Mathematical Best Fit Algorithm for Energy Distributions in VO Context

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Project Setup

Name

Mathematical fitting algorithms for Energy Distributions in VO context

Aim

To implement an algorithm that looks for the theoretical model that best fits a given Spectral Energy Distribution (SED)

Tutors

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Virtual Observatory

- Its aim is to offer seamless access to astronomical data worldwide

Astronomers → Multiple data centers → Analysis and Visualization tools

Multiple data centers ↓

Standard framework ↓

Delivering and publishing services

Virtual Observatory (cont.)

- **In order to fulfill this aim the International Virtual Observatory Alliance (IVOA) was created in June 2002**

  - **Data** -management
    -analysis
    -distribution
    -interoperability

  - **Data Access Layer (DAL)**
    -working group within IVOA
    -standards for remote observational data access

Simple Spectral Access Protocol (SSAP) → **To define a uniform interface to spectral data**

Virtual Observatory (cont.)

- **Theory Group**

-interest group within the IVOA

-formed en January 2004

-define requirements needed for a full interoperability between observations and models

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Theoretical Spectrum Access Protocol (TSAP)

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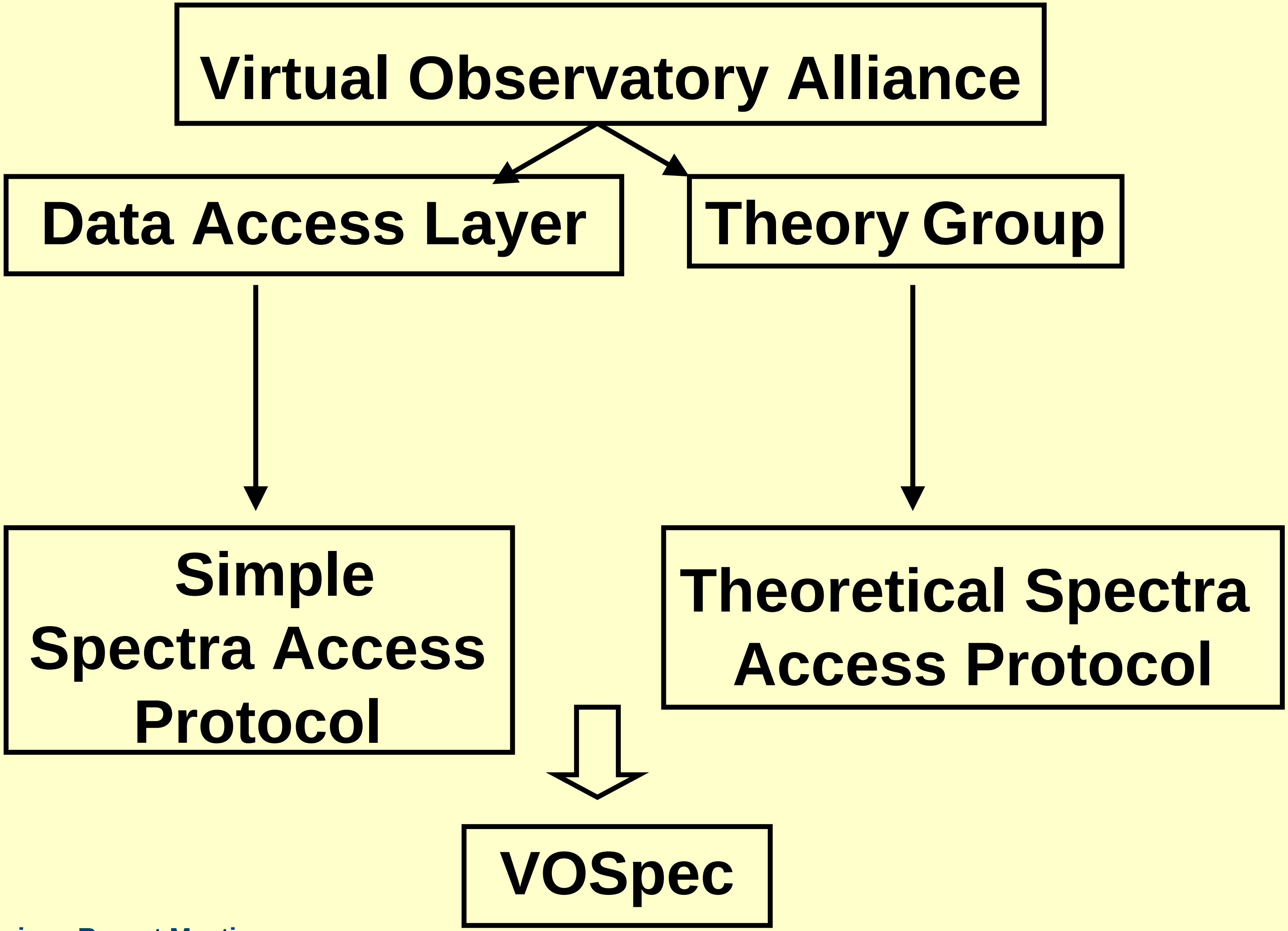
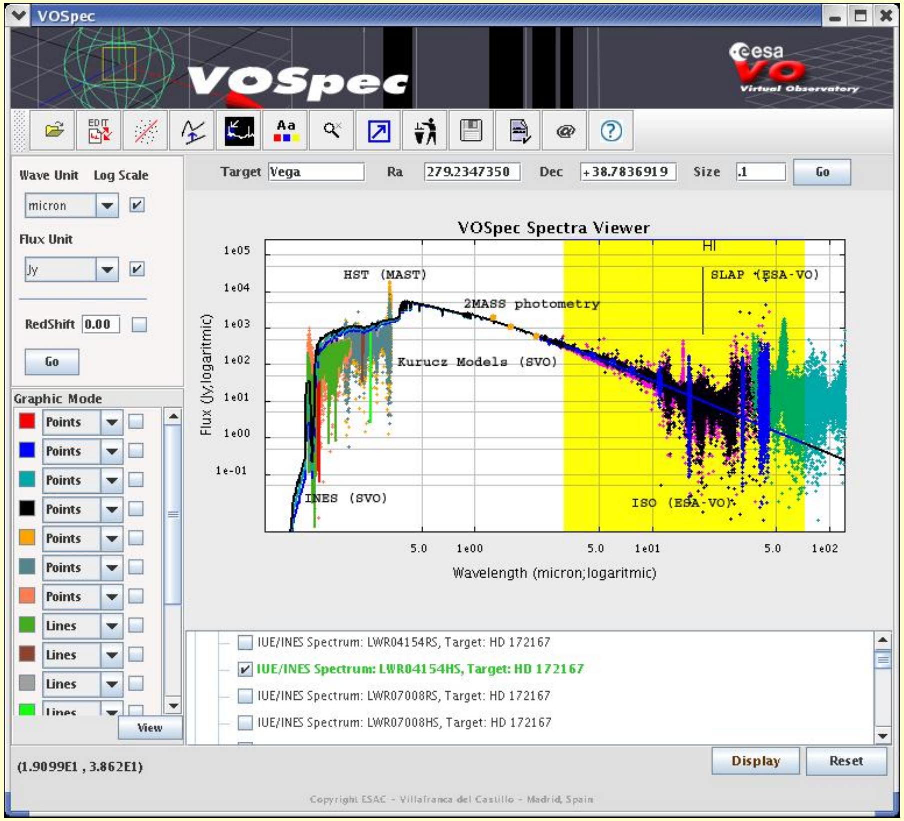
Incorporate theoretical models to the VO

