



Enabling Grids for E-  
scienceE

# Pharmacokinetics on Contrast Agents in Abdominal Cancer

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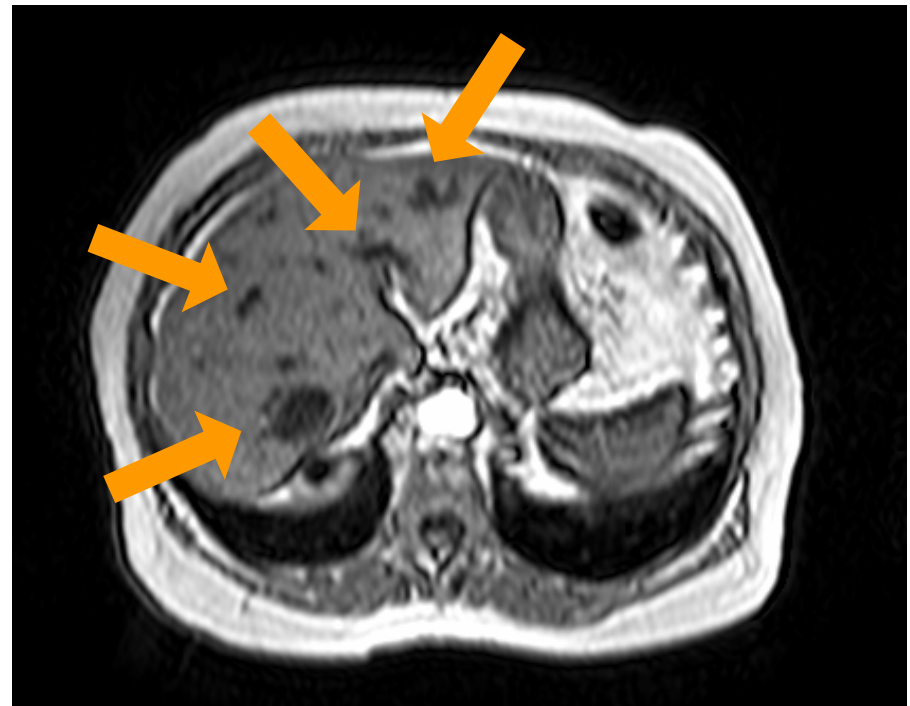
[www.eu-egee.org](http://www.eu-egee.org)



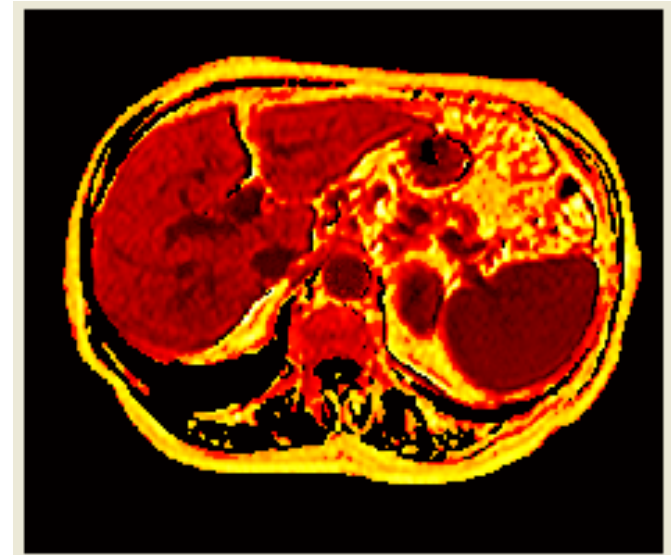
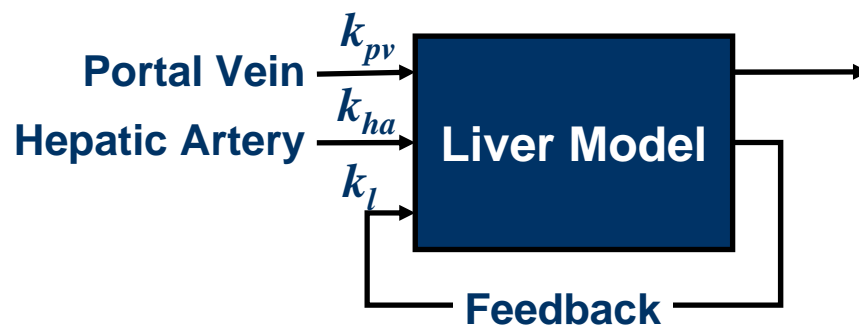
INFSO-RI-508833

- **Short Introduction of the Problem and Motivation.**
- **Brief Details of the Application.**
- **Live Demo.**
- **Analysis of the Results and Performance.**
- **Questions and Answers.**

- A Lesion is Detected in an MRI Study of a Patient.
- Malignant and Benign Lesions have Similar Appearance in Medical Images and It is Difficult to Conclude with a Diagnosis with High Degree of Sensitivity and Accuracy.
- The Final Analysis is the Biopsy.
- But Biopsy is Traumatic.
- This Delay in the Diagnosis Causes Patient Anxiety in Cases with Reasonable Uncertainty.



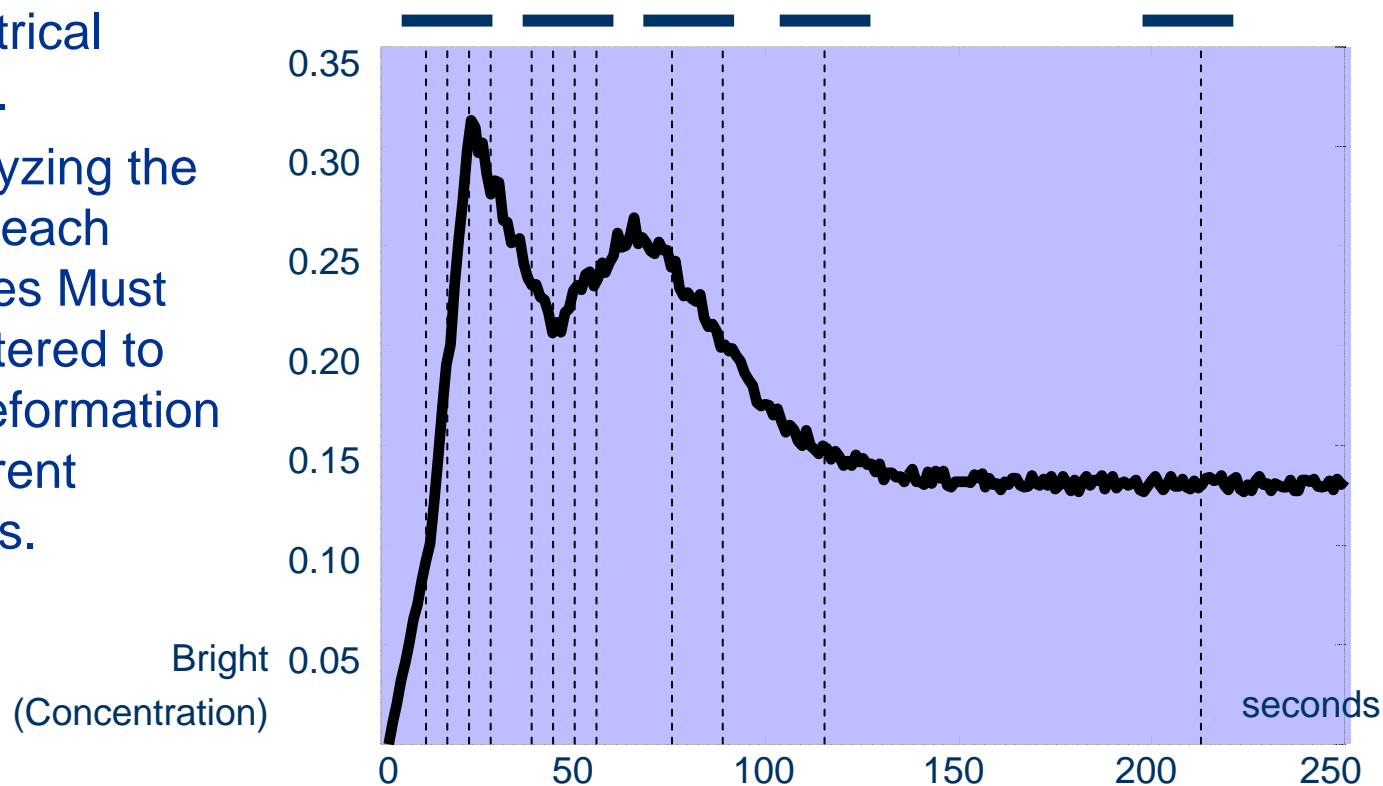
- **Characterization of the Tissular Nature by the Analysis of the Evolution of Contrast in a Time Series.**
- **Tumours Generate the Growing of Vessels Around the Tumoural Mass.**
- **Different Tissues Define Different Constants for Recycling and Flow Rate of the Physical Models.**
- **Those Constants can be used for the Creation of Parametric Images.**



