enabling the e-Scientist

ICENI: An Integrated Grid Environment for Component Applications

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From Computational Grids to e-Science

- The Grid: complex networked resources
  - Don't know which resources will be available and when
  - Potentially fragile resource connectivity and availability
  - Link instruments / storage / computation / HPC
- E-Science: higher-level applied use of these resources
  - Complex applications have to retain performance
    - Analysis of very large distributed data sets
    - Coupled execution for multi-physics or visualisation
  - Ease of use for domain specialists
    - For the Developer – higher level abstractions
    - For the User – higher level interaction, e.g. portals, PSE's
  - Better utilisation of resources and improve throughput
  - Support scientific collaboration and knowledge management

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Building Computational Communities

- Need to federate resources from real organisations
  - Express ownership and retain control
  - Grid resources are 'not' free – accountability / payment!
  - Manage the resources as a single unit
- Computational Communities (a.k.a. Virtual Organisations)
  - Share and combine heterogeneous resources
  - Ensure transparency by hiding complexity from the user
  - Optimise resource utilisation for all jobs and users
  - Easy to contribute (and withdraw) resources
- Collect and retain information relating to:
  - The resources
  - The applications
  - The users

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ICENI

The Iceni, under Queen Boudicca, united the tribes of South-East England in a revolt against the occupying Roman forces in AD60.

- IC E-Science Networked Infrastructure
- Developed by Grid Middleware Group, London E-Science Centre
- Collect and provide relevant Grid meta-data
- Use to define and develop higher-level services

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Open Extensible Technologies

- XML used to define:
  - Resource, application, user meta-data
  - Protocol between different services in the system
- Java used to construct the framework, run-time representation and interfaces to the assembled components
- Jini used to provide a wide-area transport layer that supports dynamic discovery and join
- Examining SOAP, WSDL, UDDI, .NET, SunONE etc.

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Need Higher Level Knowledge

- Resources:
  - Availability, capability, environment, access
- Application:
  - Composition, behaviour, performance

  Related talk: Anthony Mayer,
  Thursday 2.00, A201/205
- User:
  - Who, what, when, where

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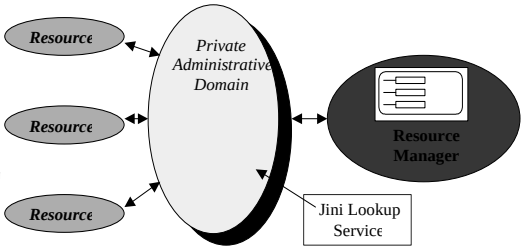
Managing Internal Resources

- The resources advertise their capabilities to a private domain
- Extensible resources abstractions:
  - Computational resources
  - Storage resources
  - Software resources
  - …
- Annotate using XML



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The Domain Manager

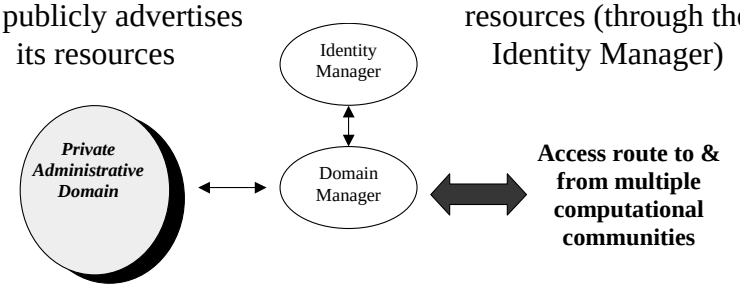
Sole route between the private and the public areas of the infrastructure

Private ➔ Public

Imposes local usage requirements and access and publicly advertises its resources

Public ➔ Private

Authenticates requests to use the local resources (through the Identity Manager)



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Trusting Organisations & Users

- Recognise three entities: individuals, groups and organisations (or domains)
- Entities verified through the Identity Manager using public key certificates (X.509)
- Locally managed access control list determine which entities have access to local resources
- Non-local users can be mapped to individual, single, or guest accounts (resource dependant policy)

