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GriPhyN Annual Report for 2001-2002

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GriPhyN Collaboration

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GriPhyN Annual Report for 2001 – 2002

The GriPhyN Collaboration

NSF Grant 0086044

Data Intensive Science

Paul Avery	University of Florida	Co-Director
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1 The GriPhyN Project

1.1 Introduction and goals

GriPhyN is a collaboration of information technology (IT) researchers and experimental physicists who aim to provide the IT advances required to enable Petabyte-scale data intensive science in the 21st century. The goal of GriPhyN is to increase the scientific productivity of large-scale data intensive scientific experiments through a two-pronged Grid-based approach:

- Apply a methodical, organized, and disciplined approach to scientific data management using the concept of *virtual data* to enable more precisely automated data production and reproduction.
- Bring the power of the grid to bear on the scale and productivity of science data processing and management by developing automated request scheduling mechanisms that make large grids as easy to use as a workstation.

Virtual data is to the Grid what object orientation is to design and programming. In the same way that object orientation binds method to data, the virtual data paradigm binds the data products closely to the transformation or derivation tools that produce data products. We expect that the virtual data paradigm will bring to the processing tasks of data intensive science the same rigor that scientific method brings to the core science processes: a highly structured, finely controlled, precisely tracked mechanism that is cost effective and practical to use.

Similarly for the Grid paradigm: we see grids as the network OS for large-scale IT projects. Just as today the four GriPhyN experiments use an off-the-shelf operating system (Linux, mainly), in the future, our goal is that similar projects will use the GriPhyN VDT to implement their Grid. The road to this level of popularization and de facto standardization of GriPhyN results needs to take place outside of and continue beyond the time frame GriPhyN; hence the partnerships that we will create between GriPhyN and other worldwide Grid projects are of vital importance.

One of GriPhyN's most important challenges is to strike the right balance in our plans between research – inventing cool stuff – and the daunting task of deploying that "stuff" into some of the most complex scientific and engineering endeavors being undertaken today. While one of our goals is to create tools so compelling that our customers will beat down our doors to integrate the technology themselves (as they do with UNIX, C, Perl, Java, Python, etc), success will also require that we work closely with our experiments to ensure that our results do make the difference we seek. Our metric for success is to move GriPhyN research results into the 4 experiments to make a difference for them, and demonstrate the ability of science to deal with high data volumes efficiently.

Achieving these goals requires diligent and painstaking analysis of highly complex processes (scientific, technical, and social); creative, innovative, but carefully focused research; the production of well-packaged, reliable software components written in clean, modular, supportable code and delivered on an announced schedule with dependable commitment; the forging of detailed integration plans with the experiments; and the support, evaluation, and continued improvement and re-honing of our deployed software.

This report is being written at the start of GriPhyN's 21st month of funding. Our research efforts in the areas of virtual data tracking and request execution have now borne fruit, and the virtual data toolkit has been created and proven as an effective technology dissemination vehicle. We demonstrated several important GriPhyN research developments at Supercomputing 2001 in Denver in November 2001, including the application of virtual data management and grid request planning and execution facilities, and real science scenarios drawn from CMS and LIGO. We have since demonstrated large virtual-data-enabled pipelines running galaxy cluster finding algorithms on Sloan Digital Sky Survey data, and have modeled virtual data techniques and tracking databases on ATLAS Monte Carlo collision event simulations. We have moved the CMS event simulation environment close to production readiness by greatly increasing the event production rates and reliability.

We have started continued to push our CS research forward, particularly in the areas of extending the scope of the virtual data paradigm, designing the dimensions of a policy-cognizant request management mechanism, enhancements to Condor and DAGman for efficient and reliable request execution, fault tolerance metrics and implementation strategies, and request execution strategies for gird storage services, and advanced models for incremental grid query planning and execution.

Our project has been steadily managed by a Project Coordinator (Mike Wilde of U Chicago/Argonne) and Deputy Project Coordinator (Rick Cavanaugh of U Florida) that have devoted significant time to the GriPhyN effort. Technical support for the project and for the development, and enhancement of web communication resources and conferencing facilities has been supplied by staff at the University of Florida.

During this time, we have held two collaboration wide meetings, at which students and postdocs made significant contributions, as well as numerous smaller meetings for CS research groups and CS-experiment interactions. The report below discusses these topics in more detail.

2 Activities and Findings for 2000–2001

2.1 Technical Progress

In general, technical progress over the past year can be summarized as follows: we gave the concept of virtual data a solid underpinning, and created a concrete roadmap for its evolution; we conducted extensive and detailed analysis of the data flows within a portion of each of the 4 GriPhyN experiments, concluding that virtual data will fit and can play a useful role; and we created and packaged the first virtual data toolkit and have leaned from this a great deal about how to integrate, package, distribute, and support this toolkit. Lastly, we have started forward-looking CS research in several areas: grid fault-tolerance; policy paradigms for grid resource allocation and scheduling, and data grid architecture to support advanced request planning.

The virtual data roadmap is elaborated in Section 3.6.1 of this report. With an initial implementation in hand and a long-term vision in mind, we engaged all four GriPhyN experiments in an in-depth dialog on the application of virtual data. From these discussions and numerous working, planning, and design sessions, we created specific plans to deploy virtual-data-based solutions in each one.

During the past 12 months, we have seen our first real applications of virtual data, including real processing pipelines for CMS (Monte Carlo simulations) and SDSS (galaxy cluster finding). These integrations of complex, actual application code with simple virtual data mechanisms have both demonstrated the applicability and utility of the virtual data paradigm and mechanism, and have also helped us see more clearly how to enhance and extend the paradigm. In the next few quarters we intend to see additional successful, realistic applications across all four experiments.

In this last reporting period we have also integrated and release the first several versions of the Virtual Data Toolkit, described below in Section 5, and created a mechanism for its support. While this initial toolkit contains pre-existing components, it will serve as the vehicle for delivering the subsequent products of the GriPhyN research effort.

The technical progress of the project is described in detail in Sections 3 through 7 and Appendix I of this report.

2.2 Creation of Working Grid Testbeds

The creation of grid testbeds for the different experiments has been accomplished to validate the main premise of the Virtual Data Toolkit (which is to provide simple, effective tools for building grids) and to provide the necessary infrastructure for research and development of grid-enabled software. Much work has been invested to demonstrate that the grid testbeds are able to provide the quality results required by the experiments. In some cases, emphasis has been placed on stressing the grid testbeds by submitting "at scale" production requests. This work has been remarkably successful and is more thoroughly described in the iVDGL Annual Report June 2001 - June 2002 [GriPhyN 2002-11].[1]

2.3 Education and Outreach

The GriPhyN Education and Outreach Program, closely tied to that of iVDGL, has been actively working on a wide variety of activities in the past 12 months. These are detailed in Section 8 of this report, and include: the creation of significant educational and outreach materials on the web; the development of Tier-3 centers at minority-serving institutions, with student participation that has yielded not only excellent educational opportunities, but also valuable feedback to GriPhyN technology developers; the development of tools to provide easy access to exciting scientific data for educational purposes at a wide variety of levels; the engagement of the EOT-PACI effort in coordination with GriPhyN and iVDGL activities; the planning of research opportunities among the GriPhyN CS and Experiment projects for undergraduate students; and a variety of other talks, presentations, and projects.

2.4 Coordination with other Projects

Over the past year, a symbiotic relationship amongst the three U.S. grid projects, GriPhyN, iVDGL, and PPDG has emerged and has led to a fruitful collaboration now known as the “Trillium”. This increased coordination has brought a convergence of ideas, allowing targeted research and development to proceed in conjunction with broader infrastructure deployment and testing. One good example of inter-project coordination is the decision to jointly manage releases of the Virtual Data Toolkit with the iVDGL. Inter-project coordination, including coordination with the European Data Grid Project, is discussed in more detail in the iVDGL Annual Report June 2001 – June 2002 [GriPhyN 2002-11][1].

2.5 Supercomputing Demonstrations

Several major GriPhyN accomplishments were demonstrated at Supercomputing 2001, held in Denver, Colorado.

One demonstration involved a Virtual Data System, including prototype virtual data language (VDL), applied to CMS Monte Carlo simulations. The Virtual Data System was able to track the dependencies of CMS data files and transformations (via CMS applications) between data files. As such, it was able to regenerate any (missing or deleted) derived CMS data file on demand across a grid testbed.[2]

Another accomplishment involved a CMS system for distributed analysis over the Grid. The demonstration involved a client/server application that allowed particle physicists to interactively analyze 105 GB of physics event data stored in two `tier 2 centers' that were part of a Virtual Data Grid system.[3] The demonstration showed key elements of a Data Grid system that CMS requires.[4]

Finally, LIGO demonstrated a prototype application of virtual data and of grid request planning and execution. This demonstration exposed much of the GriPhyN infrastructure. In particular, a 'Virtual Data Request' was formed by a broker on behalf of the client; this request was then sent to a Planner, which planned the necessary computations and data movements based on the resources available at Caltech, UWM and the SC2001 show-floor. The plan was then sent to Condor-G for execution, computation was initiated and monitored, and the result delivered to the client.[5]

For SC2002, the following demonstrations are currently being considered:

- An integrated Monte Carlo production system with virtual data tracking based on the second generation "Chimera" virtual data system. This system will be used to produce events for both the ATLAS and CMS projects, using simulation applications unique to each of those projects.
- The first application of virtual data to distributed HEP analysis, using example applications and scenarios also drawn from both ATLAS and CMS.
- A LIGO data analysis example which utilizes the Chimera virtual data system for tracking data derivations.
- A galaxy cluster finding application drawn from SDSS, with grid-based visualization on large multi-screen display panels.
- Illustrations of the concept of a virtual data browser.

2.6 Meetings

Members of the collaboration engaged in a large number of meetings for information sharing, project planning, architectural design, information dissemination and exchange, and cross-project coordination. A representative, but probably still incomplete list is presented here.

2.6.1 GriPhyN Collaboration All-Hands Meetings

- October 15-17, 2001 – ISI, Marina Del Rey, CA
- January 7-9 2002, University of Florida, Gainsville FL
- May 2002, Argonne National Laboratory, Argonne, IL

2.6.2 GriPhyN Special-focus meetings

- CS Research Coordination meeting, University of Chicago, August 3 2001
- ATLAS Project Meetings with GriPhyN Representation
    - ANL– Feb 10-11 2002 (Wilde representing)
    - BNL – May 6-7 2002 (Wilde representing)

- BU – June 12 (Wilde, by telecon)
- ANL – 4 database design sessions – Q1-2002 w/ Frank, Gardner, Malon, Vaniachine, Wilde

- LIGO and Virtual Data at ISI, all week design sessions (Deelman, Mehta, Vahi, Voeckler, Zhao, Wilde) – March 2002
- CMS Caltech – Oct 2001 – Steenberg, Litvin, Wilde
- CMS & EDG – Visit to CERN – Jan 29-30 2002 (Wilde, Wildish, Stickland, Grandi, Lefebure, Holtman, Innocente, Gagliardi, Jones)
- CMS CERN – June 2002 (Cavanaugh, Voeckler, Graham, Lefebure, Grandi, et al)
- DESY – Jan 2002 (Wilde, Ernst, Wolf)
- Numerous meetings at FNAL with SDSS – approx 5 (Foster, Wilde, Voeckler, Zhao, Kent, Annis)
- Numerous meetings at FNAL with CMS – approx 7 (Wilde, Voeckler, Zhao, Graham, Amundson, Pordes, Musaffar)
- Numerous meetings with ANL ATLAS staff – approx 3 – (Malon, Vaniachine, May,Wilde, Voeckler, Zhao)

2.6.3 GriPhyN Representation at other Project meetings

- PPDG – Workshop on Replication and Data Transfer – Madison Wisconsin Aug 2001
- PPDG – Replication Workshop – JLab, Jan 10, 2002
- PPDG – All Hands Toronto Canada – (W GGF4) – January 2002
- PPDG – Scheduling Workshop – FNAL – May 2002
- PPDG – Interactive Data Analysis Workshop – LBL, June 2002
- Distributed Teragrid Facility – Project Kickoff – ISI, Marina Del Rey CA– 27 Nov 2001
- Distributed Teragrid Facility Application Meeting – April 2002, Argonne National Laboratory

2.6.4 GriPhyN Advisory Board meetings

The External Advisory Committee (EAC) consists of nine members, with Messina and Reed acting as co-chairs:

Paul Messina	Caltech	Director, Center for Advanced Computational Research
Bill Johnston	LBNL	Director, NERSC
Fabrizio Gagliardi	CERN	Project Leader, EU DataGrid
Jim Gray	Microsoft	Microsoft Research
David Williams	CERN	Former Head, CERN IT Division
Joel Butler	Fermilab	Former Director, Fermilab Computing Division
Dan Reed	NCSA	Director, NCSA Alliance
Fran Berman	SDSC	Director, SDSC
Roscoe Giles	Boston U.	Head of EOT-PACI

The EAC met with the GriPhyN project team for an open all-hands review on Jan 7, 2002. The material presented at that review[6] and the committee's report on the project's progress[7] are available on the GriPhyN web site. In general, the committee concluded that very good progress had been made and that the project was on track to deliver successful results. Valuable suggestions were made and are being followed by the project.

3 CS Research activities

Computer science research during the first nine months of the GriPhyN project has focused on three main activities:

- Construction of two releases of a virtual data system, which includes a virtual data catalog
- Request planning and execution: algorithms and architectural issues
- Understanding the architectural interactions of data flow and work queuing and scheduling

In addition, the first phases of research work has begin on:

- Understanding fault tolerance for the grid: metrics and strategies
- Policy definition and implementation strategies
- Characterization of data grid workloads in GriPhyN application domains

We review the progress in each of these areas in the following sections, organized by institution.