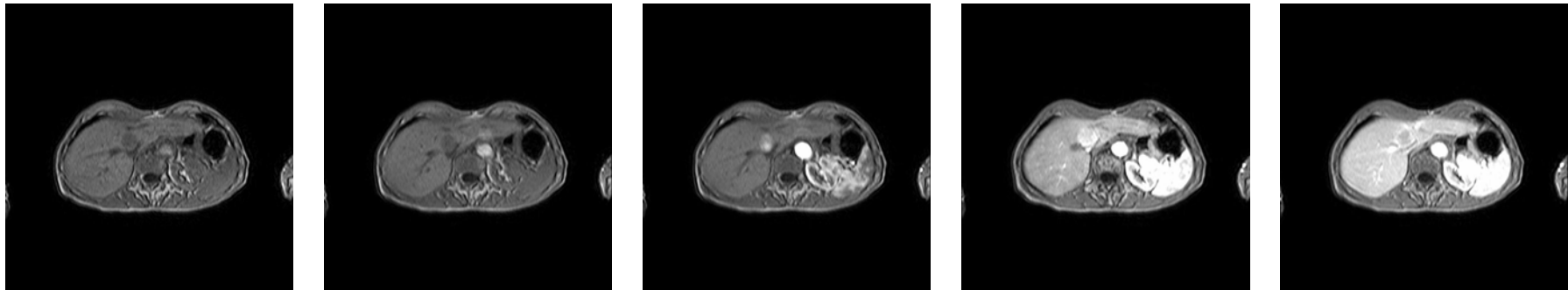
- **Pharmacokinetics in Contrast Evolution is a Hot Topic in Medical Research (845 Articles for Liver in PubMed).**
- **The Work is a Result of a Collaboration Among Four Research Groups (Radiologists, Chemical Engineering and Medical Informatics).**
- **The Problem is User-Driven with a High Interest by the Industry.**
- **The Objective is to**
  - Validate the Theory of the Model.
  - Work in 3D.
  - Demonstrate the Relation of the Constants and the Tissular Nature.
  - Create a New Image Modality.
- **The Model can be Used, with the Proper Tuning, to Other Areas where Vessel Growing is Significant (such as Infertility).**

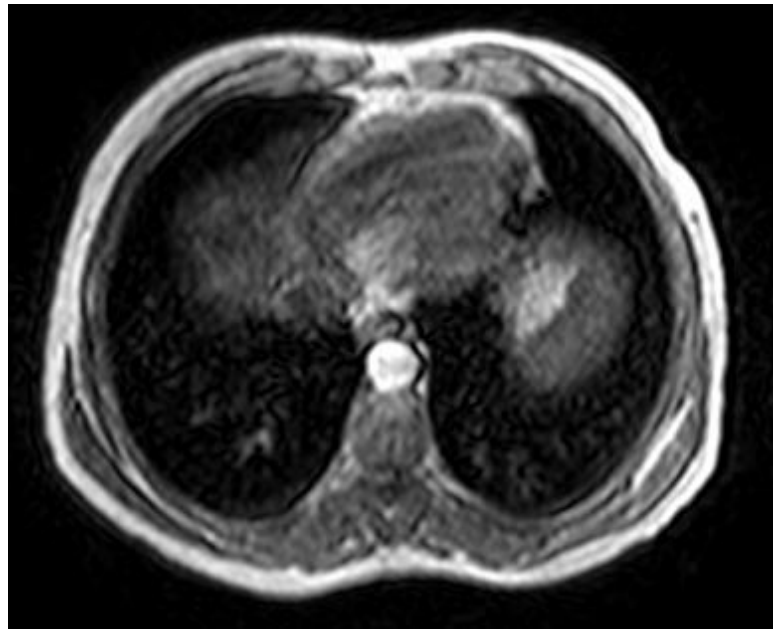
- **Description**

- The Process Requires Obtaining a Sequence of MRI Volumetric Images.
- Different Images are Obtained in Different Breath-holds.
- The Movement of the Abdomen is Unavoidable and Relevant when Voxels have Sub-millimetric Dimensions.
- Before Analyzing the Variation of each voxel, Images Must be Co-registered to Minimize Deformation due to Different Breath Holds.

