PROGRESS IN EMULATION FOR RADIATIVE TRANSFER MODELING AND MAPPING

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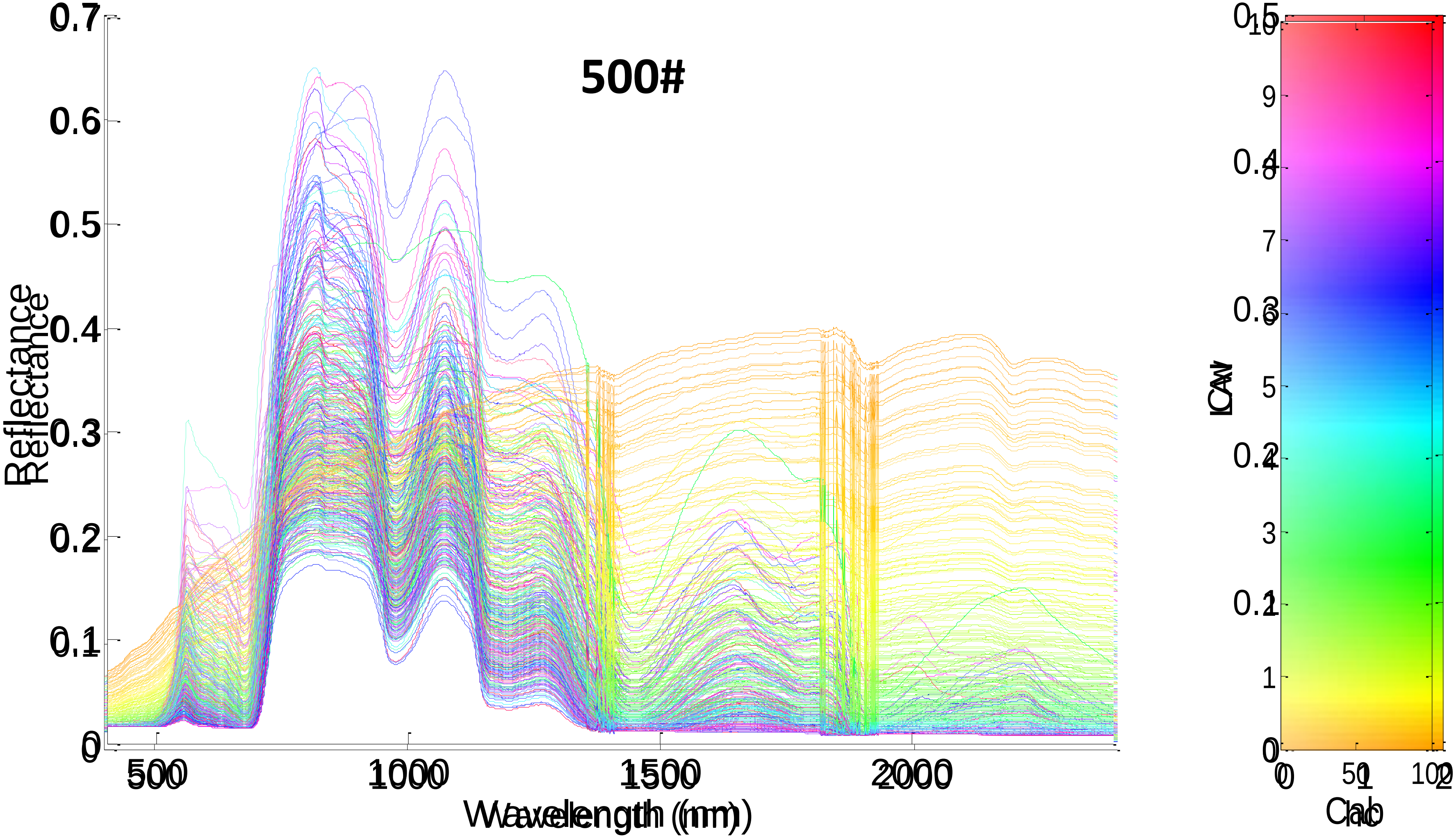
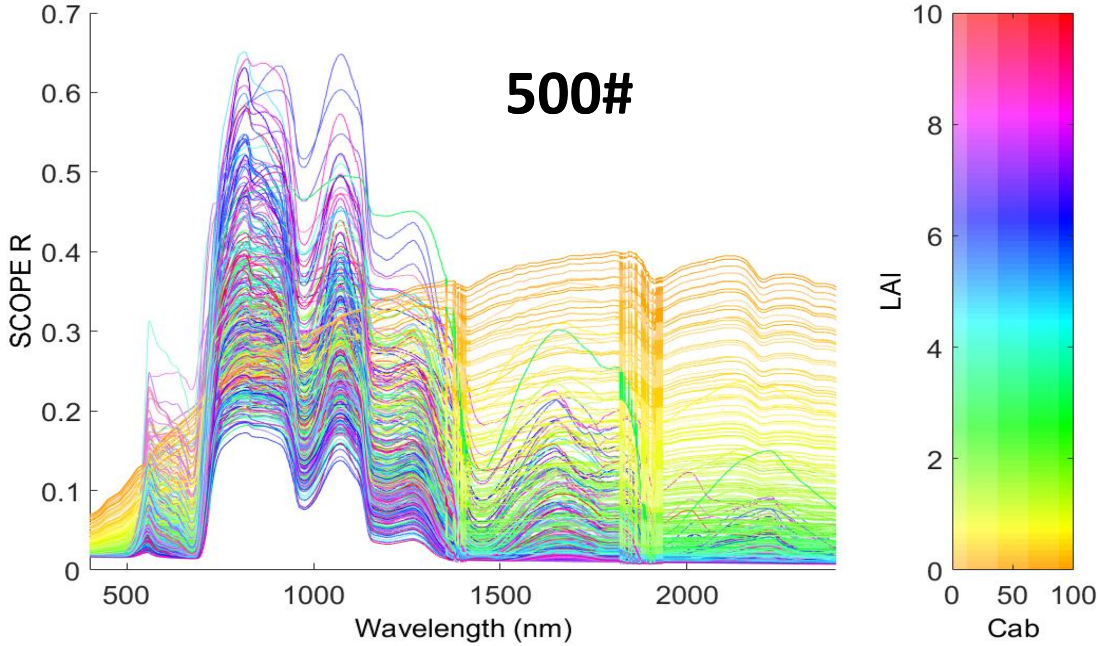
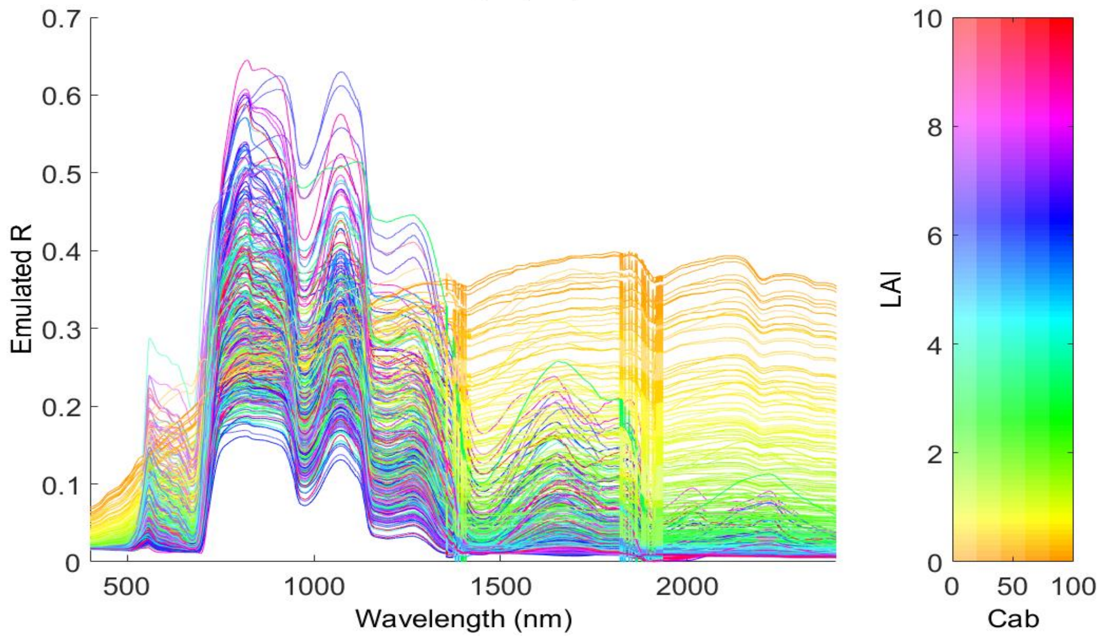

500#
Reflectance
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
500
1000
1500
2000
Wavelength (nm)
Cab

Any difference? Which model would you choose?

37 min



SCOPE
(RTM)



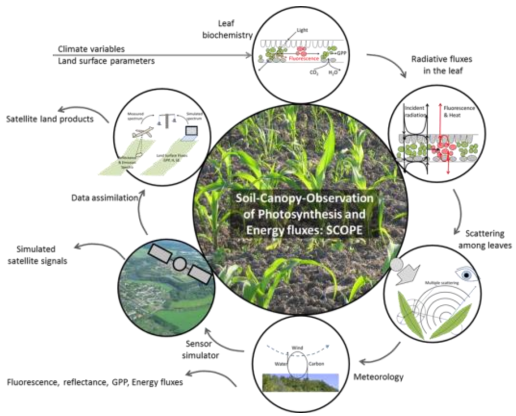
0.2 s

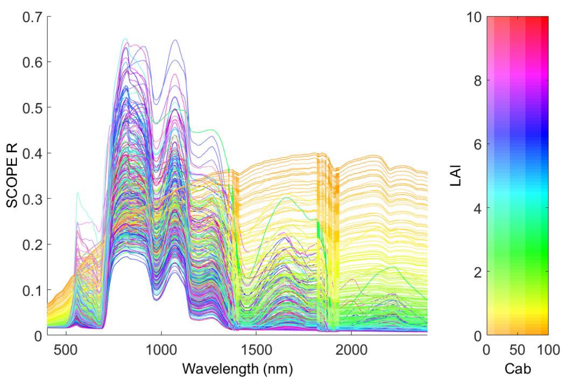
Emulator
(emulated SCOPE)

BACKGROUND

Advanced RTMs: generation of a large LUT (>1000#)