Activities for the LIGO and SDSS experiments are described under the CS research institutions with which those experiments collaborate most closely – for LIGO, ISI, and for SDSS, the University of Chicago.

3.1 Information Science Institute of USC (including work on the LIGO Experiment)

3.1.1 Virtual Data Catalog Design

For the past year we have focused on realizing the concepts of Virtual Data particularly in the context of LIGO but also as it applies to other experiments. In collaboration with University of Chicago, we have laid out an architecture composed of a collection of catalogs which will work together provide transparency with respect to data location and materialization. Some of the catalogs, such as the Replica Catalog, which maps logical filenames to their physical instances are part of the standard Globus software. Other catalogs, such as the Transformation Catalog which maps need to developed.

In the past year, ISI has designed a Transformation Catalog, which can be used to store information about logical transformations and their physical instances (installed, binary, source). This catalog can be used to locate the appropriate executable for a given architecture or if one is not available the source code for a desired transformation. The initial design can be found in the GriPhyN report 2001-17.[8] We are currently in the process of finalizing the design and schema for the catalog and expect to have the catalog implemented in the next few months.

3.1.2 Demonstration of LIGO's Virtual Data Concepts

In November 2001, we have demonstrated the initial Virtual Data concepts in the context of the LIGO experiment. The overall design of the prototype is shown in Figure 1.

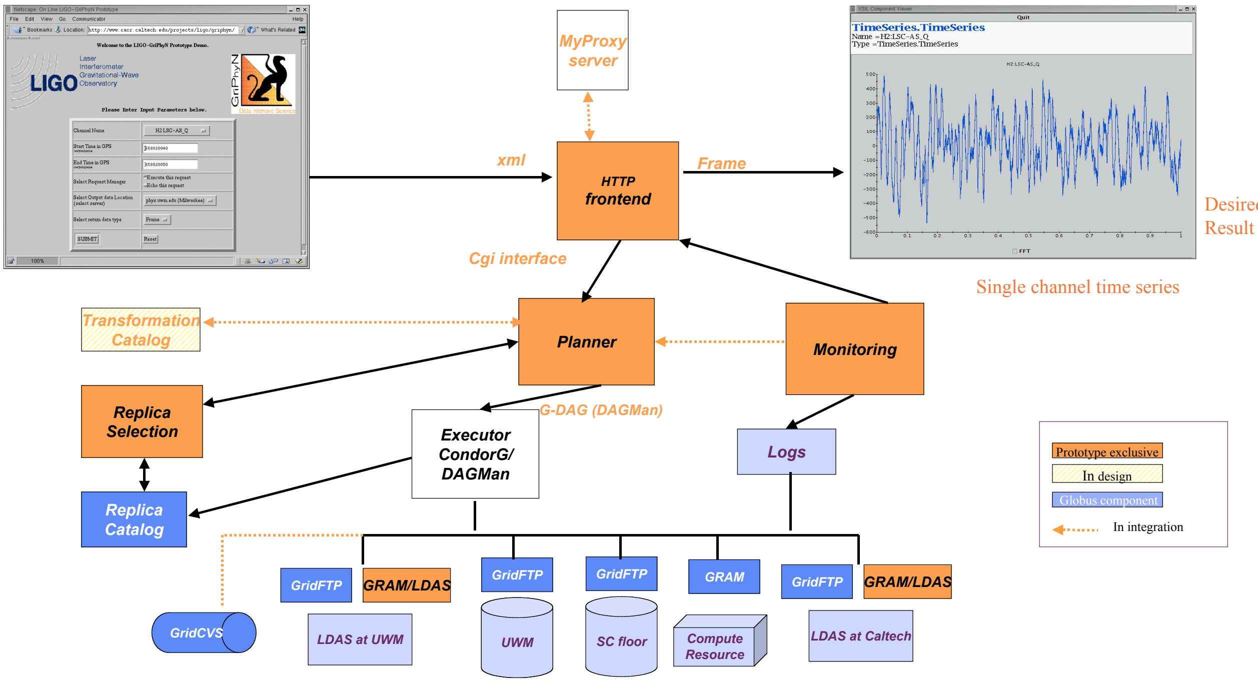

Figure 1: GriPhyN/LIGO Prototype Overview Demonstrated at SC 2001.

The prototype was designed to work in the context a Virtual Data scenario, where the user can request data products such as the seismometer channels for 3 days in April 2001. For each requested data the system would then needs to:

- Determine if the data product is instantiated, if so where, if not, how to compute it.
- Plan data movements and computations required to obtain all results
- Execute this plan.

The detailed prototype functionality was as follows:

- User inputs request using a web browser. User can specify:
  - Data channel name
  - Time of interest
  - Desired output data location
- Request is transformed into XML
- Request Interpreter: Understand an XML-specified request
- Acquire user's proxy credentials
- Replica Selection: Consult replica catalog for available data, select replica "closest to the desired output location"

- Request Planner:
    - If data available: plan necessary data movement
    - Else: Construct a plan to produce data not available, including execution location selection. Select input data location ("close to compute resources"), schedule data movements etc…
    - Specify plan in DAGMan format (a Condor-G specification format)
- Request Executor: submit DAGMan specified plan to Condor-G
- Return requested data to the user specified location in Frame format
- Provide a graphical view of the data by using the XSIL frame viewer.

In addition to demonstrating the transparency with respect to data location and data materialization, we have also achieved the integration of software such as Globus components and Condor-G. We have also designed and implemented the Globus interfaces to the LIGO Data Analysis System (LDAS[9]). Using these interfaces, we were able to stage data in and out of the system and schedule jobs to be executed within the LDAS environment.

3.1.3 Request planning

The request planner developed within the SC 2001 prototype was a planner that identified an appropriate course of action given the current location of the data in the system. This type of planner however, although adequate for the demonstration, does not provide the necessary flexibility we seek for a general solution.

As part of the research into request planning, we have investigated the usefulness of AI planning techniques. AI planners seeks to build control algorithms that enable an agent to synthesize a course of action that will achieve its goals. In classical planning the objective is to achieve a set of defined goals expressed as positive and negatives literals. The planners normally take two inputs.

1. The facts file which is the current view of the world and describes the initial state of a system and its resources.
2. The domain file which has information about the various types used in the system and the various predefined actions that can be done on the resources of the system to achieve a desired result.
3. An optional the control file which puts restrictions on the kinds of decision a planner may make.

We have evaluated two commonly used AI planners, such as Blackbox and FF, and have found that they have some disadvantages:

- There is no way to represent a time model for the planners. One cannot satisfy the duration of an action or specify time constraints on either goals or actions. All actions are modeled as if they are instantaneous and uninterruptible.
- One cannot specify resource consumptions or requirements.
- There is no ability to model uncertainty--the initial state of the world and actions are assumed to be certain.

- There is no provision for providing a goal with optimization factors.

In summary, we concluded that neither Blackbox nor FF are ready to use as they are for the purposes of request planning within GriPhyN. We are continuing researching and developing request planning solutions that would meet GriPhyN's requirements. Our goal is to start with a simple planner and increase its level of complexity as we develop more sophisticated solutions.

Currently, we have integrated a simple planner with the Virtual Data System—Chimera. This planner takes an abstract DAG specified by Chimera and builds a concrete DAG which can then be executed by Condor-G. In the abstract DAG the locations of where the computation is to take place nor the location of the data are specified. The planner consults the replica catalog to determine which data specified in the abstract DAG already exists and reduces the DAG to only the minimum number of required computations and data movements. Finally, the planner transforms the abstract DAG into a concrete DAG where the execution locations and the sources of the input data are specified. This DAG is then sent to Condor-G for execution.

3.1.4 Fault tolerance

We are currently designing a framework in which we provide a means of identifying the likelihood of failure of particular Grid components. Our approach combines information related to the success or failure of various tasks running on the Grid with prior information about the possible causes of a failure. This information is used to determine the most likely faulty component when there is possibility of a failure in the system. Currently, our assumptions are that the system has an estimate of the amount of time required to accomplish various tasks. This estimate might be a range rather than an exact number and we consider its upper bound to be the maximum amount of time that the task will take to complete if there is no possibility of failure in the system. We also consider the non-completion of a task within this amount of time to be a possible failure and use information about the completion or non-completion of other tasks that are scheduled simultaneously on the same set of resources to determine the possible cause of the non-completion of the task in question. In this work, we have used the Bayesian Belief Networks to update these probability distributions as new information is collected about the behavior of the system. The updated probabilities reflect the most likely cause of a failure. Information about the most likely faulty component in the system will allow us to generate better plans for fulfilling user's requests or scheduling repair and maintenance on the system.

3.1.5 Future Plans

Our plans for the next year focus on four main areas.

- Development of more sophisticated planning techniques. We plan to increase the level of complexity and sophistication of the planner by taking into account current system information provided by such services as the Globus MDS and the Network Weather Service. We will also implement and integrate the Transformation Catalog into the planning system to enable the planner to determine the suitable execution locations for the data analysis.
- Support a larger set of LIGO's Virtual Data products. We have identified the LIGO's pulsar search as an important representative problem for the LIGO community. The search includes data analysis both in the time and Fourier domains. We will develop a model for the data products used in the search and will populate Chimera with the necessary information.

- As part of expanding the set of Virtual Data products we will develop a Metadata catalog which interfaces to Chimera and allows for the identification of data products, raw and derived with the use of application-specific metadata attributes.
- Support for the execution of jobs which are commonly executed within the LDAS system. Many sophisticated LIGO analyses are currently conducted within the LIGO Data Analysis System. In order to fully make use of the Grid environment, we need to be able to export the LDAS analysis onto the wide area environment.

3.2 Northwestern University

The work at Northwestern University, conducted by Valerie Taylor, associate professor, and Lin Yin (post-doctoral researcher, started March 2002), has focused on monitoring and analyzing the performance of the ATLAS experiment, in particular the Atlfast simulator. Using the auditors available within Athena, the Atlfast simulator was analyzed in terms of different generators and identifying the time attributed to the different algorithms for the different generators. At this time, we are working closely with some key ATLAS researchers at LBL to provide performance feedback on the simulator. Another goal of this work is to use the Prophesy Infrastructure to develop performance models for the simulator that can aid in evaluating different execution environments by the replication manager. The performance data is available to researchers via a dedicated website and the Prophesy database.

Future work is focused on detailed monitoring of the ATLAS experiments, identifying where time is spent within the different algorithms used in each experiment. This work entails utilizing the Prophesy Infrastructure to instrument some of the algorithms. The result of this work will be detailed performance models for the replication manager as well as performance feedback for the algorithm developers and ATLAS researchers. Work is also in progress for incorporating the monitoring work into a demo for SC 2002.

This work is described in three publications: *PAIDE: Prophesy Automatic Instrumentation and Data Entry System*, IASTED Conference on Parallel and Distributed Computing, August 2001; *Prophesy: Automated Performance Analysis of Distributed Applications*, invited paper to the Active Middleware Services (AMS) Workshop, August 2001; and *Using Kernel Couplings to Predict Application Performance*, to appear in HPDC-11, July 2002.

3.3 San Diego Supercomputing Center

Personnel on this project are Xufei Qian, Amarnath Gupta, Arun Jagatheesan, Arcot Rajasekar, Bing Zhu, Reagan Moore.

Data management is driven by competing requirements: improvement of access to data for use within computations, data sharing between collaborators, and management of the long term storage and organization of material within collections. The Storage Resource Broker[10] has focused on high-level grid services for the creation and management of collections that are distributed across multiple storage systems, either for data sharing or for long term management. The SRB manages distributed data through the use of storage repository abstractions that define a uniform set of operations for manipulating data, and through the use of information repository abstractions that define a uniform set of operations for manipulating catalogs in databases. These abstractions are implemented using a logical name space that is organized as a collection hierarchy. The result is the ability to generate generic virtual data catalogs. Within the GriPhyN project, the SRB technology is being used to prototype data sharing environments for CERN, prototype generic virtual data catalogs, and prototype distributed data collections. A grid-enabled version of the SRB collection management is being developed that interoperates with GSI authentication and GridFTP transport services. The major research goal is the integration of knowledge management for describing virtual data products on top of the collection management systems.

Virtual data catalogs can be modeled as an instance of a knowledge space that describes the relationships between simulation output files and the associated applications. By applying generic knowledge management systems, it is possible to extend the definition of virtual data to include knowledge about the underlying data models, physical constraints, and application relationships. SDSC technology is being used to create generic knowledge spaces. The components include template-based relationship identification, relationship management, and inference rule generation. The three principal efforts at SDSC include demonstration of a virtual data catalog, knowledge management tool development, and Storage Resource Broker (SRB) development.

A virtual data catalog was implemented using the SDSC Metadata Catalog (MCAT). Templates were developed that support the extraction of virtual data relationships from a VDL file, and the ingestion of the relationships into an MCAT catalog. Arbitrary queries are supported against the catalog. To facilitate interaction with the collection, WSDL interfaces were created for selected data manipulations. The system forms a simple version of a knowledge space in which relationships are restricted to input/output file semantic equivalences.

A generic knowledge management system was developed that extends the concepts behind virtual data catalogs to support creation of inference rules for applying relationships. The relationships are stored in a relational database and characterized by their dependence on a data model, by application constraints, by logical semantic rules for describing semantic relationships, and by data model methods. Note that the logical semantic rules are effectively "relationships" about "relationships". Tools were developed to extract relationships from the database, and convert them into logical inference rules. This effectively makes it possible to build an application from a generic description of the underlying relationships and constraints.

The SRB data handling system was extended to support digital entities, including files, directories, tables, SQL command strings, and URLs. This capability can be used to register knowledge relationships and virtual data. The mySRB web interface was developed to demonstrate manipulations of digital entities within a logical name space. The name space is organized as a collection hierarchy, with each sub-collection and each object able to be characterized by unique attribute sets. This makes it possible to build a virtual data catalog that contains not only the descriptions of the data creation process, but also the underlying relationships and the resulting output files. The integration of the generic knowledge management system with the MCAT catalog is the next step.

