



Enabling Grids for E-science

Pharmacokinetics on Contrast Agents in Abdominal Cancer

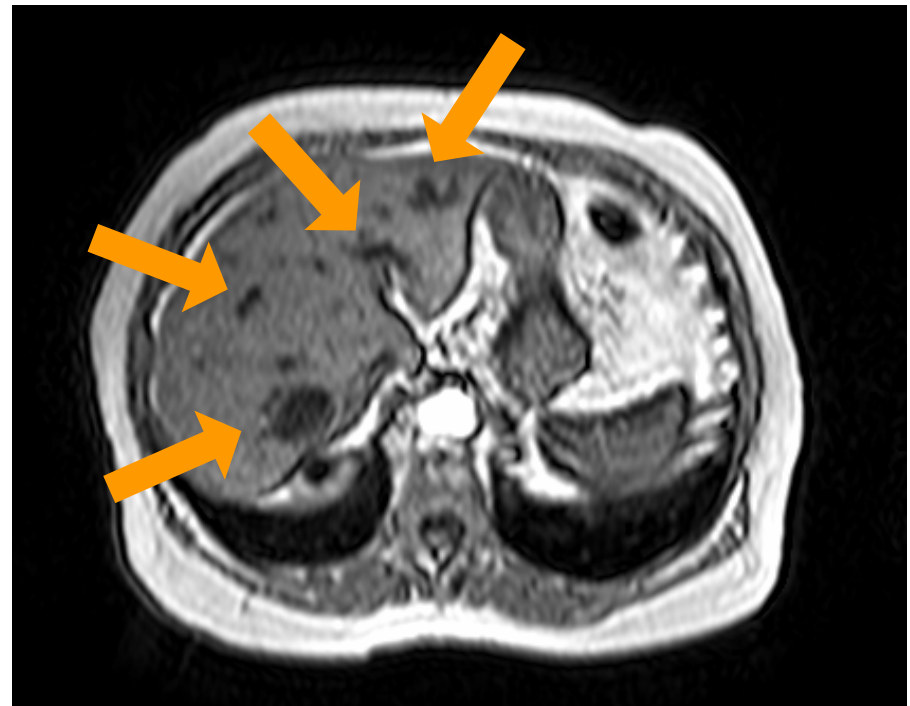
Technical University of Valencia
Ignacio Blanquer

www.eu-egee.org

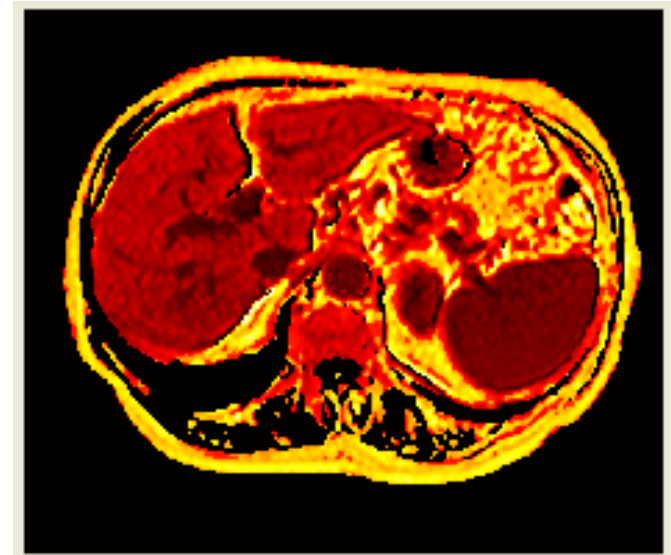
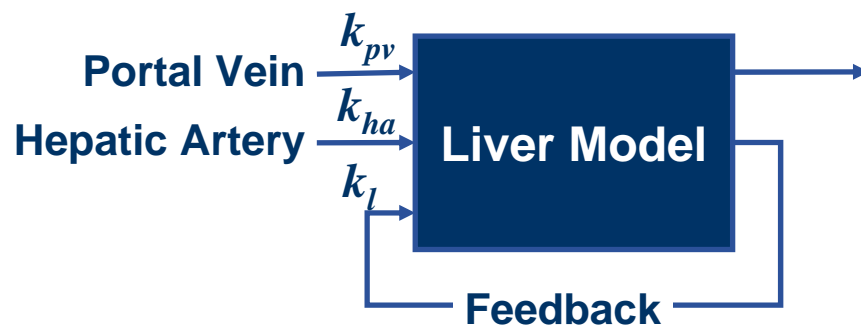


- **Short introduction of the problem and motivation.**
- **Brief details of the application.**
- **Live demo.**
- **Analysis of the results and performance.**
- **Questions and answers.**

- 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.



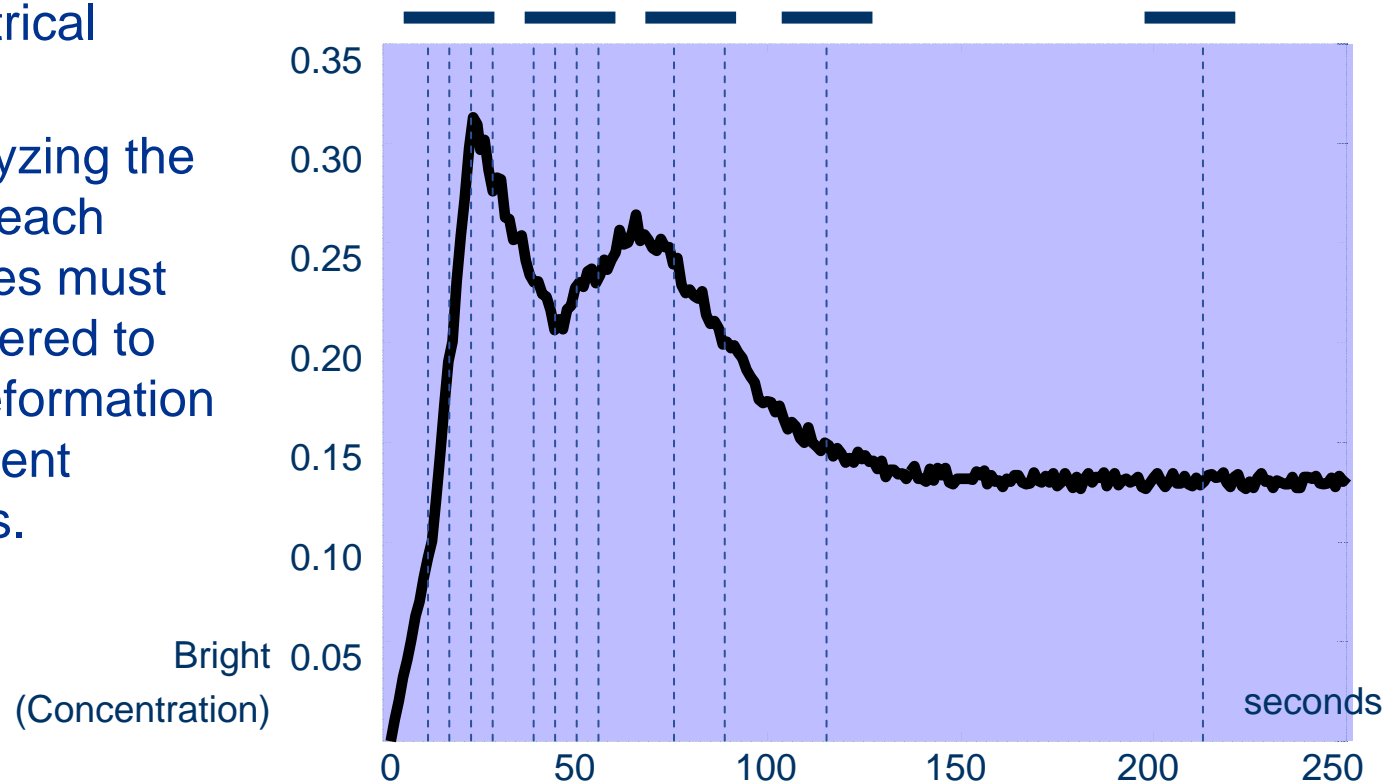
- Characterization of the tissular nature by the analysis of the evolution of contrast in a time series.
- Tumours generate the growing of vessels around the tumoural mass.
- Different tissues define different constants for recycling and flow rate of the physical models.
- Those constants can be used for the creation of parametric images.



