

# Developing a Science Gateway for Physical Activity Lifelong Modelling & Simulation

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**Health Economics (2)**

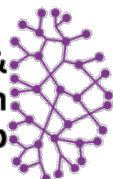
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**University of Catania, Italy**

**Modelling &  
Simulation  
Group**



# Outline

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- Who we are
- Open Science and Data Infrastructures
- PALMS Case Study

# Who we are: Modelling & Simulation Group

<https://tinyurl.com/ycdylsk8>

Modelling &  
Simulation  
Group

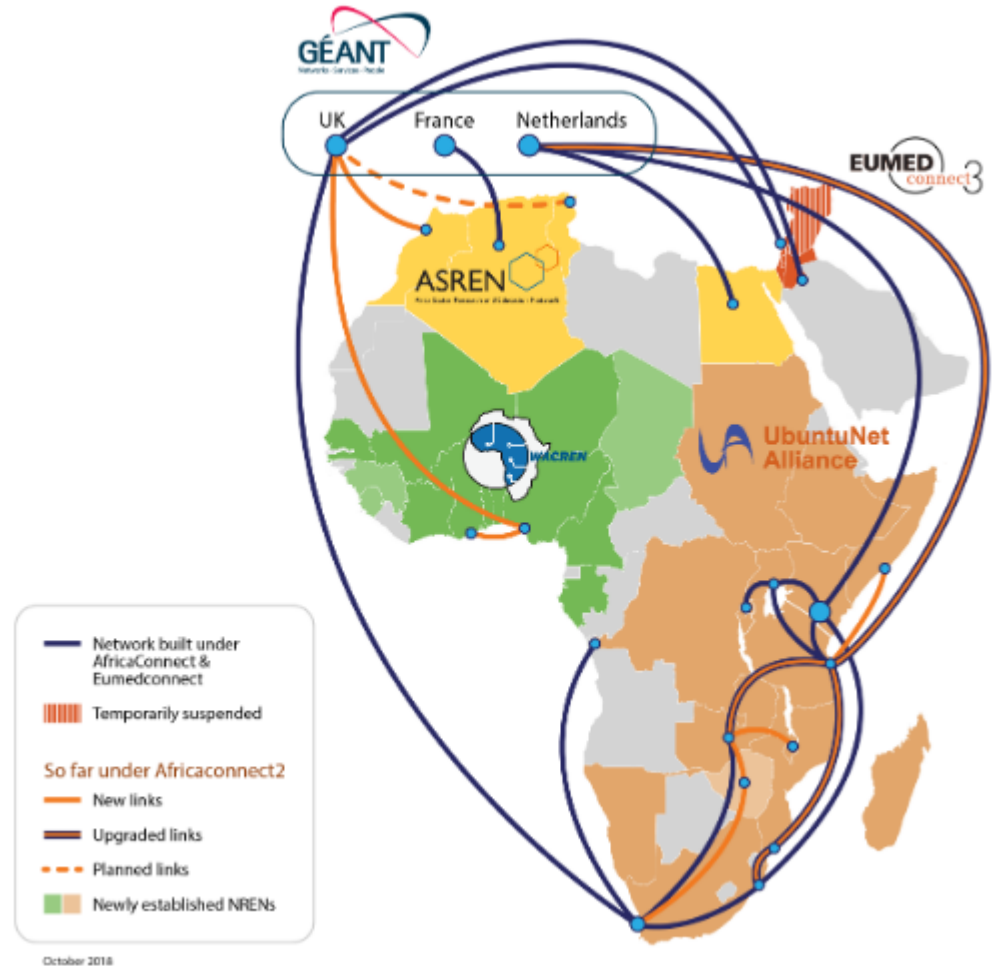


- Industry
  - High Performance Simulation
    - Ford, Saker Solutions, Sellafield, SISO (Standard SISO-STD-006-2010)
  - Cloud-based Simulation
    - CloudSME, CraftBrew, COLA, numerous industrial cloud-based services
- Africa
  - e-Infrastructures for Africa
    - el4Africa, Sci-GaIA, TANDEM NREN Roadmap , numerous African NREN services
- Modelling & Simulation
  - Pathway simulation
    - Tamoxifen, Prostate Cancer, Atrial Fribulation, Physical activity intervention (PALMS)
  - Refugee migration simulation
    - FLEE suite
- Education – Modelling & Simulation
  - Courses
    - NATCOR, PG, UG, Taster workshop (e.g. Cape Town)
  - Student projects
    - Hillingdon Hospital, NASA Simulation Worldwide Exploration Experience
- Local engagement
  - Advising residents on traffic analysis (e.g. HS2)

