

How new communities can get access to the HPC-driven DEISA infrastructure

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www.deisa.eu

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RI-222919



HLRS



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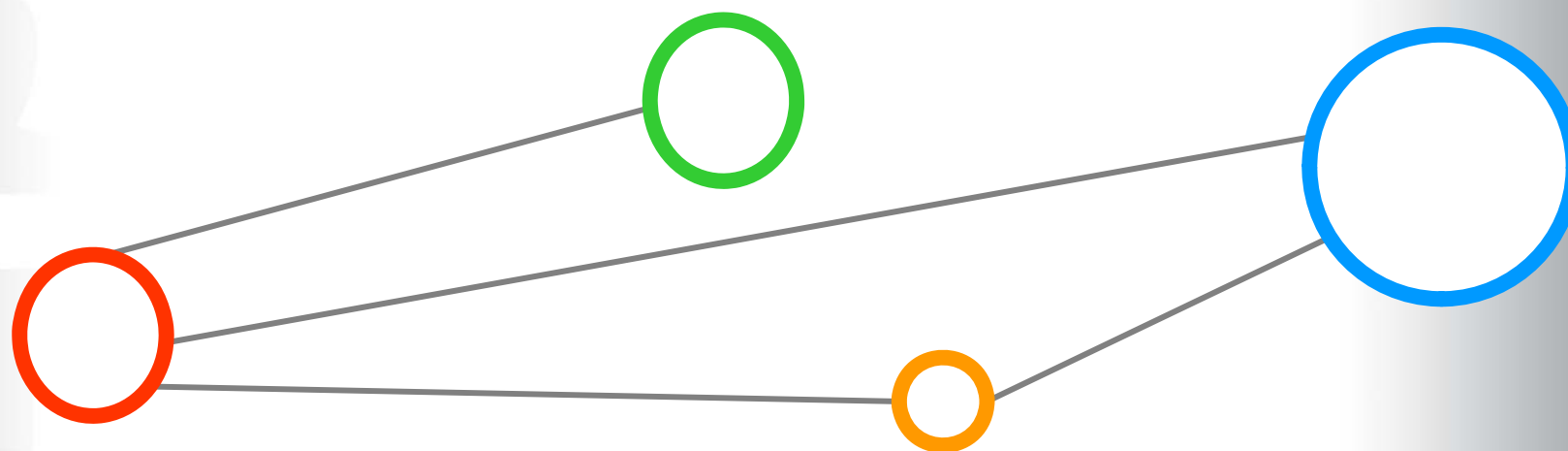
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Outline

- DEISA 101
- Different Paradigms HTC/HPC
 - Paradigms HTC & HPC
 - Future Trends & Interoperability
- DEISA Extreme Computing Initiative
 - DECI Project Examples & Application Categories
- DECI Proposals
 - DECI Operation Process & Proposal Creation
- DEISA Virtual Communities
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- References & Acknowledgements

DEISA 101



DEISA Infrastructure



[1] DEISA

- DEISA is an EU FP7 Research Infrastructure Project
- Consortium of national supercomputing centres
- Aims to advance computational sciences in the area of High Performance Computing (HPC)
- Providing access to HPC resources for researchers all over Europe independent of national boundaries
- Deploys and operates a persistent, production quality, distributed supercomputing environment
- Using the **UNICORE** Grid middleware for multi-site workflows and chains of different computations

