

**Programme for Research-Development-Innovation on  
*Space Technology and Advanced Research - STAR***

Software development and  
integration for access to  
large-scale atomic databases  
and analysis applications

**DATOM**

V. Stancalie

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- **Coordinating organization**
  - National Institute for Laser, Plasma and Radiation Physics (INFLPR)
  
- **Project manager**
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- **Short description of the project**

- Support for physics related x-ray astrophysical observations providing large scale relativistic atomic data for the Fe-peak elements (Co, Ni, Fe) and for the light elements such as C, N, O or Ar;
- Model the plasma emission spectra under extreme conditions;
- Design and development of an advanced graph-based database for storing large amounts of data; the data communication system;
- Expose system functionality through a Web portal.

- **Project goal**

- Large-scale atomic data calculation and related spectral modeling;
- Advanced graph database for data representation and data processing;
- Web Portal for data and application access.

- Objectives

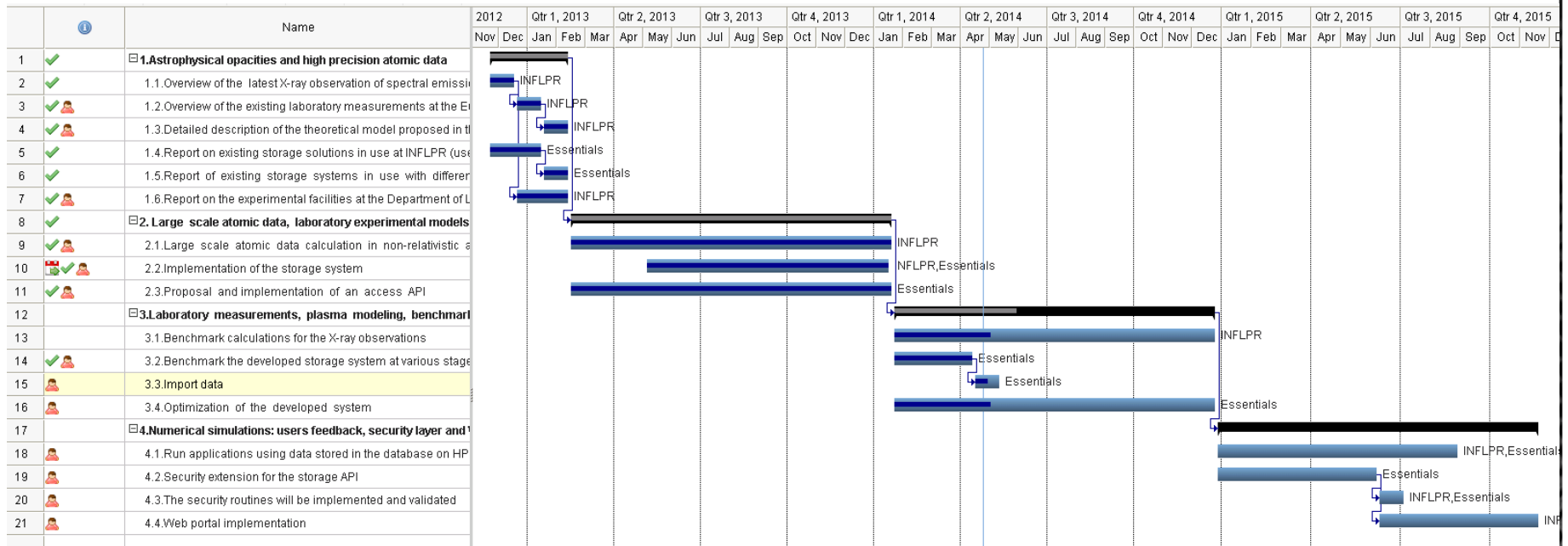
- 1. Theoretical computations;
- 2. Laboratory measurements and plasma modeling;
- 3. Numerical simulations and databases;
- 4. Advanced graph database for data representation and data processing;
- 5. Web Portal.

