



# Deploying Multiscale Applications on European e-Infrastructures



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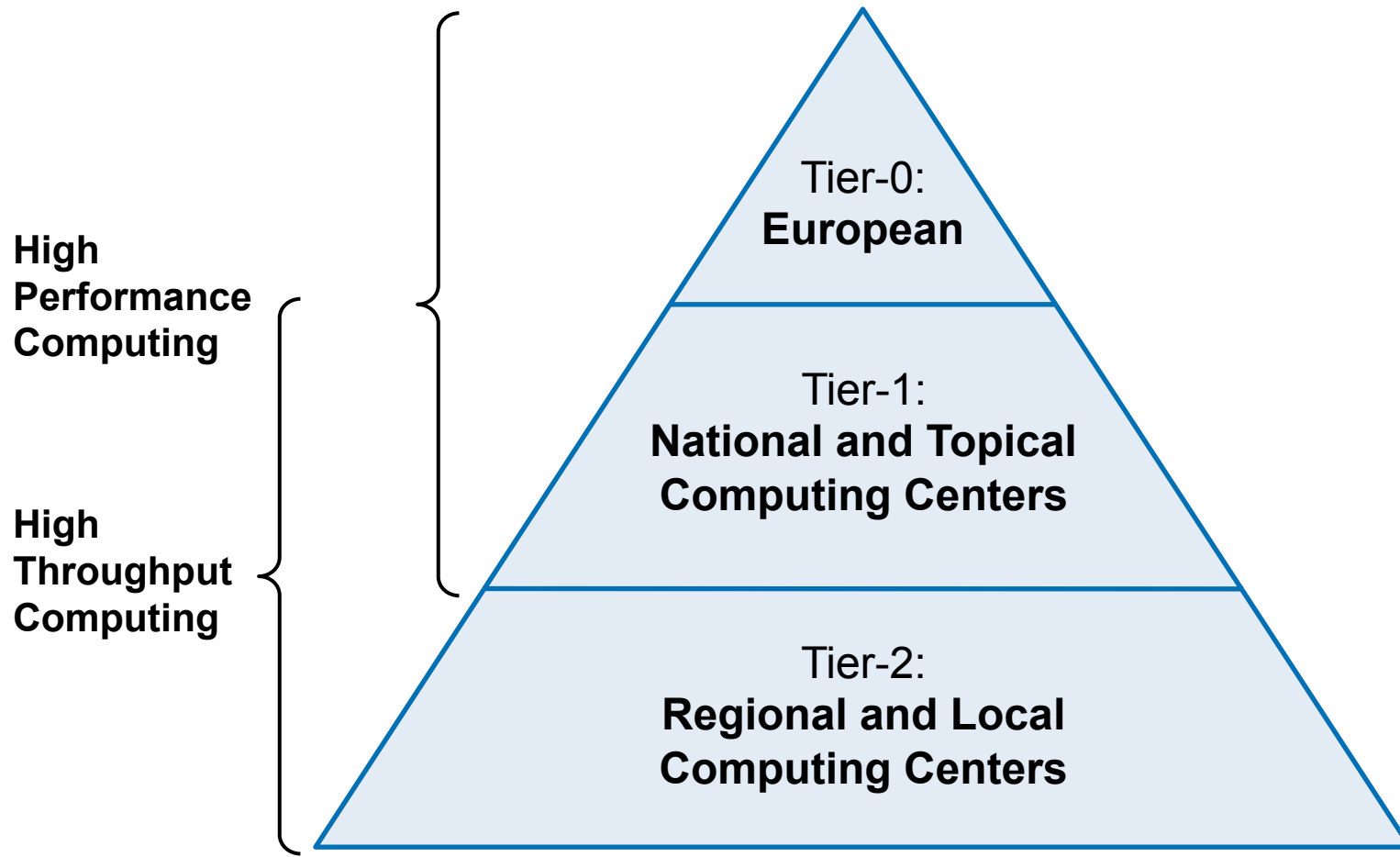
Ilya Saverchenko

