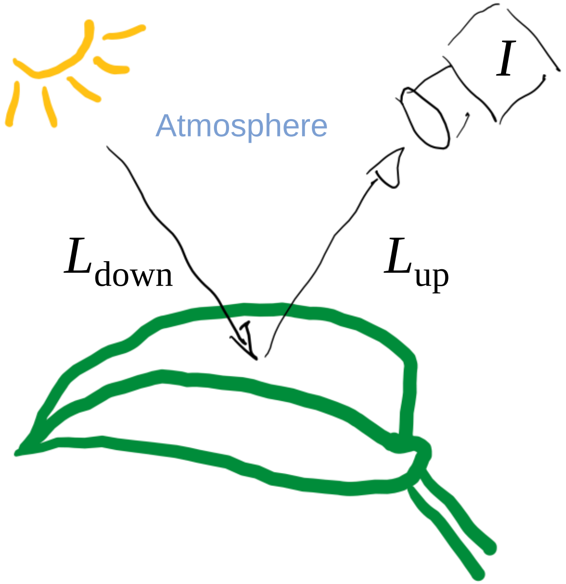
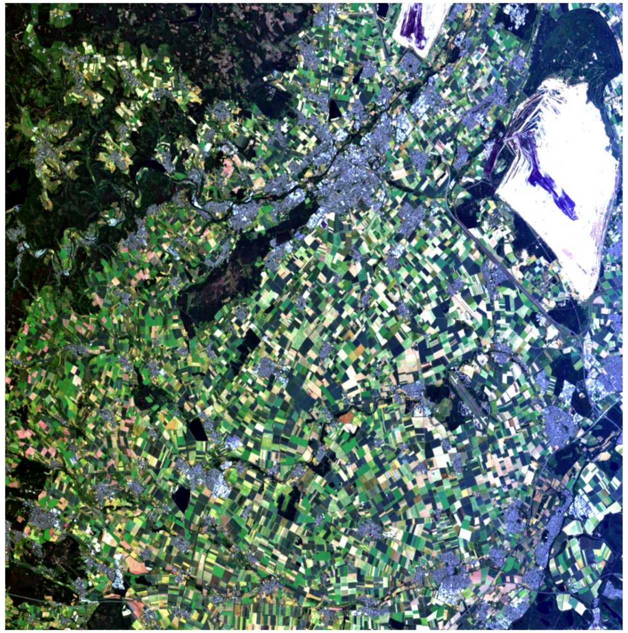
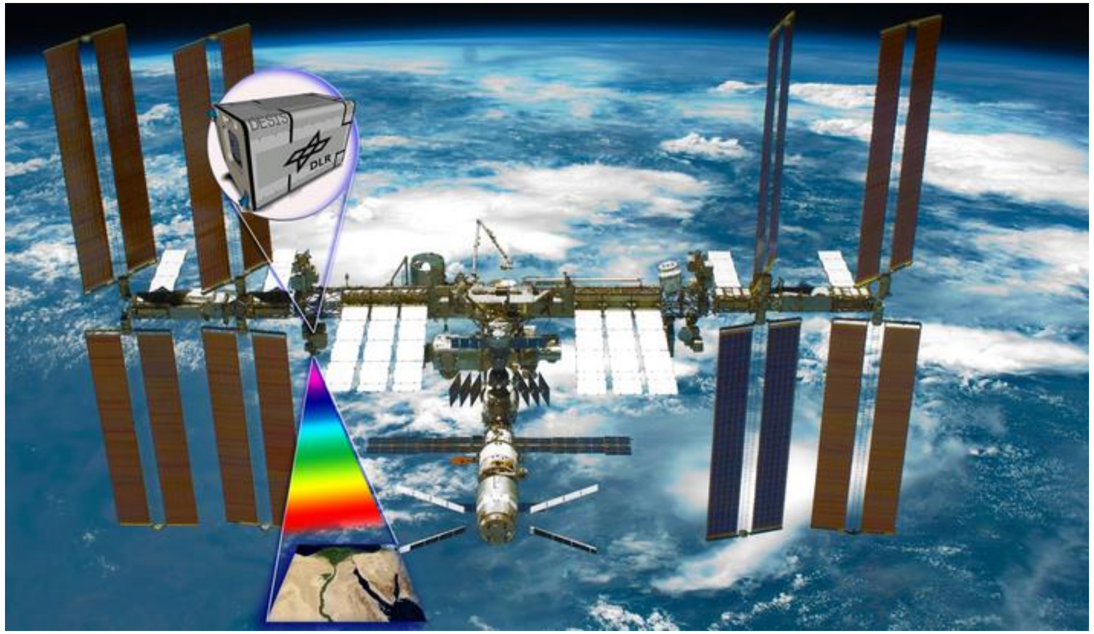






A DEEP-LEARNING-BASED METHOD FOR THE RETRIEVAL OF SUN-INDUCED PLANT FLUORESCENCE FROM AIRBORNE AND SPACEBORNE HYPERSPECTRAL IMAGERY

Hanno Scharr, Data Analytics and Machine Learning, Forschungszentrum Jülich

Helmholtz Association

Mission: Research towards answering major and pressing questions of science, society, and industry

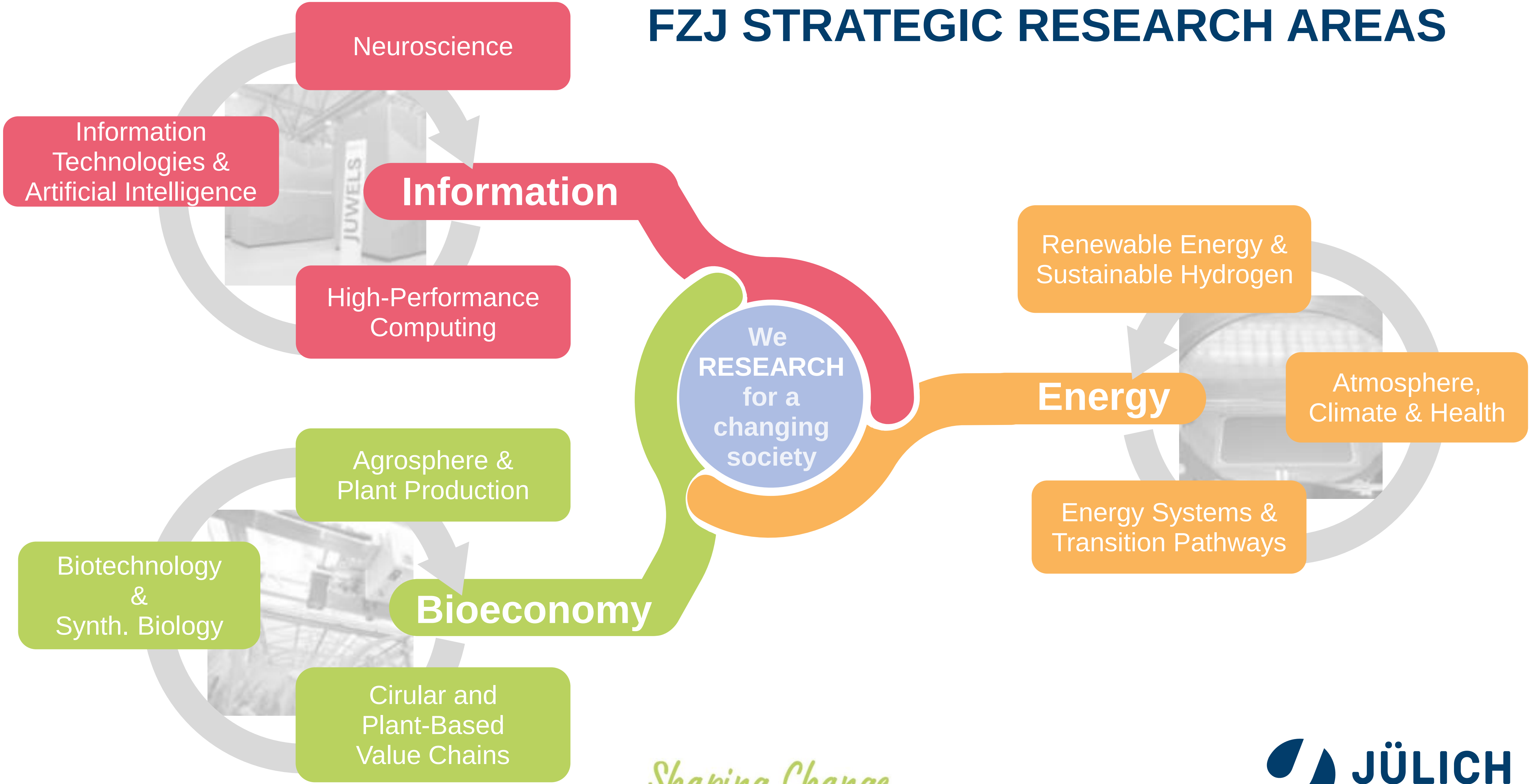
- 18 national labs
- 46,000 employees
- 14,500 international guest researchers
- 6B€/a budget

Forschungszentrum Jülich at a glance

> 7000 staff, 14 Institutes, 1.0B€/a budget, 1.7km² campus

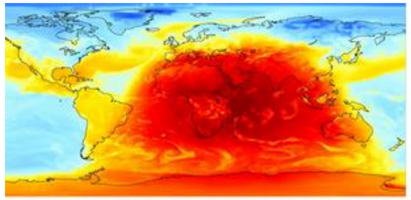
JÜLICH
Forschungszentrum

FZJ STRATEGIC RESEARCH AREAS



Institute of Climate and Energy Systems (ICE)

Climate Institutes at Jülich




ICE-3: Troposphere (~110 staff)

- Explores the chemistry of the troposphere
- Performs global observations
- Simulates atmospheric chemistry and transport processes by numerical models

ICE-4: Stratosphere (~60 staff)

- Chemistry, dynamics, and microphysics of the stratosphere and tropopause
- Role of these layers in the climate system

Atmospheric Research at Jülich

From Observations to Process Understanding to Earth System Models: Troposphere and Stratosphere

Atmospheric Research at Jülich

Atmospheric Observations

- Field campaigns with strategic partnerships
- Leading roles in EU infrastructures

Atmospheric Process Understanding

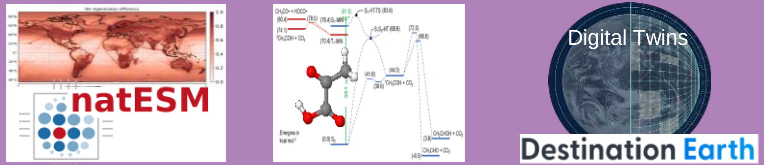
- Holistic understanding by simulation of atmospheric processes at atmospheric conditions

Predictability of Air Quality and Climate Warming in the changing Earth and Energy systems

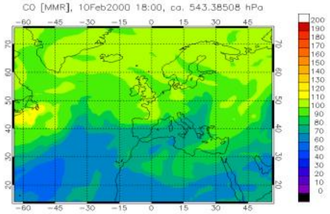
High Quality Data / Instrument Development

- State-of-the art, high-quality (new) instrumentation
- Provision of quality-controlled FAIR data
- Use of new instruments by (industry) partners

Theory / Earth System Model Development



- Exascale-ready model development
- Exploring machine learning approaches
- Connecting to energy system modelling

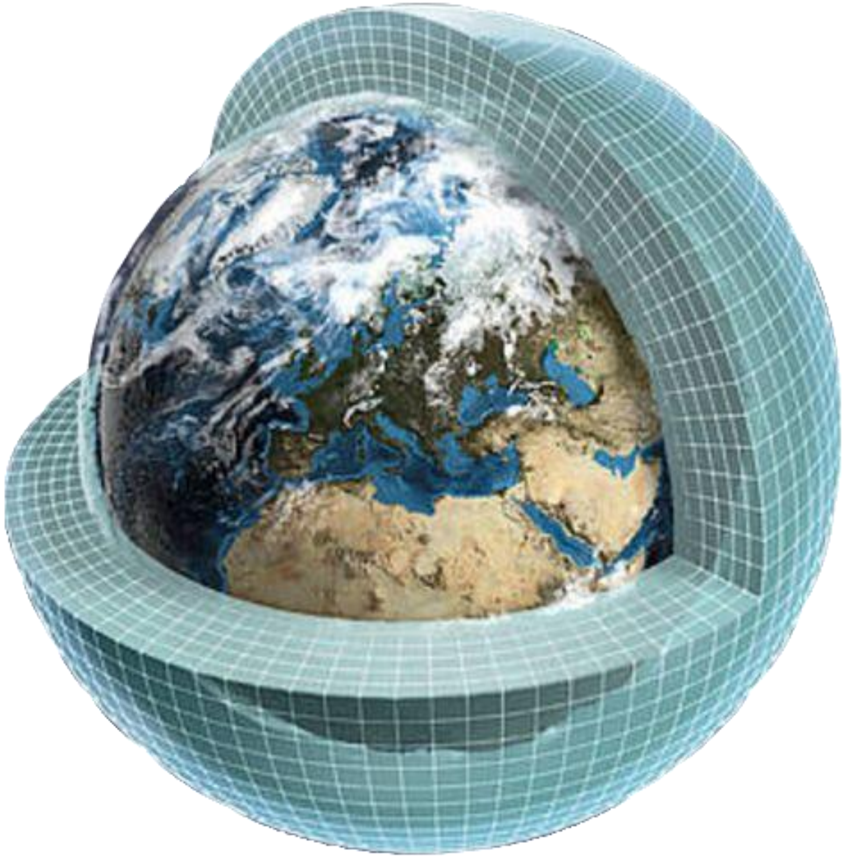


Operational chemical weather forecast
Copernicus Atmospheric Service, IPCC

JÜLICH Forschungszentrum

Traditional Earth System Modelling

Atmosphere dynamics



[Bildquelle](#)

Variables: $\{\mathbf{v}, p, T, \rho, q\}$

$$\frac{d}{dt}\mathbf{v} = -2\mathbf{\Omega} \times \mathbf{v} - \frac{1}{\rho}\nabla_3 p + \mathbf{g} + \mathbf{F}$$

Conservation of momentum (Navier-Stokes)

$$C_v \frac{d}{dt}(\rho q) + p\frac{d}{dt}\left(\frac{1}{\rho}\right) = J$$

Conservation of energy (1st Law of Thermodynamics)

$$\frac{\partial}{\partial t}(\rho) = -\nabla_3 \cdot (\rho \mathbf{v})$$

Conservation of air mass

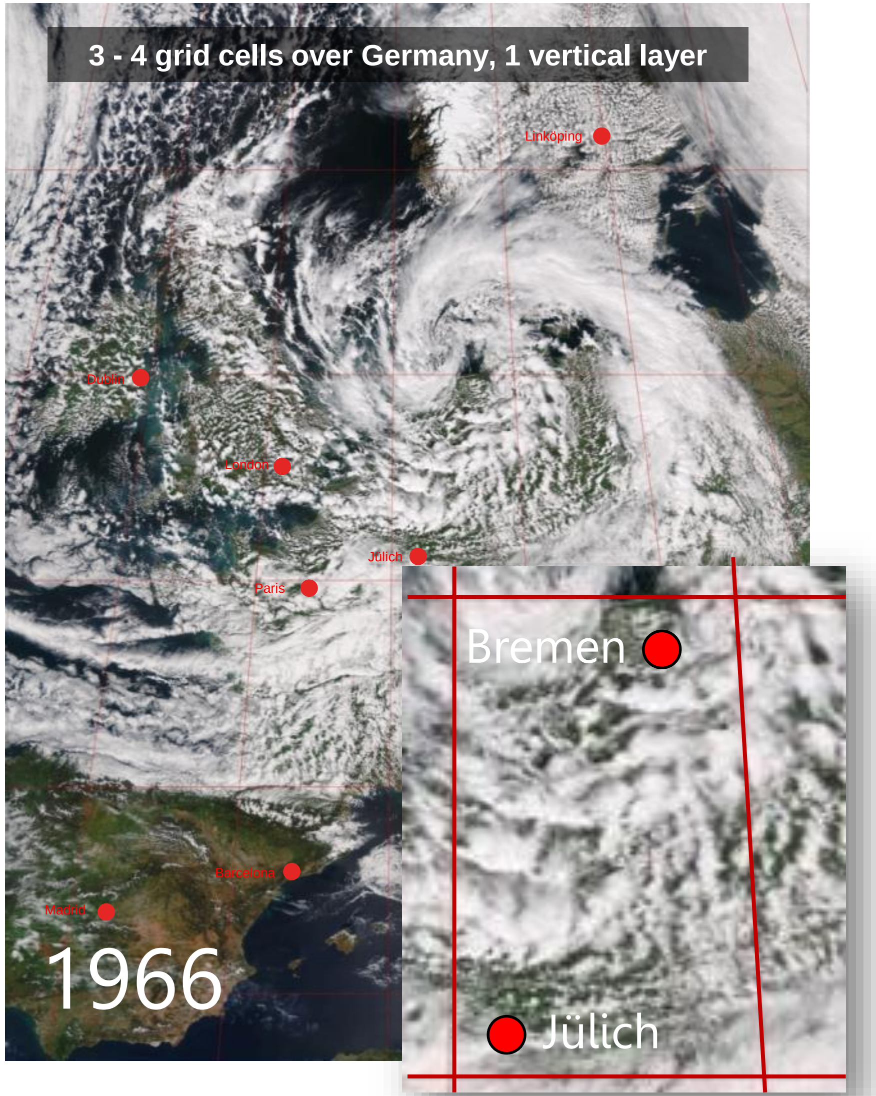
$$\frac{\partial}{\partial t} = -\nabla_3 \cdot (\rho \mathbf{v} q) + \rho\,(E - C)$$

