## 1 EUROSPEC: At the interface between remote sensing and

# 2 ecosystem CO<sub>2</sub> flux measurements in Europe

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#### **Abstract**

Resolving the spatial and temporal dynamics of gross primary productivity (GPP) of terrestrial 8 ecosystems across different scales remains a challenge. Remote sensing is regarded as the solution 9 to upscale point observations conducted at the ecosystem level, using the eddy covariance (EC) 10 technique, to the landscape and global levels. In addition to traditional vegetation indices, the 11 photochemical reflectance index (PRI) and the emission of solar-induced chlorophyll fluorescence 12 (SIF), now measurable from space, provide a new range of opportunities to monitor the global 13 carbon cycle using remote sensing. However, the scale mismatch between EC observations and the 14 15 much coarser satellite-derived data complicates the integration of the two sources of data. The solution is to establish a network of *in situ* spectral measurements that can act as bridge between EC 16 17 measurements and remote sensing data. In situ spectral measurements have been already conducted for many years at EC sites, but using variable instrumentation, setups, and measurement standards. 18 19 In Europe in particular, in situ spectral measurements remain highly heterogeneous. The goal of EUROSPEC Cost Action ES0930 was to promote the development of common measuring protocols 20 21 and new instruments towards establishing best practices and standardization of these measurements. In this review we describe the background and main tradeoffs of in situ spectral measurements, 22 23 review the main results of EUROSPEC Cost Action, and discuss the future challenges and 24 opportunities of in situ spectral measurements for improved estimation of local and global estimates of GPP over terrestrial ecosystems. 25

- 27 Keywords: Carbon balance, Chlorophyll Fluorescence, COST Action, Flux Measurements, ICOS,
- Optical Sampling, Proximal Sensing, Remote Sensing, Spectral Reflectance, Greenness, SpecNet,
- 29 FluxNet, Vegetation Indices.

#### 1 1. Introduction

2 Accurate quantification of carbon fluxes across space and time is of primary importance to climate scientists, land use managers, and policymakers (Beer et al., 2010; Ciais et al., 2014; Joos et al., 3 2001). Carbon budgets can be estimated with high accuracy at the ecosystem level (e.g. Clement et 4 al., 2012; Grace et al., 2006; Zanotelli et al., 2015) but global estimates of Gross Primary 5 6 Productivity (GPP) and carbon balance in terrestrial ecosystems still have high levels of uncertainty 7 (Alton, 2013; Balzarolo et al., 2014; Beer et al., 2010; Enting et al., 2012; Jung et al., 2011; Keenan et al., 2012; Piao et al., 2013). The primary method used to measure the net flux of carbon dioxide 8 (CO<sub>2</sub>) between the Earth's surface and the atmosphere is eddy covariance (EC) (Aubinet et al., 9 2000; Baldocchi, 2008; Goulden, 1996). The EC technique has dramatically improved our 10 understanding of inter and intra annual variations in the carbon fluxes at the ecosystem level 11 12 (Baldocchi, 2008). However, upscaling these local observations to the landscape and regional level remains a challenge. Because EC measurements require sites with moderate to low slopes, there is 13 a bias towards certain topography and ecosystem types (Göckede et al., 2008). In addition, the 14 footprint of EC measurements is not constant and varies with wind direction and speed, 15 16 measurement height, and vegetation structure (Schmid, 2002; Vesala et al., 2008). Although footprint size can be controlled to some extent with tower height, the resulting data may still 17 represent different vegetation communities depending on time-varying wind direction. Footprint 18 analysis (e.g. Kormann and Meixner, 2001) is required to cope with this source of variability that 19 complicates the interpretation of flux data. Despite these limitations, the global number of active 20 flux sites exceeds 500 and is constantly increasing (Schimel et al., 2015). The question remains as 21 to how to better upscale these point measurements to the landscape, regional and global scale. 22

Given that most of the factors affecting carbon fluxes have strong spatial and temporal components it is difficult to envisage upscaling without the use of remote sensing data, the only means to provide regular and spatially continuous observations of the Earth surface. One of the most widely applied approaches to assimilate remotely sensed data is to estimate GPP through a light use efficiency (LUE) model (Monteith, 1972; Reichstein et al., 2014; Ruimy et al., 1994):

where GPP is expressed as a function of the incident photosynthetically active radiation (PAR), the fraction of this PAR that is eventually absorbed by vegetation (fAPAR), and the efficiency by which absorbed PAR is used to assimilate atmospheric CO<sub>2</sub>, termed the light use efficiency (LUE) (Hilker et al., 2008a). The fAPAR in Eqn 1 is a function of canopy chlorophyll content or green

biomass (i.e. more chlorophyll results in more absorption). It is important to note that fAPAR in 1 2 Eqn 1 corresponds to green fAPAR, in contrast to total canopy fAPAR where both photosynthetic and non-photosynthetic elements such as wood contribute to PAR absorption. Green fAPAR has 3 been widely estimated using reflectance-based vegetation indices as proxy, notably the Normalized 4 Difference Vegetation Index (NDVI) derived from red and near-infrared (NIR) reflectance (Rouse 5 et al., 1973; Tucker, 1979). These vegetation indices correlate better with green fAPAR than with 6 7 total fAPAR because their spectral formulation can significantly discriminate green from non-green 8 elements (Gamon et al. 1995). However, canopy structural factors, background properties, or sun-9 target-sensor geometry can complicate the estimation of green fAPAR with vegetation indices (Di Bella et al. 2004; Gamon 2015, Knyazikhin et al.2013). Vegetation indices (VIs) have been 10 11 successfully used to track seasonal dynamics in GPP in ecosystems characterized by strong seasonal dynamics in green biomass such as croplands, grasslands, broadleaf forests (Gitelson et al., 2006, 12 13 2008, 2012; Harris and Dash, 2010; Peng and Gitelson, 2012; Rossini et al., 2010).