# Outline

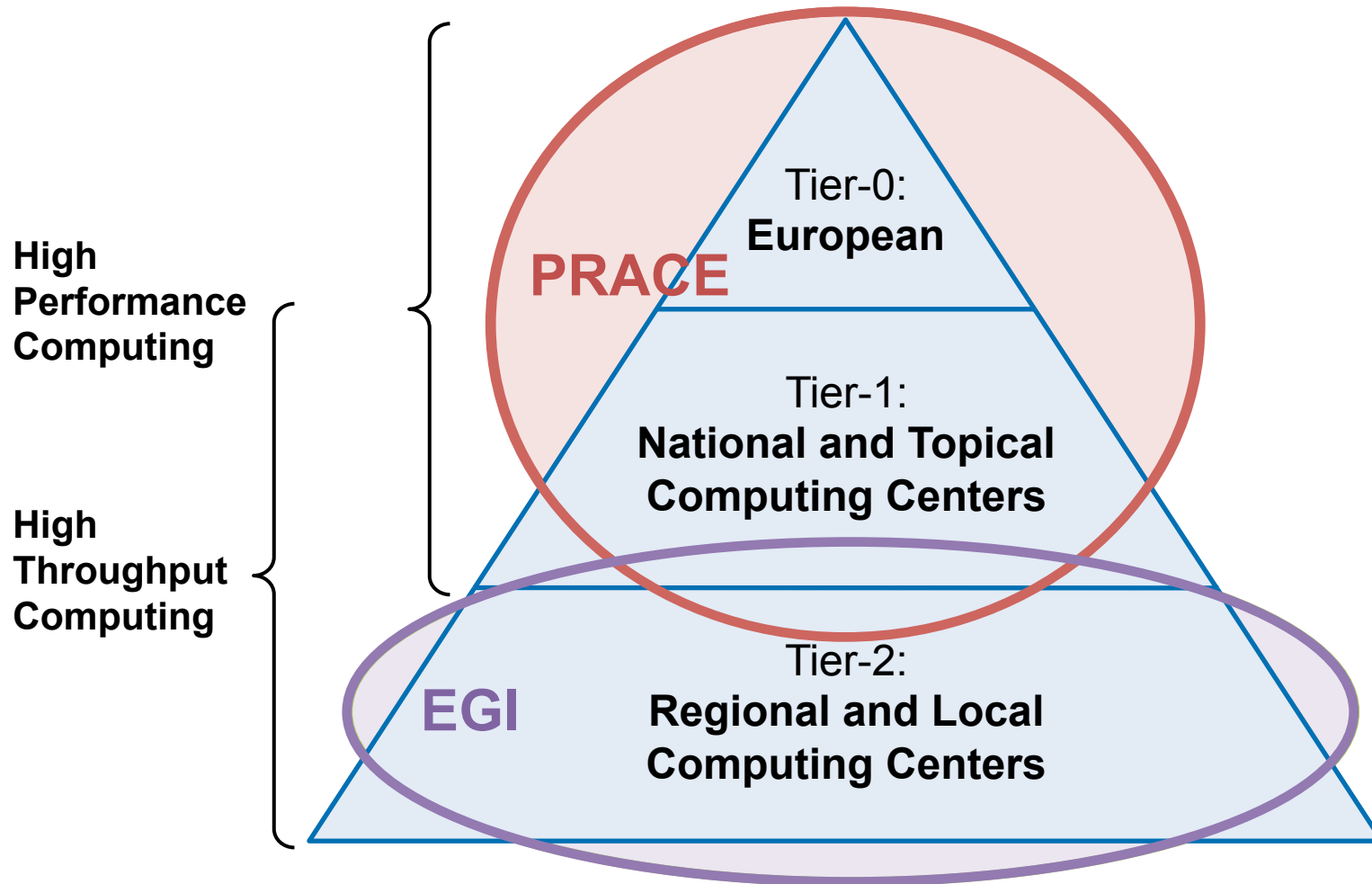


- European e-Infrastructure Ecosystem
- European e-Infrastructures
  - MAPPER
  - EGI
  - EUDAT
  - PRACE
- Tools and services for multiscale computing