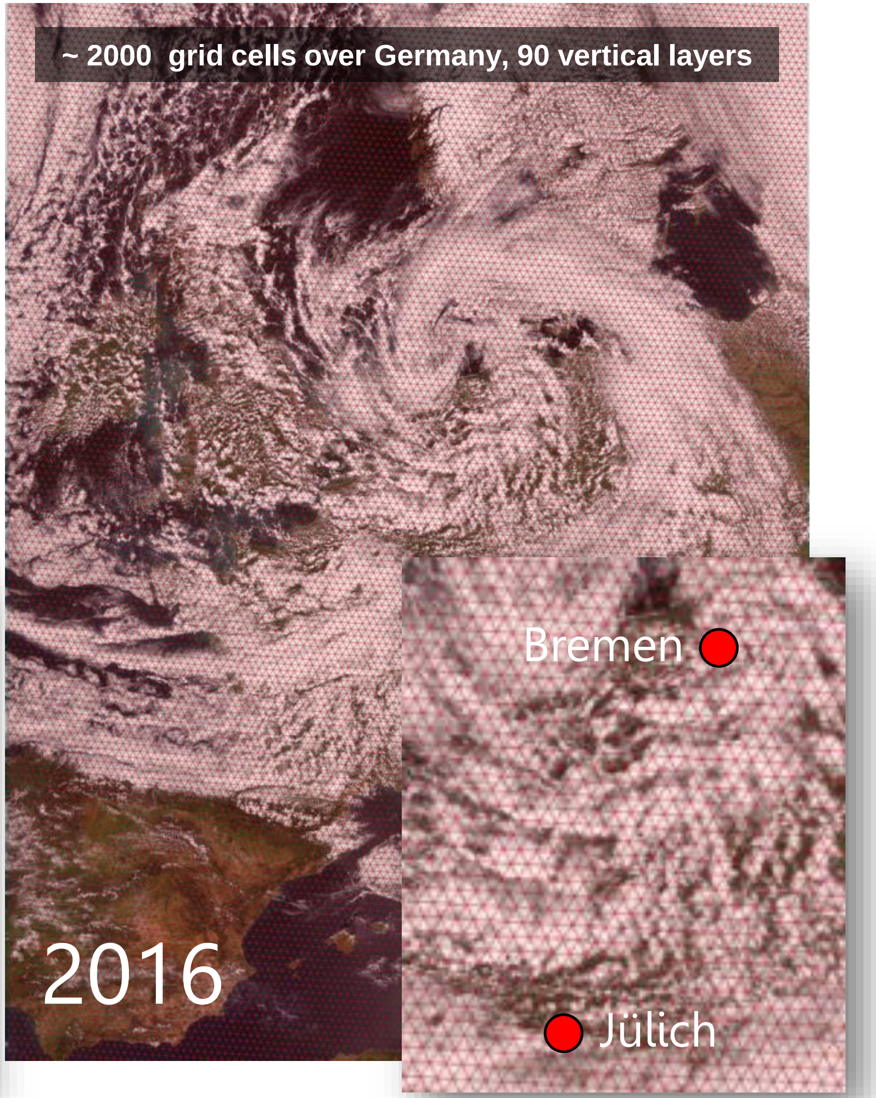
Continuity of water vapor mass

$$p = \rho R T$$

Equation of state (Ideal gas law)

Progress in numerical weather forecasts





Increased compute power

1967 : 0,7 Mflops

1976 : 130 Mflops (Cray-1)

1990 : 23 Gflops (NEC)

2002 : 36 Tflops (NEC)

2009 : 1 Pflops (JUGENE)

2021*: 73 Pflops (JUWELS Booster)

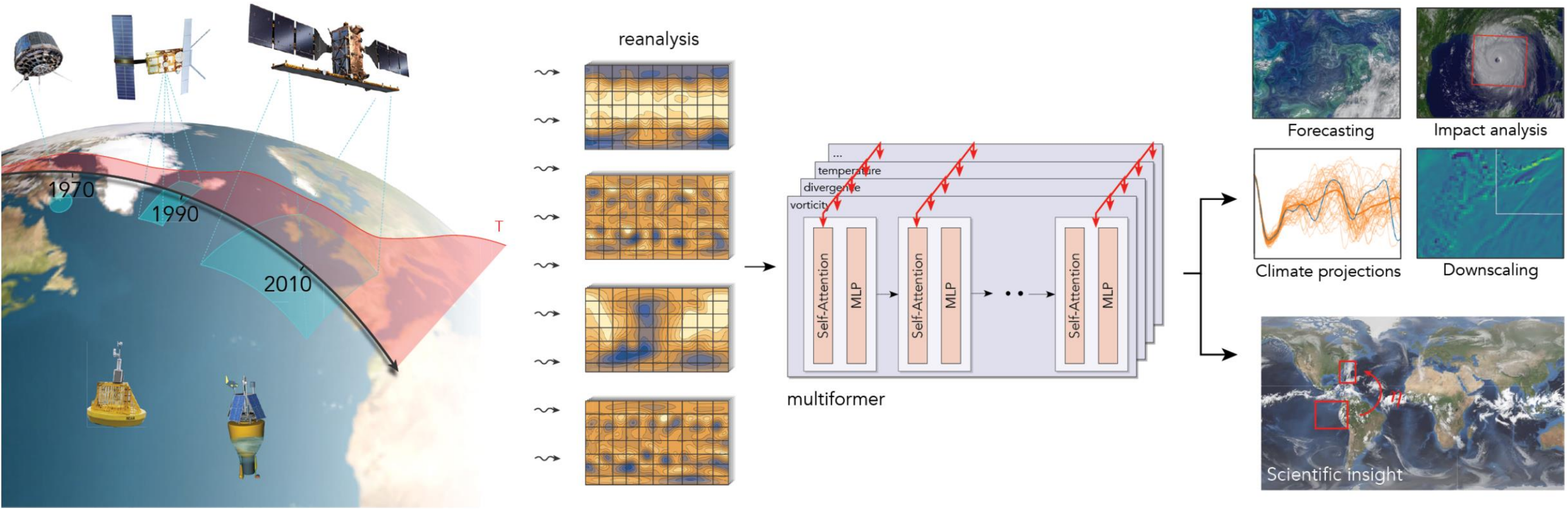
2025*: >90 Eflops (JUPITER)

* Accelerator technology (GPUs)

Current resolution of the DWD weather models: global = 13 km, regional = 2,1 km

AtmoRep: A stochastic model of atmosphere dynamics

Trained using large scale representation learning (Masked Auto-Encoder)



Lessig et al. https://arxiv.org/abs/2308.13280

Martin Schultz, Earth System Data Exploration Group, JSC

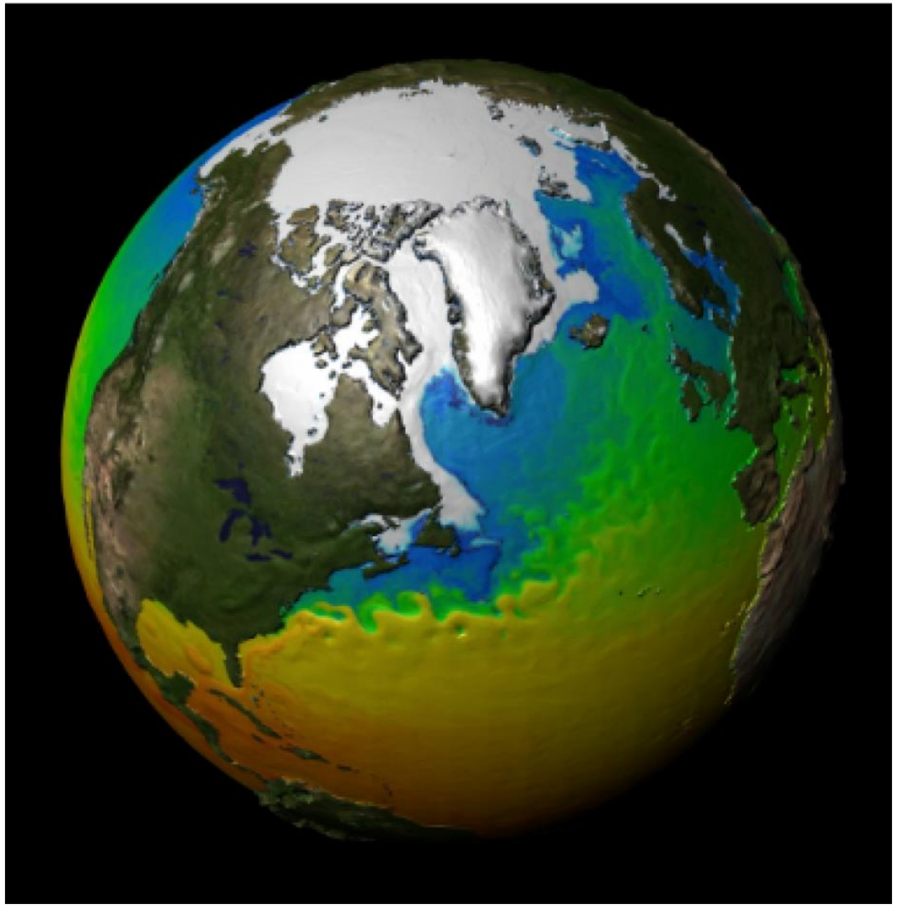
ECMWF: European Center for Medium Weather Forecast

ECMWF CERN JÜLICH Forschungszentrum JÜLICH SUPERCOMPUTING CENTRE

HClimRep: Helmholtz Foundation Model for Climate Science

Will be the first Earth system foundation model including the troposphere, stratosphere, ocean, sea ice, and hydrology

- **Seasonal-to-decadal** AI-based simulations
- First **climate-capable** foundation model, incorporating
  - multiple grids and resolutions,
  - atmosphere-ocean-sea ice coupling, and a
  - wide range of available data
- **Generalization across tasks**
  - support for prediction, data assimilation,
  - uncertainty quantification, and counterfactual scenarios
- **Downstream applications** demonstrate potential for future climate research and services



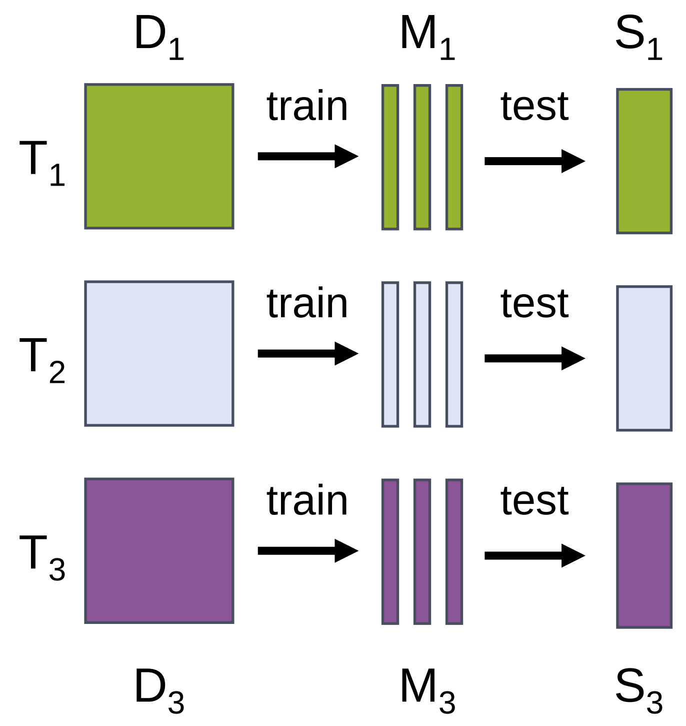
source

Lead: Jülich, IAS/JSC, Martin Schultz
Project start 2024, duration 36 months

FOUNDATION MODELS

State of the Art: Predictive and Generative AI with large Foundation Models

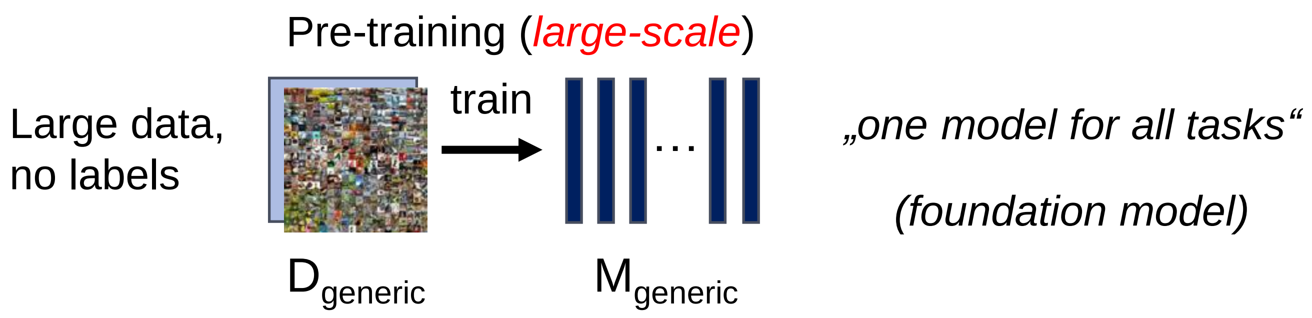
Classic supervised machine learning



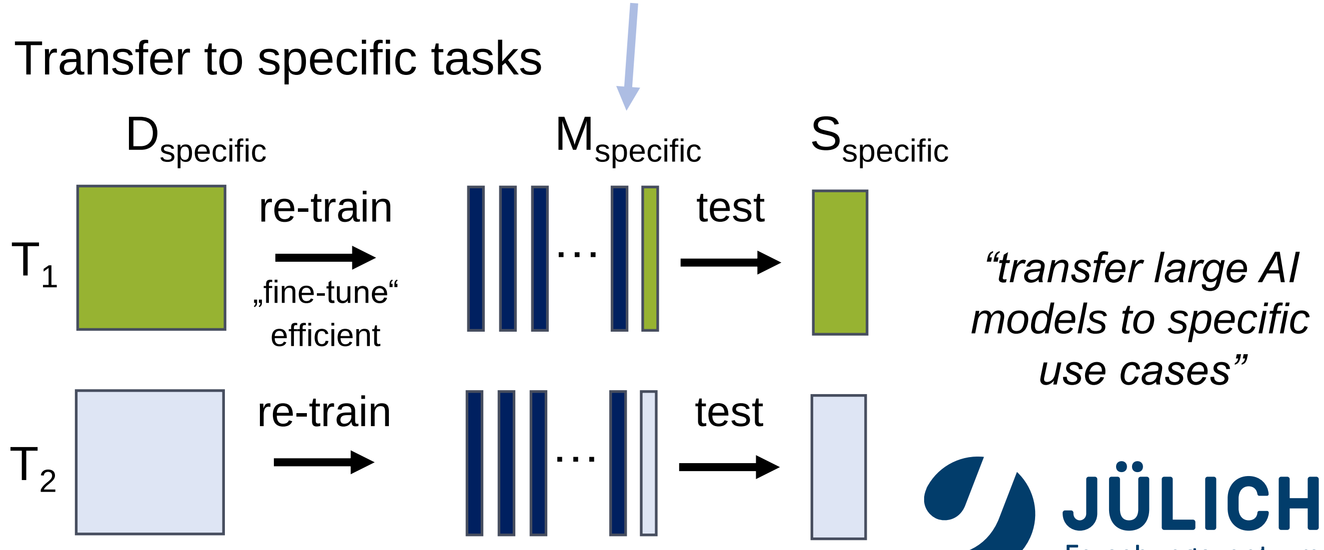
- poor generalization and transfer
- labeled data for each task
- no model re-use