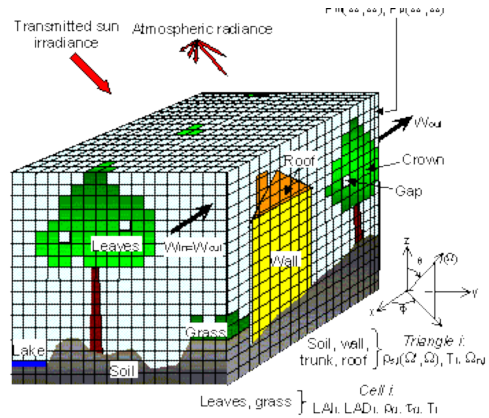
SCOPE

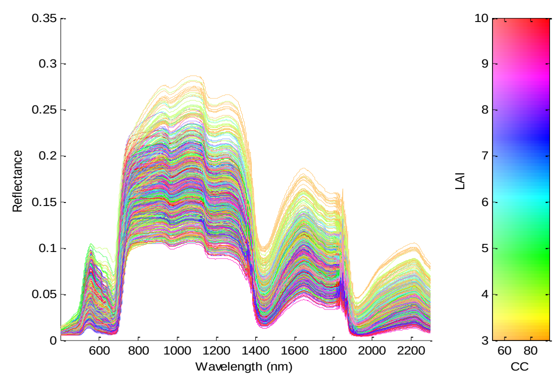


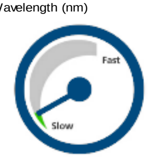


Hours

DART

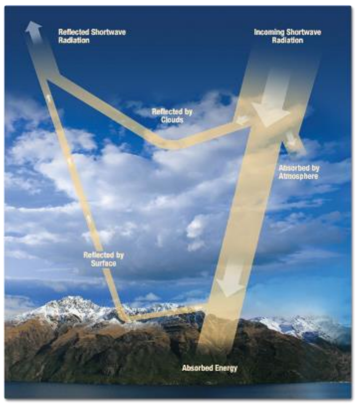


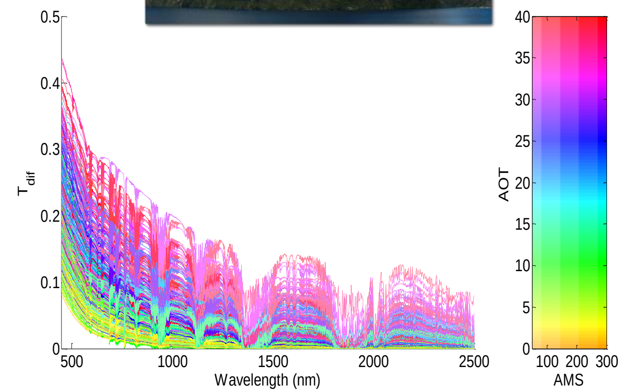




days

MODTRAN





>days

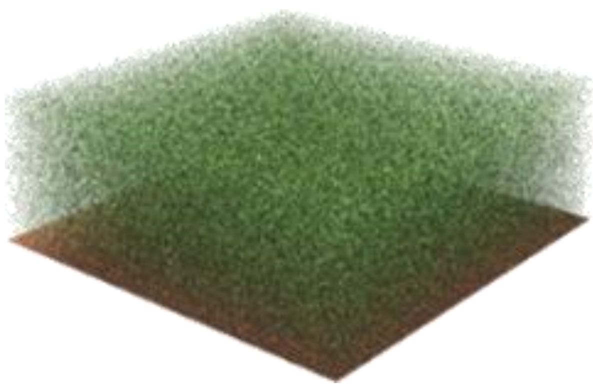
Advanced RTMs: *more realistic but slow*

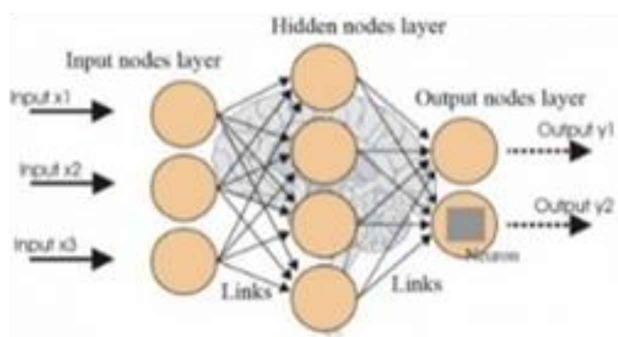
Emulation of RTMs

<u>Emulators</u> are statistical models that approximate the processing (input-output) of a physical model (e.g. RTM) - at a fraction of the computational cost:

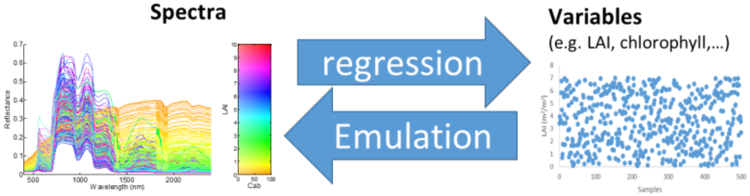
making a statistical model from a physical model

RTM | **Machine learning** | **Emulator**

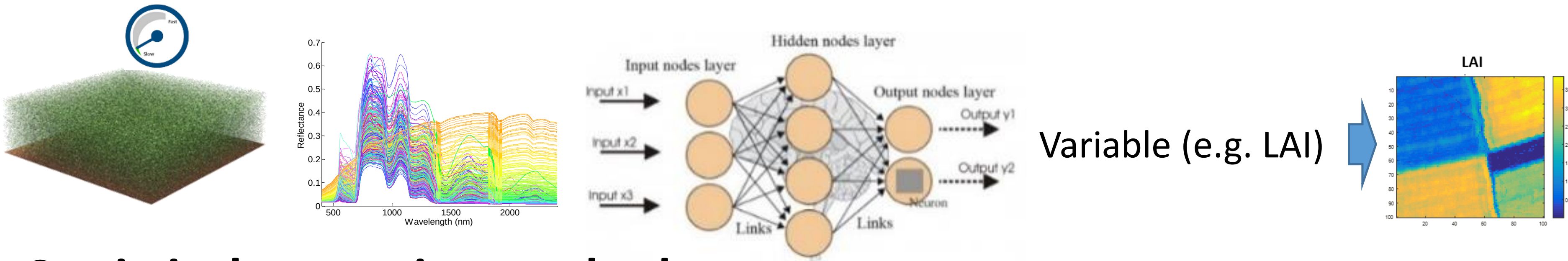




Regression vs. Emulation:



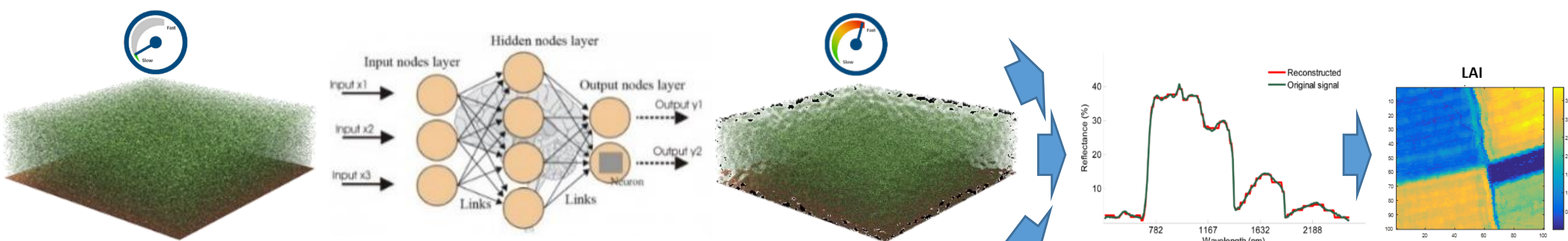
Common use of machine learning in optical RS:



Statistical regression method:

- Variable/data-driven, black box, 1 output, portability is questionable

Emulation in optical RS:



Replace RTM:

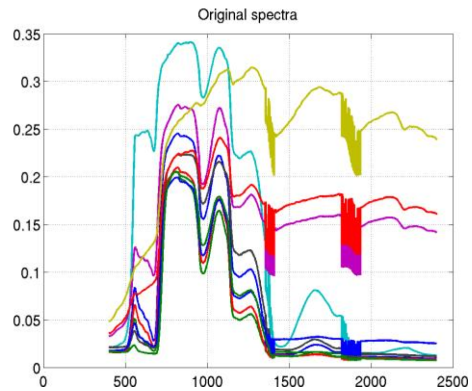
- Multiple applications, e.g. inversion
  - ✓ Radiometric method: Spectral fitting
  - ✓ Portable: generally applicable

"spectral redundancy" is a blessing

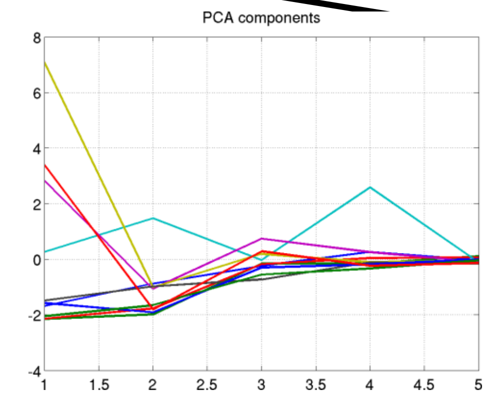
Processing steps emulation

Input (variables + spectra) → Splitting into training/validation → PCA on spectra → MLRA training looping over components → Prediction of components → Reconstruction of spectra → Validation → Emulator

PCA on spectra



$$Sc = U \cdot X$$

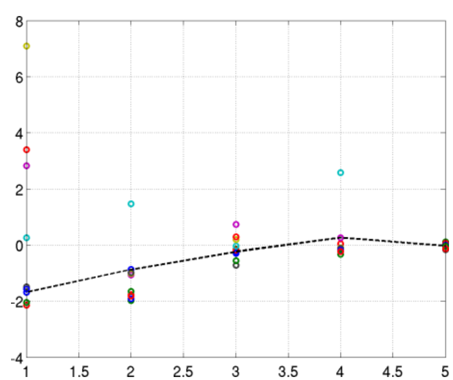


MLRA training looping over components

$$W = (Y + \lambda I)^{-1} \cdot Sc$$

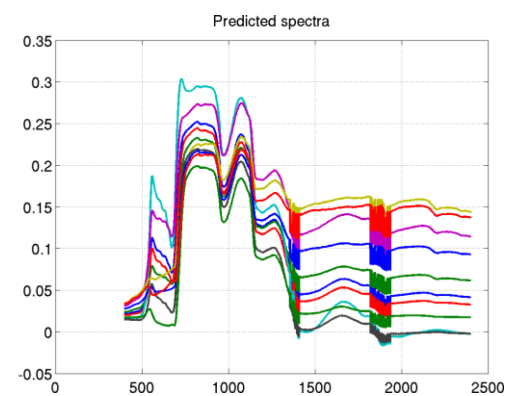
Prediction of components

$$Sp = Sc \cdot W$$



Reconstruction of spectra

$$Xr = U^{T} \cdot Sp$$



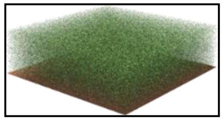
Validation → Emulator

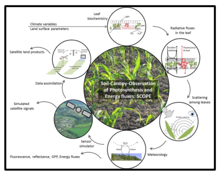
Emulator toolbox

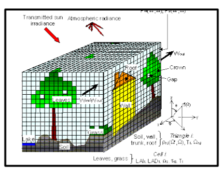
http://ipl.uv.es/artmo/

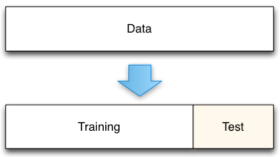
With ARTMO's emulation processing chain any RTM can be converted into an emulator.

