

# Knowledge discovery in astrophysics: massive data sets, virtual observatory and beyond

*astrophysics and the data tsunami*



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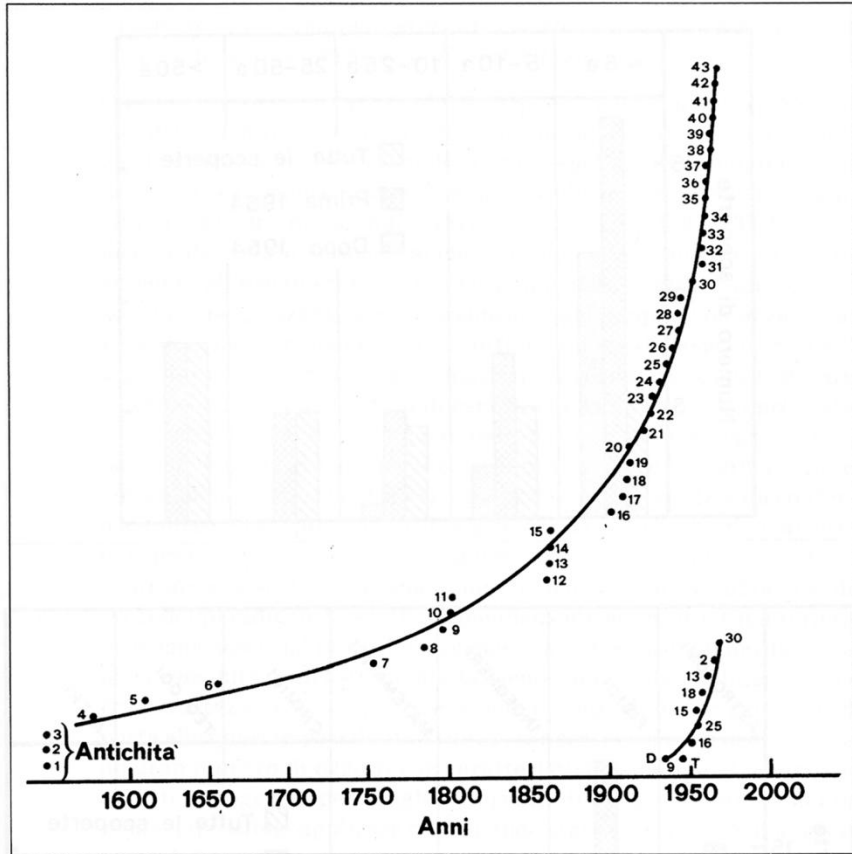
2 - Department of Physical Sciences - University Federico II Napoli

# An overview of the topics:

- Information Technology revolution and science in the exponential world
  - The Virtual Observatory: a new type of a scientific research environment
    - Massive data sets and a new scientific methodology
      - DAME project: Data Mining and Exploration
        - Some general considerations on the future



# Discoveries in astronomy

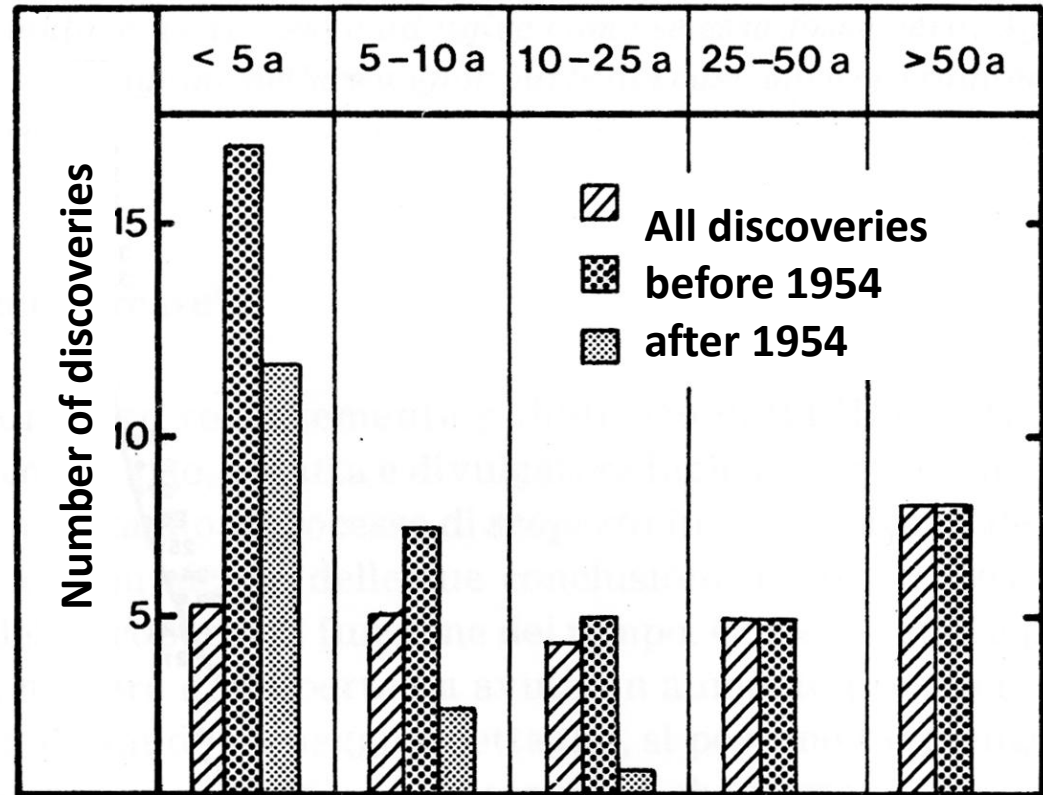


From M. Harwit, *Cosmic discoveries*

1. Stars
2. Planets
3. Novae
4. Comets
5. Satellites
6. Rings
7. Galactic clusters
8. Galaxy clusters
9. Interplanetary dust
10. Asteroids
11. Binary stars
12. Variable stars
13. Planetary nebulae
14. Globular clusters
15. HII regions
16. Cold ISM
17. Giant stars
18. Cosmic rays
19. Pulsating variables
20. White dwarfs
21. Galaxies
22. Expansion of universe
23. Cosmic dust
24. Supernovae/novae
25. Gas in galaxies
26. SN remnants
27. Radiogalaxies
28. Magnetic variables
29. Flare stars
30. Intergalactic magnetic fields
31. X stars
32. X background
33. Quasar
34. CMB
35. Masers
36. Infrared stars
37. X galaxies
38. Pulsar
39. Gamma background
40. IR galaxies
41. Superluminal sources
42. GRB
43. Unidentified radio sources
44. ...
45. ....

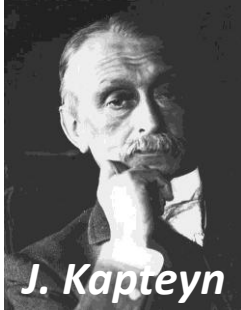
# The role of technology

Most discoveries take place immediately after a technological breakthrough

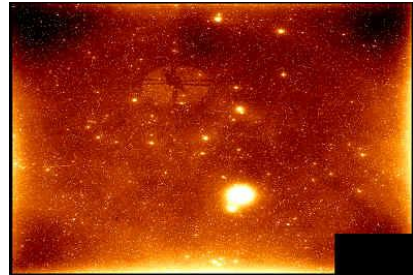


# An historical perspective

**1910**  
Final settling of stellar statistics, by the work of Kapteyn, Oort, etc.)  
**S.I.L.**



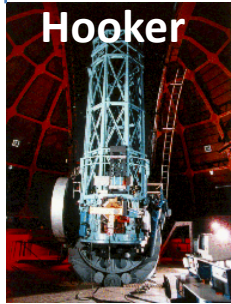
**1960's**  
Photographic wide field plates (PSS)



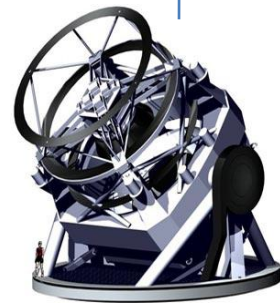
**XXI century**  
Renaissance of statistical astronomy (synoptic surveys)

**Rush for the larger and the bigger**

20's



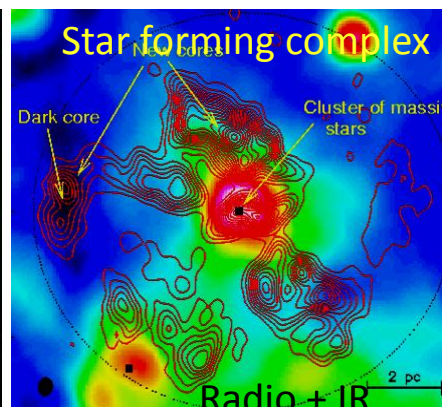
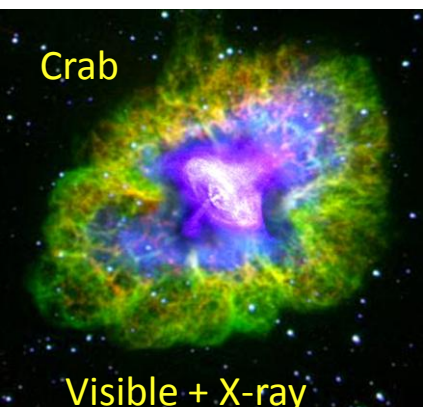
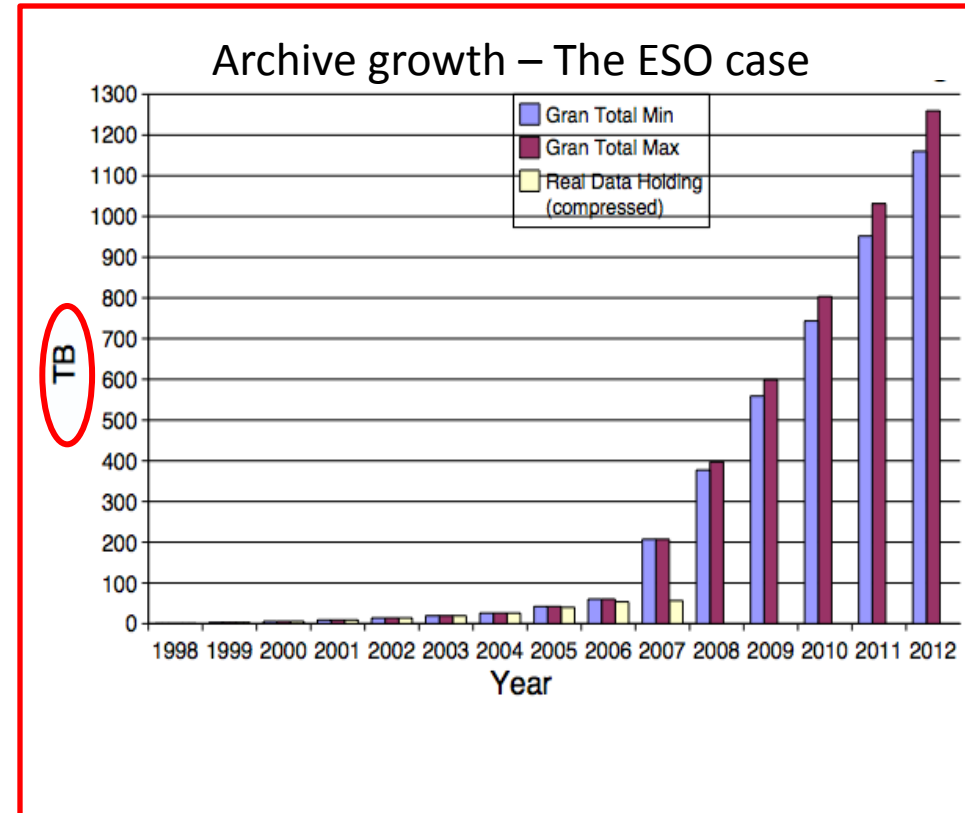
**80's**  
Virtual Obs.



Few objects, few  $\lambda$ 's, heterogeneous data

# Astrophysics as a data rich science

- Telescopes (ground- and space-based, covering the full electromagnetic spectrum)
- Instruments (telescope/band dependent)
- **Large digital sky surveys** are becoming the dominant source of data in astronomy: ~ 10-100 TB/survey (soon PB), ~  $10^6$  -  $10^9$  sources/survey, many wavelengths...
- **Data sets many orders of magnitude larger, more complex, and more homogeneous than in the past**



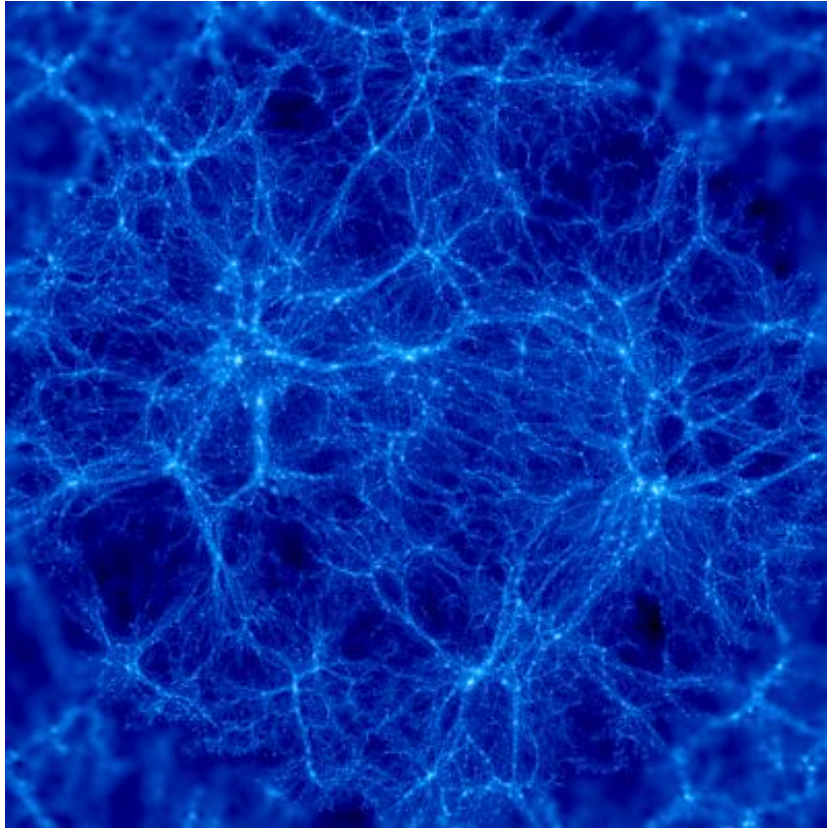
**Panchromatic Views of the Universe:  
Data Fusion - A More Complete, Less Biased  
Picture**