- Estimated results

- The project uses the R-matrix method in atomic physics and provides atomic data for atoms and ions, cross sections and rates for elementary processes in laboratory and astrophysical plasma.
- Laboratory measurements of spectroscopic data. With this respect, the aim of the project is high precision first, then completeness supporting benchmark state-of-art theoretical calculations with experiments for: Photoionization – Accelerator based Advanced Light Sources (Reno/Berkeley, Aarhus, Paris); Recombination – Heavy ion storage rings (Heidelberg, Stockholm); Electron-Ion Scattering – Electron Beam Ion Traps (Livermore, NIST).
- The proposed graph system aims at improving both data access and data storage. It is a new kind of data representation that allows for parallel computing due to multiple storage servers employed combined with data storage in binary files.

- Human resources involved
  - Specialized human resources as well as young scientists are involved in numerical simulation
  - two project managers (from CO and P1)
  - scientific researchers
  - software analysts
  - programmers
  
- Start date of the project / End date of the project
  - 19.11.2012 – 19.11.2015

## ■ Work plan of the project

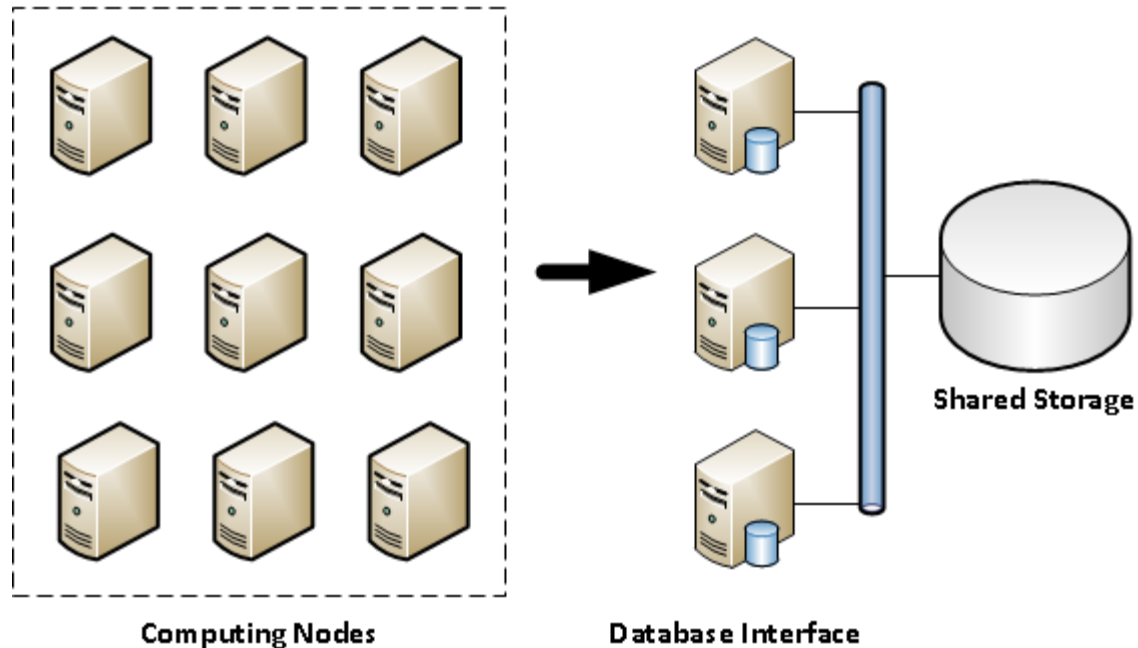


- Work proceeds as planned;
- All tasks scheduled to end until now were completed;
- A skeleton system is in place;
- Data calculations were performed and some of them are imported in the skeleton system;
- Work is focusing on optimization of the system, testing and correction of bugs.