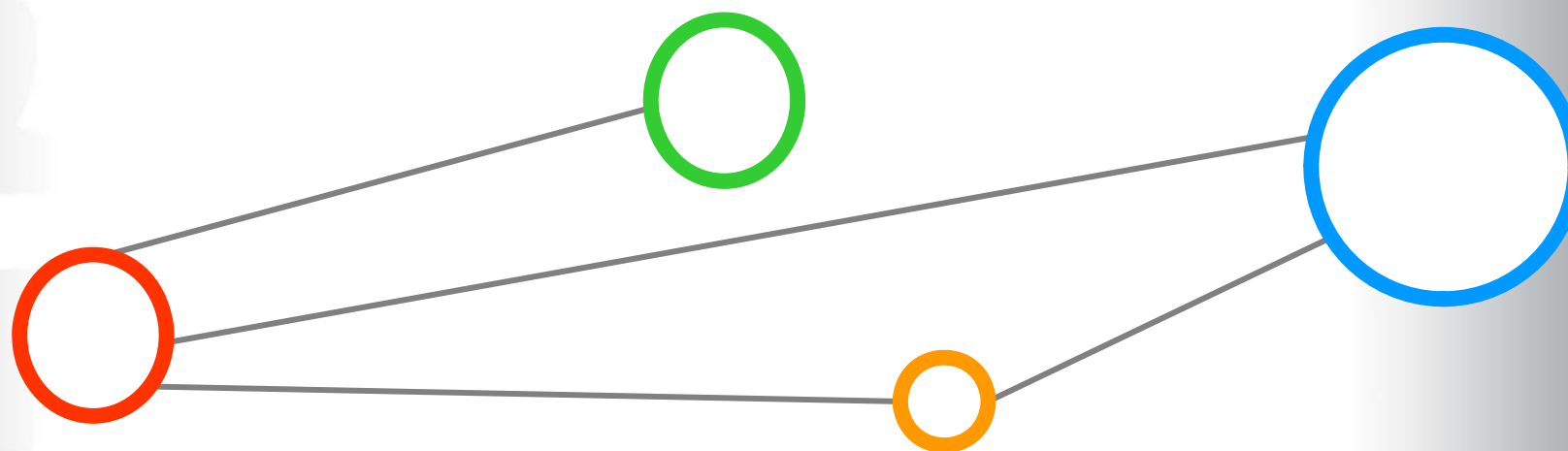


[4] UNICORE



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Different Paradigms HTC/HPC

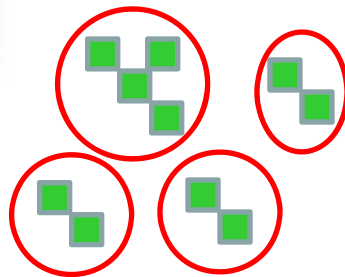


HTC – Computing Paradigm

- High Throughput Computing (HTC)



- *used by ,embarassingly parallel applications‘*
- *cpus/cores not well interconnected*
- *relatively cheap compared to HPC resources*
- *cpus/cores often physically distributed*
- *high availability → ,free/idle cycles‘*
- *access may be granted by beeing part of well-known Virtual Organizations (VOs)*

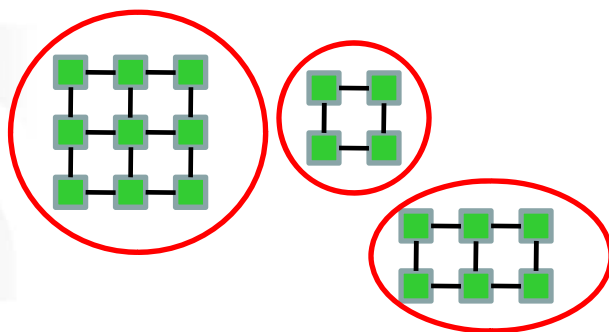


HPC – Computing Paradigm



- High Performance Computing (HPC)

- *used by massively parallel applications*
- *cpus/cores well interconnected*
- *good interconnection leads to costly resource*
- *physically often concentrated in centres*
- *no free cycles, mostly ,n times overbooked‘*
- *access only possible if scientific proposal passed evaluation process → ,time grants‘*



Future Trends in HPC/HTC

eGee

eGI

[8] EGI



Distributed
European
Infrastructure for
Supercomputing
Applications



PRACE

[9] PRACE

- HPC/HTC difference will remain
- HTC infrastructures & resources
 - European Grid Initiative (EGI)
 - National Grids aligned in the EGI infrastructure → Sustained Grid
 - Evolution of infrastructure(s) such as EGEE
- HPC infrastructures & resources
 - Partnership for Advanced Computing in Europe (PRACE) → Petascale systems
 - National HPC centres aligned in PRACE
 - Evolution of infrastructure(s) such as DEISA
 - Element of HPC ecosystem ESFRI strategy

