Physics and Earth Science User Communities of Armenian National Grid Initiative

Hrachya Astsatryan[1], Vladimir Sahakyan[2], Yuri Shoukourian[3], Sargis Mkoyan[4], Norayr Akopov[5], Hrachya Asatryan[6], Gagik Kryuchkyan[7], Areg Mickaelian[8], and Lusine Sargsyan[9]

[1, 2, 3] Institute for Informatics and Automation Problems,
National Academy of Sciences of the Republic of Armenia,
1, P. Sevak str., Yerevan 0014, Armenia
{hrach, svlad, shouk}@sci.am

[4, 5, 6] Yerevan Physics Institute,
2, Alikhanyan Brothers str.,Yerevan 0036, Armenia
{sako, akopov, hrachia}@yerphi.am

[7] Yerevan State University,
1, Alex Manoogian str., Yerevan 0025, Armenia
kryuchkyan@ysu.am

[8, 9] Byurakan Astrophysical Observatory,
National Academy of Sciences of the Republic of Armenia,
Byurakan 0213, Aragatzotn province, Armenia
aregmick@aras.am

Abstract. The main purpose of this article is to present the results and activities of physics and earth sciences heavy user communities of Armenian National Grid Initiative (ArmNGI) using computational or storage resources of Armenian National Grid infrastructure (ArmGrid).

Keywords: ArmNGI, ArmGrid, Grid, eInfrastructure, Hermes, Monte Carlo, QCD, IVOA, ArVO, Quantum Informatics, CMAQ, WRF

1 Introduction

eInfrastructures are one of the key enablers of scientific research and of the development of Information Society in Europe. Enabling large-scale innovative research to be conducted through collaboration of distributed teams of scientist across the European Research Area paves the way towards a long-term vision of a sustainable, transparent, ubiquitous electronic infrastructure open to a wide range of scientific user communities. The grid infrastructure is recognized today in Europe and worldwide, together with the highspeed networking, as one of the basic components of the eInfrastructure of research and education and soon of the entire knowledge-based society. In the years, a number of targeted initiatives funded by the European Commission via its RTD programmes have contributed to ameliorating the state of eInfrastructures in Armenia. Taking into account the importance, the interested parties including the State Committee of Science, Presidium of the National Academy of Sciences (NAS RA), Yerevan Physics Institute (YerPhi), Institute for Informatics and Automation Problems of the National Academy of Sciences (IIAP NAS RA), Yerevan State University (YSU), State Engineering University of Armenia (SEUA) and Armenian e-Science Foundation strive to work together towards establishment of the ArmNGI [1]. The ArmNGI represents an effort to establish a sustainable distributed computing infrastructure in Armenia. The Governmental decision was adopted in April 2010 on the set up the ArmNGI Foundation. The main purpose of this article is to present the efforts and activities of Armenian heavy user communities in physics and earth sciences using computational or storage resources of Armenian distributed computing infrastructures, particularly the resources of ArmGrid.

2 Armenian Grid Infrastructure

In 2004, the first high Performance computing cluster (Armcluster) in the South Caucasus region had been deployed in Armenia [2] which consists of 128 Xeon 3.06GHz (64 nodes) processors. The cluster achieved 523.4GFlops performance by HPL (High Performance Linpack) test. Now ArmGrid infrastructure (gLite middleware) consists of seven Grid sites located in the leading research and educational organizations of Armenia. Apart from computing (416 cores) and storage resources, core Grid services which enable seamless access to all resources are provided to national users. The first Armenian national VO ARMGRID.GRID.AM has been established and registered in the Grid operations centre database in May 2009 [3]. Users can register and view their membership details trough VOMS admin web portal [4]. The nodes of the Grid sites are interconnected by Myrinet and Infiniband High bandwidth or Gigabit networks.

Many international projects, such as the projects funded by International Science and Technology Centre (Development of Scientific Computing Grid on the Base of Armcluster for South Caucasus Region, Development of Armenian-Georgian Grid Infrastructure and Applications in the Fields of High Energy Physics, Astrophysics and Quantum Physics) and EU Framework Programmes (South East European eInfrastructure for regional eScience) have contributed to deploy the above mentioned infrastructure. The core of European Grid Initiative (EGI) [5] is the establishment of sustainable eInfrastructures, either within individual countries sustained by national funding to support national research communities and coordinated by NGIs, or within international research communities. Armenia is a member of EGI and actively takes part in all activities within the EGI.

3 Armenian Heavy User Communities in Physics and Earth Sciences

In this part, it is given brief information about Armenian heavy user communities in the different directions of physics and earth sciences.