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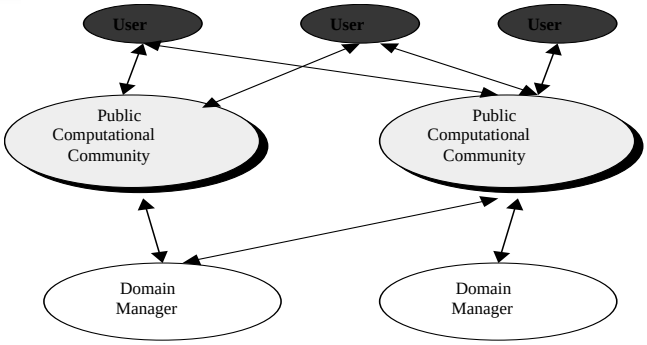
Interaction with the Computational Community



The Computational Community allows Users & Domain Managers to advertise their capabilities and requirements.

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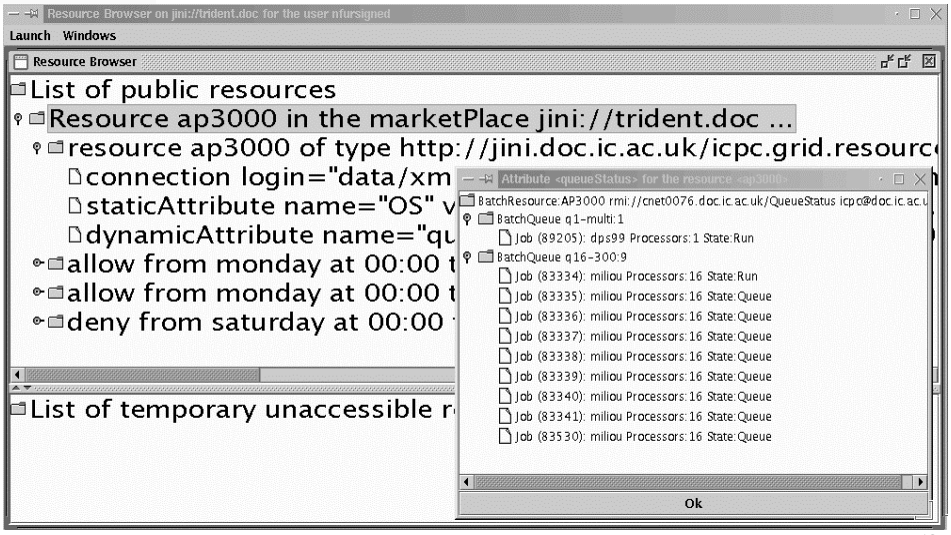
The Resource Browser GUI



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Resources in a Computational Community

A resource might be:

- *Available* → shown with all its public attributes and access policies. It's possible to get the values of the dynamic attribute(s) and to connect to the resource
- *Temporary unavailable* → only the access policies are shown
- *Always unavailable* → no information is shown

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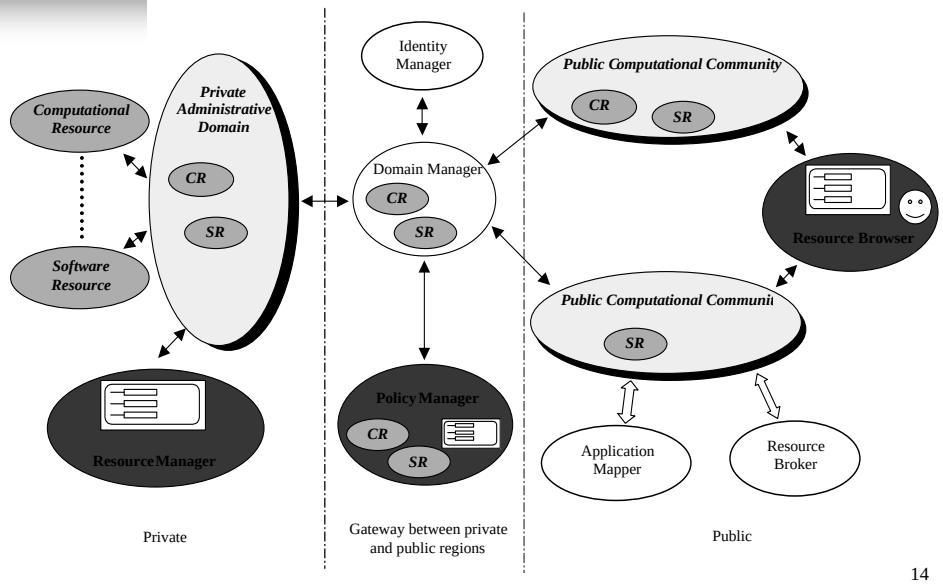
ICENI Architecture