HPC/HTC Interoperability



[7] IGIIW



[6] GIN

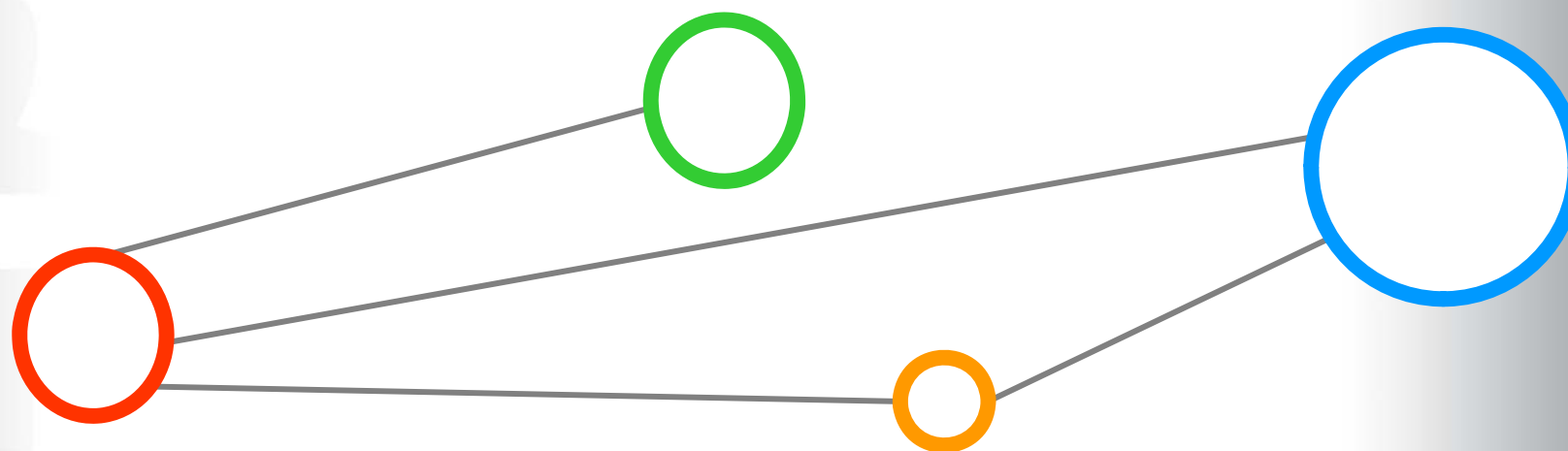


[5] PGI



- Int. Grid Interop* Workshops (IGIIWs)
 - Co-located with e-science conference series
- OGF Grid Interoperation Now (GIN)
 - Grid Applications (often jointly HTC and HPC)
 - Multi-physics, multi-scale applications
- OGF Production Grid Infrastructure (PGI)
 - Standardization of relevant OGF standards
 - Based on production experience of GIN
- HPC+HTC on large-scale resources
 - High amount of HTC jobs may run on future large-scale resources together with HPC
 - E.g. HTC jobs on BlueGene/P systems with up to 1 Petaflop/s (~200.000 cores)

DEISA DECI



DEISA Extreme Computing Initiative

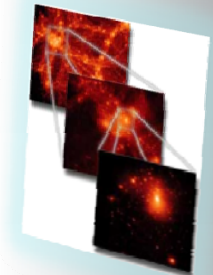
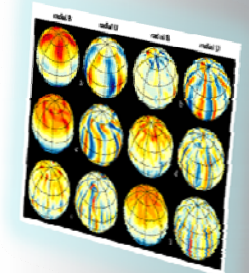


[2] DECI

- Launched in May 2005 by the DEISA Consortium
- Work to advance computational sciences in Europe
- Enable a number of 'grand challenge' applications in all areas of science and technology
- Enabling and operating new challenging supercomputing applications
- Leading, ground breaking applications that deal with complex, demanding and innovative simulations
- Enable applications that would not be possible without the DEISA infrastructure
- Applications benefit from exceptional HPC resources