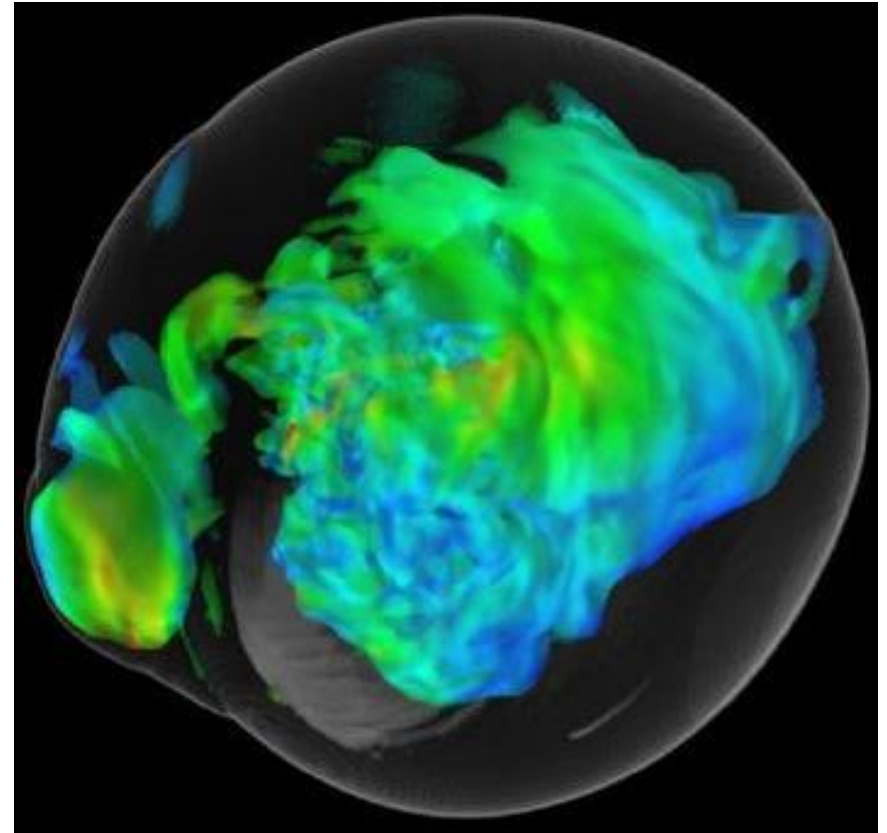


## 2. The astronomical data tsunami:

Theoretical Simulations Are Becoming More Complex and Generate TB's of Data ...



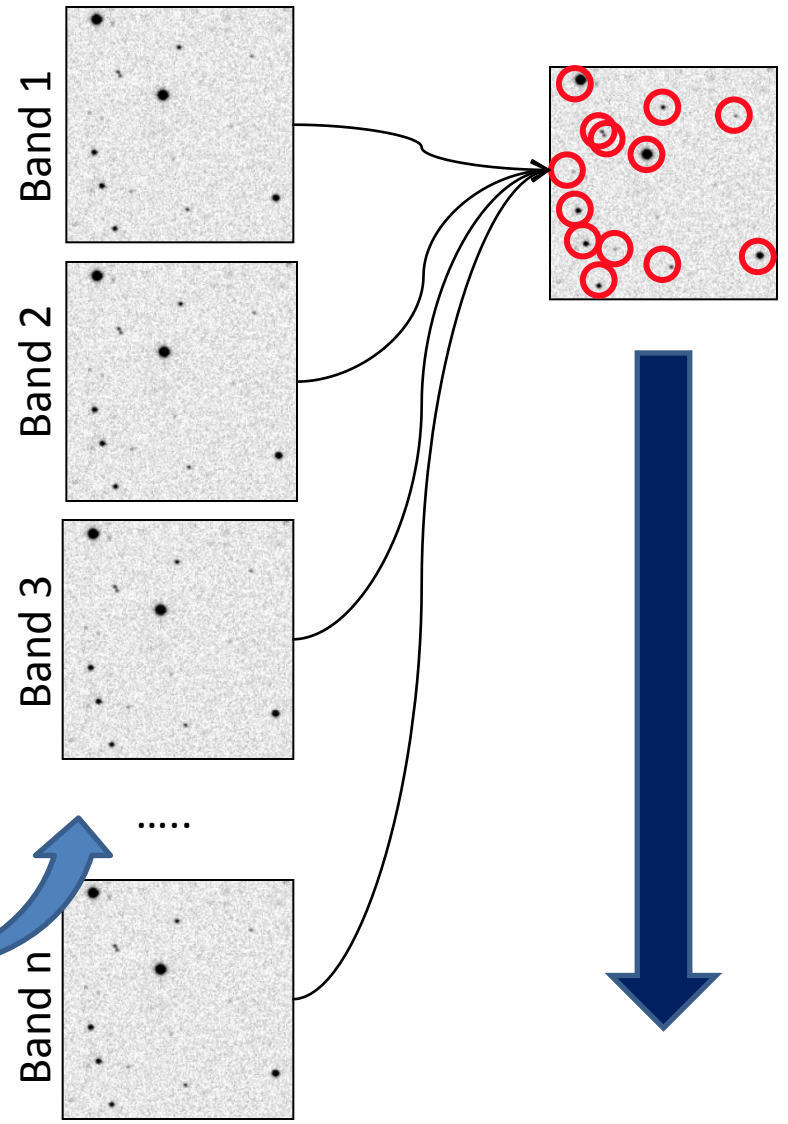
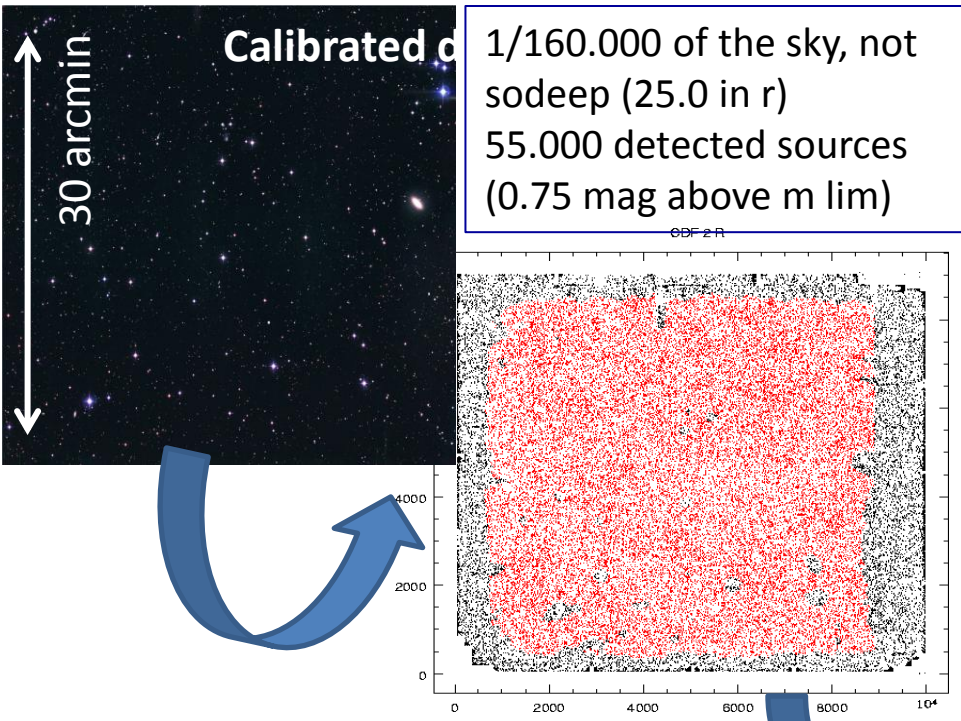
Structure formation in the Universe



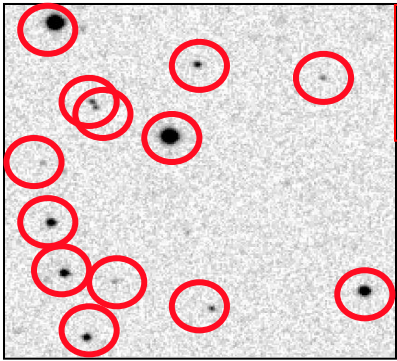
Supernova explosion instabilities

Comparing the massive, complex output of such simulations to equally massive and complex data sets is a non-trivial problem!

# 3. The data complexity: the parameter space



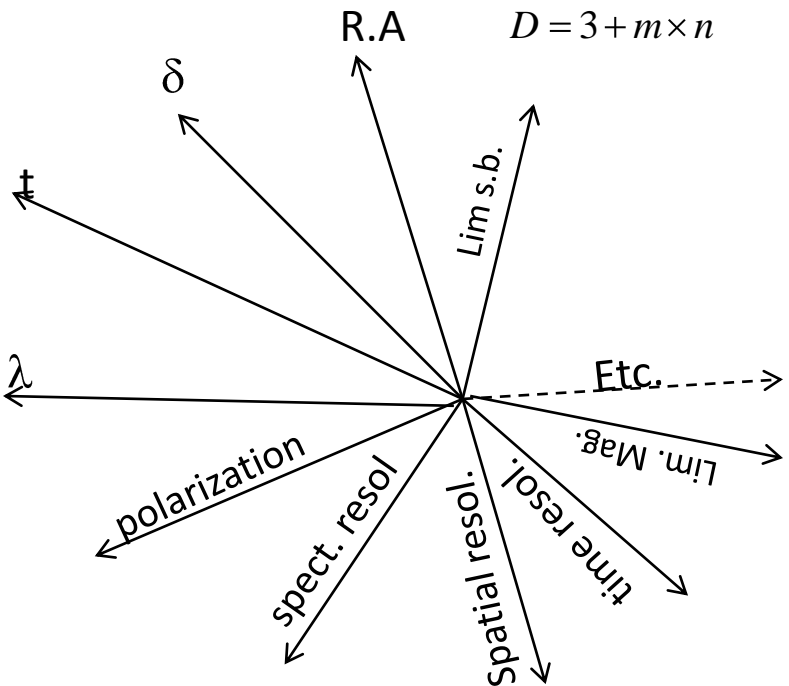




Detect sources and measure their attributes  
(brightness, position, shapes, etc.)

$p = \{\text{isophotal, petrosian, aperture magnitudes, concentration indexes, shape parameters, etc.}\}$

$$\begin{aligned}
 p^1 &= \{R^1, \delta^1, t, \lambda, \Delta\lambda_1, f_1^{1,1}, \Delta f_1^{1,1}, \dots, f_1^{1,m}, \Delta f_1^{1,m}\} \\
 p^2 &= \{R^2, \delta^2, t, \lambda, \Delta\lambda_1, f_1^{2,1}, \Delta f_1^{2,1}, \dots, f_1^{2,m}, \Delta f_1^{2,m}\} \\
 &\dots \\
 p^N &= \{R^N, \delta^N, t, \lambda, \Delta\lambda_1, f_1^{N,1}, \Delta f_1^{N,1}, \dots, f_1^{N,m}, \Delta f_1^{N,m}\} \\
 D &= 3 + m \times n
 \end{aligned}$$



**PARAMETER SPACE**

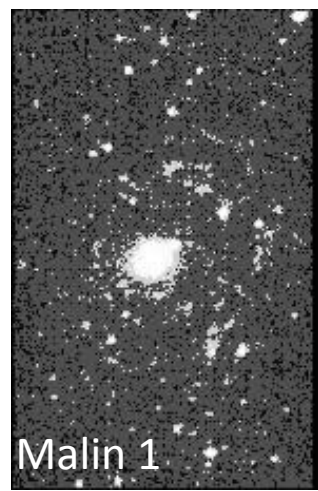
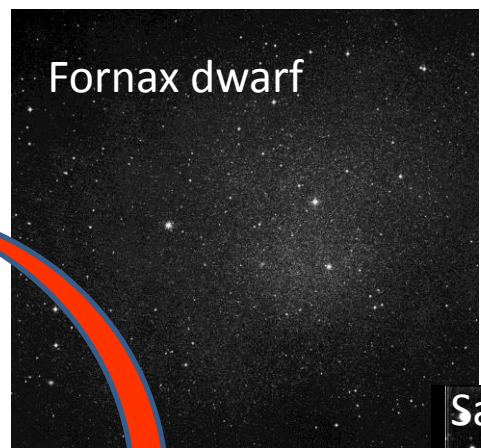
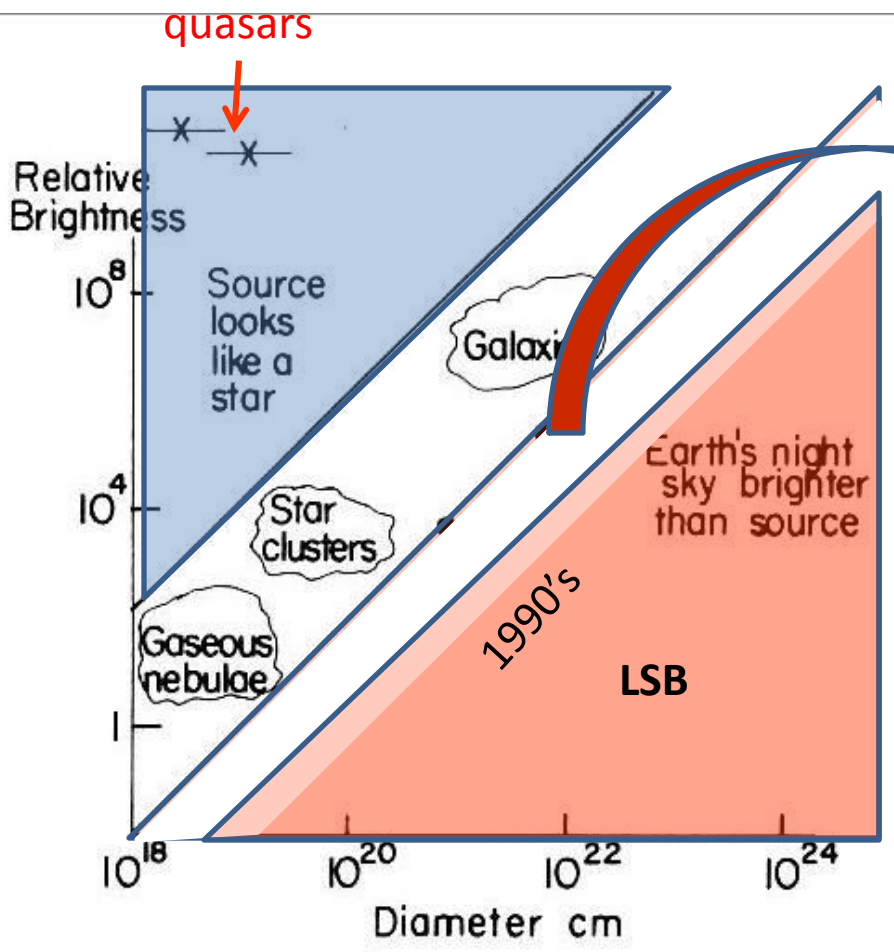
From the Data Mining point of view, any observed (simulated) datum  $p$  defines a point (region) in a subset of  $\mathbb{R}^N$ .