In ecosystems dominated by evergreen species, the seasonal variation in GPP can be strongly 14 controlled by LUE in addition, or instead of, fAPAR (e.g. Garbulsky et al., 2008; Gamon, 2015). 15 The LUE term is usually estimated as the product of the potential maximum LUE ( $\varepsilon_{max}$ ) and an 16 environmental scalar (f) expressing the influence of one or several environmental stress factors 17 18 constraining  $\varepsilon_{max}$ . For example, in the MODIS GPP product (Running et al., 2004), LUE is estimated by using a plant functional type or biome-dependent  $\varepsilon_{max}$ , and climate variables 19 20 describing the environmental scalar f (i.e. air temperature and vapour pressure deficit). The problem of this approach is that maximum LUE depends only on vegetation type (Xiao et al., 2004a,b; Zhao 21 22 et al., 2005), while inter-seasonal variability due to plant phenology and photosynthetic dynamics (Lagergren et al., 2005) is only considered via the instantaneous effect of the environmental scalar, 23 which cannot reproduce the slow response dynamics of vegetation. 24

Importantly, LUE generates optical signatures that can be measured with optical remote sensing instruments mounted on airborne or satellite platforms. These signatures are the photochemical reflectance index (PRI), and the emission of solar-induced chlorophyll-a fluorescence (SIF) by vegetation. The PRI uses the reflectances at 531 and 570nm to capture the temporal dynamics in LUE via variations in the xanthophyll-cycle pigments and the relative ratio of carotenoids to chlorophyll found in foliage (Gamon et al. 1992; Porcar-Castell et al. 2012; Wong and Gamon 2015). The PRI has been successfully estimated from sensors mounted on multiple platforms including towers, aircrafts and satellites (e.g. Drolet et al., 2005; Garbulsky et al., 2008; Nichol et al. 2002). In contrast, SIF are photons of red/far-red light (660-800nm) emitted during the first steps

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- of photosynthesis. Accordingly, the emission of SIF is expected to depend on both fAPAR and LUE
- 2 (Porcar-Castell et al. 2014). Despite the challenge of measuring SIF, due to the small intensity of
- 3 the signal relative to that of the reflected light, recent technical advances make it now possible to
- 4 estimate SIF from towers, aircrafts and satellites (Frankenberg et al., 2011; Guanter et al. 2007;
- 5 Joiner et al., 2011; Porcar-Castell et al., 2014; Rossini et al., 2010; 2015). Overall, the growing
- 6 number of satellite missions with enhanced capacity to retrieve PRI and SIF at increasing spatial
- 7 and temporal resolutions (e.g. Clevers and Gitelson, 2013; Frankenberg et al., 2014; Guanter et al.
- 8 2015; Guan et al., 2015) open up new possibilities to improve carbon models and upscale EC data.
- 9 Noting that the relationship between NDVI and fAPAR tends to saturate at high canopy densities
- 10 (Myneni and Williams, 1994; Olofsson and Eklundh, 2007) also other approaches have been used to
- estimate vegetation carbon uptake. For example, the Enhanced Vegetation Index (EVI) (Huete et
- al., 2002) efficiently describes the seasonal variability in GPP across both dense and sparse
- vegetation canopies (Schubert et al., 2010, 2012; Sims et al., 2006; Sjöström et al., 2011; Xiao et
- al., 2004a, 2004b; Xiao et al., 2010). More recently, the plant phenology index (PPI) (Jin and
- Eklundh, 2014) has been shown to be linearly related to green leaf area index (LAI), and better
- 16 related to seasonal GPP variations than NDVI and EVI of coarse-resolution MODIS data at
- 17 northern latitudes. This illustrates the value of investigating the relationship between carbon uptake
- and spectral information in flux footprint areas beyond the LUE model depicted in Eqn 1.
- 19 Integrating satellite and EC data into large scale carbon models is not straightforward. The spatial
- 20 mismatch between EC measurements and coarser grid-cell information in models and most satellite-
- derived remote sensing data adds significant uncertainty (Chen et al., 2012; Oren et al., 2006). The
- 22 large viewing angle of many satellite products, e.g. MODIS, results in ill-defined and variable
- footprint areas leading to additional geometric uncertainties (e.g. Tan et al., 2006). Furthermore,
- 24 airborne and space-borne data needs to be corrected for atmospheric absorption and scattering
- effects (Karpouzli et al., 2003; Richter, 2011), a process that again can add further uncertainty
- 26 (Drolet et al., 2005; Hilker et al., 2009). All these physical limitations could be substantially
- 27 reduced by including *in situ* long-term spectral measurements to the network of EC flux sites
- 28 (Gamon et al., 2010; Hilker et al., 2009).
- 29 Coordinated *in situ* spectral measurements require a network of stable sensors that follow the same
- 30 measurement standards, calibration protocols, and have traceable technical specifications to allow
- 31 across-site comparisons. Following the example of the EC Fluxnet community
- 32 (http://fluxnet.ornl.gov/), SpecNet (www.specnet.info) was set to cover the needs for networking

- and standardization of optical measurements across flux sites (Gamon et al., 2006, 2010). Although
- 2 the geographical coverage of SpecNet collaborators is constantly increasing the network was until
- 3 very recently strongly biased towards North American sites. The European community of scientists
- 4 conducting optical measurements remained highly dispersed and heterogeneous. It is in this context
- 5 that the EUROSPEC COoperation in Science and Technology (COST) Action ES0903 (http://cost-
- 6 es0903.fem-environment.eu/) originated in 2009 and operated until 2013. European COST Actions
- 7 are four year projects aimed at promoting trans-national cooperation and networking among
- 8 scientists and engineers across Europe and beyond (see <a href="www.cost.eu">www.cost.eu</a> for further details).
- 9 The goal of EUROSPEC COST was to promote the development of common measuring protocols
- and new instruments for *in situ* spectral measurements, bringing together scientists and industries in
- order to increase the reliability, value and cost-efficiency of such measurements. This was done so
- that field-installed spectral sensors could be used as "bridge" between the EC and optical remote
- sensing communities.
- 14 The Action was divided in four Working Groups (WG): WG1, network and state-of-the-art
- characterization. The goal was to characterize the variability of spectral measurements and methods
- being used across flux sites in Europe. WG2, intercomparison and standardization of instruments.
- 17 The goal was to characterize the sources of variability between sensors, methods and protocols.
- 18 WG3, New instruments. The goal was to promote the development of new instruments that better
- match sensor design, specifications, cost and purpose. And WG4, upscaling methods. The goal was
- 20 to evaluate challenges and tools to upscale point observations to the footprint area and beyond.
- 21 The main objective of this review is to contextualize and synthesize the accomplishments made
- during EUROSPEC and to identify a number of challenges and opportunities for the near future.
- We review the main outcomes from EUROSPEC. We describe the background of *in situ* long-term
- 24 spectral measurements and their main tradeoffs, followed by presenting the main results of each
- 25 EUROSPEC WG and by a final discussion on future challenges and opportunities of these
- 26 measurements.