DECI Project Examples

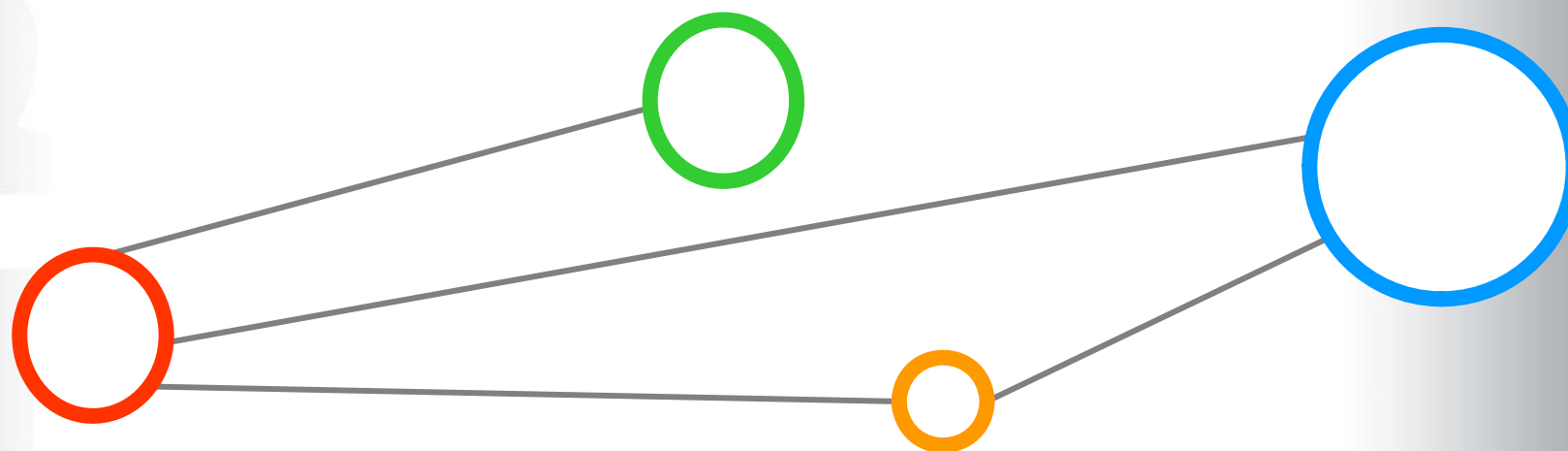
- **3C4WTS → Large scale Wind Turbines**
 - Computational Fluid Dynamics (CFD), Wind Turbines, Aerodynamic Design
- **3DEarth**
 - Numerical modeling of geodynamical processes
- **AntiEflx**
 - Bacterial resistance against antibiotics research
 - Computational Biophysics
- **AQUILA → Cosmological simulation**
 - Hydro-dynamics, earth system science
- **Dratchet → Particle transport studies**
 - fluid-structure interactions, multi-physics simulations