$$p \in \mathbb{R}^N \quad N \gg 100$$



# Every time you improve the coverage of the PS....

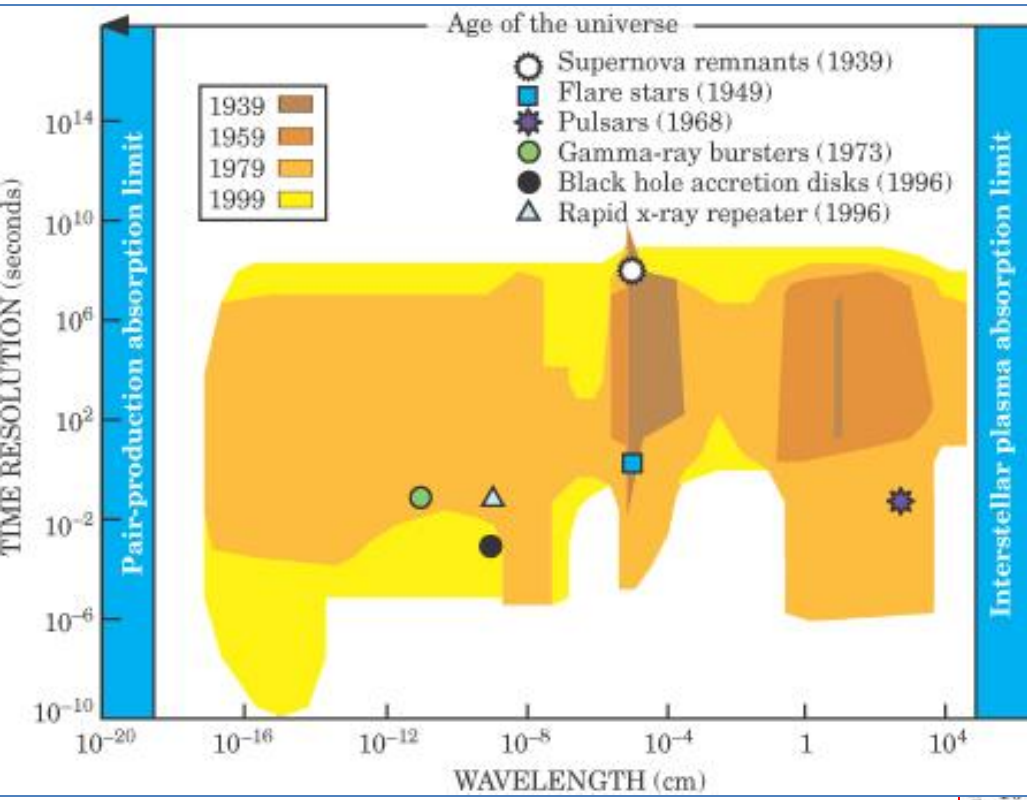
Every time a new technology enlarges the parameter space or allows a better sampling of it, new discoveries are bound to take place



Discovery of Low surface brightness Universe

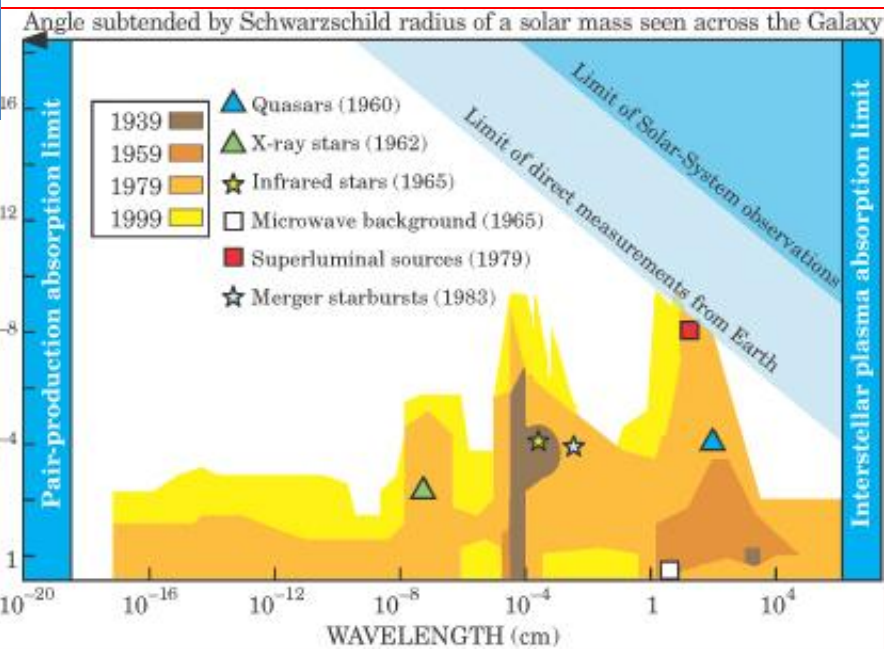


# Improving the coverage of the Parameter Space - II



Projection of parameter space along (time resolution & wavelength)

Projection of parameter space along (angular resolution & wavelength)

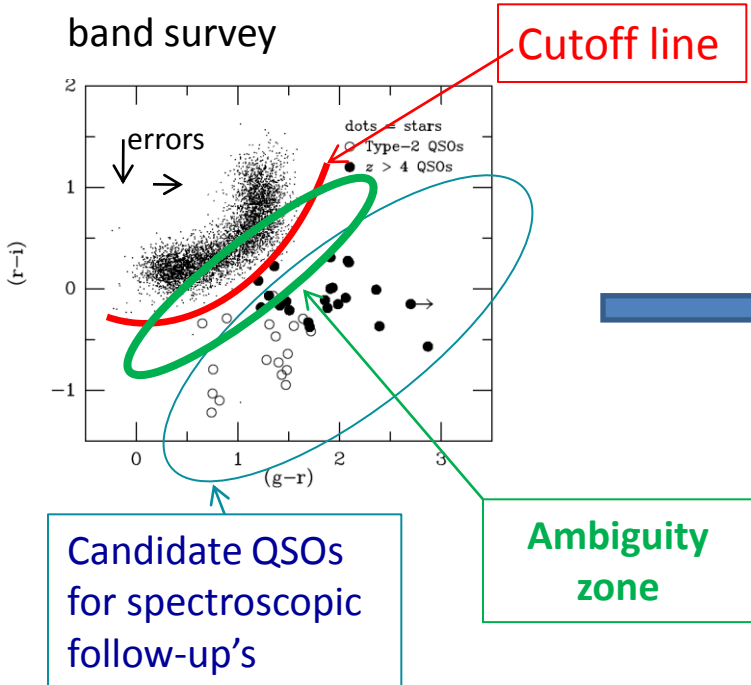


Angle subtended by Schwarzschild radius of a solar mass seen across the Galaxy



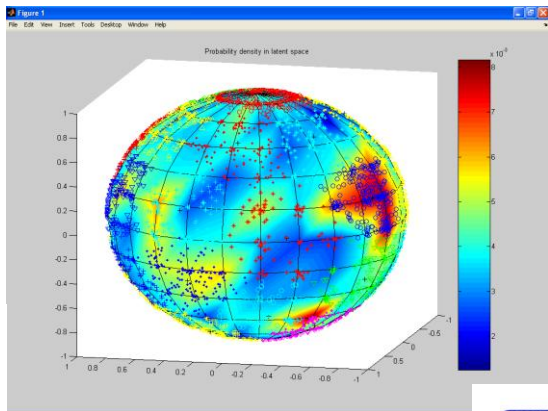
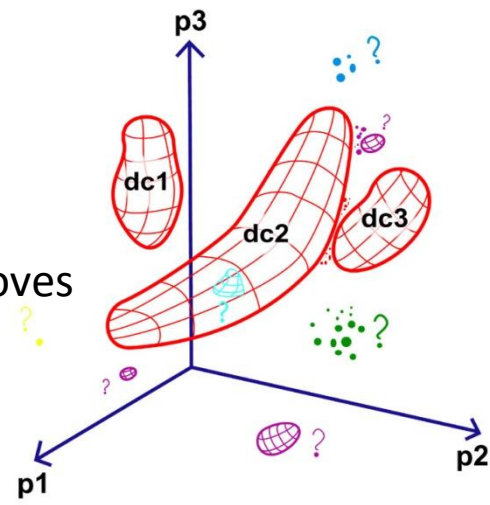
# More dimensions allow better disentanglement

Traditional way to look for candidate QSO in 3 band survey



Adding one feature improves separation...

A Generic Machine-Assisted Discovery Problem: Data Mapping and a Search for Outliers



PPS projection of a 21-D parameter space showing as blue dots the candidate quasars. Notice better disentanglement



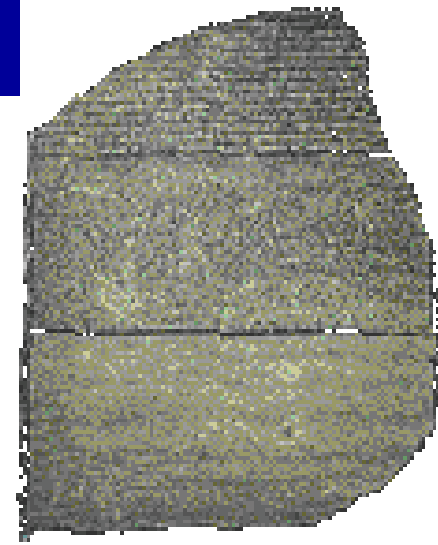


**And now, the question is....**

**Where to search ... for the next discoveries?  
And what has mathematics got to do with it?**

# Considerations on the next breakthroughs

- We have reached the physical limit of observations (single photon counting) at almost all wavelength...
- Detectors are linear & all electromagnetic bands have been opened



## Hence

Our capability to gain new insights on the universe will depend mainly on:

- Capability to recognize patterns or trends in the parameter space (i.e. physical laws) being not limited by human 3-D visualization
- Capability to extract patterns from very large multiwavelength, multiepoch, multi-technique parameter spaces



➔ ***Most data will never be seen by humans!***

The need for data storage, network, database-related technologies, standards, etc.

Information complexity is also increasing greatly

➔ ***Most knowledge hidden behind data complexity is lost***

Most (all) empirical relationships known so far depend on 3 parameters ....  
Simple universe or rather human bias?

➔ ***Most data (and data constructs) cannot be comprehended by humans directly!***

The need for data mining, KDD, data understanding technologies, hyperdimensional visualization, AI/Machine-assisted discovery

# The answer is Data mining ... matching Donald Rumsfeld's epistemology

*There are known knowns,  
There are known unknowns, and  
There are unknown unknowns*

## Classification

Morphological classification of galaxies  
Star/galaxy separation, etc.

## Regression

Photometric redshifts

## Clustering

Search for peculiar and rare objects,  
Etc.

Donald Rumsfeld's  
about Iraqi war



## Extracting knowledge

The scientific exploitation of a multi band, multiepoch (K epochs) universe implies to search for **hidden patterns**, trends, etc. **among N points in a DxK dimensional parameter space**:

**MASSIVE, COMPLEX DATA SETS with:**  
 **$N > 10^9$ ,  $D \gg 100$ ,  $K > 10$**

**The computational cost of Data Mining:**

N = no. of data vectors, D = no. of data dimensions

K = no. of clusters chosen,  $K_{\max}$  = max no. of clusters tried

I = no. of iterations, M = no. of Monte Carlo trials/partitions

K-means:  $K \times N \times I \times D$

Expectation Maximisation:  $K \times N \times I \times D^2$

Monte Carlo Cross-Validation:  $M \times K_{\max}^2 \times N \times I \times D^2$

Correlations  $\sim N \log N$  or  $N^2$ ,  $\sim D^k$  ( $k \geq 1$ )

Likelihood, Bayesian  $\sim N^m$  ( $m \geq 3$ ),  $\sim D^k$  ( $k \geq 1$ )

SVM  $\sim (N \times D)^3$



**Lots of  
computing  
power**





# Need for a new science: Astroinformatics

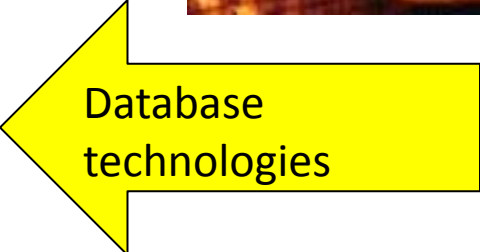
## Knowledge Discovery in Databases



**Data Gathering** (e.g., from sensor networks, telescopes...)

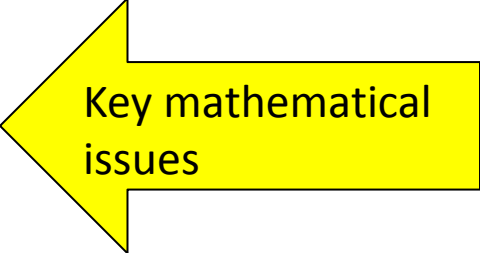
→ **Data Farming:**

- Storage/Archiving
- Indexing, Searchability
- Data Fusion, Interoperability, ontologies, etc.