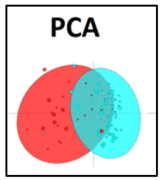
Input (variables + spectra) → Splitting into training/validation → PCA on spectra → MLRA training looping over components → Prediction of components → Reconstruction of full spectrum → Validation → Emulator

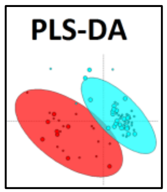


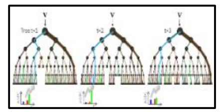


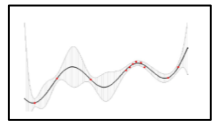


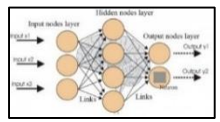


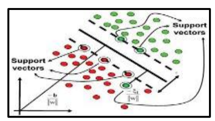


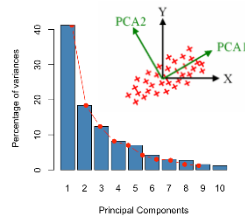








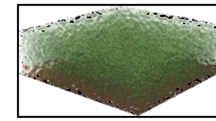




$$Xr = U^{T} \cdot Sp$$

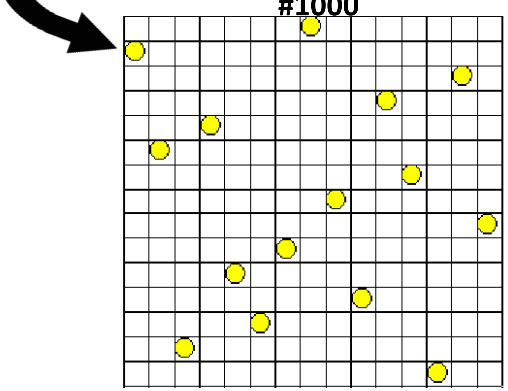
$$RMSE = \sqrt{\sum \frac{(y_{pred} - y_{ref})^2}{N}}$$

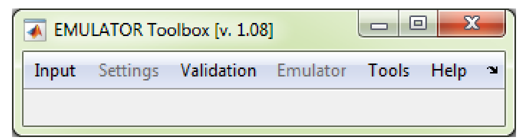
$$NRMSE = \frac{1}{Y_{max} - Y_{min}} \sqrt{\frac{\sum_{i=1}^{N} (Y_i - \hat{Y}_i)^2}{N}},$$



Latin Hypercube Sampling (LHS)

#1000





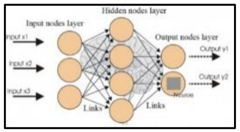
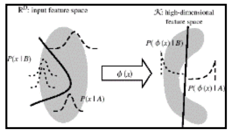
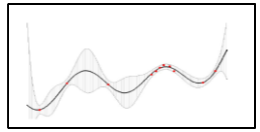
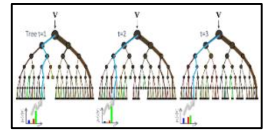
Input → Settings → Validation → Emulator

- Input
  - RTM data
  - Txt data
    - Select project
    - Edit settings
- Settings
- Validation
  - New
  - Load
- Emulator
  - RTM vs Emulator
  - LUT Emulator
  - Txt Emulator
  - Scene Emulator
- Tools
  - Save
  - Load
  - Manage tests
    - Delete
    - Rename
  - Options
  - View figure
  - Plot LUT
  - Residual analyzer
  - Statistical analyzer
  - Import
  - Scene comparison
- Help
  - Show Log
  - User's manual
  - Installation guide
  - Disclaimer

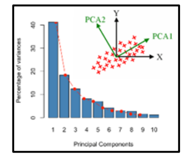
Rivera, J.P., Verrelst, J., Gómez-Dans, J., Muñoz-Marí, J., Moreno, J., Camps-Valls, G. (2015). An Emulator Toolbox to Approximate Radiative Transfer Models with Statistical Learning. Remote Sensing. p. 7, 9347-9370.

Emulators great idea… what about accuracy?

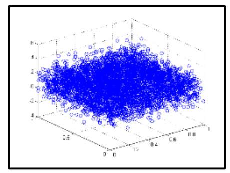
1) Role of machine learning regression algorithm?

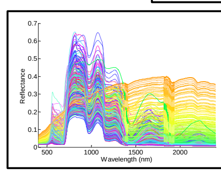
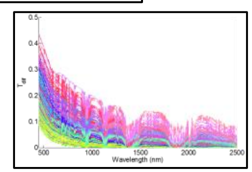
2) Role of dimensionality reduction (DR) method?



3) Role of LUT size training?



4) Role of data type?

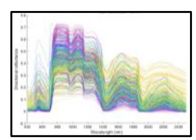
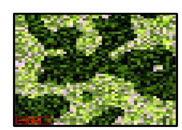
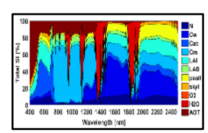
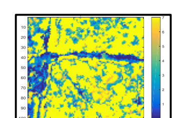



All these factors determine emulation accuracy. Some testing is required*

If OK with losing some accuracy, various applications are opened:

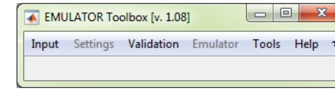
Fast RTM output generation

1. ***Fast scene generation***
2. ***Fast global sensitivity analysis***
3. ***Fast inversion***

* Verrelst, J., Rivera Caicedo, J.P., , Muñoz-Marí, J., Camps-Valls, G., Moreno, J. (2017). SCOPE-Based Emulators for Fast Generation of Synthetic Canopy Reflectance and Sun-Induced Fluorescence Spectra. Remote Sensing. 9(9), 927.

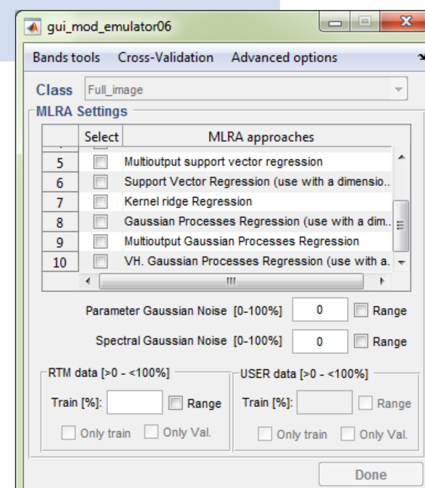
Latest developments in Emulator toolbox:



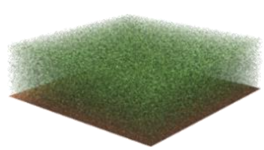
- **New ML algorithms implemented:**
  1. Multi-output support vector regression
  2. Multi-output Gaussian process regression

In total 9 ML algorithms implemented in toolbox.

Random Forests (TreeBagger) (RF TB)	Kernel Ridge Regression (KRR)
Random Forests (Fitensemble) (RF FE)	Gaussian Process Regression (GPR)
Neural Network (NN)	Multi-output GPR (MGPR)
Support Vector Regression (SVR)	Varational Heteroscedastic GPR (VH GPR)
Multi-output SVR (MSVR)	

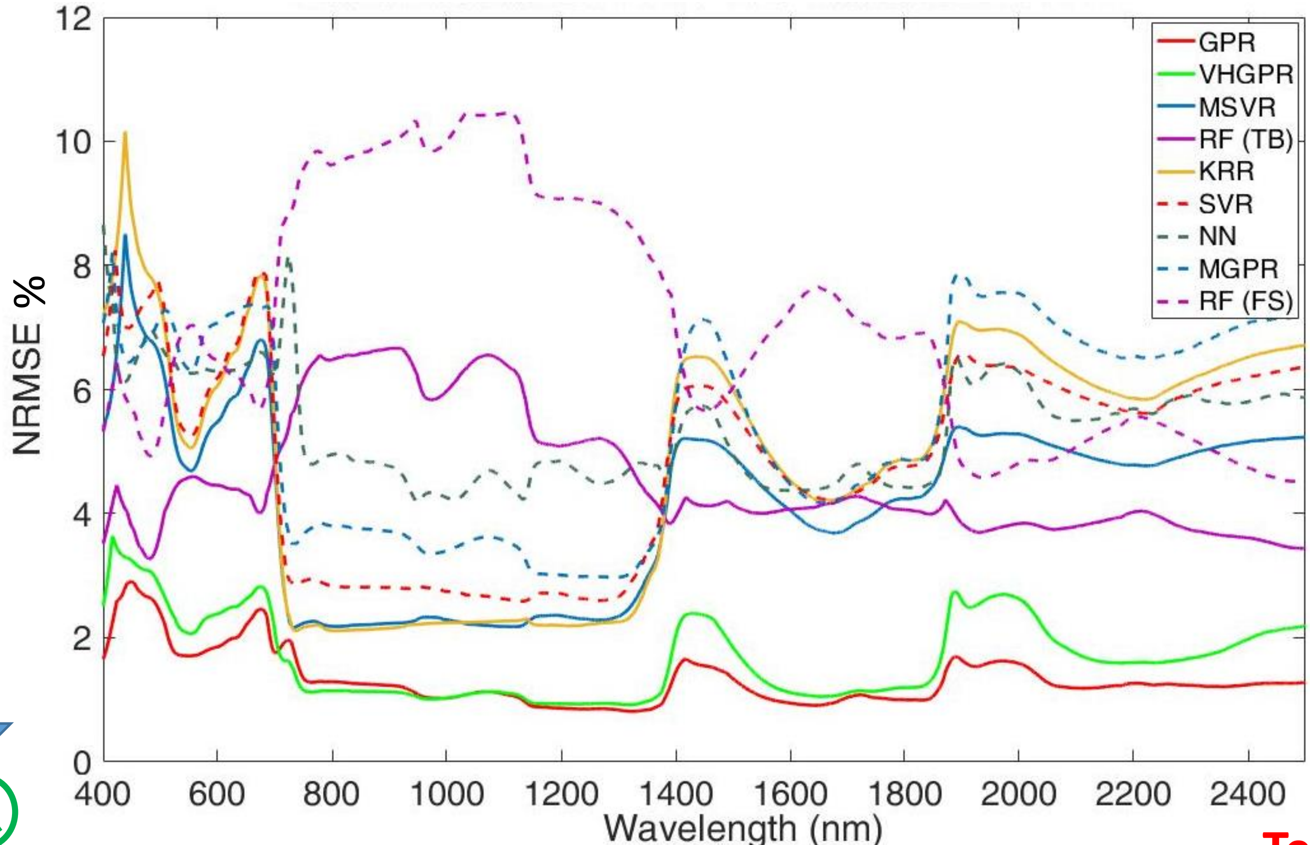


<u>Experimental setup:</u>



- **PROSAIL 1500 LHS** simulations, all variables ranged
- **20 PCA** and 70/30 training-testing data splitting