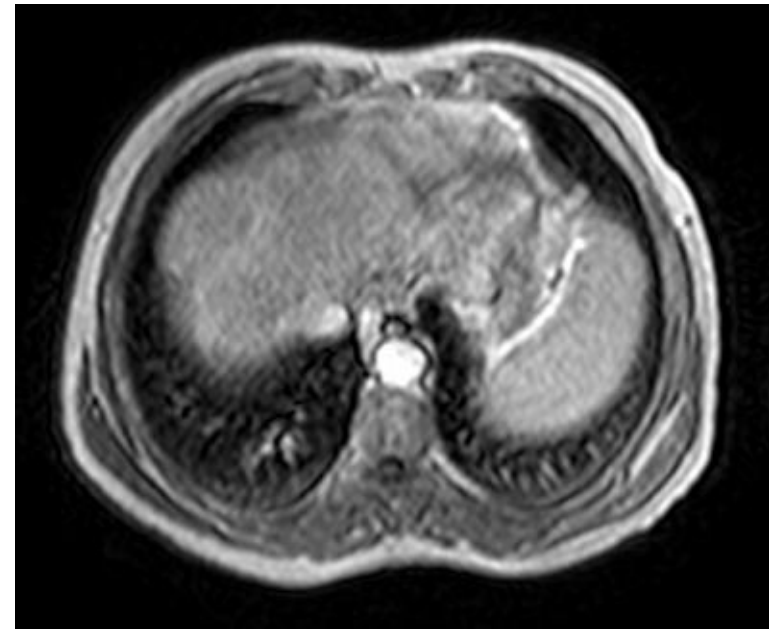


- **The Area of the Abdomen Requires the use of Deformable Registration Methods.**
- **Much More Computationally Intensive than Rigid Affine Registration.**
- **Moreover, Registration Must be Very Accurate to Reduce the Artefacts on the Interpolation, Leading to Test Different Parameters.**
- **The Total Computational Cost of a Clinical Trial of 20 Patients is Around 100 CPU Days.**





**MRI Volume at  
Timestep 1**

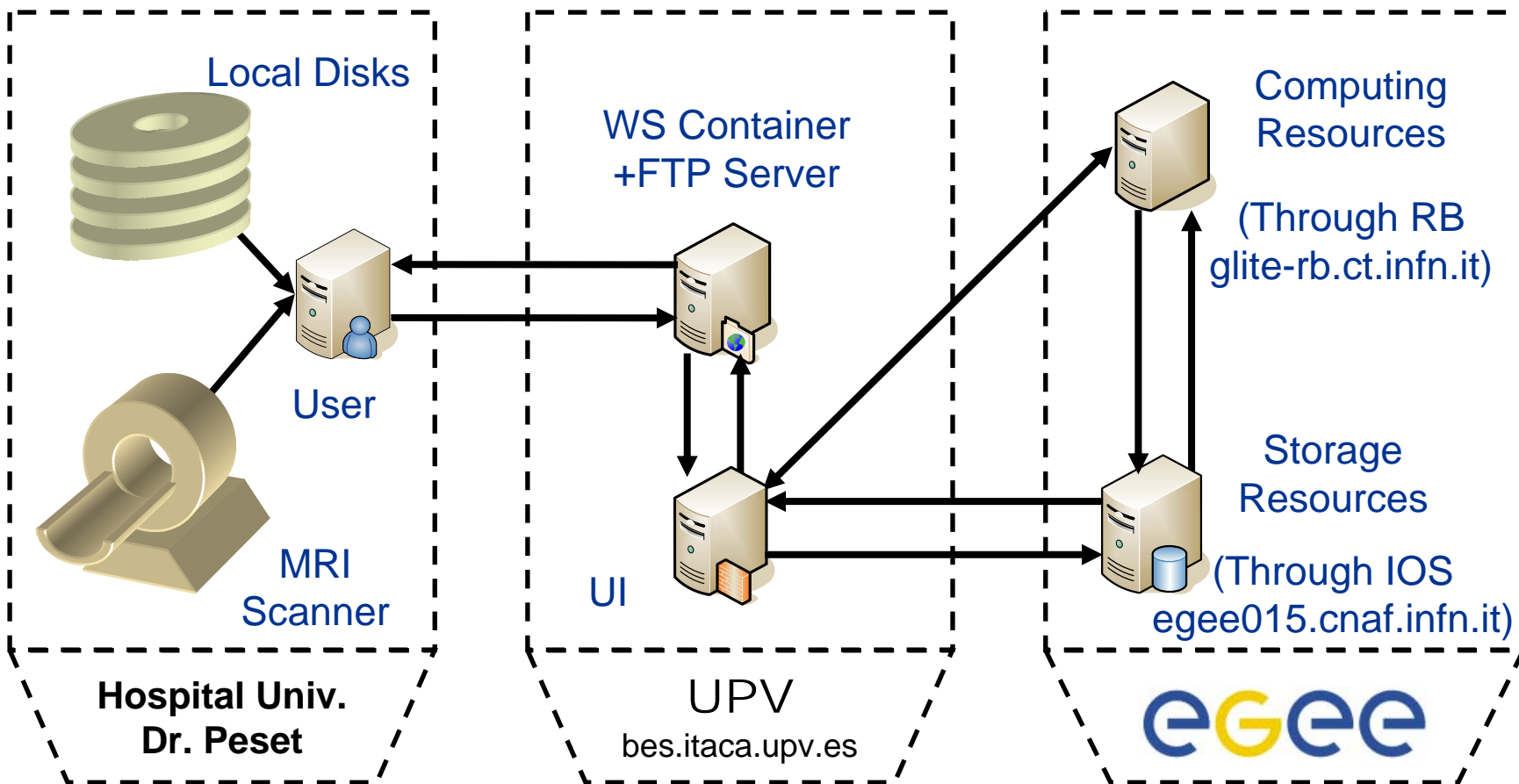


**MRI Volume at  
Timestep 13**



- **Performance**
  - Use of the Grid to Provide the Computational Power.
  - >> Use a Large Grid Infrastructure
- **Usability**
  - Reduce the Complexity of Grids by Using a Friendly Interface.
  - Provide an Interface Open to its Integration in Other Applications.
  - >> Implement a Web-Services Based Portal.
- **Security**
  - Deal With the Risks of Using Remote Resources.
  - >> Anonymise and Access Control.
- **Reliability**
  - Production Capability.
  - >> Provide Intelligence on Selecting the Sites.