#### 2. In situ long-term spectral measurements: principles and trade-offs

- 28 Remote sensing measurements can be collected from platforms that may operate at variable
- 29 distance from the Earth's surface: from satellites for regional-global extent measurements, to field
- 30 spectrometers mounted on top of towers for close-range *in situ* measurements. In between these two
- 31 scales are airborne platforms including piloted and unpiloted aircraft, kites and blimps that can

- 1 measure at multiple scales depending on height. In EUROSPEC we focused on long-term in situ
- 2 optical measurements conducted from EC towers.
- 3 There are a number of important differences between close-range in situ measurements and the
- 4 traditional remote sensing from aircraft or satellites. *In situ* measurements, sometimes referred to as
- 5 proximal sensing, are conducted at short distances and are to a large extent free from the
- 6 atmospheric absorption and scattering effects that affect traditional remotely sensed data (Cheng et
- al., 2006; Meroni et al., 2009; Thenkabail et al., 2002). *In situ* measurements can be used to track
- 8 the spectral properties of individual biological elements (leaves, shoots, plants, homogeneous
- 9 canopies) while traditional remote sensing tends to measure at coarser scales where multiple
- species, soil and non-vegetated areas may contribute to the measured signals. Most importantly, in
- 11 situ measurements can provide data at high-temporal resolution, something that cannot be
- accomplished with traditional remote sensing. All these characteristics make *in situ* measurements
- ideal to study and disentangle the link between optical signals and carbon flux dynamics, as well as
- 14 for calibrating and validating satellite data and atmospheric correction algorithms (Brook and Ben-
- 15 Dor, 2015; Czapla-Myers et al., 2015; Hilker et al., 2009).
- 16 In situ spectral measurements involve the measurement of the down-welling (incoming) and up-
- welling (both reflected and emitted) radiation fluxes from the Earth surface. These measurements
- can be conducted with variable setup and approaches and the optimal solution will depend on the
- 19 purpose, characteristics of the site and amount of resources available.

#### 2.1 Single vs Dual Field of View (SFOV vs DFOV)

- 21 Measurements of down-welling and up-welling radiation can be carried out either in sequence
- 22 (when a single sensor or spectrometer is used), or simultaneously (when two separate sensors or
- 23 spectrometers are used) (Fig. 1). These are also addressed as single beam/field-of-view (SFOV) or
- dual beam/Field of view (DFOV) configurations, respectively, and have their own advantages and
- 25 disadvantages (See Table 1). A SFOV system is generally configured with a single sensor (or
- spectroradiometer) and will be generally cheaper to set up than a DFOV using two sensors. Having
- a single sensor means also that there is no need to inter-calibrate the sensor pair. However, long-
- term and unattended measurements with a SFOV system face the challenge of automating a single
- 29 sensor/spectrometer to measure both down-welling and up-welling radiation. This automation
- usually involves moving parts (e.g Meroni et al., 2011; Sakowska et al., 2015), which may become
- a problem for long-term field operation under certain environments and entail a time delay between
- 32 up-welling and down-welling measurements, which in turn may generate noisy data under cloudy

conditions. Similarly, DFOV systems have also associated advantages and disadvantages. Because 1 2 radiometric measurements are temperature-sensitive (Saber et al., 2011), DFOV based on two spectrometers are particularly sensitive to temperature. A practical solution is to keep the two 3 sensors at constant temperature, e.g. by housing them in a temperature-controlled enclosure (e.g. 4 (Drolet et al., 2014), but this might not be always possible due to power limitations. Also, regular 5 intercalibration of the two sensors will be essential in DFOV measurements (see e.g. Anderson et 6 7 al., 2006; Gamon et al., 2015; Jin and Eklundh, 2015). Additionally, long-term measurements with 8 a DFOV may be constrained by aging-dependent degradation of the two sensor heads (see Section 9 3.2.4). These limitations were partly overcome with new DFOV systems developed during 10 EUROSPEC that include a single spectrometer (see Section 3.3). The advantage of a DFOV system 11 is that it guarantees quasi simultaneous measurements of down-welling and up-welling radiances, each within a few hundred milliseconds of the other and may be easier to automate because do not 12 13 require moving parts to shift from up-welling to down-welling measurements. Importantly, systems such as the Piccolo and SIF-Sys (developed during EUROSPEC and described in section 3) share 14 15 the benefits from both SFOV and DFOV systems as they include a single spectrometer but make use of bifurcated fibre optics to sample two fields of view (Fig. 1). 16

#### 2.2 Multispectral vs Hyperspectral Sensors

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18 Spectral information can be acquired at different spectral resolution, which depends on the sampling intervals (discrete or continuous) and the width of the spectral bands (Fig. 2). Accordingly, spectral 19 20 measurements can be classified into multispectral or hyperspectral. Multispectral sensors measure a limited number of spectral bands, from two to five bands found for example in the SKYE SKR-21 22 1800 or 1860 sensor series (Skye Instruments Ltd, UK) the Decagon-SRS series (Decagon devices Inc, WA, USA) or the Cimel five-band sensors (Cimel Electronique, FR), or up to 16 bands found 23 24 in the Cropscan MSR16R (Cropscan Inc. MN, USA) (Balzarolo et al., 2011; Sakowska et al., 25 2014). The bandwidth of these sensors (in terms of full width at half the maximum response, 26 FWHM) is in the order of 10 nm or greater and the sampling across a specific spectral range is 27 typically discrete (Fig. 2). These sensors are typically manufactured using optical filters, light emitting diodes (LEDs) and photodiode detectors (Norton, 2010; Ryu et al., 2010). These sensors 28 are characterized by relatively low cost (from a few hundred to a few thousand euros/dollars), ease 29 of maintenance, weather-proof design, and low power consumption. Hence, they are useful and 30 affordable instruments for deployment at flux tower sites for extended periods of time. In addition, 31 32 their relatively low cost allows mounting of several sensors in different positions to study spatial heterogeneity. Multispectral sensors can be deployed to measure a number of vegetation indices 33

- 1 (e.g. NDVI or PRI) to track and study vegetation phenology and seasonality. They can also be used
- 2 to produce satellite calibration and validation data, provided that their spectral configuration can be
- 3 related to that of the spaceborne sensor.