## ■ Implementation status of the project

- Based on previous year's work on analyzing existing storage systems and formulating requirements for the Graph Database storage engine, work was focused on **actual implementation of the system.**
- Storage system based on data blocks with specific access mechanisms
- API based on web service calls
  - using REST for speed

## Implementation status of the project: Database connectivity



### Basic top-level API:

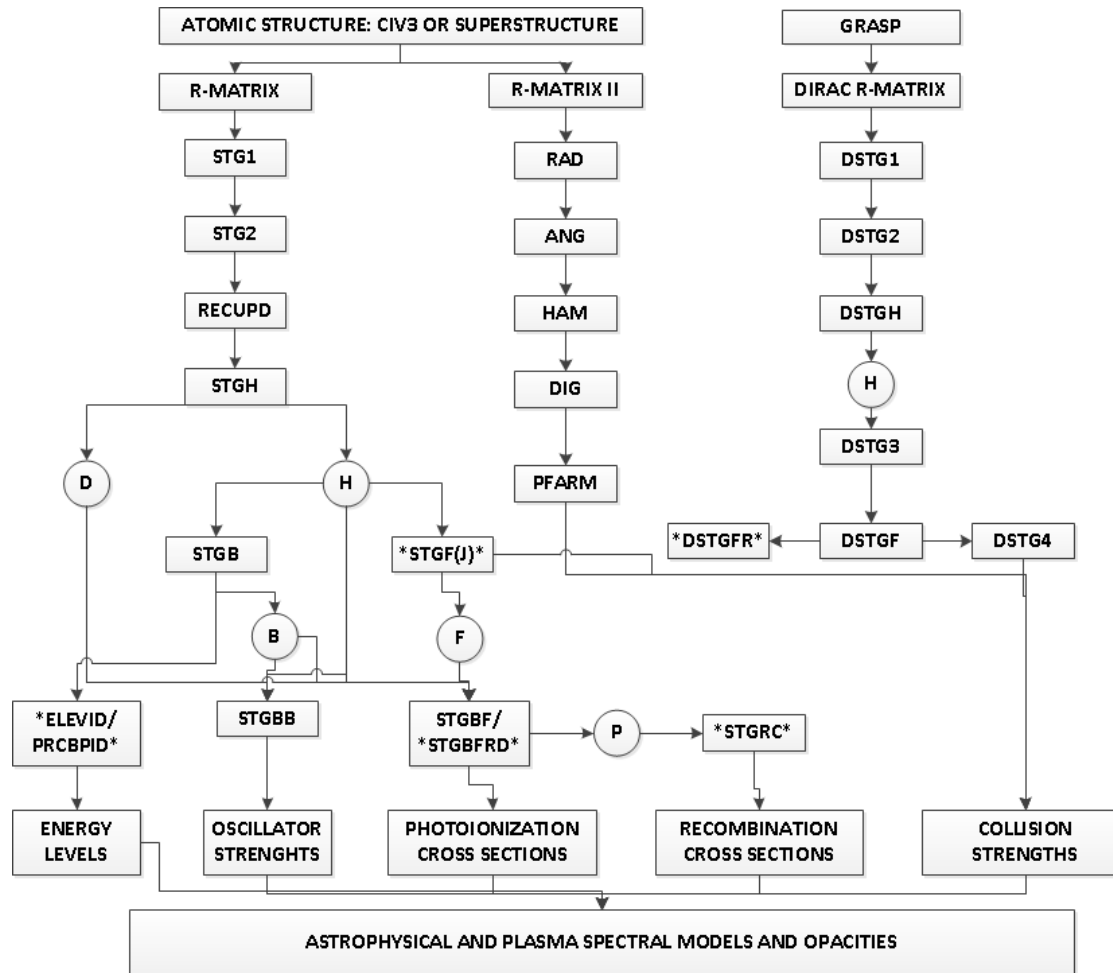
- **INSERT (n1,n2,relation)**: inserts a new relation between two nodes
- **COMPUTE (graph algorithm)**: computes a graph algorithm on the database (closeness, indegree, centrality,...)
- **GET (condition)**: retrieves nodes based on condition (either from a relation or based on computed values)



