



Partnership for International Research and Education
A Global Living Laboratory for Cyberinfrastructure Application Enablement

Interface for Drug-Protein Targeting Specifics Project

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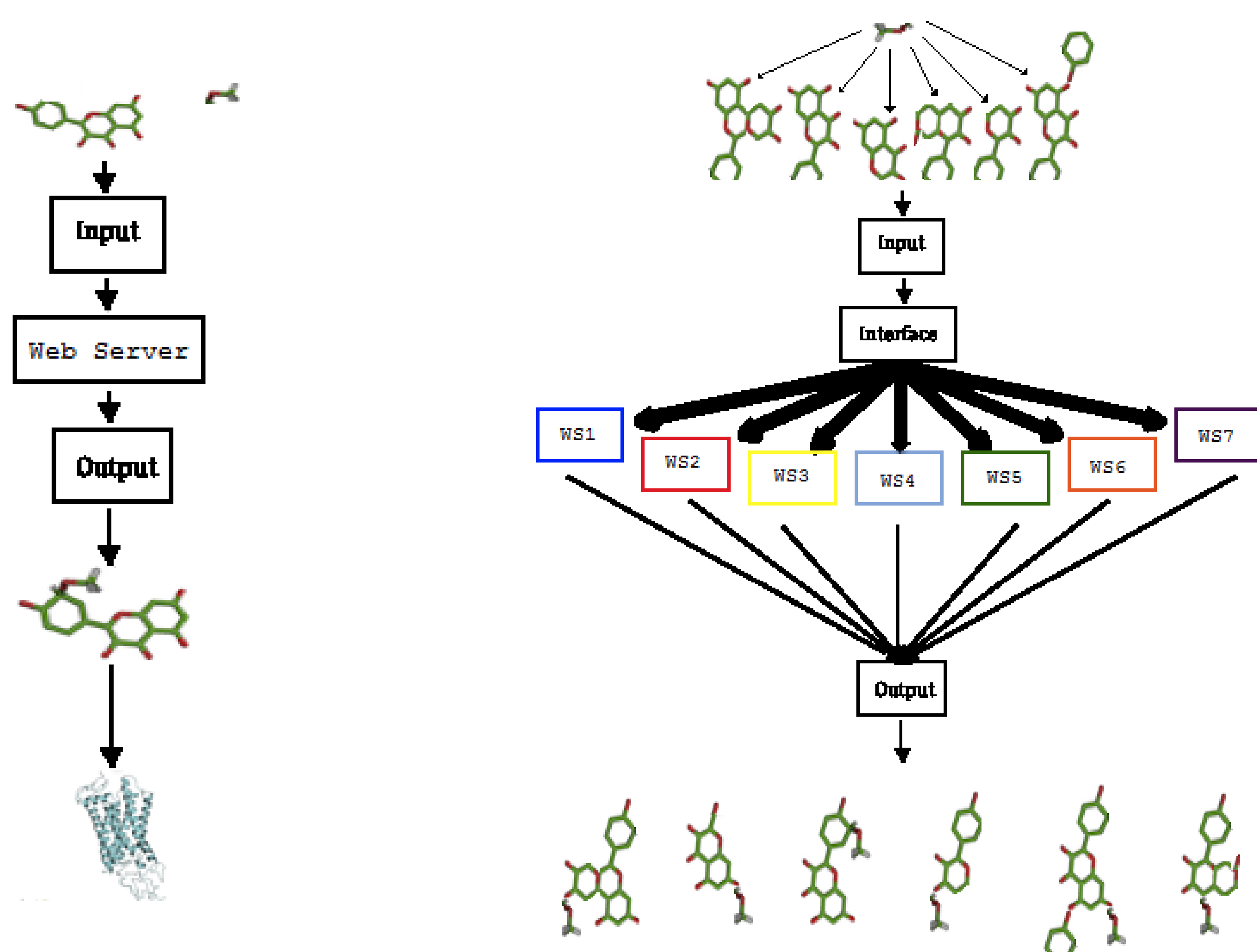
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I. Research Overview and Outcome

Concept

Protein docking web servers are one of the online tools used by biochemists to research the geometry of proteins when a ligand(smaller protein) binds with them. The web servers accept one ligand and one protein as input to do the calculations that result in a file or files that describe the geometry of binding sites of the ligand on the protein. My research consisted of designing an interface that could accept one ligand and up to six proteins and submit them in pairs to up to seven protein docking web servers simultaneously. Each web server receives up to six pairs, one ligand paired with each of the six proteins.