4 In contrast, hyperspectral sensors (more often addressed as spectrometers, or spectroradiometers 5 when they are radiometrically calibrated) can measure hundreds of spectral bands, often 250 or more, with bandwidths usually less than 10 nm full width at half maximum (FWHM) and sampling 6 7 intervals from less than 1 nm to 10 nm depending on configuration (Fig. 2). The obvious advantage 8 of hyperspectral sensors is that they can resolve more detailed features of the vegetation (Milton et al., 2009) and serve to estimate parameters that require higher spectral resolution, such as the 9 emission of chlorophyll fluorescence (Meroni et al., 2009). Moreover, since hyperspectral 10 information can be resampled to coarser spectral resolutions, data from hyperspectral systems can 11 be flexibly convoluted to match spectral bands of different remote sensors (Olsson et al., 2011) 12 increasing its value as a source of satellite calibration and validation data. In addition, hyperspectral 13 14 data can be used to mine new spectral band combinations to match different ecosystem variables (e.g. Balzarolo et al., 2015; Heiskanen et al., 2013; Inoue et al., 2008; le Maire et al., 2008; Milton 15 et al., 2009; Tagesson et al., 2015; Wang et al., 2011; Yao et al., 2010). Milton and coworkers 16 (2009) presented an extensive review of how hyperspectral proximal sensing, or field spectroscopy, 17 18 has developed and listed the most commonly available field spectrometers. Spectrometers are very complex opto-electro-mechanical instruments and tend to be expensive, from a few thousand 19 20 Euros/dollars for optical benches measuring in the VNIR, to several tenths of thousands for field instruments measuring in the VNIR and the SWIR. The common limitation of all these 21 22 spectrometers is that they are not designed for unattended or long-term field operation. Accordingly, users need to build their own weatherproof housing, power supply, automatic 23 datalogging, and control units (see next section). As a result, the overall cost of these user-made 24 systems is difficult to quantify because in addition to off-the-shelf components they involve plenty 25 26 of in-house skilled technician hours. Field spectrometers are also more susceptible to physical 27 damage (due to their inherent complexity), and are more difficult and expensive to automate for continuous or periodic logging applications. In addition, these systems tend to be considerably 28 larger and heavier than their multispectral counterparts, presenting a structural challenge to their 29 deployment on flux towers. Despite these limitations, the number of such measurements is rapidly 30 increasing (Drolet et al., 2014; Huber et al., 2014; Pacheco-Labrador and Martín, 2015; Rossini et 31 al., 2012; Sakowska et al., 2015). 32

### 1 2.3 Instrument Configurations: hemispherical-conical, bi-conical and bi-

### 2 hemispherical

- 3 Reflectance factors relate the radiant flux reflected by a target surface to the radiant flux incident on
- 4 it and they can be measured using different instrument configurations (see Schaepman-Strub et al.,
- 5 2006 for a full mathematical explanation of the different factors and terms). Three main instrument
- 6 configurations have been applied to in situ field measurements to quantify incoming and reflected
- 7 radiation and estimate reflectance factors: bi-conical, hemispherical-conical and the bi-
- 8 hemispherical configurations (Fig. 1).
- 9 Hemispherical-conical measurements use a foreoptic diffuser assembly, designed to have a cosine
- 10 response at changing solar zenith angle to estimate down-welling irradiance, and a conical foreoptic
- for upwelling measurements which can be installed at nadir or off-nadir. The hemispherical-conical
- configuration lends itself to both multispectral and hyperspectral measurements from flux towers.
- 13 Bi-conical measurements rely on a diffuse white reference panel, typically of Spectralon®
- 14 (Labsphere Inc., NH, USA), reflecting down-welling solar radiant flux, normally viewed from nadir
- through a fixed angularly limited (conical) field-of-view foreoptic, to provide the reference
- measurement. The potential limitation of using a reference panel is that it needs to be kept clean and
- stable over time which may become a challenge in the field due to particle deposition (but see
- Sakowska et al., 2015 in Section 3). In practice, because both direct and diffuse light contribute to
- 19 the up-welling signal reflected from the reference panel when measuring under field conditions,
- 20 field data obtained in a bi-conical instrument configuration can be used to derive hemispherical-
- 21 conical reflectance factors (HCRF) (Schaepman-Strub et al., 2006).
- 22 Bi-hemispherical measurements use a foreoptic diffuser to capture both down-welling and up-
- welling irradiance. Bi-hemispherical measurements require a nadir-view installation for both sensor
- 24 heads and have the great advantage of enabling the sampling of a wider area. The main limitation of
- 25 this configuration is that while the hemispherical-conical measurements can be taken by observing
- 26 the canopy at nadir or off nadir, all viewing directions (both nadir and off-nadir) contribute to the
- 27 bi-hemispherical measurements (Meroni et al., 2011). For this reason, bi-hemispherical
- 28 measurements tend to be more sensitive to variations in illumination geometry compared to
- 29 hemispherical-conical measurements collected with a nadir view particularly for large illumination
- 30 zenith angles.

#### 3. EUROSPEC Main Results

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#### 3.1. Network and State-of-the-art characterization

- 3 When research questions become global, as in the case of global carbon cycle monitoring,
- 4 networking becomes a key methodological element to ensure consistent implementation of
- 5 measuring protocols, data sharing and management. One of the objectives of EUROSPEC was to
- 6 contribute to build up a distributed European spectral sampling network to foster data sharing in
- 7 order to better understand relationships between optical responses of vegetation and carbon cycle.
- 8 In situ long-term spectral measurements at flux towers are still accomplished with instruments that
- 9 are of variable design and performance, use different configurations, are installed with contrasting
- 10 geometries, and are conducted with different calibration or quality assessment regimes. In
- 11 EUROSPEC, we conducted a detailed review of proximal sensing measurements based on the
- 12 responses to a questionnaire obtained from groups working at 40 flux tower sites in Europe
- including two sites from Africa and Australia (Balzarolo et al., 2011). In situ measurements
- included SFOV and DFOV systems; bi-hemispherical or hemispherical-conical configurations, and
- both multispectral and hyperspectral sensors. The study portrayed the lack of consensus on what are
- the most suitable proximal sensing systems and methods to support EC measurements. No
- standards were being applied in terms of system performance (e.g. non-linearity in response, signal-
- 18 to-noise ratios, and cosine response of down-welling radiant flux foreoptics); measurement
- 19 geometries (e.g. hemispherical vs conical and their combinations); different foreoptic field-of-
- views; installation geometry (e.g. nadir or off-nadir; height of sensor above target surface), or
- 21 calibration regimes (e.g. regularly calibrated by manufacturer, calibrated in situ or even not
- regularly calibrated) (Balzarolo et al., 2011). The lack of regular calibrations was presented as a
- 23 fundamental limitation to overcome in order to produce high quality data, reliability of time series
- 24 analysis and to enable inter-comparison of results between network sites, e.g. Integrated Carbon
- Observation System (ICOS) sites (https://www.icos-ri.eu/). At the end of EUROSPEC, the need to
- standardize these measurements still exists.
- 27 Balzarolo et al. (2011) suggested also that two possible levels of instrumentation could be
- 28 considered. The first; termed the Basic Standard, would include only multispectral broadband
- 29 sensors to estimate selected vegetation indices. The second, termed Advanced Standard, would
- augment these multispectral sensors sites with hyperspectral sensor systems. The question remains
- as to what specific instruments and sensors would be more appropriate in each case. Anderson et al.
- 32 (2013) conducted a field intercomparison experiment to assess the reproducibility of measurements