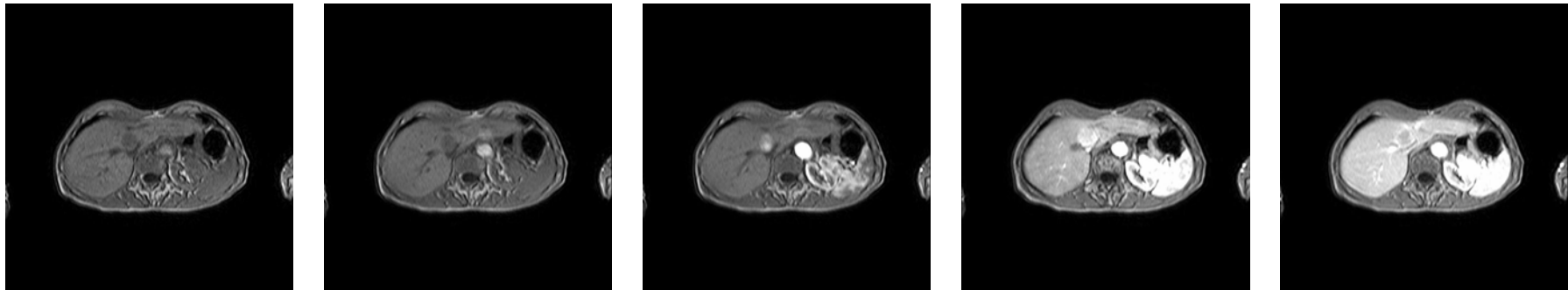
- **Pharmacokinetics in contrast evolution is a hot topic in medical research (236 articles for “Contrast diffusion and liver” key words in PubMed).**
- **The work is a result of a collaboration among four research groups (radiologists, chemical engineering and medical informatics).**
- **The problem 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).**

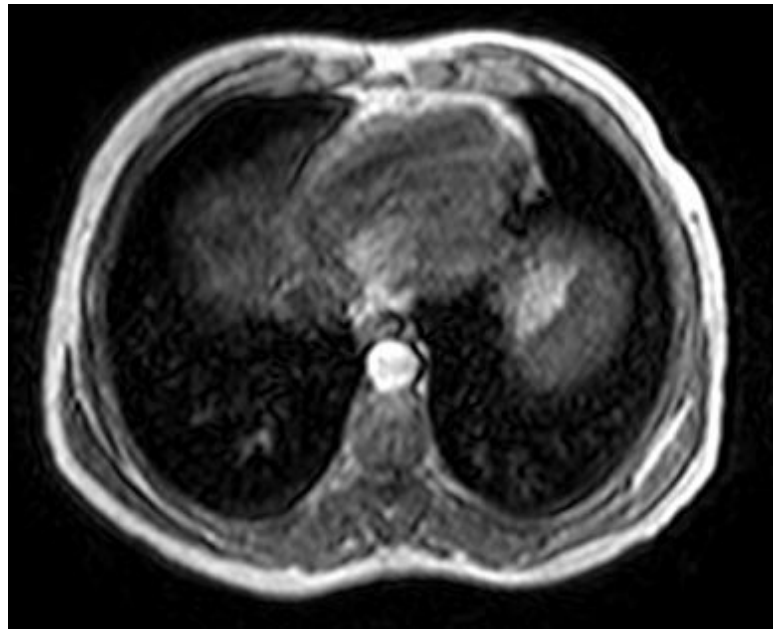
- **Description**

- 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-millimetrical dimensions.
- Before analyzing the variation of each voxel, images must be co-registered to minimize deformation due to different breath holds.

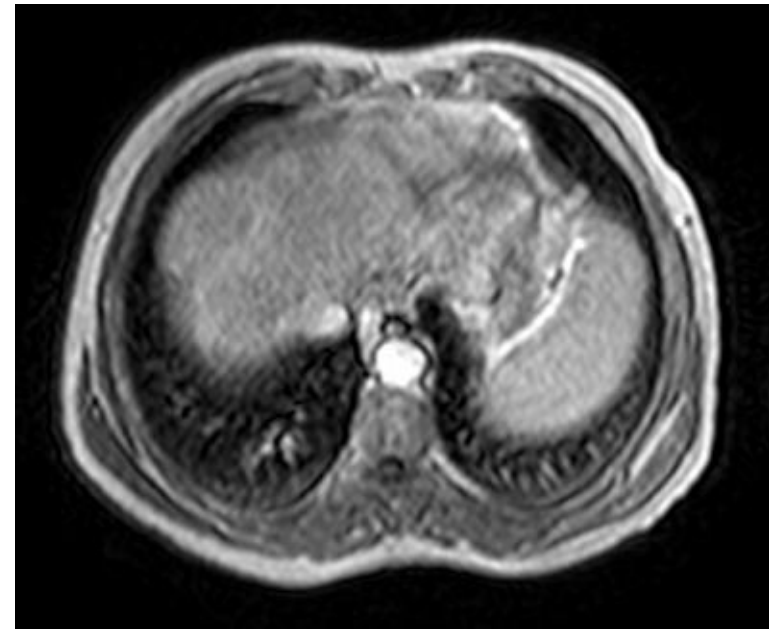


- The area of the abdomen requires the use of deformable registration methods.
- Much more computationally intensive than rigid affine registration.
- Moreover, registration must be very accurate to reduce the artefacts on the interpolation, leading to test different parameters.
- The total computational cost of a clinical trial of 20 patients is around 100 CPU days.