Project environment

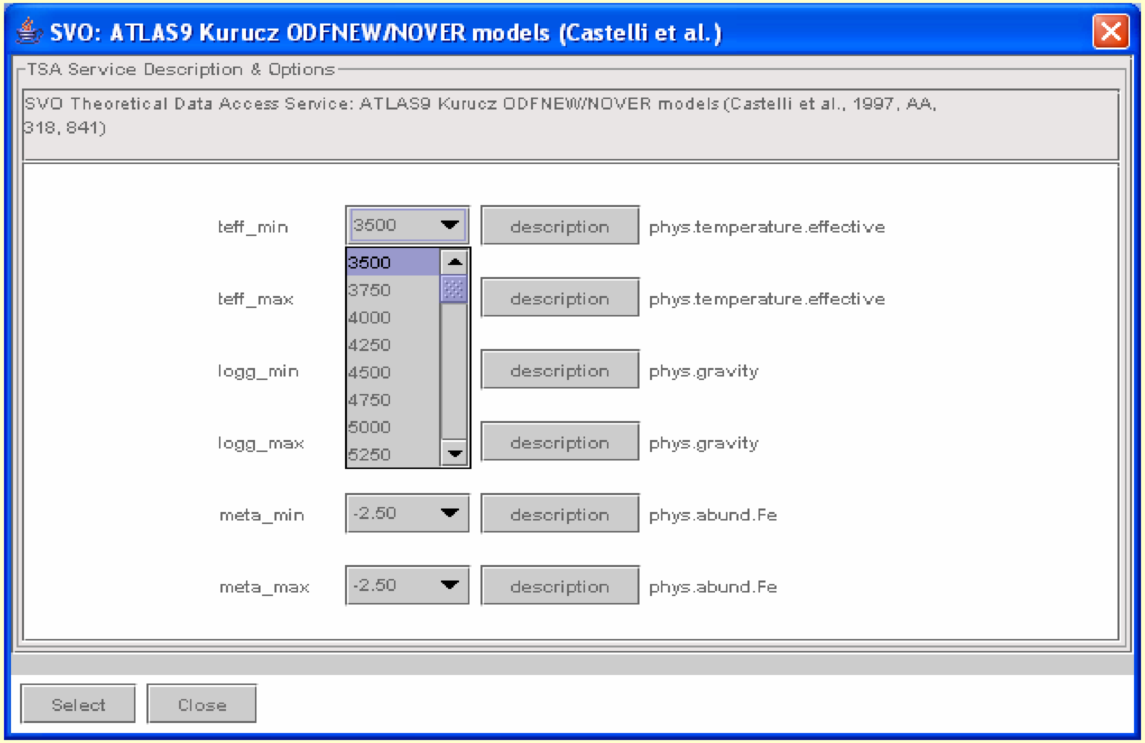


VOSpec

- Tool for handling
  - VO compliant spectra through **SSAP**
  - Theoretical models through **TSAP**
- Handling spectra with VOSpec:
  - Display and superimpose spectra
  - Automatic unit conversion through dimensional analysis
  - Multi-wavelength analysis
  - Polynomial/Black Body/Gaussian fitting



Why Best Fit?



Currently to find the model that best fits a given SED:

- **Choose parameters manually**
- **Inspect result visually ("Chi-by-eye")**
- **Modify parameters manually**
- **Reinspect visually**
- **Loop…..**

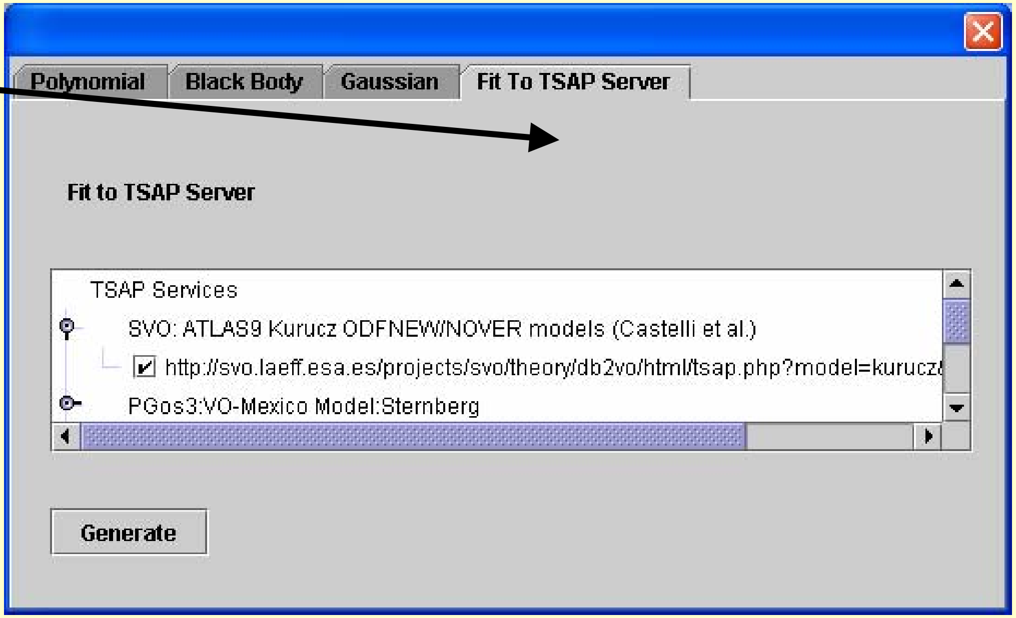
New approach

Best Fit finds the model

automatically

Best Fit brief description

- ❑It is going to be integrated as a new fitting utility in **VOSpec**



- ❑**Java** language

- ❑Aim

Find the theoretical model that best fits the SED

Best Fit brief description (cont.)