- 1 collected by different sensors used at flux tower sites. The analysis showed that lower-cost
- 2 spectroradiometer systems performed similarly to more costly models and suggested that cost-
- 3 effective and accurate measurements in the PAR range can also be acquired using lower-cost
- 4 instrumentation. Similar conclusions were obtained by Harris et al. (2014) when they compared the
- 5 performance of lower-cost multispectral sensors with a reference spectroradiometer to estimate the
- 6 photochemical reflectance index (PRI). Another conclusion of these studies was the importance of
- 7 characterizing sensor properties to allow inter-comparison of results between sensors and sites (see
- 8 next section). Further long-term field instrument intercomparisons will be needed before final
- 9 conclusions can be drawn from these studies.
- 10 EUROSPEC managed to establish an active network including scientists from 28 countries from
- Europe and beyond. This network remains active under a new COST Action (OPTIMISE-ES1309)
- and under the umbrella of SpecNet. Together we hope to continue promoting the standardization
- and implementation of optical measurements across flux sites.

#### 14 3.2 Sources of variability

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- 15 Limited consideration had been given to the comparability of spectral measurement protocols and
- systems before EUROSPEC (but see Castro-Esau et al., 2006; Pfitzner et al., 2011). Because the use
- of the same type of sensor in all sites is not realistic, and perhaps neither desirable as it would
- 18 undermine the development of new sensors, we need to examine the factors that influence the
- variability in the data collected with different sensors. In EUROSPEC we dealt with a number of
- 20 these factors: linearity of spectrometer response, impact of cosine diffusers and reference panels,
- 21 effect of sensor FOV, and temporal stability of measurements and calibrations.

#### 3.2.1 Linearity of spectrometer response

- 23 Linearity refers to the linear relationship between the signal generated by a radiation sensor and the
- 24 impinging light power. Any dependence of this relationship on third or more variables leads to a
- 25 systematic error in the measurements which needs to be characterized and corrected. Pacheco-
- Labrador et al. (2014) and Pacheco-Labrador and Martín (2014) assessed the linearity of one of the
- 27 commercial field portable spectroradiometers, the Unispec-DC (PP Systems) currently used in
- unattended systems at EC sites (Hilker et al., 2010; Pacheco-Labrador and Martín, 2015), finding
- 29 that both the gray level measured and also the integration time had an effect on linearity. They
- 30 showed that non-linearity could be a significant problem in hyperspectral proximal sensing,
- 31 especially for *in situ* and long-term unattended measurements. The impact of gray level-dependent

non-linearities may be significant when estimating narrow band indices, such as the photochemical 1 reflectance index (PRI), and therefore cannot be left uncharacterized and uncorrected (Pacheco-2 Labrador and Martin, 2014). The impact of non-linearity can be minimized avoiding the most non-3 linear region of the dynamic range. In turn, non-linearities related with the integration time affected 4 also the characterization of other instrumental artifacts (Pacheco-Labrador et al., 2014). This 5 dependence, previously reported in cameras (Ferrero et al., 2006) but not in field 6 7 spectroradiometers, is significant when the integration time is close to the readout time of the sensor (i.e. a photodiode continues to collect photons during the time when the signal is being processed 8 9 (the readout time), producing an extra signal that is added to that obtained during the integration 10 time). Despite that integration-time dependent non-linearities have been characterized only in the 11 Unispec-DC (Pacheco-Labrador and Martín, 2015) it would be recommendable to avoid integration times close to the instrument readout time, unless the integration-time dependent non-linearity has 12 13 been characterized.

#### 3.2.2 Cosine diffusers and reference panels

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Irradiance (i.e. downwelling radiant flux) can be measured with cosine corrected foreoptics pointed vertically up, or with a diffuse white reference panel (see Fig. 1). Importantly, the materials, calibration status, and method selected to measure irradiance may have an impact on the result. Biggs et al. (1971) highlight the need for a properly designed foreoptic to avoid spectral variations caused by changing sun azimuth and zenith angles. Malthus and Mac Lellan (2010) demonstrated that the material selected for the foreoptic diffuser can significantly affect the spectra with angular/wavelength dependencies and a poor cosine response. Similarly, they reported that the performance of cosine diffusers in the Short Wave Infrared (SWIR) tends to be very poor with high signal attenuation above 1400 nm (Malthus and Mac Lellan, 2010), and suggested that a diffuse reference panel will provide a better cosine response than a cosine-corrected foreoptics. Importantly, because reference panels present and angular-dependent time degradation at such wavelenghts, especially when used in the field (e.g. Anderson et al., 2002; Georgiev and Butler, 2007) (Fig. 3), recalibration and regular maintenance is essential. Recalibration requires a dedicated laboratory facility as demonstrated by Georgiev et al. (2011) for the SWIR region of the solar spectrum. In turn, Labsphere, the manufacturers of Spectralon® provide guidance on how to clean reference panels. Consequent care, careful cleaning and recalibration of reference panels are essential to minimise error propagation and uncertainties when conducting spectral measurements.