Performances emulators: accuracy & CPU



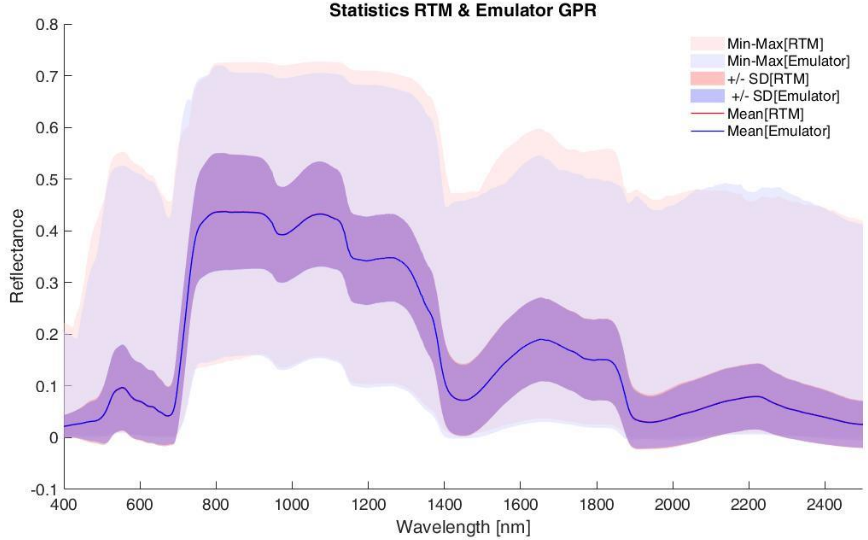
MLA	Time train (s) (#1050)
GPR	179
VH.GPR	724
MSVR	52
RF (TB)	32
KRR	4
SVR	2106
NN	42
MGPR	12
RF (FS)	21

Testing time (#450): <1 s

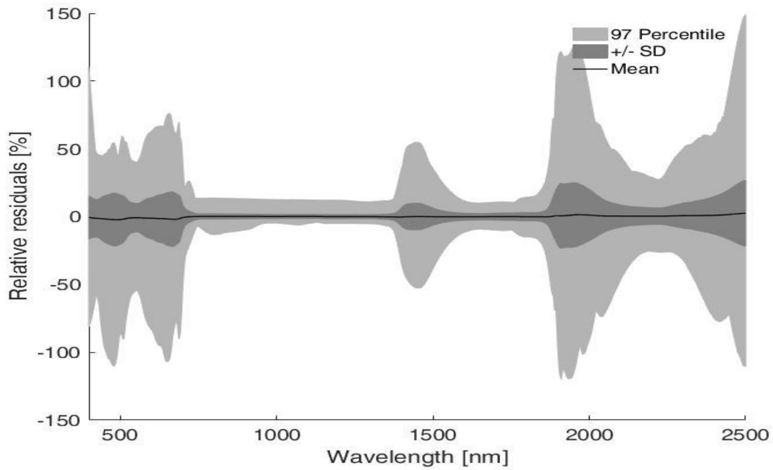
GPR very accurate (<2%)

Validation GPR emulator

Overview statistics emulator vs validation



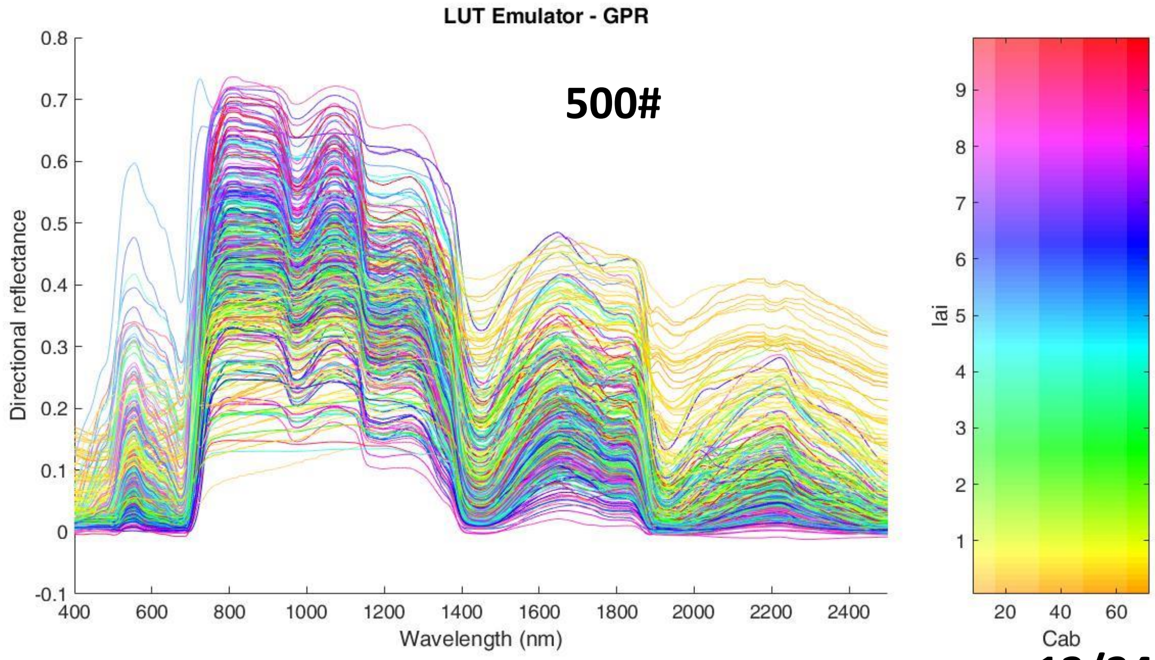
Residuals



- Mean and SD perfectly matching.
- Some small mismatch in boundaries.

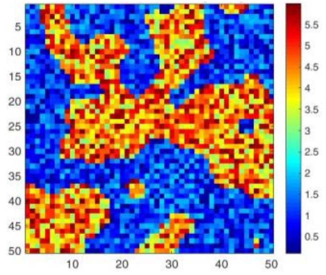
Running GPR emulator:

1.0 s

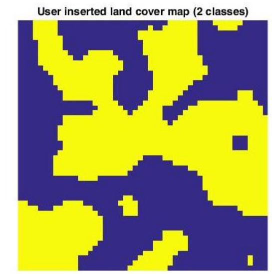


Applications (1/3)

Scene generation

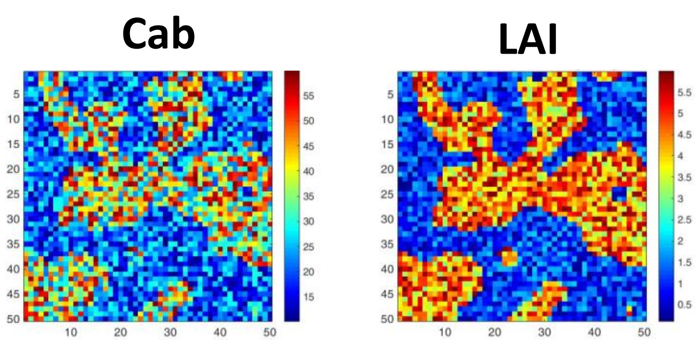


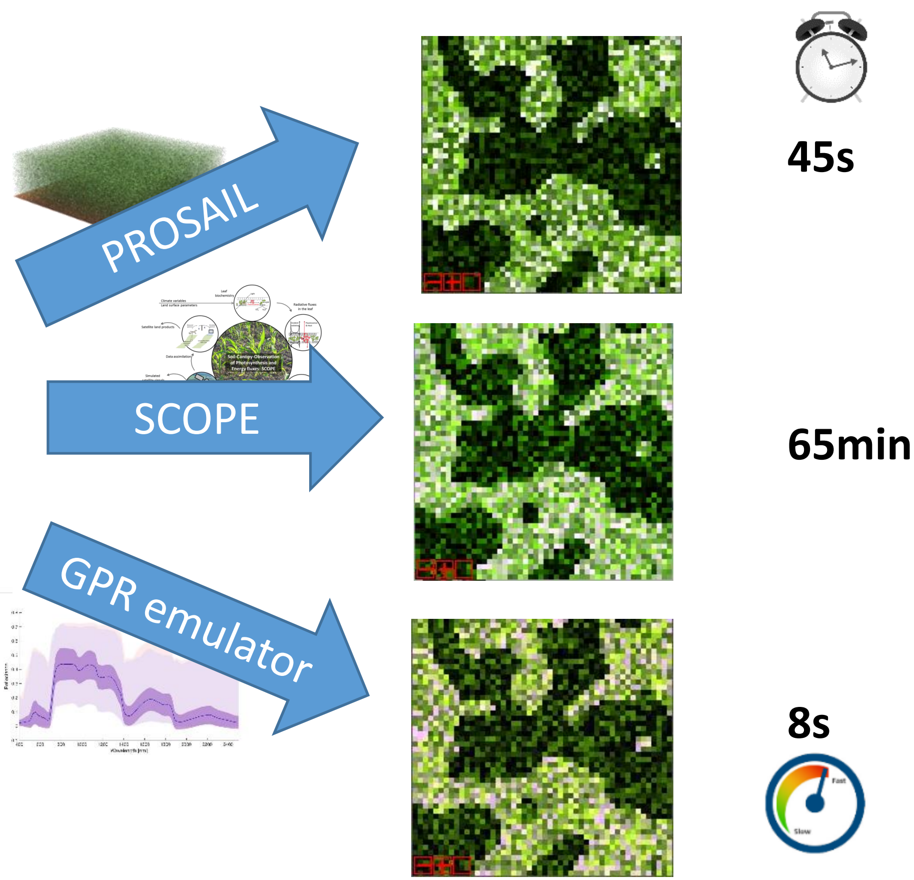
Emulation for Scene generation



- GPR emulator applied for scene generation
- Compared against RTM scenes: PROSAIL & SCOPE