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Higher Levels of Abstraction

- Developer
  - Create numerical implementations
  - Provide performance & implementation meta-data
  - Extensible abstract objects or interfaces
- Scientist
  - Add domain specific knowledge to implementations
  - Define (new?) component interfaces
  - Specify component meta-data
- End-User
  - Customise component instances
  - Application defined by interacting component instances
  - Use components in local (or remote) repositories

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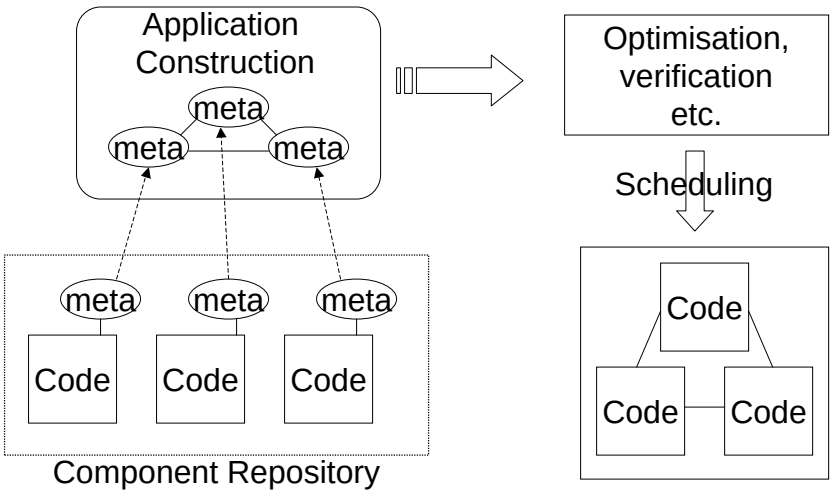
Separating Meta-Information from Implementation



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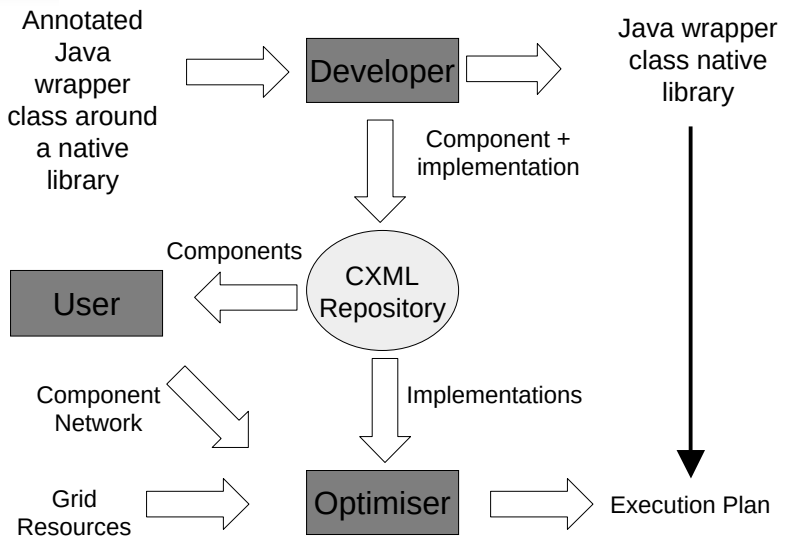
CXML – Component Meta-Data