- 1 Selection of reference panel material is also very important. Manufacturers of reference panels for
- 2 spectroscopy such as LabSphere (Spectralon ®) or SphereOptics (Zenith polymer ®) use a sintered
- 3 fluoropolymer manufactured to have a very high reflectance, possibly in excess of 96% and
- 4 approximate a Lambertian reflectance across the 400 nm to 2,500 nm spectral region. Alternatively,
- 5 low cost PTFE sheets (i.e. Teflon) can be purchased at lower cost. However, PTFE sheets have
- 6 lower reflectance, approximately 80%, and have higher specular reflection. Also, because PTFE
- sheets are not manufactured to be used as 'references' there may be variability between individual
- 8 sheets and wavelength dependent reflectances may be unknown. Overall, PTFE sheets are not
- 9 recommended as field spectroscopy reference standards.
- 10 Similarly, the material and design of cosine receptors affect the estimation of hemispherical
- reference factors (Malthus and MacLellan, 2010) and consequently, the indices derived from them.
- 12 Therefore, significant and unquantified uncertainties will be introduced when comparing data from
- sites that used different cosine receptors or sites characterized by a different range of Solar Zenith
- Angles (SZA). For example, for SZA greater than 60° variation in reflectance factors obtained with
- different cosine receptors can exceed 20%. This effect is reduced when considering normalized VIs,
- and it depends on the spectral distance between bands selected for the VI calculation (Julitta, 2015).
- 17 Again, characterization of the properties of cosine diffusers and regular maintenance/replacement
- should be included inside the measurement routine.

#### 3.2.3 The fields-of-view of field spectrometers and multispectral sensors

- 20 Field spectroscopists normally assume that the Earth surface sampled by a non-imaging
- spectrometer with a limited FOV foreoptic is spatially delimited by the solid angle specified by the
- 22 manufacturer, and that the response across the surface delimited by the FOV is the same for all
- points inside the given FOV (Castro-Esau et al., 2006; Ferrier et al., 2009; Murphy et al., 2005;
- Nichol and Grace, 2010). In practice, the spectral response within FOV of a field spectrometer is
- 25 not constant (i.e. certain areas within the FOV contribute more to the signal than others)
- 26 (MacArthur et al., 2012, Eklundh et al. 2011), this can be determined by the viewing angle and the
- 27 instrument's Directional Response Function (DRF) (CIE, 1987) which can be characterized. The
- 28 DRF will be affected by both the internal design of the spectrometer (e.g. open path or fiber optic
- transfer to individual detectors) and the foreoptics used. When measurements of heterogeneous
- 30 surfaces were simulated using the measured DRFs, significant differences were found between
- 31 simulated reflectance factors and those expected from the manufacturers' specifications (Mac
- 32 Arthur et al., 2012). Even when less optically complex spectrometers, measuring only across the

VNIR region are considered, the Earth surface sampled is not necessarily that inferred from the manufacturers' specified FOV included solid angle (Caras et al., 2011). The manufacturers of some spectrometers now offer optical elements within their foreoptic mounts to defocus the foreoptics and thereby homogenize the light received (e.g. the ASD FS pistol grip "scrambler"), or have improved the optical components used to minimize 'chromatic aberrations' and heterogeneities and again, homogenize the light received prior to it being distributed to the detectors (e.g. SVC HR-2014i spectrometers). Therefore, the spectrometers' response should be more closely represented by a Gaussian or Cauchy response, albeit centre-weighted, with all areas within the FOV represented in the integrated measurement. These limitations affect the estimation of reflectance factors measured from heterogeneous Earth surfaces (Mac Arthur et al. 2013) because the sample area is ill defined and unknown but systematic sampling errors appear. In contrast, multispectral field sensors normally comprise of individual foreoptics/detector assemblies for each spectral band and subsequently have less complex optical paths than their hyperspectral counterparts, and each sensor can be more reasonably assumed to have a center-weighted and Cauchy response, though this response is also affected by the viewing angle of the instrument (Eklundh et al., 2011). For a more detailed discussion of the FOV and DRF of field spectrometers and multispectral sensors we refer readers to Mac Arthur et al. (2012) and Eklundh et al. (2011), respectively.

#### 3.2.4 Temporal stability of measurements and calibrations

The temporal stability of the measurements and the calibrations are essential factors to be considered when conducting long-term *in situ* spectral measurements. Factors such as diurnal or seasonal fluctuations in temperature, gradual particle deposition onto optical parts (e.g. cosine diffusers or reference panels), or any other processes causing a temporal drift in the functioning of will interact with the measured signals and calibrations. In turn, the impact of these factors will depend on the signals we are measuring and the instrumentation we use. For example, because the impact of these factors may be wavelength-dependent it may interfere with the estimation of reflectance indices. Similarly, in DFOV systems constructed around two sensors, the differential impact of these factors in each sensor may also introduce significant errors. Unfortunately, the quantitative characterization of these sources of variability, and the establishment of a set of recommendations, remains a key question after EUROSPEC and clearly requires further attention. We briefly introduce the topic and present some indicative data that we hope will help the reader to understand the importance of temporal stability.

- 1 Stability issues can be grouped around two points: The temporal stability of the calibration or cross
- 2 calibration of a sensor pair; and thermal stability of the measurements.
- 3 1) Temporal stability of the calibration/cross calibration. Sensor calibration against a source of
- 4 known spectral and radiometric properties is needed to derive radiometric units and control for
- 5 spectral shifts in sensor response. Similarly, cross calibration of two sensors (e.g. Gamon et al.
- 6 2015, Jin and Eklundh 2015) is essential for deriving reflectance factors using two different sensors
- 7 (e.g. DFOV systems) and to control for between-sensor variability. Importantly, particle deposition,
- 8 component aging, or partial damage of sensor components such as optical fibers, may cause a
- 9 change in these calibrations which we need to detect, quantify and correct for. For example, the
- temporal degradation of the white reference panel becomes a critical issue in systems such as the
- ASD-WhiteRef (See Section 3.3), which thanks to the system design was found to be insignificant
- 12 (maximum of 2% differences at 400nm) over the measuring period (Sakowska et al. 2015). In the
- absence of additional information, the general recommendation is to start with an intensive
- calibration/cross-calibration scheme and adjust the frequency later on when the stability of the
- calibrations for the specific field conditions is known. Key questions that the user should consider
- are: what is the temporal drift in calibration for the specific sensors and measuring conditions? what
- is the impact of this drift on the resulting signal/indices? and what is the optimal calibration/cross
- 18 calibration frequency?
- 19 2) Thermal stability. Changes in temperature may have an impact on both the intensity and the
- 20 spectral information of the measured signal. Accordingly, characterizing the temperature stability of
- 21 a spectral system and its impact on the signal we seek to measure, is a critical step when designing
- 22 and deploying *in situ* spectral measurements. For example, the radiometric response to temperature
- 23 in silicon diodes is more pronounced in the NIR compared to the visible. Saber et al. (2011)
- 24 characterized the percentage change in the response a spectrometer relative to its response at the
- calibration temperature (20 °C) and found a variation of -0.13 % / °C at 30 °C that was constant
- between 400 and 700 nm but increased to +0.2 % / °C at 30 °C at 1050 nm. Similarly, Pacheco-
- 27 Labrador et al. (2014) characterized the effect of temperature on the signal and the spectral
- 28 calibration of two sensors in a DFOV system based on a pair of Unispec DC spectroradiometers, for
- 29 the range of temperatures between 13.9 °C and 46.1 °C, finding higher variation in the NIR,
- between -10 % to 21% (relative to 30 °C) compared to variations between -1 % to +4 % below 750
- 31 nm. Clearly, the spectral component of this temperature dependencies do not only affect the
- 32 quantification of radiometric quantities, but also the comparison of the quantities measured at
- different wavelengths. This is especially critical when estimating VIs or solar-induced chlorophyll