Typical data processing flow for a Protein Docking Web Server

Data Processing Flow for our original concept interface

Project continuation and other practical applications of this concept

Next Phase

- Test and debug against each server
- Gather output into a repository
- Devising a data processing unit

Other Practical Applications

- Automated testing (site vulnerabilities)
- Submission to modeling servers

Methodology

- Research which languages have libraries for handling post requests.
- Use online tools to determine the parameters required by the target website to submit posts.
- Choose a language and find out how to write the POST requests in that language using its libraries.
- Write the interface form.
- Write the code to prepare and assemble the parameters needed for the requests.
- Write the code to submit the request.
- Test the code. Things we need to find (once the researcher prepares correct protein and ligand files):
 - Does our code post successfully to each protein docking web server?
 - Does the protein docking web server produce an output file or files?

Current stage of project and first test results

Web Server	Response from server	Errors
ClusPro	not logged in	Closing connection #0
3DGarden	unknown	Closing connection #0
PatchDock	results will be mailed	Closing connection #0

Developmental Resources

- Language
 - PHP
- Library
 - cURL
- Web
 - XAMPP server(local to web)
 - Apache server(web to web)

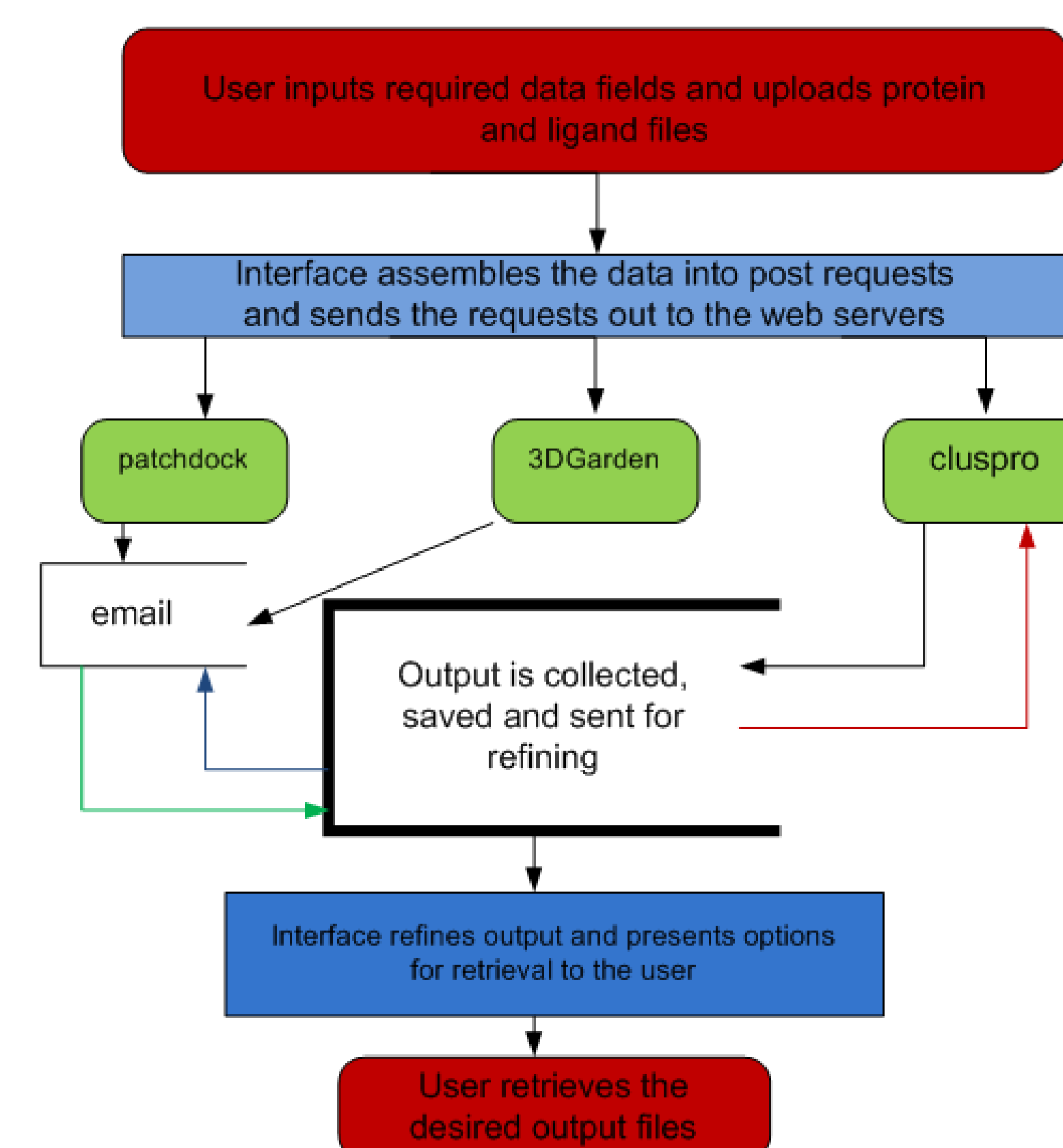
cURL functions used

- curl_init()
- curl_setopt()
- curl_exec()
- curl_close()

Outcome

A change in requirements on week six resulted in a decrease in my available research time. As a consequence my research advanced only as far as the first testing stage. This stage calls for assuring that the interface can submit one pair of ligand/protein files to each of the selected web servers and obtain the same response we would if we submitted them manually. Three web servers were chosen: Clus Pro, 3DGarden and PatchDock. Separate and independent tests on each of them yielded three different results. The flowchart below represents the final version that I could attain after another PIRE participation.

Projected operational interface



II. International Experience

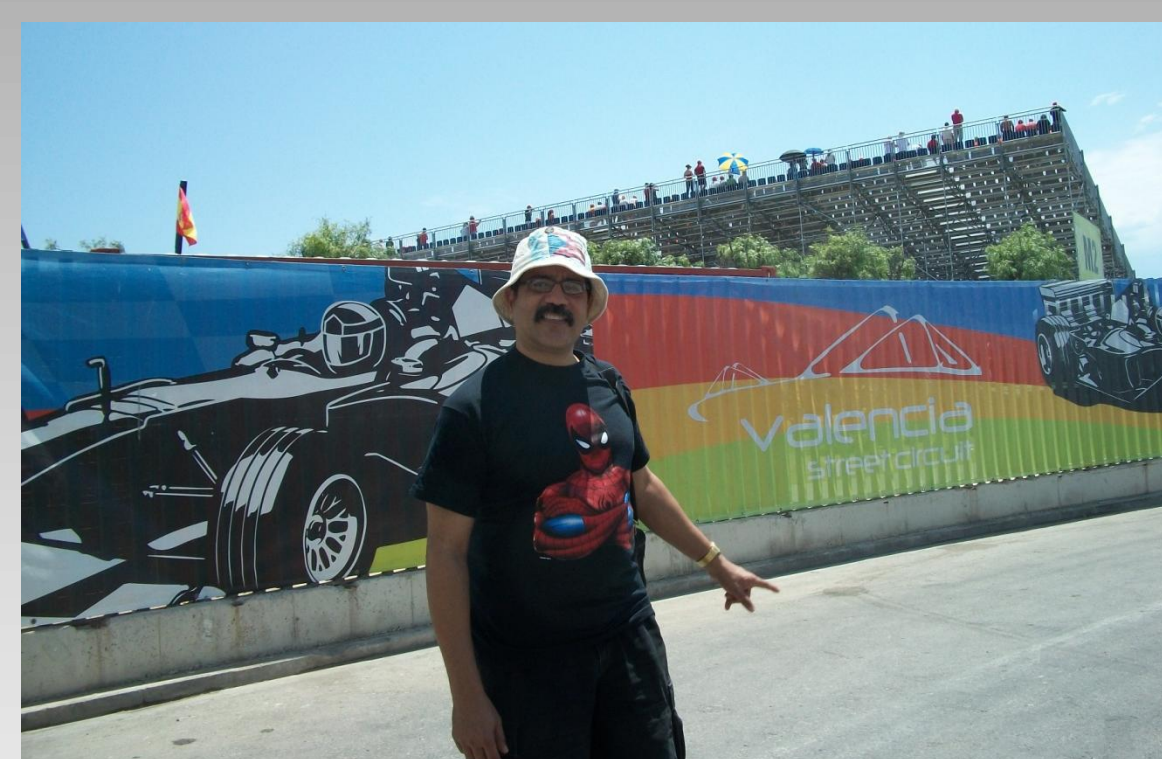
Thanks to PIRE I had the opportunity to be in Spain to witness the fervor of the people of this beautiful country when celebrating three international sporting events: The European Soccer Cup, the World Cup of Soccer, and the Valencia Formula Circuit.

I was able also to participate in two local patron saint celebrations: the sardine beach cookout and the "Fiesta de San Juan". I learned that traveling to research sites abroad should be part of a researcher's agenda, and that collaboration with researchers of different cultures not only enriches us culturally but it nurtures and expands our intellect.