3.4 University of California at Berkeley

GriPhyN research at UC Berkeley Computer Science during the past year has focused on two topics:

- Infrastructure support for interactive data analysis
- Understanding the relationship between Virtual Data and database views

Research conducted at Lawrence Berkeley Laboratory Scientific Data Management Group focused on policies for storage management in systems with widely varying latency, such as tertiary systems and wide-area networks and data grids.

UCB CS Participants and Collaborators: Michael Frankin (PI), David Liu (Ph.D. student), Asha Tarachandani (M.S. student, graduated 6/02), Sarika Agrawal (Undergrad), Honfai Cheng (Undergrad)

LBL SDMG Participants and Collaborators: Arie Shoshani, Ekow J. Otoo, Frank Olken and Donghui Guo.

3.4.1 Interactive Query Processing using Partial Results on the Grid

Much of the existing software infrastructure for the grid assumes a "batch" style of interaction, where scientists submit a processing request and must then wait for the entire result of the request to be computed. While the grid can help reduce the processing time for such requests from months to hours or days, such delays are not suitable for scientists' most common task, namely, data analysis. In our work, we are seeking to move away from this batch mode of processing and to allow grid users to have interactive response times for their data analysis tasks. Interactive response has the potential to revolutionize the way that scientists approach the data analysis task, much in the same way that interactive data analysis has impacted other domains such as business planning, drug discovery, and information retrieval.

The support of interactive processing impacts the entire software stack, from the need to provide appropriate user interfaces to visualize and manipulate data, to the need to allow fine-grained interaction and pipelining between the steps in the data processing workflow. To date, we have focused on the lower levels of the software stack, looking at how to perform resource allocation, scheduling, and interaction at a fine-grain among data processing tasks. We have constructed a prototype implementation called "Telegrid" that uses the Condor package to run multiple jobs but uses a new fine-grained scheduler to stream partial results back to the user. These results are then fed to a user interface module that allows the display of incrementally improving results. Advantages of this system include: 1) the early identification of outliers and other regions of interest, 2) interruption of jobs that appear not to be providing the desired result, and 3) fast survey of a larger area of the data space.

The initial results of this work have been presented at several meetings including the GriPhyN all hands meeting in April 2002, and the PPDG Interactive Data Analysis Tools meeting at Berkeley in June 2002.

3.4.2 Virtual Data and Database Views

In the GriPhyN project, Virtual Data is the term used to denote derived data that may be cached on the grid. Even though Virtual Data can always be derived from raw data, caching it will make it readily accessible for satisfying requests more efficiently. The primary goal of Virtual Data is to improve the performance of the grid. In databases, View Materialization is a well-established technology that also has the goal of improving performance and shares the same concept of result caching. In this project, we first surveyed the literature underlying these two techniques and then compared and contrasted both their goals and their implementations. We then focused on how the schemes and methods used in View Materialization can be applied in the context of the GriPhyN project.

The result of this study was a set of recommendations for modification and extension of the virtual data concept that would allow the exploitation of well-established implementation and optimization techniques from the materialized view literature. These recommendations included:

1. Extend the Virtual Data Language (VDL) to allow specifications of semantics and performance information about the application code.
2. Extend VDL to include a type system.
3. Extend VDL to include high-level data manipulation operators that can be used to express scientific computations.
4. Investigate specific database techniques such as extensibility APIs in Object-Relational Database Systems as a way to provide extensibility in the GriPhyN project.

These recommendations were discussed at a meeting on Virtual Data held in June 2002 at the University of Chicago with GriPhyN participants and a select group of database researchers. The study is presented in detail in the paper *A comparative study of Virtual Data and View Materialization*, University of California, Berkeley, June 2002.

3.4.3 Policies for Data Grid Storage Resource Management

Work carried out on the GriPhyN project involved the design and implementation of Policy Advisory Module (PAM) to be used as an integral software tool of a Storage Resource Manager (SRM)[11] in a data-grid. While an SRM is the principal middleware for coordinating multiple file requests over an interconnected network of storage resources, the decision as to which file requests should be scheduled next, and which file must be evicted from the cache of a particular SRM when space is needed, is made by PAM. Towards this goal, we carried out the following activities:

1) Studied various cache replacement policies used in main memory caching, disk caching, and web-caching to determine which replacement algorithm would best address the caching requirements in an SRM. The main results achieved are:
   a) The use of average access cost per reference as a new metric for evaluating disk caching policies.
   b) Derivation of two new replacement policies for file eviction from the cache.
2) Implementation of a simulator for evaluating different cache replacement policies. Using both synthetic and real workload of file accesses, we concluded that the proposed new replacement policies perform better under the average access cost per reference metric than the traditional replacement policies. These should therefore be the appropriate replacement policies for disk caches in SRMs. The main results of our studies are presented in the extended abstract of a paper[12] to appear in the 2002 Supercomputing Conference.
3) Implementation of a simulator that combines scheduling policies of file requests and the file replacement policies at each site of a storage resource manager. The work is still ongoing. This work also provides a test-bed for the code being developed for PAM and forms the basis for the design of the Application Programmer's Interface (API), that is being developed for communicating between a PAM and an SRM.

This work is described in the paper *Disk cache replacement algorithms for storage resource managers in data-grids*, to be presented in the Supercomputing Conference, 2002.

3.5 University of California at San Diego

The UCSD CSE group has been working on issue of fault-tolerance in GriPhyN. Our work has been focused on two activities:

First, we have been working to identify which part of the architecture is most exposed to the failures that one would reasonably expect to occur in systems like GriPhyN. Most of the services that we have considered are easily made resilient through well-known techniques such as primary-backup, checkpoint-restart. and fault isolation for user code. The part of the GriPhyN architecture that has the largest exposure is the translation of an abstract DAG into a concrete one. This part, which both measures system information and constructs a plan based on this information, has several vulnerabilities and can be made more robust with at least three different techniques. We have been working on understanding the efficacy of these approaches.

Our second activity concentrates on one of the three techniques: replication techniques for making progress when the sysetm is partitioned. Lacking a clear example from GriPhyN, we have been working on a well-known problem: master-worker computation. We believe that this problem will arise in concrete DAGS in GriPhyN which will exhibit considerable concurrent activities. We have:

- Examined several protocols (that have appeared in PODC) that have been developed to be optimal for an important metric: the number of times a task is executed. If a task is started on a processor that partitions away from the rest of the system, then it will be necessary to restart the task on another processor rather than wait an unbounded time for the results from the original execution. The specification of these protocols are carefully stated to isolate this metric without admitting otherwise useless solutions (such as executing all tasks on the master's processor) and without adding additional requirements (such as minimizing turnaround time).
- These protocols use *group membership*, which is a well-known protocol that allows processes to agree on the composition of *connected components*: maximal subsets of processors that can mutually communicate. We have been evaluating the efficiency of these protocols and of group membership in a real wide-area setting via simulation. To drive this simulation, we have been using traces that have been generated at MIT as part of the RON (*Reliable Overlay Network*) project. Early results indicate that group membership should exhibit poor performance in practice. We are working on obtaining more accurate wide-area network traces, both from the RON project and from another project at MIT under the leadership of Idit Keidar.
- We have developed some simple protocols for master-worker computation in a wide-area network that, while not optimal, should in practice do well in reducing the number of redundant task computations. Under simulation they appear to work well. We have been implementing these protocols as a new version of the Condor Master/Worker tool.

3.6 University of Chicago (includes Sloan Digital Sky Survey)

3.6.1 Virtual Data Research and Tools

A key area of research at Chicago was the exploration of the virtual data paradigm and the design and implementation of a toolkit to make virtual data facilities generally available to the GriPhyN collaboration and other projects.

Two generations of a Virtual Data System (VDS) were designed and implemented. The first, VDS 0, was a prototype, consisting of a simple textual interface language, the Virtual Data Language, or VDL, along with an interpreter for this language and a database to store persistent VDL definitions.[13] The VDL allowed for the specification of simple transformations and derivations, and provided a basic mechanism for the definition of parameter passing. Using this VDL we are able to implement a 4-statge CMS Monte Carlo Event simulation pipeline, and generate real events. We also developed a simple "canonical application", *keg* (or, Kanonical Example for GriPhyN), which allowed us to simulate more complex data dependency derivation chains. Using the VDL and keg, we were able to construct and test DAGs with hundreds of nodes and relatively complex topologies.

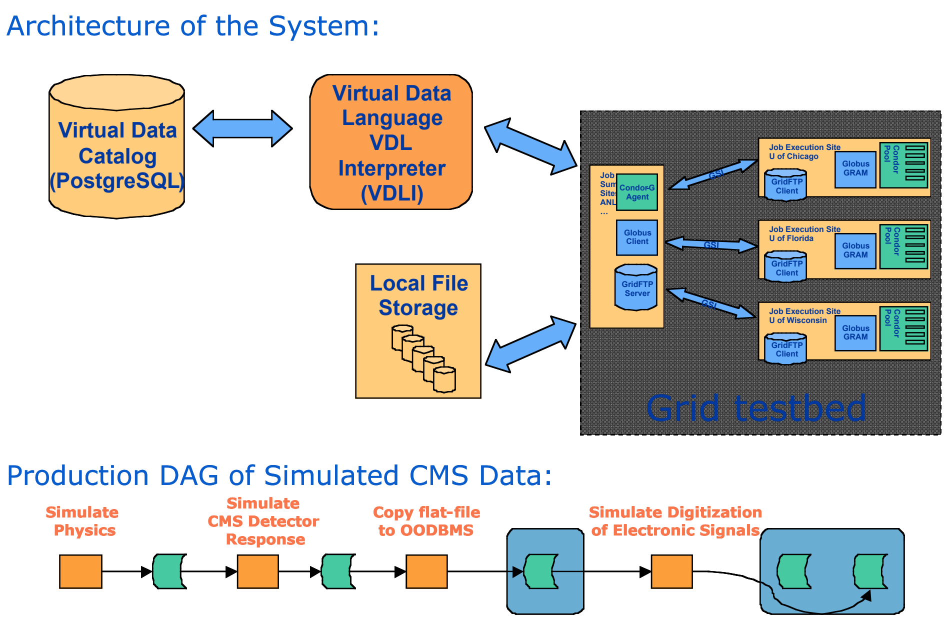

Figure 2: CMS Monte Carlo production system with VDS-0

A significant effort then went in to the definition of VDL 1, which was designed to be a widely deployable and usable VDL implementation. The VDL language was enhanced, and was specified in both a textual and XML format. The textual version is intended for use in the manual creation of VDL definitions, for use in tutorial, discussion, and publication contexts. The XML version is intended for use in all machine-to-machine communication contexts, such as when VDL definitions will be automatically generated by application components for inclusion into a VDL definition database.

The VDS-1 system, (Figure 3) which we have now named Chimera[14], is implemented in Java, and currently uses a very simple XML text file format for the persistent storage of VDL definitions. Its virtual data language provides a simple and consistent mechanism for the specification of formal and actual parameters, and a convenient paradigm for the specification of input parameter files. VDS-1 will be packaged and released during Summer 2002 to support application integration experiments and demonstrations later in the year.

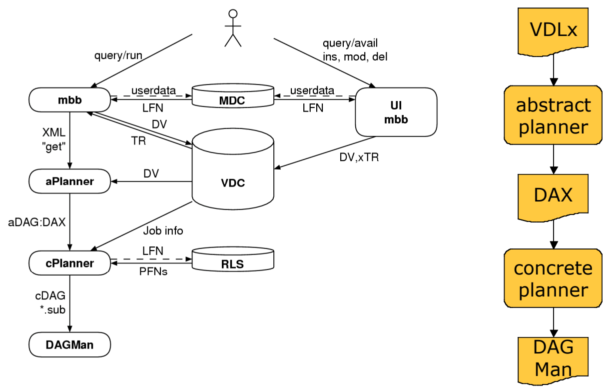

Figure 3: VDS-1 System

A large number of VDL language extensions have been proposed and studied, and are in varying states of specification, design and implementation. These include:

- compound transformations, to enable transformation designers to compose sophisticated transformations from simpler ones in much the same manner as functions are composed in a typical programming language
- Virtual Transformations A very exciting avenue currently being explored is that of datasets and virtual transformations. While transformations in VDL 1 consume and produce *files*, most application scientists seeks to work in terms of datasets, which are typically a logical construct that abstract away file boundaries. A dataset may consist of multiple files, or of a slice of a single file. They can be represented in multiple ways, ranging from a simple set of files of identical format, to a set of files with special purpose file types, indexing databases, etc.
- Instance tracking of derived data products. The model currently does not differentiate between multiple instances of the same derivation (perhaps generated at different times and/or at different sites). We propose to extend the model to track transformations, derivations, and instantiations.
- The handling of multi-modal data (flat, relational, object, and XML) in a uniform manner.
- The expansion of our model of what transformation consists of, to include more details of the transformations precise version, its dependent virtual operating environment (e.g., a detailed list of shared library modules on which the transformation depends) and a model to represents how multiple versions of the transformation are to execute on different processor types and operating system environments.

3.6.2 Sloan Digital Sky Survey Challenge Problem Progress

In this effort we applied virtual data and Data Grid concepts to the SDSS application of cluster identification. The challenge problem, addressed by researchers at Fermilab (Annis, Kent) and Chicago (Zhao, Voeckler, Foster, Wilde), is that of identifying clusters of galaxies, which are the largest gravitationally dominated structures in the universe. This problem involved the use of complex, existing applications developed for the Astrotools framework.