- 1 fluorescence where two or more spectral bands are combined. In these cases, seasonal changes in
- 2 temperature could, if not properly addressed and corrected, mask the physiological component of
- 3 the signal or even generate spurious dynamics (e.g. Pacheco-Labrador et al. 2014). Key questions
- 4 that the user should consider are: How do changes in temperature affect sensor/spectrometer
- 5 output? what is the impact on the resulting signal/indices? What are the wavelenght/sensor
- 6 dependent thermal responses? If needed, how to control and correct for thermal stability for the
- 7 selected application?

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#### 3.3. Development of instrumentation for continuous field measurements

- 9 Conducting in situ long-term spectral measurements in the field is not straightforward. In addition
- 10 to a number of logistic and infrastructural requirements, long-term field measurements require
- instrumentation specially designed and conceived for the task. One of the goals of EUROSPEC was
- to identify the main requirements of such sensors and to promote the development of new dedicated
- instrumentation. As part of these activities we organized a Science-Industry Interaction Meeting
  - where EUROSPEC scientists got together with representatives of the "spectrometry" industry
- 15 sector. A number of general requirements for field optical sensors were identified and are
- summarized in Box 1. In addition, industry representatives raised the issue of how to cover the non-
- 17 recurring engineering costs associated with instrument development. The possibility of establishing
- partnerships and seeking funding for joint collaborative projects between science and industry was
- 19 suggested, particularly to produce prototypes for new instruments.
- 20 Four different hyperspectral systems were identified during EUROSPEC for continuous proximal
- sensing from EC towers in Europe (Fig. 4): 1) A temperature-controlled spectrometer system for
- 22 continuous and unattended measurements of canopy spectral radiance and reflectance (UNIEDI
- 23 System) developed by the University of Edinburgh (Drolet et al., 2014) that has been operating at
- the FluxNet Hyytiälä site (<a href="http://fluxnet.ornl.gov/site/447">http://fluxnet.ornl.gov/site/447</a>) in Southern Finland since March 2010.
- 25 2)The Multiplexer Radiometer Irradiometer (MRI) developed by the Remote Sensing of
- 26 Environmental Dynamics Laboratory, Dipartimento di Scienze dell'Ambiente e del Territorio e di
- 27 Scienze della Terra, Università degli Studi Milano- Bicocca (Italy) and deployed for relatively short
- periods (weeks to months) in the context of different projects (Bresciani et al., 2013; Cogliati et al.,
- 29 2015); 3) the HyperSpectral Irradiometer (HSI) also developed by the previous group which has
- 30 operated in the field from 2009 to 2011 (Meroni et al., 2011; Rossini et al., 2012, 2014); and 4) the
- 31 AMSPEC-MED system, a version of the automated, multiangular spectroradiometer system
- 32 AMSPEC II (Hilker et al., 2010) modified by the Environmental Remote Sensing and Spectroscopy

#### Box 1. General Requirements for in situ long-term optical sensors

- Waterproof (should withstand direct rain)
- Robust design: external parts withstanding tension
- Avoidance of holes and cavities (perfect place for birds and insect nests)
- Attachments for easy field installation
- Minimum payload (threshold depending on application)
- Minimum size (threshold depending on application)
- Low power consumption (threshold depending on site infrastructure)
- Maximize long-term stability of optical parts (i.e. filters, diffusers, etc.) to minimize recalibration frequency
- For global networks: Operating temperature range matching the wide thermal distribution of terrestrial plant species, from -50°C to 50°C. For local measurements: temperature range matching local variation.
- High thermal stability
- Linear sensor response
- High signal-to-noise ratio
- Optimal cosine directional response function
- Logic user interface and easy to program systems
- · Remote access to data and system control

2 Laboratory (SpecLab), Spanish National Remote Sensing (CSIC) and the Centro de Estudios

3 Ambientales del Mediterráneo (CEAM) in Spain. The system has been operating at Las Majadas

4 Fluxnet site in Spain (<a href="http://fluxnet.ornl.gov/site/440">http://fluxnet.ornl.gov/site/440</a>) since August 2013 (Pacheco-Labrador and

5 Martín, 2015).

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7 The first three systems are based on commercially available spectrometers from Ocean Optics,

8 relatively low cost and compact optical benches housed in temperature controlled environments and

operated by dedicated software. The main difference between each of these systems lies in their

design.

11 The UNIEDI system (Fig. 4A) has a hemispherical-conical configuration, and is a DFOV system

that uses a pair of spectrometers (Ocean Optics, USB2000+) with one spectrometer measuring up-

welling radiance through a FOV limited foreoptic (24.8 deg) and the other spectrometer measuring

down-welling irradiance using a cosine corrected diffuser. One limitation of this system is that,

despite that both spectrometers are kept at constant temperature using a temperature control system

(Drolet et al., 2014), regular intercalibration of the two spectrometers is essential to account for

