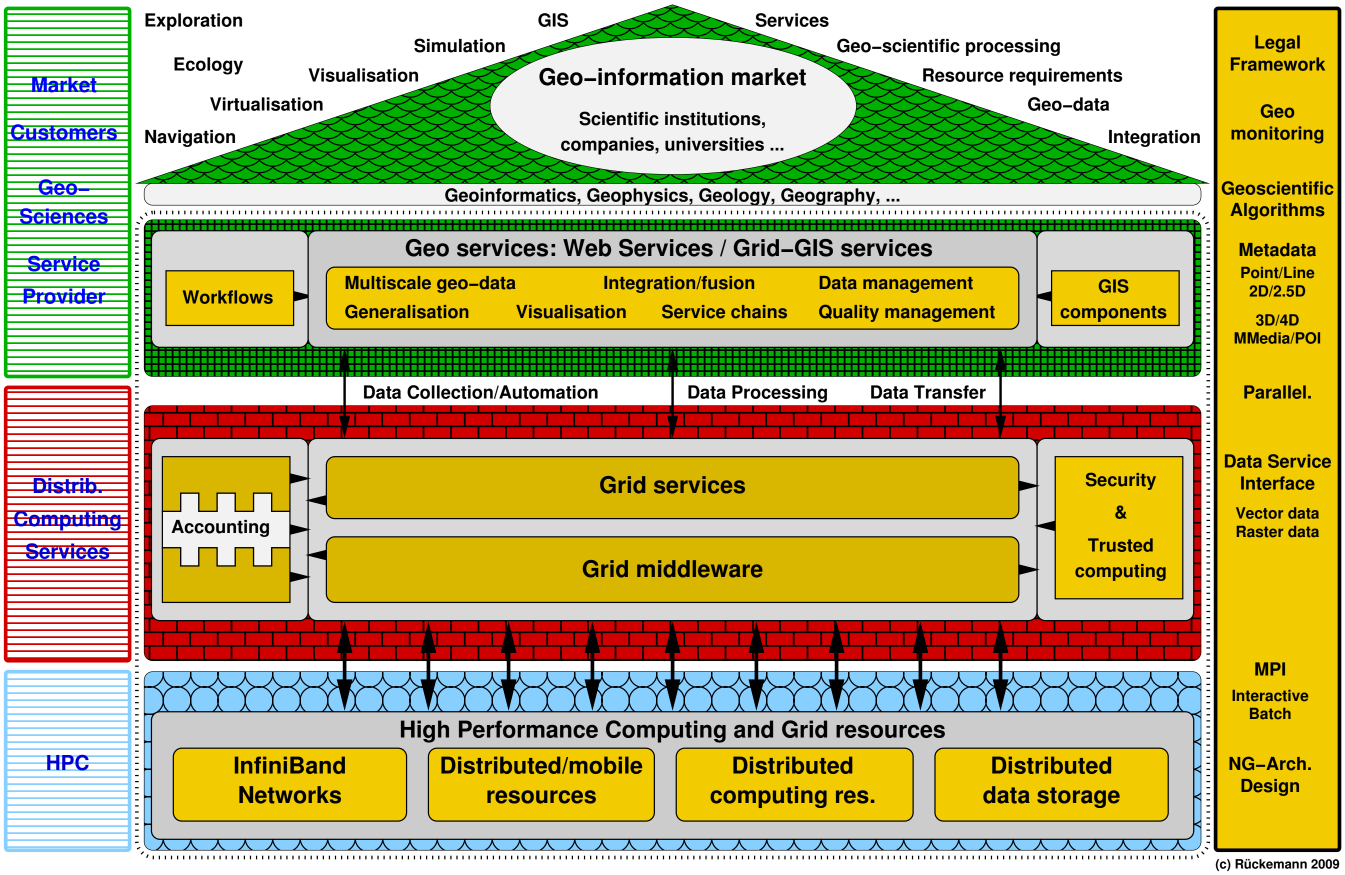

Figure 8. Future directions for service-oriented Distributed and High Performance Computing (“Grid-GIS house”).

11.3. Disciplines

Three key player collaboration sections from High Performance Computing and Distributed and Grid Computing, from services and technical development, and from Geosciences are currently building the next generation of information and computation system as shown in Figure 8.

- For the HPC and distributed resources section top level (blue) HPC computing companies are engaged. Next generation architectures and standards, for example hardware and network configuration, batch, and MPI, for using, accessing, and managing backend resources are the most prominent goals. Cooperations like DEISA [22] and PRACE [23] expedite the evolution and visibility of the core factors for the overall European resources.
- For Distributed Computing services, Grid and Cloud (red) various organisations and activities regarding services and technology will be important [24], [25], [26], [27], [28], [29], [30], [31]. A number of requirements regarding Security are exposed to be handled in interdisciplinary context [32], [33], [34], [35], [36]. For building a market ready network of partners a flexible accounting is most important. Regarding accounting, an integrated solution with complex accounting units suitable for this scenario has been proposed [2] considering suitable components [37], [38], [39], [40].
- On the level of market and services (green) various key players cover science and research, as for geosciences and exploration. A lot of work has been done in the previous years in the disciplines of geophysics, seismics, seismology als well as regarding oil and gas in order to exploit High End Computing resources [41], [42], [43], [44], [45], [46], [47], [48], [49], [50], [51], [52]. The work has already begun on parallelisation of geoscientific algorithms for parallel processing. The future work will bring the essentials of these disciplines together in order build an information and computing system for the exploration sciences.

Currently there are no comprehensive frameworks available, directly comparable to the Grid-GIS house. On this top level for the next years, legal as well as technical aspects are most important for integration of national an international geospatial data integration (GDI / SDI) frameworks like GSDI, INSPIRE, GDI-DE, GMES, GEOSS and Public Sector Information (PSI) into these concepts.

12. Summary and concluding remarks

In this article the implementation and employment of dynamical applications for use with Distributed and High Performance Computing resources has been presented. The concept relies on source code based scripting applications for utilising computing resources for specialised information systems and e-Science. Event-driven object graphics are based on Active Source, which has been developed within the GISIG actmap-project.

Based on the current framework, efficient access to distributed computing resources from HPC to Grid Computing can be achieved. Design and configuration in most cases of HEC has to consider the hardware and network components, too. Standardising interfaces helps to simplify the problems of resource usage and encourage developers and users to build new parallel networking applications. Overcoming these obstacles using Distributed and HPC resources for dynamical application, the step currently done is to implement platforms with commercial support for integrating these features into future applications.

The higher-level result is, that it will only be possible to accomplish the goal of a flexible integrated information system for geosciences and exploration using distributed High End Computing resources if partners from computing, services, and various geoscience disciplines will collaborate. With this goal and based on the extended Grid-GIS house, building an high end international information computing system for the exploration sciences is currently under way.

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