

# Web-Lar

First project results

# Task assignements

Extension of the LAR.js and LAR-DEMO.js projects with convex cells

- Andrea Somma
- Elisa Lamberti
- Fabio Cumbo

Integration of the matrix computation webservice

- Fabrizio Rebecca
- Luca Menichetti (Group Leader)

Integration of PDB visualization service

Oscar Eijsermans

Andrea Somma assigment: 1-A, 1-B
Elisa Lamberti and Fabio Cumbo assigment: 2-A, 2-B



#### Description

Extension of the LAR.js and LAR\_DEMO.js projects with convex cells

#### **Summary**

- 1. Implementation of the cartesian product function between convex cell
  - Integration of the lar.js project with the *larProduct* function, which will allow to do the product between convex cells
- Reimplementation of the "extract" function, generalizing it to make it work on cells with general shape
  - Implementation of the *larFacets* function in the lar.js project, currently provided with an extraction function that works only on simplexes.

#### **Brief explanation**

The lar.js wasn't provided of:

- Cartesian product between convex cells
- Extract function

#### Solution

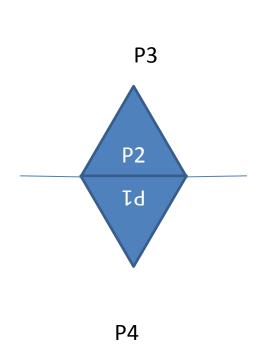
So, the actual workflow for points 1 & 2 for today's demo was to:

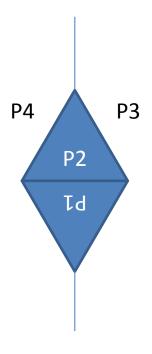
✓ Implement the lar.py functions "larProduct" & "larFacets" using dense matrixes, in lar.js.

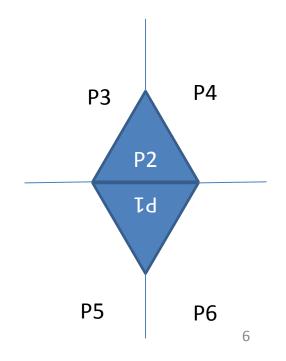
Actually, we have readapted those functions and we have implemented a "beta version", which works well with simple models.

#### To Do

- > Other test and examples for Cartesian product
- External space partitioning for larFacets: How to do that? What the criteria?









**Fabrizio Rebecca** assigment: communication **Luca Menichetti** assigment: handler

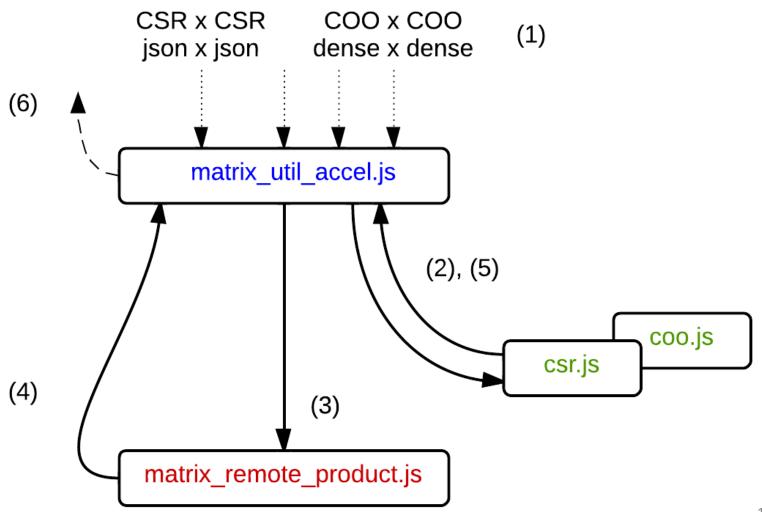


#### Description

Create a webservice that provides fast matrix operations on the network

#### **Summary**

- 1. Localization of code's sections that use matrix operations
  - Replacement with a call to an external procedure (\*interface\*)
- 2. Creation of a proper layer that implements the computation of matrix's operation hiding the logic implementation
  - Definition of a matrix\_util\_accel.js layer (responsable to handle format or encoding, such as csr, coo, json)
  - Realization of a HttpRrequest with the matrix computation webservice using Representational state transfer REST in the **matrix\_remote\_product.js** layer (This layer is also responsable to manage the answer, with an opportune decoding in order to satisfy the spefics)
- 3. Setup a web service that offers such operation online
  - available with node.js;
  - acquisition of the request using REST;
  - executing the computations (OpenCL) and forwarding the results;
  - create a domain name in which will be available such services online





Oscar Eijsermans assigment



#### Description

#### Integration of WebMOL and WebPDB projects

#### **Summary**

- 1. Identify the structure and functionalities of WebPDB and WebMOL
  - Data structure and communication protocols
- 2. Identify the connections between the two projects
  - Make changes where necessary
- 3. Merge the two projects in one project

#### WebMOL-WebPDB interaction:

- **step 1** install CouchDB and Node.js
- **step 2** install node modules and configure the database
- step 3 populate the database with proteins
- step 4 start the WebPDB rest service
- step 5 start WebMOL and input the id of the desired protein

