

# Virtual Research Environment for value-added services in national and regional NRENs: case studies

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## Abstract

Case studies are presented for the role of national and regional NRENs beyond connectivity, encompassing computing (grid, cloud and High-Performance computing) services and big data management services. The case studies are the recently started VI-SEEM and MAGIC projects. The VI-SEEM project, started in October 2015, unifies the existing e-Infrastructures in South-East Europe (SEE) and the Eastern Mediterranean (EM), including Grid, cloud, and High-Performance Computing resources. It does so in order to better utilise synergies, for an improved service provision within a unified Virtual Research Environment (VRE) to be provided to the scientific user communities in this large region. The overall objective is to provide a user-friendly integrated e-Infrastructure platform for scientific communities in Climatology, Life Sciences, and Cultural Heritage for the SEE and EM regions; by linking networking, computing, data, and visualization resources, as well as services, software and tools. The Virtual Research Environment provides the scientists and researchers with the support in the full lifecycle of scientific research: accessing relevant data necessary for their research, using it with provided codes and tools to carry out new experiments and simulations on large-scale e-Infrastructures, and producing and integrating new knowledge and data - which is stored and shared within the same VRE. The project is founded on the service-oriented data-driven approach, where a specific set of activities deals not just with simple e-Infrastructure data storage (live, dropbox-like), but includes the support for the full data lifecycle for the 3 target communities. The value-added computing services provided to the researchers include grid and cloud computing, as well as large-scale High-Performance Computing platforms, with a set of management tools provided for the unified management of computing resources. All project services will be provided through a service catalogue. Similarly the MAGIC project, started in May 2015, aims to adopt a service-oriented approach to advertising specifically the NREN cloud services, and this approach will be implemented through a compatible service catalogue, based on the GEANT cloud catalogue: thus the envisaged MAGIC cloud catalogue is also briefly discussed.

## Keywords

Virtual Research Environment, Service catalogues, Grid computing, Cloud computing, High-Performance computing, Data management.

## 1.0 Introduction

In the last decade, a number e-Infrastructure initiatives were crucial for enabling high-quality research by providing networking and computational resources, application support and training, in both South East Europe (SEE) and Eastern Mediterranean (EM) and have supported the European vision of inclusive and smart growth, based on knowledge and innovation, enriching the European Research Area. These initiatives have helped to reduce the digital divide and brain drain in Europe, by ensuring access to regional e-Infrastructures– in total 20 countries in the region. National and regional networks have been set up, as well as national and regional computing platforms, providing different types of value-added computing services to NREN users and beyond.

The VI-SEEM project (<https://vi-seem.eu/>), started in October 2015, unifies these existing e-Infrastructures in SEE and the EM, including Grid, cloud, and High-Performance Computing resources. It does so in order to better utilise synergies, for an improved service provision within a unified Virtual Research Environment (VRE) to be provided to the scientific user communities in the this large region. The overall objective is to provide user-friendly integrated e-Infrastructure platform for scientific communities in Climatology, Life Sciences, and Cultural Heritage for the SEE and EM regions; by linking networking, compute, data, and visualization resources, as well as services, software and tools.

## 2. Architecture for integrated e-Infrastructure services

The integrated platform will encompass all layers including the networking and computing resources, and adding the specific data (and related data management services), software and tools relevant for the regional multi–disciplinary communities. The diagram below depicts this integration over layers across the 3 target communities.