- Worldwide collaboration
- >£3m research funding
- >£3m industrial savings and revenue
- Many world first software and systems
- High impact research for society

# Projects

- BELIEF I & II (2006-2010)
  - EU e-Infrastructures dissemination
- FEAST (2010)
  - Study/basis for AfricaConnect programmes
- ERINA4Africa (2009-2011)
  - Value of e-Infrastructures to Africa
- eI4Africa (2012-2014)
  - Science Gateways and e-Infrastructures for Africa
- Sci-GaIA (2015-2017)
  - Open Science for Africa (via e-Infrastructures)
- TANDEM (2015-2017)
  - Capacity building for NRENs in West and Central Africa
- ADI-Engage (2018+)
  - African Data Infrastructure engagement programme



# African Open Science – key elements

- Open Access Publishing (Green)
  - Publish then self-archive it in an open access repository where it can be accessed for free (e.g. in an institutional repository or a central repository such as PubMed Central)
  - Embargo period (check via SHERPA/RoMEO)
- Open Data
  - Self-archive in open access repository
  - Compliant with FAIR data principles (<https://www.force11.org/group/fairgroup/fairprinciples>)
- Open Software
  - Self-archive in open access repository (e.g. GitHub)
  - Make available via science gateway
- Clear licencing/sharing agreement
  - e.g. Creative Commons
- Link outputs to scientist via DOIs and researcher registry
  - e.g. ORCID

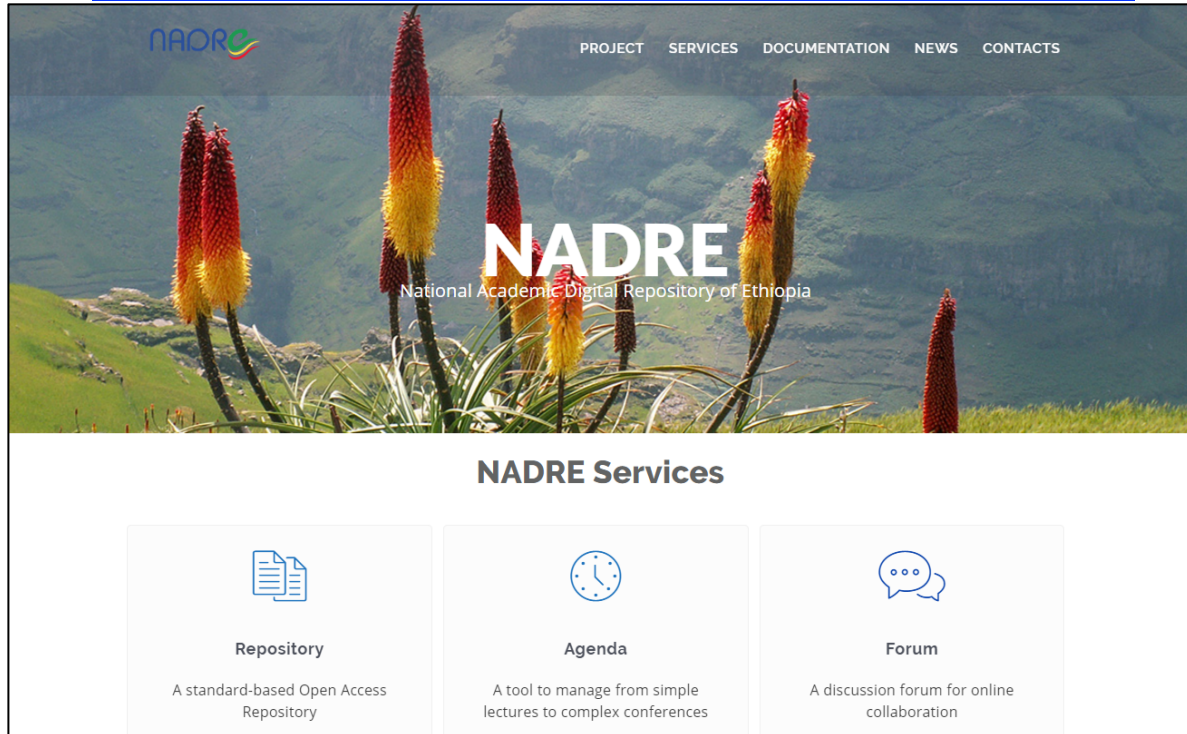


# Example:

## African Open Publishing – with Ethiopian NREN EtherNet

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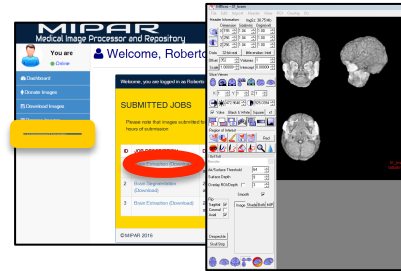
<https://nadreweb.ether.net.edu.et>



# Science Gateways

Open Science applications supporting research communities in Nigeria, Ghana, Ethiopia, Kenya, Tanzania and South Africa that impact Global Challenge research

- Computational Chemistry
- Public Health
- Genomics
- Agriculture
- Medical Imaging
- Phytomedicine
- Power Systems
- Climate Change
- General Open Science
- More being added!