The SDSS software environment, in which the “maxBcg” (maximum-likelihood brightest cluster galaxy) cluster-finding algorithm is implemented, was integrated with Chimera and a test grid was constructed, as shown in Figure 5. The work summarized here is described in a paper accepted for SC2002 and for which a detailed extended abstract is available[15]. Much of this description is derived from that paper.

In this research, we treated cluster catalogs as derived data that are constructed from base data (galaxy catalogs), with the contents of a particular cluster catalog depending on the cluster location algorithm used and on the parameter choice for the algorithm. We used the Chimera virtual data system to generate cluster catalog data. We demonstrate our ability to encode interesting algorithms and to track the materialization of both final cluster catalog data and useful intermediate products. We addressed, and obtained promising answers to, the following questions:

- Can we represent the transformations of the problem in the virtual data catalog?
- Will the overhead of managing the VDC be easier than doing this work in an ad-hoc fashion?
- Will the derived data be traceable in the manner expected?
- Will the computations map onto effective DAGs for efficient grid execution?
- When code or data changes can we identify dependent re-derivations?
- Will the virtual data paradigm enhance overall productivity?

In the integrated system that was developed, bulk background data production can be readily performed in parallel with interactive use. In this mode, the virtual data grid acts much like a large-scale cache. If a data product is produced through the batch process before it is needed interactively, then at the time of the interactive request no computations need be scheduled to produce it. If a data product is requested before the batch process has produced it, the required derivations will be executed on demand, and the results stored, eliminating the data item from the batch process work list.

The maxBCG algorithm consists of five file-based transformations. The input and output files of each stage form a natural dependency graph, as shown in Figure 4, where the nodes represent data files and the arrows the transformations listed below. The first stage and second stage are straightforward in that each output file corresponds to one input file. The third and fourth stages operate on a “buffer zone” around the target field, and the bcgSearch stage (transformation 3) needs to take both field files and brg files as inputs. The transformations are:

- *fieldPrep* extracts from the full data set required measurements on the galaxies of interest and produces new files containing this data. The new files are about 40 times smaller than the full data sets.
- *brgSearch* calculates the un-weighted BCG likelihood for each galaxy (the BRG likelihood, unweighted by galaxy count, is used to filter out unlikely candidates for the next stage)
- *bcgSearch* calculates the weighted BCG likelihood for each galaxy. This is the heart of the algorithm, and the most expensive step.
- *bcgCoalesce* determines whether a galaxy is the most likely galaxy in the neighborhood.
- *getCatalog* removes extraneous data and stores the result in a compact format.

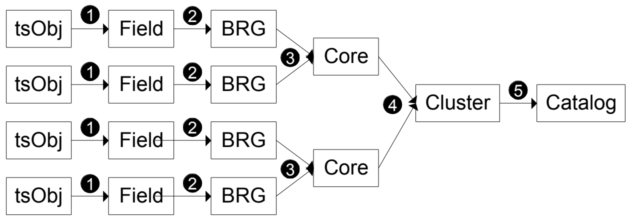

Figure 4: SDSS cluster identification workflow graph.

An important aspect of Chimera is the management of the input files containing complex input parameters. Instead of keeping all of these detailed parameters in the Chimera database, we built transformations in Chimera that take the primary changeable parameters as arguments and incorporate those parameters into *parameter file templates*, which contain numerous seldom-changed parameters, and generate complete parameter files as output. These transformations are then incorporated into the user application DAG to generate the parameter file used by the code. We only need to maintain a few templates, which can be instantiated unlimited times. With this technique, the Chimera database contains (in its derivation records) all parameters required to rerun the derivation.

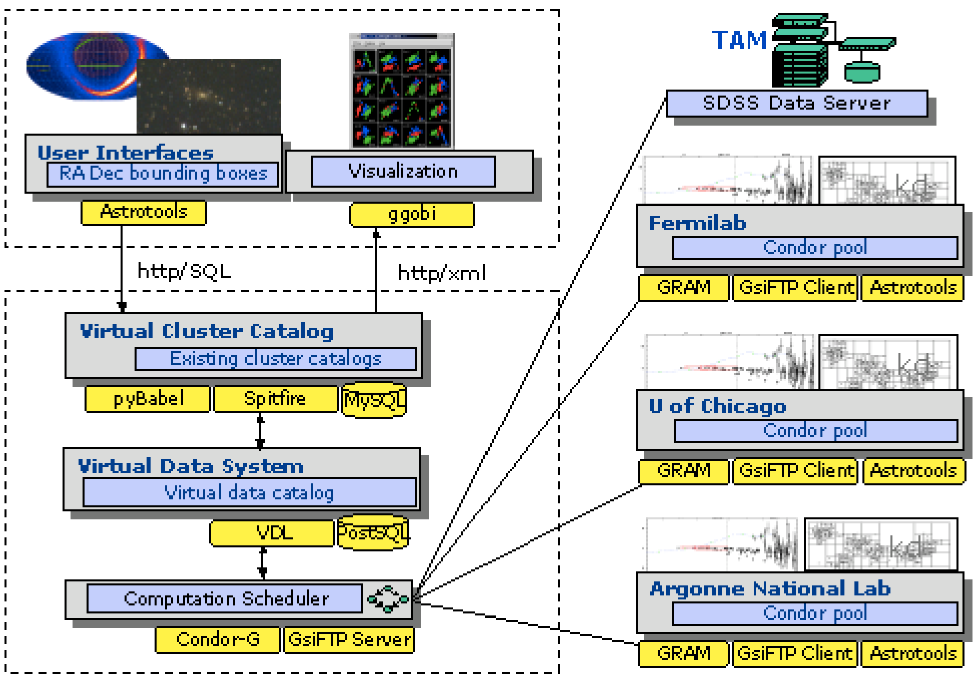

Figure 5: Architecture for integration of Chimera into SDSS environment for cluster-finding.

3.6.3 Exploration of policy-based resource sharing and allocation mechanisms

We have started a research effort, over the past six months, to study the paradigm of policy-based resource sharing in a virtual data grid context. This effort is in support of a fundamental goal of the GriPhyN project: to enhance scientific productivity by allowing scientists to express grid requests in terms of the data products they desire to produce, and to be able to initiate such requests on the grid in a manner that treats the grid as a simple but enormously powerful workstation. The latter of these two capabilities, we expect, will be derived from the ability to create highly-intelligent grid scheduling mechanisms which allocate resources for both interactive and batch-production work *in a manner that is cognizant of resource utilization policie*s which take into account the *apportionment of grid resources between different user communities*, and for different purposes.

Our work in this area of policy-driven scheduling includes creating paradigms for specifying resource apportionment on a grid, taking into account the scaling factors for heterogeneous resources, and the averaging of resource shares over large time quanta, the ability to use "left over" shares of resources for effective purposes, and the ability to account for and charge for the use of grid resources.

This work has led us to explore the nature and representation of virtual organizations, physical organizations, and of grids themselves. We are exploring the representation of a "grid" as a concrete entity between physical and virtual organizations, to serve as a resource aggregator and distributor. We are trying to apply the Community Authorization Service in the role of policy storage within this architecture.

Initial experiments have been conducted into the implementation of fair-share scheduling mechanisms within Condor and PBS. Our preliminary results from this work indicates that it will be readily possible to schedule grid work in such a manner that resources are apportioned according to role- and group-based policies, and that such models can be readily extended to the grid level.

3.6.4 Resource and Replica Discovery

In a wide area computing system, it may be desirable to create remote read-only copies (replicas) of data elements (files)—for example, to reduce access latency, increase robustness, or increase the probability that a file can be found associated with idle computing capacity. A system that includes such replicas requires a mechanism for locating them. We thus define the replica location problem: given a unique logical identifier for desired data content, determine the physical locations of one or more copies of this content. We further define a replica location service (RLS) as a component that maintains and provides access to information about the physical locations of copies. This work is described in *Giggle: A Framework for Constructing Scalable Replica Location Services* (to be presented at SC2002).

A related research effort explored a decentralized, adaptive mechanism for replica location in wide-area distributed systems. Unlike traditional, hierarchical (e.g, DNS) and more recent (e.g., CAN, Chord, Gnutella) distributed search and indexing schemes, nodes in this location mechanism do not route queries, instead, they organize into an overlay network and distribute location information. This work was published in *A Decentralized Adaptive Replica Location Service*, to be presented at HPDC-11, July 2002.

Other related research at Chicago argues for a decentralized solution for resource discovery in grid environments and presents a framework to analyze different request forwarding strategies in various resource sharing environments. This effort was described in *On Fully Decentralized Resource Discovery in Grid Environments, IWCG, November 2001.*

3.6.5 Replica placement mechanisms

Research on this topic considered how to schedule large jobs which need large input data files, for high energy physics experiments. We built a simulator, *ChicSim*, that helps evaluate different scheduling and replication strategies in the context of Grids. Our studies indicate that decoupling replication and scheduling strategies works to efficiently use Grid resources and decrease response times of users. Results are reported in *Decoupling Computation and Data Scheduling in Distributed Data-Intensive Applications* to be presented at HPDC-11, July 2002.

Related to replica placement, we have also studied protocol-performance aspects of bulk file transfers. This work was reported in a poster for SC2001: *Transport Level Protocols Performance Evaluation for Bulk Data Transfers*.

3.6.6 Research in the application of Peer-to-Peer techniques to the Grid

As part of our efforts to understand what aspects of the perr-to-peer model might benefit large distributed scientific collaborations, one of our studies focused on small-world patterns in scientific collaborations. The findings here argue for exploiting usage patterns when building P2P overlay networks. We have sketched a preliminary but still incomplete solution for building and exploiting small world overlay networks for file retrieval. This was described in *Locating Data in (Small-World?) Peer-to-Peer Scientific Collaborations,* presented at the 1st International Workshop on Peer-to-Peer Systems, March 2002.

The Gnutella network was studied as a potential model for file sharing in large scientific collaborations. The open architecture, achieved scale, and self-organizing structure of this network make it an interesting P2P architecture to analyze. The main contributions of this macroscopic evaluation are: (1) although Gnutella is not a pure power-law network, its current configuration has the benefits and drawbacks of a power-law structure, (2) we estimate the aggregated volume of generated traffic, and (3) the Gnutella virtual network topology does not match well the underlying Internet topology, hence leading to ineffective use of the physical networking infrastructure. This research is reported in: *Mapping the Gnutella Network: Properties of Large-Scale Peer-to-Peer Systems and implications for System Design, IEEE Internet Computing, vol. 6, no. 1, January-February 2002*.

Further research in P2P resource discovery was reported in *A peer-to-peer approach in resource discovery in grid environments*, to be presented at HPDC-11, July 2002. Our poster *On Fully Decentralized Resource Discovery in Grid Environments* will further explore that issue at the same conference.

Our research reported in *Improving Data Availability through Dynamic Model-Driven Replication in Large Peer-to-Peer Communities,* May 2002, suggests a dynamic model that helps nodes in a peer-to-peer system decide when to replicate files, with the view of maintaining an availability threshold for each file in the system. We test the performance of our model with simulations of large peer-to-peer networks. The model helps nodes to adapt to unreliable network conditions, by creating additional replicas as and when needed.

3.6.7 Creation of test grids at ANL and UC

To support much of the research reported above, work was conducted at Chicago to create test grids for challenge-problem work, using condor pool resources at the U of Chicago, Argonne, Wisconsin, and U of Florida. These research grids were used for informal and flexible experimentation work (in contrast to the more formal and controlled USCMS and USATLAS test grids).

3.7 University of Wisconsin

The University of Wisconsin CS department has focused on leading three major efforts, two of which are described in other sections of this report:

- In collaboration with the CMS experiment and the UW Physics department, has been pursuing the goal of an integrated CMS Event Simulation Production system. The results of this work are described in Section 7 and the press release presented in Appendix I.
- Has led and staffed the integration, release and support of the first several version of the Virtual Data Toolkit. This work is described in Section 5.
- Has conducted architectural research on data grid architecture, and led cross-group dialogs aimed at creating an architectural consensus among GriPhyN researchers and across other closely related projects.

A research effort conducted at Wisconsin, which will play an important role in the GriPhyN deployments, the NeST[16] grid data storage component, is described below.

To take advantage of storage resources available across the wide area, members of the Condor project are designing and implementing a Grid storage appliance. NeST (Network Storage Technologies) is a flexible software-only storage appliance designed to meet the storage needs of the Grid. NeST has three key features that make it well-suited for deployment in a Grid environment. First, NeST provides a generic data transfer architecture that supports multiple data transfer protocols, and allows for the easy addition of new protocols. Second, NeST is dynamic, adapting itself on-the-fly so that it runs effectively on a wide range of hardware and software platforms. Third, NeST is Grid-aware – it has features that are necessary for integration into Grids, such as storage space guarantees, mechanisms for resource and data discover, and user authentication.

NeST is an open-source, user-level, software-only storage appliance. Compared to current commercial storage appliances, NeST has three primary advantages: flexibility, cost, and Grid-aware functionality. NeST achieves this increased flexibility with its generic data transfer architecture that concurrently supports multiple data transfer protocols including GridFTP, HTTP, and NFS. This architecture is similar to the virtual file system layer in many operating systems and allows new protocols to be easily added as the Grid evolves. Because it is open-source and software-only, NeST provides a low-cost alternative to commercial storage appliances; the only costs incurred are the raw hardware costs for a PC with sufficient storage. NeST architecture is illustrated in Figure 6.