→ **Data Mining** (or Knowledge Discovery in Databases):

- Pattern or correlation search
- Clustering analysis, automated classification
- Outlier / anomaly searches
- Hyperdimensional visualization



→ **Data understanding**

- Computer aided understanding
- KDD
- Etc.



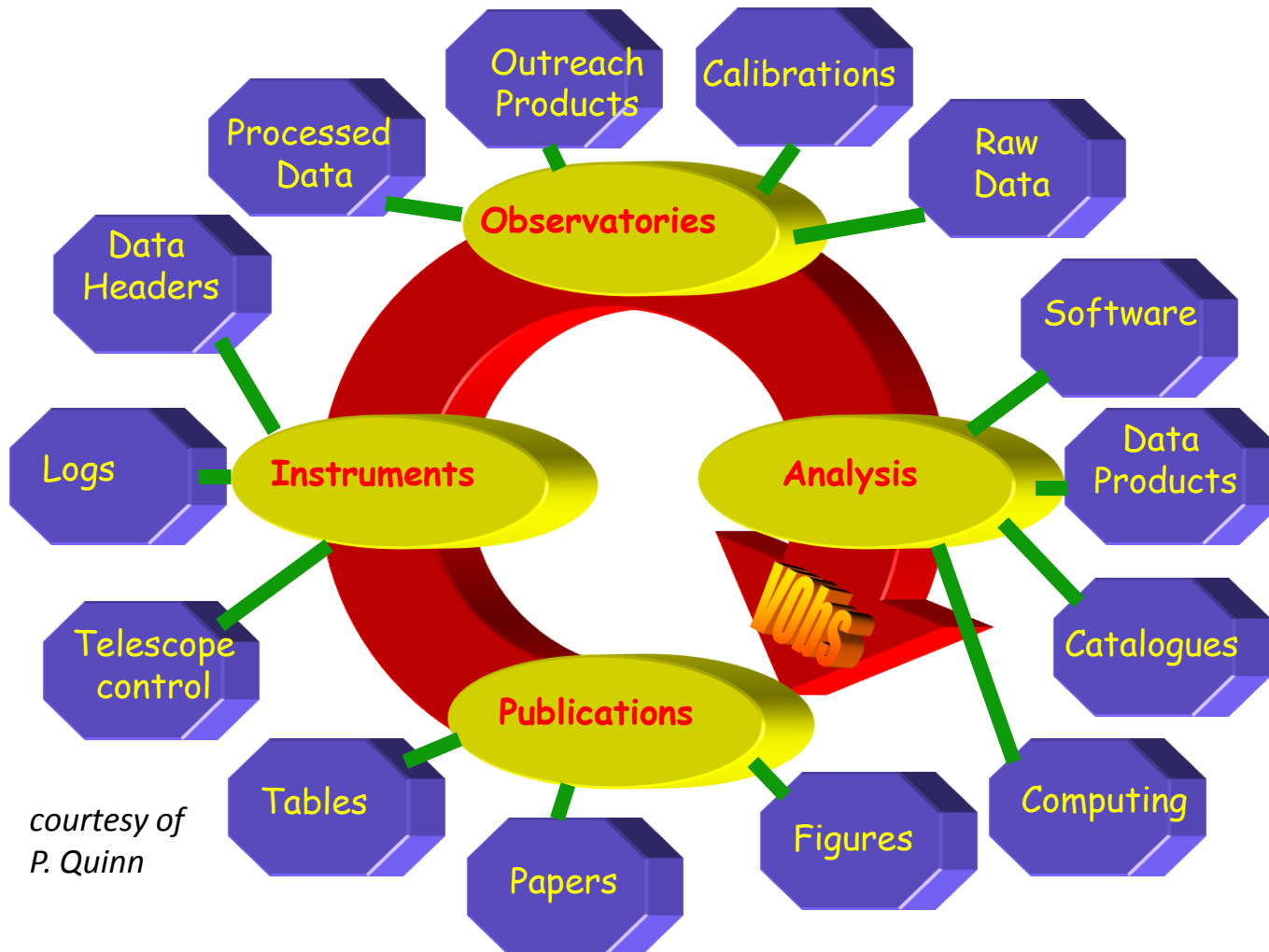
→ **New Knowledge**





# VOBs Represents a New Type of a Scientific Organization for the era of information abundance

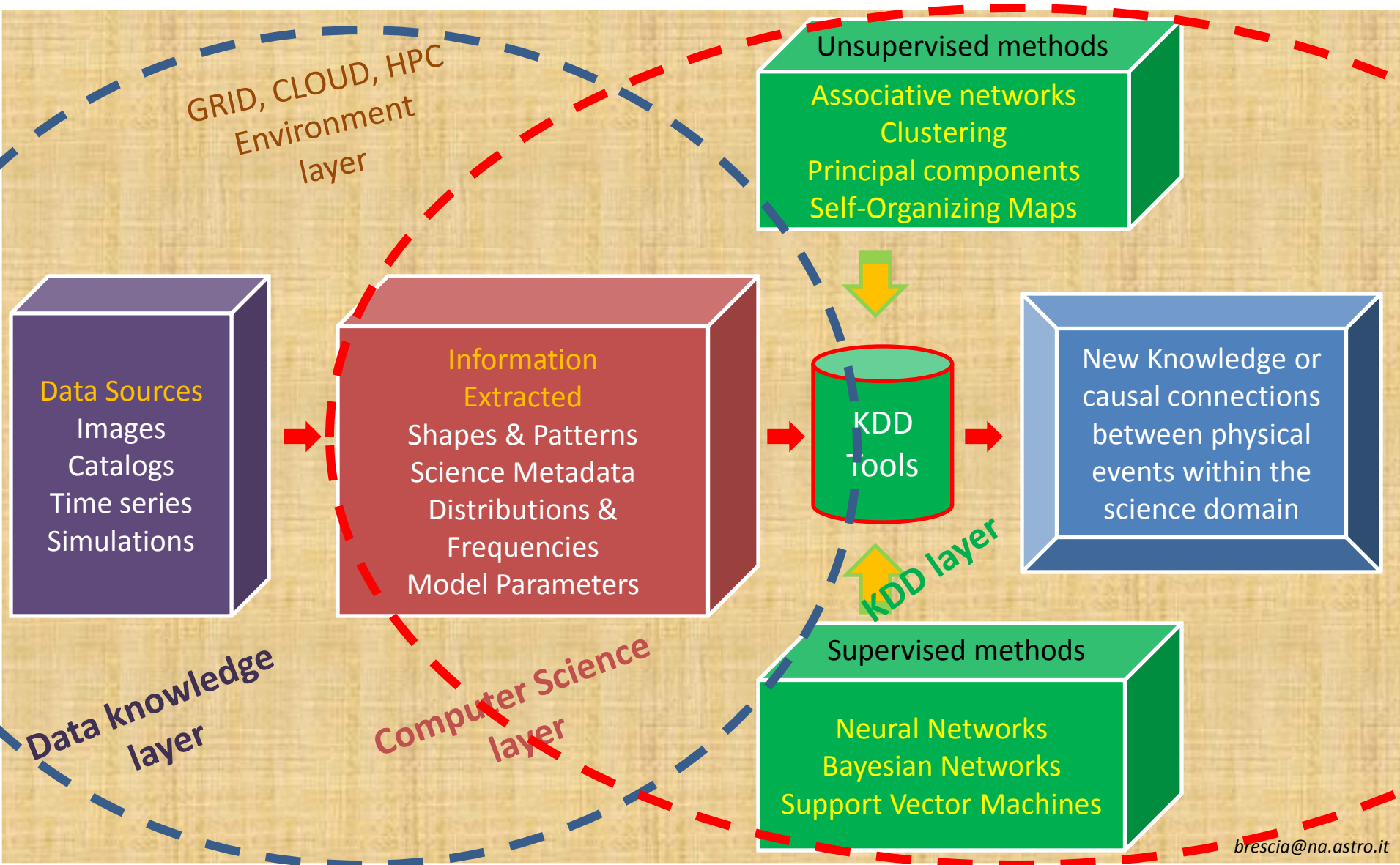
- It is inherently ***distributed***, and web-centric
- It is fundamentally based on a ***rapidly developing technology*** (IT/CS)
- ***It transcends the traditional boundaries*** between different wavelength regimes, agency domains, etc.
- It has an ***unusually broad range of constituents*** and interfaces
- It is inherently ***multidisciplinary***



courtesy of  
P. Quinn

# Vobs standards and infrastructure

## Data mining level





# What is DAME



DAME is a joint effort between University Federico II, INAF-OACN, and Caltech aimed at implementing (as web application) a scientific gateway for data analysis, exploration, mining and visualization tools, on top of virtualized distributed computing environment.

<http://voneural.na.infn.it/>

Technical and management info  
Documents  
Science cases  
Newsletter

<http://dame.na.infn.it/>  
Web application PROTOTYPE

Name	Science case	Mode
pp200	pp200	pp200
PROBABISOR	pp200	pp200
ACQUAZ	pp200	pp200
DM2000	pp200	pp200
MAE	pp200	pp200
pp200	mpregression	mpregression
Test	mpclassification	mpclassification
India	pp200	pp200

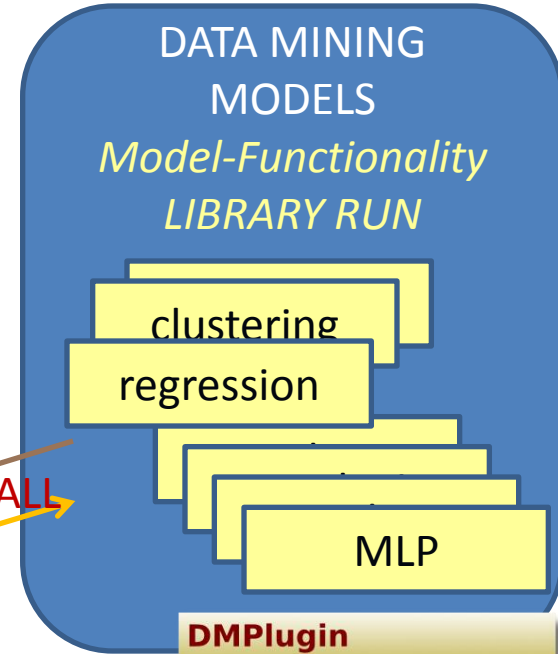
# The DAME architecture



*user*



Client-server AJAX  
(Asynchronous JAVa-  
XML) based;  
interactive web app  
based on Javascript  
(GWT-EXT);



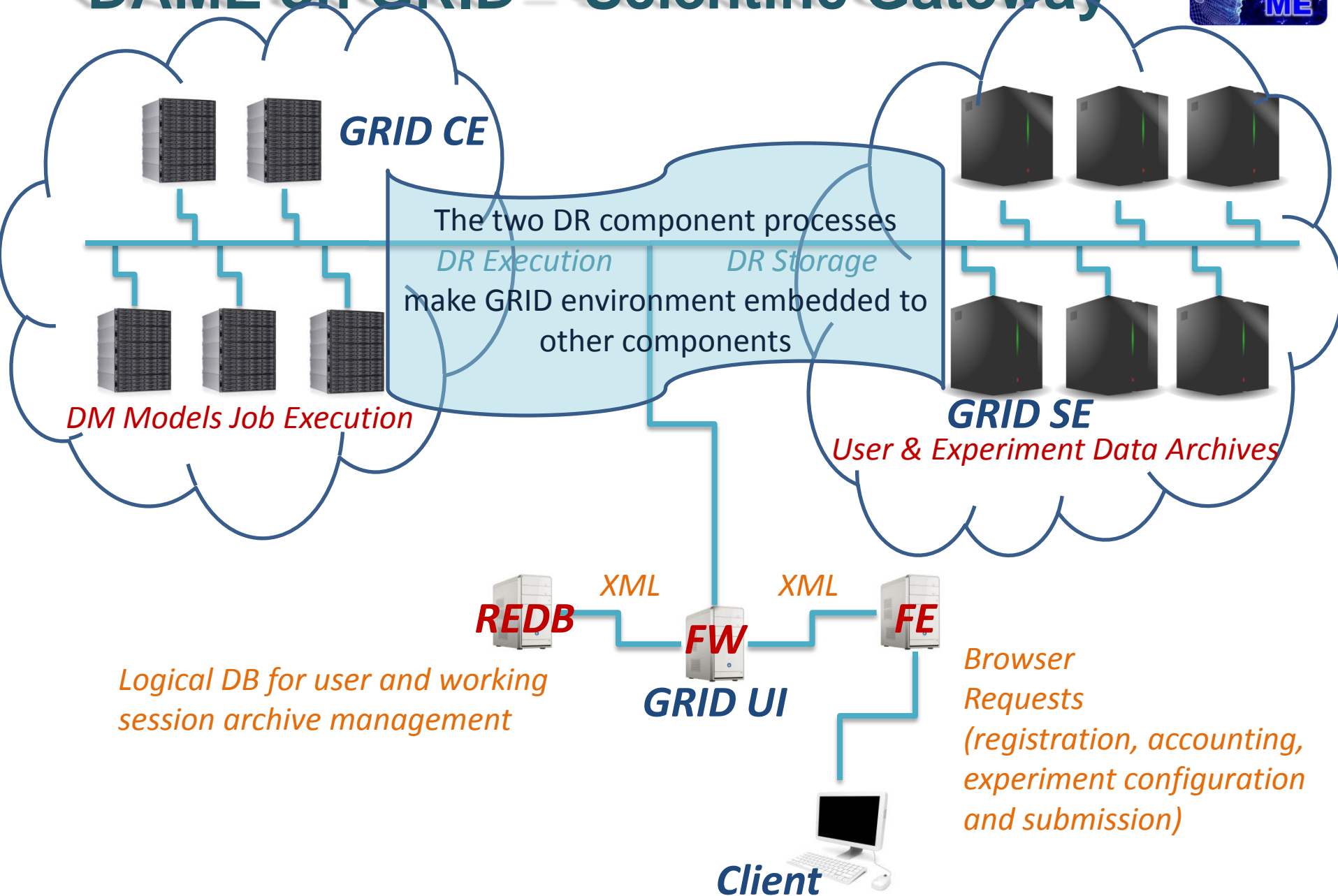
HW env virtualization;  
Storage + Execution LIB  
Data format conversion



Restful, Stateless Web Service  
experiment data, working  
flow trigger and supervision  
Servlets based on XML  
protocol



# DAME on GRID – Scientific Gateway



# How to spread the word within the community

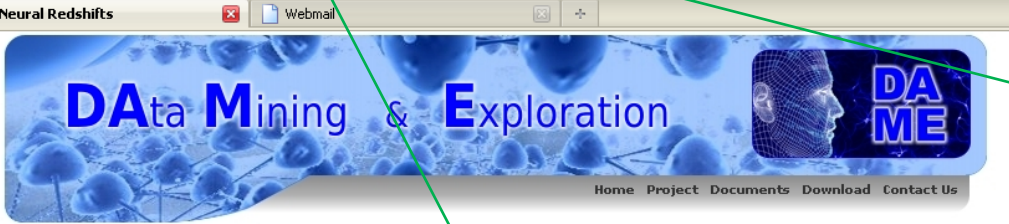
In parallel with the Suite R&D process, all data processing algorithms (foreseen to be plugged in) have been massively tested on real astrophysical cases.