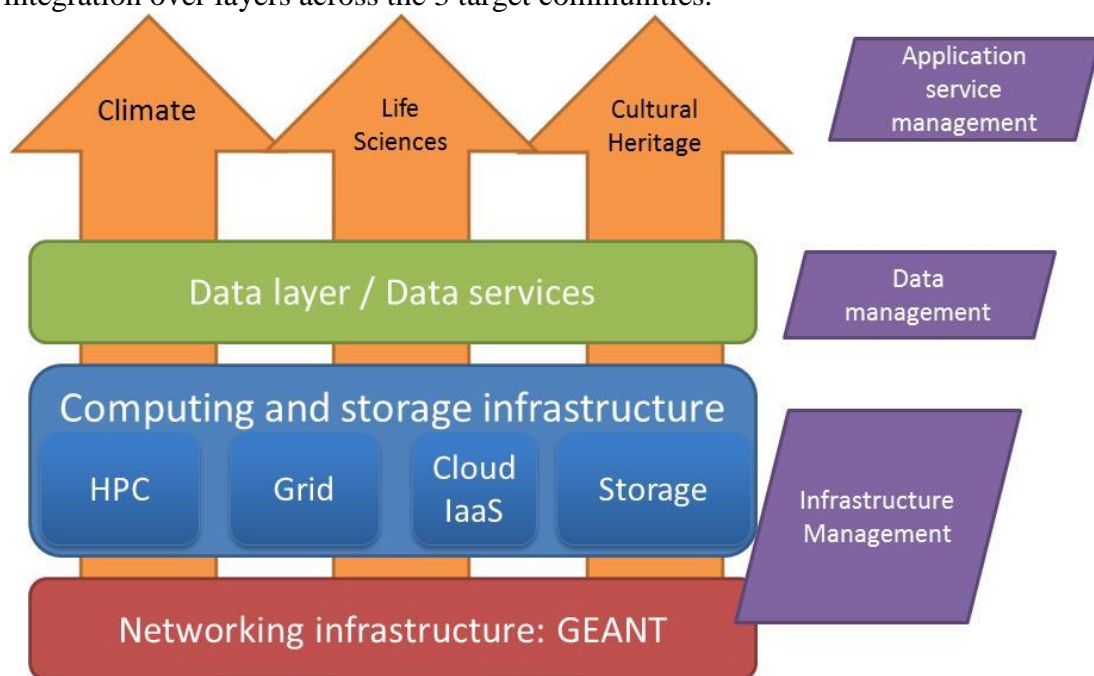


Figure 1 - VI-SEEM conceptual architecture

Overall objective is to provide user-friendly integrated e-Infrastructure platform for Scientific Communities in Climatology, Life Sciences, and Cultural Heritage for the SEEM region; by

linking compute, data, and visualization resources, as well as services, software and tools. The detailed objectives include the following, also giving an indication of size of the infrastructure and the spread of its services.

- Provide scientists with access to state of the art e-Infrastructure - computing, storage and connectivity resources - available in the region; and promote additional resources across the region. Size of infrastructure – 21500 CPU cores, 325000 GP-GPU cores and 18500 Intel Xeon Phi cores of HPC, 2900 grid cores, 10500 cloud VM cores, 11 PBytes of storage (of which dedicated 5-15% , 10-15%, 5% and 10% respectively).
- Integrate the underlying e-Infrastructure layers with generic/standardised as well as domain-specific services for the region. The latter are leveraging on existing tools (including visualization) with additional features being co-developed and co-operated by the Scientific Communities and the e-Infrastructure providers, thus proving integrated VRE environments. The approach will be service-driven in terms of service components and definitions, and their invocations. 10 domain-specific services and 25 codes are envisaged.
- Promote capacity building in the region and foster interdisciplinary approaches, with minimum of 39 distinct applications and 45 research teams using the VRE.
- Provide functions allowing for data management for the selected Scientific Communities, engage the full data management lifecycle, link data across the region, provide data interoperability across disciplines: with minimum of 30 distinct data sets.
- Provide adequate user support and training programmes for the user communities in the SEEM region: 18 dissemination events organized by the project with total of 1000 persons targeted, 12 training events organized by the project with 300 persons targeted.
- Bring high level expertise in e-Infrastructure utilization to enable research activities of international standing in the selected fields of Climatology, Life Sciences and Cultural Heritage. There are 70 expected publications in project lifetime, 30 after project end, as well as 50 presentations at the selected events.

### 3 Scientific communities served

The initiative focuses on 3 distinct communities of crucial importance for the region. The breakdown of the types of the applications is shown in the table below, and the details of the communities and their use of e-Infrastructure services described further down.

Climate	Life Sciences	Cultural Heritage
Regional Climate Modelling	Modeling and Molecular Dynamics (MD) study of important drug targets	Digital Libraries
Global Climate Modelling	Computer-aided drug design	Interactive Visualization Tools
Weather Forecasting	Analysis of Next Generation DNA sequencing data and RNA profiling data	Semantic Referencing
Air Pollution/Quality	Data mining to identify prevalent diseases/mutations in the SEEM region	Image Classification
Model Development	Image processing for biological applications	Modelling of Built Environments and

		Advanced Representation Techniques
Visualization, Datasets, etc.	Computational simulation of DNA and RNA	Scientific simulation of materiality and systems' properties
	Synchrotron data analysis	Geo-referencing Tools
		Bioarchaeology