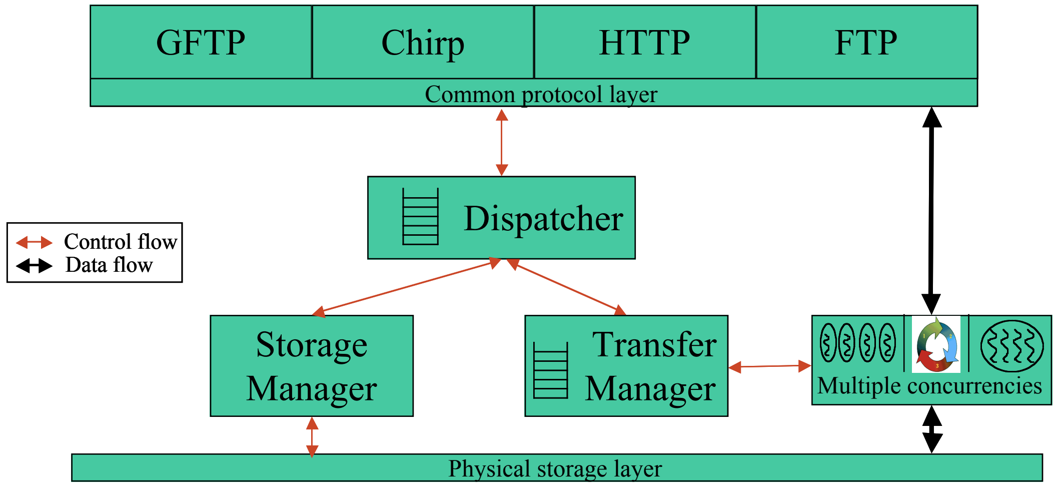

Figure 6: NeST Architecture

Finally, NeST has been designed from the outset to be a Grid-aware storage appliance. Key features, such as storage space guarantees, mechanisms for resource and data discovery, user authentication, are a fundamental part of the NeST infrastructure. This functionality is designed to enable NeST to integrate smoothly into higher-level job schedulers and distributed computed systems. Storage space guarantees are provided by "lots," which allow users to claim space and logically group files together. Lots have leases, which allow proper garbage collection to be performed lazily by the NeST. NeST advertises statistics about itself using ClassAds, and these advertisements can be used by scheduling systems for optimizations. User authentication is handled by all of the supported protocols and NeST to allows different security policies, such as “only allow users with proper GSI certificates”. Lastly, Nest uses stride scheduling to provide configurable levels of service between the different protocol classes. NeST’s interaction with Grid scheduling is illustrated in Figure 7.

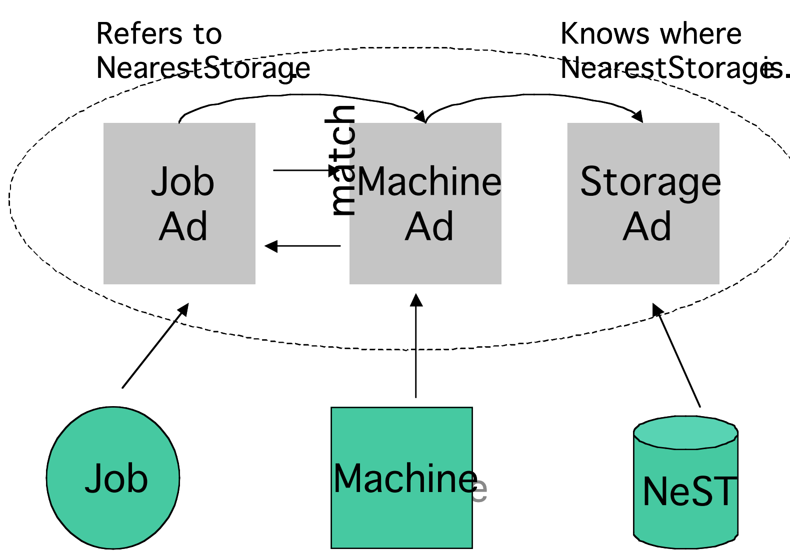

Figure 7: NeST and Grid Scheduling

NeST version 0.9 is currently available at http://www.cs.wisc.edu/condor/nest; we plan on releasing version 1.0 by the end of 2002. We have deployed Nest on several sites across the wide area, in order to experiment with realistic scenarios. Our future goals for the development of NeST include extending the stride scheduler to distinguish between individual users and groups instead of just the different protocols. We are also working on developing grids of cooperative NeSTs to maximize availability and reliability as large datasets are shared across the wide-area.

4 Joint GriPhyN-iVDGL-PPDG Monitoring Group

Initial steps in organizing a monitoring effort were taken during this period. A web site was created[17], available at http://www-unix.mcs.anl.gov/~schopf/pg-monitoring/ , as were a mailing list and archives. This group is currently being lead by Jennifer Schopf and Brian Tierney. Jennifer is a researcher at Argonne National Lab, and is strongly involved in the Globus MDS[18] and monitoring efforts in the Global Grid Forum. Brian Tierney is a researcher at LBNL, and was recently funded by Mary Anne Scott through PPDG. Brian has been working in the field of monitoring and Grid computing for many years now, including as a lead for the performance effort in PPDG and the lead architect for the NetLogger work.

4.1 Use cases

The first goal for this group was to define use cases for requirements gathering. We did this by first defining a template, and then by requesting use cases from the experimentalists involved in this effort. To date we have 19 of these covering a wide range of examples from testing a network for stability to evaluating the progress of an application. Jennifer Schopf presented this work[19] at the Internet2 End-to-End Performance Initiative Measurement Workshop in January 2002. This work was also part of the talk[20] she gave for the LCG kick-off meeting in March 2002.

4.2 Requirements document

Serious work started on developing a draft requirements document[21] for grid-level monitoring issues. We are currently waiting feedback from several experiments, and hope to have a new draft of this by mid-July.

4.3 Meetings and Re-scoping

This group met informally as part of the GriPhyN meeting in January, and were tasked by the VDT people tasked us with defining a set of sensors to be deployed in the various application testbeds as part of VDT. However, at the PPDG meeting in February it was realized that that goal was really one of fabric management, and work in that area was being done by many members of the PPDG monitoring community already, and what was needed was a better plan for how to interface these various fabric-level monitoring systems to a grid-level monitoring system, such as the Globus Monitoring and Discovery Service (MDS). A new version of the charter[22] has recently been advertised to the group.

This re-focusing will involve the use of the currently being defined unified schemas being developed by the Glue-Schema group (discussed below), the development of needed sensors or information providers to allow inter-operable deployment of this information, and a joint GIIS set-up for this group which has already been set up by Dantong Lu, BNL.

4.4 Glue Schema work

In early March the JTB started a group to define, publish, and enable the use of common schemas for interoperability between the EU physics grid projects (focusing on EDG and DataTag) and the US physics Grid projects (focusing in on PPDG, GriPhyN and iVDGL). Brian and Jenny are coordinating this effort.[23] This work is part of the Grid Laboratory Uniform Environment (GLUE) Phase I task.[24]

This effort will provide a basis from which to understand short, medium and longer term needs and definitions, and will encourage coordinated progress, and increased communication between these groups. No one set of schemas are being adopted, rather a new, unified schema is being developed; with the goal of having schemas defined for use in LDAP, SQL and XML.

The first step is to define common schemas to describe Compute Elements (CE), Storage Elements (SE), and Network Elements (NE), to be used by the MDS and R-GMA Grid Information Services. The goal is to have common schemas defined, deployed, and tested in time for the EU DataGrid Testbed 2 release in September 2002. Common schemas for monitoring and notification events are being address by the Global Grid Forum DAMED working group, and will be addressed later by iVDGL and DataTag.

As of June 2002, the CE schemas are finished, and implementation of them in the Globus and EDG information providers has begun. A test of these is planned for late July. We have started work defining the Storage elements, and have recruited expert help for this from Arie Shoshani and John Gordon.

5 VDT – The Virtual Data Toolkit

In the past year, we have integrated, tested, released, and supported the initial releases of the Virtual Data Toolkit[25] (VDT). This work was led and primarily staffed by the University of Wisconsin.

5.1 Pacman

In our early stages of planning the VDT, we needed to chose a method to deliver the VDT to end users. After consideration of various options, we chose to use Pacman.[26] Pacman has several important features.

- Pacman stores software in caches, which are trusted centrally located software repositories.
- Pacman allows individual pieces of software to be installed in any manner. Each piece of software can be an RPM, a tarball requiring compilation, or can require custom installation. Pacman allows the VDT developers to list the commands needed to install each piece of software. This allows us to quickly assemble diverse pieces of software into a cohesive package.
- Pacman provides features to simplify life for system administrators, such as generating web pages that describe the software that has been installed.
- Pacman provides features to simplify life for users, such as creating shell scripts to set up a user's environment for using the software.

5.2 Versions of the VDT

Version 0.5 was descriptive: it described what software was planned for version 1.0 of the VDT. It allowed us to gain valuable feedback from Griphyn and iVDGL members.

Version 1.0 was our first full release. It used the Pacman software, developed within the Atlas project, to package the software. It included Globus 2.0 beta, GDMP 2.0, Condor 6.3.1, and Classads 0.9.2.

Version 1.1 was our next release. It was identical to Version 1.0, except that it replaced GDMP 2.0 with GDMP 3.0.

Version 1.1.1 was our next release, and it substituted Globus 2.0 final for Globus 2.0 beta. It also included a new version of Pacman that included new features suggested by users.

5.3 Feedback From Users

After the release of VDT 1.0 and VDT 1.1, we received lots of feedback from users. Not only did we get feedback from Griphyn participants (particularly the USCMS testbed project), but we received excellent feedback from the European Data Grid, which performed an extensive review of Pacman and the VDT.

Feedback we received guided the release of Version 1.1.1 and the version of Pacman that accompanied it.

5.4 Release strategy

After the release of Version 1.1, we developed a release strategy for the VDT. Versions with an odd minor version number (such as 1.1, 1.3, and 1.5) are considered development versions. They are meant for early adopters and testers. Versions with an even minor version number (such as 1.2, 1.4, and 1.6) are considered stable versions. They have received interoperability testing that assures us that the individual pieces of software are stable and work well together. As of this writing, we are still developing our testing procedures, and expect them to be defined in the near future.

5.5 Future VDT releases

In the near future, we will release version 1.2 of the VDT, which will be a stable version of the VDT, as verified by our testing procedures.

We expect new software to be included in the VDT in the near future. In particular, we expect development versions of Chimera, the virtual data system, to be included.

After we finish the development of the testing procedures to produce the stable releases of the VDT, we will develop tests that people can use to verify that a VDT installation has been properly installed and configured.

5.6 Cooperation with the iVDGL Core Software Group

We have been working closely with the iVDGL Core Software Group. In fact, the Griphyn VDT group and the iVDGL Core Software Group have informally merged into a single group, because of our need to work together closely. We have telephone conference calls every other week.

6 ATLAS Research Activities

ATLAS GriPhyN work in Year 2 has followed a two-prong approach. The first was to develop experience running distributed ATLAS applications using existing grid middleware technology and toolkits as packaged by VDT. The principal aim here was to adopt, implement and develop software and infrastructure which had immediate use and value to ATLAS. Support for ATLAS Data Challenges (DC) occurring towards the end of Y2 was identified as the best target for this purpose. The second was to concurrently develop concepts, semantics, and architectures for a prototype virtual data system appropriate for the ATLAS event store architecture and analysis framework. Here coordination with the ATLAS core database development group (both at US and international levels) has been important. We discuss progress on both these fronts briefly in this review. Where possible, a coordinated approach with other U.S. Grid projects, namely PPDG and iVDGL, has been followed.

6.1 Virtual Data for Monte Carlo Production

The Argonne ATLAS database group developed and delivered an infrastructure for early application of GriPhyN virtual data concepts and techniques to ATLAS data production. A prototype was deployed in the spring of 2002 for evaluation in the context of the 2002 ATLAS data challenges. The prototype is currently being used successfully by groups at Argonne, Brookhaven, and CERN for data challenge event generation and detector simulation.

Production job options for physics event generation and production scripts for detector simulation were recast as parameterized transformations to be cataloged, with the resulting parameterizations represented as derivations. This work was implemented in a manner chosen to be compatible with the impending release of the Chimera system. The ATLAS database group plans to build a repository of its production "recipes" using Chimera and the GriPhyN Virtual Data Language later this year. This repository will provide the raw material for ATLAS virtual data browser and portal work underway at Indiana and Chicago. An example of the virtual data flows that we intend to focus on are shown in Figure 8.

The ATLAS virtual data effort has identified new requirements for the GriPhyN CS research program with its needs for random number seed and {run number, event number} management in the parameterization of cataloged transformations. ATLAS and Chimera researchers are working together to define and develop these extensions.