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User Information

- Security
  - Need secure trusted identity for use on the Grid
  - Need to define what it can be used for
- Application
  - Develop through visual programming
  - Drag & drop functionality from elsewhere
- Policy
  - Restrict where the application runs
- Accounting
  - Which project (account) and how much?
  - Defining resource exchange rates

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Exploiting The Meta-data

- The Computational Community contains information:
  - On resource capability, usage and access policy
  - On the user's job and their application's capability
- Uses this information to ensure:
  - The user's job is run as specified (e.g deadline)
  - All resources are fully utilised (if possible)
  - The mapping of jobs to resources is 'optimal'

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Higher-level Grid Services

- Application Mapper
  - Uses resource and application information to optimise resource selection for an application

    (e.g. are 16 PC processors better than 8 Alpha processors?)
- Resource Broker
  - Uses computational economics to balance priorities

    (e.g. 16 underused PC processors may cost less for longer than 8 over subscribed Alpha processors)
  - Factor queue length into resource selection

    (e.g. Will a slow unloaded resource provide shorter job turnaround time than a faster but heavily loaded resource?)

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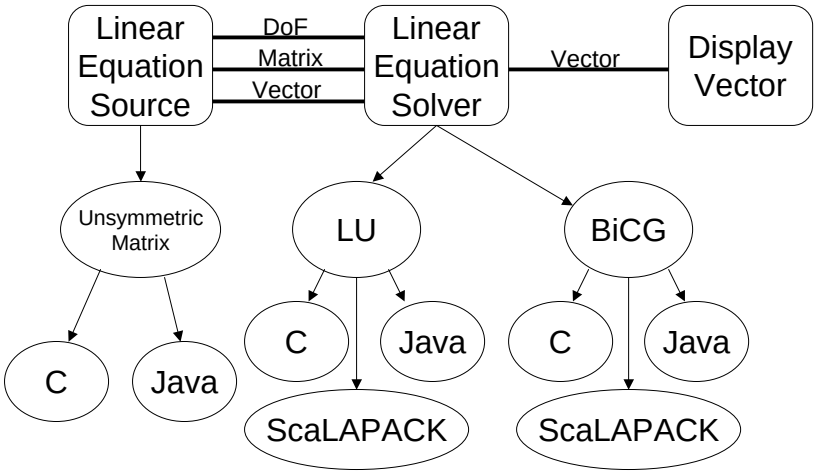
Example: Linear Solver



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Local Computational Community

System	Processor	Number	Language	Solution
PC (Linux)	AMD 900MHz	1	Java + C LAPACK	LU + BCG LU
Atlas	Alpha 667MHz	1,4,9	ScaLAPACK	LU + BCG
AP3000	UltraSparcII 300MHz	4,9,16	ScaLAPACK	LU + BCG

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Dynamic Resource Cost

System	Cost Model 1	Cost Model 2
PC (Linux)	80	80
Atlas	475	425
AP3000	100	100

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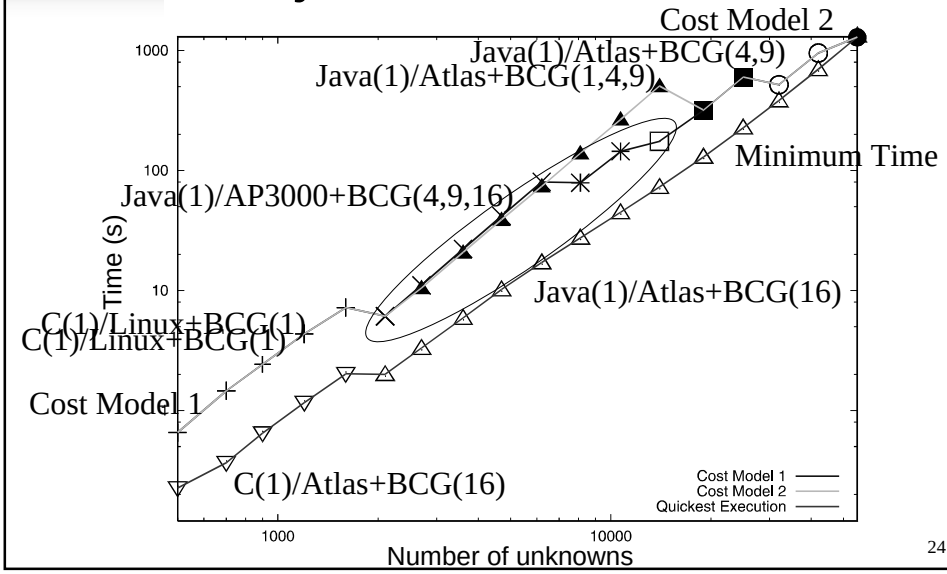
Influence of Resource Selection Policy on Execution Times