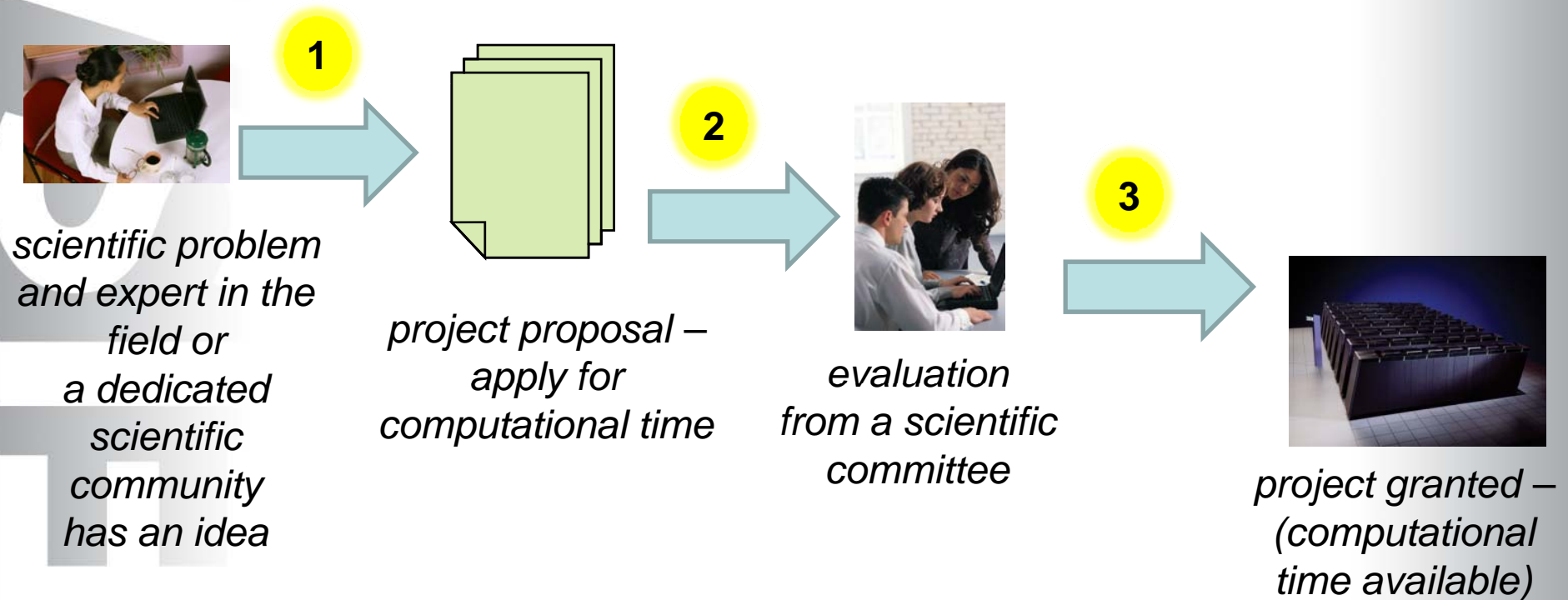
DECI Application Categories

- Int. collaborations with scientific teams that access cpus/cores of supercomputers in different countries
 - Benefits: common global file systems, joint data repositories
- Extreme computing demands for projects requiring a dominant fraction of a single supercomputer
 - Benefits: one big HPC system instead of 2-3 smaller cluster
- Workflow applications involving at least two or even more HPC platforms and/or different HPC resources
 - Benefits: use UNICORE for chain of computations
- Coupled applications involving more than one HPC platform using co-allocation methods
 - Benefits: simultaneously running different codes in parallel

DECI Proposals



How do communities get access?



- Reminder: Process necessary because HPC resources are very costly and highly demanded
 - There are typically no 'idle supercomputers'
 - Such systems are typically even 'overbooked'

DECI Operation Process Overview

- New communities create a scientific proposal 1
 - A call for proposals is launched every year
 - Templates are available at the DECI Web-site
- Evaluation of the proposals is carried out by so-called National Evaluation Committees 2
 - DEISA Executive Committee takes final decisions based on the recommendation of the national committees
 - Projects are chosen on the basis of innovation potential
 - Scientific excellence and HPC relevance is important
- Approved proposals get computational time 3
 - Community run jobs directly using their 'time grants'
 - Some may be scheduled to run at given time windows

First steps for new communities

- Get in contact with the national partners of the Applications Task Force (ATASKF) 
 - ATASKF is a team of leading experts in HPC and also in Grid computing (i.e. multi-site jobs)
 - ATASKF provides consultancy needed to enable the user's adoption of the DEISA research infrastructure
 - Experts help users to design and adapt applications to the DEISA infrastructure
 - Only general information: ataskf@deisa.eu
- Create a DECI Project Proposal taking the guidance of the ATASKF members into account 
 - DECI Project Proposal should follow the template provided on the DECI Web-site