3.1 Monte Carlo production for the HERMES

During past several years the HERMES collaboration has studied various aspects (like the extraction of the spin density matrix elements, coherence length and nuclear transparency effects [6-9]) of the electro-production of exclusive ρ^0 mesons using hydrogen, deuterium and various nuclear unpolarized and polarized targets with 27.5 GeV electron (positron) beam at HERA accelerator (DESY, Hamburg). One of the interesting phenomenon, which can be extracted from the data accumulated by HERMES experiment, is well known effect of color transparency predicted by QCD, which is based on the picture of quark-antiquark pair content of ρ^0 meson, and the inverse-proportionality of the cross section of such pair production to the photon virtuality (Q^2). This effect is expected to be well defined measuring the cross section ratio of exclusively produced ρ^0 mesons on nuclear targets related to those measured on hydrogen target. In order to perform such analysis one need to provide extensive Monte Carlo (MC) studies to estimate different characteristics like the acceptance of used detector, the resolution over various kinematical variables etc. A set of special studies to take into account possible attenuation of hadrons produced in nuclear matter were performed. The developed model will be used to modify the physics generator for future Monte Carlo massive production. Various tests of physics generator to be used for this massive production have been performed. Also the optimization of a software framework to manage the submission of Monte–Carlo jobs using MPI (Message Passing Interface) with copies of all necessary specific HERMES software packages, like HMC (digitalization of charged tracks), HRC (reconstruction of tracks) etc., have been done. The package (with the required CERN libraries) has been ported on the Grid infrastructure by using the YerPhi Grid (AM-04-YERPHI) site for the experiments. A full massive MC chain of HERMES jobs (event generation, reconstruction, etc) have been tested. About 15 millions fully reconstructed MC events are produced, which will be used to provide necessary physics analysis of accumulated HERMES data.

Another important MC related subject is the matrix generator, based on solid theoretical ground, like Kolmogorov's K-systems [10], has been started to adopt with the usage of parallel arithmetic in order to provide very high speed of generation. It allows generation of arbitrarily large consequences of pseudorandom numbers, which could be used as a coordinates of multi-dimensional vectors for any high dimensional physics problem. The modified (optimized) matrix generator was already checked, using well known statistical tests like multidimensional Kolmogorov discrepancy and χ^2. Such pseudorandom generator with parallel arithmetic option will be extremely important to solve a wide class of multi-dimensional problems with the use of Monte-Carlo method, and related not only to high energy physics, but also to different disciplines like: seismology, biophysics, weather prediction etc.

3.2 The calculation of QCD corrections for $B \to X_s\gamma$

More than 15 years after their first direct observation, radiative B decays have become a key element in the program of precision tests of the Standard Model (SM) and its extensions. The inclusive decay $B \to X_s\gamma$ is particularly well suited to this precision program thanks to the low sensitivity to non-perturbative effects. The first estimate of the $B \to X_s\gamma$ branching ratio within the Standard Model at the next-to-next-to-leading order (NNLO) level was published some years ago [11]. The central values of the theoretical prediction and of the experimental average are compatible at the 1.2^{σ} level, while both the theoretical and experimental uncertainties are very similar in size (about 7%). Since the experimental uncertainty is expected to decrease to 5% by the end of the B-factory era, it is also desirable to reduce the theoretical uncertainty accordingly. In this work we calculated the contribution to the $B \to X_s\gamma$ decay of two-loop diagrams coming from O_7 - O_8 operator interference (see fig.1) at $O(\alpha_s^2)$ order. These corrections are one of the elements needed in order to complete the calculation of the branching ratio for the radiative $B \to X_s\gamma$ up to NNLO at order $O(\alpha_s^2)$. We use IBP equations and AIR program to reduce the number of integrals on internal momenta and 3 or 4 particle phase space parameters. To get the photon energy endpoint behavior it is necessary to keep the regulator $S^{-\varepsilon}$, where s is the hadron invariant mass squared and ε is dimensional regularization parameter (d=4- 2 ε). The result can be presented in form of series on inverse powers of ε. Near the endpoint on photon energies we used plus distributions to get results where endpoint singularities are separated. The remaining Master Integrals we calculate using numerical integrations methods. We use 8 kernels of YerPhI computing cluster to calculate most complicated integrals in the Feynman parameter space, as well as in phase space. We use Mathematica 7 symbolic programming language to develop corresponding programs. From the phenomenological point of view, it is interesting to estimate the effect these corrections on the theoretical prediction for the $O(\alpha_s^2)$ branching ratio. Our conclusion is that they effect from these corrections are of order - 0.13 % for μ =2.34 GeV and -4.91% for μ =5 GeV of central value of theoretical prediction [11].

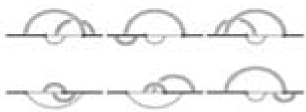

Fig. 1. Some of Feynman diagrams corresponding to O_7 - O_8 operator interference.