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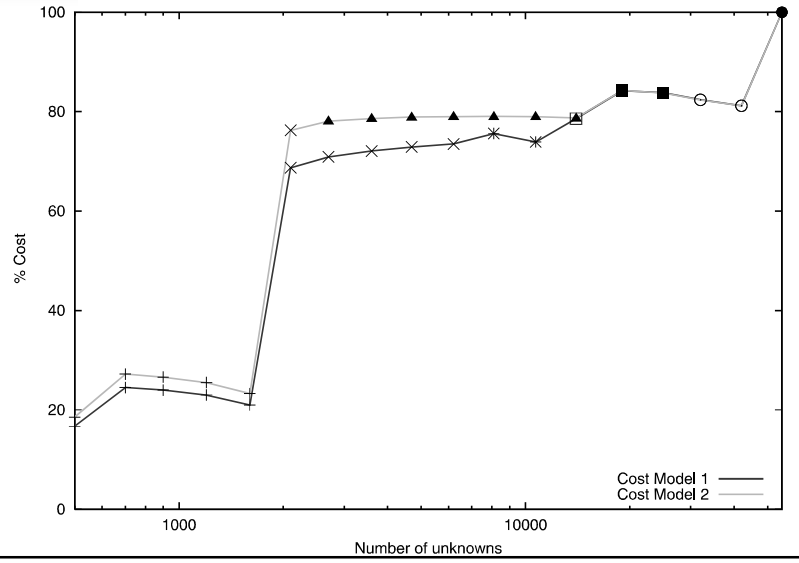
Cost savings relative to minimum time



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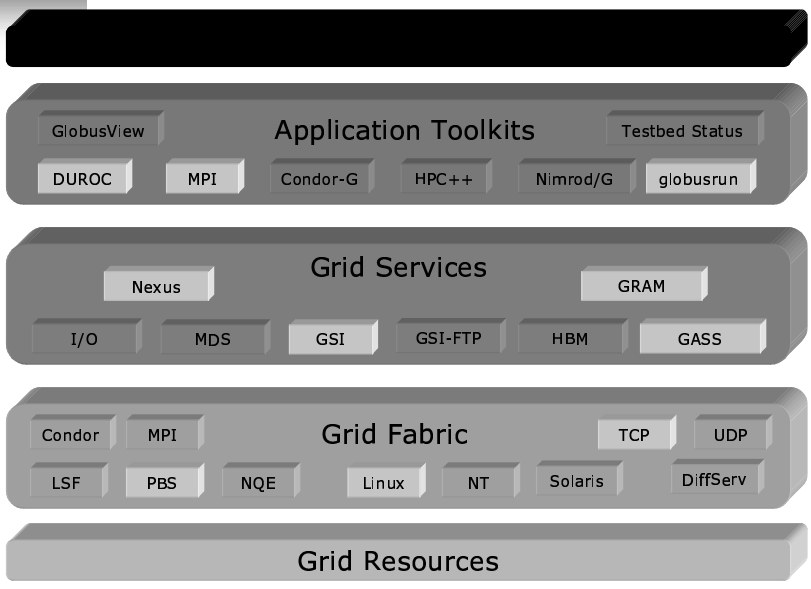
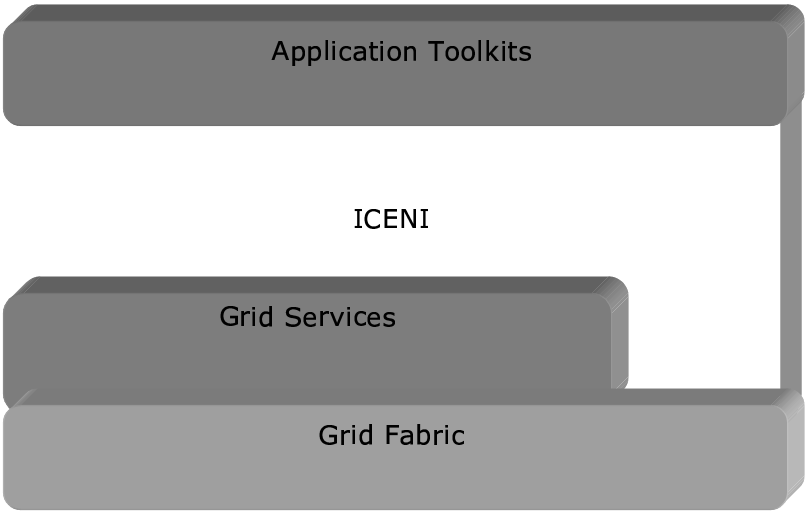
Layered Grid Architecture