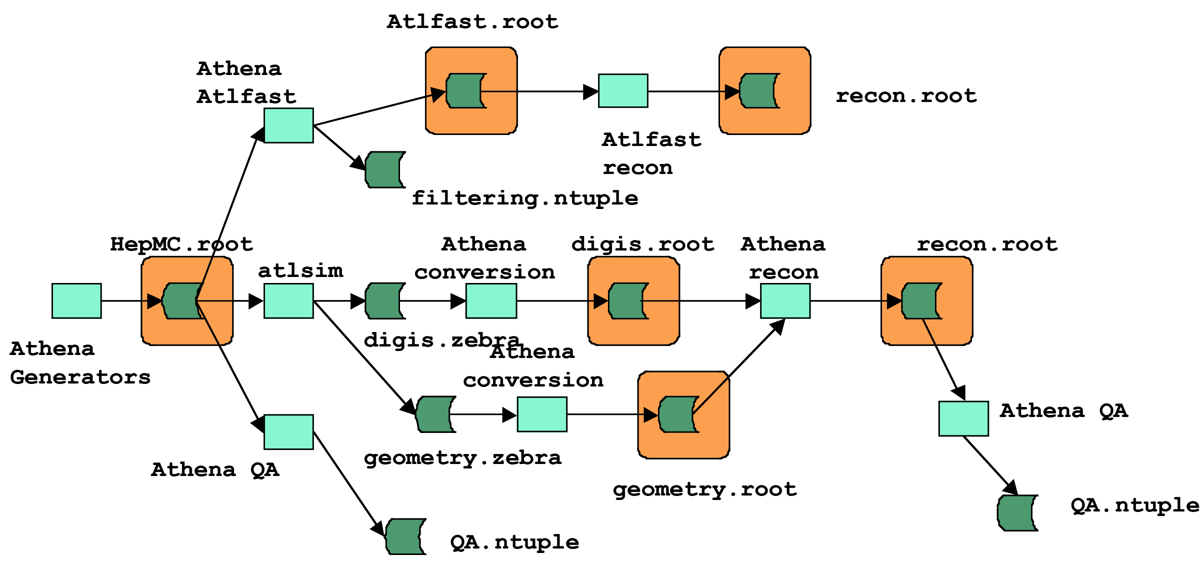

Figure 8: Envisioned Virtual Data Flow for Athena Modules

6.2 Grappa

Work continued at Indiana University on the Grappa job submission portal for the US ATLAS Testbed. Grappa is an acronym for Grid Access Portal for Physics Applications.[27] This work supports U.S. ATLAS Grid WBS 1.3.9 (Distributed Analysis Development) work breakdown deliverables. The preliminary goal of this project was to provide a simple point of access to Grid resources on the U.S. ATLAS Testbed.[28] The project began in May 2001. A demonstration of this software was made at the ATLAS Software Week in March 2002 and at ATLAS Testbed workshops at UT Arlington (April) and Boston University (June). The demonstration showed the first instance of Athena grid-wide job submission on the US Testbed. Jobs producing Monte Carlo simulation events from the PYTHIA event generator followed by the ATLAS fast simulation program (ATLFAST) were submitted to several sites on the testbed using a web-based job submission interface. Globus tools such as GSI for user credentials, GRAM for job submission, Condor and fork job managers were invoked on the prototype Tier 2 centers at Indiana University and Boston University, the Tier 1 grid test node at Brookhaven Lab, and an AFS-enabled grid node at Oklahoma University. Resources (sites, job queues) could be selected from a portal "notebook". Simple job monitoring was accomplished by queries to the site gatekeepers, which check and reported the GRAM status. Physics results were written out in the form of ntuples, and were fetched automatically back to the user's work area. Web reporting of histogram output was automatically generated by invoking PAW kumac files from a Java servlet.

6.3 Virtual Data Portal

We have begun extending the work of Grappa to provide a user interface to virtual data. If virtual data with respect to materialization is to be realized, a data signature fully specifying the environment, conditions, algorithm components, inputs etc. is required. These will be captured by using the Virtual Data Language (VDL) and Virtual Data Catalog (VDC), and the components that make them up are cataloged and a data signature is a unique collection of these components constituting the 'transformation' needed to turn inputs into output. Grappa could then interface to the data signature and catalogs and allow you to 'open' a data signature and view it in a comprehensible form, edit it, run it, etc. Take away the specific input/output data set(s) associated with a particular data signature and you have a more general 'prescription' or 'recipe' for processing inputs of a given type under very well defined conditions, and it will be very interesting to have catalogs of these -- both of the 'I want to run the same way Bill did last week' variety and 'official' or 'standard' prescriptions the user can select from a library. A preliminary architecture for the Virtual Data System for ATLAS/Athena is shown below.

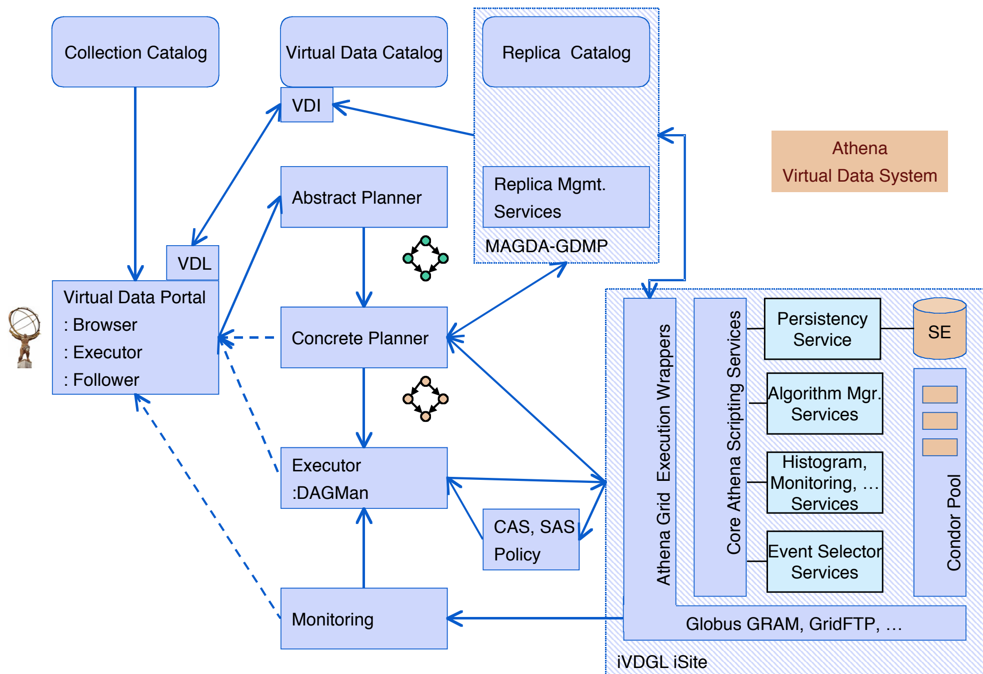

Figure 9: Preliminary Architecture for ATLAS/Athena Virtual Data System

6.4 Pacman

If ATLAS software is to be smoothly and transparently used across a shifting Grid environment, we must also gain the ability to reliably define, create and maintain standard software environments that can be easily moved from machine to machine. Such environments must not only include standard ATLAS software via CMT (Code Management Tool) and CVS (Code Versioning System), must able also include a large and growing number of "external" software packages as well as Grid software coming from GriPhyN itself. It is critical to have a systematic and automated solution to this problem. Otherwise, it will be very difficult to know with confidence that two working environments on the Grid are really equivalent.   Experience has shown that the installation and maintenance of such environments is not only labor intensive and full of potential for errors and inconsistencies, but also requires substantial expertise to install and configure correctly.

To solve this problem we have proposed to effectively raise the problem from the individual machine or cluster level to the Grid level. Rather than having individual ATLAS sites work through the various installation and update procedures, we can have individual experts define how software is fetched, configured and updated and publish these instructions via "trusted caches." By including dependencies, we can define complete named environments which can be automatically fetched and installed with one command and which will result in a unified installation with common setup script, pointers to local and remote documentation and various such conveniences. Since a single site can use any number of caches together, we can distribute the expertise and responsibility for defining and maintaining these installation procedures across the collaboration. This also implies a shift in the part of Unix culture where individual sites are expected to work through any installation problems that come up in installing third party software. The responsibility for an installation working must, we feel, be shifted to the "cache manager" who defined the installation procedure to begin with. In this way, problems can be fixed once by an expert and exported to the whole collaboration automatically.

Over the past year we have used an implementation of the above ideas called "Pacman" to define standard ATLAS environments which can be installed via caches. This included run-time ATLAS environments, full development environments and project specific user defined environments. In parallel, we have been working with the VDT distribution team and with Globus to develop a second-generation solution to this problem that can be more easily integrated with the rest of the GriPhyN Grid tools.

7 CMS Research Activities

The CMS group within the GriPhyN collaboration includes Caltech, Florida, FNAL, UCSD, and Wisconsin, and has been actively pursuing several GriPhyN activities that are described below.

7.1 US-CMS Test Grid Development and Deployment

A small scale US-CMS Test Grid[29] has been built to provide the necessary infrastructure for research and development of grid-enabled software for CMS. The test grid offers approximately 30 dedicated processors (1 GHz each) distributed across the five different CMS institutions participating in GriPhyN. In addition, the test grid is based upon the GriPhyN Virtual Data Toolkit (VDT) and was the first such grid to deploy the VDT. As such, it validated the main premise of the VDT, which is to provide simple, effective tools for building grids. Work to ensure availability of services and monitoring have resulted in a heart beat tool which uses the Grid Data Movement Package[30] (GDMP) to periodically move files around the test grid.

In addition, ongoing deployment and evaluation of several monitoring tools is currently underway, including: the Globus Meta-Directory Service (MDS), the Condor Hawkeye[31] monitoring service, and the FLexable monitoring frAMework for scalable systEmS[32] (FLAMES) from Iosif Legrand of Caltech.

7.2 Virtual Data and Distributed Monte Carlo Production

In the area of production of simulated CMS data, much work has been done in studying and prototyping Virtual Data concepts and technologies into CMS Monte Carlo Production. This effort cumulated in a demonstration at Super-computing 2001 entitled "Virtual Data for Real Science"[33] and showed that even an early implementation of the GriPhyN Virtual Data Catalog could already successfully track the dependencies of CMS data files and CMS application transformations between data files. In particular, the demonstration was able to regenerate any (missing or deleted) derived data file (across a test grid) on demand.

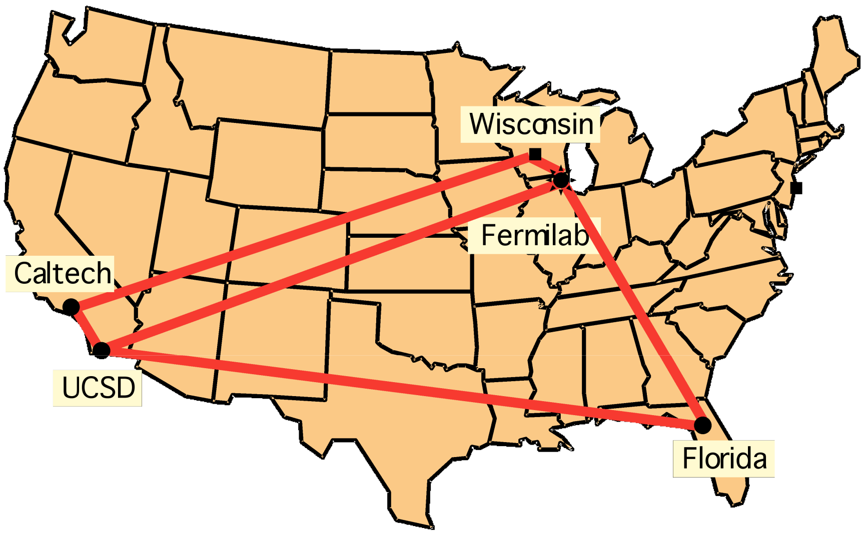

Figure 10: US-CMS Test Grid

In addition, considerable effort has been devoted to deploying an operational tool on the test grid for the distributed production of CMS Monte Carlo simulated data, known as MOP (see Figure 11). MOP (which is based upon Globus, Condor-G, and DAGMan) is loosely integrated with a set of shell scripts (known as IMPALA) that are currently used by CMS for Monte Carlo production as well as the Grid Data Movement Package (GDMP). The requirement for, and the pursuit of, a stable, robust grid platform have successfully provided valuable information to the core-grid middle-ware developers concerning scalability and reliability in an actual grid production environment. In June, the MOP system, running on the test grid, passed a milestone by successfully carrying out the first ever "at scale" production of simulated CMS data (over 100 000 simulated events, fully validated for official use by CMS physicists world wide) on a grid (see Appendix I).

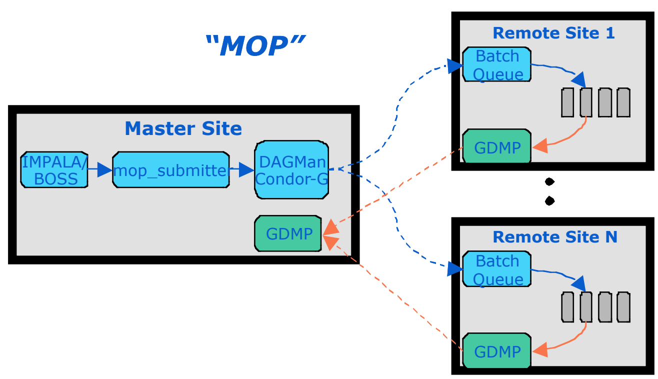

Figure 11: Monte Carlo Production Architecture (MOP)

7.3 Grid-enabled Distributed Analysis Research

Studies in the area of physics data analysis led to a demonstration at Super-computing 2001 entitled "Bandwidth Greedy Grid-enabled Object Collection Analysis for Particle Physics."[34] This work employed a client/server application that allowed particle physicists to interactively analyze over a hundred GB of physics event data stored at two "tier 2 centers" which took part in the demonstration. The work successfully showed several key elements of a future CMS Data Grid (see reference) including seamless, easy access to data using virtual data at the object level and grid technology.

Substantial activity has been devoted to the creation of a Grid-enabled data Analysis Environment (GAE) for CMS. Much of the work has focused on using web services to access CMS data. CMS data stored in an OODBMS are converted into reduced data formats, known as AOD or TAG data, and stored into an RDBMS. Physicists may then remotely query and analyze the AOD/TAG data in the RDBMS using various web services and optionally stored RDBMS procedures for improved efficiency.

Prototype systems have been developed both for Oracle9i and SQLServer, using large reconstructed simulated datasets produced by the ORCA (Object Reconstruction for CMS Analysis) program. An analysis using traditional ntuples to explore LHC physics involving "Jets and Missing Transverse Energy" signatures has been chosen, the data has been converted to TAGs and AODs with a schema generated from the Entity Relationship diagram describing the ntuples, and these objects have then been loaded into Oracle9i and SQLServer databases at Caltech and CERN. Prototypical web services have been written to access and query these object collections.