German soccer fans celebrating their team's showing at the European Soccer Cup

me at the Valencia Formula I Circuit



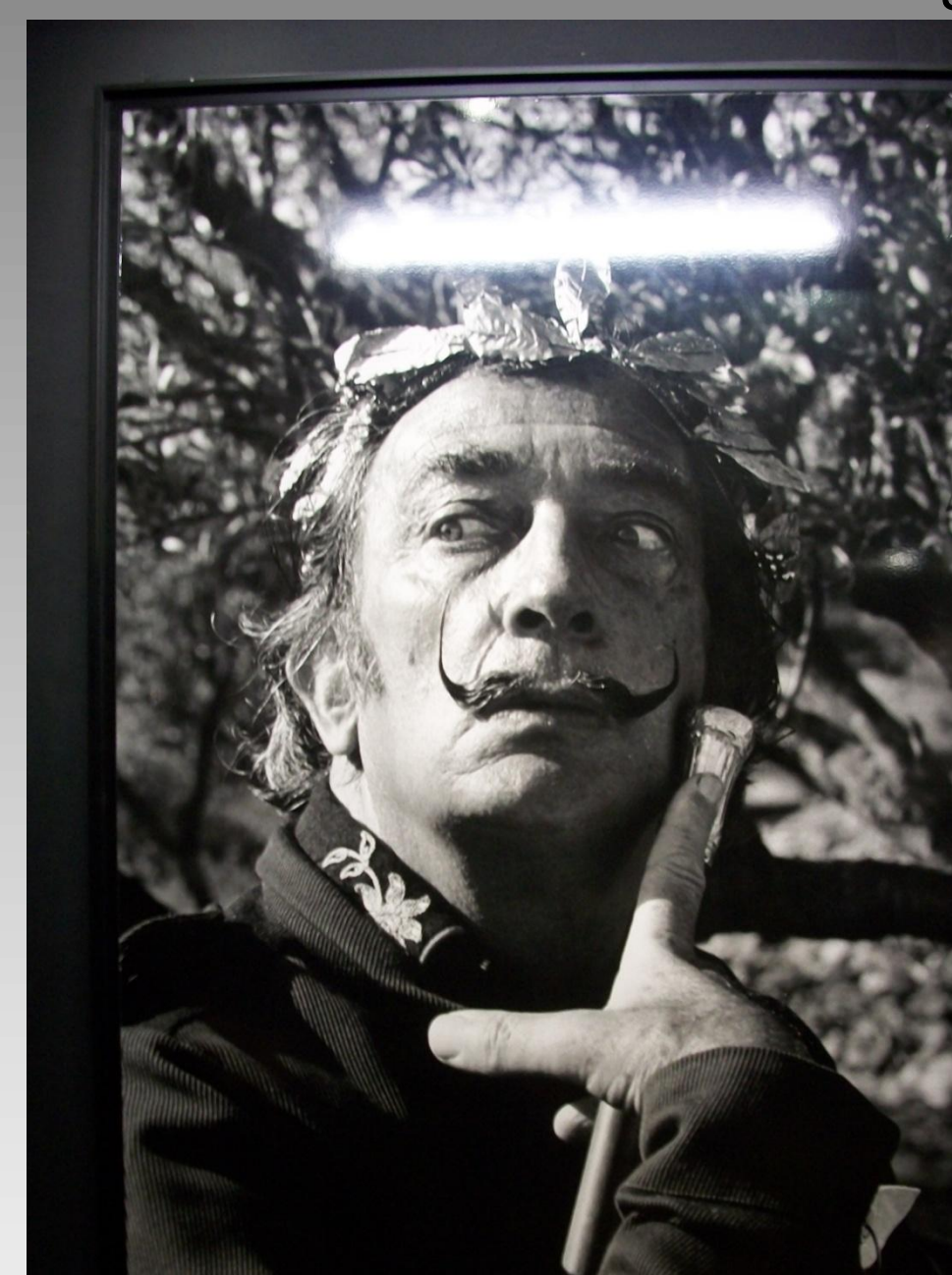
I will never forget the view from our balcony at dusk, nor will I forget my trip to Salvador Dali's house.



Barcelona from Mount Puig



Outdoor cafes are a common sight in Spain



Glass Castle inside "El Retiro Park" in Madrid



Salvador Dali, a view from inside his house, and the beach at Roses(also left)



III. Acknowledgement

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