Foundation models: generic transferable learning

1. Self-supervised pre-training of large-scale models



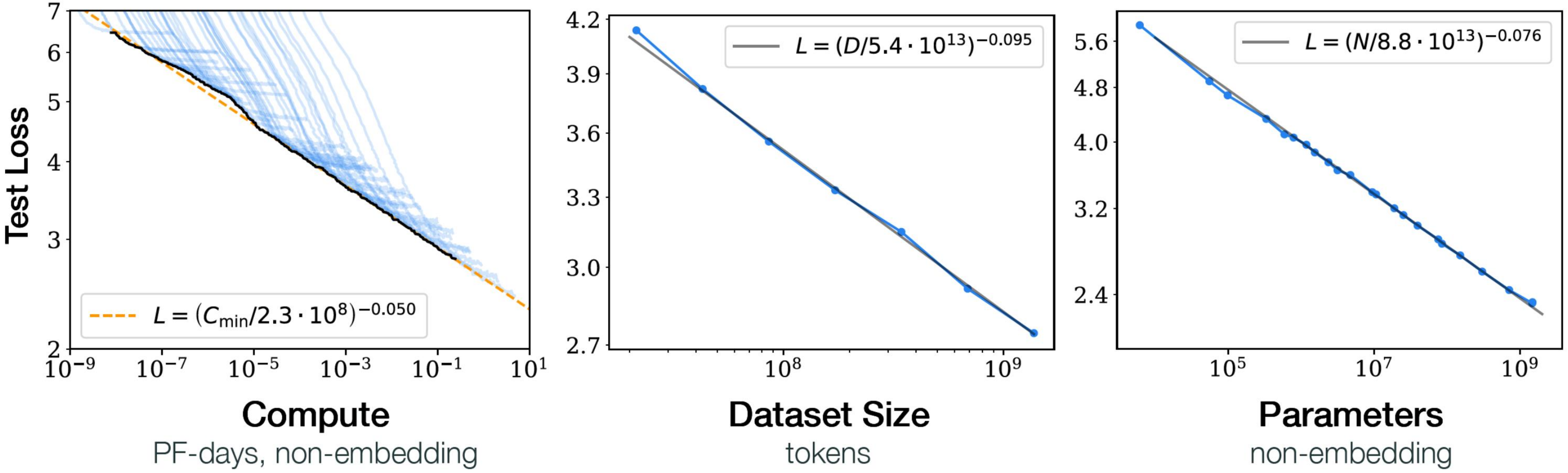
2. Transfer to specific tasks



FOUNDATION MODELS

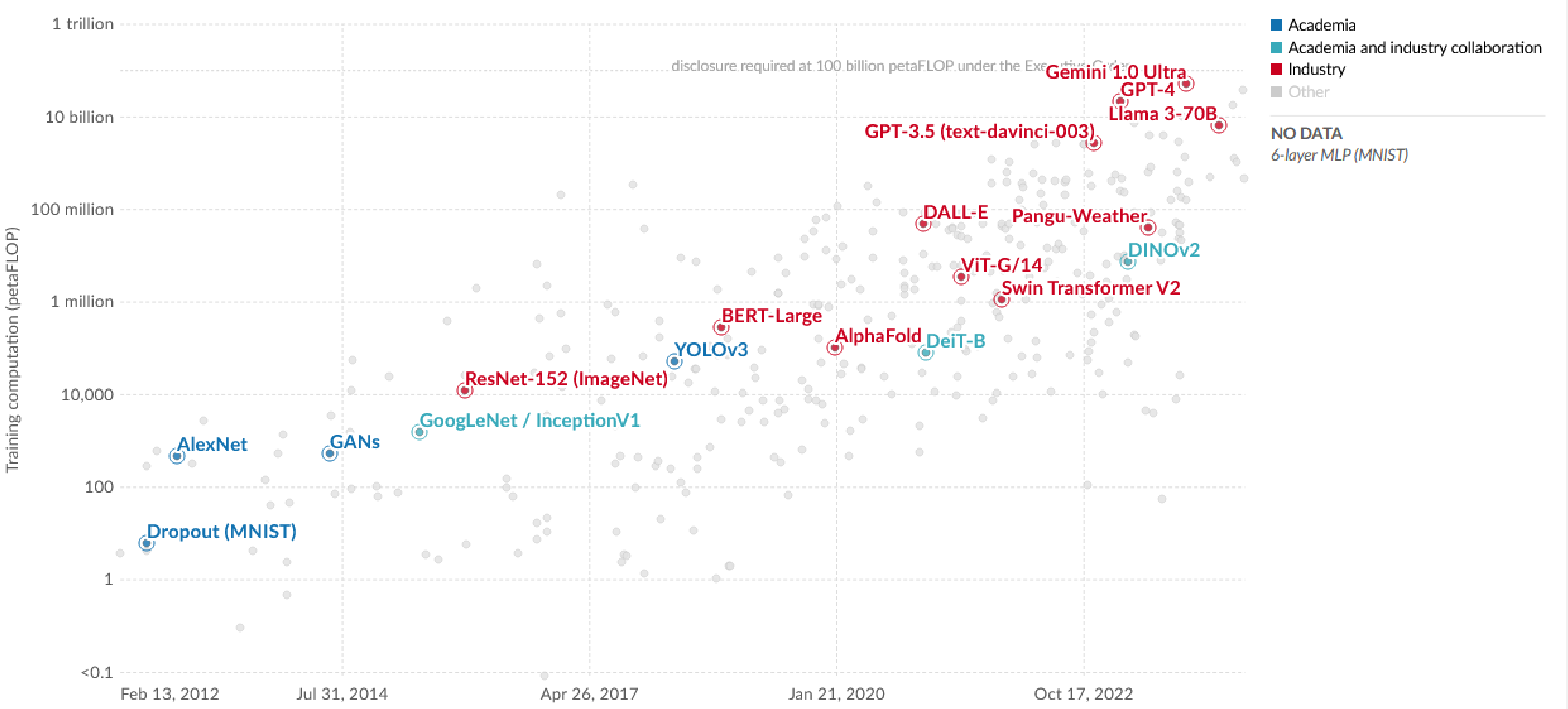
Scaling Laws in AI

- **Scaling Laws**: larger model, data and compute scale during pretraining lead to **stronger generalization and transferability**
- **No change** in algorithmic procedure. Just scale up and important generic functions – e.g. generalization - get better



Source: Kaplan et al. 2020, https://arxiv.org/abs/2001.08361

Trend: larger models, larger data, larger compute

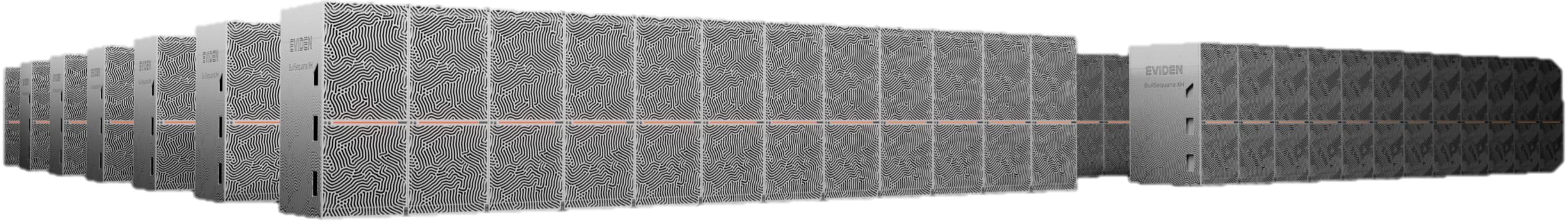


Source: https://ourworldindata.org/grapher/artificial-intelligence-training-computation

HAPPENING NOW: JUPITER Ascending

A MODULAR EXASCALE COMPUTER

93 ExaFLOPS of AI | 1.0 ExaFLOPS for HPC | 24,000 GH200



EuroHPC Joint Undertaking

ParTec MODULAR SUPERCOMPUTING

Bundesministerium für Bildung und Forschung

EVIDEN an atos business

Ministerium für Kultur und Wissenschaft des Landes Nordrhein-Westfalen

NVIDIA

JEDI

JUPITER EXASCALE DEVELOPMENT INSTRUMENT

JEDI

Energy efficiency: rank 1 world-wide

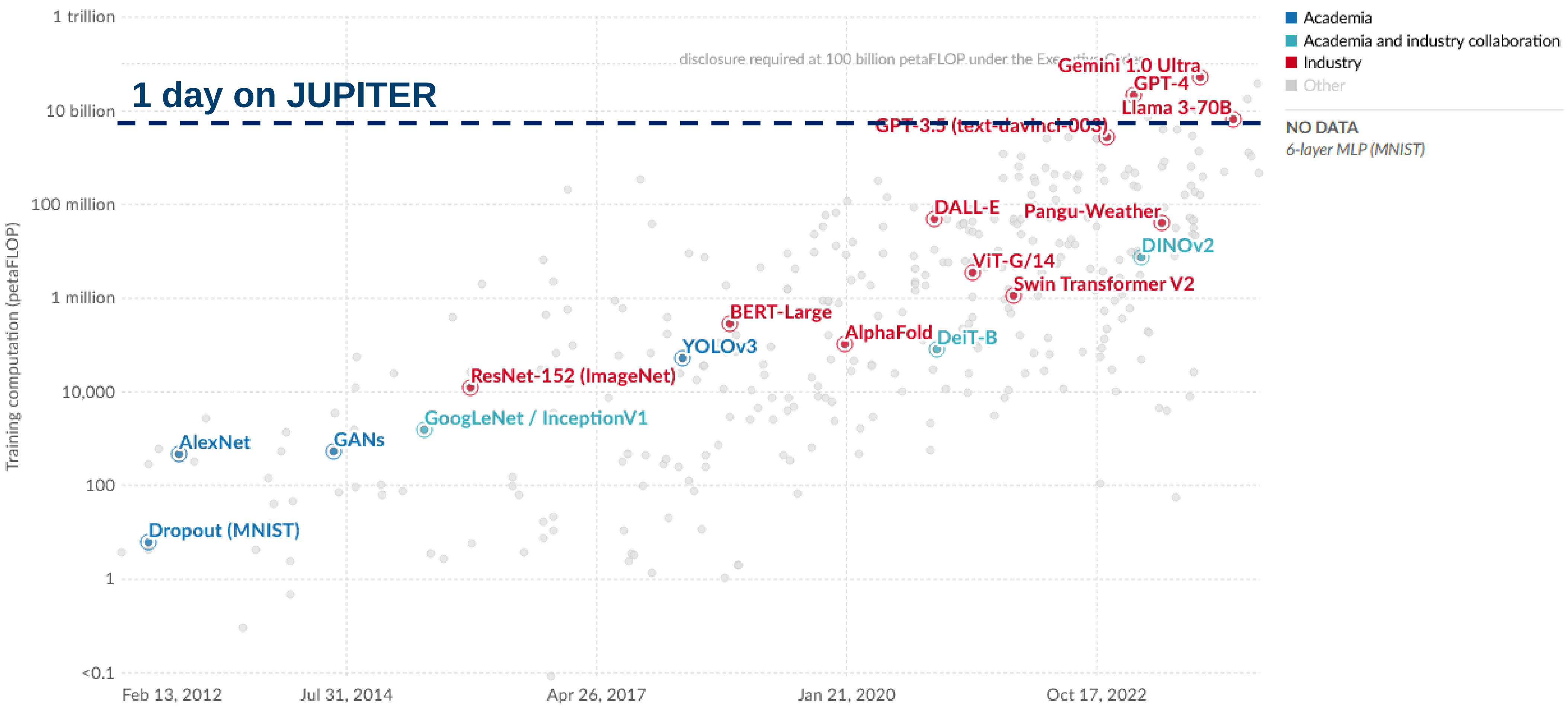
Rank	TOP500 Rank	System	Cores	Rmax (PFlop/s)	Power (kW)	Energy Efficiency (GFlops/watts)
1	189	**JEDI** - BullSequana XH3000, Grace Hopper Superchip 72C 3GHz, NVIDIA GH200 Superchip, Quad-Rail NVIDIA InfiniBand NDR200, ParTec/EVIDEN EuroHPC/FZJ Germany	19,584	4.50	67	72.733

JUNE 2024

TOP500 The List.

JUPITER AI Performance Estimate: 93 exaflop/s

State of the Art: Predictive and Generative AI with large foundational models



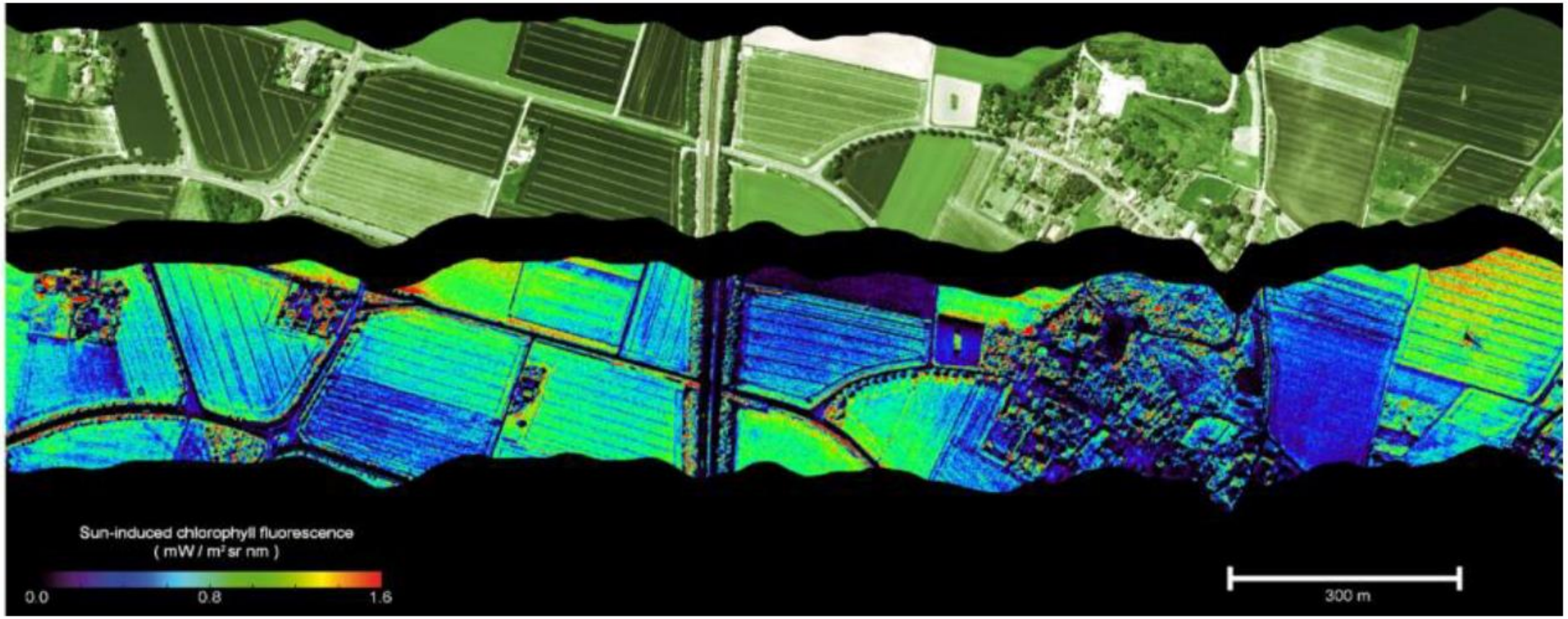
Source: https://ourworldindata.org/grapher/artificial-intelligence-training-computation

ML-based Fluorescence Retrieval from Optical Satellite Data

Helmholtz AI project FluoMap with IBG-2: Plant Sciences and German Aerospace Center (DLR)

Infer Plant Fluorescence from Hyperspectral Imaging Data

- Fluorescence contains information on status of plant photosystem, i.e. photosynthetic activity.
- Available on **close range and flat terrain** e.g. using spectral fitting method (SFM), i.e. physical model fitting.