The **Climate Modelling** and weather forecasting community has traditionally very strong computational needs. In particular, the integration of various computational resources such as HPC and Grid jointly with data infrastructure that is addressed in VI-SEEM greatly supports research and operational activity of regional relevance. The community targeted here is active in a wide range of research activities. Perhaps the largest focus is on regional climate modelling and weather forecasting, where local weather and regional climate phenomena are investigated. This is complemented by global climate modelling where the impact of global phenomena on the regional climate is the focus. The results of both are crucial to predict extreme weather in the region and understand the future trends of the regional climate. Another strong field of related research is the study of air pollution that includes the influence on the climate and human health. These activities jointly enable the assessment of the impact on regional climate due to climate change. Climate impact studies provide the analysis of the upcoming change on humans, the environment and society that is so crucial for policy makers. Complementing the research activities above are code development to help improving simulation methods and also visualization, which is crucial for the analysis of the enormous amount of data created in simulations, but also important for the communication of results to policy makers in particular and the wider public in general. The activities pursued based on tools to be provided through VI-SEEM have strong synergies, both geographically and thematically, and all require a neat integration of data and computing resources.

The Climate Scientific Community will specifically benefit from the combination of HPC and Grid computing jointly with the storage facilities as it heavily relies on data from very scattered locations. The VRE will collect a comprehensive list of commonly used databases and provide direct access where possible. Jointly with code repositories and training material for climate models, the VRE will create a highly productive working environment for Climate scientists from the 19 different research groups distributed over 13 countries. Additionally, some of these users have pledged to make accessible local data through the VRE. The data management provided through the VRE will enable the community to professionally host and share the data.

Regarding the **Cultural Heritage**, the SEEM region is renowned for its ancient civilizations. It is also an area of major socioeconomic and cultural developments during the medieval and early modern periods. In this context, the cultural heritage of the region is of central importance for the whole of humanity. Yet, these rich traditions and their study are under threat by contemporary political developments and conflicts. This Scientific Community aspires to invest in advanced computational tools in order to build an appropriate VRE for the collection and study of the historical artefacts and build scientific interaction that transcends ethnic boundaries and conflict. The current state-of-the-art of the field is that no common models and software platforms are developed due to the lack of access to the required resources and support. This limitation renders the users unable to explore the potential of bespoke software for big data applications, which is necessary for the establishment of universal platforms that would perform as cross-disciplinary test labs. This project can act as a catalyst in strengthening links among key players in the field bringing users currently

working autonomously together. Great potential is identified for research groups that have not used large scale computing before. Linking these to experienced groups will significantly improve productivity.

The project aims to improve the research capabilities of the CH community by providing access to an e-Infrastructure with critical components needed for the advancement of the field such as access to Cloud Infrastructure as a Service, data repositories and visualization. Given the wealth of the historical artefacts of the SEEM region, there is a demonstrated interest for researchers across Europe for integrated repositories and data access. This facility will promote collaboration not only among groups in SEEM but also with groups across Europe enabling ground-breaking research to be accomplished. Beyond the data needs, VI-SEEM will also facilitate the slow transition of the CH community towards computational more intensive activities. Examples for these trends are the high detail rendering of 3D modelling, and efforts to simulate environmental influence on historical buildings. The CH community also includes the combination of advanced content management systems and computational intensive workflows and querying. The training and user support program will be critical for the adaptation of advanced computational approaches by the CH community that is not as advanced as compared to the other two scientific domains. The established VRE will enable ground-breaking research in CH not only involving regional users but across Europe. We thus expect an increase in the number and quality of publications and presentations. The CH Scientific Community of VI-SEEM consists of 14 research institutes from 9 countries (including those outside the catchment area).

Regarding **Life Sciences** community, advances in computational infrastructure during the last decade have facilitated the development of biological data analysis for big data and computational biology as key research methodologies in both academia and industry. The use of computers in biology has enabled our better understanding of mechanistic aspects in health and disease and has accelerated the development of novel therapeutics. In this proposal, the Life Sciences Research Community is chosen because of its central role in achieving a higher quality of life in the SEEM region. The aim of the VRE is to create and provide the necessary services over a capable infrastructure to facilitate research for understanding of disease mechanisms in the SEE and EM populations. The overall goal is analysis of datasets by using integration of data within the VRE that could ultimately lead to regional characteristics that would assist the effort for developing personalized medicine in SEE and EM. Project participants and related institutes will assist in data collection and analysis, run and optimizing computational codes and using the research results to understand the molecular basis of diseases associated with SEE and EM areas with projections to develop personalized therapies. By bringing their own expertise into the consortium, the VRE partners will intersect their research interests in order to achieve the common goal in an interdisciplinary approach. Such an undertaking would require the use of computational resources for a) data production, b) data analyses, b) storage, d) visualization.