In addition, a remote data access framework, known as Clarens[35], has been developed to enable analysis of CMS data distributed over wide-area networks. Clarens is based on a client/server approach and provides Web-based services for physicists to run their own CMS analysis and AOD/TAG creation codes on CMS data. The Clarens server is linked against the standard CMS data analysis software libraries, while the (relatively light) Clarens clients are end-user specific; client implementations currently exist for several generic data analysis tools including, C++, Python, Java, PHP, and the ROOT Data Analysis Framework[36]. The envisioned architecture is depicted below (Figure 12).

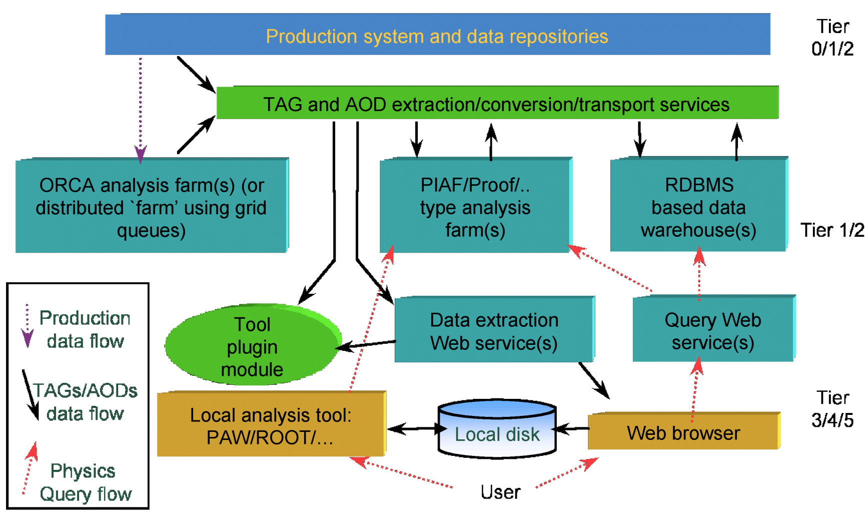

Figure 12: Prototype Architecture for the CMS Grid Analysis Environment

7.4 CMS Grid Requirements Analysis and Implementation

Particular attention has been given to documenting CMS requirements for grid computing. One resulting report[37] details the expected medium term grid infrastructure, which is to be developed by the Grid Projects in conjunction with CMS over the next two to three years. Another report[38] provides a reference model of how virtual data concepts will likely fit within a CMS data grid. Such research, which has proven vital to the planning of tasks, will continue as CMS refines and redefines its software environment.

Specifically, a short term CMS grid implementation plan for 2002 has been defined.[39] As part of this short term plan, a prototype Virtual Data Grid System[40] (VDGS) is currently being developed based upon the documented CMS grid requirements[41] and upon the GriPhyN Data Grid Reference Architecture[42], or DGRA. The prototype system implements a virtual data catalog as well as simple planners and grid execution services from the VDT. The purpose of this VDGS prototype implementation is to provide a reference grid integration of current CMS software applications with existing grid technology and to test the viability of the DGRA for CMS needs. To ensure realistic CMS scenarios for testing and to discover unforeseen bottlenecks in a grid production environment, actual CMS Production requests for Monte Carlo simulated data will be processed through the prototype system. In addition, distributed data analysis tools, such as Clarens, will be integrated with the prototype VDGS allowing users to analyze the simulated data. This will provide valuable feedback to developers of the CMS Grid-enabled environment for data analysis as well as the infrastructures for production of simulated data. The CMS-GriPhyN team plans demonstrate the prototype Virtual Data Grid System at Super-computing 2002 (see Figure 13).

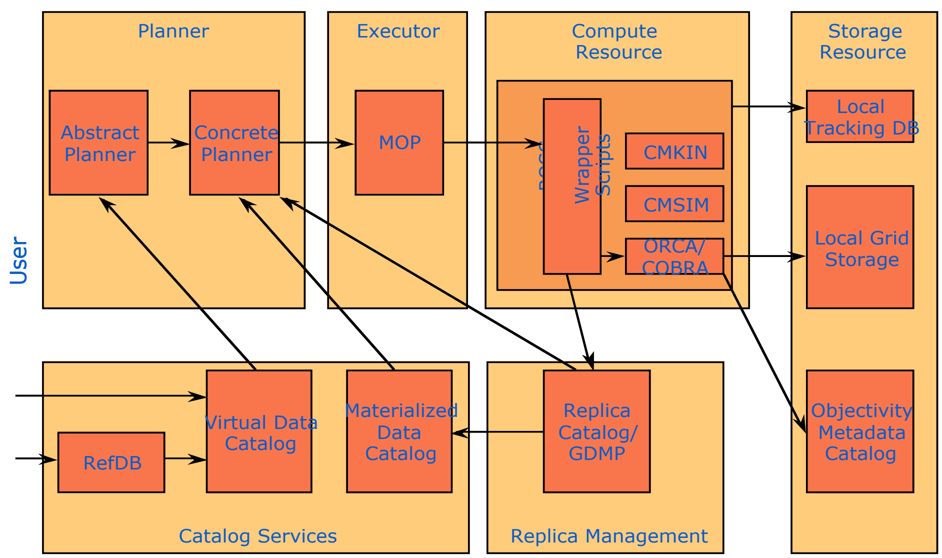

Figure 13: Prototype CMS Virtual Data Grid System Architecture

Finally, Virtual Organization issues related to account management and policy enforcement are being investigated. Once a centralized account management agreement (and infrastructure) is in place, Virtual Organization management scripts can be deployed to dynamically create grid-mapfiles for multiple Virtual Organizations. A prototype VO management infrastructure is expected to be in place on the US-CMS Test Grid during the Summer of 2002. Parallel work involving policy enforcement and user authorization within a multiple VO environment is expected to be performed over the Summer with a simple implementation deployed on the US-CMS Test

Grid by the end of the Summer. It is then hoped to combine, for testing purposes, the US-ATLAS and US-CMS Test Grids into a single multi-VO environment for a specified period of time.

8 Education and Outreach Status and Progress

The scope of the Education and Outreach (E/O) program of the GriPhyN and iVDGL projects is to enhance grid-related research capabilities of faculty and students at other universities and institutions. In particular, it intends to promote learning and inclusion via the integration of faculty and (K-12, undergraduate, and beginning graduate) students at a diverse set of minority and under-represented institutions (MSI) into the scientific program of participating physics and computer science experiments.

In Spring 2002, three MSIs (called Tier3 centers) received funds from the iVDGL project for hardware and personnel to upgrade or construct small (32-node) clusters, thus bringing a large number of additional minority students directly into contact with large-scale grid research. These Tier3 centers are: The University of Texas at Brownsville (UTB), a Hispanic Serving Institution (HSI) involved in LIGO research (LSC member Institution), Hampton University (HU), a Historically Black College and University (HBCU) involved in ALTAS/CMS research, and Salish Kootenai College (SKC), a Tribal College that has recently joined the LCS (LIGO Scientific Collaboration).

Associated with each Tier3 center are E/O work team members, consisting of Manuela Campanelli (UTB), Keith Baker (HU), Tim Olson (SKC), and several undergraduate and graduate students (e.g. Jose Zamora and Sean Morris at UTB, Howard Brown at HU, etc.). To facilitate the coordination of the E/O activities among the various Tier3 centers, Manuela Campanelli is leading the E/O program for both the GriPhyN and iVDGL projects, integrating the two into a single E/O effort. Keith Baker is serving as co-lead deputy. Team members collaborate to the overall effort by actively interacting with each other (through mail lists, regular telecons and meetings), leveraging existing E/O programs (such as SkyServer, EOT-PACI, QuarkNet, etc.), and collaborating with the E/O efforts in other national projects (e.g. PPDG, etc.) and international projects in Europe (e.g. DataGrid, etc.) and possibly in Asia and South America.

8.1 Education and Outreach Web site

As one of her first projects, Manuela Campanelli developed a web site for E/O activities ("GriPhyN Education and Outreach Center"[43]), linked from the main GriPhyN and iVDGL web pages. This web site currently contains basic educational material about data grids and the participating physics experiments, and provides some technical support information (e.g., documentation, user manuals, how-to guides, etc.) for grid software (like Globus, Condor, and the VDT). In the last 6 months, this site has been continually improved to provide more detailed information about the E/O activities in GriPhyN and iVDGL and other similar educational programs. It also contains a list of talks given by various GriPhyN and iVDGL members and course development activities that are on-going at various GriPhyN/iVDGL institutions. The E/O web site will soon be expanded to provide examples of scientific projects for students at various educational levels, which can be linked directly to the E/O activities of existing programs, such as SkyServer, EOT-PACI, QuarkNet, which are described in later sections.

8.2 Construction and grid-enabling the Tier3 centers

During Fall 2001, UTB completed the construction of a 96-node Linux cluster. Although constructed primarily to analyze LIGO data, it is also being used as a testbed for GriPhyN/iVDGL software, thus introducing Hispanic minority students at UTB to distributed computing and grid-related technology. During Spring 2002, UTB undergraduate students Jose Zamora and Sean Morris (with the help of Scott Koranda at the University of Wisconsin, Milwaukee) learned how to install an initial version of the VDT on the cluster. UTB also hired another graduate student, Santiago Pena, who will be working jointly with Jose Zamora and Sean Morris, to test newer versions of the VDT. The aim is to be able to participate in joint LIGO-grid testbed together with other interested Tier 2 centers. UTB has also been in contact with Ahktar Mahmood (UT Pan American) and Kaushik De (UT Arlington) in order to help them grid-enable their clusters.

In addition, Tim Olson (SKC) has been attending several cluster construction workshops and plans to attend more meetings this upcoming fall. He will start a detailed planning of the construction of the SKC Linux cluster by this summer.

8.3 E/O Meeting

On March 1, 2002, Manuela Campanelli organized the first GriPhyN/iVDGL E/O Meeting at UTB. The meeting successfully spread the news about GriPhyN and iVDGL to UTB students and faculty, and to local high school and middle school teachers and students. There were a number of talks given by GriPhyN/iVDGL researchers (e.g., Paul Avery, Jordan Raddick, Scott Koranda), and an inauguration of the UTB cluster "Lobizon" attended by UTB administration and local newspaper reporters. The meeting also served as an opportunity to begin to coordinate the E/O activities among the various Tier3 Centers participating in GriPhyN/iVDGL.

It was decided then that E/O meetings will be held at least once or twice a year, and will rotate locations between UTB, HU, SKC, and possibly other Tier3 centers. HU has expressed interest in hosting the next meeting (possibly in Fall 2002) while high school teachers participating QuarkNet activities are still on campus.

Manuela Campanelli also proposed holding an E/O workshop in conjunction with one of the "All-hands GriPhyN/iVDGL Meetings." This would allow a more direct and larger participation of minority students at such a meeting, without needing additional travel money for students. UTB has volunteered to host such a meeting in 2003.

8.4 SkyServer

SkyServer is a project lead by Alex Szalay (Johns Hopkins University) and Jim Gray (Microsoft) to provide Internet access to the public of SDSS data for both astronomers and for science education. This project is well under development, and it appears to be an excellent educational tool. During the E/O meeting at UTB in March 2002, Carol Lutsinger and Andy Miller (elementary and middle school teachers in Brownsville) talked to Jordan Raddick (Web designer and contact person for E/O in SDSS) about testing SkyServer[44] projects in their classrooms. Tim Olson is now also using Skyserver as an SDSS educational tool in his astronomy and astrophysics courses at SKC.

8.5 EOT-PACI

The EOT-PACI program (Education, Outreach, and Training Partnership for Advanced Computing Infrastructure[45]) has expressed interest on ways to link the E/O activities of

GriPhyN/iVDGL with their program. In the past 4 months, Roscoe Giles (EOT Team Leader), Scott Lathrop, (EOT Program Manager), Mary Bea Walker (Associate Director for EOT at NCSA), and Valerie Taylor (PI of the Coalition to Diversify Computing and senior investigator in the GriPhyN project) have been actively in contact with Manuela Campanelli to discuss some initial ideas for a possible collaboration. These include: (a) joint participation at major educational conferences and All-Hands meetings, (b) exploring opportunities for workshops on GriPhyN/iVDGL tools/resources with the Advanced Networking with Minority Serving Institutions (ANMSI), and (c) linking our respective E/O web sites to on-line tutorials.

8.6 QuarkNet

QuarkNet[46] is an ambitious (and highly successful) NSF-funded program that introduces large numbers of high school students across the US to particle physics research techniques. High school teachers attend an eight-week summer program for intensive study at host institutions where they work closely with particle physics faculty and staff. These teachers then take their experience (and enthusiasm) from this program back to their classrooms after the end of the summer. Keith Baker, who is the lead person for HU and a principal investigator for QuarkNet, is currently serving as a direct link between the QuarkNet, ATLAS/CMS and GriPhyN/iVDGL E/O programs. Ken Cicere (a QuarkNet investigator) and Howard Brown (an undergraduate student) at HU are helping Keith in this effort.

8.7 REU supplement

In order to give more undergraduate students the opportunity to participate in grid-related research at GriPhyN/iVDGL institutions, Manuela Campanelli has begun preparations to submit a proposal for an NSF Research Experience for Undergraduate (REU) supplement. James Williams and John Hicks at Indiana University, Ruth Pordes at Fermilab and Bruce Allen at the University of Wisconsin, Milwaukee have already expressed interest in providing projects and mentoring students during the summer months. Proposed projects include: (a) having students develop a scaled-down, simple to install VDT that high school teachers and students could use to grid-enable a small cluster or single computer, (b) automating hardware monitoring and account management on large Linux clusters, and (c) using grid tools for automated file replication. Manuela plans to submit the proposal in Fall 2002.