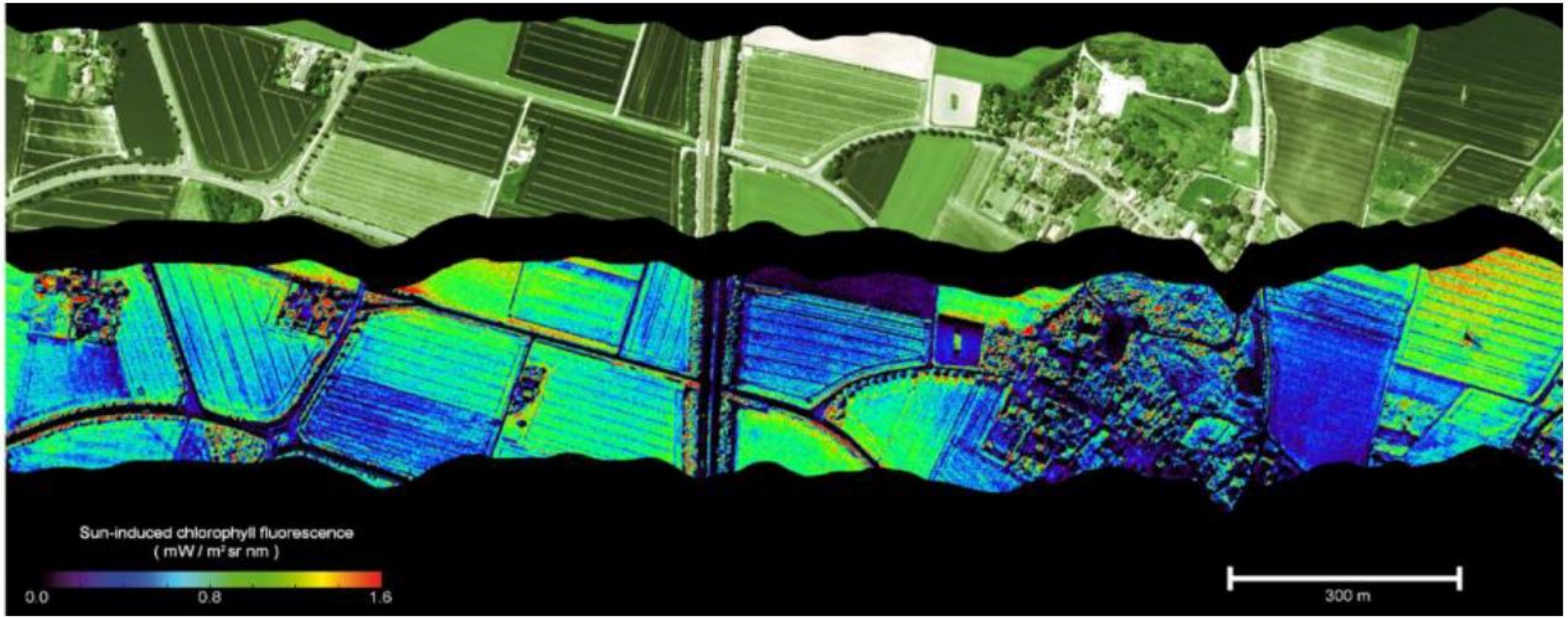


ML-based Fluorescence Retrieval from Optical Satellite Data

Helmholtz AI project FluoMap with IBG-2: Plant Sciences and German Aerospace Center (DLR)

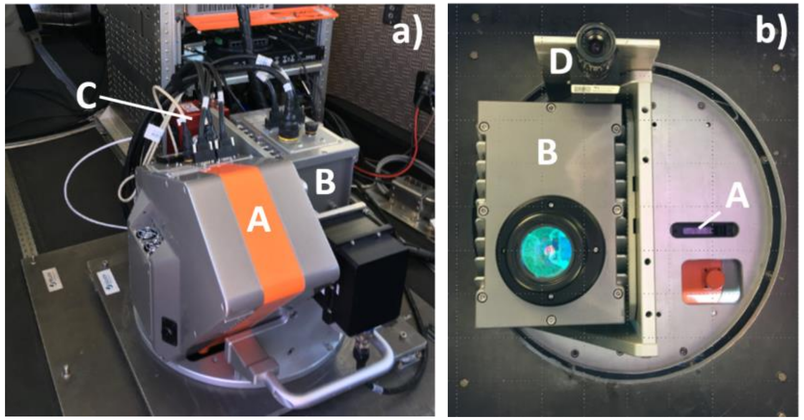
Project goal

- Devise method allowing to use satellite data for SIF retrieval – consider elevation and atmosphere
- High risk: Use spectrally low resolved DESIS data

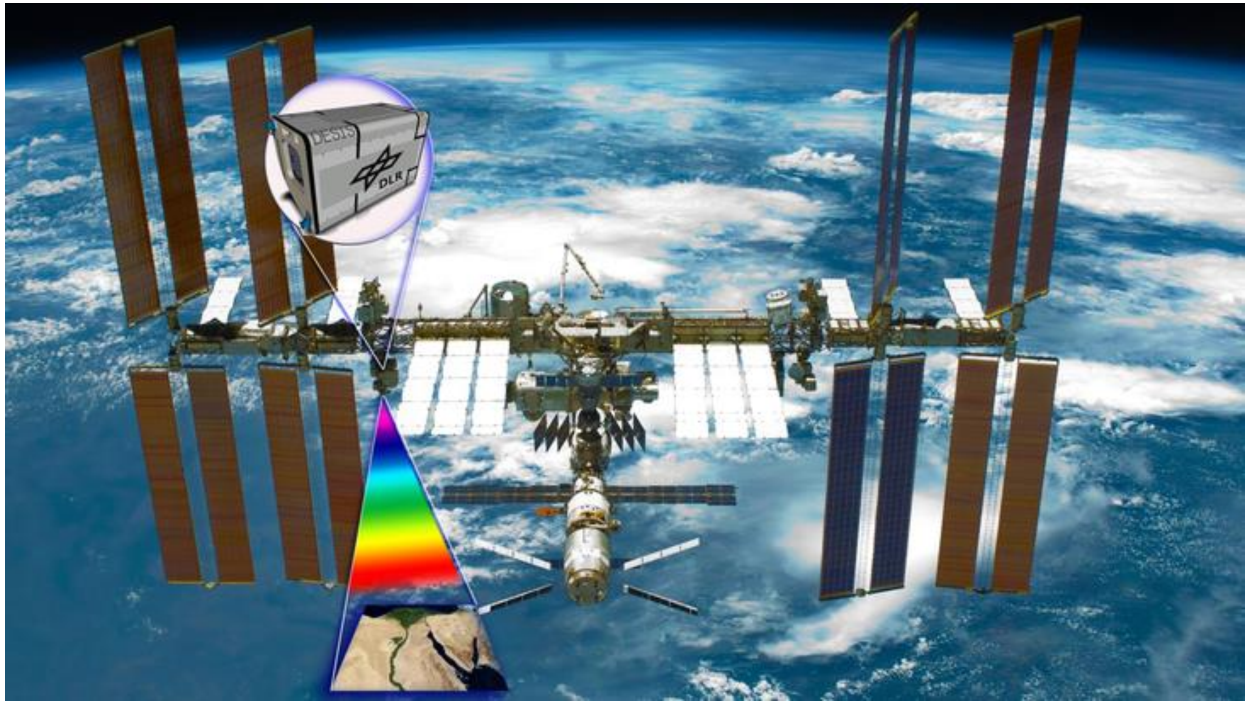


DLR JÜLICH Forschungszentrum

Hyperspectral imaging sensors: DESIS on ISS and HyPlant for FLEX



HyPlant airborne hyperspectral imaging sensor. Precursor for FLEX
Operated by FZJ, IBG-2

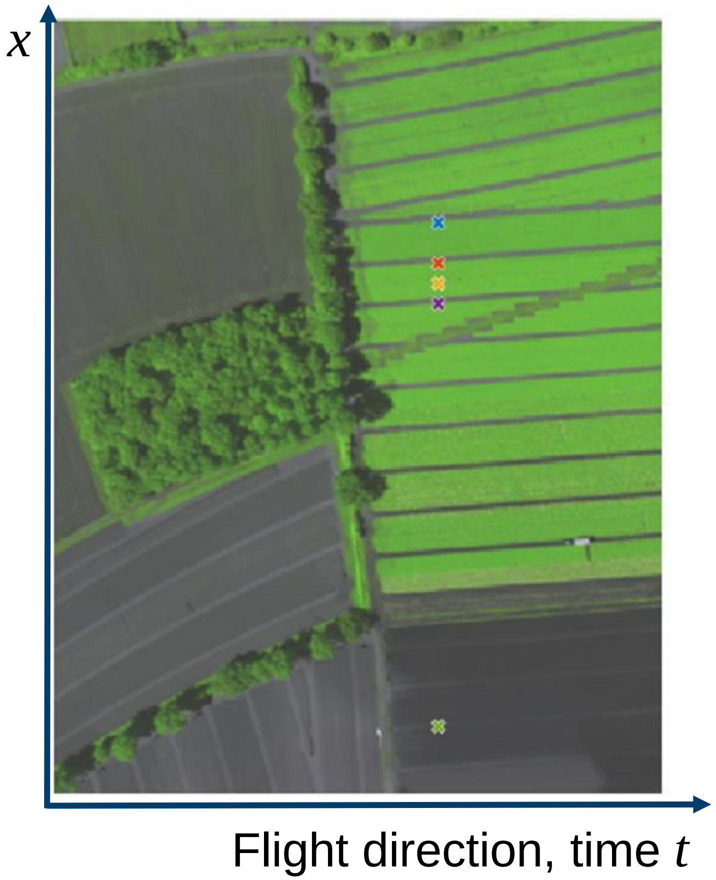


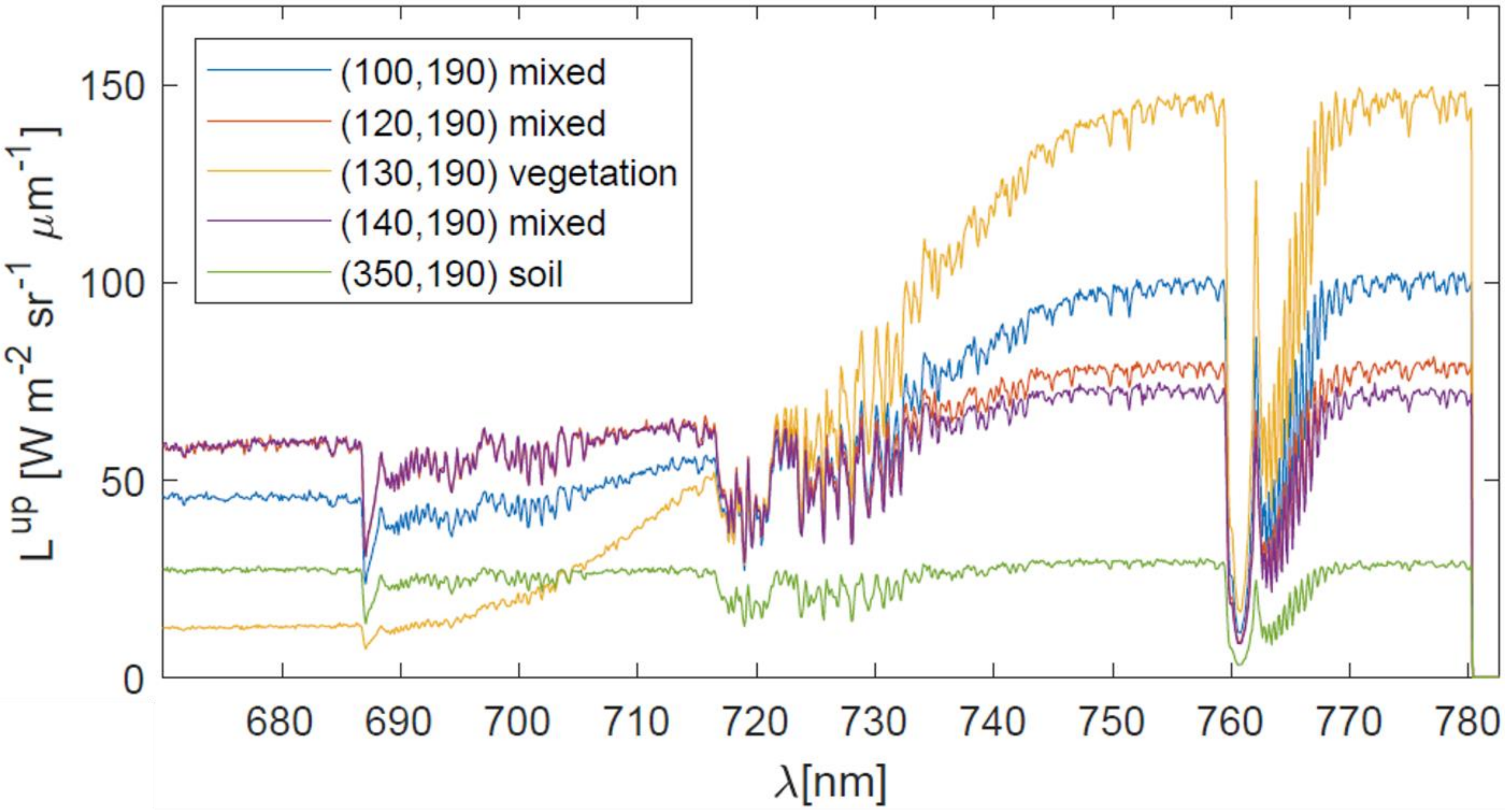
DESIS (DLR Earth Sensing Imaging Spectrometer) on ISS

- Good coverage of earth – high impact in environmental sciences
- Lower spatial and spectral resolution than HyPlant data

Spatio-spectral Images from HyPlant

Line sensor operated in push broom fashion

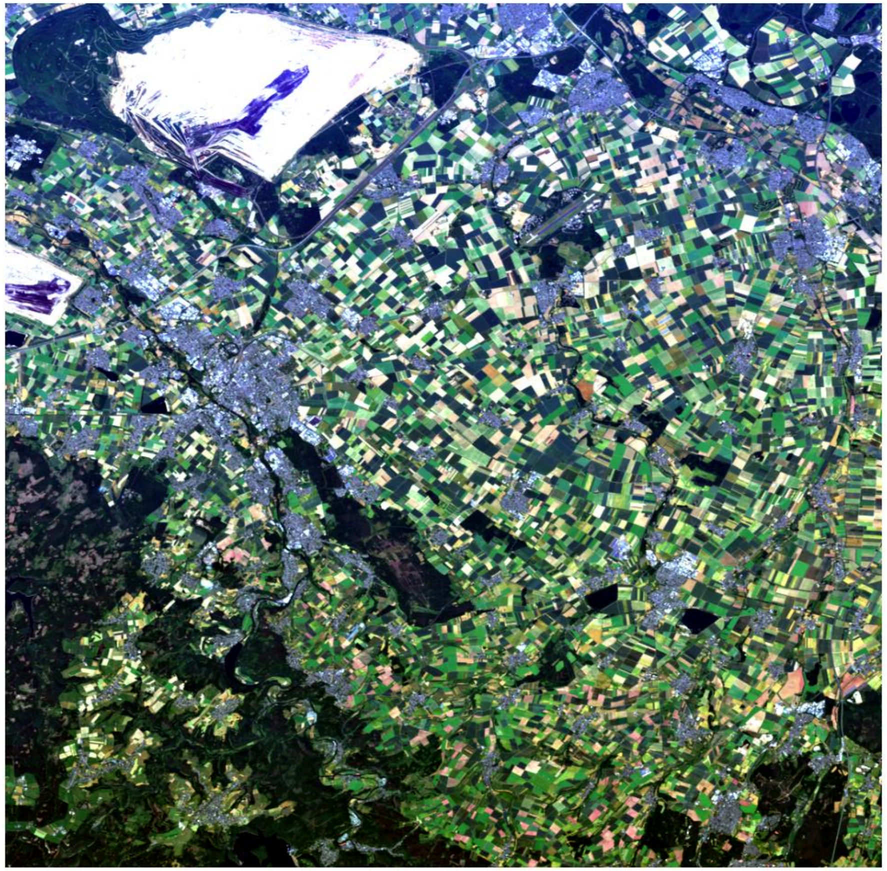




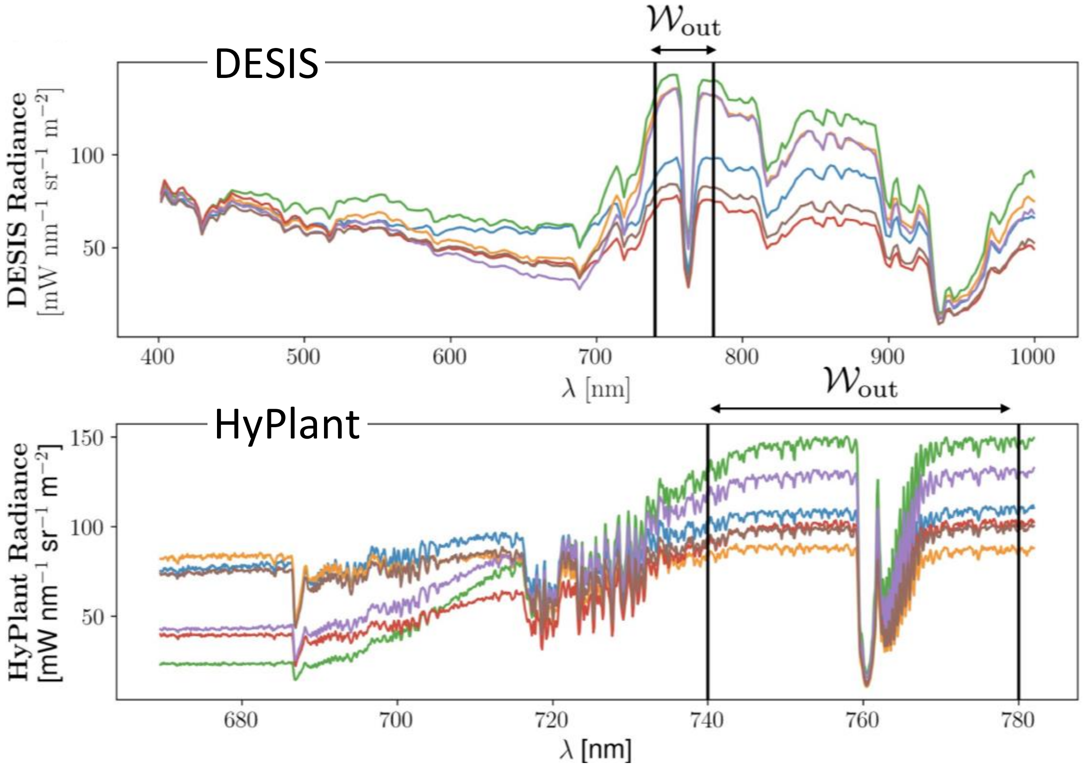
DESIS data as compared to HyPlant imagery