[2] DECI



National Partners of ATASKF

- **Finland**
 - CSC, Espoo, Finland: Juha Fagerholm, juha.fagerholm@csc.fi
- **France**
 - IDRIS, Orsay, France: Pierre Francois Lavallee, lavallee@idris.fr
- **Germany**
 - FZJ, Juelich, Germany: Marc-Andre Hermanns, m.a.hermanns@fz-juelich.de
 - HLRS, Stuttgart, Germany: Thomas Boenisch, boenisch@hlrs.de
 - LRZ, Garching, Germany: Matthias Brehm, brehm@lrz.de
 - RZG, Garching, Germany: Hermann Lederer, lederer@rzg.mpg.de
- **Italy**
 - CINECA, Bologna, Italy: Giovanni Erbacci, g.erbacci@cineca.it
- **Spain**
 - BSC, Barcelona, Spain: David Vicente, david.vicente@bsc.es
- **United Kingdom**
 - ECMWR, Reading, UK: Umberto Modigliani, umberto.modigliani@ecmwf.int
 - EPCC, Edinburgh, UK: Gavin Pringle, gavin@epcc.ed.ac.uk
- **Netherlands**
 - SARA, Amsterdam, Netherlands: Wim Rijks, wimr@sara.nl

Concrete DECI Project Proposal



- Create a proposal following a provided template...
 - Contact of principal investigator
 - Further investigator from different institution
 - Cooperating institutions
 - Research area
 - Types of requirements
 - Overall resource requirements (e.g. total # of CPU hours)
 - Requirements for a typical run (e.g. # CPUs / jobs)
 - Data repository demands
 - Necessary application enabling



DEISA



2

Proposal for a challenging project within the DEISA Extreme Computing Initiative

DEISA is an EU FP7 Research Infrastructure Project to advance computational sciences in the area of supercomputing in Europe.

The DEISA Extreme Computing Initiative is aiming at leading, ground breaking applications in selected areas of science and technology dealing with complex, demanding, innovative simulations with a label of excellence from at least one national evaluation committee.

The initial focus on "Grand Challenge" applications with only little or moderate application enabling work for the DEISA environment has been expanded to include medium to long term support for important complex application enabling.

Please mail this **Proposal** to the DEISA Executive Committee execomm@deisa.eu (and in cc to: ataskf@deisa.eu) not later than **June 30, 2008**.
For technical questions please contact the DEISA Applications Task Force ataskf@deisa.eu

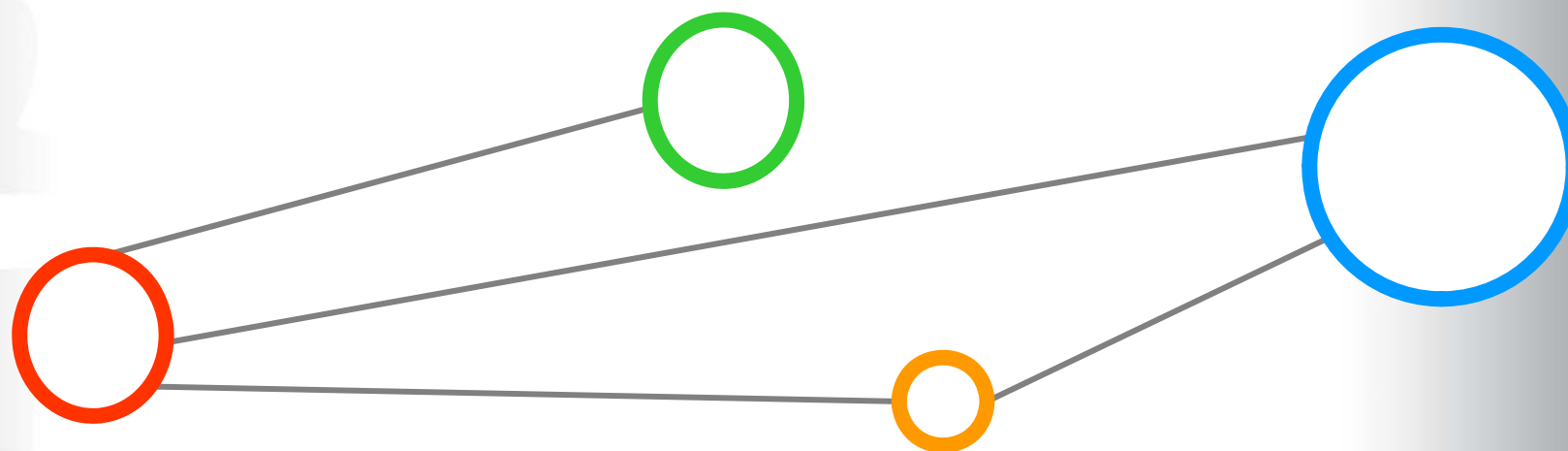
Project Title	
Project Acronym (up to 8 characters)	
Name of Principal Investigator	