<http://voneural.na.infn.it/>

Technical and management info

Documents

Science cases



Links

- Shakbazian groups in the SDSS
- Photometric redshift for SDSS galaxies
- Documents
- Public Outreach
- Science Papers

## A method for the extraction of photometric QSOs candidates

In this page, you will find a description of the method for the extraction of photometric QSOs candidates described in the paper "Quasar candidates selection in the Virtual Observatory era" from D'Abrusco et al. submitted to MNRAS (preprint).

The inspiring principle of this work is the application of statistical and data-mining techniques to obtain a clustering of astronomical sources inside a photometric parameter space and fully characterize the distribution of different types of sources inside this parameter space. This concept has been applied to the problem of the selection of QSOs candidates from broadband photometric data by exploiting the availability of large spectroscopic bases of knowledge (BoK: i.e., samples of sources with a reliable classification).

The procedure for the extraction of candidates can be summarized as follows:

- A BoK consisting of a sample of stellar sources with spectroscopic classification is clustered inside the colour parameter space. This BoK is drawn from the catalogue of photometric sources from where, at the end of the process, the new QSOs candidates will be extracted.
- Several possible partitions of the distribution of sources of the BoK inside the colour space are produced by a combination of two clustering algorithms: PPS and NEC.
- The members of each cluster of each different partition are labelled using the BoK classification.
- Amongst all the possible partitions in the colour space, the one allowing the best separation between clusters populated mainly by confirmed QSOs ("successful" clusters) and clusters populated mainly by contaminants is considered.
- The new candidates QSOs are selected as the photometric sources which are associated, in the colour space, to the "successful" clusters by a suitable distance definition.

The details of the method and algorithms can be found in the paper.

The catalogues of QSOs candidates extracted from the SDSS DR7 photometric survey can be downloaded [here](#).

Links

- Shakbazian groups in the SDSS
- QSO candidates in the SDSS
- Documents
- Public Outreach
- Science Papers

## Evaluation of photometric redshifts using neural networks

Download the catalogues!

The work discussed here represents the natural evolution of a previous attempt described in these pages and presented in the 2002 and 2003 papers. The final result, namely the redshifts for a large subsample of the galaxies present in the SDSS are downloadable [here](#). This work was part of the Ph.D. Thesis of Raffaele D'Abrusco and has been published in *Ap.J* (2007).

The main idea behind the work is to exploit the huge data wealth of the SDSS to train a supervised neural network to recognize photometric redshifts. The details of the work can be found in this paper. In short the procedure can be summarized as it follows:

- The training, validation and test sets are built using the SDSS spectroscopic subsample. This sample is almost complete at  $m(R) < 17.7$ , while for fainter magnitudes it includes mainly Luminous Red Galaxies or LRG's.
- A first MLP is trained at recognizing nearby ( $z < 0.25$ ) objects from distant ( $0.25 < z < 0.5$ ) ones.
- Then two networks are trained in the two different redshift ranges and the optimal architecture is found by varying the NN parameters
- The resulting redshifts show a trend which is corrected by applying an interpolative correction.
- Once the three NN have been trained the photometric data are processed for the whole galaxy sample and the photometric redshifts are derived.

The whole procedure outlined above is repeated independently for all objects in the MAIN GALAXY sample of the SDSS and for the LRG's only. The resulting catalogues can be downloaded [here](#).

The main results can be summarized as it follows.

1. The method leads to an r.m.s. error (evaluated on the test set only) better than any other method so far appeared in the literature.

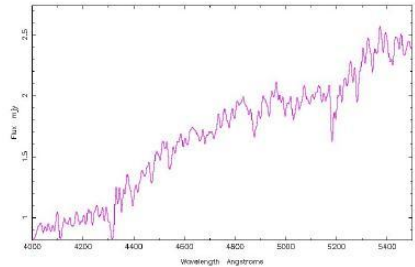
Reference	Method	Data	$\Delta z$	$\sigma$	Range
Csabai et al. (2003)	SED fitting CWW	EDR		0.0621	
Csabai et al. (2003)	SED fitting BC	EDR		0.0509	
Csabai et al. (2003)	interpolative	EDR		0.0451	
Csabai et al. (2003)	bayesian	EDR		0.0402	
Csabai et al. (2003)	empirical, polynomial fit	EDR		0.0318	
Csabai et al. (2003)	K-D tree	EDR		0.0254	
Suchkov et al. (2005)	Class X	DR-2		0.0340	
Way & Srivastava (2006)*	Gaussian Process	DR-3		0.0230	



# An EXAMPLE: photometric redshifts of SDSS galaxies

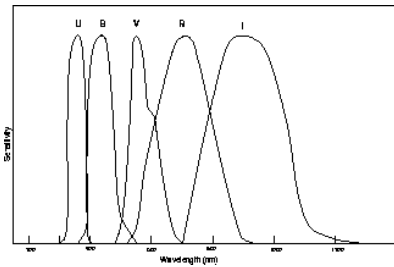


$$z \times c \equiv \frac{\Delta \lambda}{\lambda_0}$$



Galaxy spectrum -  $F(\lambda)$

**X**



Photometric system -  $S_i(\lambda)$

**=**

$$m_U = -2.5 \log_{10} \frac{\int F(\lambda) S_U(\lambda) d\lambda}{\int S_U(\lambda) d\lambda} + c_U$$

$$m_B = -2.5 \log_{10} \frac{\int F(\lambda) S_B(\lambda) d\lambda}{\int S_B(\lambda) d\lambda} + c_B$$

Etc...

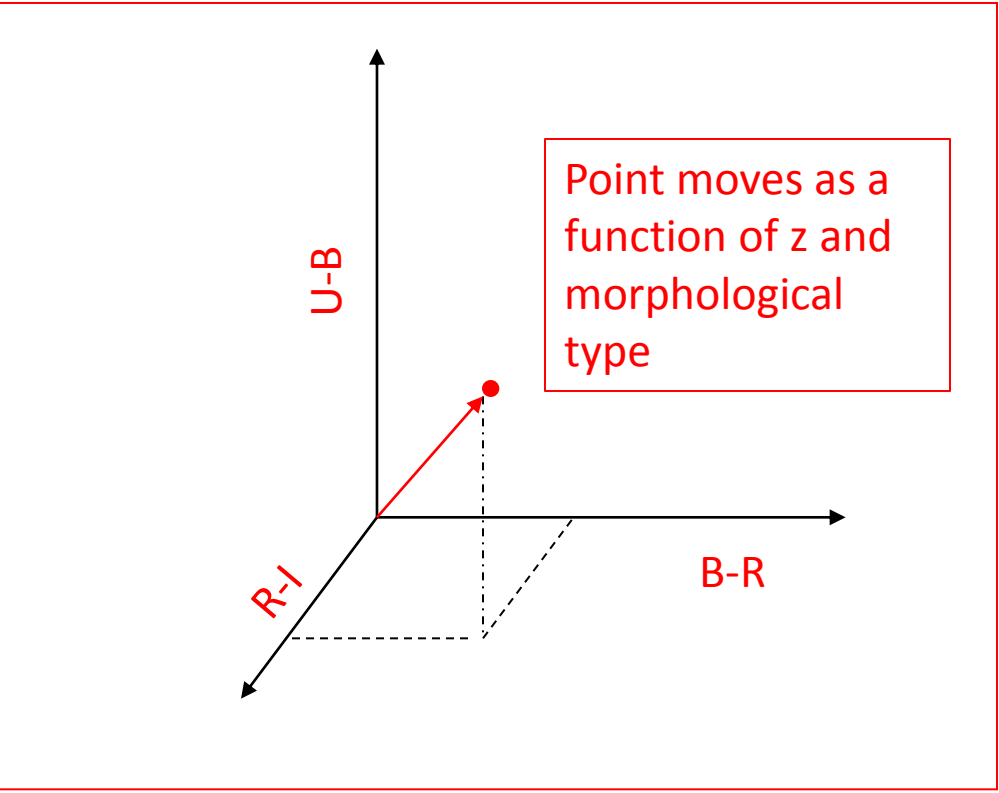


**Color indexes**

$U - B \equiv m_U - m_B$

$B - R \equiv m_B - m_R$

*etc.*



**Phot-z are an inverse problem**

# Photometric redshifts: the DM approach



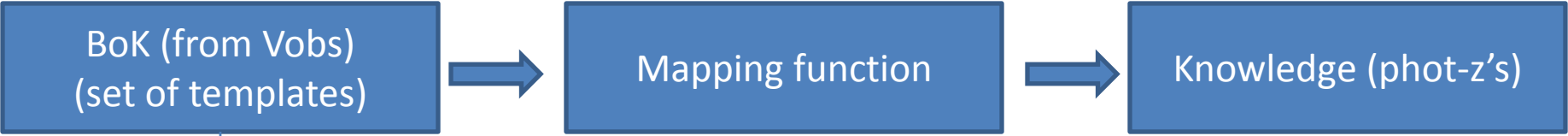
Photometric redshifts are always a function approximation hence a DM problem:

$\mathbf{X} \equiv \{x_1, x_2, x_3, \dots, x_N\}$  input vectors

$\mathbf{Y} \equiv \{y_1, y_2, y_3, \dots, y_M\}$  target vectors  $M \ll N$

**BoK = Base of Knowledge**

find  $\hat{f}: \hat{\mathbf{Y}} = \hat{f}(\mathbf{X})$  is a good approximation of  $\mathbf{Y}$



Observed Spectroscopic Redshifts

Synthetic colors from theoretical SEDs

Synthetic colors from observed SED's

.....

Knowledge always reflects the biases in the BoK.