<https://mipar.sci-gaia.eu/about/>



<https://phg.sci-gaia.eu>



*Developed through freely available international Hackfests ( available from [www.sci-gaia.eu](http://www.sci-gaia.eu))*

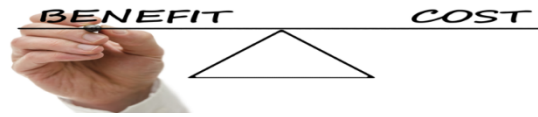
# PALMS Case Study

- Transition of African societies into ‘sedentary’ lifestyle
- Burden on Africa:
  - Over 85% of NCD related mortality globally (58 million deaths)
  - Cumulative economic losses of US\$7 trillion over the next 15 years
- Strategic pathway to achieving UN’s 2030 Sustainable Development Goals.
- Current evidence base lacks ‘policy relevance’
- PALMS model as a basis for evidence-based policy making:
  - GHS: evidence-based cost-effectiveness
  - Local/regional authorities: return on investment from any sector locally within 1-5 years





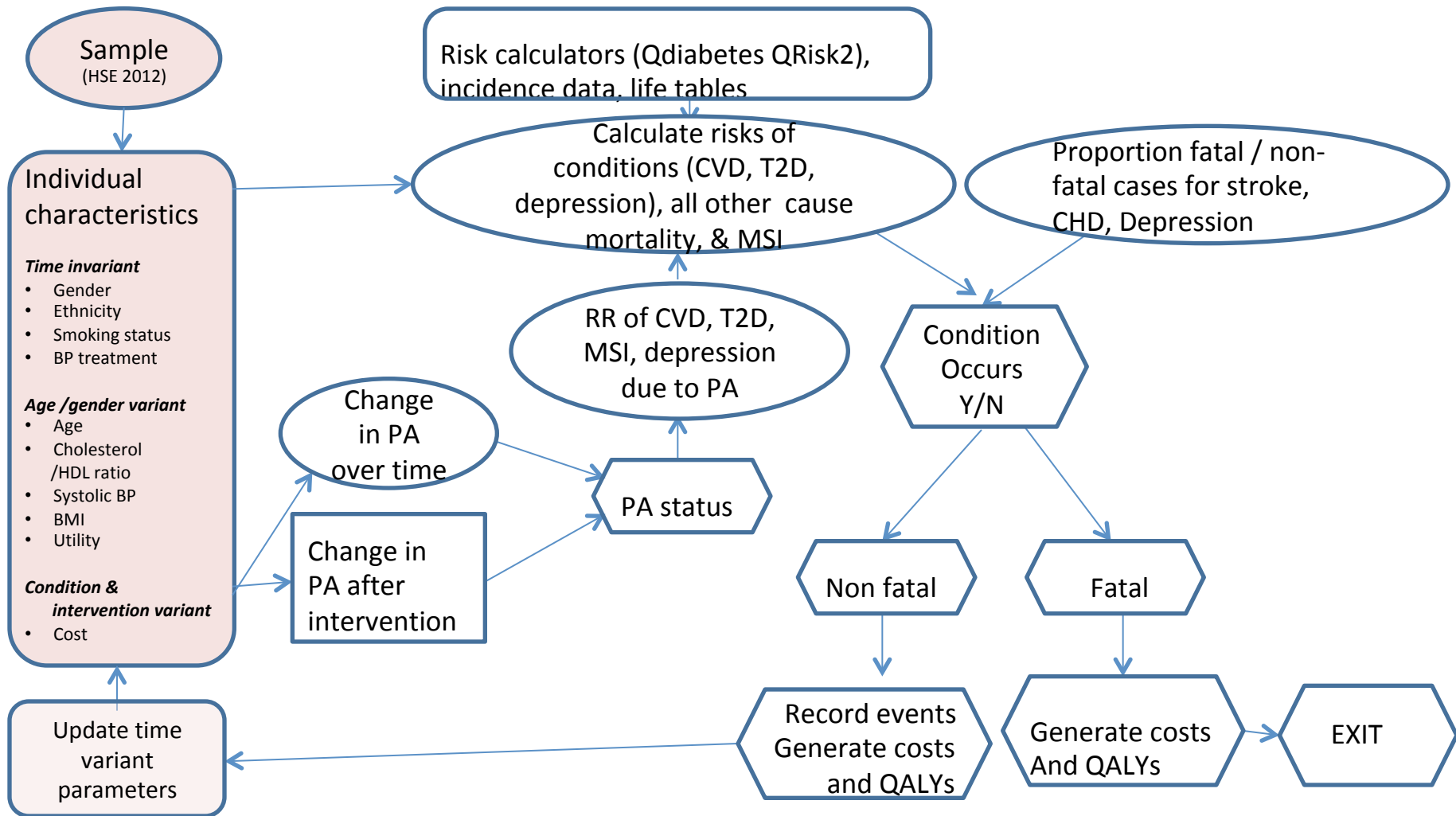
# Aim



Policy relevant cost-effectiveness modelling of cross-sectoral interventions that increase physical activity

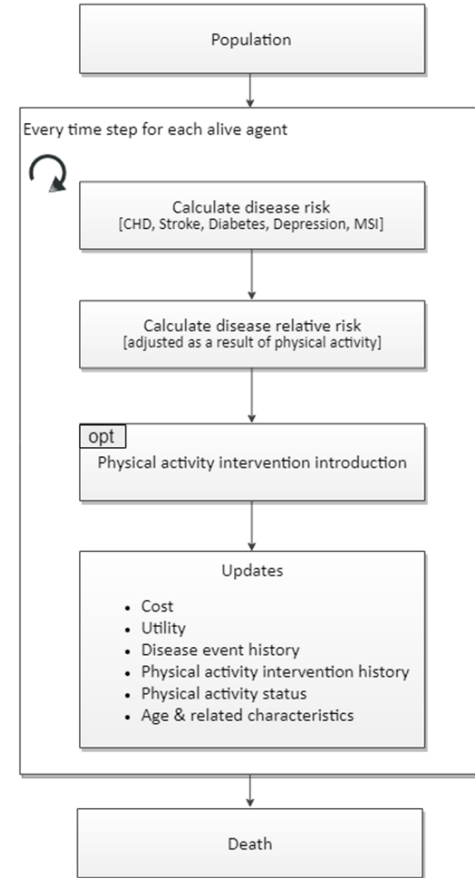
To support decision-making for policy and practice ...

- Which effective interventions are most **efficient**?
  - Which **age groups** is it most efficient to target?
  - Identify **future research targets** to improve decision-making