DECI Support

- ATASKF complements the traditional user support for established users of the DEISA infrastructure
- Key task in deploying and maintaining a so-called Common Production Environment across all sites
- Other ATASKF activities that support DECI projects
 - ‘Hyper-scaling’ of parallel applications
 - Design of workflow applications
 - Design of coupled and Grid applications
 - Enabling data-intensive applications
- Scientists that would like to use interoperability between HTC & HPC (Grids/resources/applications)
 - Contact: Morris Riedel (m.riedel@fz-juelich.de)

DEISA Virtual Communities

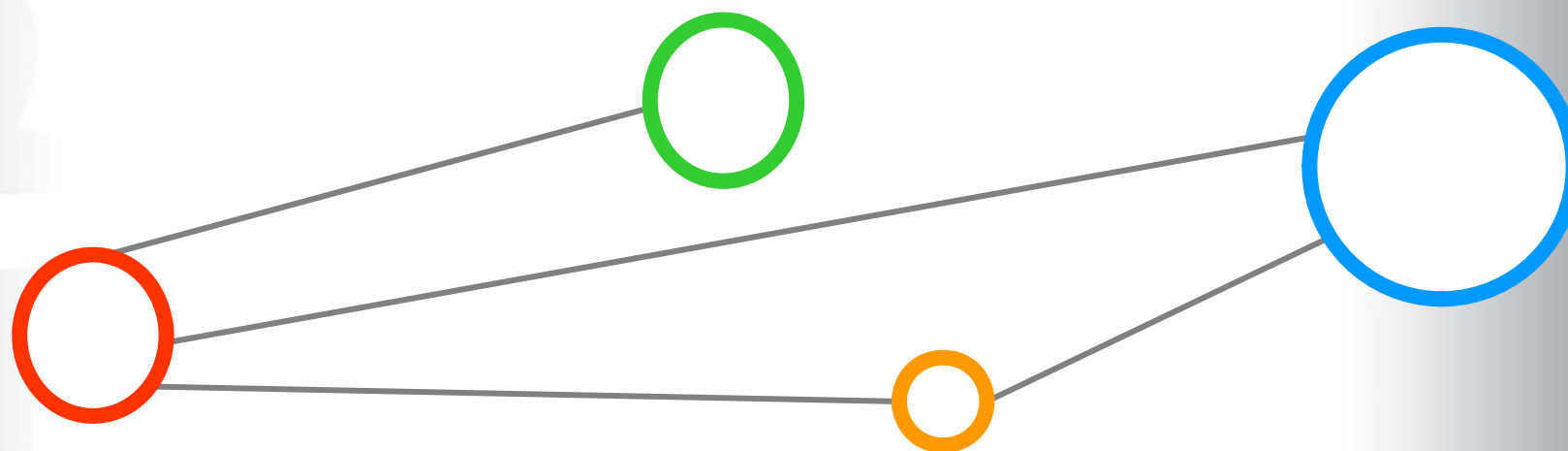


DEISA Virtual Communities

[3] DEISA Virtual Communities

- Established communities can reply to a call of expression of interest
- New virtual communities should download the template file and contact deisa2-coordinator@rzg.mpg.de
- Slightly different evaluation process from DECI
- Examples of a structured science community with DEISA HPC support are...
 - The European fusion community
 - Pre-studies towards the Virtual Physiological Human (VPH)
 - Others like climate/earth system research, astrophysics & cosmology, life sciences & materials sciences,...
 - The initiative is open for communities from other disciplines