## ■ Implementation status of the project : users' specific requirements

- Energy levels and radiative rates for transitions in Cr-like Co IV have been obtained in different relativistic approximations. Discrepancies in energies are noted with the NIST listings for many levels;
- We have performed several sets of calculations: a) 1334 levels included, b) 21 992 levels included, c) 59 190 levels included, d) 71 528 levels included into configuration interaction model.
- Development of storage system:
  - IBM HS22V Blade complemented the INFLPR Infrastructure offering a platform for the software development in the current Project
  - Current implementation of the access API has known bugs
    - Will need to correct these issues
- Data access speed is a key factor
  - More tests will be performed
    - Data access routines optimization

- Implementation status of the project : users' specific requirements



- Relativistic and Non-relativistic R-matrix Codes for Atomic Processes, Currently used on our ATOMIC Computing facility
  - Used as data source for computations and supplying data to the storage system

## ■ Risk analysis and contingency plan (lessons learned)

No.	Risk	Prob. (L,M,H)	Impact (L,M,H)	Effect on Project	Risk Reduction Actions Proposed & Actual	If it happens: Triggers & Actions Proposed & Actual
3	Volume of change requests following testing extending work on each phase.	Medium	Medium	Delays	Agree specification. Agree priorities. Reasonable consultation on format	<b>Triggers:</b> swamped with changes; delay in signing off items. <b>Actions:</b> managerial decision on importance, technically feasibility and observance of time constraints.
4	Poor capture of full User requirements.	Medium	High	Failure to meet minimum requirements. Failed delivery.	Focus on User Requirements capture at start of project	<b>Triggers:</b> feedback from Users <b>Actions:</b> monitor through project meetings, feedback from testers.
5	Poor data quality	High	Medium	User will find system difficult to use unless data quality has been addressed	Data clean up - correction and removal of duplicates	<b>Triggers:</b> poor data <b>Actions:</b> only use records which have good quality basic set
7	Loss of power or internet connection during data import/access	Medium	Low	Import operations may need restart; Delays.	Check for scheduled outages. Test equipment/network connection prior to import operations.	<b>Triggers:</b> data import fail/incomplete <b>Actions:</b> re-schedule the import session
9	Loss of budget funding	Low	High	Not enough funding to complete all tasks	Participate to presentations, conferences	<b>Triggers:</b> reduction in project budget <b>Actions:</b> managerial decision on what can be implemented based on importance of items
10	Unable to make secure connections for data transfer	Low	Medium	Unable to properly test the system using private data	Make sure network equipment at both ends is compatible; ensure high-speed network connections	<b>Triggers:</b> unable to establish VPN connections; connections go down unexpectedly <b>Actions:</b> find alternatives; managerial decision on public data that can be used for testing

■ So far no unexpected problems

■ More risks for the next phases of the project (during/after data import)

## ■ Project's contribution to the goal of the STAR Programme

- By producing a system able to handle large amounts of data, such as those collected by ESA missions, organizations using this new storage and classification system have an advantage for actively participating in the analysis of ESA released data.
- Large scale atomic data calculation and laboratory measurements could provide contribution towards the GREAT-ESA-ESF project supporting spectroscopic studies for GAIA mission.

- Dissemination activities

- Publication of scientific papers:

- “Electron collisions with Fe-peak element CoIV: A computational grand challenge” Rom. Rep. Phys. (2013)
    - “ State selective photo-recombination cross sections in Be-like Al and C ions” The European Physical Journal D (2013)67:223
    - “Complements to the theoretical treatments of the electron collision with Co<sup>3+</sup>: an R-matrix approach” J. of Spectroscopy (2013) ID 820635

- Participation in conferences and presentations:

- Conferința științifică anuală a Programului “Tehnologie Spațială și Cercetare Avansată - STAR” (2013)
    - Conferința științifică anuală a Programului “Tehnologie Spațială și Cercetare Avansată - STAR” (2014)

- A web portal is planned for a later stage of the project

- Conclusions

- Planned activities for the current stage of the project were completed as scheduled
- No outstanding issues were identified at this moment with regard to project implementation