**Interpolative**  
Uneven coverage of parameter space

**SED fitting**  
Unknown or oversimplified physics  
Unjustified assumptions

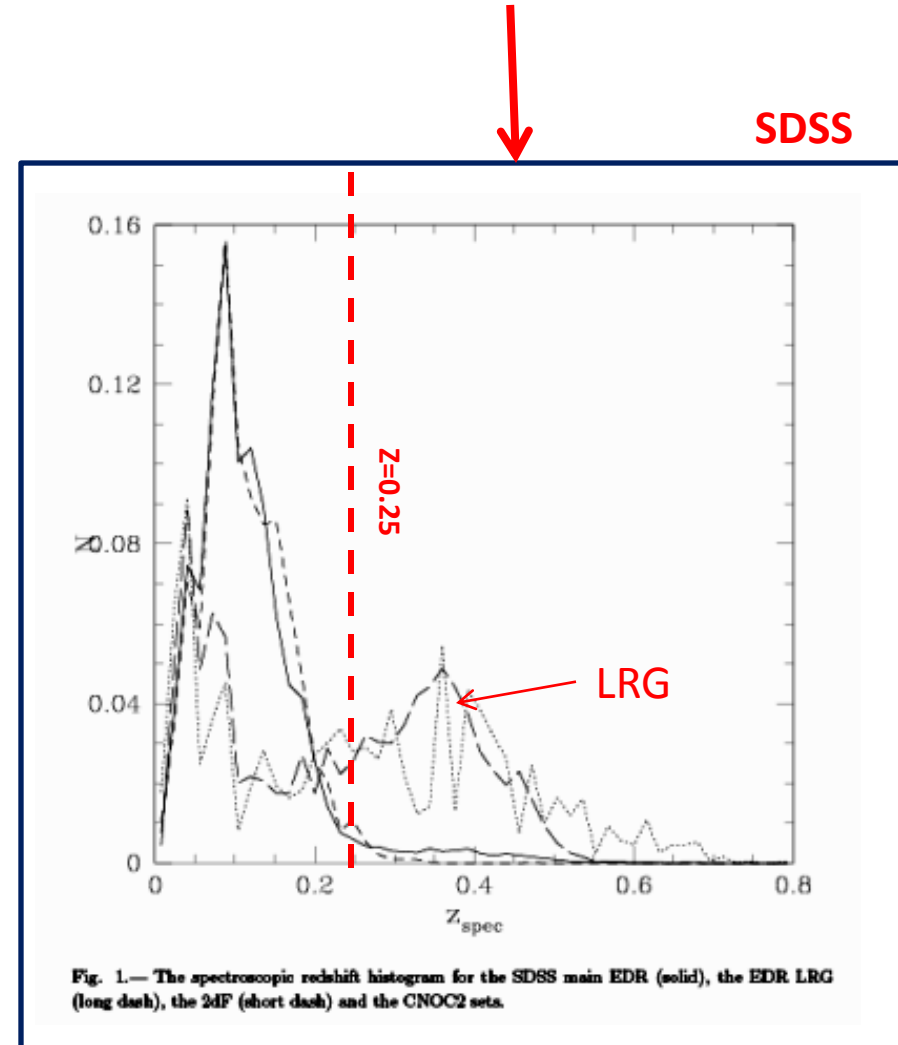
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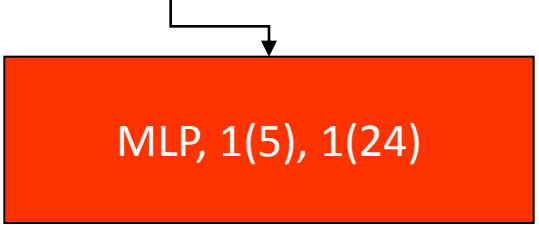
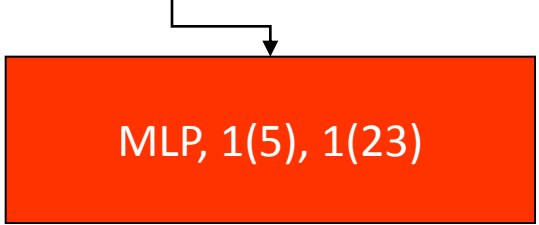
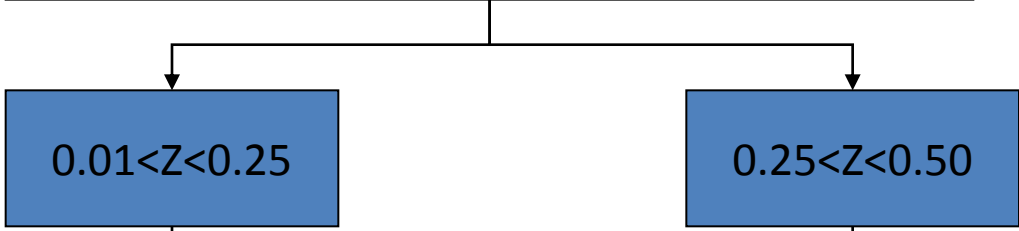
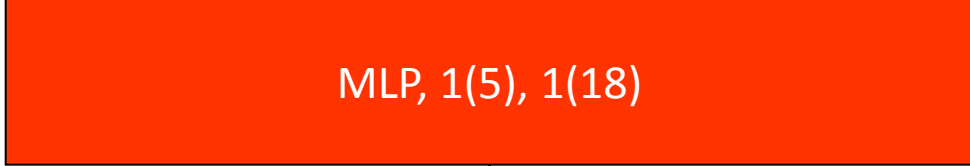
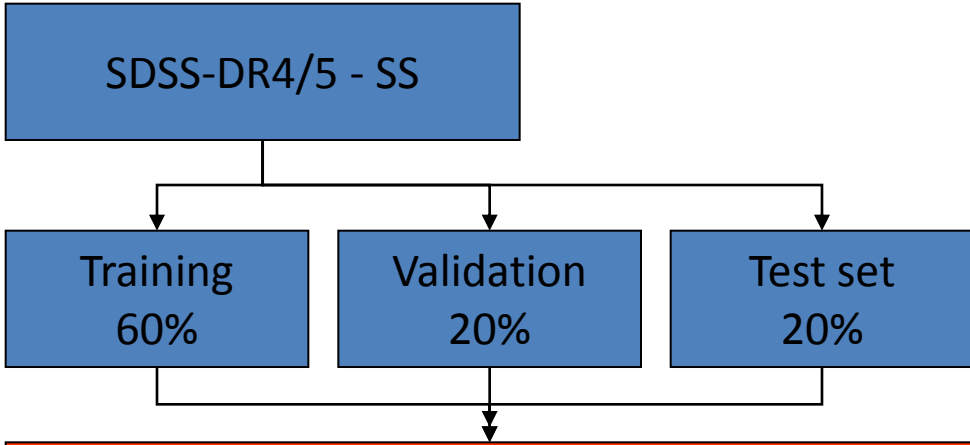
# Data used in the science case:

**SDSS:**  $10^8$  galaxies in 5 optical bands;  
 BoK: spectroscopic redshifts for  $10^6$  galaxies → **Spectroscopic BoK**  
 BoK: incomplete and **biased**.

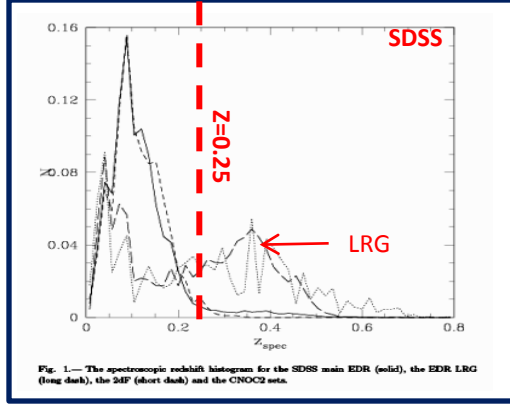
**UKIDSS: overlap with SDSS**  
 3 infrared bands.

**GALEX: overlap with SDSS**  
 Ultraviolet bands;

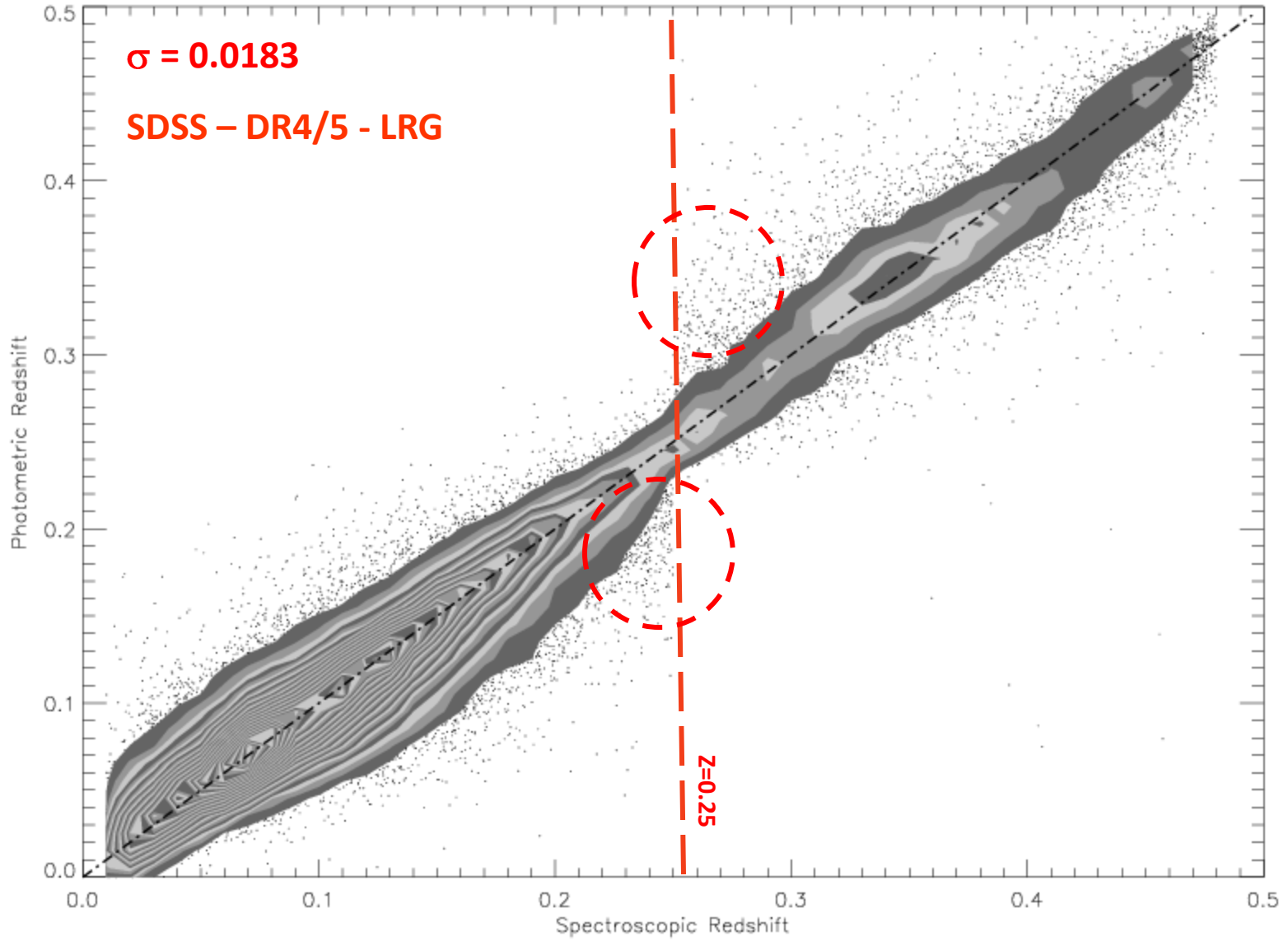




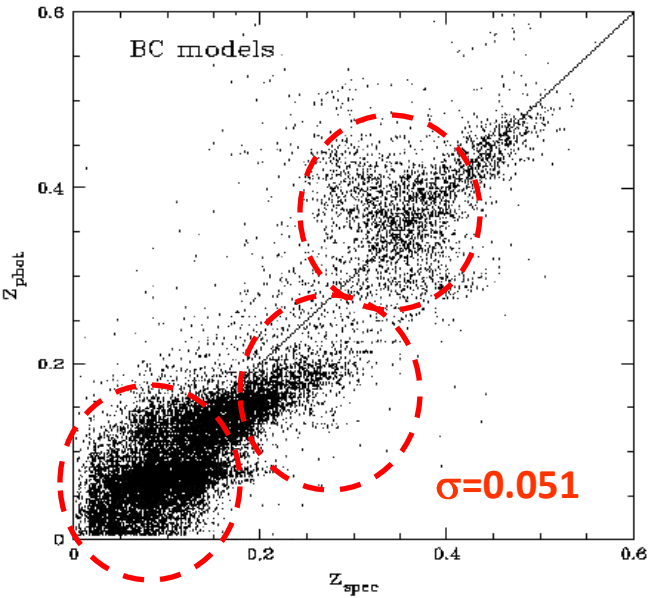
→ 99.6 % accuracy





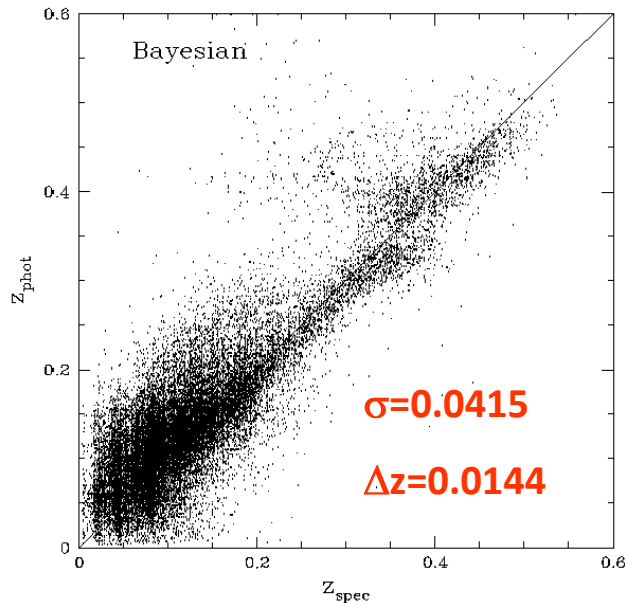


# Traditional approaches: interpolation based on BoK



## BoK from Spectral Energy Distribution (SED) fitting

Templates from synthetic colors obtained from theoretical SED's  
Mapping function from simple interpolation



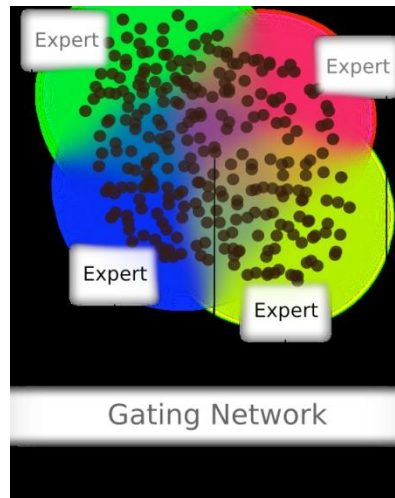
## BoK from Spectral Energy Distribution (SED) fitting Interpolative

Templates from synthetic colors obtained from theoretical SED's  
Mapping function from Bayesian inference



# What do we learn if the BoK is biased:

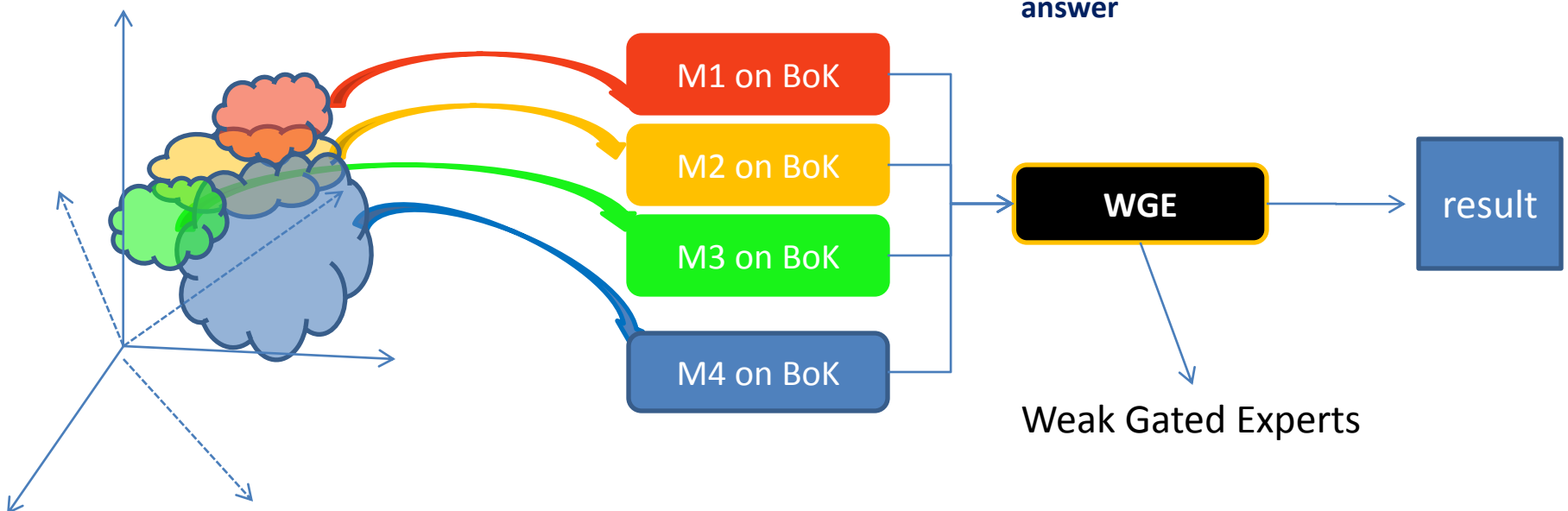
- At high z LRG dominate and interpolative methods are not capable to “generalize” rules
- An unique method optimizes its performances on the parts of the parameter space which are best covered in the BoK