Parameter	Symbol	Units	Class 1	Class 2
Leaf area index	LAI	m^2/m^2	Uniform: 3 - 6	Uniform: 0 - 2
Chlorophyll a+b content	C_{ab}	$\mu g/cm^2$	Uniform: 20 - 60	Uniform: 10 - 35





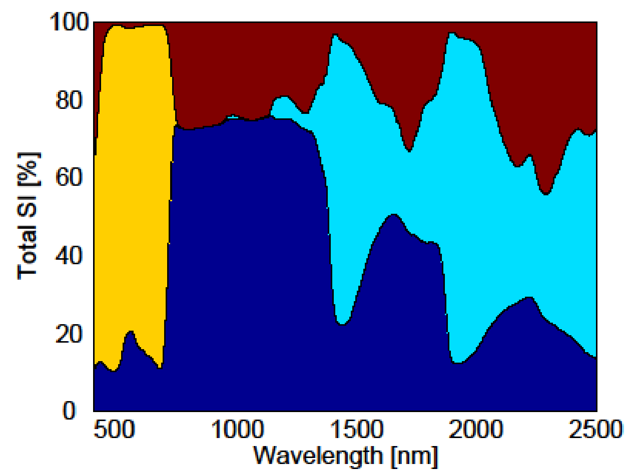
See Talk TU4.R9.5 for emulation of real scenes

Applications (2/3)

Global Sensitivity Analysis (GSA)

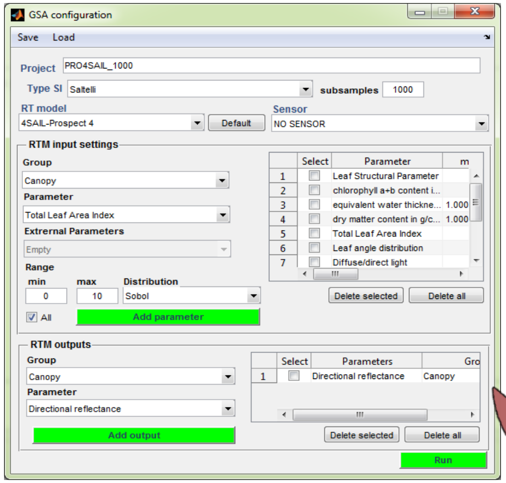
GSA techniques quantify the relative importance of each input parameter to model outputs.

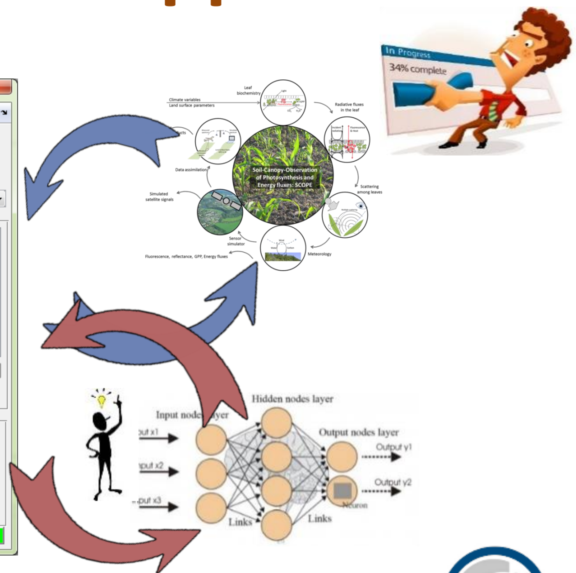
PROSPECT 4



Emulators applied into GSA: PROSPECT-4

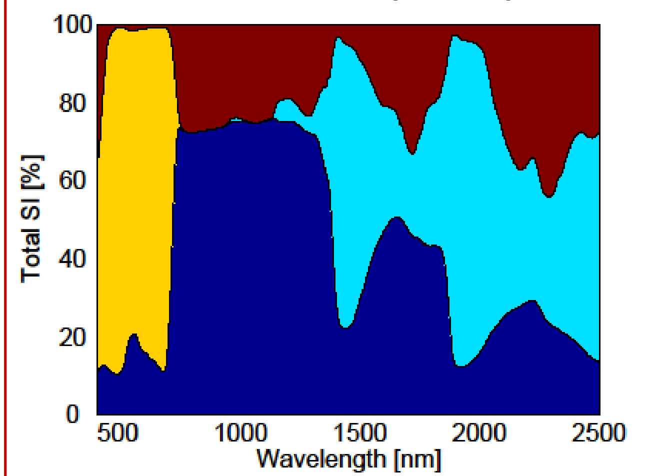
ARTMO's GSA toolbox



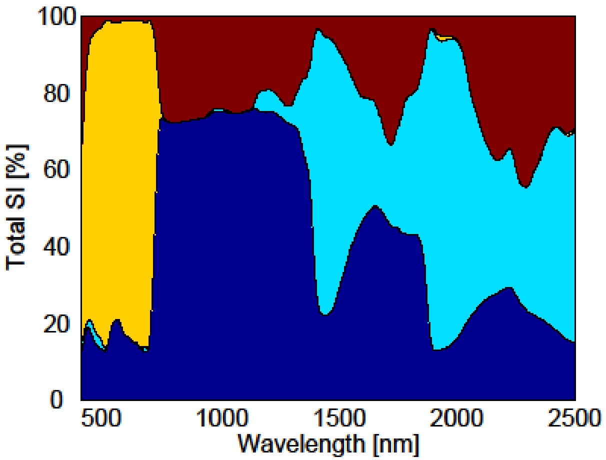


X 2

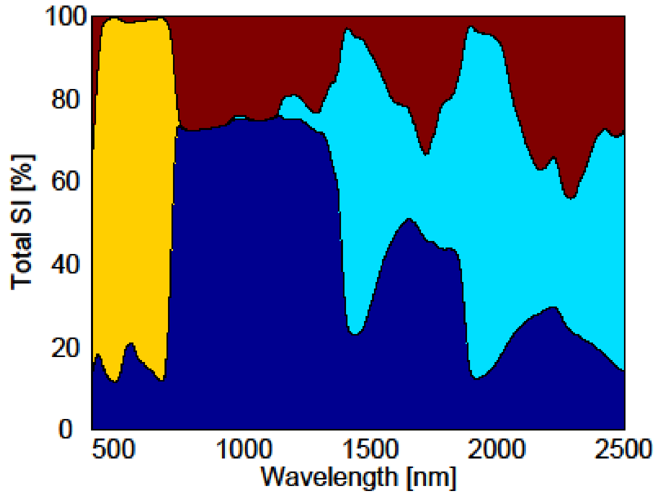
PROSPECT-4 (122 s)



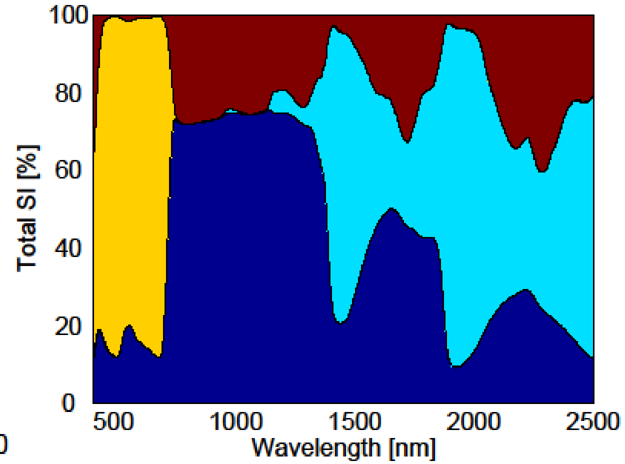
KRR (55 s)



NN (55 s)



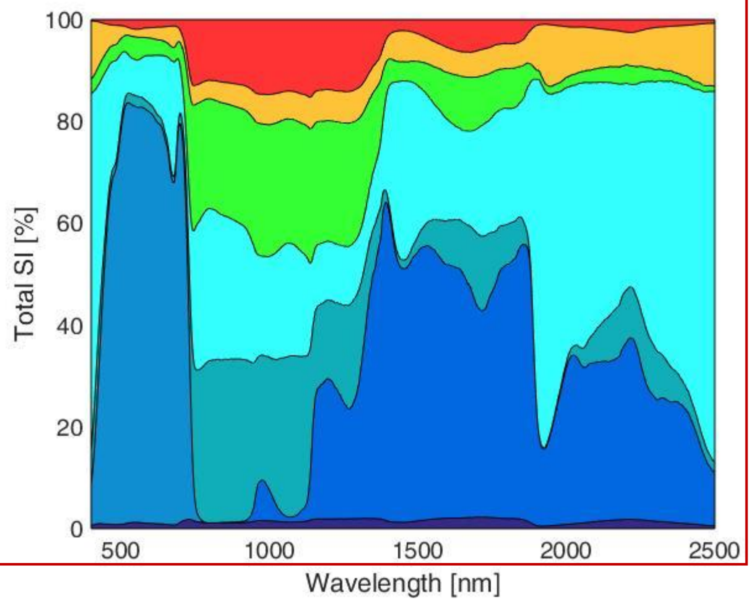
GPR (58 s)