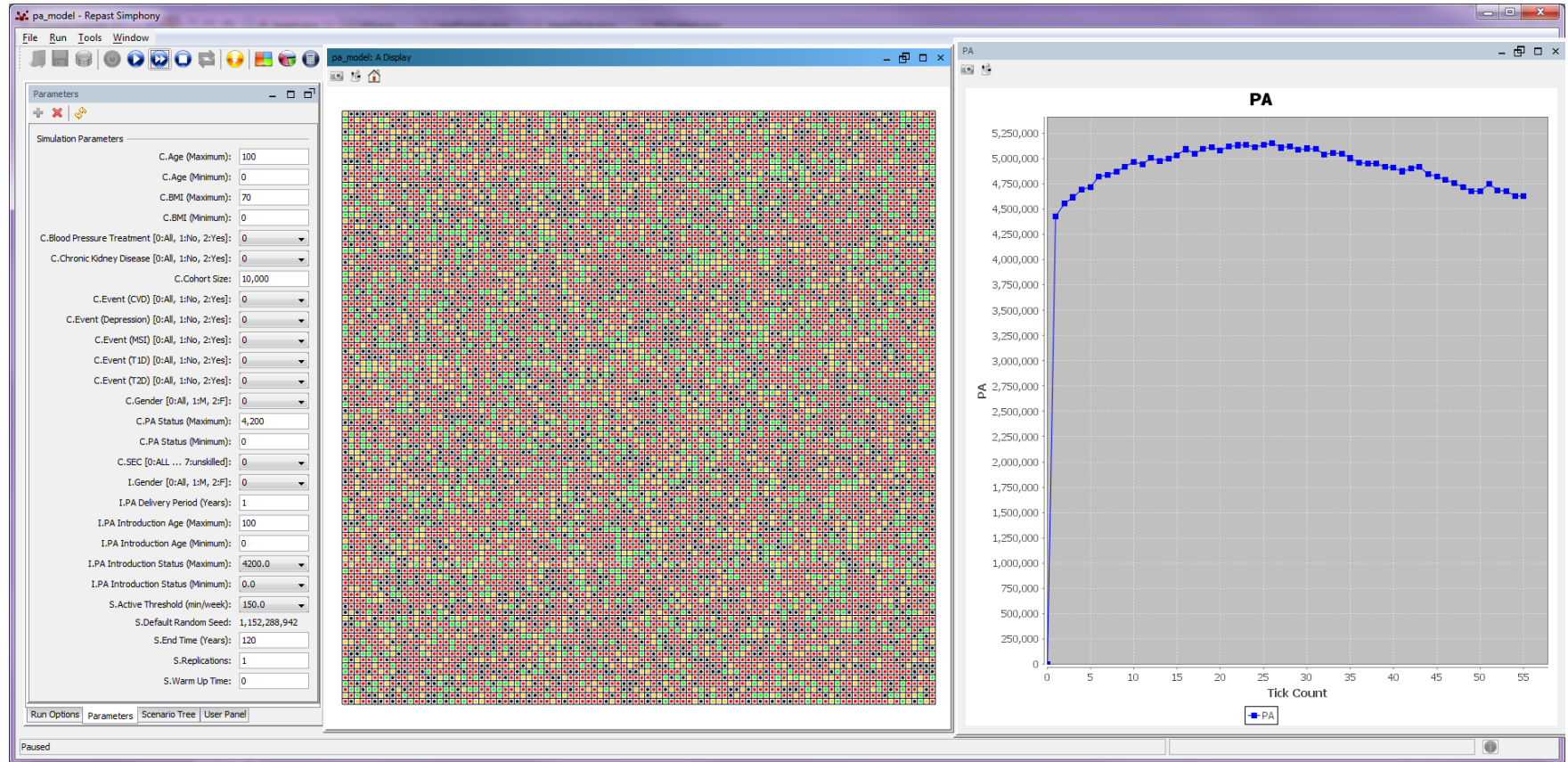


# PALMS: Physical Activity Lifelong Modelling & Simulation

- Selection of population
- Follow the population through their lifetime
- As time progresses
  - Estimate risk for diseases
  - Adjust this risk as a result of the physical activity status
  - Optional: introduce intervention
  - Update individual history
  - Update aggregated values
- At the end of the simulation
  - Output the results