→ Raw images →

← Results ←

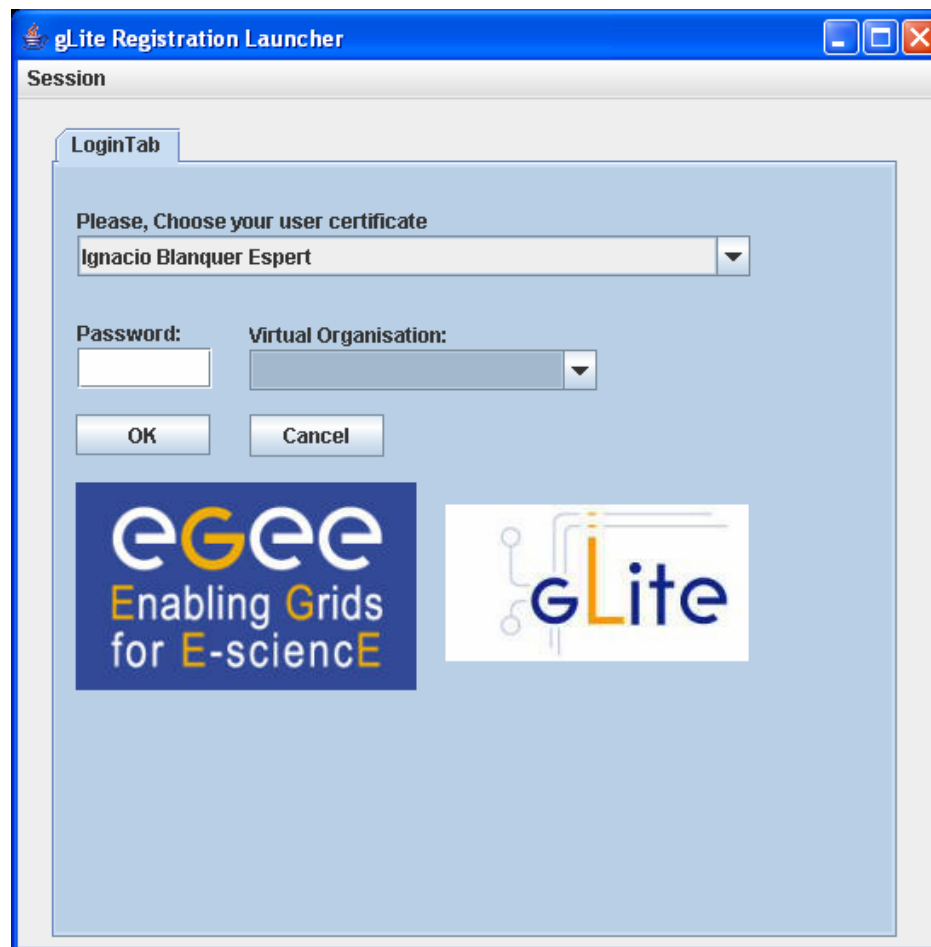
- **A Graphical User Interface has Been Created.**
- **The GUI Calls the Web Services to Implement**
  - Creating the Proxy on the Grid.
  - Transferring the Data into the Grid Storage Area.
  - Select the Ranges of the Parameters to Test:
    - Maximum Step Length for the Gradient Descent Optimisator.
    - Maximum Number of Iterations for the Optimiser.
    - Initial Scaling Factor.
    - Initial Angle for Deformation.
  - Create the JDLs and Define the Arguments for the Scripts of Each Job
    - One Job per Registration and Per Combination of Parameters.
  - Monitoring of the Evolution of a Set of Jobs.
  - Downloading the Output of All the Jobs in a Group with a Single Click.

- **First Development of a Version on LCG**
  - Good Performance and Large Scale.
  - Need for Improved Privacy on the Data.
  - Testing Lead to the Improvement of the Site Selection.
  - Final Version runs on LCG 2.4.0 - 2.6.0.
- **Evolution to a Version on gLite**
  - Shares the Same Interface and 90% of the Code.
  - Migration of Commands and Inclusion of Access Control.
  - Inclusion of Configuration Files.
  - Evolution from gLite 1.3 to gLite 1.4.