1000#/variable

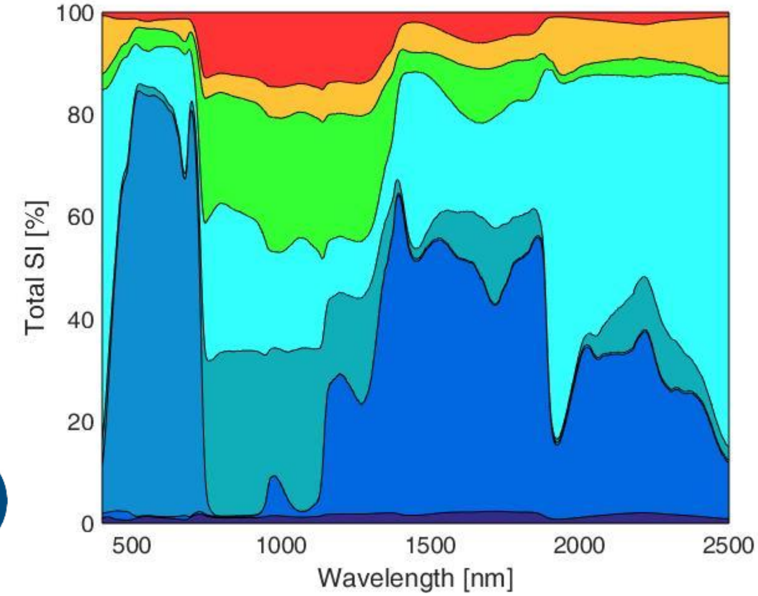
PROSAIL

4SAIL (103 s)

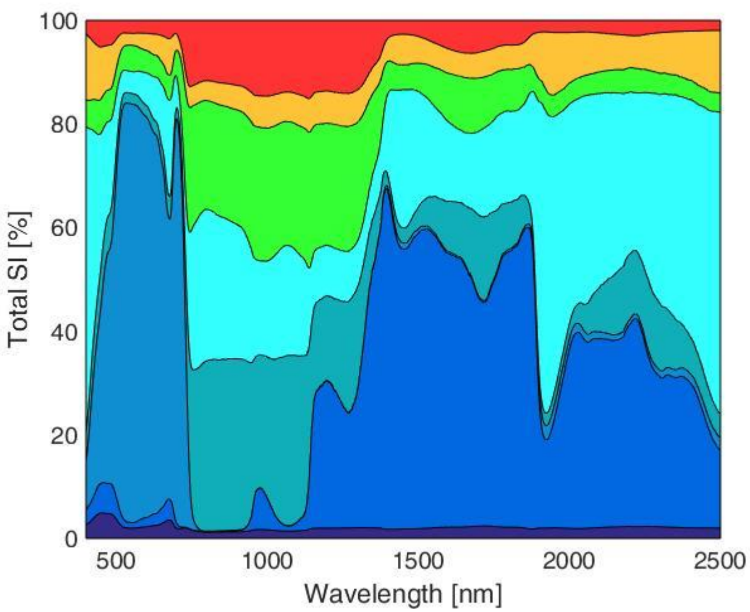


X 3

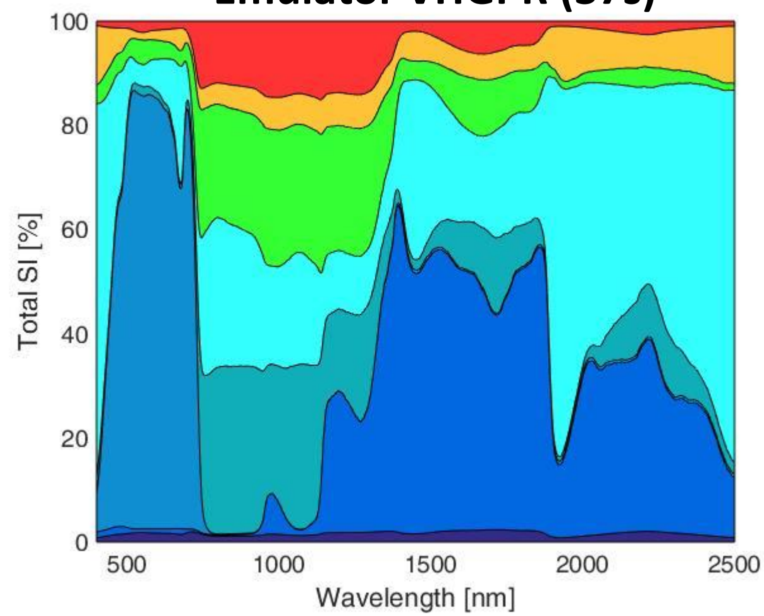
Emulator GPR (32s)



Emulator KRR (28s)



Emulator VHGPR (37s)

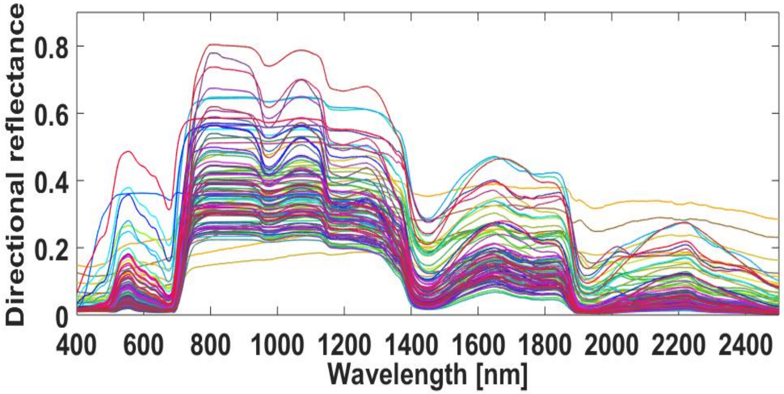


1000#/variable

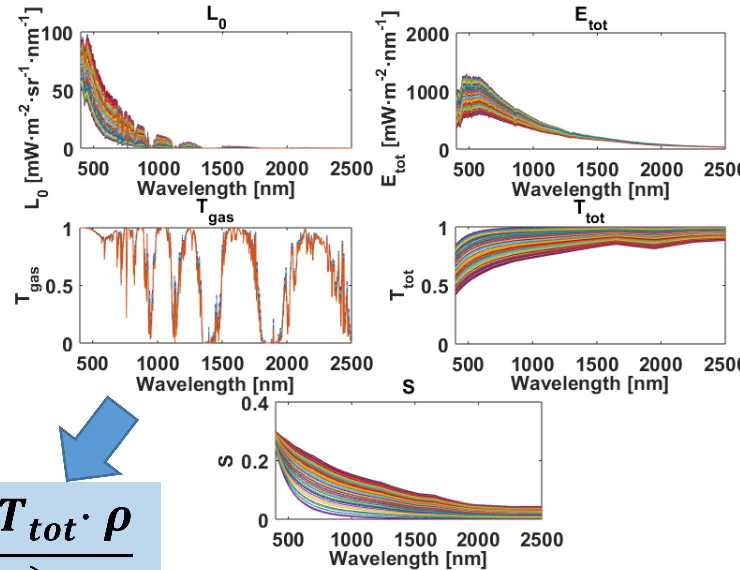
N Cw Cab Cm LAI LAD soil coeff SZA

Applying emulation to L_{TOA} (1/3)

50 PROSAIL spectra

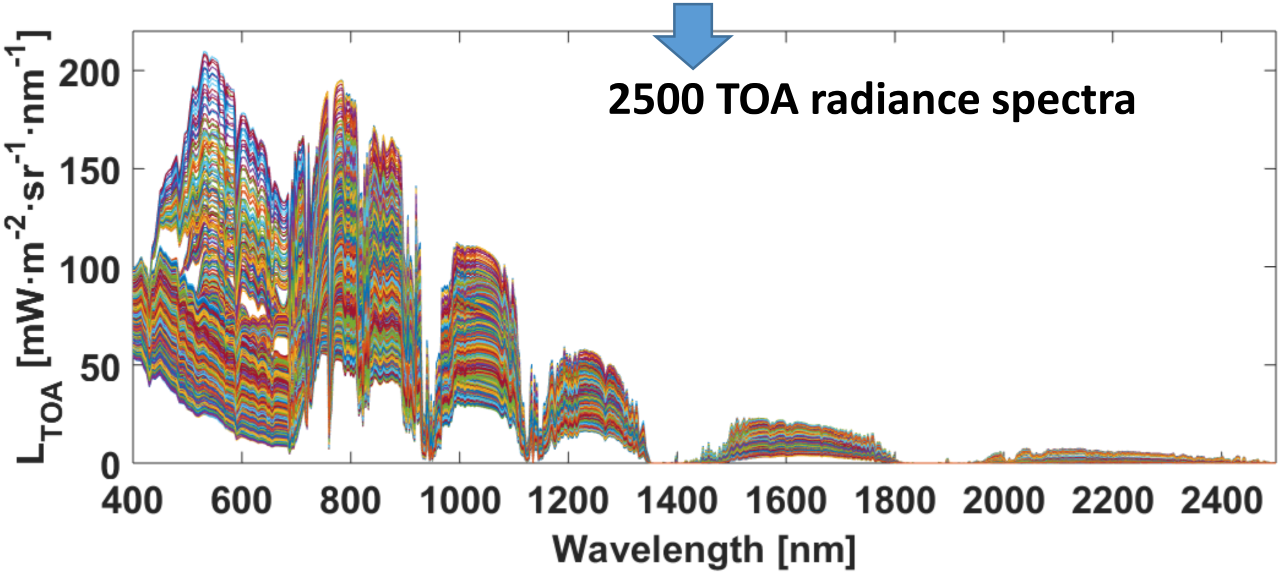


50 6S spectra



$$L_{TOA} = L_0 + \frac{T_{gas} \cdot E_{tot} \cdot T_{tot} \cdot \rho}{\pi(1 - S\rho)}$$