The exponential growth and availability of data from patients of the SEEM region and beyond have led to the “big data” era. Patient data sets are markedly large and complex, which renders their processing laborious using traditional data processing applications. The associated data analysis challenges include capture, curation, analysis, search, sharing, storage, transfer, and visualization. This trend to larger data sets is due to the additional information derivable from analysis of a single large set of related data, as compared to separate smaller sets with the same total amount of data, allowing correlations to be found in order to prevent and understand diseases. The participating countries have a keen interest to analyse and use big data for the understanding and prevention of diseases prevalent in the SEEM region. The cross border/cross region nature of human disease requires data and local

knowledge sharing over a wider SEEM area: the LS Scientific Community of VI-SEEM consists of 12 research institutes from 10 different countries of the region.

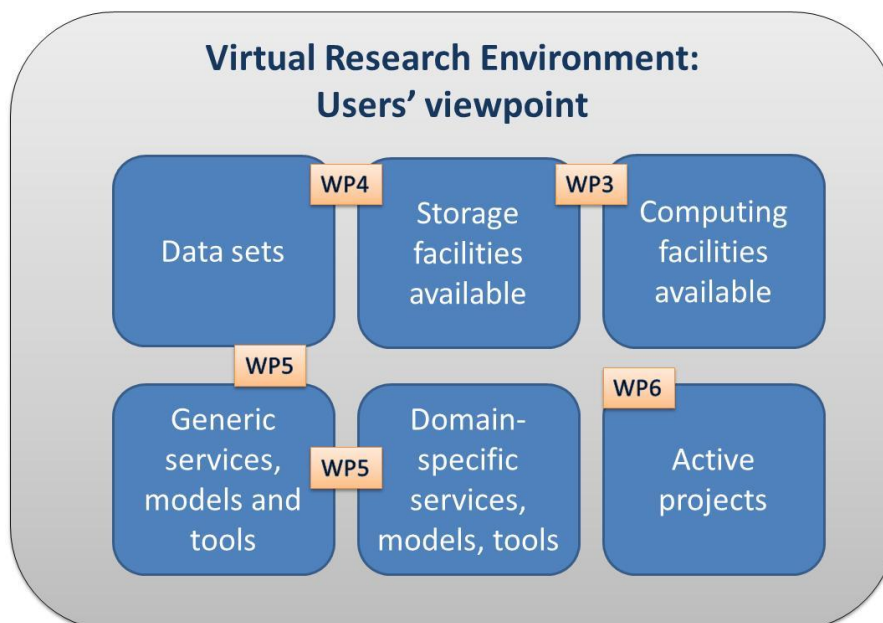
#### 4. Technical activities

The activity on **e-Infrastructure services** provides the unified underlying state-of-the-art e-Infrastructure for the benefit of the Scientific Communities. The underlying components include networking, computing (HPC, Grid, Cloud), storage, and standard interfaces to these. Issues of dynamic provisioning, access to combination of resources for the same project / application, monitoring and accounting for different types of resources will be specifically tackled. Thus, integrated high-quality services will be provided to end users, by supporting the regional e-Infrastructure, fused with end-user VRE services.

**Data Management Lifecycle** activities deals with Data lifecycle support for VRE and Scientific Communities including data storage (live, dropbox-like), data archiving, data manipulation, collaborative access, domain specific interfaces to storage, data annotation and citation, metadata, PIDs, etc. All these are state-of-the-art services which will enable the users to conduct high-quality research with the relevant data. Semantic knowledge representation and ontologies will be used where appropriate to enable data reuse from different services and applications, thus ensuring knowledge sharing, separation of domain from operational knowledge.

The activity on "**Domain-specific services and support**" deals with domain-specific services in 3 target regional communities. These services include community-specific content management systems, workflow engines, collaborative tools, etc; as well as specific community-related codes, analysis tools and visualization components. This WP will provide the link for integration of these services with the e-Infrastructure backbone, and will be following the data management principles supported in the data activity. Finally, it will provide user support. The activity will gather together large number of data sets, codes, models and tools and fine-tune these to provide smooth and coherent VRE access to the end user. In this manner, it will both quantitatively and qualitatively improve the overall end-user perception of the underlying services provided by the project.