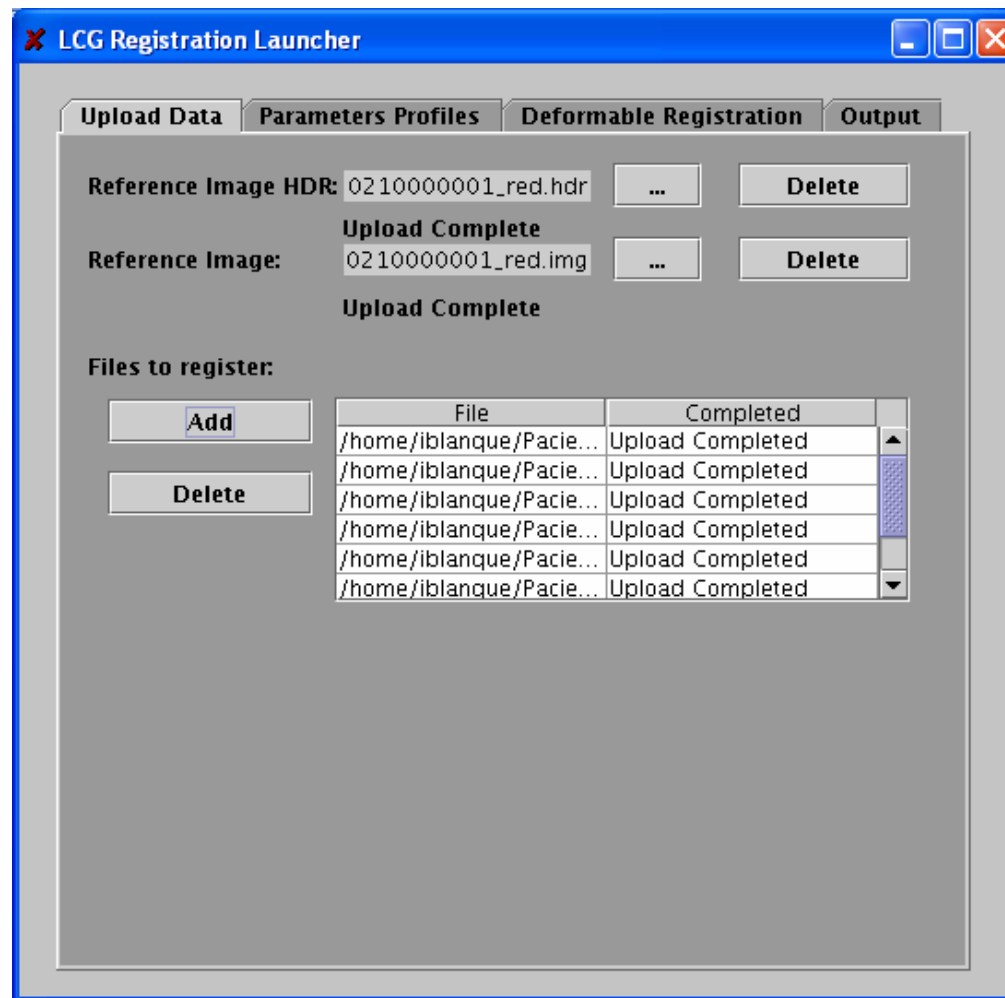


**Demo**

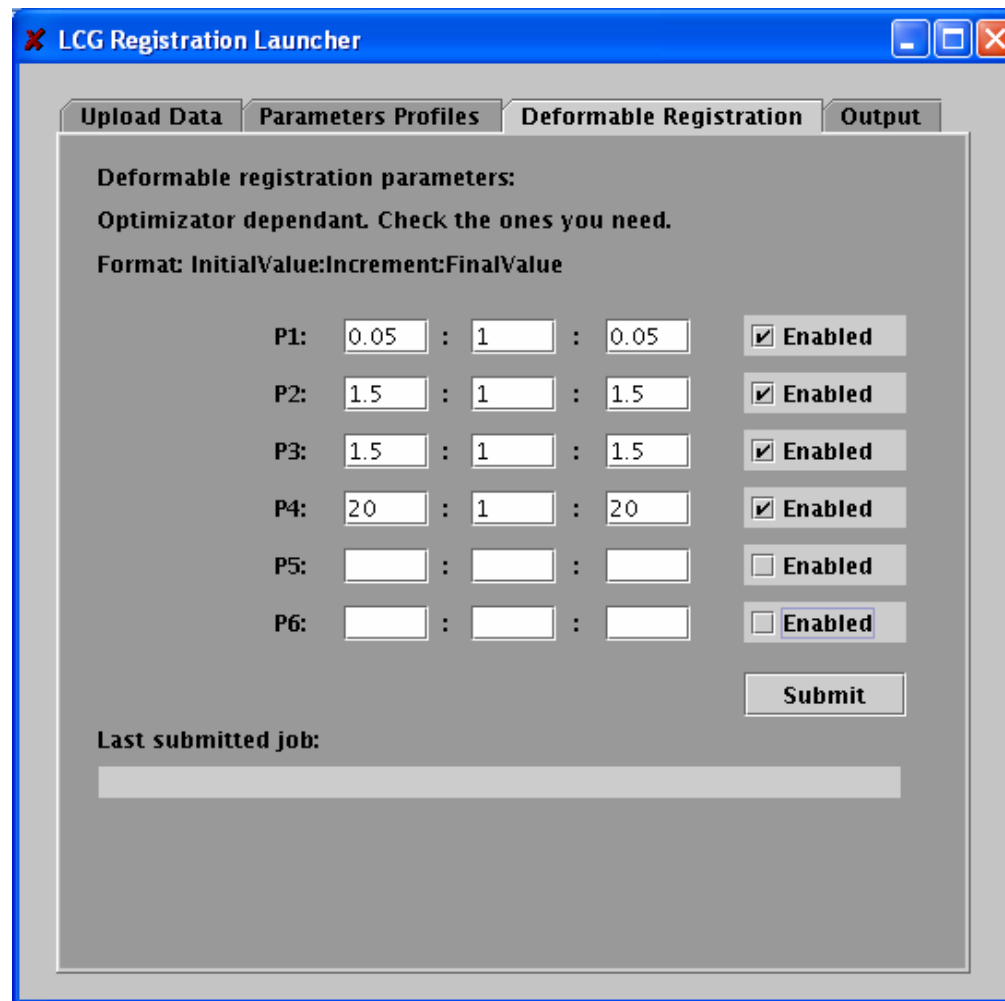
- Password for Accessing a Pre-loaded Certificate.



- **Uploading Reference and Deformable Medical Studies in Analyze Format.**
- **Register the Files on the Grid and Stores the LFN for the Scripts Creating the Jobs.**



- Both the JDL Files and the Necessary Scripts to Copy Locally the Input Data and Start the Co-registration.
- Create All the Instances Necessary for the Combination of Parameters.
- The Executable File is Easily Upgradeable to Test Different Methods.



**LCG Registration Launcher**

Upload Data Parameters Profiles **Deformable Registration** Output

Deformable registration parameters:  
 Optimizator dependant. Check the ones you need.  
 Format: InitialValue:Increment:FinalValue

|     |      |   |   |   |      |   |
|-----|------|---|---|---|------|---|
| P1: | 0.05 | : | 1 | : | 0.05 | <input checked="" type="checkbox"/> Enabled |
| P2: | 1.5  | : | 1 | : | 1.5  | <input checked="" type="checkbox"/> Enabled |
| P3: | 1.5  | : | 1 | : | 1.5  | <input checked="" type="checkbox"/> Enabled |
| P4: | 20   | : | 1 | : | 20   | <input checked="" type="checkbox"/> Enabled |
| P5: |      | : |   | : |      | <input type="checkbox"/> Enabled            |
| P6: |      | : |   | : |      | <input type="checkbox"/> Enabled            |

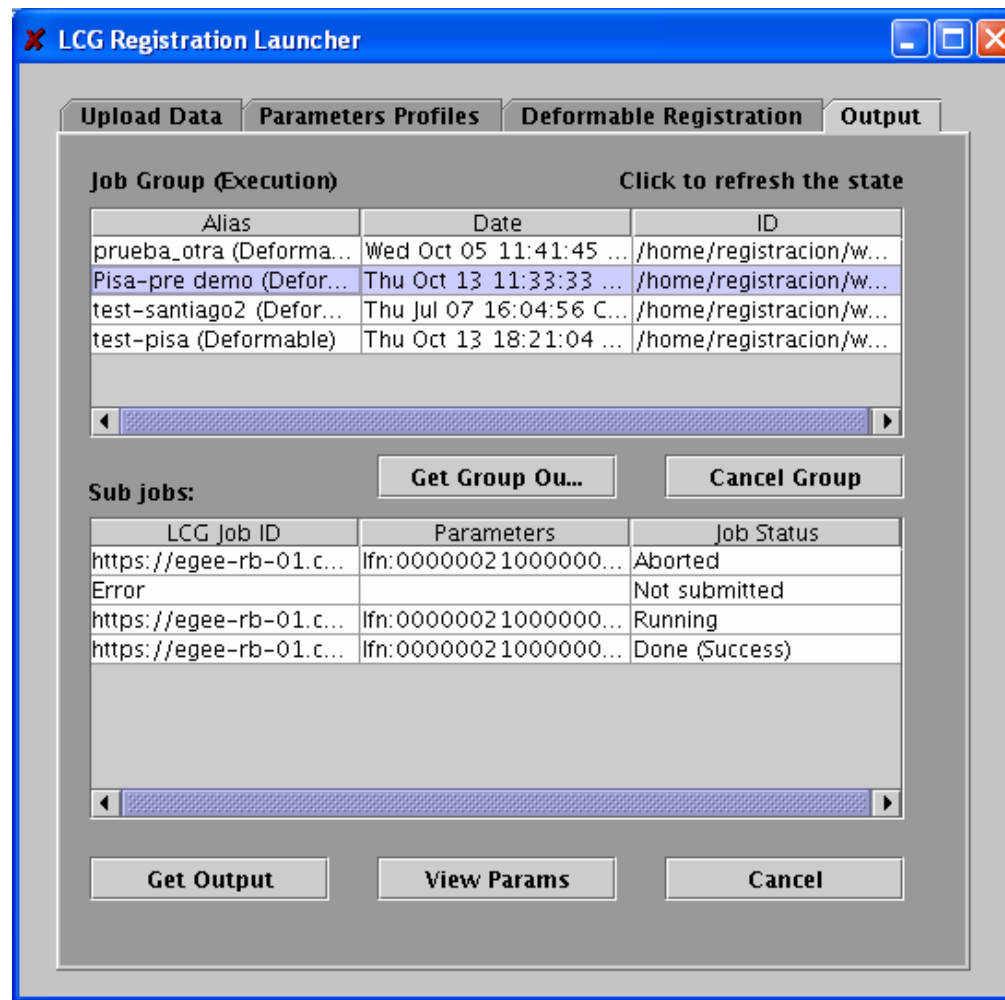
Submit

Last submitted job:

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- Submit all the JDLs Instances Through the RB and Monitoring the Jobs.
- Use a High-Level Name Identifier for the Jobs of a Group.