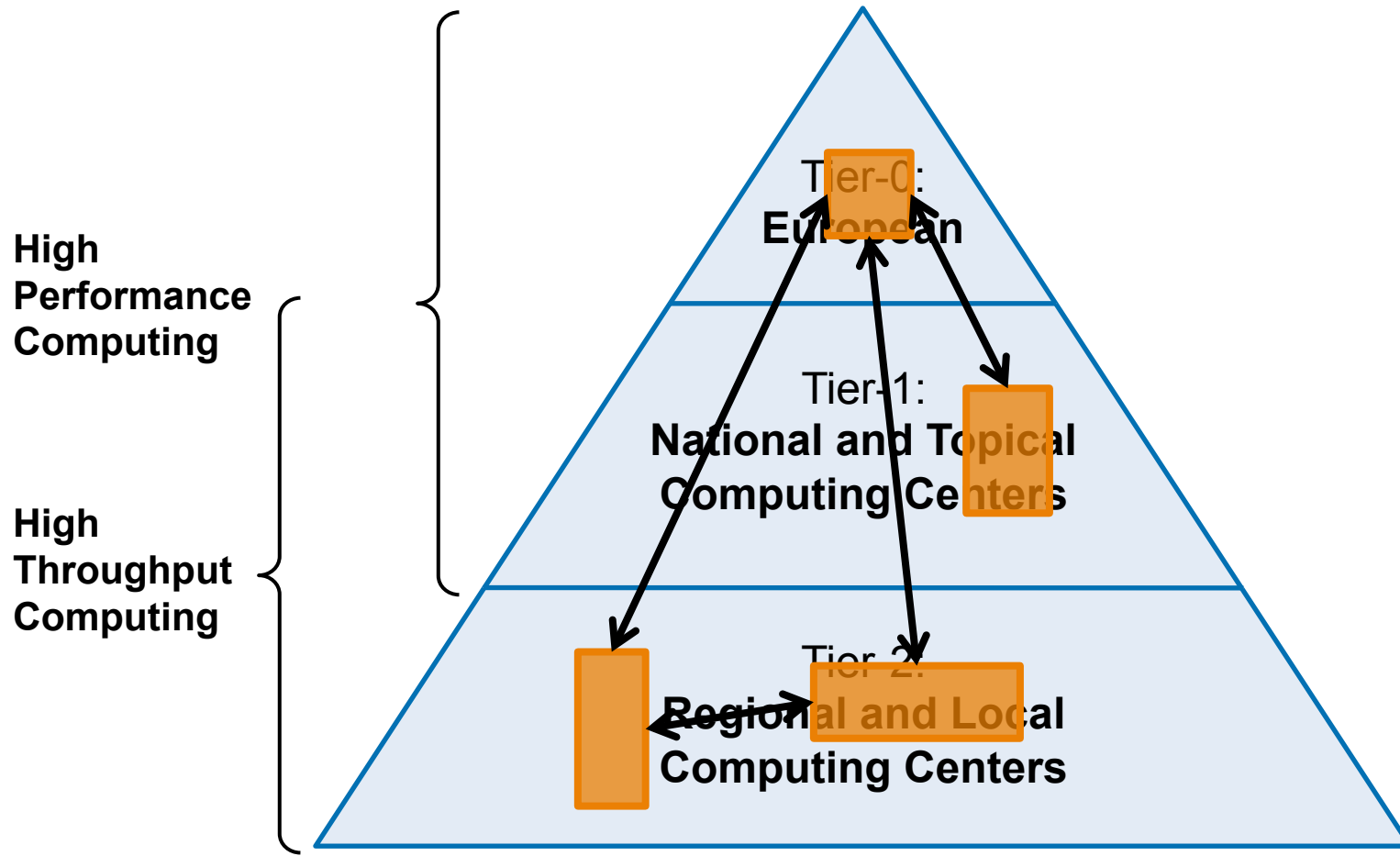
# European Computing Infrastructures



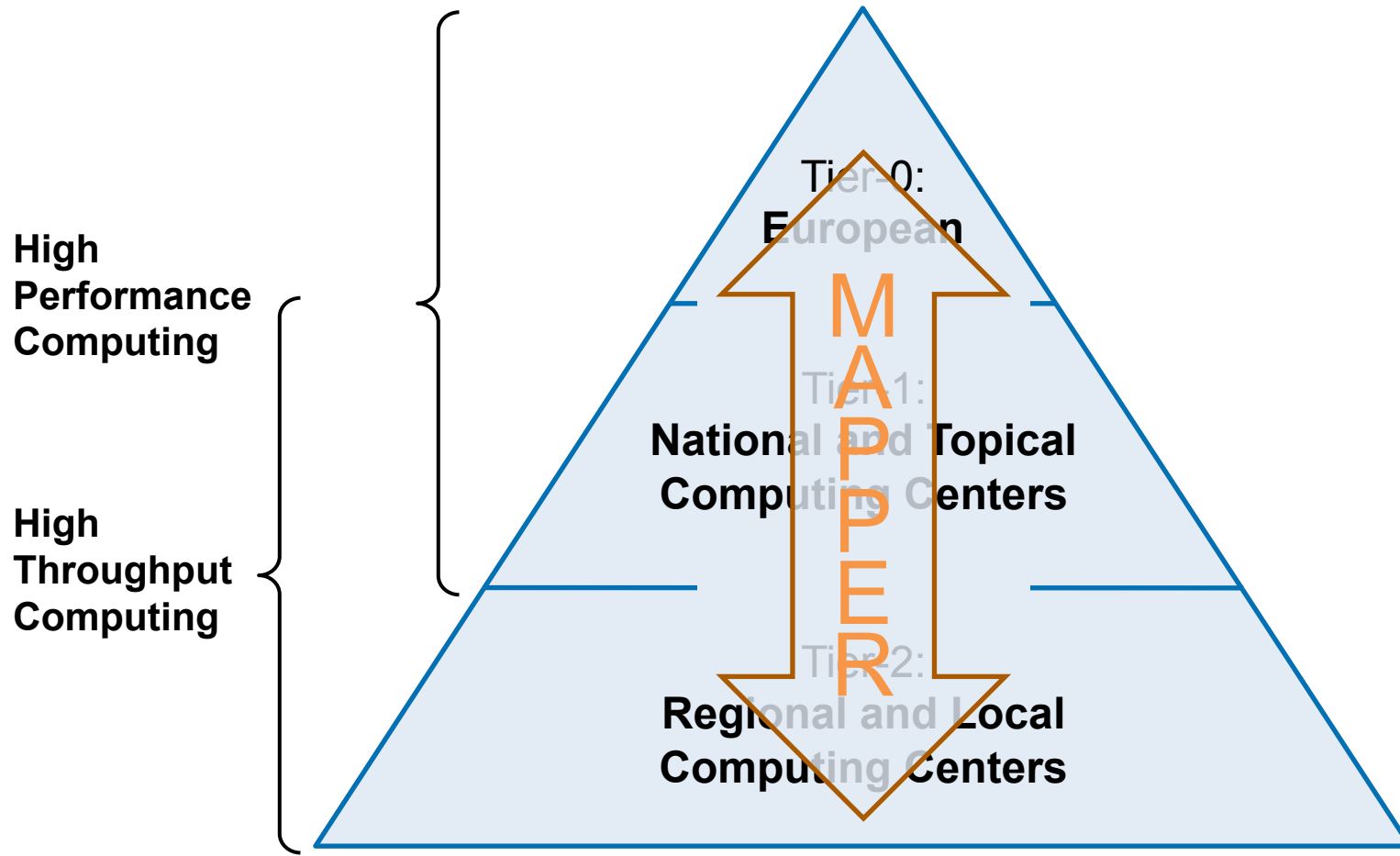
# European Computing Infrastructures



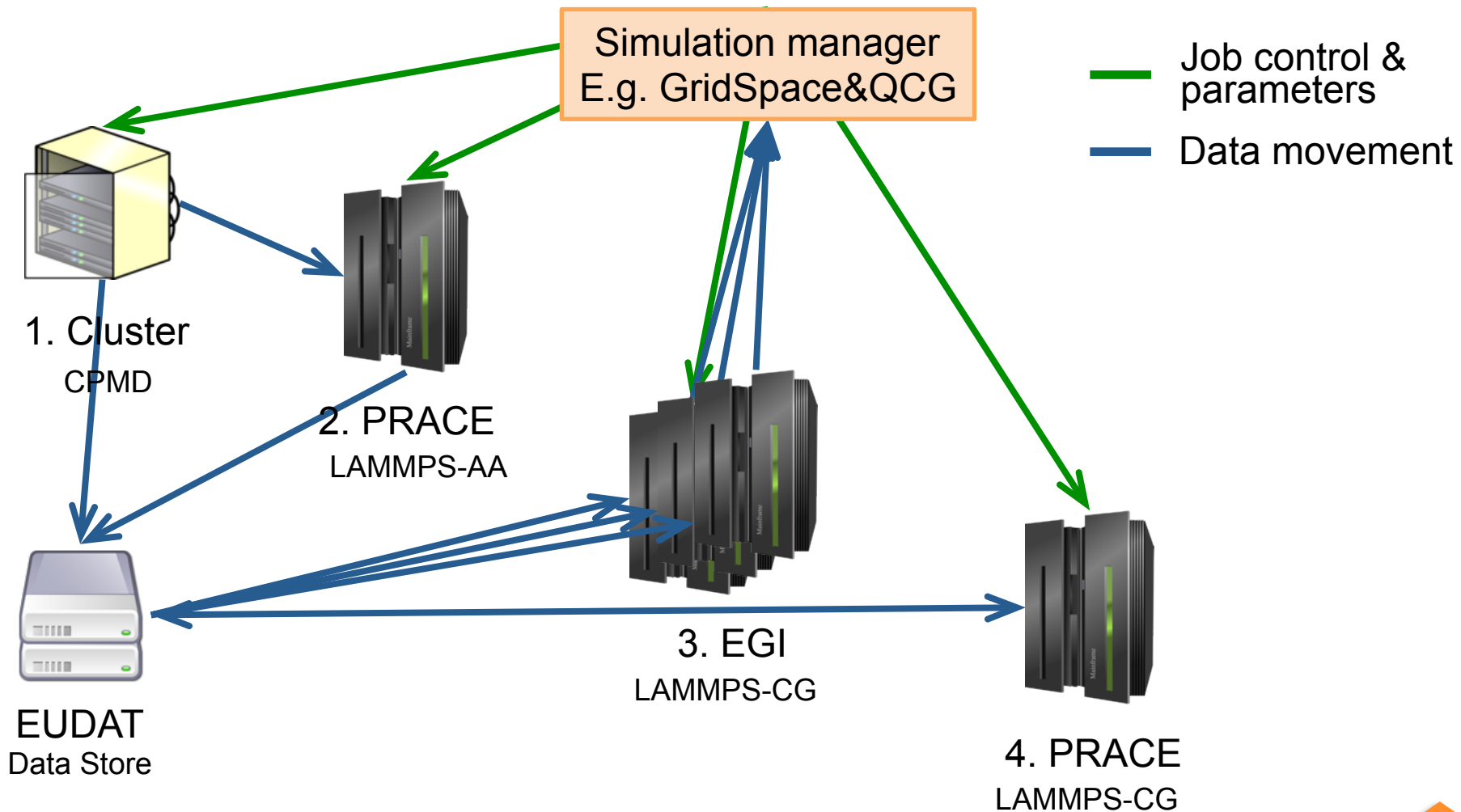
# Multiscale Computing



# Multiscale Computing



# Nanomaterial use case



# Resources & Services



- MAPPER e-Infrastructure
- European e-Infrastructures
  - EGI
  - EUDAT
  - PRACE
- National and regional service providers
- Shared academic facilities
- Local resources and services



# MAPPER e-Infrastructure



- High throughput and high performance computing resources
  - Development, testing, debugging
- Tools and services for multiscale computing
- Training materials and documentation
- Support services



- European Grid Infrastructure

Enables access to computing resources for European researchers from all fields of science, from High Energy Physics to Humanities.