Overall, the end-user will be provided with a Virtual Research Environment which can be visualized in the diagram below.



## 5.0 Service management principles

The VI-SEEM project will adopt a full service-oriented approach, where all services offered and created by the project need to be included in a service portfolio/catalogue following the service portfolio management process as defined by FitSM ([www.http://fitsm.itemo.org/](http://fitsm.itemo.org/)) with the additions and fine-tuning that is required for the VI-SEEM environment. Two distinct tools need to be used/developed: the service portfolio/catalogue management portal and the configuration/service/resource registry. The service registry will be based on the similar design such as the GN3+ Cloud Service Catalogue] (<https://catalogue.clouds.geant.net>) developed by GRNET.

Similarly, the MAGIC (<http://www.magic-project.eu>) project will build the service catalogue in order to advertise the NREN cloud services available in all world regions. It will also be based on the GN3+ Cloud Service Catalogue, which provides the Cloud Service Registration: a point through which the cloud providers can list their services: thus service operators will be able to register their services, and end-users will be able to find the offerings. The implementation provides view of Service providers, Services and Criteria per service. Edugain (<http://services.geant.net/edugain/Pages/Home.aspx>) or local account based authorization model is used for access. Components of the design of the current GN3+ Cloud Service are:

- Service Registry: central point for registering all the services with all relevant metadata associated with the services (e.g. type of service, endpoints, price information).
- Service Search: catalogue being searchable directly by end users. Users can login using their institutional credentials, but log in is not required for accessing the service. Users can see/search: services that are available to them through their IdF; services that are available to all the users of eduGain; services that are available on the platform but not to their IdF.
- Service Matrix: a single place with information for all the services available on the platform, displaying the relationships, in matrix form, between the services, the IdFs and the individual institutes.
- Service Map: a way to drill down to the services offered to a specific region.
- Service Rating: users can rate the service; ratings would not be anonymous. Comments accepted, and accessible to the respective SP.
- Service Request: users send requests to their IdF/Group/Organization for a service that is listed in the catalogue but is not available to their scientific community

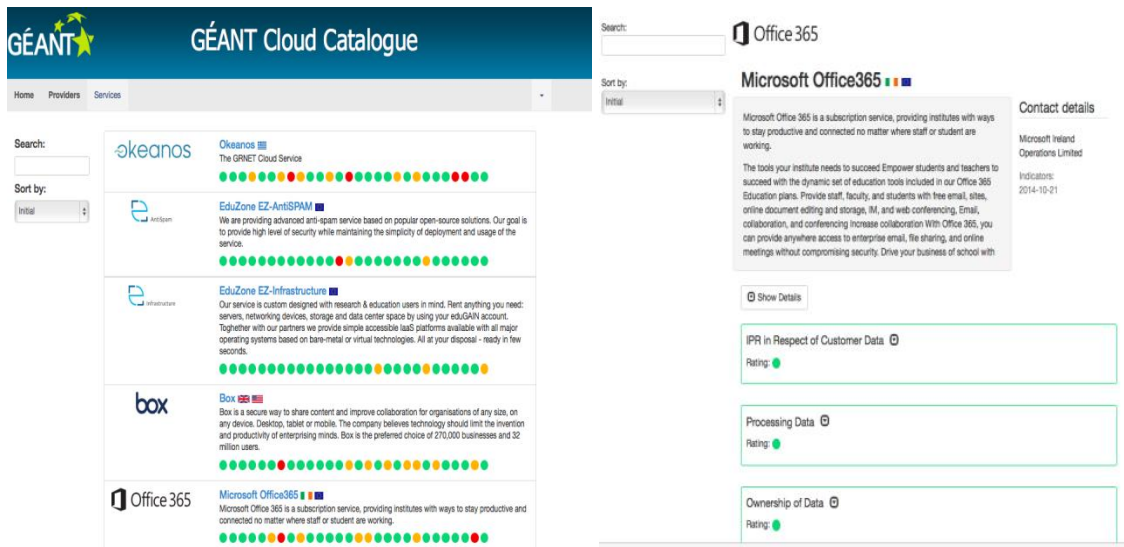


Figure 3 – Cloud catalogue

28 rating criteria are currently available in the GEANT Cloud Catalogue, including AAI, Billing, Compatibility, Concordance with National Privacy Act(s), Data Backup & Restore, Data Protection, Electronic Data Processing, External Security Audit Certificate, Governing Law, Information about the performance of the Service, IPR in respect of Customer Data, Liquidated Damage, Managing Security Incidents, Network Connectivity, Notification, Ownership of Data, Peering, Network Connectivity & Associated Costs, Portability, Processing Data, Protection of Minors as Users, Quality Review, Reporting / Metering / Sales Estimates, Requests for Data Access from 3rd Parties, Security of the Cloud Service, Service Level Agreement, Subcontractors, Supervision, User Provisioning.