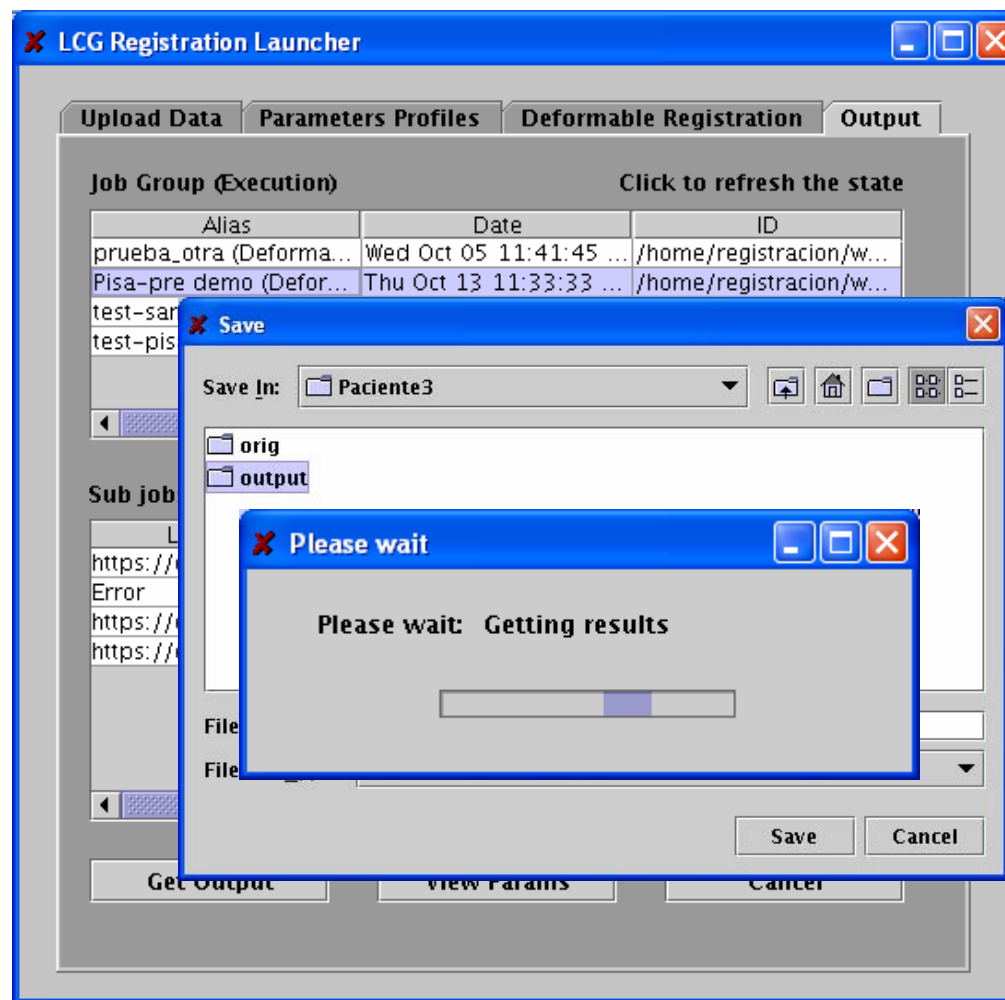
The screenshot shows the 'LCG Registration Launcher' window with the 'Deformable Registration' tab selected. It displays a table of job groups and a sub-table of individual jobs.

| Job Group (Execution)    |                          |                         | Click to refresh the state |
|--------------------------|--------------------------|-------------------------|----------------------------|
| Alias                    | Date                     | ID                      |                            |
| prueba_otra (Deforma...  | Wed Oct 05 11:41:45 ...  | /home/registracion/w... |                            |
| Pisa-pre demo (Defor...  | Thu Oct 13 11:33:33 ...  | /home/registracion/w... |                            |
| test-santiago2 (Defor... | Thu Jul 07 16:04:56 C... | /home/registracion/w... |                            |
| test-pisa (Deformable)   | Thu Oct 13 18:21:04 ...  | /home/registracion/w... |                            |

Sub jobs:

| LCG Job ID              | Parameters            | Job Status     |
|-------------------------|-----------------------|----------------|
| https://egee-rb-01.c... | lfn:00000021000000... | Aborted        |
| Error                   |                       | Not submitted  |
| https://egee-rb-01.c... | lfn:00000021000000... | Running        |
| https://egee-rb-01.c... | lfn:00000021000000... | Done (Success) |

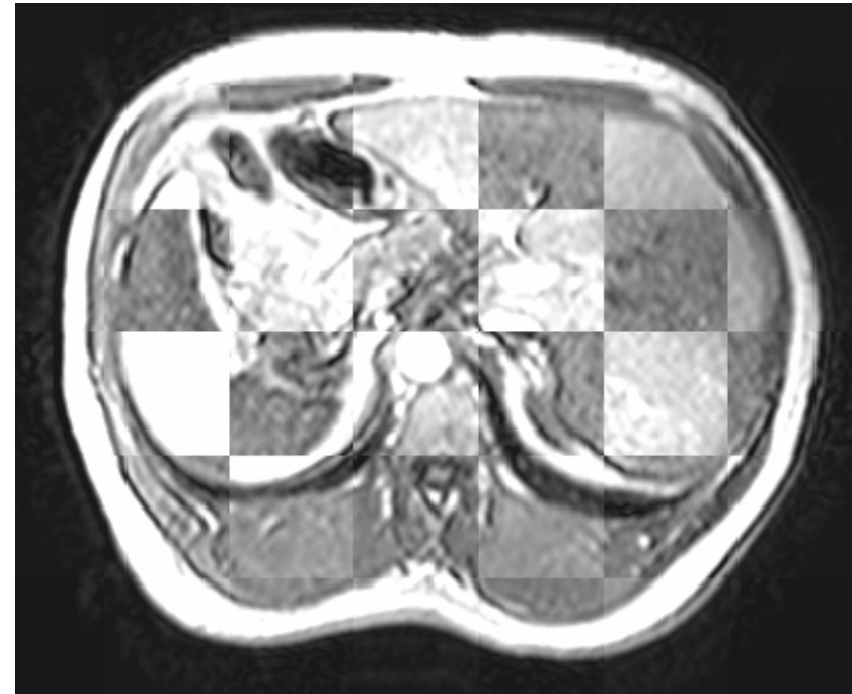
- Retrieve the Output Files from a Group of Jobs.