- Legal entity: EGI.eu

- Coordinates NGIs

- National and regional resources

- ~500 resource providers



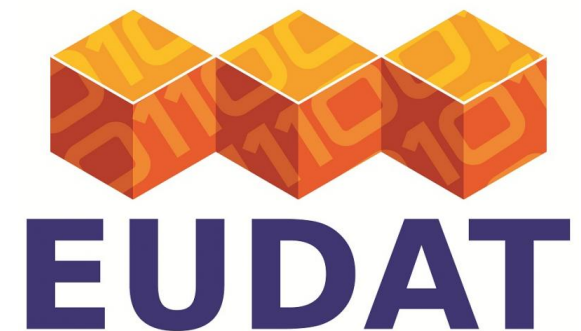


- European Data Infrastructure

Support a Collaborative Data Infrastructure which will allow researchers to share data within and between communities and enable them to carry out their research effectively.

- Tools and services for managing

- Scientific data
- Big data





- Partnership for Advanced Computing in Europe

Enable and support European scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society.

- Legal entity: PRACE AISBL





- European and national HPC resources
  - 25 members
- PRACE Tier-0
  - 6 resources
- PRACE Tier-1
  - 19 resources

# Application & Allocation



- PRACE
  - Tier-0 preparatory access
  - Tier-0 regular access
  - Tier-1 access (DECI)
- EGI
  - Virtual Organisations (VOs)
  - Virtual Research Communities (VRCs)
  - National Grid resources



- Authentication
  - Public-key infrastructure
  - Grid security infrastructure
- Authorization
  - Resources and services
- Accounting
  - Compute and storage quotas

# Middleware & Services



- Network services
- Data management
- Unified Middleware Distribution
  - QCG
- Advance reservation and co-allocation
- Workflow management
- Federated cloud services



# Training & Support



- Documentation, user guides and training material
- Application porting and enabling
- User support and help desk
- Workshops and training events

# Summary



- Communicate your requirements
- Don't hesitate to ask for support
- Foster interoperability between services
- Provide feedback
- Make friends with your regional and national computing centres
- Attend community-focused events
  - EGI Community Forum
  - PRACE User Forum



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# Useful Links: MAPPER



- MAPPER
  - <http://www.mapper-project.eu>
- MAPPER tools and services
  - <http://www.mapper-project.eu/web/guest/tools>
- MAPPER documentation and training material
  - <http://www.mapper-project.eu/web/guest/documents>
- MAPPER user support
  - [support@mapper-project.eu](mailto:support@mapper-project.eu)

# Useful Links: EGI



- EGI
  - <https://www.egi.eu/>
- EGI membership
  - [https://www.egi.eu/how-do-I/become\\_a\\_user.html](https://www.egi.eu/how-do-I/become_a_user.html)
  - [https://www.egi.eu/how-do-I/join\\_or\\_start\\_a\\_community.html](https://www.egi.eu/how-do-I/join_or_start_a_community.html)
- EGI help desk and user support
  - <https://ggus.eu>

# Useful Links: PRACE



- PRACE RI
  - <http://www.prace-ri.eu>
- PRACE Tier-0 preparatory access
  - <http://www.prace-ri.eu/Preparatory-Access>
- PRACE Tier-0 regular access
  - <http://www.prace-ri.eu/Application-Guide>
- PRACE Tier-1 DECI access
  - <http://www.prace-ri.eu/DECI-Projects>
- PRACE help desk and user support
  - <https://tts.prace-ri.eu/SelfService/>