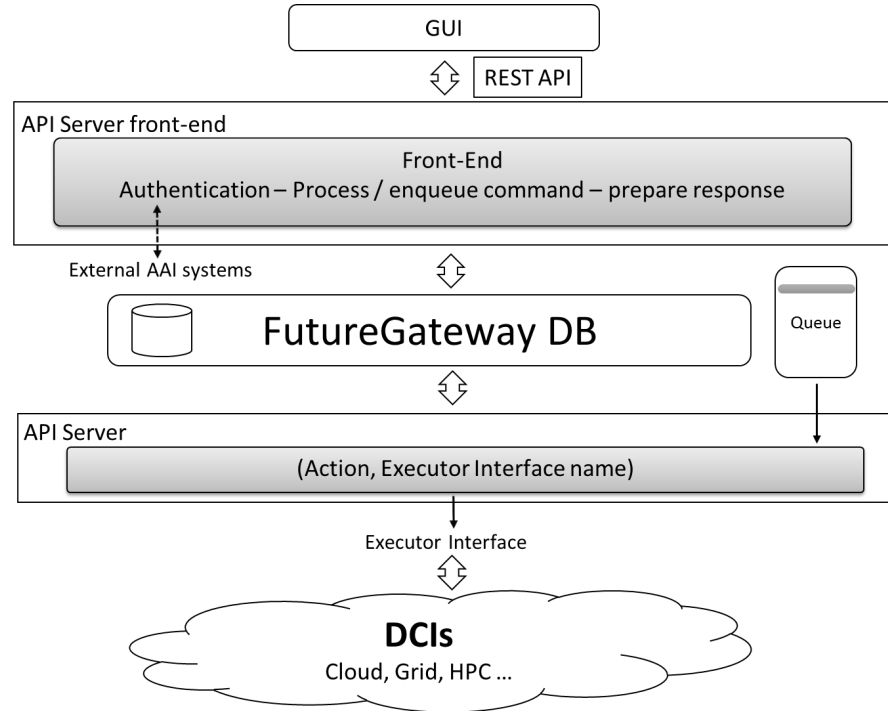


# PALMS: Graphical User Interface & Visualisation



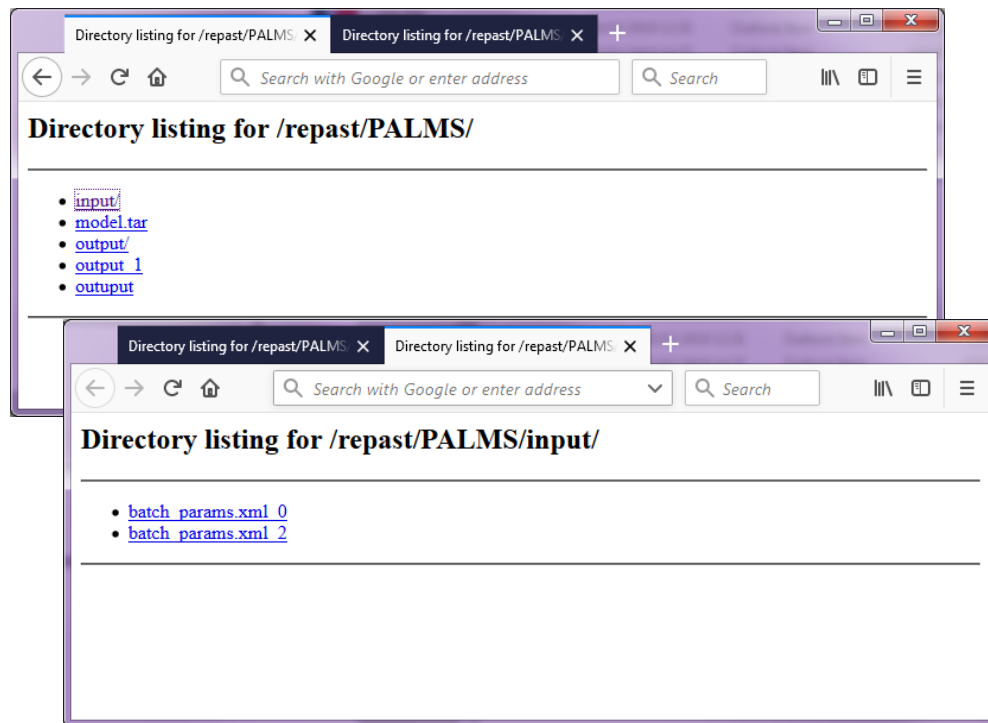
# PALMS Science Gateway Architecture

- User Interface (GUI) is a **web browser**
- Users define the inputs of simulation on the user interface
- Everything else is **hidden from the users**
- The simulation runs on Distributed Computing Infrastructures (DCIs)




# PALMS Science Gateway Inputs

- Inputs are
  - The model
  - The parameter files
- Stored in a file server



# PALMS Science Gateway



## Science Software on Demand

Sign In

Welcome Applications ▾ Propose About

R-Studio

REPAST (PALMS)

Chipster accounts

### Science Software on Demand

Science software on demand.

A selection of most common scientific applications, demonstrators and use cases.

The Science Software on Demand is a ScienceGateway service built on top of the [FutureGateway](#), it provides a selected number of general purpose scientific applications available for all registered members. With this web site, it is also possible to propose new use cases and registering them on this portal or eventually being supported to create a new dedicated ScienceGateway if necessary.


#### Applications

The top level of the application menu, provides an overview of the available applications. Each sub menu voice will redirect directly to the specific application. Only registered members can access the applications and for some of them it is also necessary to be allowed by the [EGI marketplace](#).

#### Propose

The propose menu, provides instructions for a possible integration of new use cases to integrate in this portal, or to be supported in the creation of a new dedicated Science Gateway based on the [FutureGateway Framework](#).

# PALMS Science Gateway



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# PALMS Science Gateway Authentication



Science Software on Demand

[Sign In](#)



[Welcome](#)

[Applications](#) ▾

[Propose](#)

[About](#)

## Repast (PALMS)

**Warning!** You have to sign-in to access this service.



Please contact the [user support](#) to get information and instructions about the access to this application.

Powered By Liferay

# PALMS Science Gateway Authentication



Science Software on Demand

Search



Sign In

Welcome

Applications ▾

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About

Repast (PALMS)

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Powered By Liferay

# PALMS Science Gateway Sign In Options



Check-in

Choose your academic/social account



Search...

[A. T. Still University](#)

[AAF Virtual Home](#)

[AAI@EduHr Single Sign-On Service](#)

[Aalborg University](#)

[Aalto University](#)