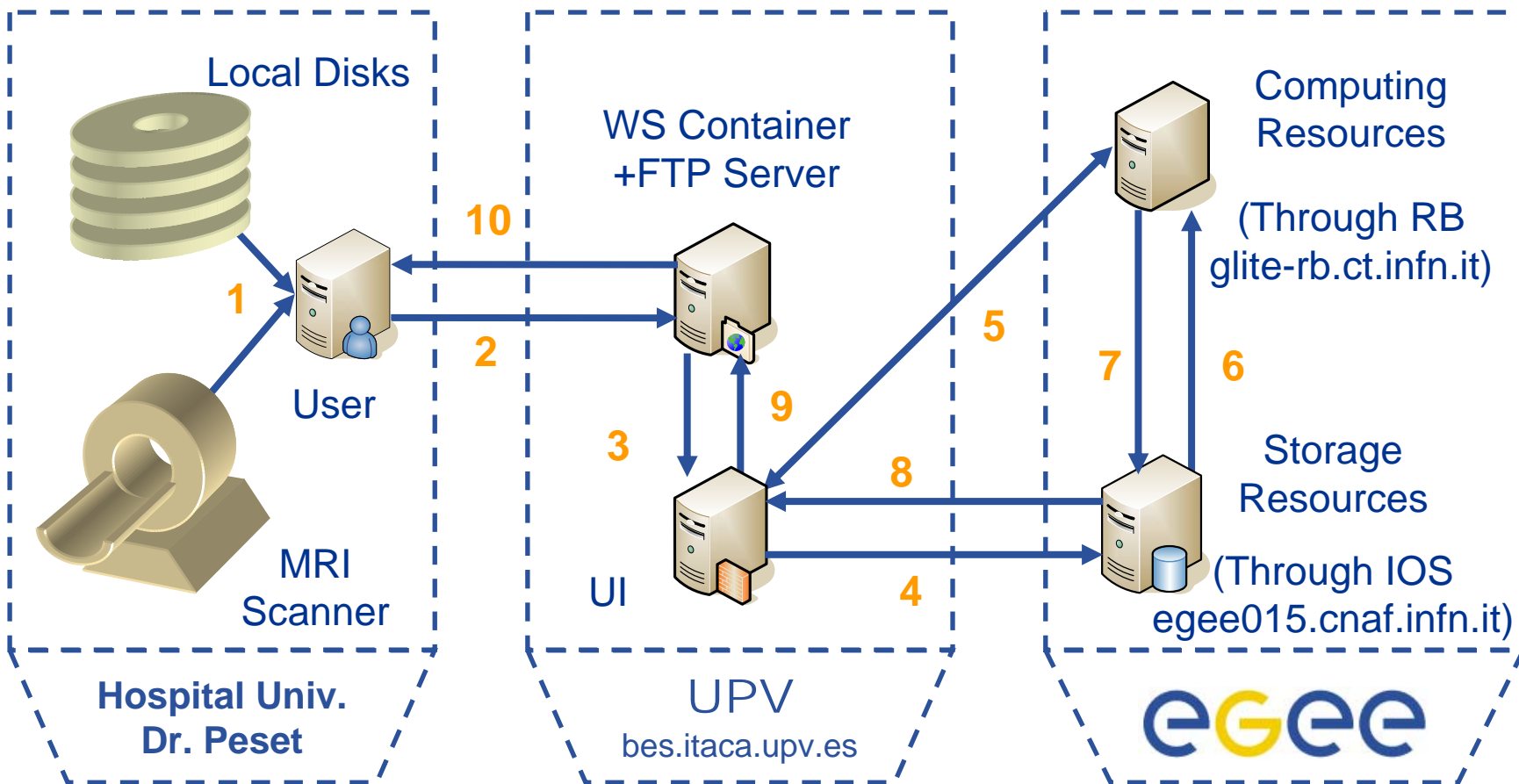
**MRI Volume at
Timestep 1**



**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.

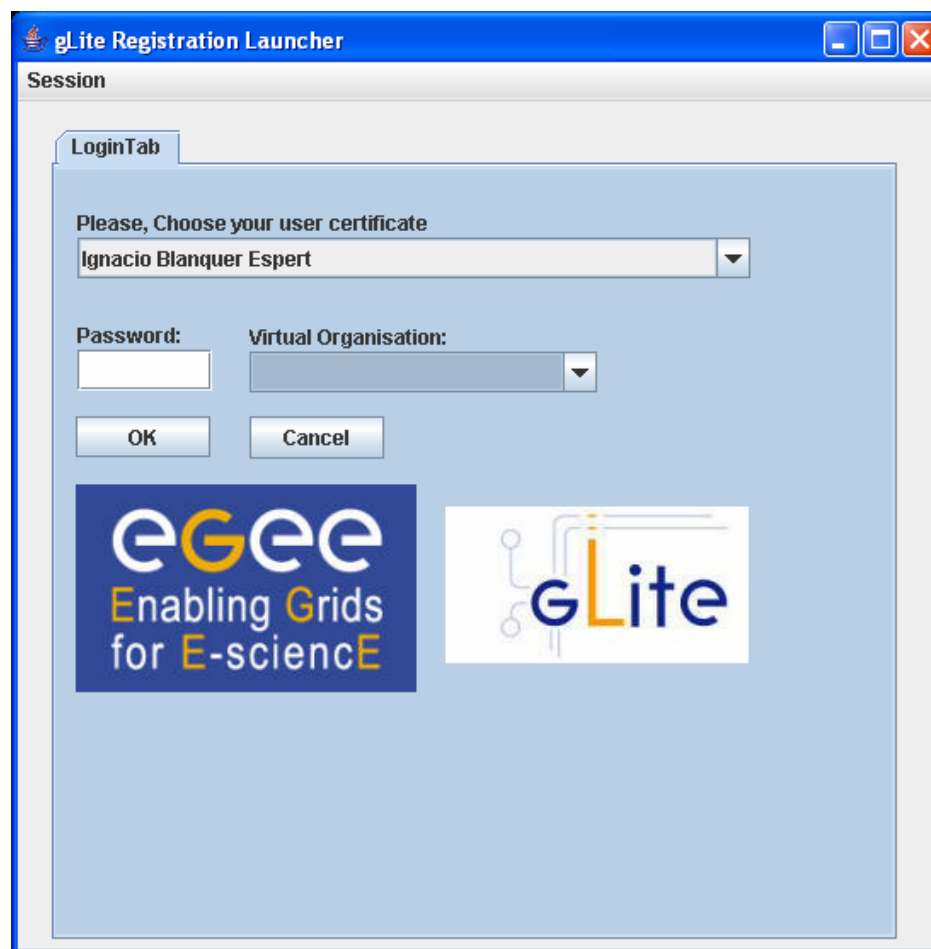


A large, yellow, rectangular button with a 3D effect and a blue border. The word 'Demo' is centered on the button in a bold, blue, sans-serif font.