HyPlant FLUO (0.5 - 2 m)

DESIS (30 m)



Spectral resolution is different (0.25 vs. 3.5 nm)



Sun Induced Fluorescence

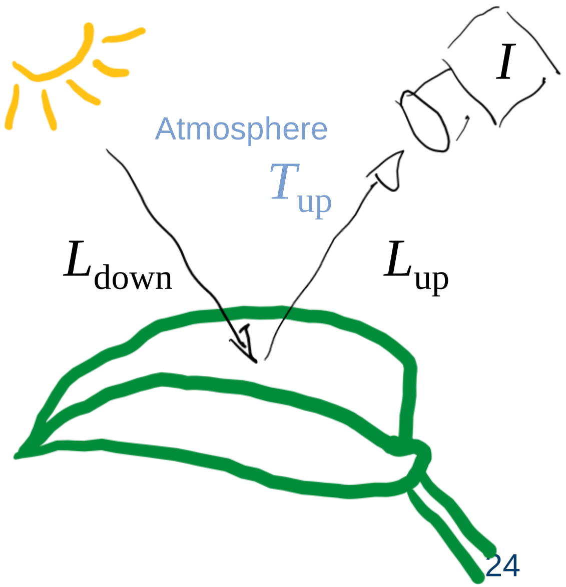
Image formation

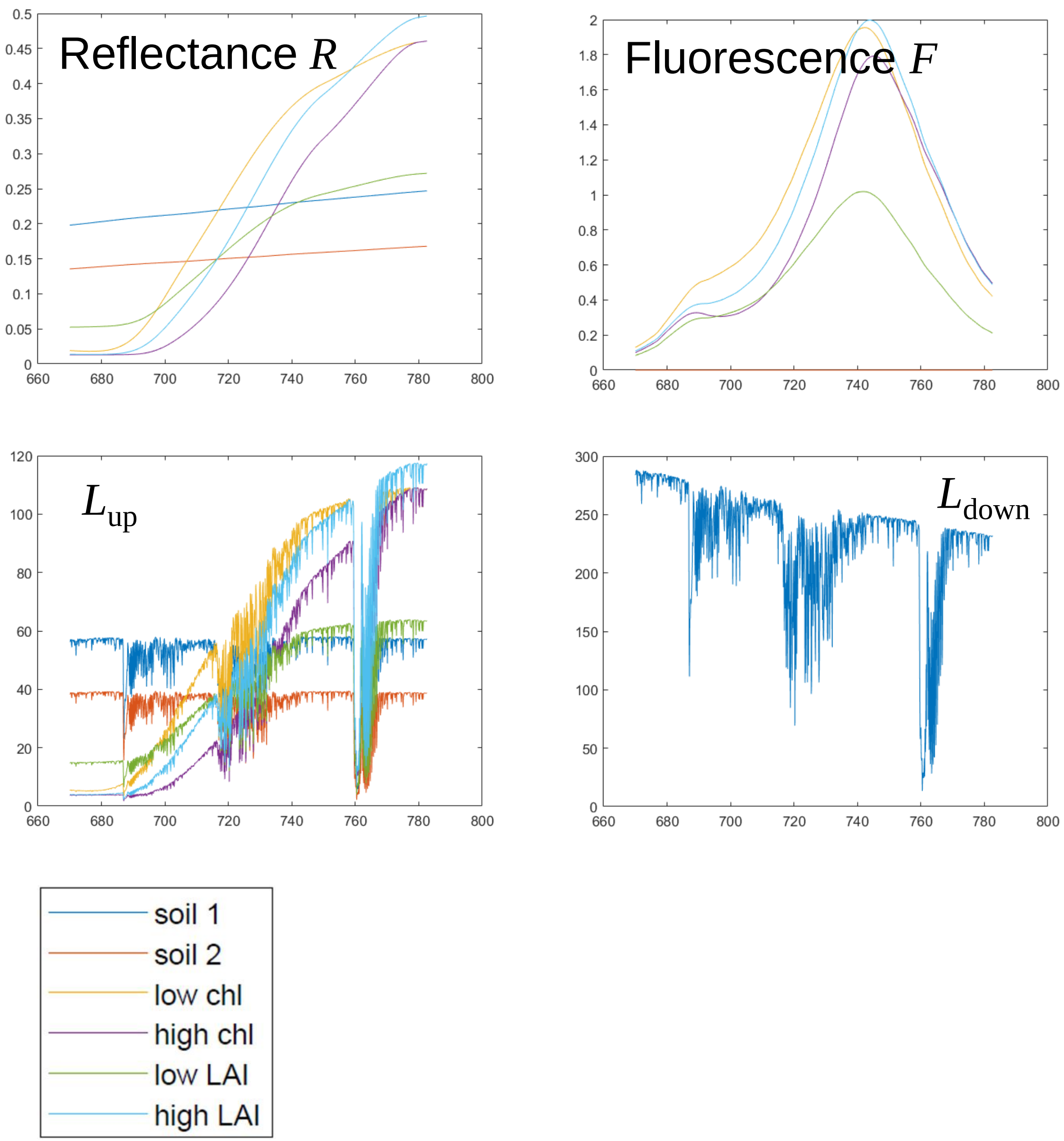
- Incoming light L_{up} goes through optics and is detected by digital sensor

$$I(\lambda,x,t) = \phi(\lambda,x) * L_{up}(\lambda,x,t) + n$$

$$L_{up}(\lambda,x,t) = T_{up}(\lambda,x,t)(R(\lambda,x,t)\, L_{down}(\lambda,x,t) + F(\lambda,x,t))$$

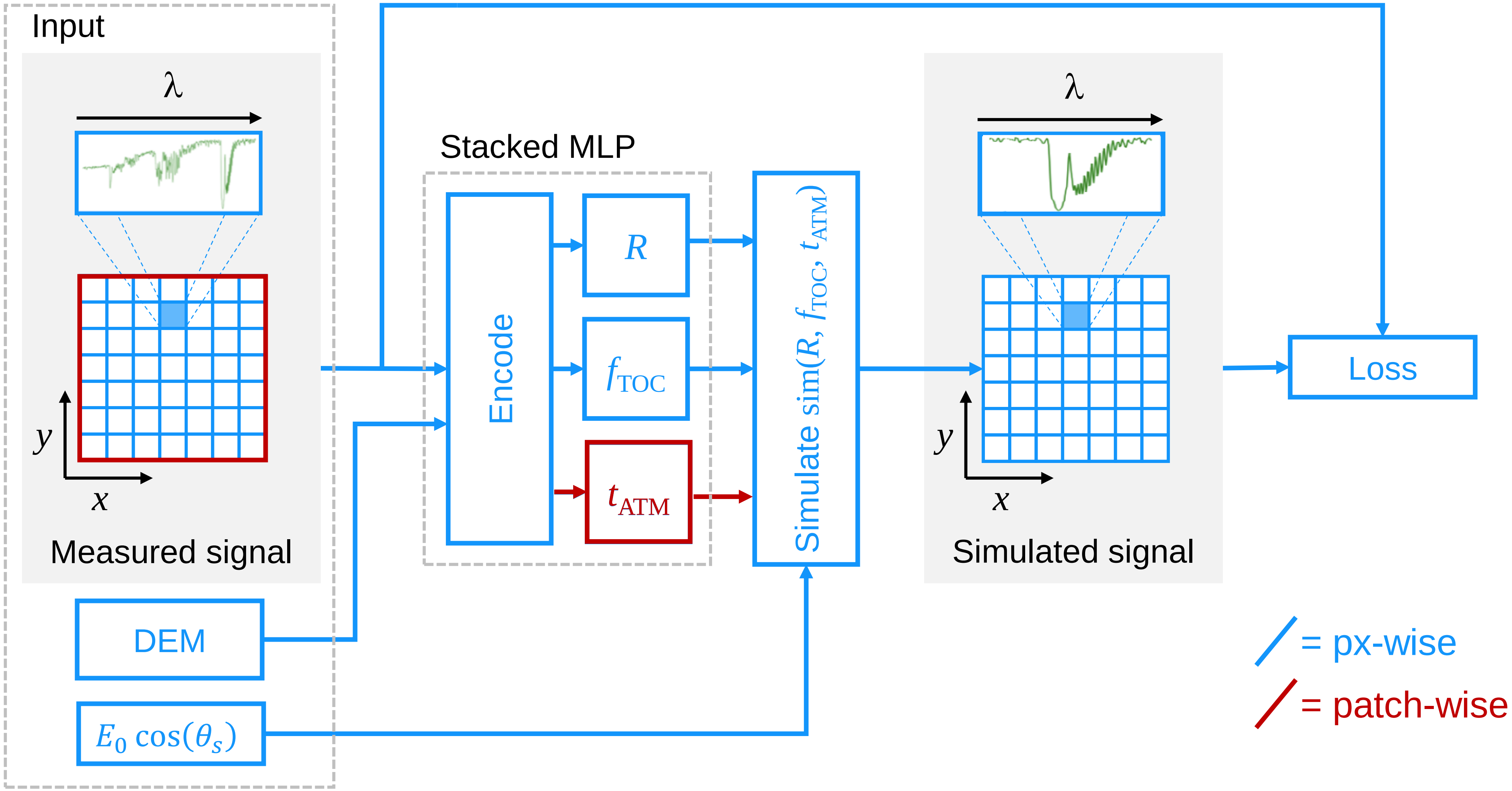
- Measured intensity I
- ϕ sensor optics, sampling
- Photon ‚shot‘ noise n
- Reflectance R
- Fluorescence F



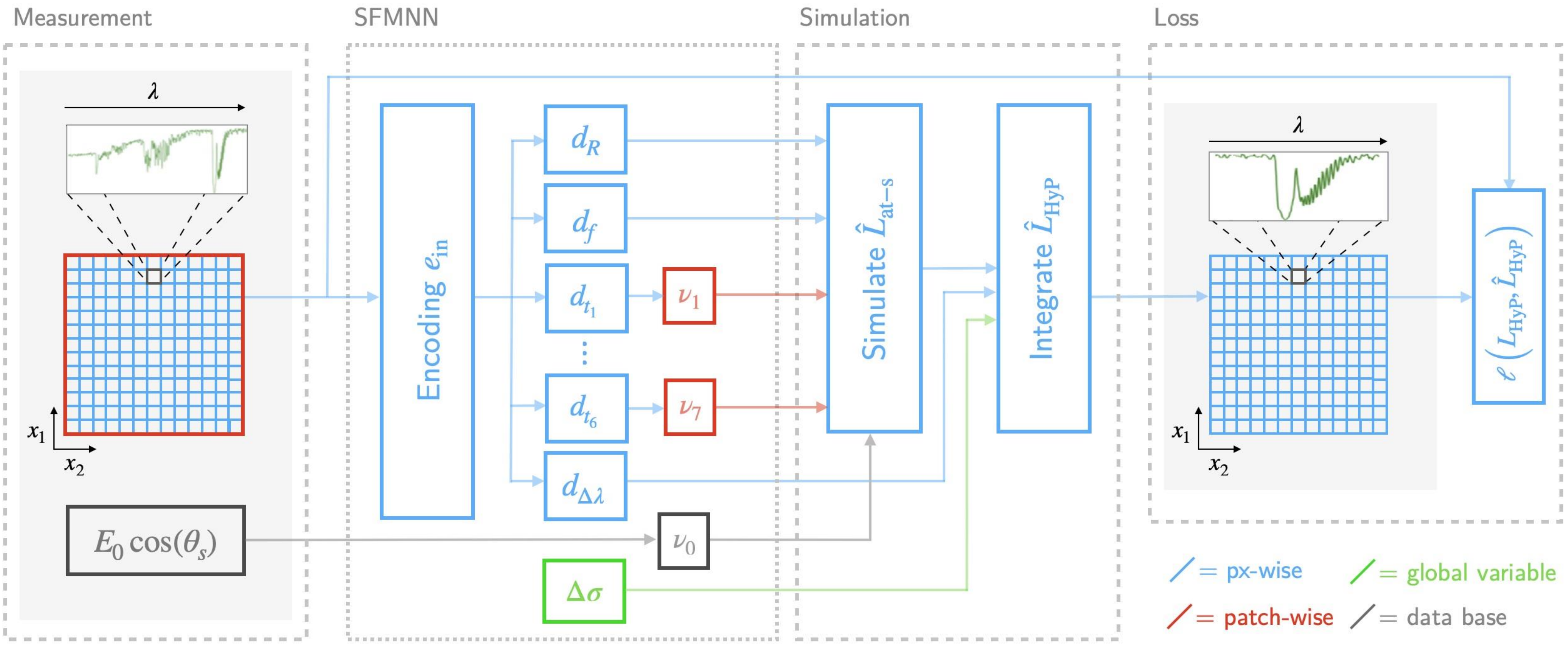


Scharr et al. (2021), Remote Sensing

Self-supervised spectral fitting



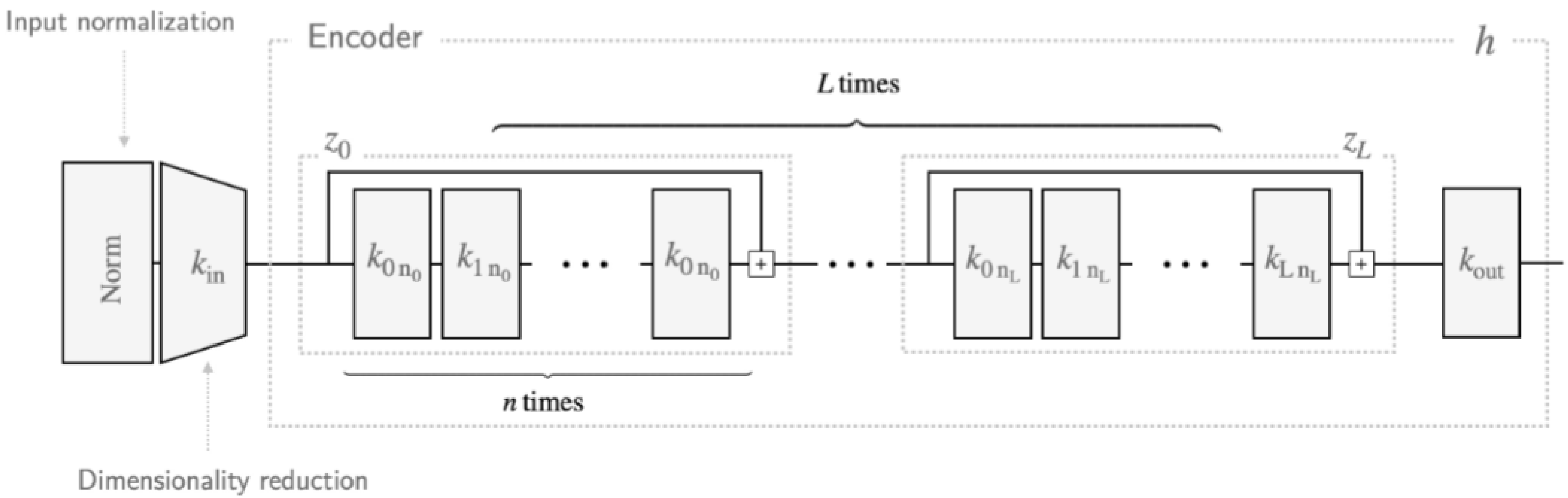
Self-supervised spectral fitting of a high-resolution simulation model to HyPlant data



Colors indicate: Atmosphere, surface material, sensor, additional measurements (sun zenith angle etc.)