- To fulfill this aim:
  - Chi-square function measures the agreement between real and theoretical spectrum
  - The best fit spectrum is the one that achieves a minimum in the Chi-square function
  - Problem in minimization in many dimensions

real **theoretical**

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - y(x_i; p_{1,\ldots,} p_M)}{\sigma_i} \right)^2$$

Different sampling

Levenverg-Marquardt method

SED
CUBIC SPLINE interpolation

Levenberg-Marquardt method

- Iterative method
- Standard technique for nonlinear least-square problems ⇒ Modified for discrete case
- Combination of → **Steepest descent method** / **Gauss-Newton method**
- **Steepest descent method**
  - Initial estimate ⇒ $\mathbf{x}_0$
  - Successive estimate ⇒ $\mathbf{x}_{i+1} = \mathbf{x}_i - c \cdot \nabla \chi^2(\mathbf{x}_i)$
  - Iterations stop when $\nabla \chi^2(\mathbf{x}_i)$ is sufficiently small
  - Hard to determine the step size
  - Slow, but guaranteed convergence

Levenberg-Marquardt method (cont.)

❑Gauss-Newton method

- Taylor expansion

$$\chi^2(\mathbf{x}+\Delta\mathbf{x}) = \chi^2(\mathbf{x}) + \nabla\chi^2(\mathbf{x})\cdot\Delta\mathbf{x} + \frac{1}{2}\cdot\Delta\mathbf{x}^T\cdot\mathbf{H}(\mathbf{x})\cdot\Delta\mathbf{x}$$

- Set the derivative of the previous expression equal to 0

Iterative equation

$$\mathbf{x}_{i+1} = \mathbf{x}_i - \mathbf{H}^{-1}\cdot\nabla\chi^2(\mathbf{x}_i)$$

- Quadratic convergence

- If the initial value is too far from the minimum convergence can fail

Levenberg-Marquardt method (cont.)

❑Steepest descent and Gauss-Newton methods are complementary in the advantages they provide ⇨ **Levenberg Marquardt Method**

$$\mathbf{x}_{i+1} = \mathbf{x}_i - c \cdot \nabla \chi^2(\mathbf{x}_i)$$

$$\mathbf{x}_{i+1} = \mathbf{x}_i - \mathbf{H}^{-1} \cdot \nabla \chi^2(\mathbf{x}_i)$$

$$\mathbf{x}_{i+1} = \mathbf{x}_i - (\mathbf{H} + \lambda \mathbf{I})^{-1} \cdot \nabla \chi^2(\mathbf{x}_i)$$

Levenberg-Marquardt method (cont.)

- **Far from the minimum**
  - Linear approximation with steepest descent method to the closest minimum
  - Adds a measure of the step in the steepest descent method