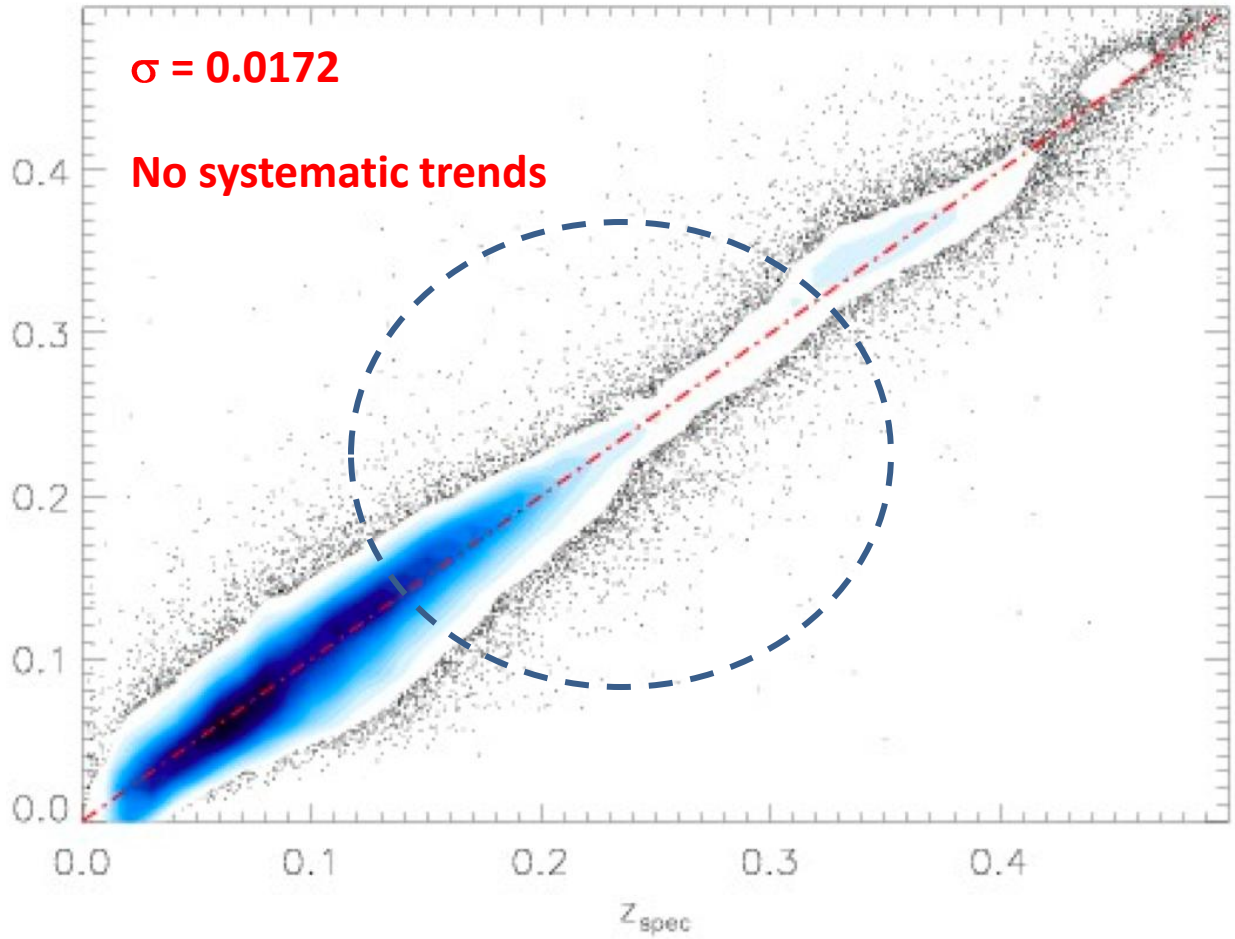
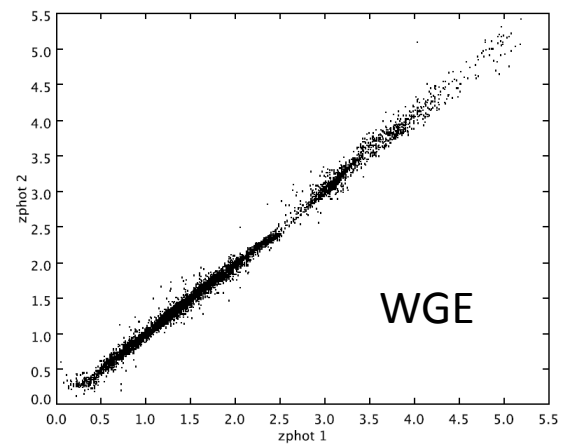
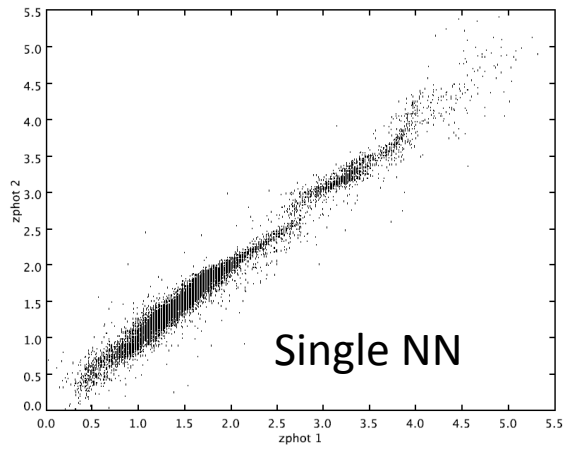


**Step 1:**  
unsupervised clustering in parameter space

**Step 2:**  
supervised training of different NN for each cluster

**Step 3:**  
output of all NN go to WGE which learns the correct answer

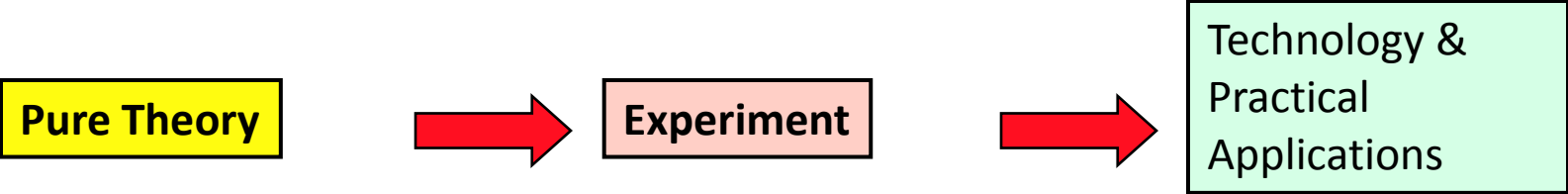




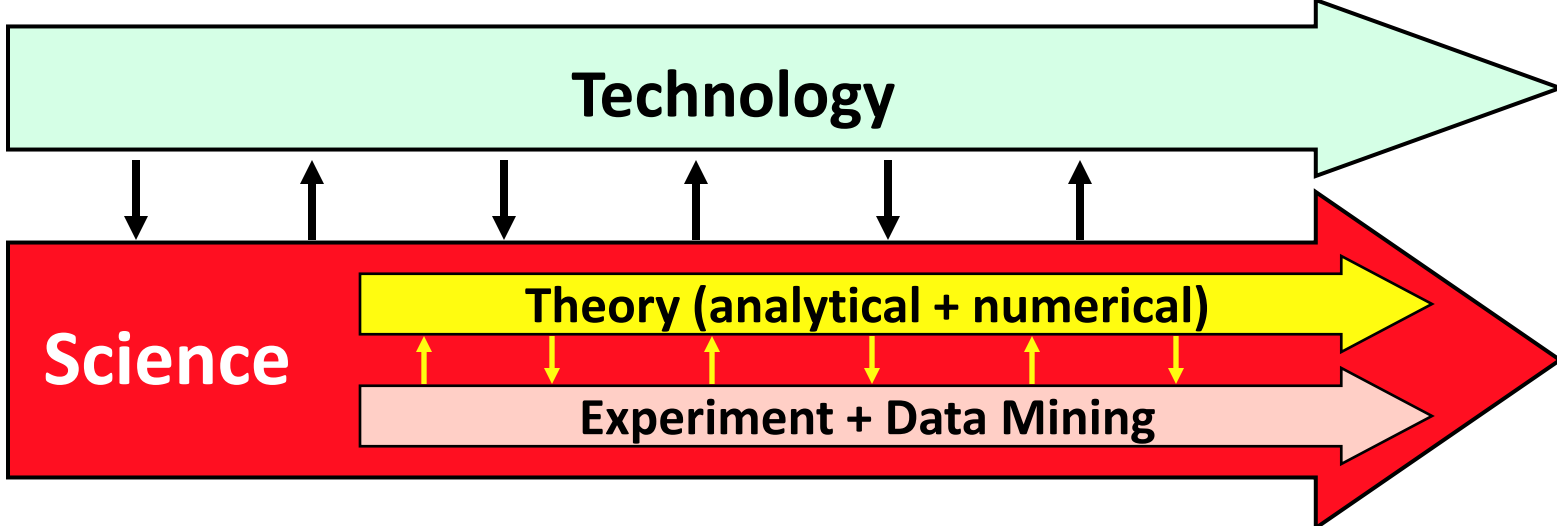


# Conclusion I. I.T. is changing the methodology of science

The old traditional, "Platonistic" view:



The modern and realistic view when dealing with complex data sets:



This synergy is stronger than ever and growing

# Open problems to be addressed soon:

- Scalability
- Robustness
- Reliability
- Choice of optimal models
- Connection: semantics -> Ontologies -> Bases of knowledge
- Visualization

# Algorithms

**Restricted choice of algorithms (MLPs, SVM, Kernel methods, Genetic algorithms (few models), K Means, PPS, SOM ...)**

*Astronomers know little statistics, forget about SPR, DM, etc... Just a few astronomers go beyond the introductory chapters of the Bishop.*

Tagliaferri et al. 2003	Ball & Brunner 2009	BoK
S/G separation	S/G separation	Y
Morphological classification of galaxies ( <i>shapes, spectra</i> )	Morphological classification of galaxies ( <i>shapes, spectra</i> )	Y
Spectral classification of stars	Spectral classification of stars	Y
Image segmentation	-----	
Noise removal ( <i>grav. waves, pixel lensing, images</i> )	-----	
Photometric redshifts ( <i>galaxies</i> )	Photometric redshifts ( <i>galaxies, QSO's</i> )	Y
Search for AGN	Search for AGN and QSO	Y
Variable objects	<b>Time domain</b>	
Partition of photometric parameter space for specific group of objects	Partition of photometric parameter space for specific group of objects	Y
Planetary studies (asteroids)	Planetary studies (asteroids)	Y
Solar activity	Solar activity	Y
<b>Interstellar magnetic fields</b>	----	
<b>Stellar evolution models</b>	----	



# Limited number of problems due to limited number of reliable BoKs

## Bases of knowledge

*(set of well known templates for supervised (training) or unsupervised (labeling) methods)*

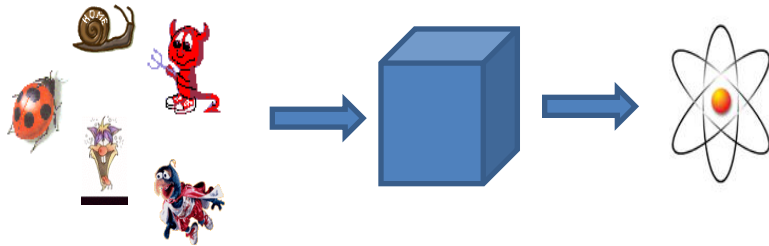
### So far

- Limited number of BoK (and of limited scope) available
- Painstaking work for each application (es. spectroscopic redshifts for photometric redshifts training).
- Fine tuning on specific data sets needed (e.g., if you add a band you need to re-train the methods)