Encoder and Decoder

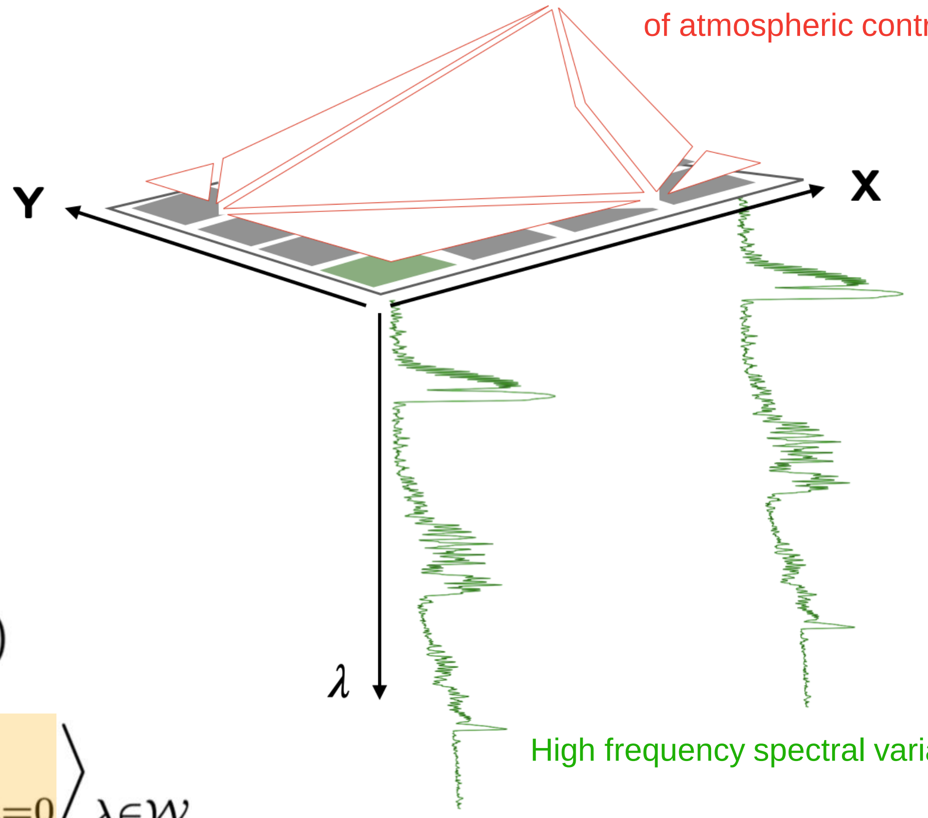
Multi-Layer Perceptron with Skip Connections



	Dims.	Rep.	D_p
Encoder e_{in}	(100, 100, 50)	(3, 3, 3)	(0.1, 0, 0)
Decoders d_v	(100, 50, 50, 50)	(3, 1, 1, 1)	(0, 0, 0)

Regularization strategies in the Loss and Architecture

- Inversion under incomplete knowledge of physical process is **ill-posed**.
- Architectural **constraint** formulation: difference in spatial variation of terms contributing to radiance signal



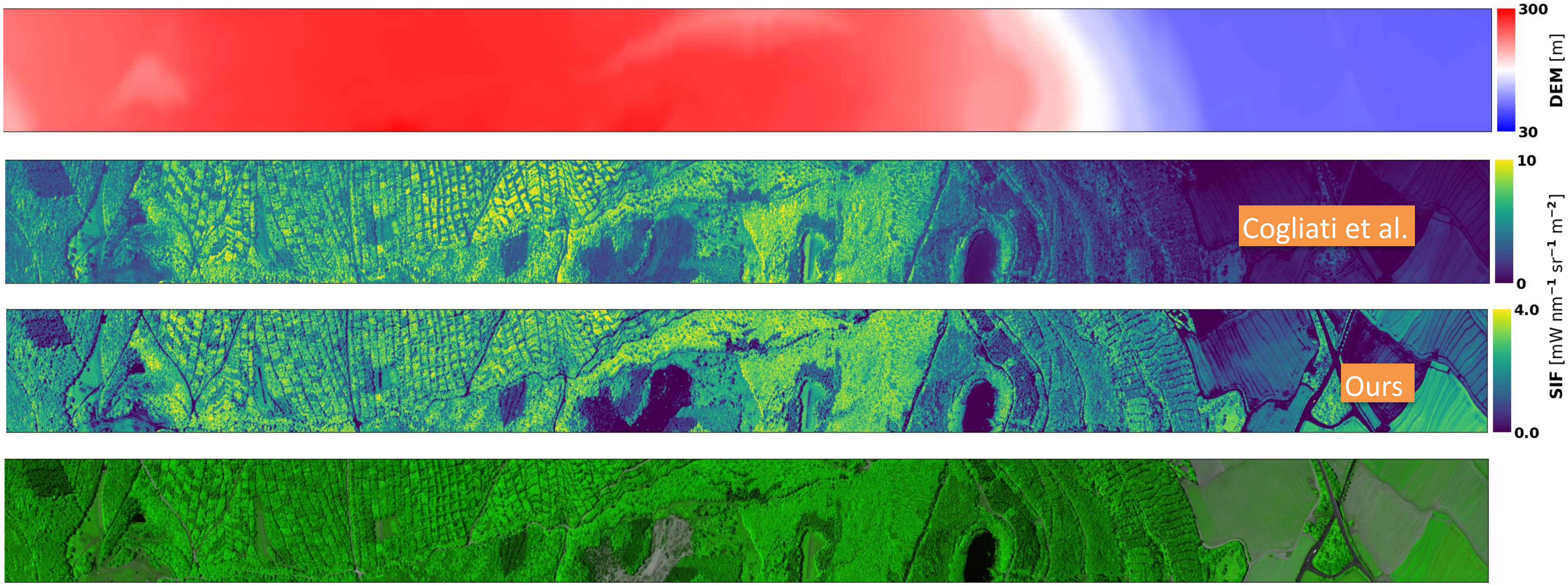
$$\ell(y,\hat{y}) = \left(\ell_{R,f} + \gamma_f\,\ell_f + \gamma_N\,\ell_{\mathrm{NDVI}} + \gamma_a\,\ell_{\mathrm{atm}}\right)(y,\,\hat{y})$$

$$= \left\langle \left(y(\lambda) - \hat{y}(\lambda)\right)^2 + \gamma_{\mathrm{f}} \left(w_\lambda \left(y(\lambda) - \hat{y}(\lambda)\right)^2 \right)_{\delta \mathrm{R}=0} \right\rangle_{\lambda \in \mathcal{W}}$$

$$+ \;\gamma_{\mathrm{N}}\;\hat{f}\;\delta\left(\mathrm{NDVI}_y \leq t\right) + \gamma_{\mathrm{a}}\;\mathrm{ReLU}(\hat{t}_{\mathrm{tot}} - 1)$$

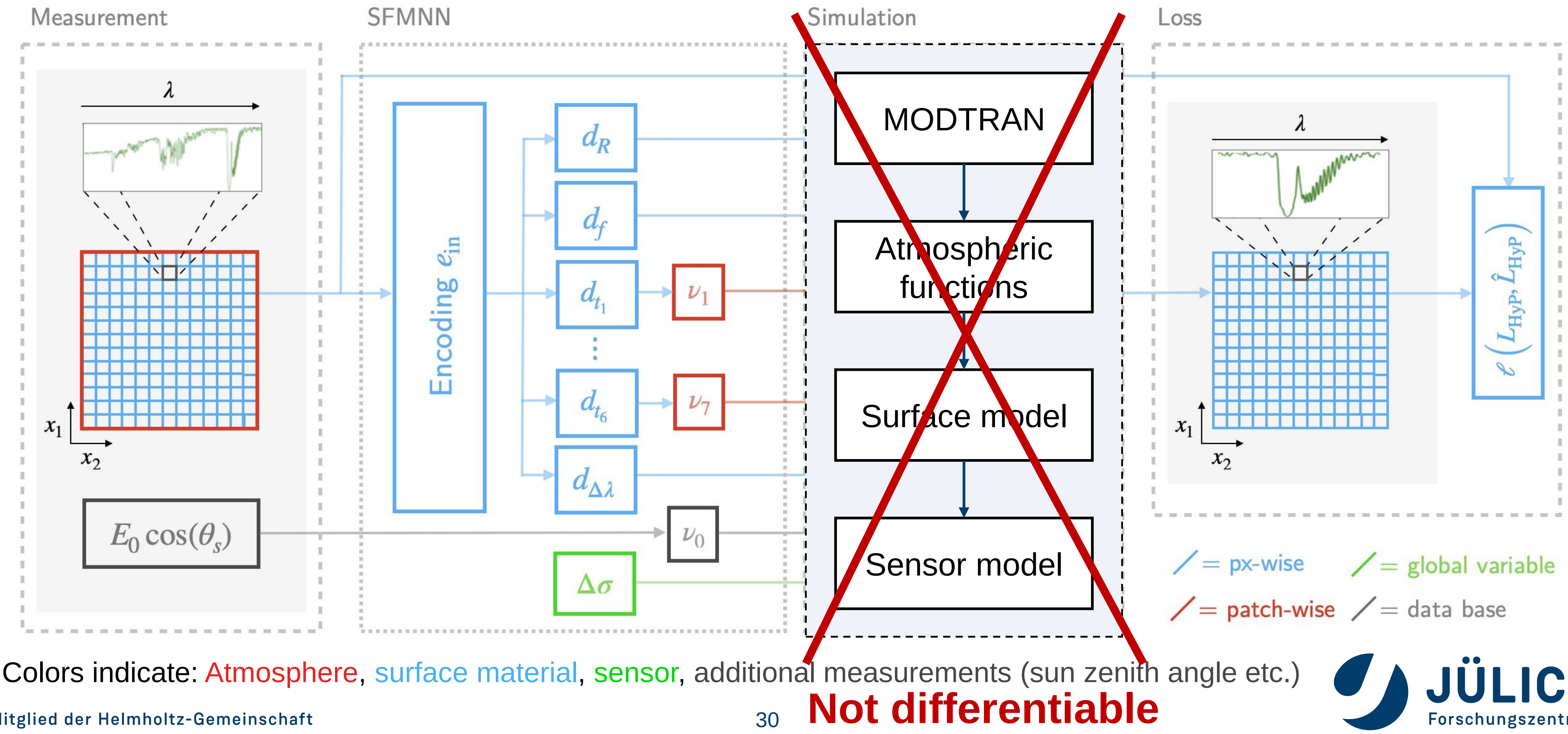
Overall residual | SNR weighting | Physiological constraint | Physical constraint

Local Atmospheric Fitting



SFM: Spectral Fitting Method (Cogliati, 2019)

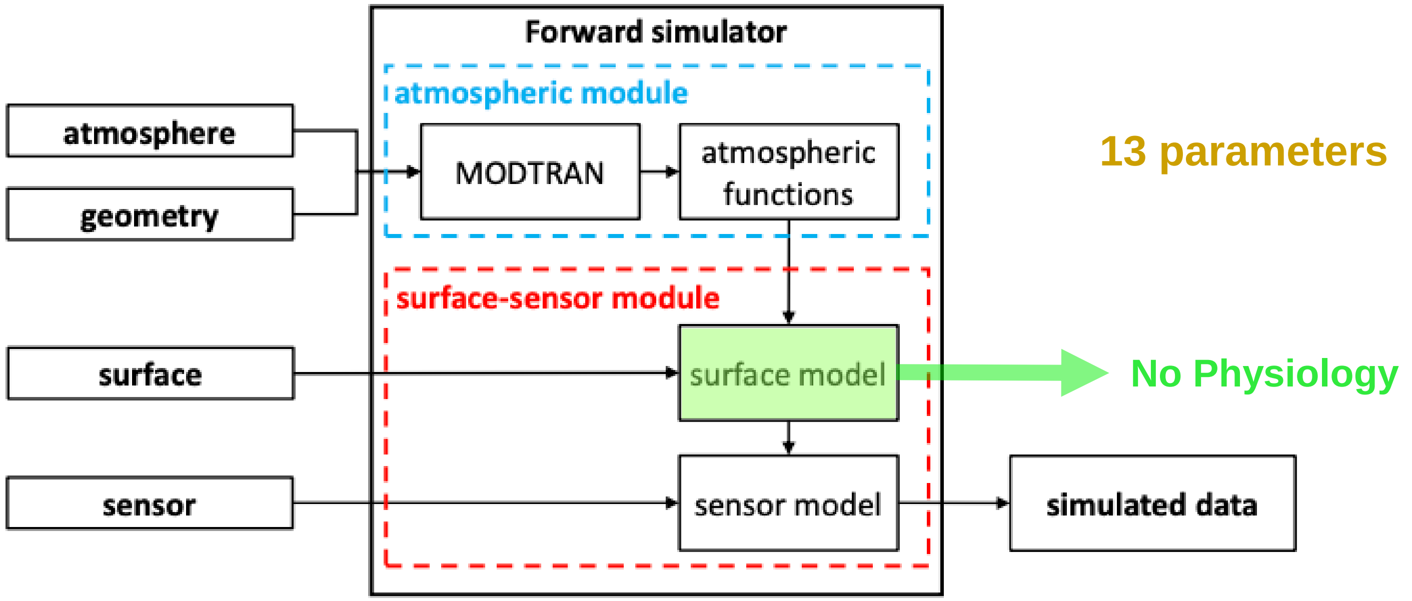
Self-supervised spectral fitting of a high-resolution simulation model to HyPlant data



Colors indicate: Atmosphere, surface material, sensor, additional measurements (sun zenith angle etc.)

MODTRAN: MODerate resolution atmospheric TRANsmission

MODTRAN6 based simulation tool to extensively sample the at-sensor radiance domain of HyPlant and DESIS



Specification	Databases	
	DESIS	HyPlant
Input dimensions	11	13
Output dimensions	13	349
Number of samples	1.2×10^7	1.5×10^7
Data size [GB]	5.6	64.7

~1-4 min/sample
~0.5M core-h overall
Halton sampling

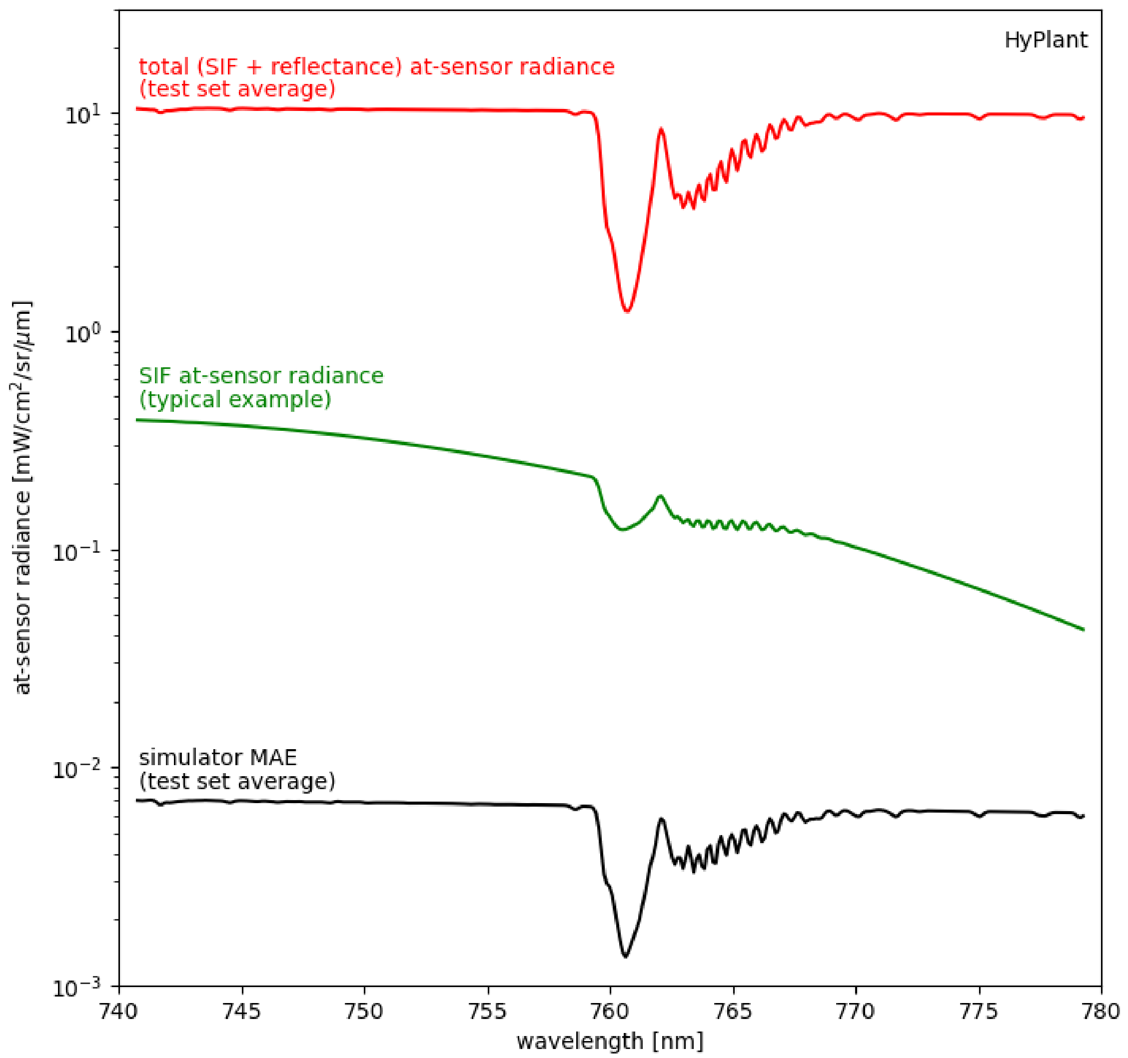
13 parameters

Parameter		HyPlant DB
Atmosphere	model	mid-latitude summer
	H_2O [cm]	0.3–3.0
	O_3 [DU]	332
	AOT_{550} []	0.05–0.40
	aerosol model	rural
	g []	[−1, +1]
Geometry	TA [°]	0–20
	SZA [°]	20–55
	RAA [°]	0–180
	h_{gnd} [m]	0–300
	h_{sen} [km]	0.659–0.691 agl 1.543–1.598 agl
Surface	ρ_{740} []	0.05–0.60
	$d\rho/d\lambda$ [nm^{-1}]	0–0.008
	F_{737}/F_0	0–8
Sensor	δ_λ [nm]	[−0.080, +0.023]
	δ_{FWHM} [nm]	[−0.040, +0.040]