## 1. Conclusion

We presented a case study for the role of national and regional NRENs beyond connectivity, encompassing computing (grid, cloud and High-Performance computing) services and big data management services. The case studies are the recently started VI-SEEM and MAGIC projects.

The VI-SEEM consortium brings together partners from 16 countries, the majority of which are the NRENs also providing cloud Infrastructure-as-a-Service storage / Virtual Machines, Grid and High-Performance Computing value-added services. The partners join forces to provide a large regional unified Virtual Research Environment to be provided to the scientific user communities in Climatology, Life Sciences, and Cultural Heritage for the SEE and EM regions. The platform links networking, computing, data, and visualization resources, as well as services, software and tools. The Virtual Research Environment provides the scientists and researchers with the support in the full lifecycle of scientific research: accessing relevant data necessary for their research, using it with provided codes and tools to carry out new experiments and simulations on large-scale e-Infrastructures, and producing and integrating new knowledge and data - which is stored and shared within the same VRE. All project services will be provided through a service catalogue. Similarly the MAGIC project aims to adopt a service-oriented approach to advertising specifically the NREN cloud services, and this approach will be implemented through a compatible service catalogue, based on the GEANT cloud catalogue: thus the envisaged MAGIC cloud catalogue is also briefly discussed.

Overall these 2 projects are flagship examples how multiple NRENs within a large region can come together and share a number of value-added services for the benefit of their

international scientific communities.

## References

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## Biographies

Dr. Ognjen Prnjat holds the position of European and Regional eInfrastructure manager in the Greek Research and Technology Network. In this role he is responsible for organizing various aspects of computing infrastructures in the South-East European region and beyond, their sustainability and seamless integration in pan-European eScience infrastructure; as well as GRNET involvement in pan-European and worldwide eInfrastructures. In the past 10 years he has acted as project coordinator for 5 EC projects in the field. Previously Ognjen was with the Department of Electronic and Electrical Engineering, University College London, where as a Research Fellow he was leading technical and project management aspects of a number of EC ACTS/IST and UK EPSRC projects in diverse fields of computing and telecoms. He holds a Bachelor of Eng. Degree in Electronics and Electrical Eng. (First Class Honours) from University of Surrey, UK, 1995; MSc (Distinction), 1996, from University College London; and Ph.D. in Telecoms from UCL, 2001.

Ioannis Liabotis is a project manager at GRNET S.A. During his 8 years at GRNET he has been involved in a series of FP6 and FP7 eInfrastructures projects related to HPC, Grids and Cloud. He has been the technical coordinator of the SEE-GRID-2, SEE-GRID-SCI and HP-SEE projects. He is currently member of PRACE Council and member of PRACE project management boards representing Greece. He has managed open calls for HPC access in Europe (DECI) and South-East-Europe (HP-SEE), and has extensive knowledge of SLA management aspects in computing environments. He obtained his Diploma in Electrical & Computer Eng from NTUA, Greece, in 1998; and his MPhil in Computation from UMIST, UK, 2000. He is technical coordinator of the VI-SEEM project.

Christos Kanellopoulos has been involved in European and National research and infrastructure projects since 2000, serving in various technical and management positions. 2000-02 he was a team leader in the project CAMPUS of Lufthansa coordinating the infrastructure rollouts at the airports of Athens, Beirut, Paris, Venice, Vienna and Zurich. 2002-12 he was the technical coordinator of the Scientific Computing Centre at the University of Thessaloniki leading the activities of the centre in more than 15 FP6 & FP7 projects in the areas of Grids, Distributed Systems and HPC. During that period he served as a WP Leader, Activity Leader and Working Group chair in various projects and fora. Since 2012 he works at GRNET in the fields of Distributed Systems, Cloud Computing & Security. Currently he is the Product Manager for the ARGO Availability & Reliability Monitoring Framework, he is leading the eduGAIN - STORK Integration Pilot in GN3Plus and he is the Security Officer for NGI GRNET and the CA Manager for the HellasGrid CA and the SEE-GRID CA, which provides services as a Catch-All CA for EGI.