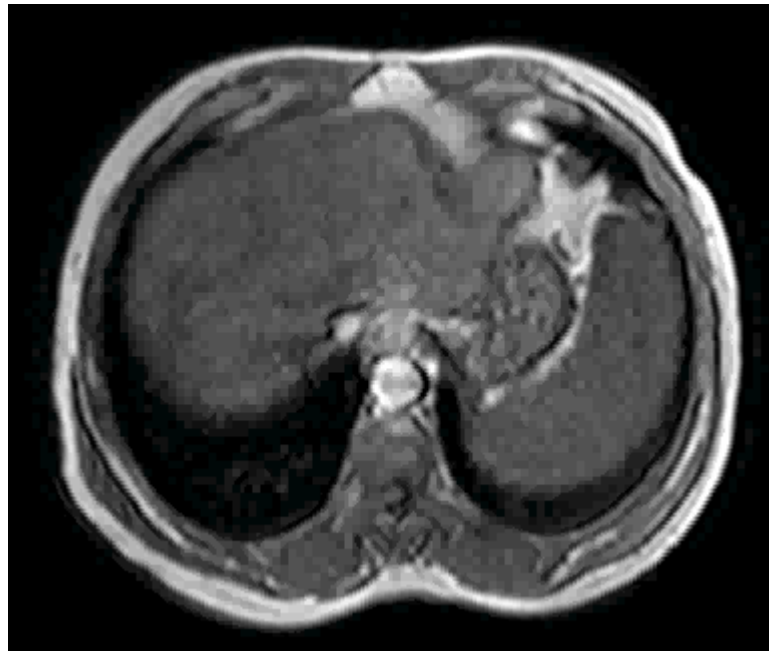
**Before Co-registration**



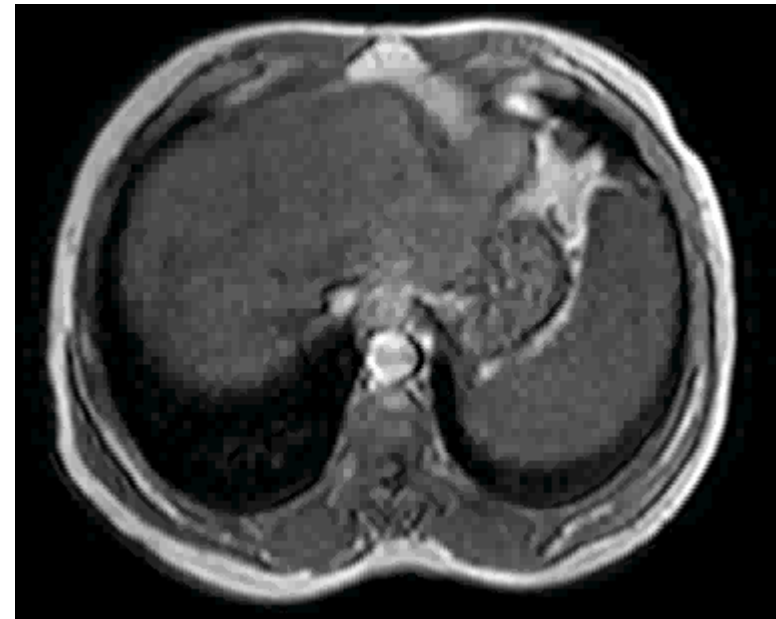
**After Co-registration**

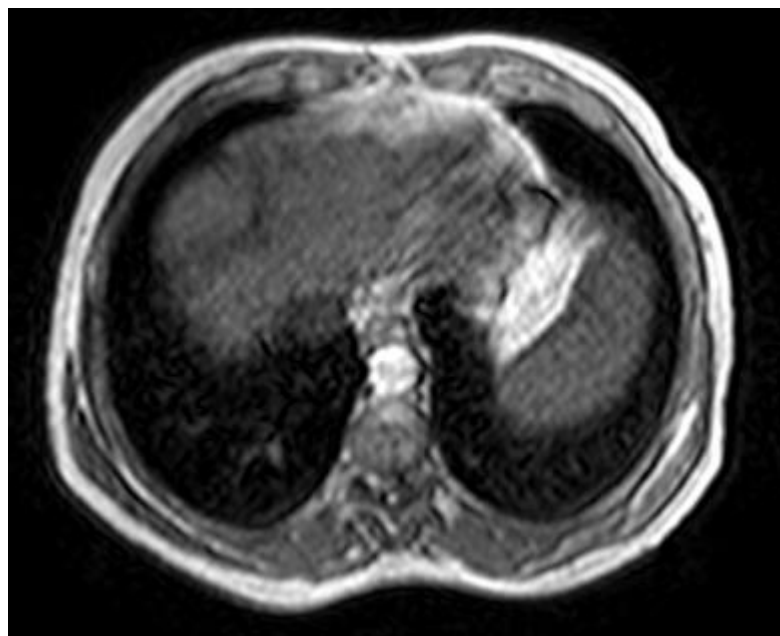


**Before Co-registration**

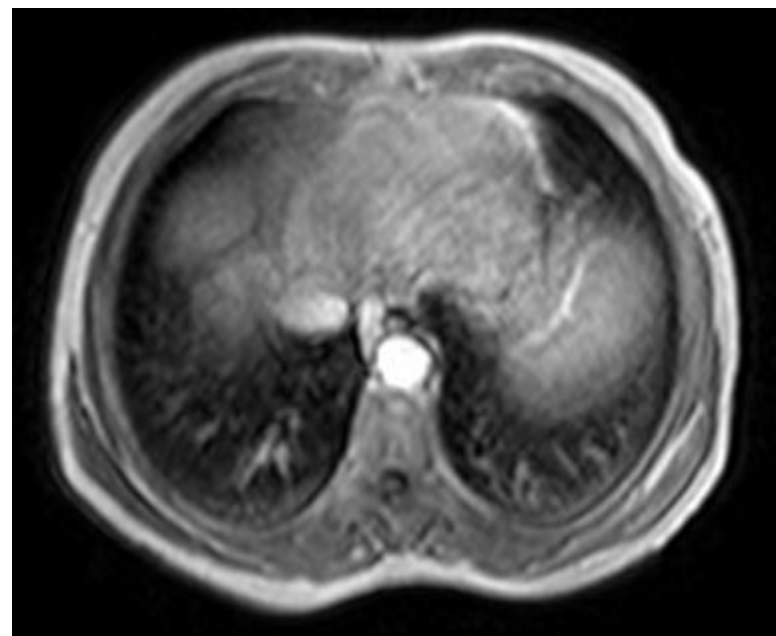


**After Co-registration**



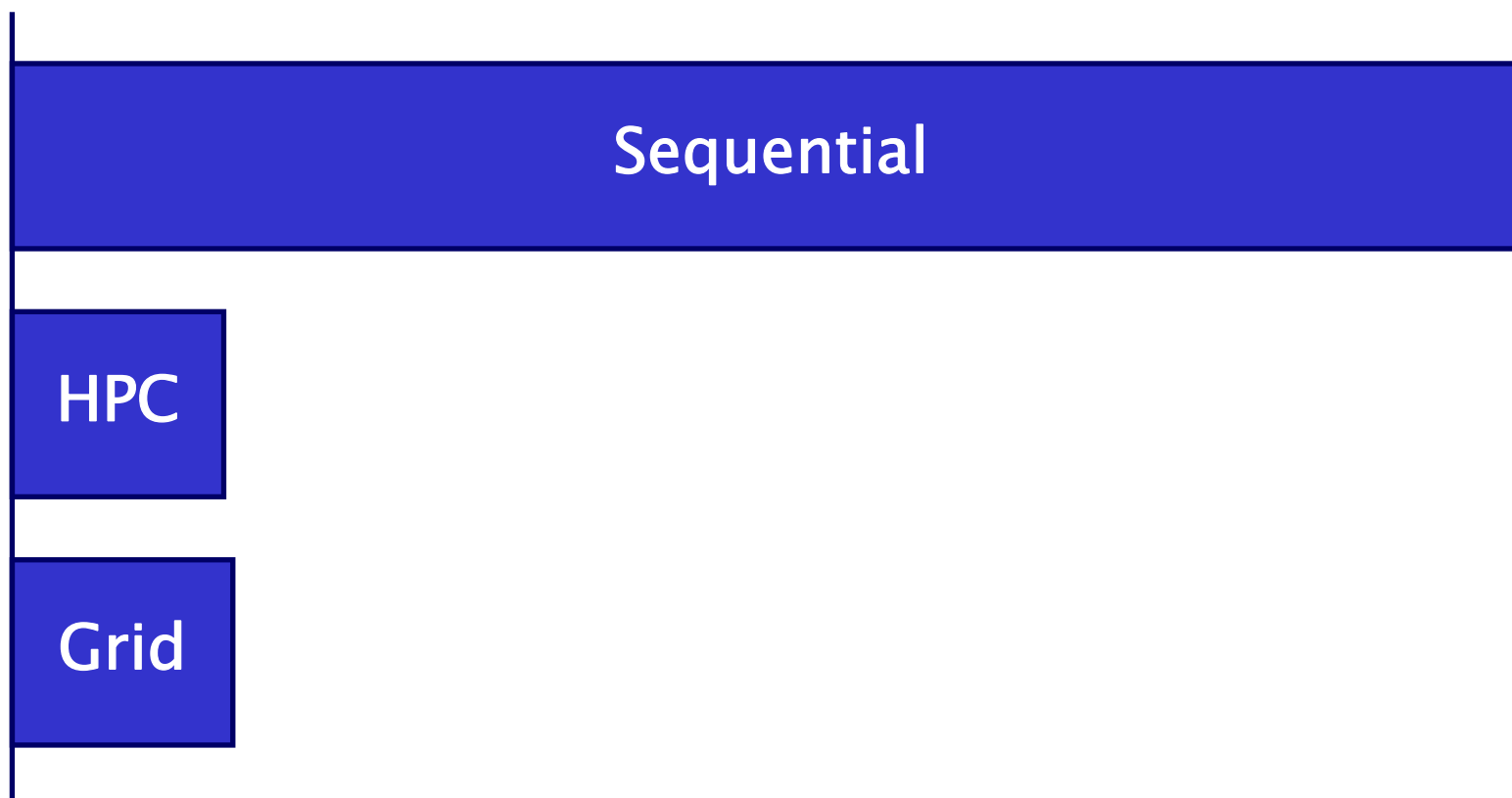


**Correg Volume  
at Timestep 1**

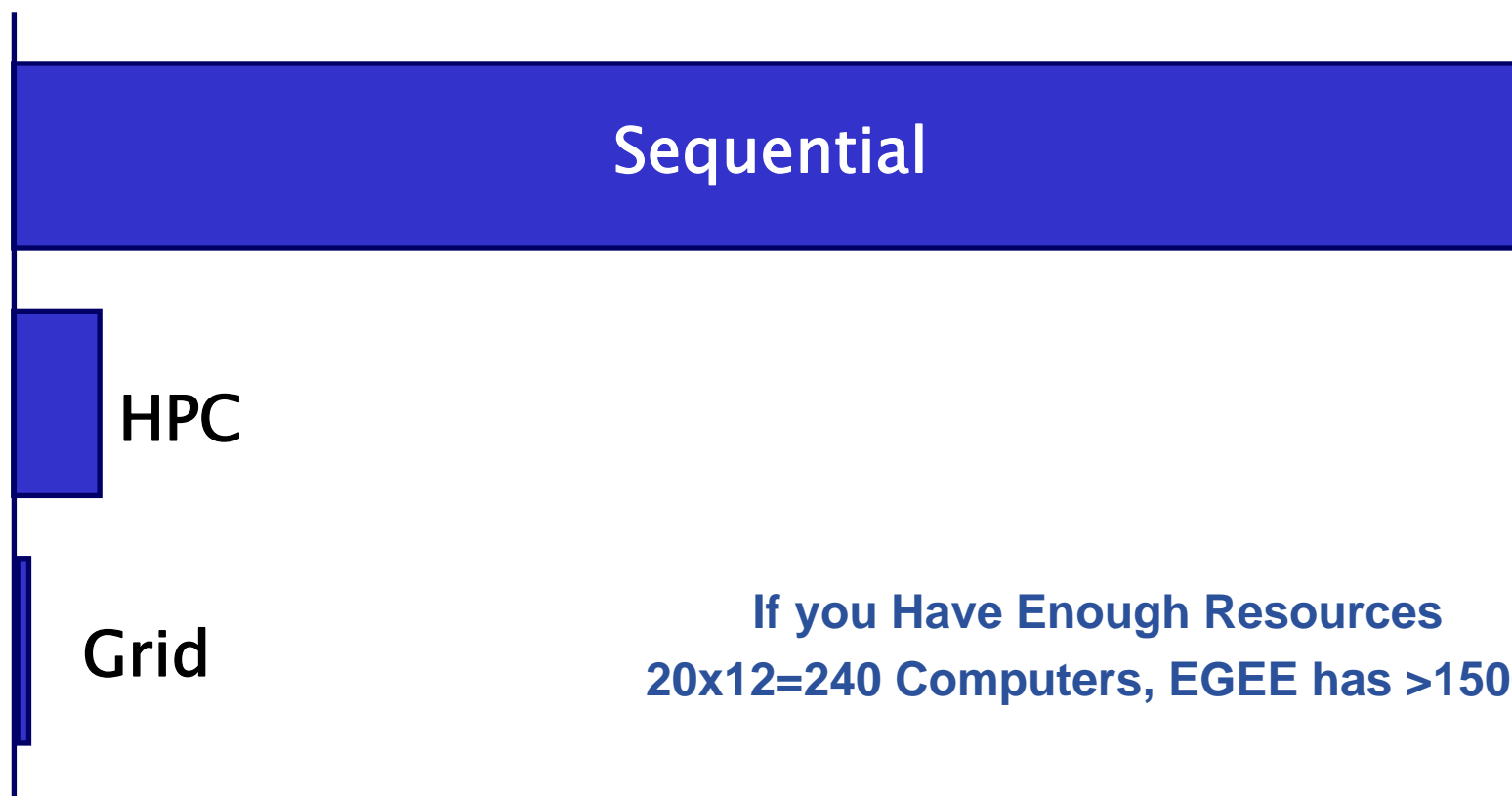


**Correg Volume  
at Timestep 13**

- **Cost of One Patient: 61h 08m.**
- **Cost Using a 20-Procs Computing Farm: 2h 30m.**
- **Computational Cost Using the Grid: 3h 10m.**



- **Cost of 20 Patients: 2331h 22m.**
- **Cost Using a 20-Procs Computing Farm: 132h 50m.**
- **Computational Cost Using the Grid: 17h 35m.**



- **Need for the Grid**
  - The Computing Requirements for a Reduced Clinical Trial of 20 Patients Exceeds the Conventional Computational Capabilities of Either a Hospital or a Research Team.
  - The Need for Computing is Not Flat and Only After the Trials.
- **Added Value of EGEE**
  - Need for a Production Platform 24x7 (Users).
  - Outstanding Improvement in the State-of-the-art Knowledge on Grid Technologies (Developers).
- **Added Value of gLite**
  - Need for Access Control in Data and MetaData.
  - Rich MetaData Management.
  - Batch-Oriented Jobs.
- **Easy to Use Interface: No Need for Grid Knowledge.**
- **Usable From Any Computer Through a Web Service.**