MODTRAN: MODerate resolution atmospheric TRANsmission

Emulator representing the simulated HyPlant and DESIS data

- Trained ML simulators of at-sensor radiances to approximate the generated databases
- Tested different models, incl. relatively shallow NNs, all trained with L2 loss,
- Best: simple fourth-degree polynomials



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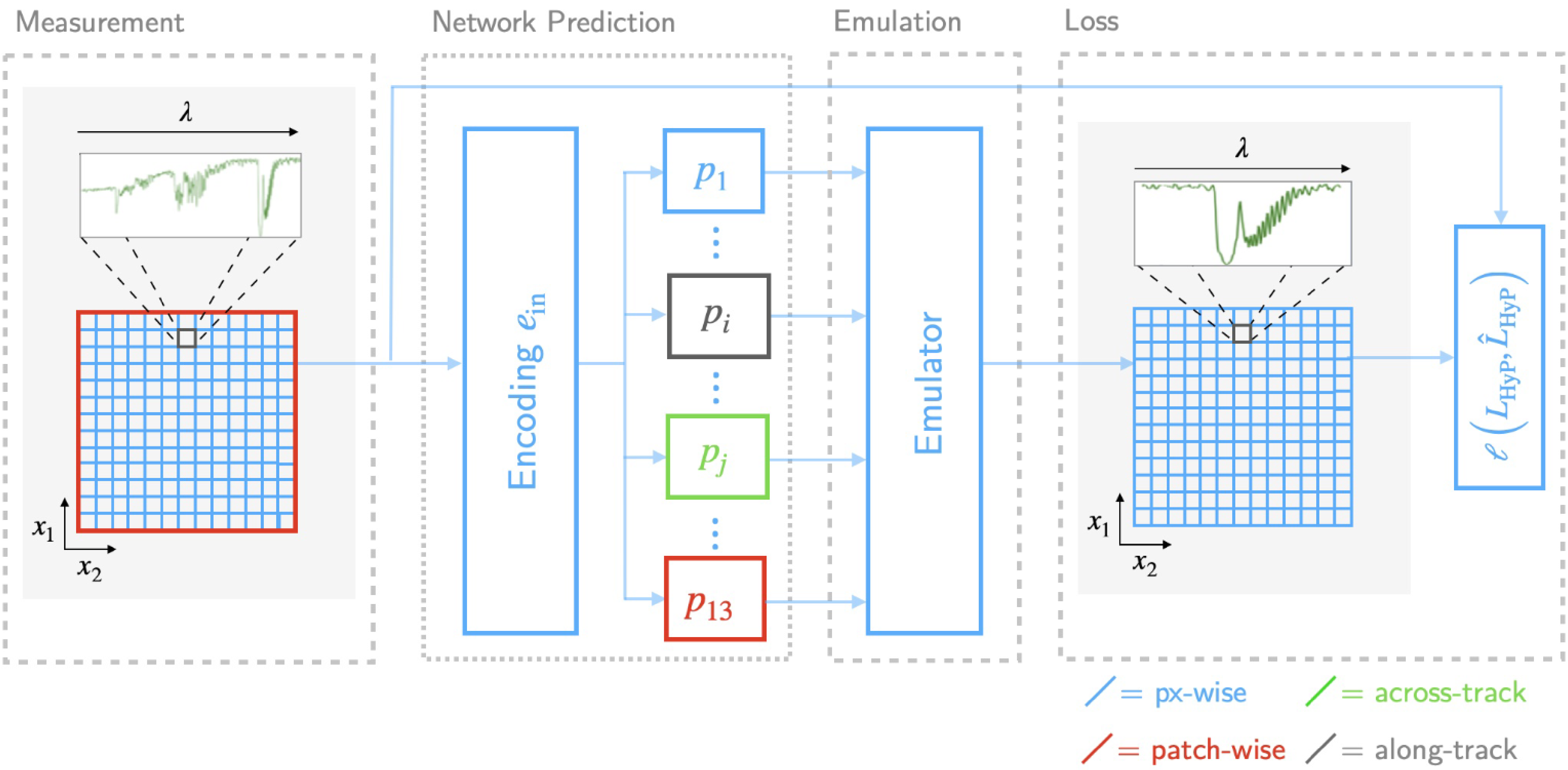
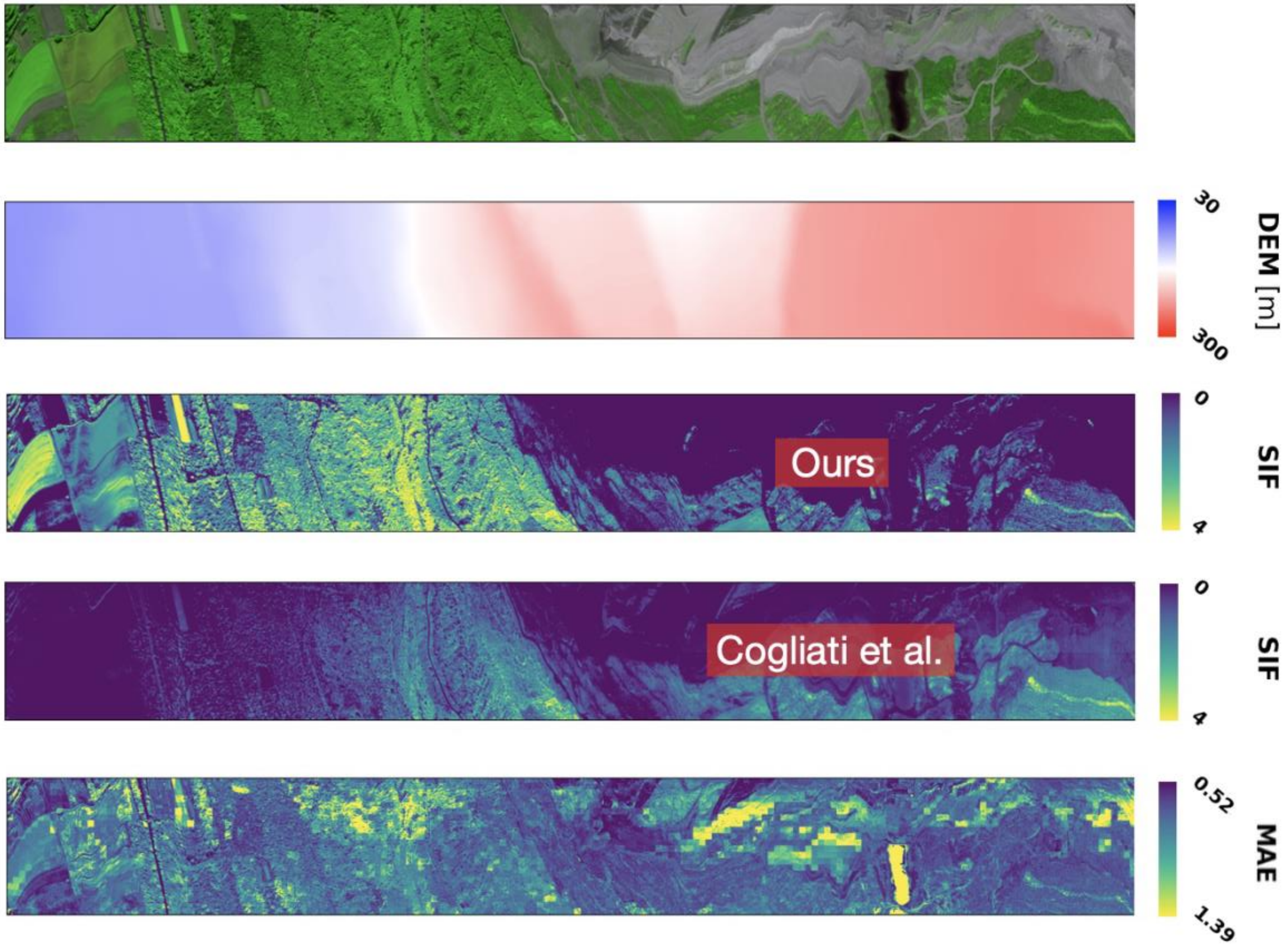
Emulator instead of Simulation in SFMNN



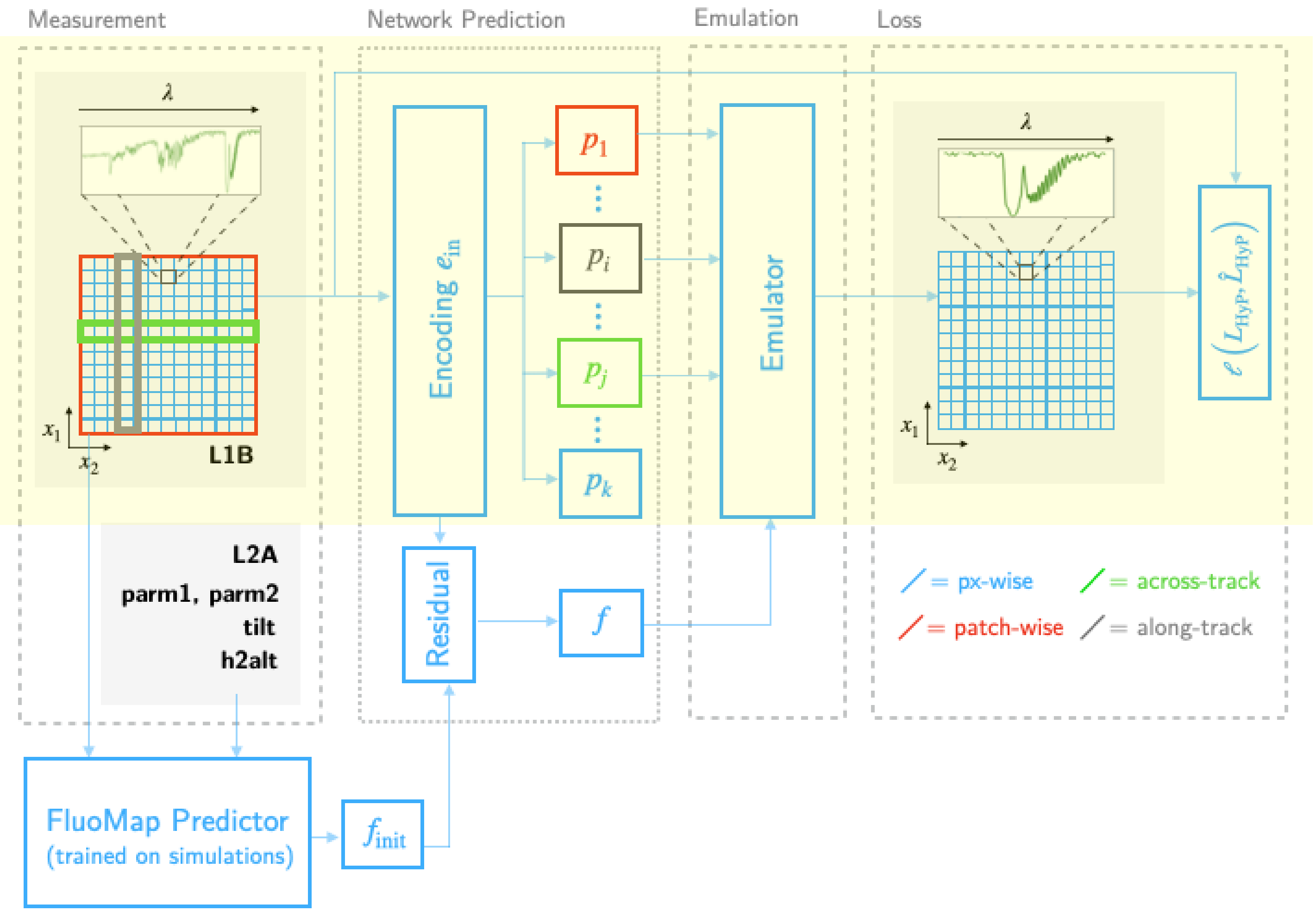


SFM: Spectral Fitting Method (Cogliati, 2019)

Integrating self-supervised and supervised approaches for DESIS SIF prediction

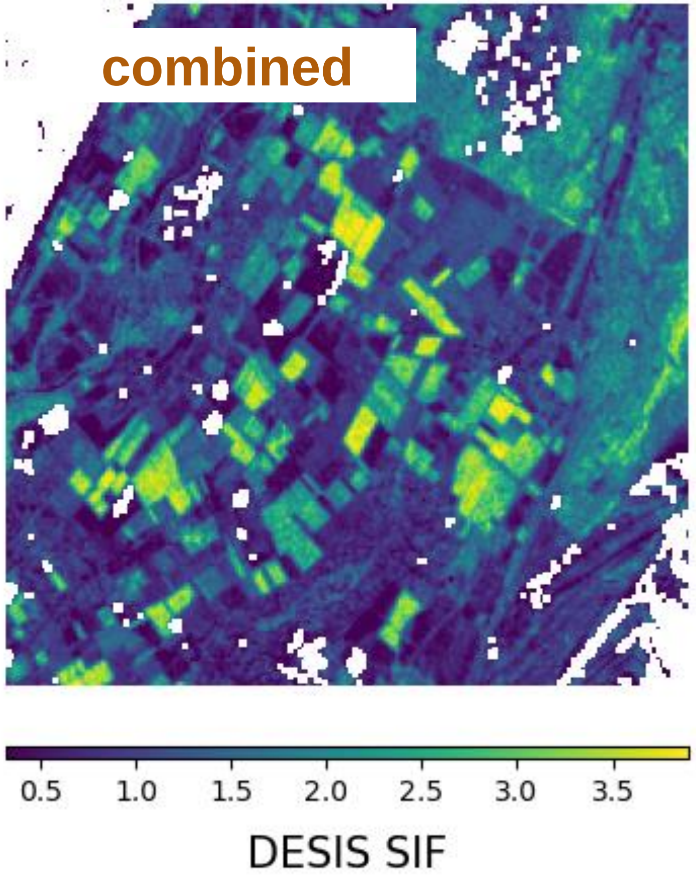
- **Integrate** constraint and label-based training
- **Use supervised** SIF predictor for an initial guess
- Train an **emulator-based SFMNN**
- **Estimate residual**: SIF residual w.r.t. the initial guess

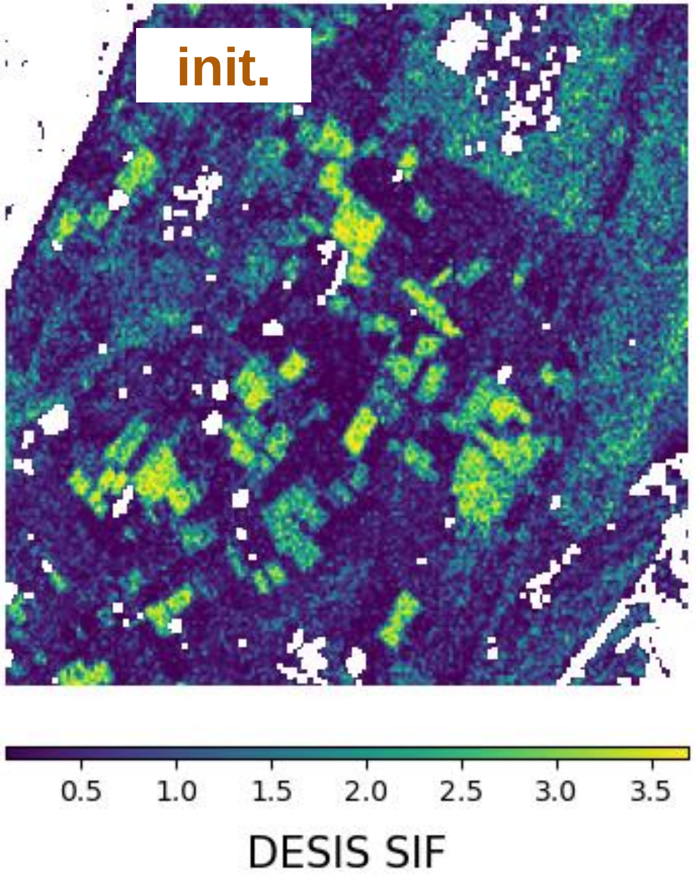
$$f = f_{\text{init}} + n_{\text{res}}(x), \ \text{with } n_{\text{res}}(x) \in [\Delta f_{\min}, \Delta f_{\max}]$$