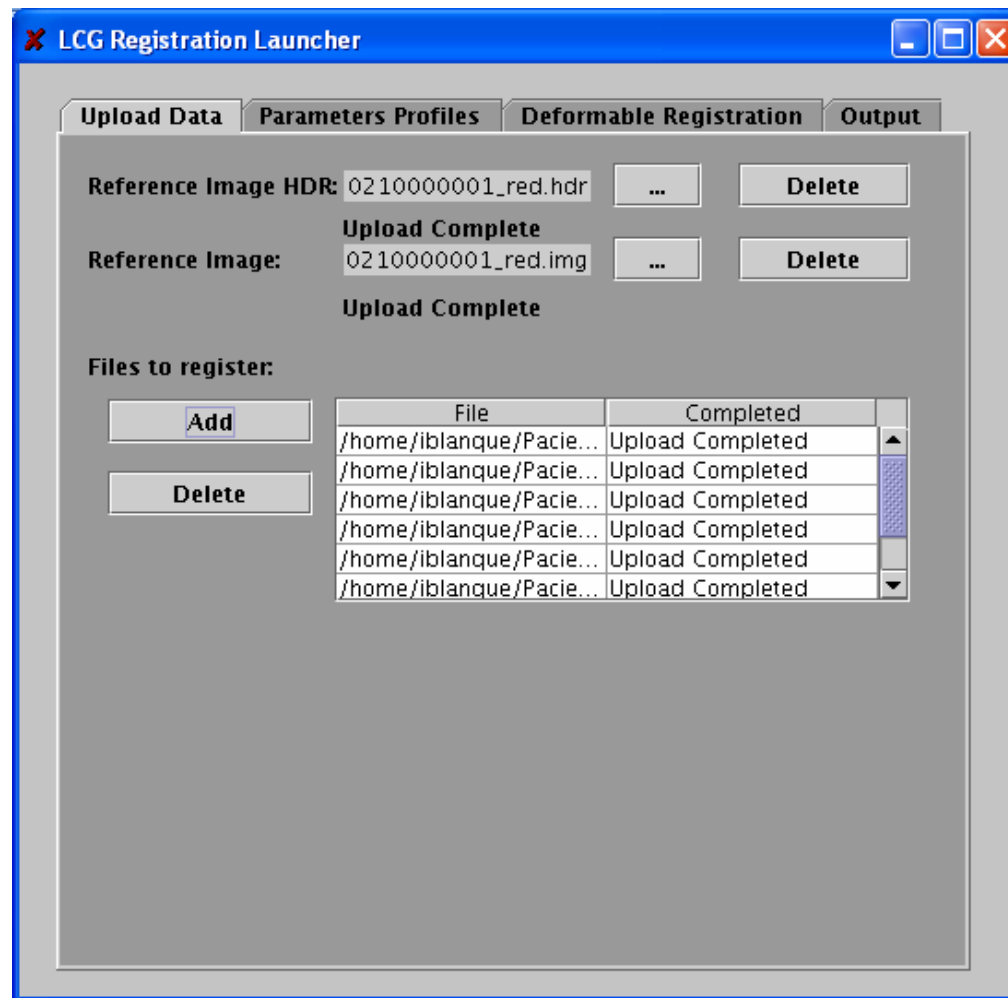
Demo

Step 1: Entering in the System

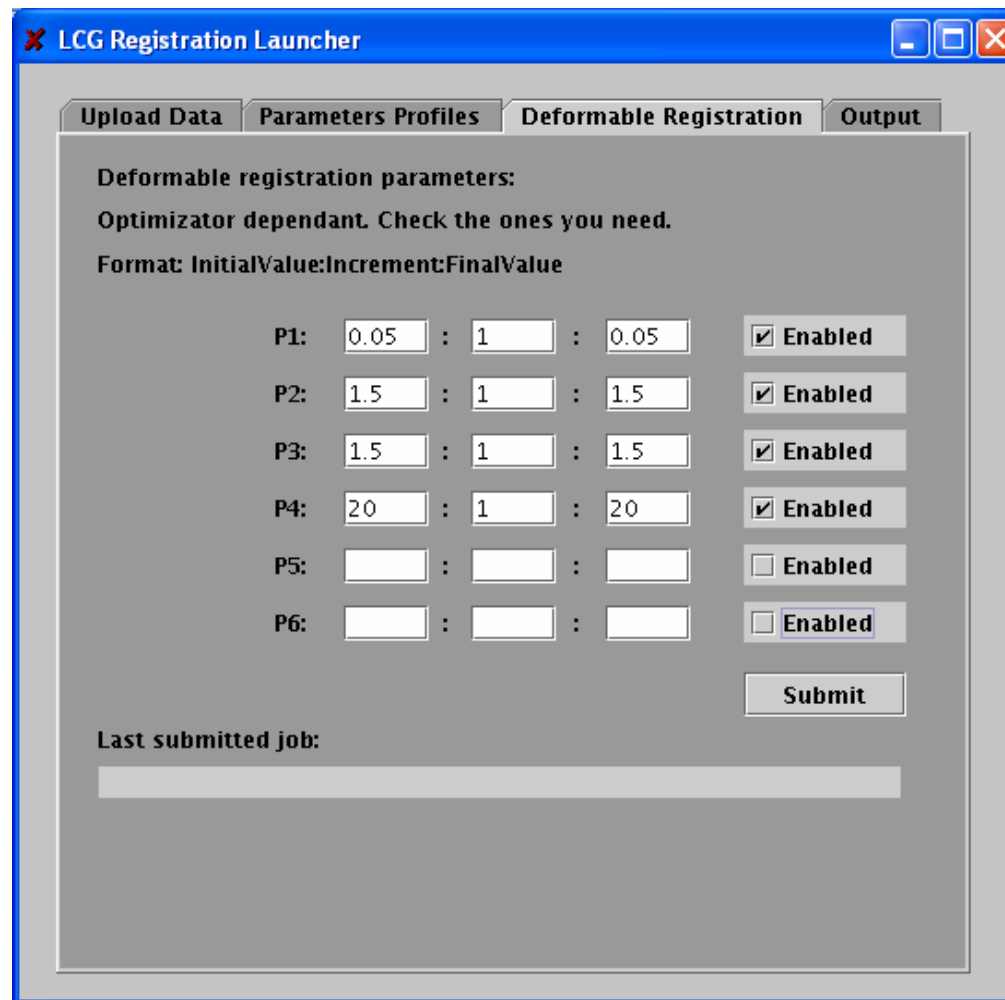
- Password for Accessing a Pre-loaded Certificate.