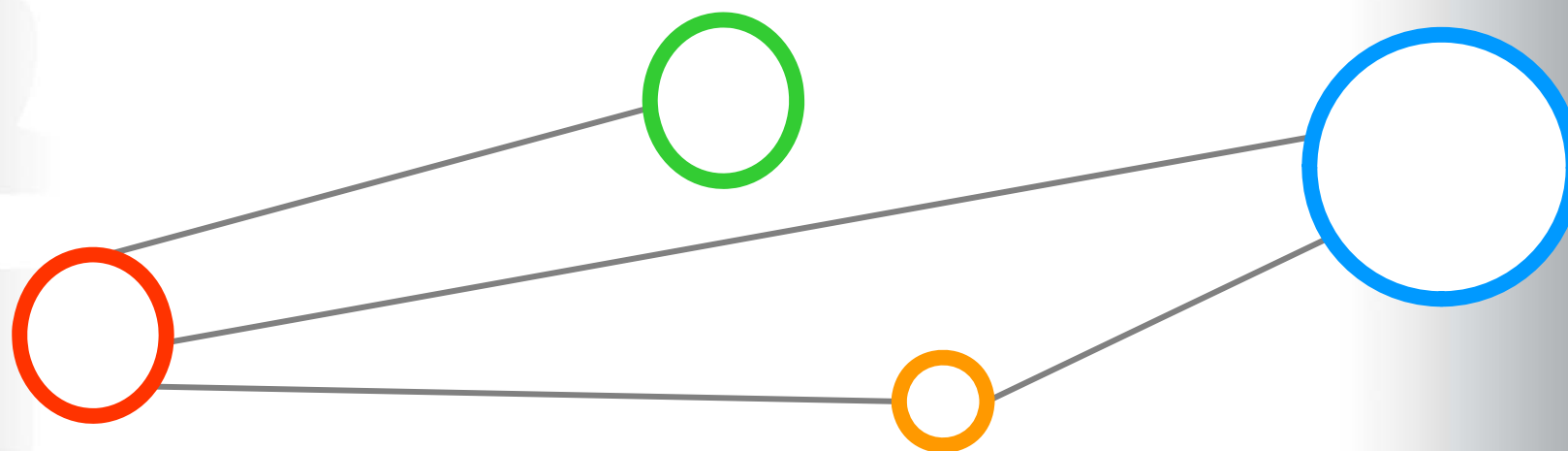
Summary



Summary

- New communities can be everytime involved
 - New communities don't have to share any HPC resources
- Think about of becoming a DEISA virtual community
- Create a DECI Proposal to get access to DEISA
 - 1: Contact ATASKF national contact point for guidance
 - 2: Use provided DECI project template for a good proposal
- Three-step process to get computational time
 - 1: Create a scientifically-driven project proposal
 - 2: Evaluation process of a scientific committee
 - 3: Computational time available once proposal granted
- **Contact ATASKF (ataskf@deisa.eu) or national contacts or consider being a virtual community**

References & Acknowledgements



References (1)

- [1] DEISA,
<http://www.deisa.eu>
- [2] DECI,
<http://www.deisa.eu/science/deci>
- [3] DEISA Virtual Communities
<http://www.deisa.eu/science/communities/overview>
- [4] UNICORE Grid Middleware
<http://www.unicore.eu>
- [5] OGF Production Grid Infrastructure Working Group
http://www.ogf.org/gf/group_info/view.php?group=pgi-wg
- [6] OGF Grid Interoperation Now Community Group
http://www.ogf.org/gf/group_info/view.php?group=gin-cg

References (2)

- [7] Int. Grid Interoperability and Interoperation Workshop
<http://www.fz-juelich.de/jsc/igiw>
- [8] European Grid Initiative Design Study
<http://www.egi-ds.eu>
- [9] Partnership for Advanced Computing in Europe
<http://www.prace.eu>

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