… + fast emulator with improved correction term for bandwise $\Delta\lambda$

SIF Prediction — Initial guess and combined approach

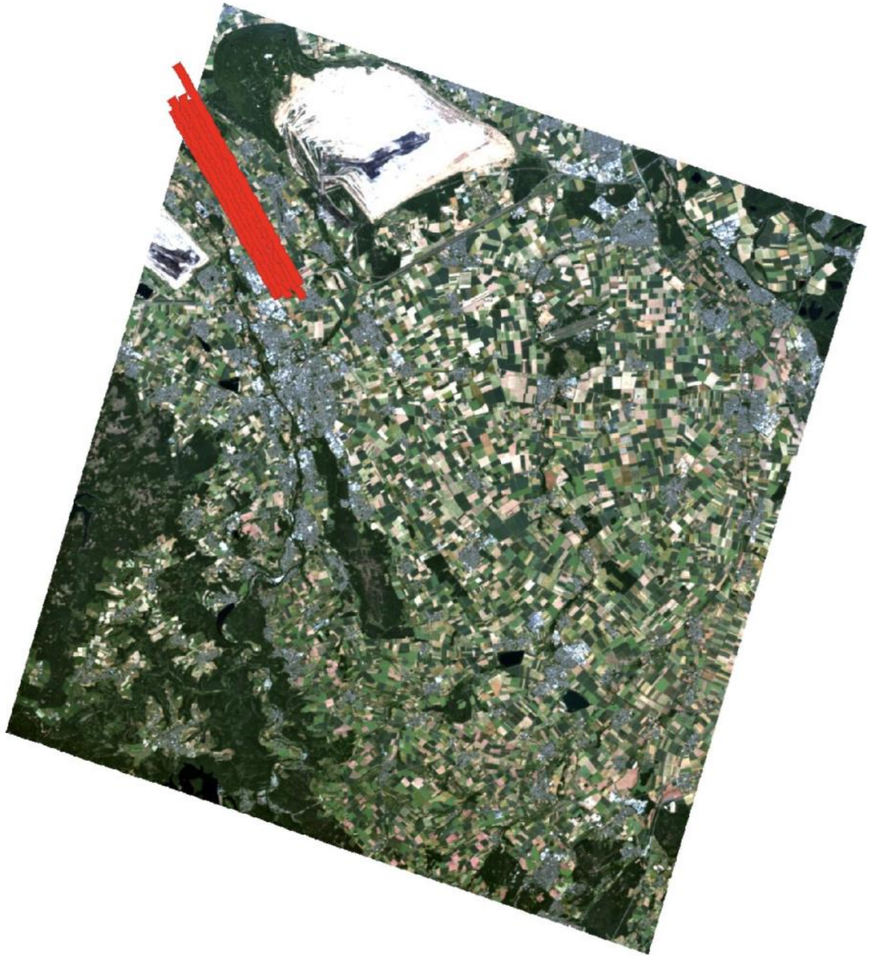




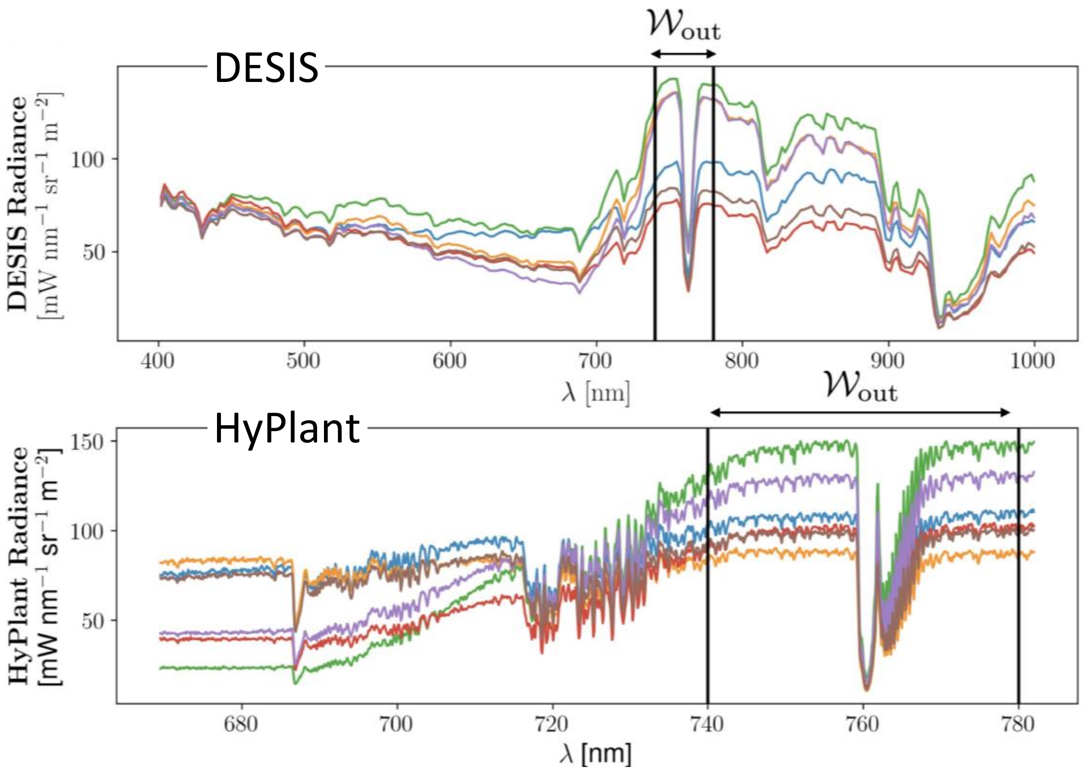
Data set of 6 DESIS acquisitions quasi-simultaneous with HyPlant campaigns

HyPlant FLUO (0.5 - 2 m)

DESIS (30 m)

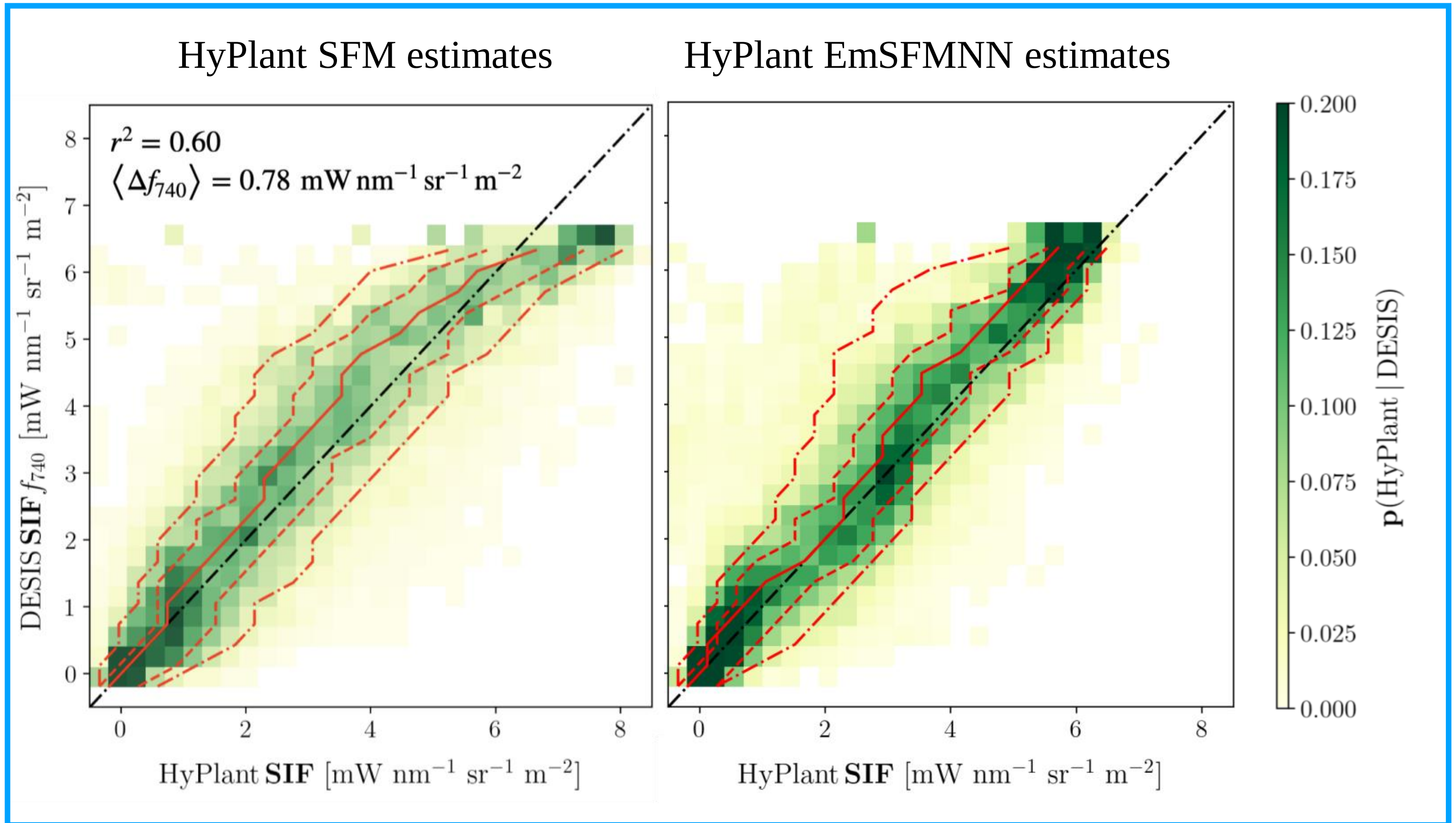


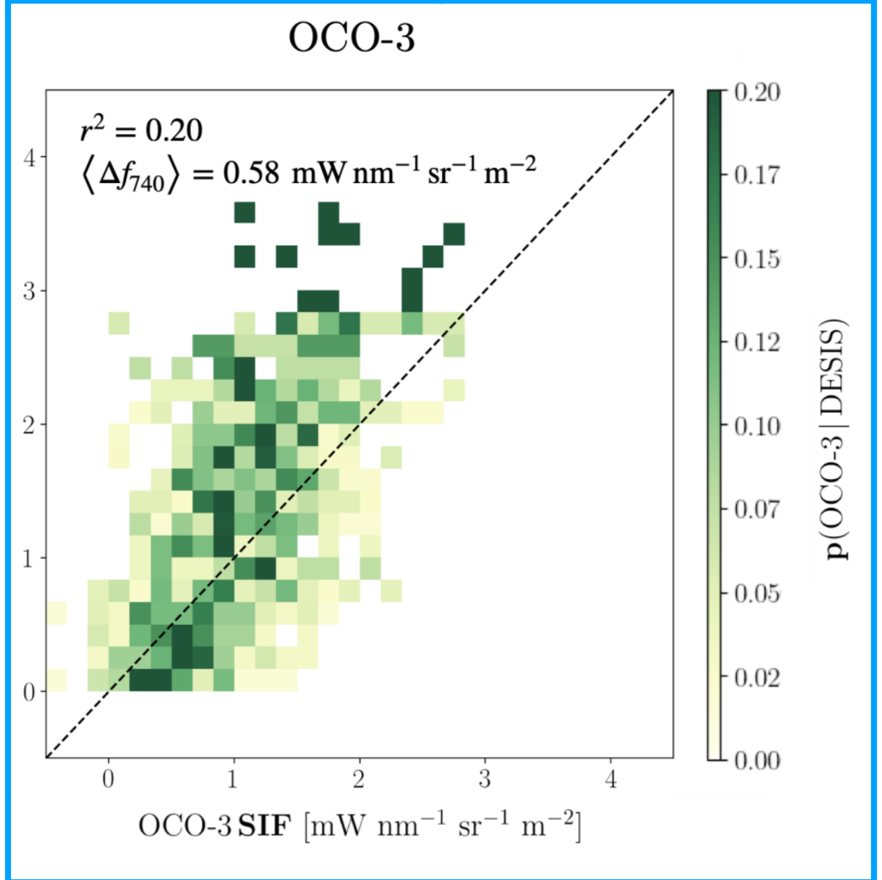
Spectral resolution is different (0.25 vs. 3.5 nm)



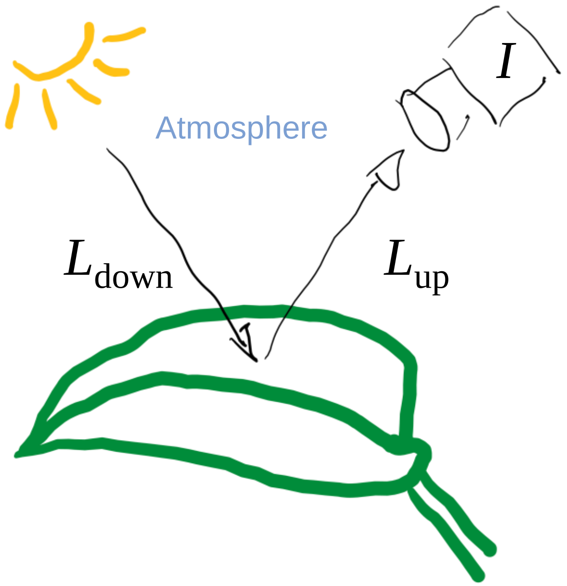
Comparison of DESIS with quasi-simultaneous HyPlant data

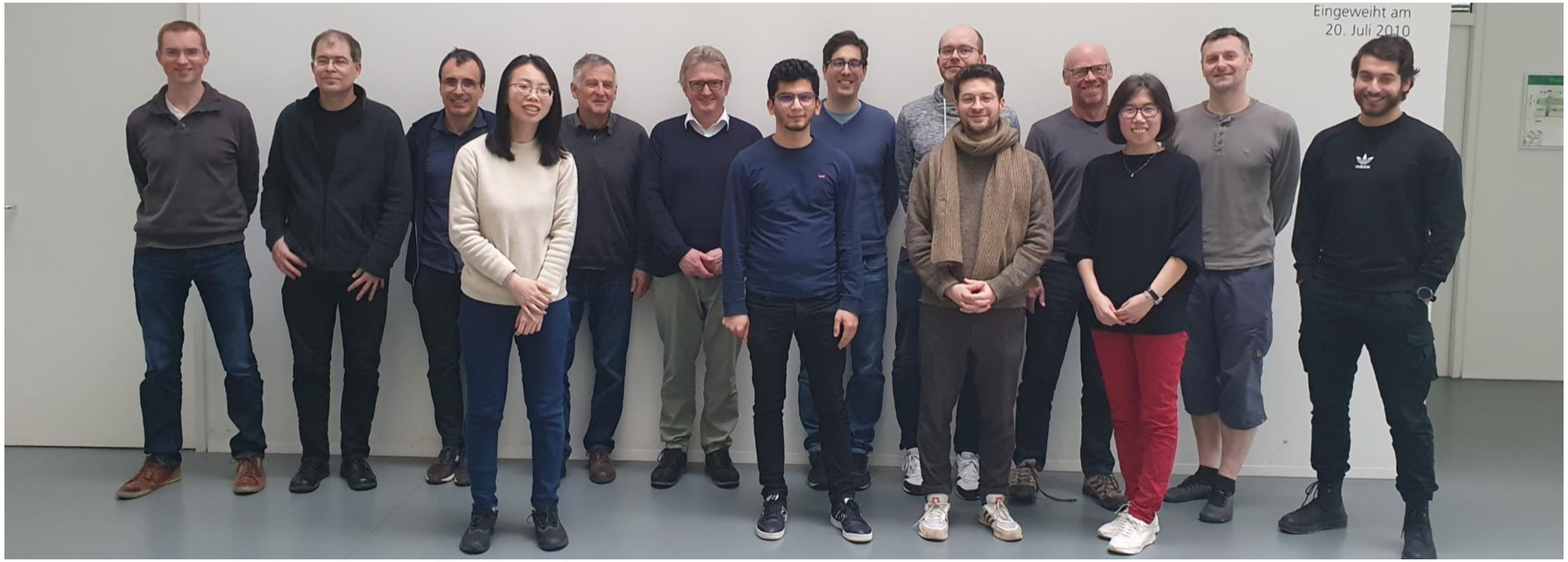
Point matches with OCO-3 data (global)





Coincident data set of DESIS and HyPlant





A DEEP-LEARNING-BASED METHOD FOR THE RETRIEVAL OF SUN-INDUCED PLANT FLUORESCENCE FROM AIRBORNE AND SPACEBORNE HYPERSPECTRAL IMAGERY

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