- **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

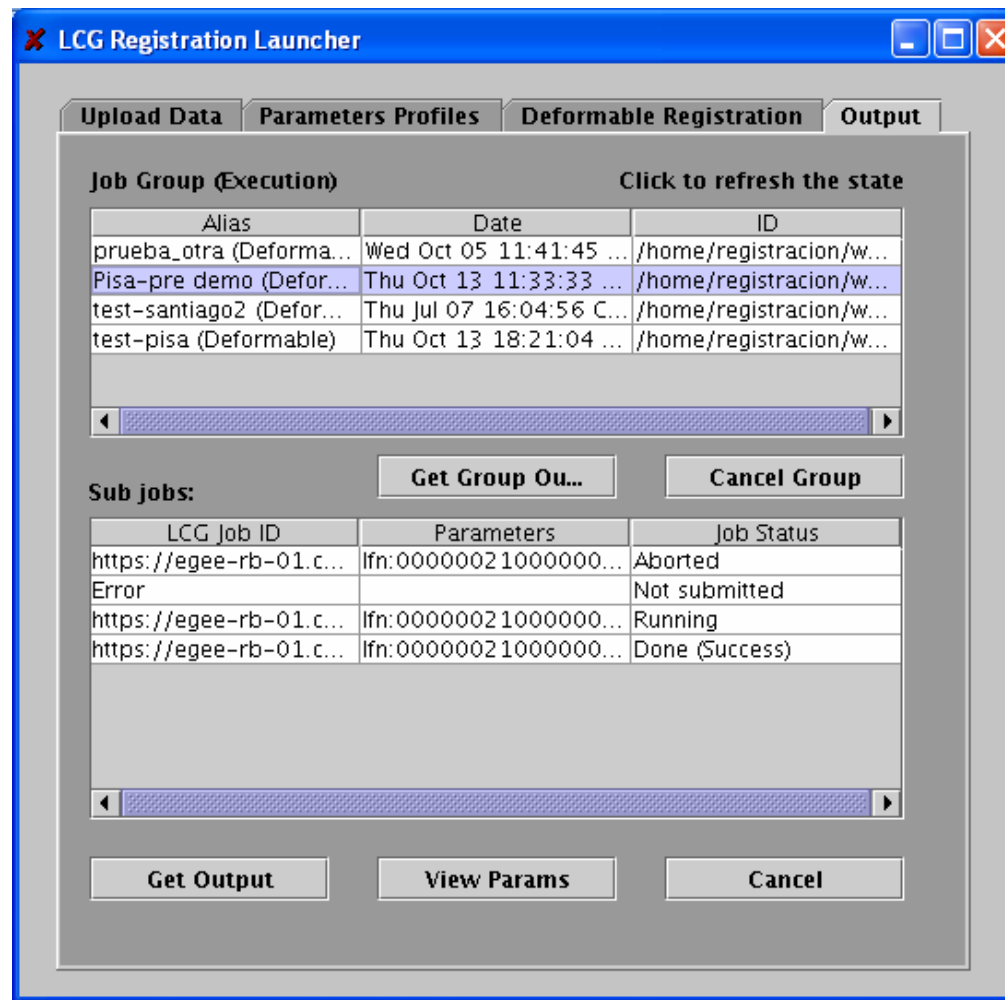
P1:	0.05	:	1	:	0.05	<input checked="" type="checkbox"/> Enabled
P2:	1.5	:	1	:	1.5	<input checked="" type="checkbox"/> Enabled
P3:	1.5	:	1	:	1.5	<input checked="" type="checkbox"/> Enabled
P4:	20	:	1	:	20	<input checked="" type="checkbox"/> Enabled
P5:		:		:		<input type="checkbox"/> Enabled
P6:		:		: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

Submit

Last submitted job:

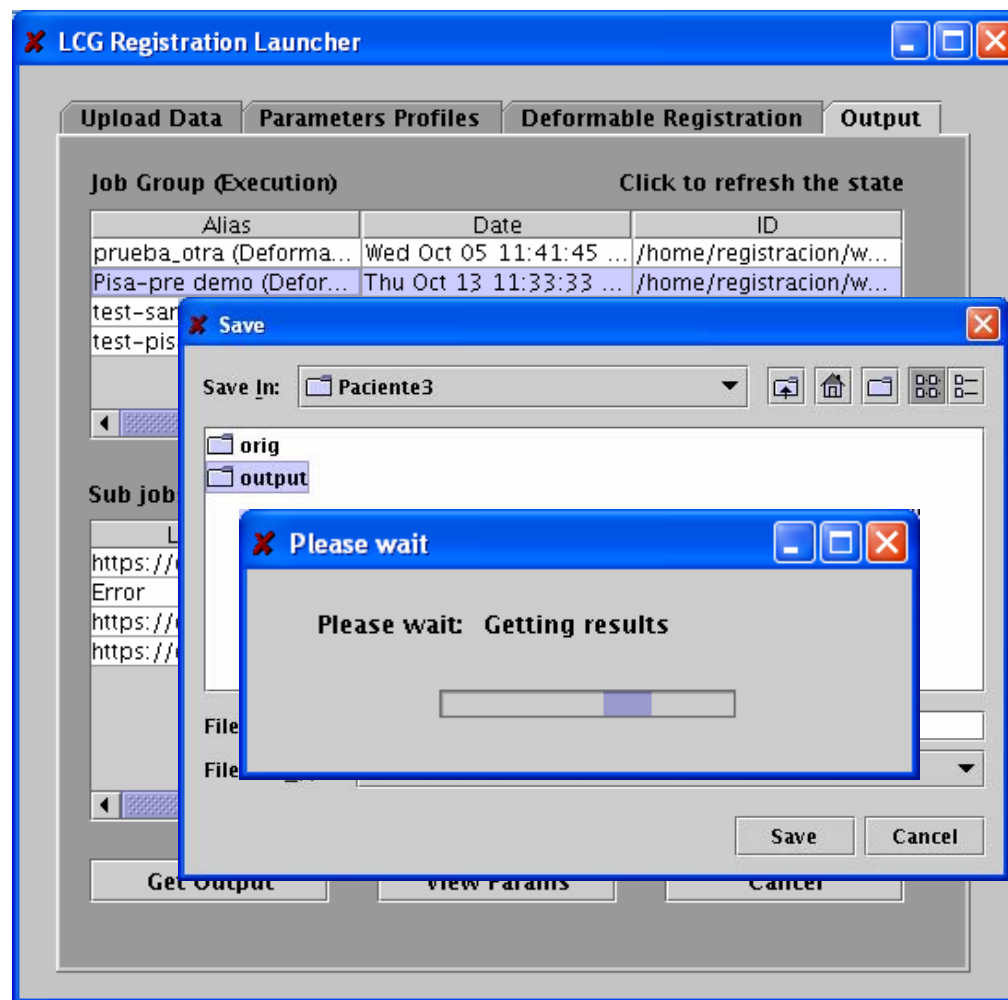
Step 4: Submitting and Monitoring Jobs

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

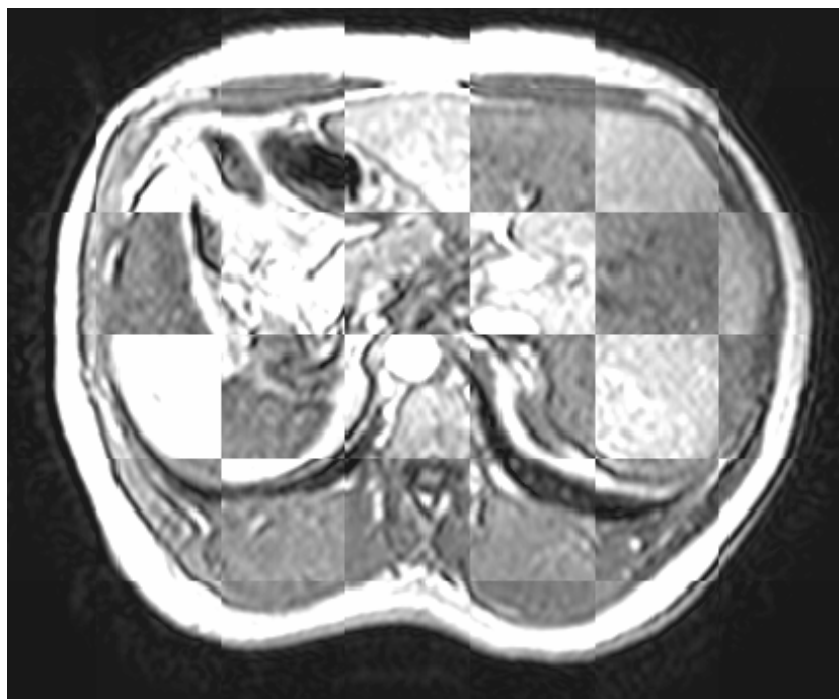


Step 5: Retrieving the Output

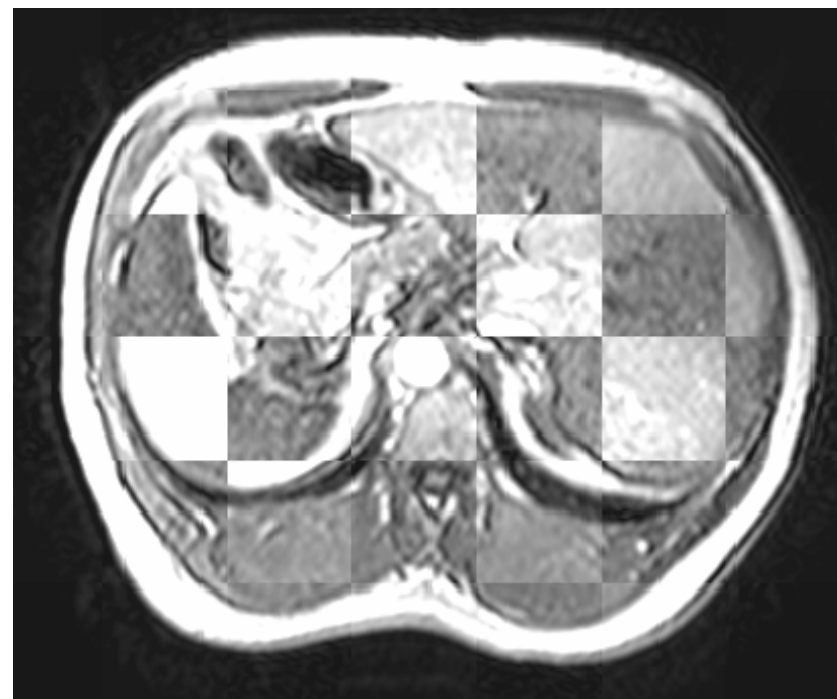
- Retrieve the Output Files from a Group of Jobs.