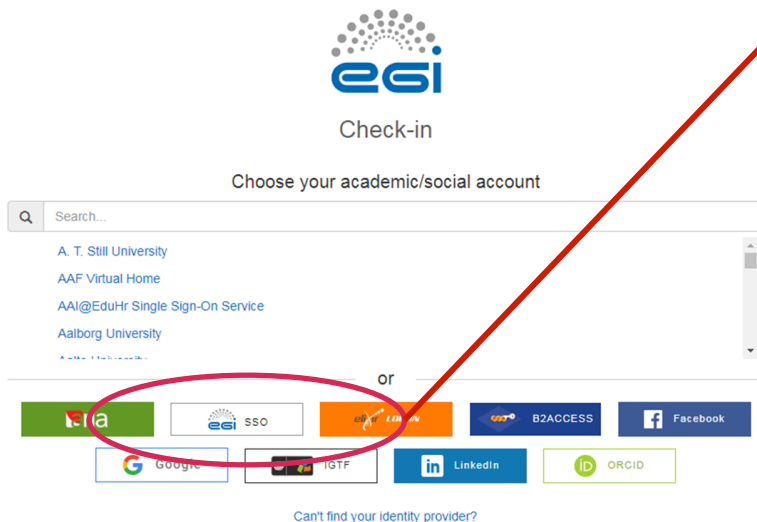
or



[Can't find your identity provider?](#)

# PALMS Science Gateway Sign In Options

- Example
  - selecting the European Grid Infrastructure (EGI) authentication service



The screenshot shows the EGI Check-in page. At the top is the EGI logo and the text "Check-in". Below this is a search bar with the placeholder text "Choose your academic/social account". A list of accounts is displayed below the search bar, including "A. T. Still University", "AAF Virtual Home", "AAI@EduHr Single Sign-On Service", and "Aalborg University". Below the list is a red circle highlighting the "or" text and a row of identity provider logos: "via", "egi SSO", "ORCID", "B2ACCESS", "Facebook", "Google", "IGTF", "LinkedIn", and "ORCID". A red arrow points from the "egi SSO" logo to the "Login" button on the right side of the page.



Login to EGI AAI Service  
Provider Proxy

Username

Password

☐ Don't Remember Login

☐ Clear prior granting of permission  
for release of your information to this  
service.

Login



Service provider proxy for all  
federated EGI services

> Forgot your password?

> Need Help?

# PALMS Science Gateway



Science Software on Demand

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Applications ▾

Propose

About

Search



AA

## Repast (PALMS)

The [repast](#) application, is a free and open source agent-based modeling toolkit that offers users a rich variety of features. In this area it is possible to execute a given model with a given set of parameters, for the (PALMS) experiment.

Model:

Parameters:

Execute

Reset



Executions

ActionDate

Status

Model

Parameters



2019-02-28T15:40:16Z

DONE

<http://jobserver2.hopto.org/repast/PALMS/model.tar> [http://jobserver2.hopto.org/repast/PALMS/input/batch\\_params.xml\\_2](http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_2)



2019-02-28T15:22:32Z

DONE

<http://jobserver2.hopto.org/repast/PALMS/model.tar> [http://jobserver2.hopto.org/repast/PALMS/input/batch\\_params.xml\\_1](http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_1)

# PALMS Science Gateway



Science Software on Demand

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AA

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Model:

Parameters:

URL of the model input

URL of the parameter files input



Executions

Action	Date	Status	Model	Parameters
	2019-02-28T15:40:16Z	DONE	<a href="http://jobserver2.hopto.org/repast/PALMS/model.tar">http://jobserver2.hopto.org/repast/PALMS/model.tar</a>	<a href="http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_2">http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_2</a>
	2019-02-28T15:22:32Z	DONE	<a href="http://jobserver2.hopto.org/repast/PALMS/model.tar">http://jobserver2.hopto.org/repast/PALMS/model.tar</a>	<a href="http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_1">http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_1</a>

# PALMS Science Gateway



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Model:

Parameters:

[Execute](#) [Reset](#)