8.8 NISBAS grant

SKC administration has submitted a proposal for the creation of a NISBAS Center for Excellence in Teaching. The focus of the proposal is to develop a training center for K-12 teachers to improve science, math, and technology education in National Indian School Board Association Schools (NISBAS). If funded, SKC will be able to hold summer workshops and national educational meetings at SKC (starting next year), where GriPhyN/iVDGL researchers could participate by giving talks and tutorials.

8.9 Other forms of dissemination

In December 2001, Manuela Campanelli released an interview about GriPhyN, iVDGL, and grid computing in general that has been published in several magazines in Germany, among them an article in the Financial Times. In March 2002, she also released an interview with the Brownsville Herald and wrote an article with Patrick Brady (University of Wisconsin, Milwaukee) in "Matters of Gravity"[47] to inform the relativity community about the advantages grid computing.

Outreach talks and presentation were given by GriPhyN team members at numerous venues around the world, ranging from Bucharest, Romania; Poznan, Poland; DESY in Hamburg, Germany; and Oak Park – River Forest High School in Illinois. We expect to increase the rate of these efforts in the future, increasing our focus on MSI's at both the secondary and college levels.

8.10 Planned E/O Activities

8.10.1 Further development of the Web site

As one of our milestones for the next year, we propose to continue the development of the "GriPhyN Education and Outreach Center".[48] In particular, Manuela Campanelli plans to use this web site to provide examples of scientific projects for students at various educational levels, which can be linked directly to the E/O activities of existing programs, such as SkyServer, EOT-PACI, QuarkNet, as described in the progress report.

8.10.2 Grid-enabling the Tier3 centers and preparation for a LIGO grid-testbed

Campanelli will also continue to instruct two undergraduate students, Jose Zamora and Sean Morris, and another graduate student, Santiago Pena, in the testing and deployment of new versions of the VDT on the UTB 96-node Linux cluster. The aim is to eventually participate in a LIGO-grid testbed, together with other interested Tier 2 centers. A possible target date for such a testbed is the 2003 Super-Computing Conference (SC2003). In preparation for this event, Campanelli plans to send her students to SC2002 and to various GriPhyN/iVDGL institutions to familiarize them with the VDT and the other grid tools that GriPhyN researchers are developing. UTB will also continue to assist two other iVDGL Tier3 centers (HU and SKC) and other interested partners (such as UT Pan American and UT Arlington), helping them grid-enable their clusters once they complete the actual construction.

8.10.3 Meetings and Workshops

HU has expressed interest in hosting the next E/O meeting (possibly in Fall 2002) while high school teachers participating in QuarkNet activities are still on campus. Campanelli has also volunteered to host an iVDGL facilities meeting in December 2002, again providing an opportunity to coordinate the E/O activities among the various Tier3 Centers.

8.10.3.1 EOT-PACI

Campanelli plans to continue her collaboration with the EOT-PACI program as discussed in the report, encouraging joint participation at major educational conferences, workshops, and All-Hands meetings, and linking the E/O web sites to on-line tutorials.

8.10.3.2 REU supplement

Campanelli plans to submit a proposal for an NSF Research Experience for Undergraduate (REU) supplement in Fall 2002. This will give additional undergraduate students the opportunity to participate in grid-related research. The success of this program will depend on the participation of GriPhyN and iVDGL institutions.

8.10.3.3 Other forms of dissemination

Campanelli, Ian Foster, Paul Avery, and Ruth Pordes are currently discussing the possibility of creating a joint newsletter for GriPhyN, iVDGL, and PPDG. The plan is to start the newsletter program in Spring 2003, publishing it two or three times every year.

9 Products Resulting from GriPhyN Work

Below is a list of publications and documents associated with GriPhyN.

Note: several of the documents listed here are discussed in more detail in Section 3.

9.1 Publications

- *GriPhyN and LIGO, Building a Virtual Data Grid for Gravitational Wave Scientists*, Ewa Deelman, Carl Kesselman, Gaurang Mehta, Leila Meshkat, Laura Pearlman, Kent Blackburn, Phil Ehrens, Albert Lazzarini, Roy Williams, Scott Koranda. to appear in the Proceedings of the High Performance and Distributed Computing Conference, 2002.
- *PAIDE: Prophesy Automatic Instrumentation and Data Entry System*, X. Wu, V. Taylor, R. Stevens, IASTED Conference on Parallel and Distributed Computing, August 2001.
- *Prophesy: Automated Performance Analysis of Distributed Applications*, X. Wu, V. Taylor, J. Geisler, Z. Lan, X. Li, R. Stevens, M. Hereld, I. Judson, invited paper to the Active Middleware Services (AMS) Workshop, August 2001.
- *Using Kernel Couplings to Predict Application Performance*, V. Taylor, X. Wu, J. Geisler, R. Stevens, to appear in the Proceedings of the High Performance and Distributed Computing Conference, 2002.
- *A comparative study of Virtual Data and View Materialization*, A. Tarachandani, M.S. Report, University of California, Berkeley, June 2002
- *Disk cache replacement algorithms for storage resource managers in data-grids*, Ekow J. Otoo, Frank Olken and Arie Shoshani, to be presented at the Supercomputing Conference, 2002. http://sdm.lbl.gov/~ekw/ftpDir/sc2002Cache.pdf.
- *Giggle: A Framework for Constructing Scalable Replica Location Services*, Ann Chervenak, Ewa Deelman, Ian Foster, Wolfgang Hoschek, Adriana Iamnitchi, Carl Kesselman, Peter Kunszt, Matei Ripeanu, Heinz Stockinger, Kurt Stockinger, Brian Tierney, Global Grid Forum Document, GGF4, Toronto, Canada February 2002, (a version of this paper will has been accepted at Super Computing 2002). http://www.globalgridforum.org/Meetings/GGF4/Docs/rep1.pdf
- *A Decentralized, Adaptive Replica Location Service*, Matei Ripeanu and Ian Foster, 11th IEEE International Symposium on High Performance Distributed Computing (HPDC-11), Edinburgh, Scotland, July 24-26, 2002. http://people.cs.uchicago.edu/~matei/PAPERS/hpdc-02.pdf
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9.3 Web site

The griphyn web site has grown in both content and usage over the past year. It serves as a document repository, meeting announcement and reservation board, and as repository of working dociuments and information for various working groups such as virtual data research and the VDT.

It has recently been extensively revised and turned into a fully database-driven dynamic site, with virtually all content coming from a database. A site-management web site has been created to enter and manage all dynamic content. This new structure enables a far grater number of project participants to modify site content in an access-controlled manner. Now, authorized individuals can post news, meetings, update a GriPhyN calendar, and create general information captions on the site. This effort will greatly enhance project communications and reduce bottlenecks in making information available to the GriPhyN community and its collaborators.

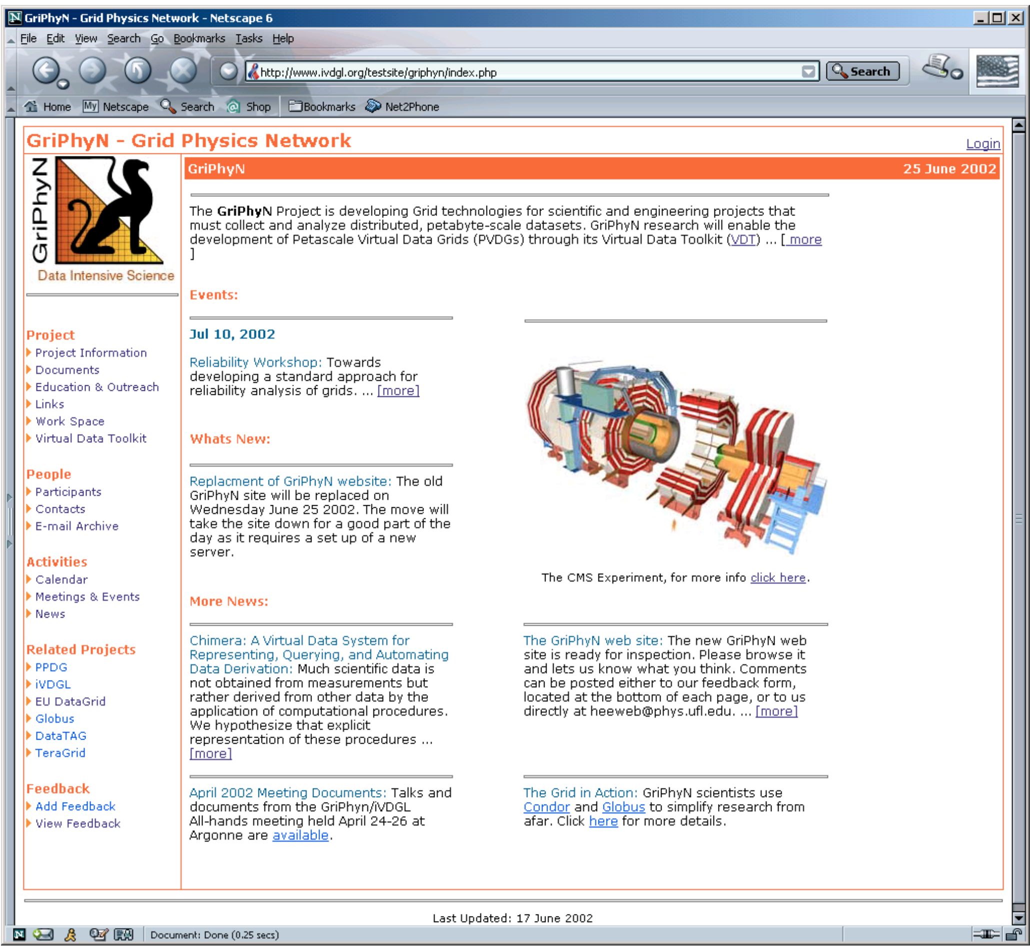

Figure 14: A screen shot of the front-page for the GriPhyN web site. The page consists of a grid of cells where general information, news and events about the project are displayed. Each "[more]" link points to the full article. The image on the right is randomly selected from a collection of images with links to more information. On the top right hand corner is the link to the user and administrator login system.

The web site has proven to be a very good coordination site for the project, so much so that its deficiencies have become noticeable over the last year. It has also become apparent that maintaining the site with up to date information requires a significant amount of work. To remedy these deficiencies while reducing the maintenance the team at Florida redesigned the site with technology that incorporates the ability to control the information-content dynamically with built in logic. Dynamic information-content which includes: news articles, event postings and meeting information, are now displayed at different times in different locations depending on a predefined date and time attribute associated with the particular news or event article. For example, articles that are out of date are relocated from both the front page and a current location page to a past location page. In addition to the dynamic information-content, the new site features a user login system, a new document server and an agenda creation tool. The user login system was designed to control access to sensitive information and define the individuals who can administer the site. The agenda creation tool allows downloads, restricted uploads and is fully integrated into the new document server. Presenters without administrator intervention will now be able to upload their own presentation and add it to the GriPhyN/iVDGL document database at the same time. We have also designed a tool to facilitate and standardize the creation of registration forms for IVDGL meetings.

The front page was significantly redesigned. It consists of a grid of cells into which is displayed general information about the project; important GriPhyN events, news and a “What’s New” article are now displayed. Each news and event articles contain information this is dynamic in the sense described above. There are also cells reserved for the display of images related to the project complete with links that point to more information about the image. Several images are stored on the site and selected for display randomly. The navigability of the site has been greatly improved by a menu bar that is located on the left side of every page displayed on the site. A screenshot is shown in the above Figure.

We plan to make some additional adjustments to the site before the end of Summer 2002. We will add more internal documents and links to other projects and bring up to date the new combined GriPhyn/iVDGL/PPPDG calendar of meetings and events.

Appendix I: PPDG-GriPhyN-iVDGL Press Release – CMS Production Milestone

Particle Physics Data Grid Collaboratory Pilot,
Grid Physics Network,
International Virtual Data Grid Laboratory
Integrating Datagrid Technology with Physics Experiment End-to-end Applications.
ppdg-exec@ppdg.net

www.ppdg.net www.griphyn.org www.ivdgl.org

Members of the CMS experiment working in concert with PPDG, iVDGL, and GriPhyN have carried out the first production-quality simulated data generation on a data grid comprising sites at Caltech, Fermilab, the University of California-San Diego, the University of Florida, and the University of Wisconsin-Madison. This is a combination of efforts supported by DOE SciDAC, HENP, MICS, and the NSF as well as the EU funded EU-DataGrid project.

The deployed data grid serves as an integration framework where grid middleware components are brought together to form the basis for distributed CMS Monte Carlo Production (CMS-MOP) and used to produce data for the global CMS physics program. The middleware components include Condor-G, DAGMAN, GDMP, and the Globus Toolkit packaged together in the first release of the Virtual Data Toolkit.

The CMS-MOP distributed production system employs a tier-like hierarchy in which a production manager at a Tier-1 center distributes production jobs to several remote Tier-2 sites. Once generated at the Tier-2 sites, the simulated data is automatically published back to the Tier-1 center as well as replicated to selected Tier-2 sites.

This integration exercise showed that the Grid still presents significant challenges in harnessing distributed resources. Issues of data and security had to be overcome, e.g. how do you get your software & data to many remote systems and know it's there? How do you get your results back? How do you allow people on the Grid to trust you?

Issues of heterogeneity and error recovery had to be addressed, - to use other sites' resources, you need to interface with many batch systems; the Grid means more errors, more crashes, more mysterious failures. Unanticipated errors were handled such as: Key machines crashing in the middle of a run; Grid credentials expiring in the middle of a run; Jobs successfully completing but their results being lost before they got sent back; Various pieces of middleware did the unexpected; The network would go down.

Despite these challenges, over 50,000 proton-proton collision events inside the CMS detector have been simulated using CMS-MOP and validated for use by CMS physicists. Production of another 150,000 simulated events is underway.

This achievement represents an extremely challenging and important milestone in the integration of grid middleware components within the current "real world" LHC computing environment!

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