3.3 Quantum Physics

In the last twenty years quantum physics gained technological interest but sometimes theoretical science is not always able to answer questions that are posed by engineers as well as analytical solutions are not always exist. For many applications in this field there is a need for effective modeling and high performance computation. Recently, a software package “Photonic Technologies” for parallel numerical simulation on the base of MPI has been developed by group of YSU [12-14] in areas of applied quantum information and laser physics. The software has been constructed on the base of numerical simulation method of quantum trajectories for studies of the wider class of open quantum systems that involve dissipation and decoherence. It is also provided a graphical user interface to make the library convenient for wide range of users. To achieve the actuality in numerical calculations the library parallel programming patterns are included. It is important that the effectiveness of the parallelization depends on the number of parallel tasks linearly due to peculiarity of quantum trajectory algorithm. This software can also provide wide range of applications in quantum optics, including atom-photon interactions in laser fields. It can be used for numerical calculations of density matrices of the systems, quasi-distributions of photonic states, Poincare section, and populations of the simple atomic states (Λ- and V-systems). The recent scientific results obtained on the base of Grid computation concern to: elaboration of new laser-like sources of entangled light beams for long distance quantum communication [15-16]; production of long lived macroscopic photonic superposition states in dissipative nonlinear systems exhibiting hysteresis-cycle and chaos [17]; calculation and investigation of quantum distributions for complex quantum dissipative systems [18].

3.4 Armenian Virtual Observatory

Armenian Astronomers are facing different kind of problems that involves data reduction and analysis, modeling of physical observations, theoretical simulations and comparison of theoretical and observed data. Byurakan Astrophysical Observatory (BAO) possesses a huge amount of astronomical information obtained during last 60 years on about 35 thousand photographic plates and films. The most valuable part of this information is the First and Second Byurakan Surveys with many millions of low-dispersion spectra. Plates with astronomical direct images or spectra are highly valuable and need a safe maintenance. On the other hand this information is not as safe as needed because the photographic emulsion is very vulnerable against various types of damages. That is why a process of digitization of this information is being implemented. One of the first and largest digitization projects in the world was the Digitized First Byurakan Survey (DFBS) [19-21] now having some 40,000,000 spectra of 20,000,000 astronomical objects (stars, nebulae, galaxies). All the digitized information has served as a base for the creation and development of the Armenian Virtual Observatory (ArVO) [22-23]. The platform of ArVO makes possible to utilize all these data including also new data obtained with our 2.6m telescope and to integrate with the International Virtual Observatories Alliance [24]. DFBS and ArVO have been ported [25] to the ArmGrid infrastructure and corresponding tools is being developed for its implementation and integration [26-27]. The huge amount of astronomical information collected at BAO and outside have very high importance for comparative and joint analyses with other data obtained in various (ground based and space) observatories. Thus, undoubtedly the VO ideology from the very beginning was and is based on the Grid technologies, as it requires a high-speed networking and tools for processing and analyses of large catalogues and other data. Similar problems arise while modeling of astrophysical phenomena dealing with multi-million objects each of those characterized by a set of physical parameters is initiated. It is absolutely certain that the more detailed models able to describe astrophysical phenomena require huge computational spaces and vast number of mathematical operations to be done in an acceptable period of the time. That is why the development of astronomy/astrophysics is completely dependent on development of the computational environment and methods.

3.5 Numerical Weather Prediction

Numerical weather prediction (NWP) [28] is a prediction based on numerical integration of the equations of motion for the atmosphere. These are the non linear partial differential equations of dynamics, thermodynamics, mass continuity and moisture conservation. There are global, hemispheric, and regional scale models. The global model involves atmospheric phenomena on the whole globe, the hemispheric one – on the half globe. The regional models are applied in a specified region and depending on the resolution used they are intended to resolve mesoscale phenomena. Efficiency in prediction is achieved by using high performance computing. Advances in NWP have been always very closely related with advances in computing sciences as NWP requires numerical calculations that are parallelizable. The computational resources needed for NWP applications are important both in terms of CPU usage and disk storage. The WRF model [29-30] is a next-generation mesoscale forecast model and assimilation system that advances both the understanding and the prediction of mesoscale precipitation systems and promotes closer ties between the research and operational forecasting communities. The model has been ported and is operationally used by Armenian Hydro meteorological centre [31] for different couples of parent-nest domains with different spatial resolutions (5 and 25km) (see fig. 2). The results have been compared with the observed values of temperature, precipitation and pressure.

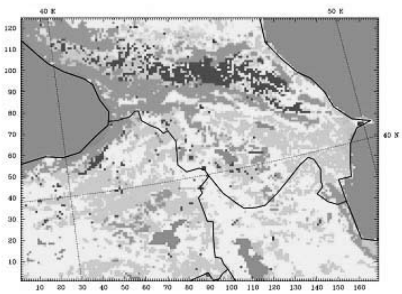

Fig. 2. The nested domain for the territory of Armenia.

3.6 Air Pollution

The usual application of three dimensional air quality models is to predict the spatial and temporal distributions of ambient air pollutants and other species. Third generation complex Eulerian models generate output concentrations by solving systems of partial differential equations. These equations define the time- rate of change in species concentrations due to a series of physical and chemical processes (deposition, emission, chemical reactions, horizontal advection, etc.). The WRF-CMAQ (Community Multi-scale Air Quality) modeling system [32] has been applied and ported on the ArmGrid by using the domain of WRF. The CMAQ modeling system has been designed to approach air quality as a whole by including state-of-the-science capabilities for modeling multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation.

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