URL of the model input

URL of the parameter files input



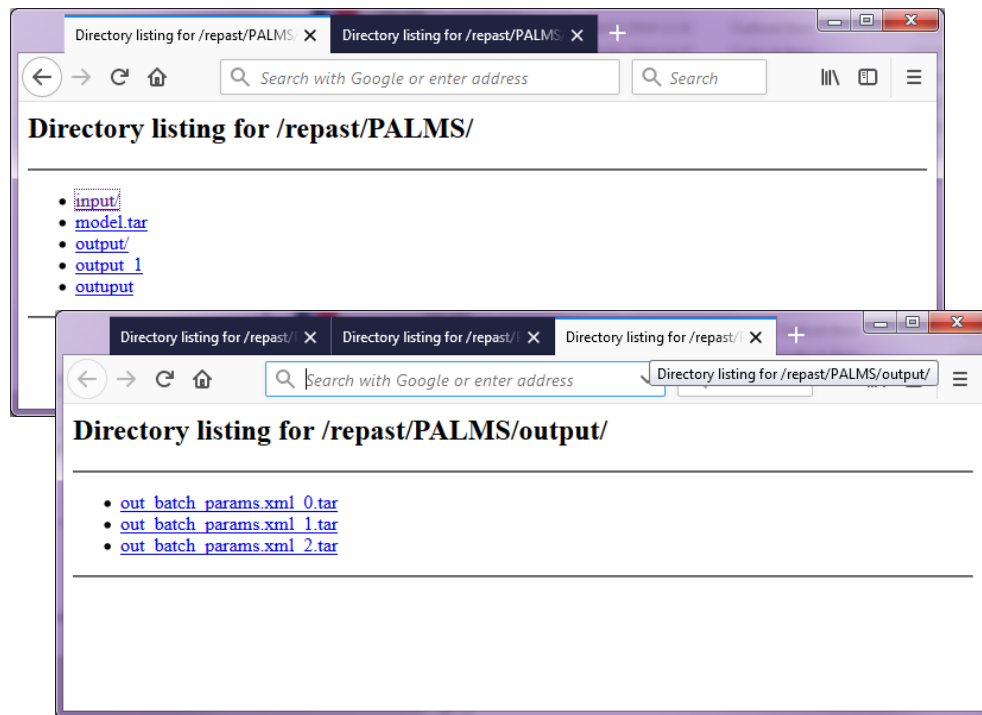
Executions

Monitoring simulation execution progress

ActionDate	Status	Model	Parameters
2019-02-28T15:40:16Z	DONE	<a href="http://jobserver2.hopto.org/repast/PALMS/model.tar">http://jobserver2.hopto.org/repast/PALMS/model.tar</a>	<a href="http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_2">http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_2</a>
2019-02-28T15:22:32Z	DONE	<a href="http://jobserver2.hopto.org/repast/PALMS/model.tar">http://jobserver2.hopto.org/repast/PALMS/model.tar</a>	<a href="http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_1">http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_1</a>

# PALMS Science Gateway Outputs

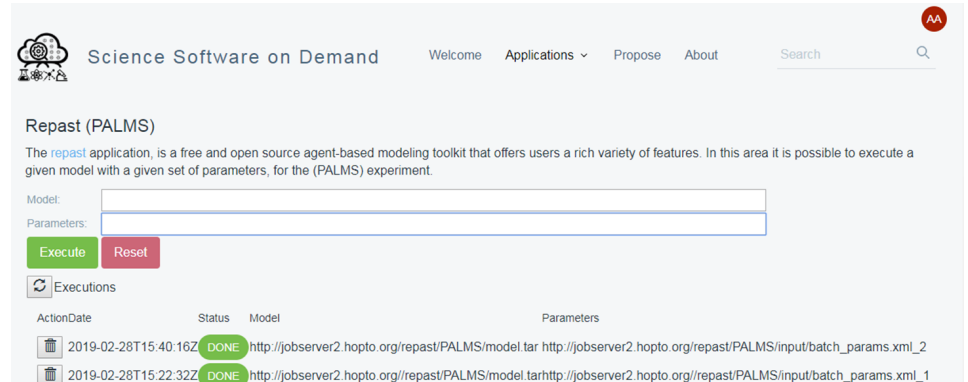
- Outputs contain all results
- Stored in a file server when job is finished
- Can be downloaded from the server





# PALMS Science Gateway Summary

- PALMS Science Gateway supports sharing and using the simulation openly
- Hides the infrastructure complexity from the user
- Does not require ICT skills to use the simulation



The screenshot displays the 'Science Software on Demand' interface for the 'Repast (PALMS)' application. The header includes a logo, the title 'Science Software on Demand', and navigation links: 'Welcome', 'Applications', 'Propose', 'About', and a 'Search' bar. The main content area is titled 'Repast (PALMS)' and contains a description: 'The [repast](#) application, is a free and open source agent-based modeling toolkit that offers users a rich variety of features. In this area it is possible to execute a given model with a given set of parameters, for the (PALMS) experiment.' Below the description are two input fields: 'Model:' and 'Parameters:'. To the right of the 'Parameters:' field are two buttons: 'Execute' (green) and 'Reset' (red). Below these fields is a section titled 'Executions' with a refresh icon. It contains a table with columns 'ActionDate', 'Status', 'Model', and 'Parameters'. The table lists two successful executions, both with a status of 'DONE'.

ActionDate	Status	Model	Parameters
2019-02-28T15:40:16Z	DONE	<a href="http://jobserver2.hopto.org/repast/PALMS/model.tar">http://jobserver2.hopto.org/repast/PALMS/model.tar</a>	<a href="http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_2">http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_2</a>
2019-02-28T15:22:32Z	DONE	<a href="http://jobserver2.hopto.org/repast/PALMS/model.tar">http://jobserver2.hopto.org/repast/PALMS/model.tar</a>	<a href="http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_1">http://jobserver2.hopto.org/repast/PALMS/input/batch_params.xml_1</a>