Exploit Layered Architecture



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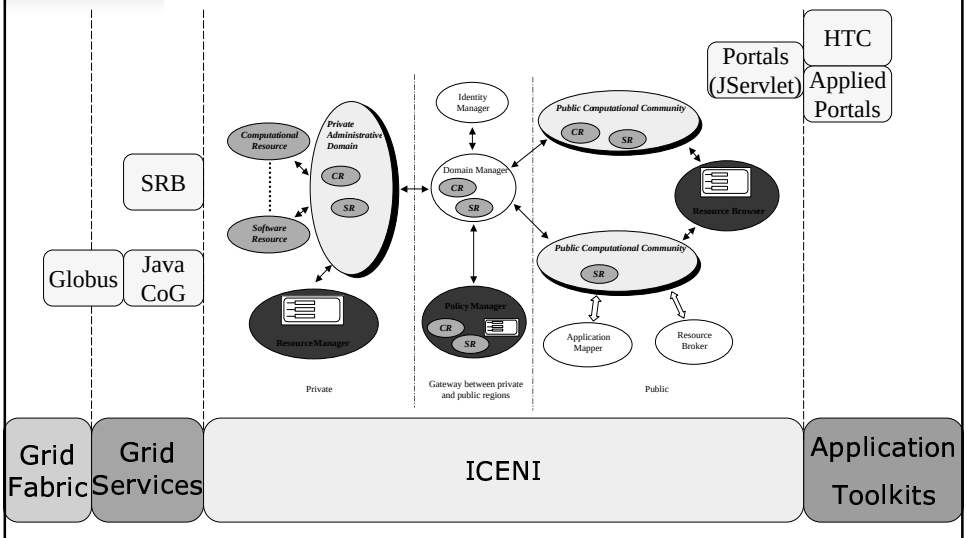
Integration with the Grid



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Summary

- To enable the e-Scientist to fully exploit the resources in the Grid we need information relating to the:
  - Resources
  - Applications
  - Users
- Represent the meta-data in an open extensible manner using XML derived syntax.
- Collect and hold the meta-data in a Java / Jini Grid middleware which has inherent fault-tolerance.
- Allow higher level services to use this meta-data to transparently guide resource allocation within the computational community for defined goals.

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Acknowledgements

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  - Anthony Mayer, Nathalie Furmento, Stephen McGough,
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  - http://www-icpc.doc.ic.ac.uk/components/
  - http://www.lesc.ic.ac.uk/
- Contact: icpc-sw@doc.ic.ac.uk
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- Related talk:Anthony Mayer, Thursday 2.00, A201/205

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