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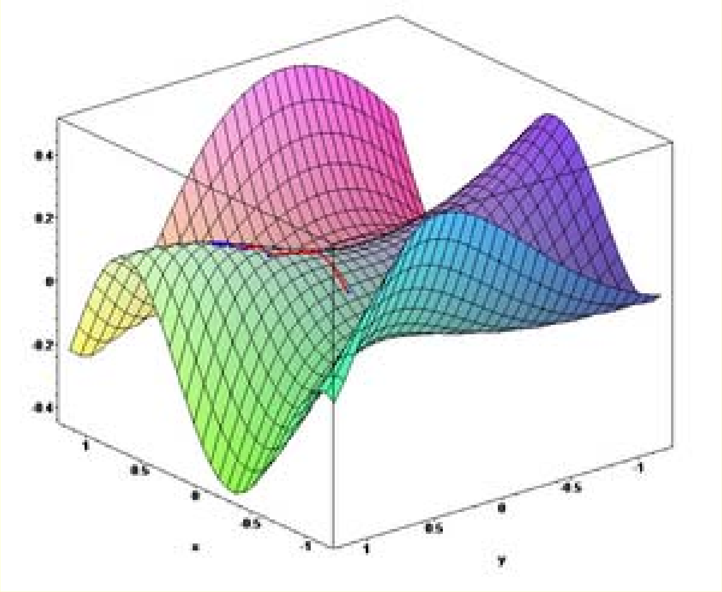
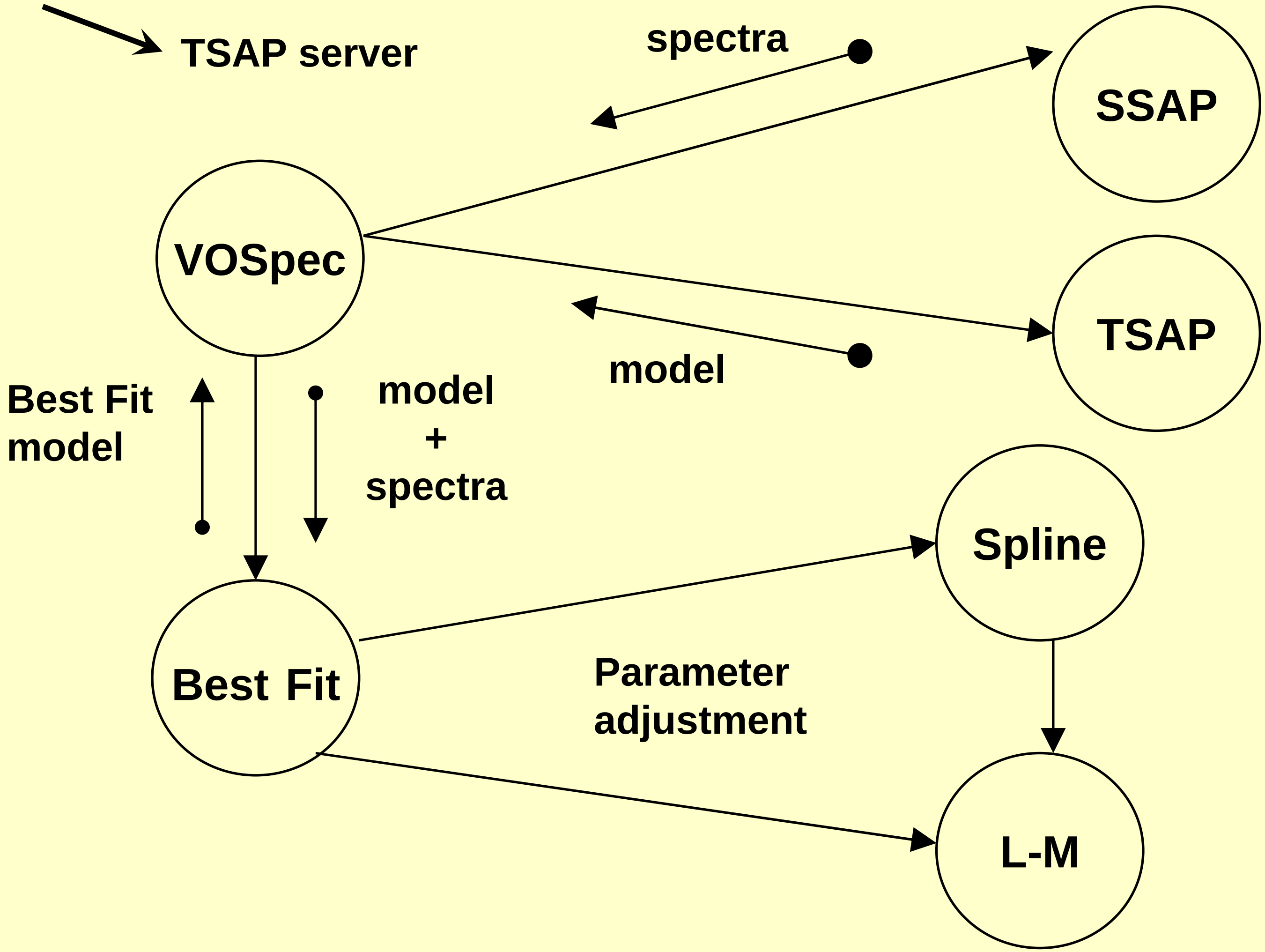
Close to the minimum
Gauss-Newton convergence



- **L-M method works well in practice**

Best Fit diagram

- Given
  - → Real spectrum from SSAP server
  - → TSAP server



Conclusions

- IVOA standards are nearly mature enough to do real science
- BF algorithm implementation using TSAP protocol increases VO functionality
- Nonlinear least-square methods (LM) are very appropriate for the implementation of the algorithm
- Very easy integration with ESA VOSpec tool