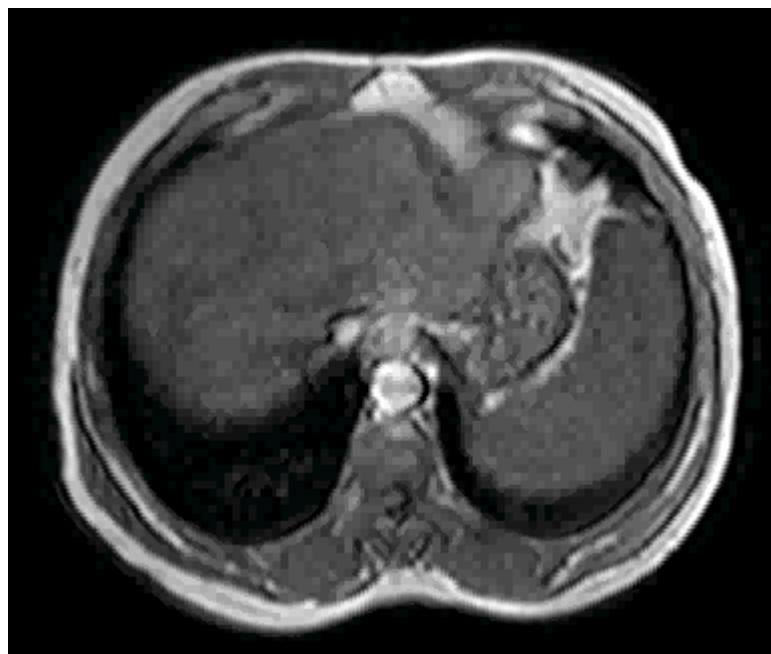
Before Co-registration



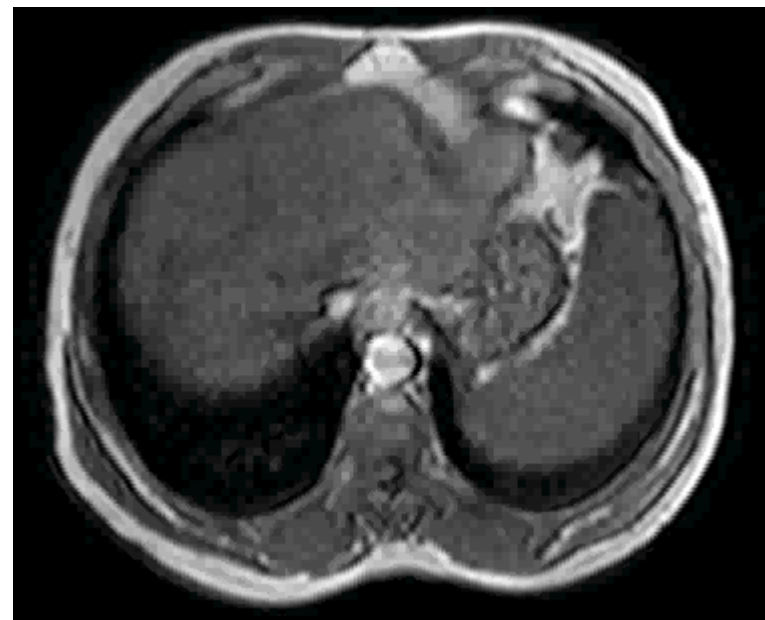
After Co-registration

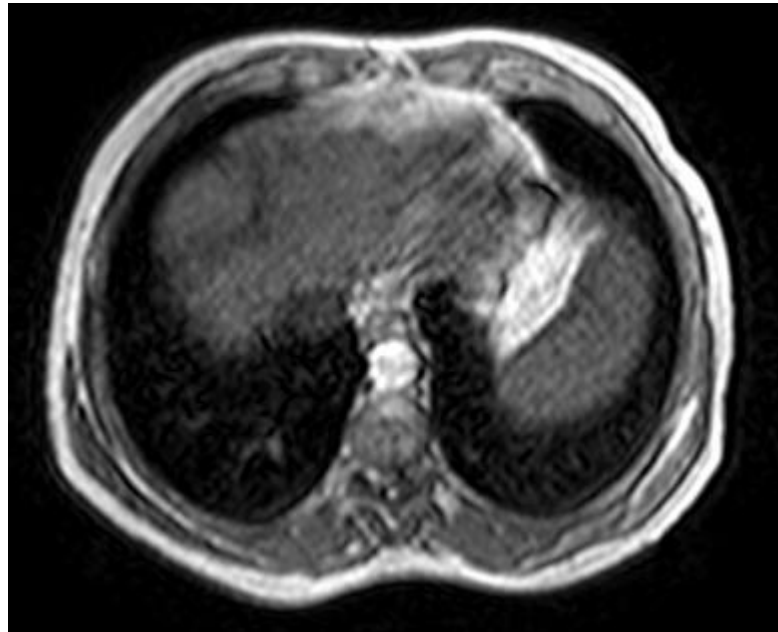


Before Co-registration

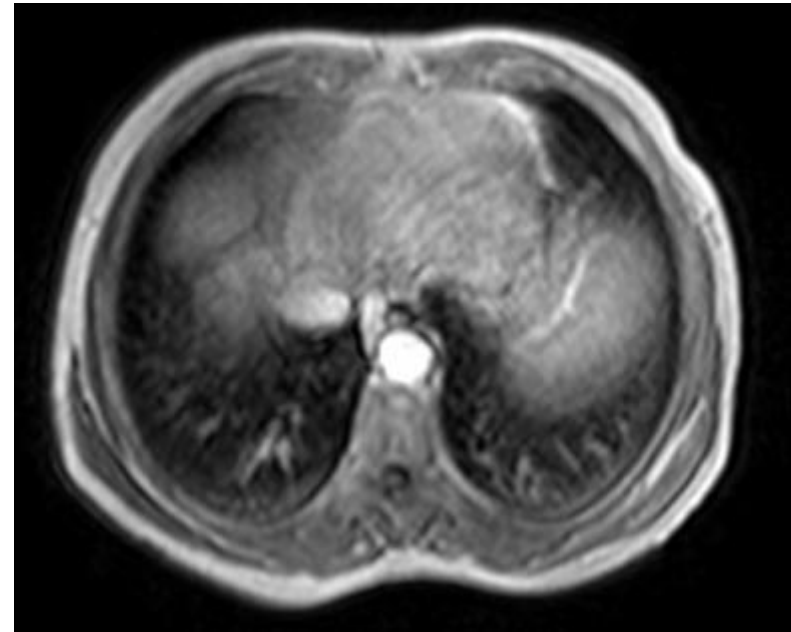


After Co-registration



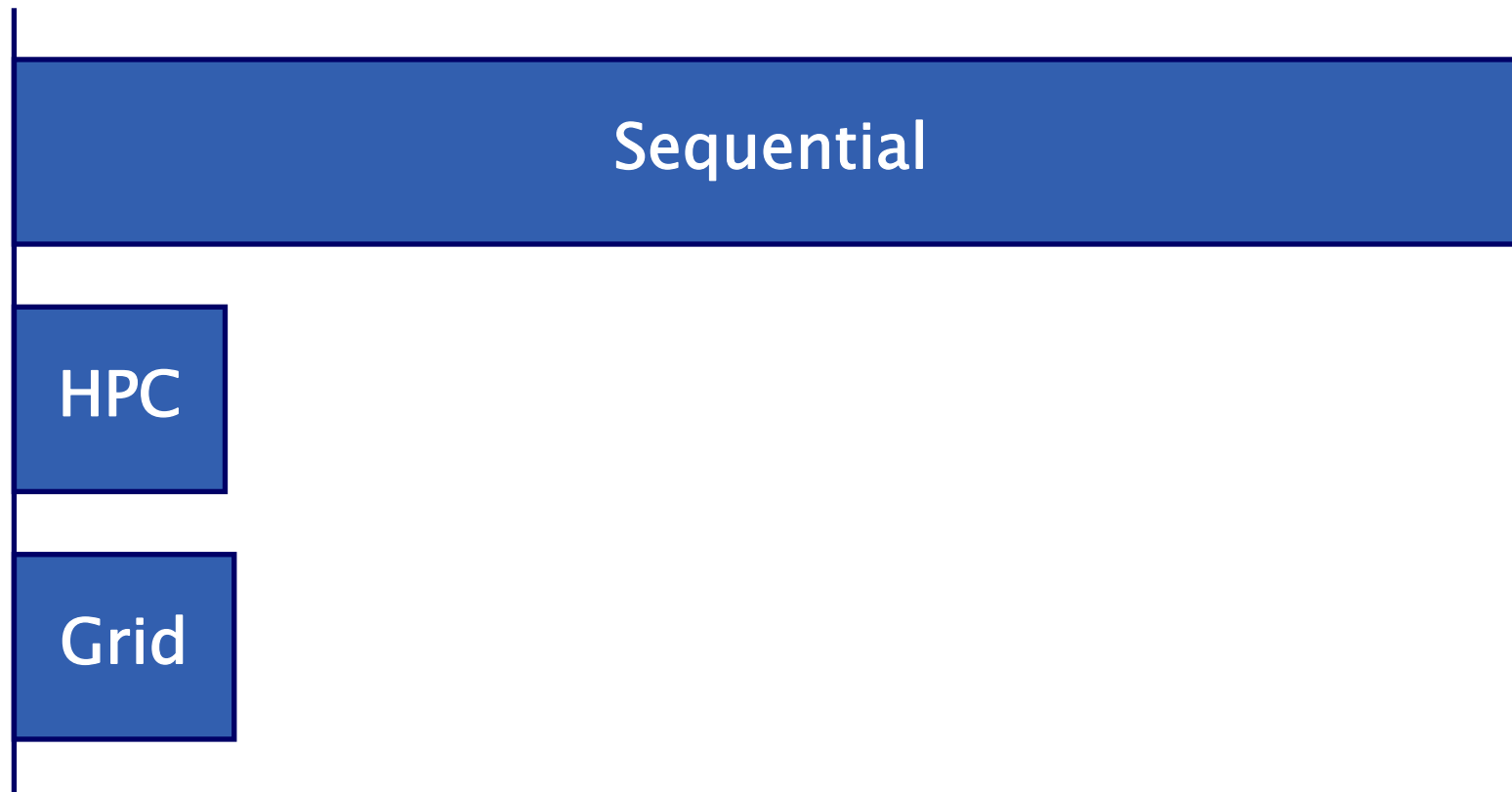


**Correg Volume
at Timestep 1**

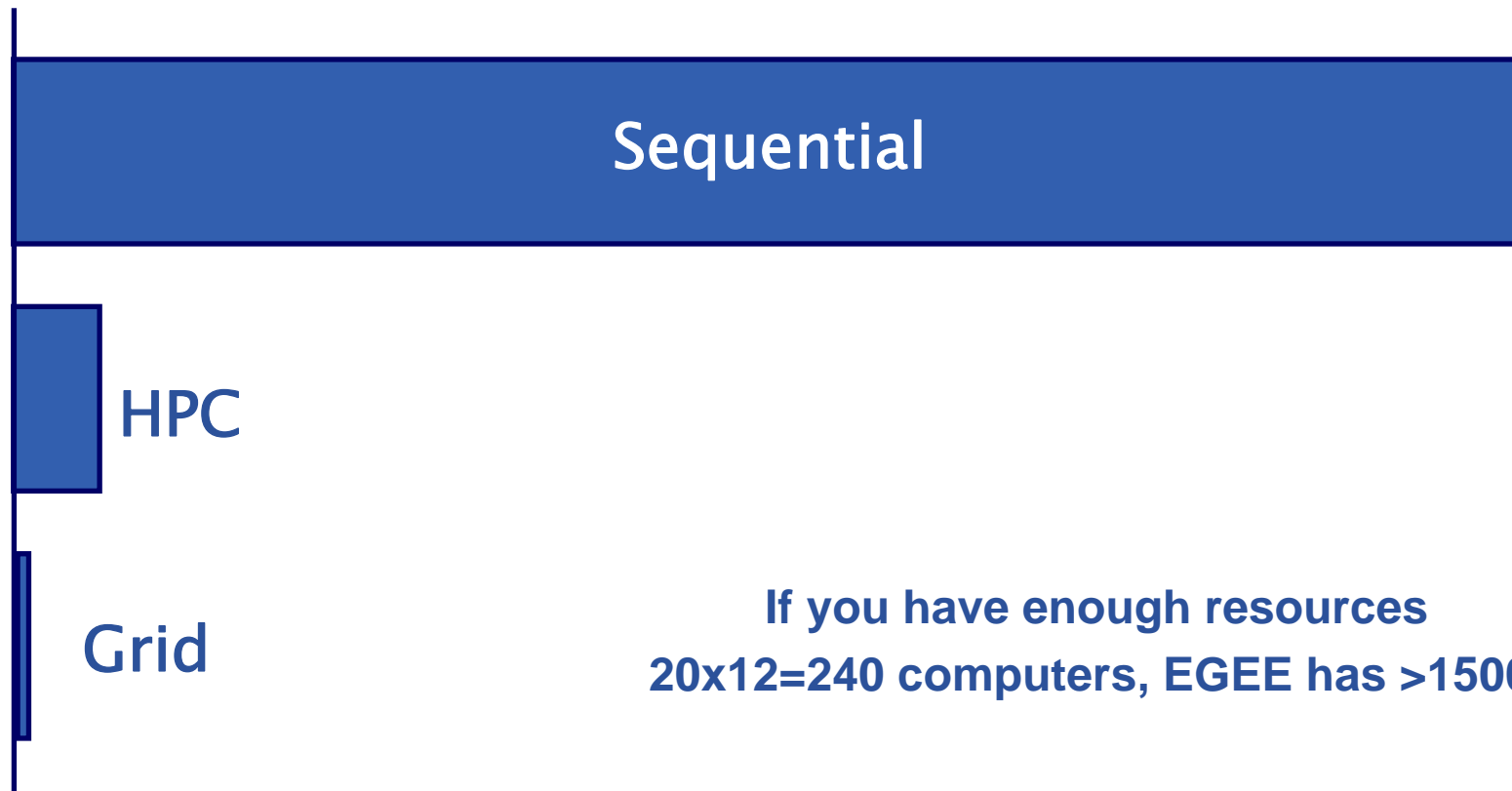


**Correg Volume
at Timestep 13**

- Cost of one patient: 44h 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.



If you have enough resources
 $20 \times 12 = 240$ computers, EGEE has >15000

- **Application Development**

- The computation of the parametrical Image is being implemented.
- It implies solving a overdetermined system of 13 equations for each pixel in the 3D image >> High computational cost.

- **Production Plans**

- Short term: Extend the clinical trial up to 50 patients (this will require about 4000 CPU hours, only for coregistering).
- Long term: Execute the tuned system for each relevant clinical case (1 case will be about 40 CPU hours, only for coregistering. Statistically, ~5 weekly cases appear at the hospital).

- **Extension to Other Areas**

- The analysis of diffusion and correlation to vessel growing has potential impact in most other tumoral localisations.
- It also has relevance in the study of adverse reaction in infertility treatments.



- **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 constant and only after the clinical 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.**