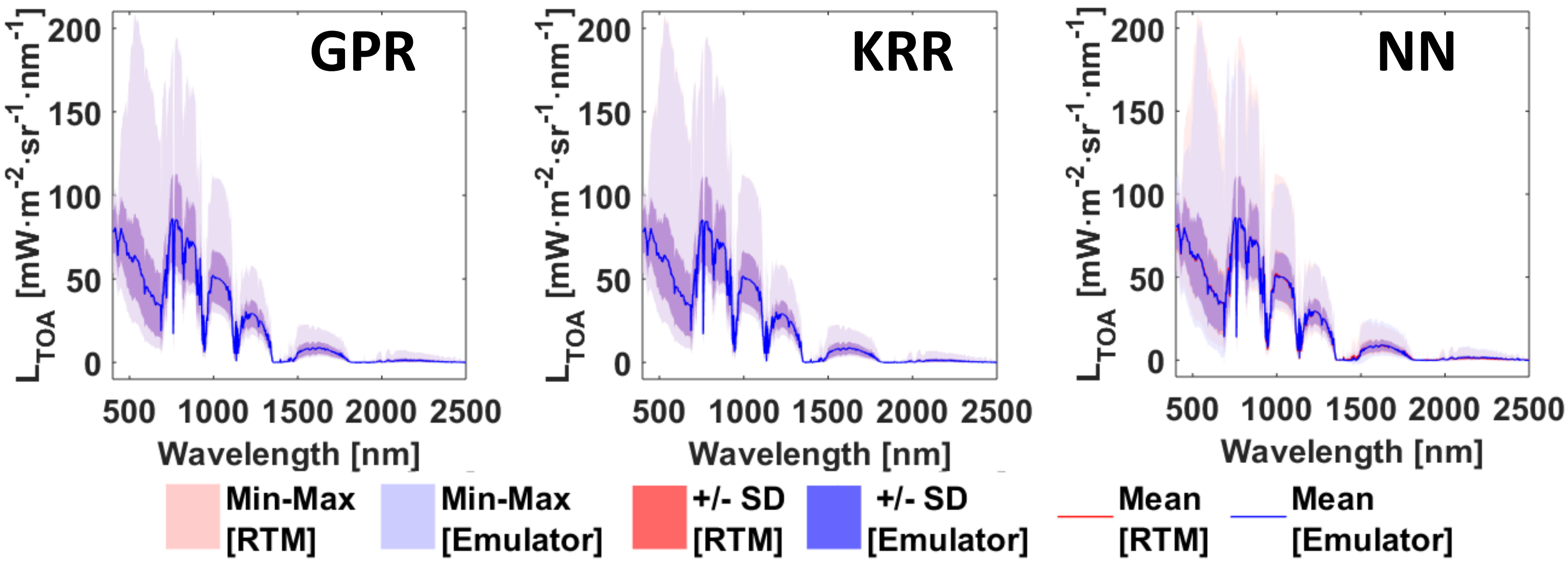
2500 TOA radiance spectra

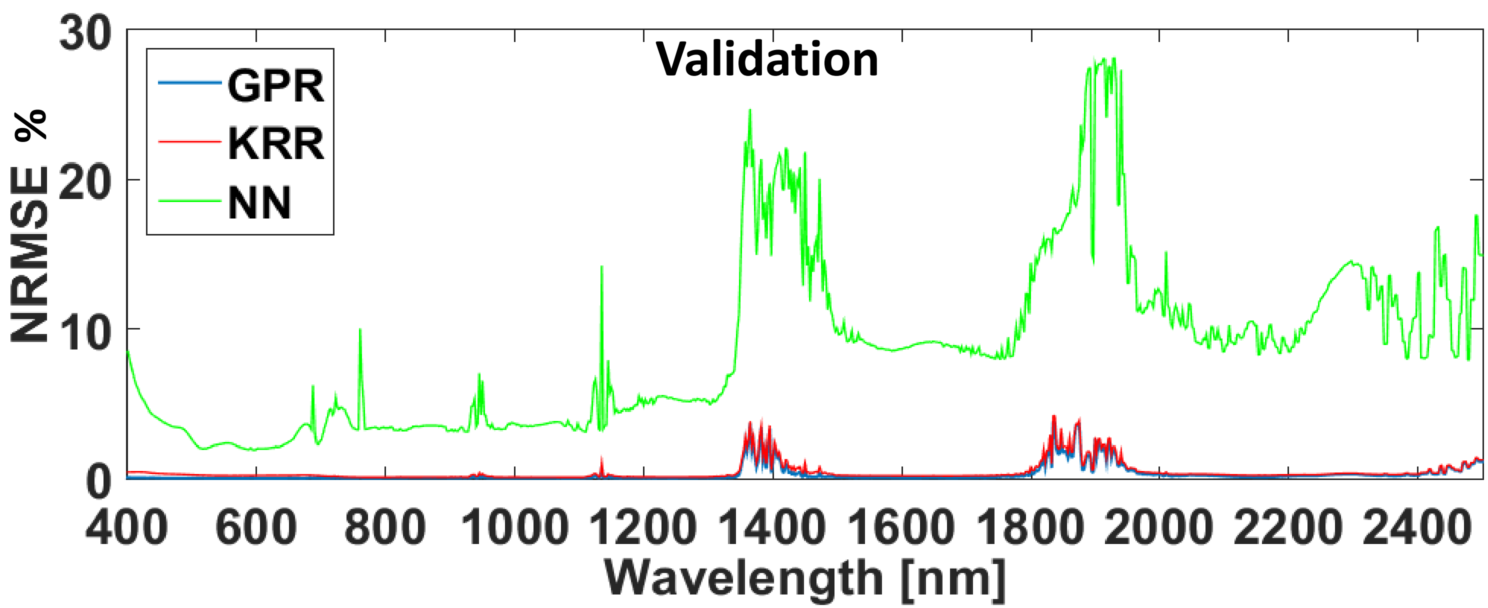


Emulator

- **30 PCA**
- **70/30% train/test**

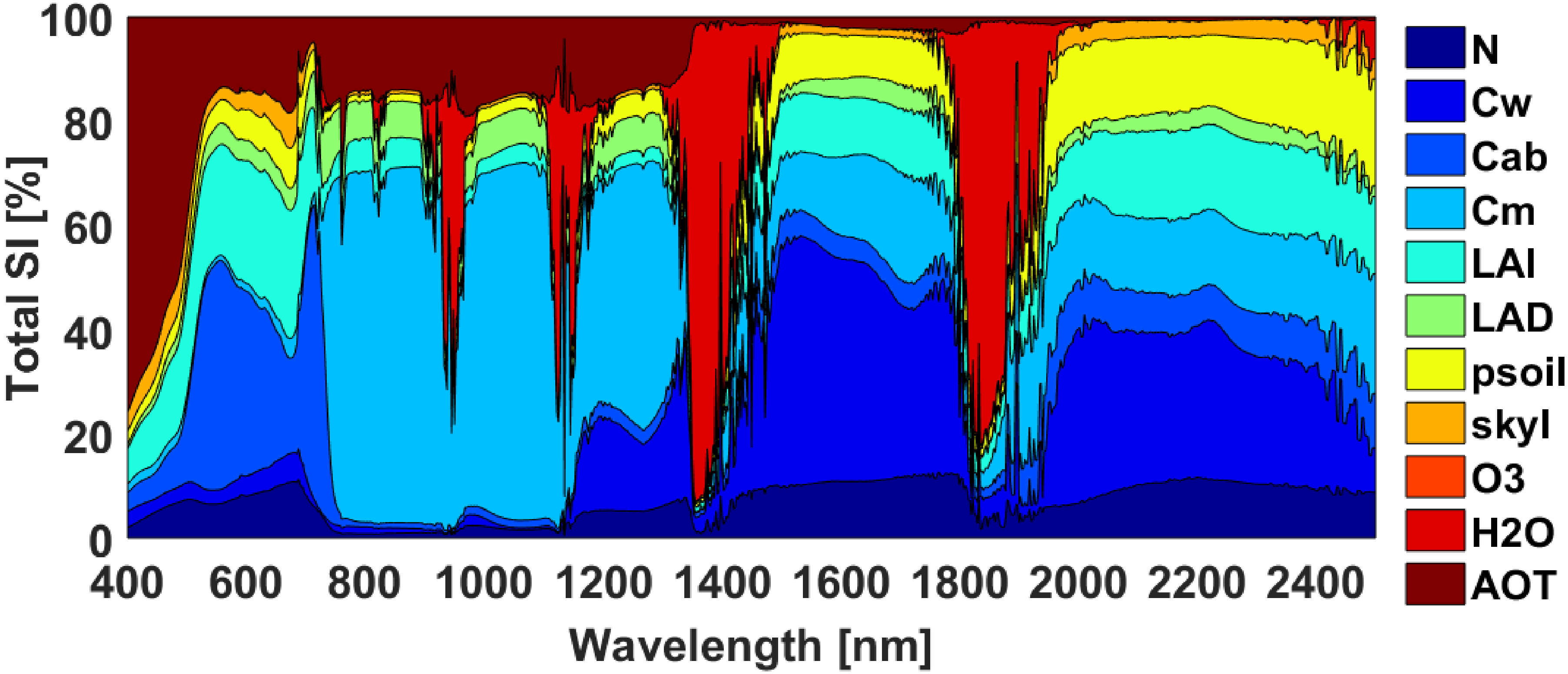
L_{TOA} Emulator results (2/3)





L_{TOA} GSA results GPR emulation (#1000/var) (3/3)

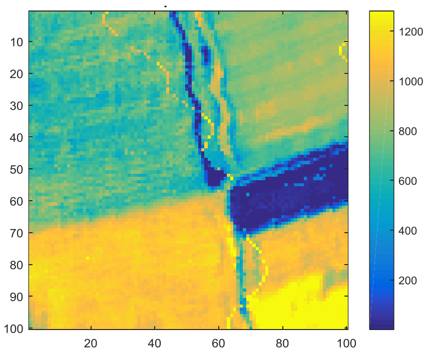
36 s



- Strong influence of AOT in visible.
- Strong influence of water absorption regions
- SWIR seems attractive for TOA retrieval of vegetation properties (hardly atmospheric effects).