# Bases of knowledge need to be built automatically from Vobs Data repositories

## Community believes AI/DM methods are black boxes

*You feed in something, and obtain patters, trends, i.e. knowledge....*

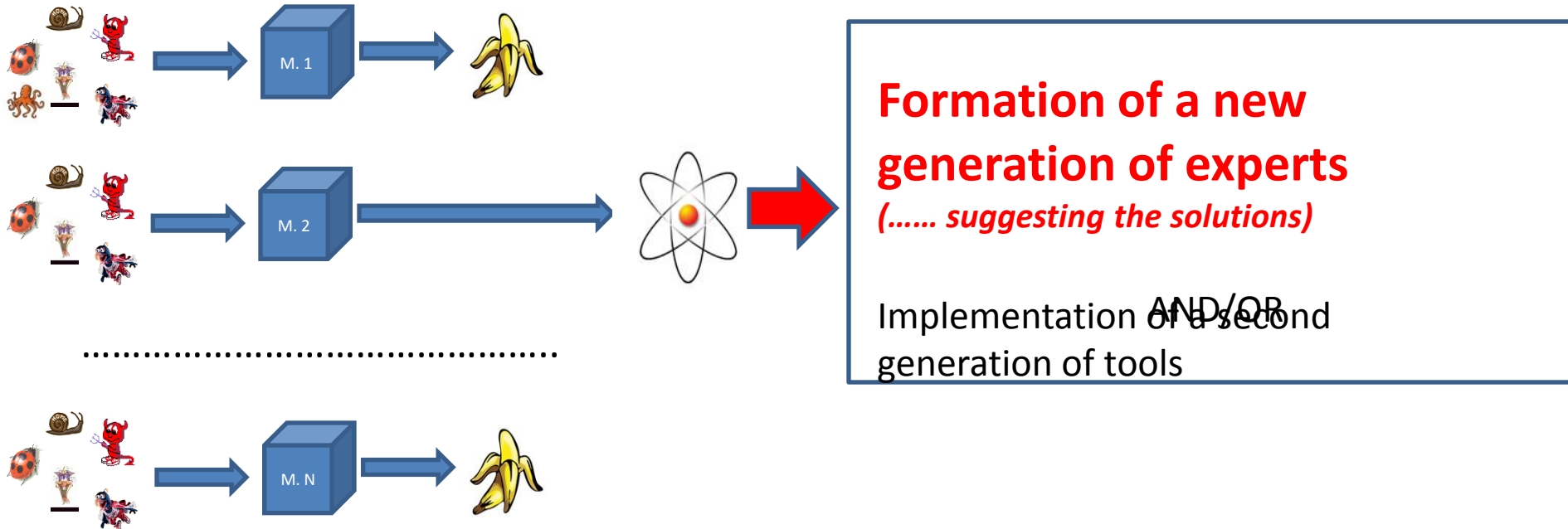




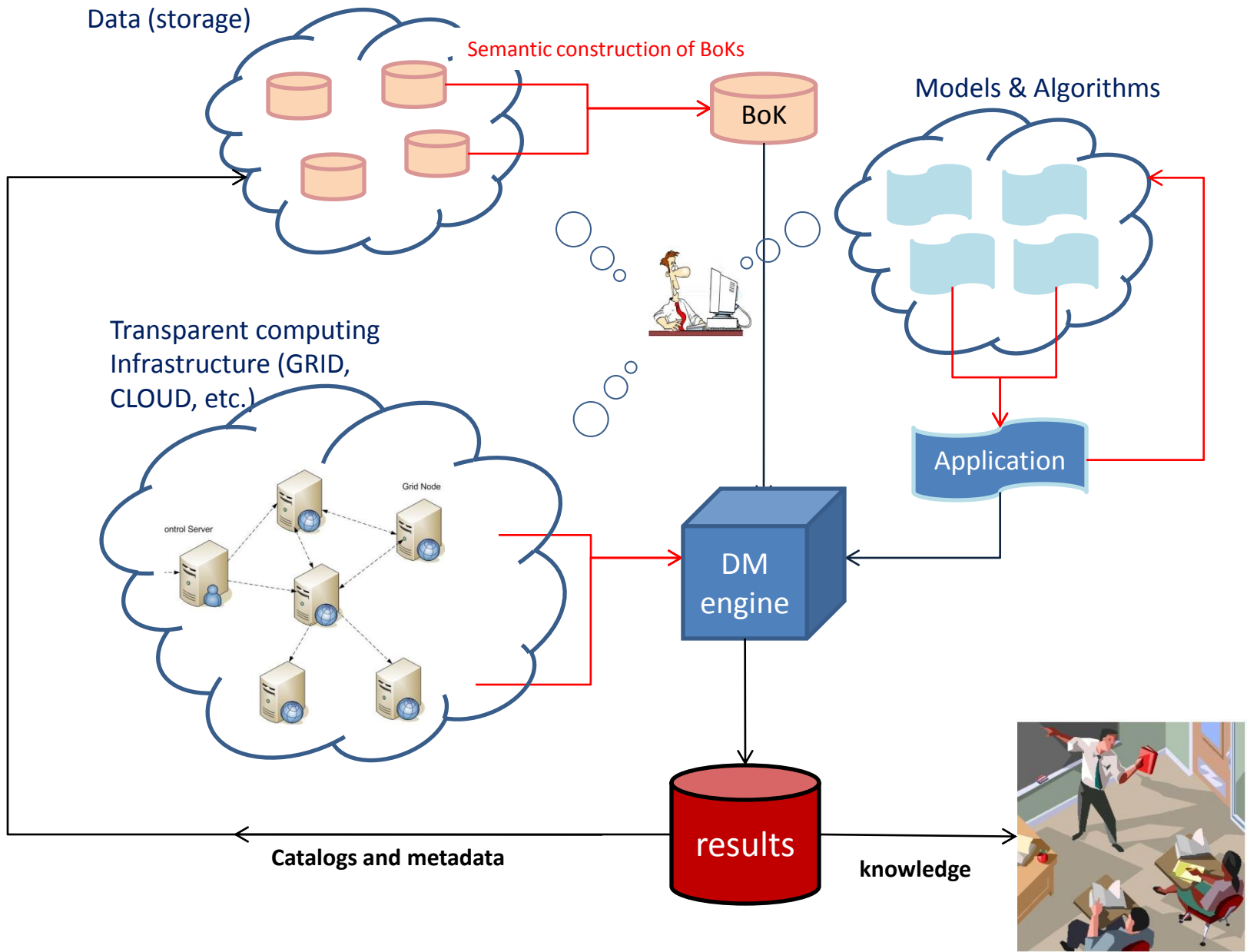
Exposed to a wide choice of algorithms to solve a problem, the r.m.s. astronomer usually panics and is not willing to make an effort to learn them ...

The r.m.s astronomer doesn't want to become a computer scientist or a mathematician (large survey projects overcome the problem)

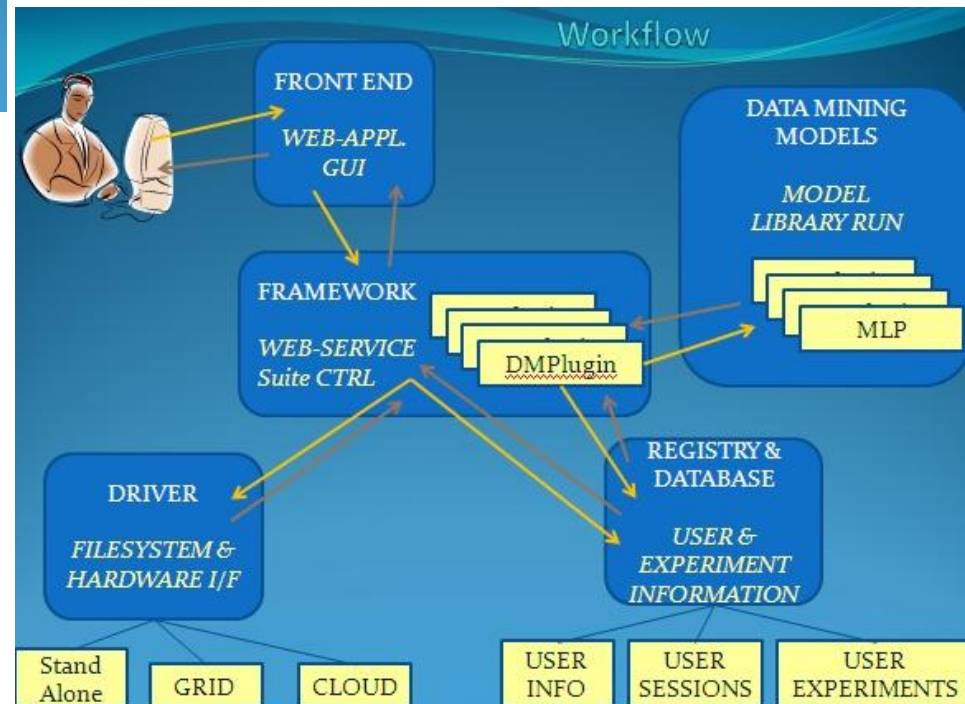
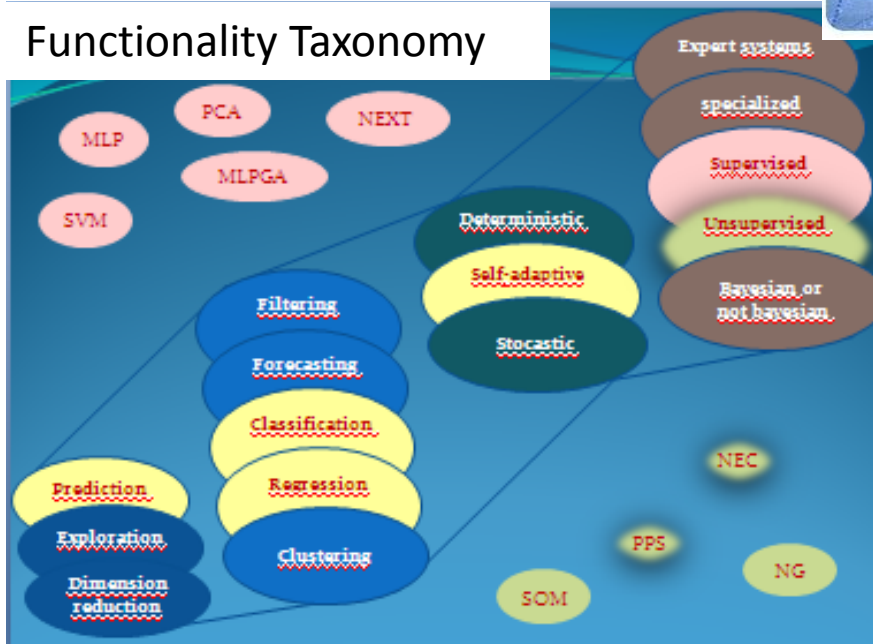
Tools must run without knowledge of GRID/Cloud no personal certificates, no deep understanding of the DM tool etc. )



# A break-down of an effective DM process



## Functionality Taxonomy



# X-informatics

## The changing methodology of science

- Data Mining, computer science, etc. have become the “fourth leg of science” (besides theory, experimentation and simulations)
  - Synergy between different worlds is required
  - Sociological issues to be solved (formation, infrastructures, and so on)

The  
**F O U R T H**  
**P A R A D I G M**

DATA-INTENSIVE SCIENTIFIC DISCOVERY

EDITED BY TONY HEY, STEWART TANSLEY, AND KRISTIN TOLLE

*Downloadable at Microsoft Research site*

The image shows the cover of the book 'The Fourth Paradigm: Data-Intensive Scientific Discovery'. The top half of the cover features a blue background with a bright light source on the left, creating a lens flare effect. The background is filled with a pattern of binary code (0s and 1s) that appears to be receding into the distance, creating a sense of depth and movement. The title 'The Fourth Paradigm' is written in a serif font, with 'The' in a smaller size and 'FOURTH PARADIGM' in large, bold, yellow capital letters. Below the title, the subtitle 'DATA-INTENSIVE SCIENTIFIC DISCOVERY' is written in a smaller, white, sans-serif font. At the bottom of the cover, the editors' names 'EDITED BY TONY HEY, STEWART TANSLEY, AND KRISTIN TOLLE' are listed in a small, white, sans-serif font. A dark blue horizontal bar at the very bottom contains the text 'Downloadable at Microsoft Research site' in a white, italicized, sans-serif font.

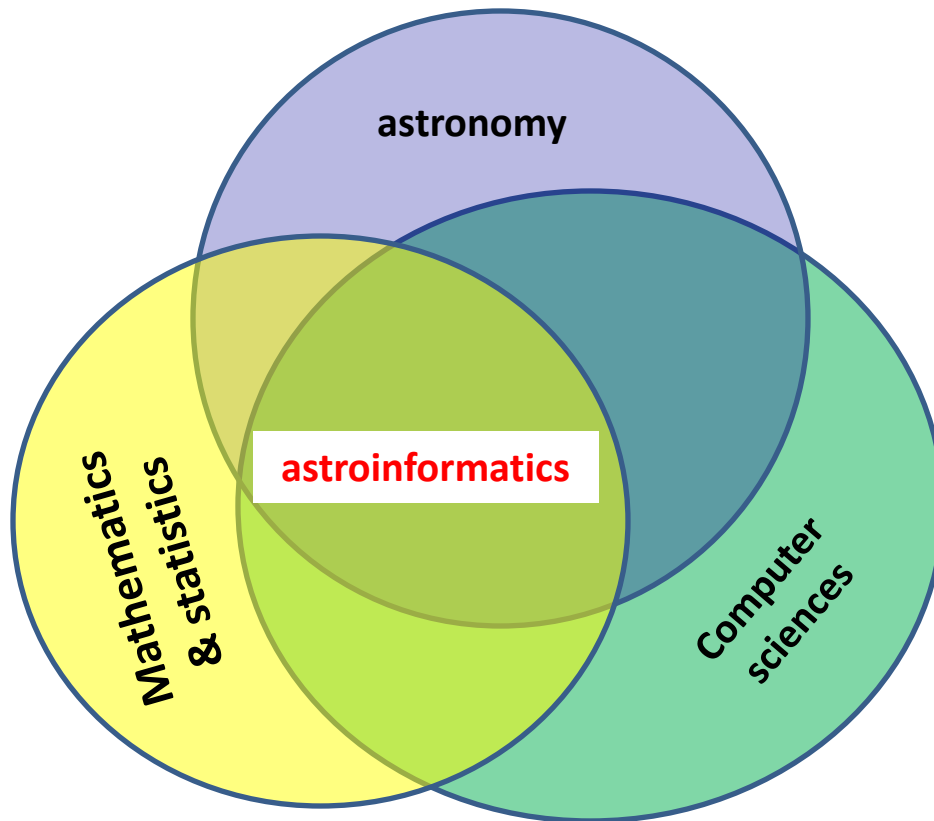
DATA-INTENSIVE SCIENTIFIC DISCOVERY

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# Experimental astronomy has become a three players game



- **astronomy:** problems, data, understanding of the data structure and biases
- **mathematics:** evaluation of the data, falsification/validation of theories/models, etc
- **computer science:** implementation of infrastructures, databases, middleware, scalable tools, etc

- **Astroinformatics:** AAS n. 215, Washington, December 2009, chairperson: K. Borne
- **Astroinformatics 2010:** Caltech (USA) June 16-19 2010; co-chairpersons: S.G. Djorgovski, G. Longo
- **Astroinformatics 2011:** UNINA – Sorrento, co-chairpersons: S.G. Djorgovski, G. Longo