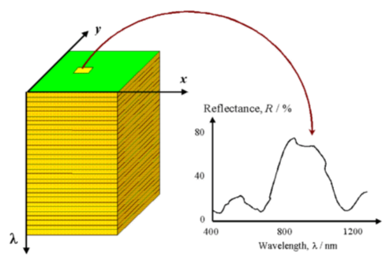
Applications (3/3)

Inversion



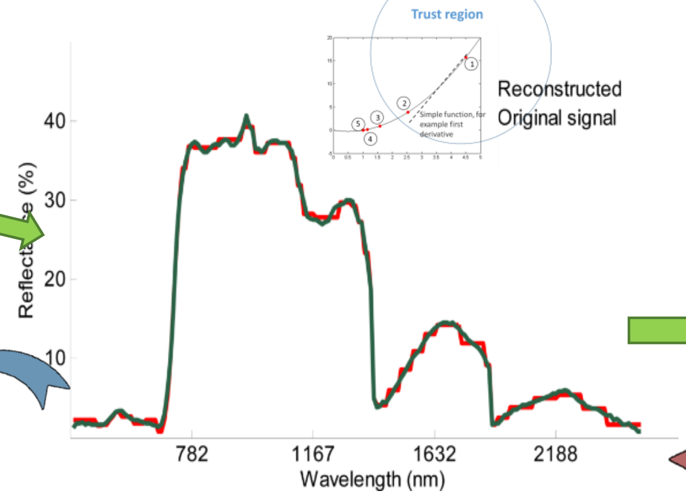
Emulators into numerical inversion

Image

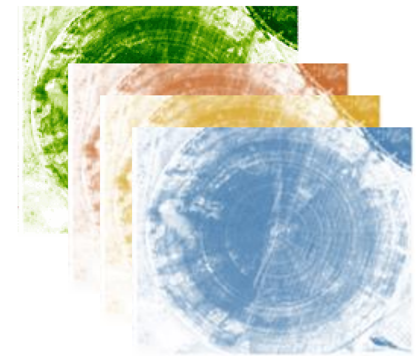


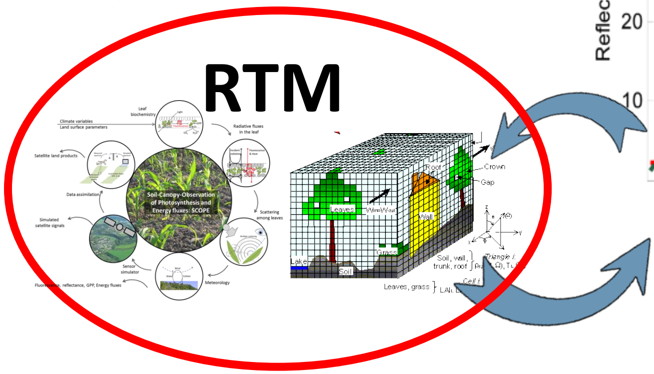
Spectral fitting:

Minimization algorithm: lsqnonlin



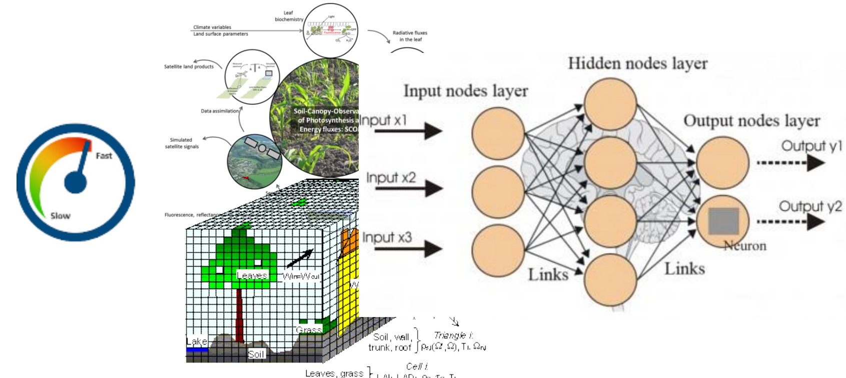
Output maps of RTM variables

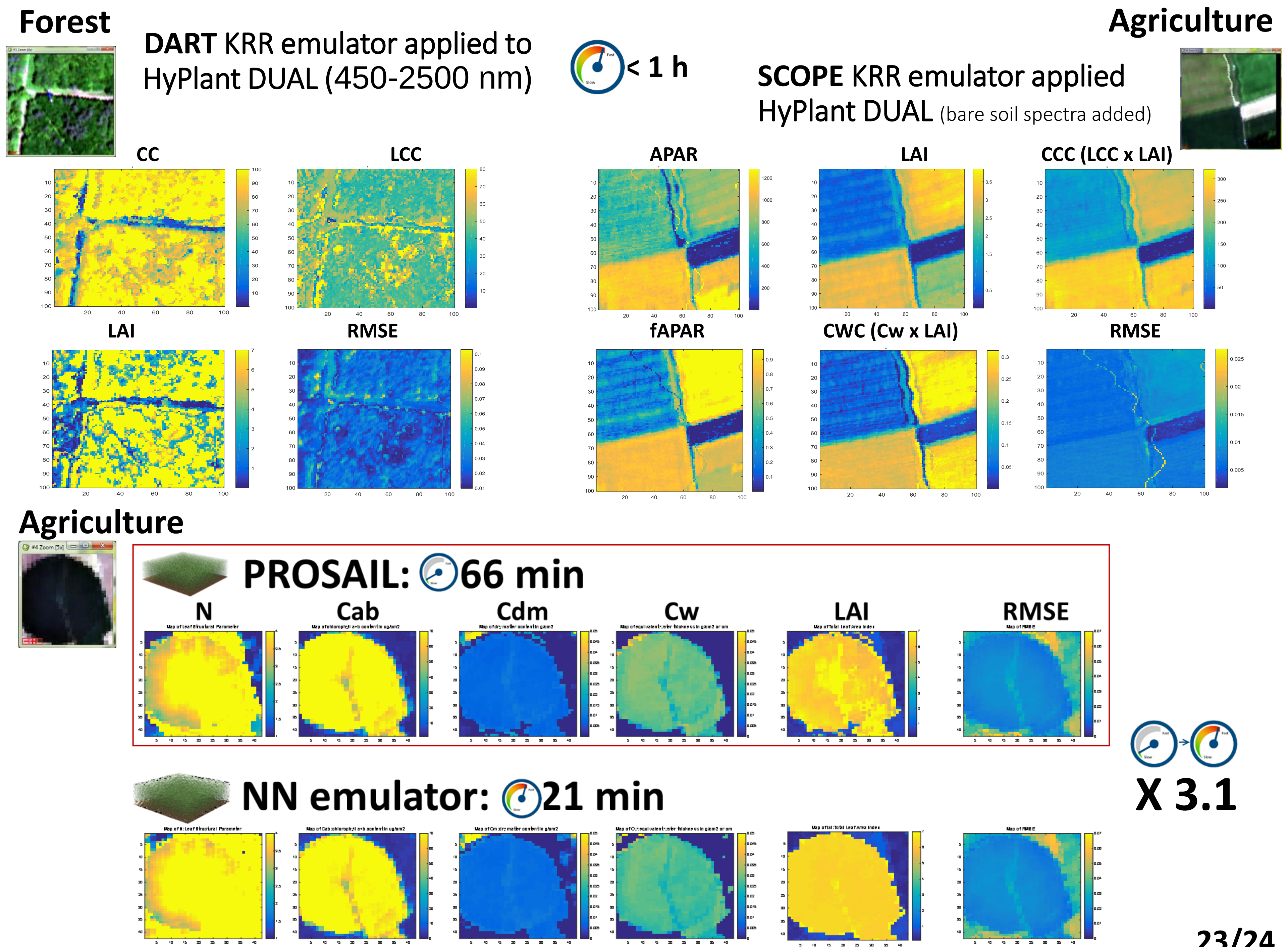




Per-pixel RTM iterations: very slow method, inapplicable to advanced RTMs.

Emulation of an RTM




Forest
DART KRR emulator applied to HyPlant DUAL (450-2500 nm)
< 1 h
Agriculture
SCOPE KRR emulator applied HyPlant DUAL (bare soil spectra added)
CC
LCC
APAR
LAI
CCC (LCC x LAI)
LAI
RMSE
fAPAR
CWC (Cw x LAI)
RMSE
Agriculture
PROSAIL: 66 min
N
Cab
Cdm
Cw
LAI
RMSE
NN emulator: 21 min
X 3.1

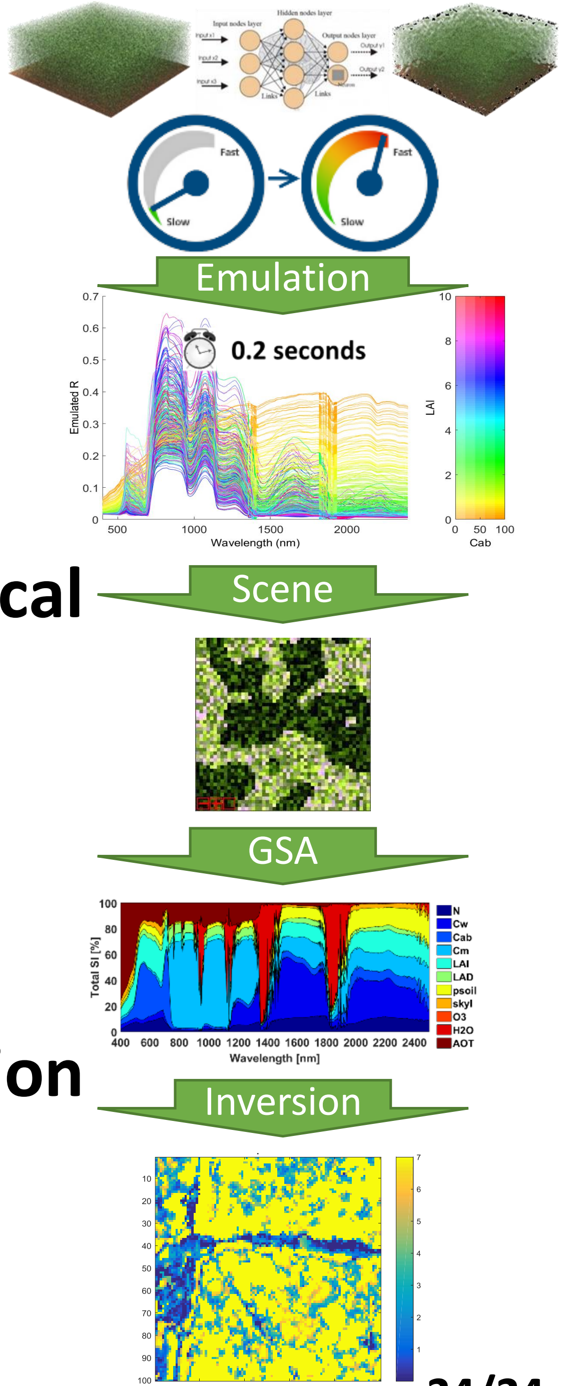
Take home messages

Emulation approximates physical models with sufficient accuracy and tremendous gain in speed.

✓ **Emulation permits fast rendering of optical images**

✓ **Emulation permits fast calculation of global sensitivity analysis**

✓ **Emulation permits fast numerical inversion of RTM against an image for biophysical variables retrieval**



Thanks!

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More talks about emulation:

1) **Jorge Vicent:** TU1.R7.4: **STATISTICAL LEARNING FOR END-TO-END SIMULATIONS** (09:30 - 09:50)

2) **Jochem Verrelst:** TU4.R9.5: **APPROXIMATING EXPERIMENTAL VEGETATION SPECTROSCOPY DATA THROUGH EMULATION** (18:10-18:30)

3) **Daniel Heestermans**: WE2.R7.5 **MULTIOUTPUT AUTOMATIC EMULATOR FOR RADIATIVE TRANSFER MODELS** (12:30-12:50)