- 1 sensor-specific time- and temperature-dependent drift in their radiometric capabilities.
- 2 Intercalibration can be done using a calibration lamp and a dark setting either in situ or in the
- 3 laboratory. In fact, Anderson et al (2006) showed that for calibrating field-based spectra collected
- 4 with a DFOV spectrometer, a field-derived intercalibration function provides the most accurate
- 5 results.
- 6 The MRI system has also a hemispherical-conical configuration, but it is a SFOV system with a
- 7 single spectrometer. A commercially available optical multiplexer is used to switch the input to the
- 8 spectrometer from down-welling to up-welling radiant flux. Irradiance can be measured through a
- 9 fibre connected to either a cosine corrected diffuser or an up-looking integrating sphere foreoptic.
- 10 Up-welling radiance is measured through a bare optical fibre with a FOV of 25 deg. The S-FLUOR
- has been more recently developed in collaboration with the Forschungszentrum Jülich GmbH based
- on the MRI design (see Fig 4B). The major technical improvements are an overall compact design
- and the integration of the cooling system within the instrument box (Cogliati et al., 2015). The S-
- 14 FLUOR has been used in the years from 2012 to 2014 as reference instrument for the HyPlant
- 15 (Specim, Finland) airborne fluorescence imager (Rossini et al., 2015). The HSI system (Fig. 4C)
- has a bi-hemispherical configuration and a SFOV and uses of a rotating optic with a cosine response
- to measure the down-welling and the up-welling radiant flux. Because both the MRI and HSI are
- 18 SFOV they present a time delay (at best multiple seconds) between the down-welling and the up-
- welling measurement. These delays may add some measurement uncertainties due to changes in sky
- 20 conditions between the individual measurements, particularly under cloudy or overcast conditions.
- 21 The AMSPEC-MED system is based on a commercial Unispec dual channel VIS-NIR
- spectroradiometer (PP-Systems, Amesbury, MA, USA) equipped with a motor driven pan-tilt unit
- 23 that allows measuring up-welling radiance in a range of zenithal and azimuthal angles. Similar to
- 24 the UNIEDI, the system is a DFOV system and, therefore, cross calibration between spectrometers
- 25 is performed regularly using a Spectralon<sup>®</sup> panel. Because the system is operated with solar panels,
- 26 temperature control is not possible due to power restrictions. Instead, temperature sensitivity of
- each of the spectrometers and its impact on the resulting hemispherical-conical reflectance factors
- 28 was characterized in the laboratory and used in signal post-processing (Pacheco-Labrador and
- 29 Martín, 2015). Note that power constraints are not system dependent but rather site specific,
- depending on power availability and site temperature range.
- In an attempt to address some of the limitation of the systems reviewed above and based on
- discussions between groups during EUROSPEC, three new approaches were developed (Fig. 5):

1) The Piccolo system, developed by the UK Natural Environment Research Council (NERC) Field Spectroscopy Facility (FSF) Geoscience, University of Edinburgh, is based on a DFOV hemispherical-conical configuration with a cosine corrected foreoptic to capture down-welling radiant flux and a configurable up-welling channel to capture up-welling radiant flux. The upwelling foreoptic can either be fitted with a view angle limited foreoptic or with another cosine corrected receptor to enable a bi-hemispherical measurement approach to be adopted (Fig. 1). The novelty of this system is the use of low weight components for decreased weight, and the use of bifurcated fibre optic with electronic shutters for decreased time delay between up and downwelling measurements (Mac Arthur et al., 2014). In addition, as both light inputs can be closed at the same time, the systems' dark current (inherent electrical noise) can be recorded and used in post processing. The Piccolo system is currently undergoing service life cycle testing and will be field trialled in a number of flux towers in the near future. In addition, the low weight and DFOV mode of this system makes it compatible with unmanned aerial vehicles (UAV) applications, opening a new range of research possibilities. 2) A similar configuration has been adopted in the SIF-Sys (Burkart et al., 2015) developed by the Forschungszentrum Jülich GmbH. The system hosts a low cost and small size spectrometer (STS-VIS, Ocean Optics, Inc., Dunedin, US) and uses also a bifurcated optical fibre with optical shutters to split the optical signal between two channels: one channel pointing to a white reference panel to measure the down-welling radiant flux and the downlooking channel measuring the radiant flux up-welling from the vegetation. SIF-Sys is specifically intended to measure SIF and, for this reason, it is equipped with a LED emitting at the wavelength of SIF (at 760 nm). The LED is placed in the instrument down-looking FOV and it is used as a reference to assess the uncertainty of passive SIF retrieval in field conditions. SIF-Sys has been tested in dedicated field experiments and will be installed at flux towers for long term and unattended data collection in the near future. 3) The ASD-White Ref system (Sakowska et al., 2015) is an automated system designed for continuous acquisition of measurements using an ASD FieldSpec spectroradiometer. The WhiteRef system was developed by the Forests and Biogeochemical Cycles Research Group, Sustainable Agro-Ecosystems and Bioresources Department, Research and Innovation Centre—Fondazione Edmund Mach, San Michele all'Adige, together with the Institute of Biometeorology—National Research Council, Firenze in Italy, and the contribution of NERC Field Spectroscopy Facility, School of Geosciences, University of Edinburgh, and has been deployed in a grassland site in the Viote del Monte Bondone in Northern Italy. The main advantage of this system is the possibility to scan in the VNIR and SWIR regions (350 nm to 2,500 nm) using a popular and commercially available spectrometer. The system is SFOV and measures in a hemispherical-conical configuration with a FOV of 25 deg. A novelty of

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- the WhiteRef system is that both, reference and vegetation target radiances, are measured by
- 2 automatically sliding a white reference panel under the fibre optic. To protect the WR panel from
- 3 light, dust, rain, insects and adverse weather conditions, the WR is kept inside a waterproof box and
- 4 ejected only during the measurements. Each acquisition is preceded by a reading of a dedicated
- 5 wetness sensor signal, and in case of rainfall or dew the reference measurements are not conducted.
- 6 In addition, to remove eventual dust/insects from the measurement surface, the WR panel is sprayed
- 7 with compressed air during each ejection and insertion phase.

### 3.4. Upscaling optical data and fluxes from the footprint to the landscape level

- 9 In situ spectral measurements are essential for the successful upscaling of optical and flux data
- across space and time. In particular, the temporal match between in situ spectral measurements and
- 11 flux data facilitates the characterization, modelling and validation of their linkage. Spatial and
- temporal scales are tightly connected with each other and neither temporal or spatial upscaling can
- be fully accomplished without giving attention to the other. Considering that the temporal link
- between optical and flux data can covered with *in situ* spectral measurements the main question is
- probably that of upscaling these signals across space from the footprint to the landscape level (Fig.
- 16 6).

- 17 In the process of integrating remote sensing data with flux measurements an assumption is
- 18 commonly made: the match between flux footprint and image pixel (e.g. Beer et al. 2010,
- 19 Tramontana et al 2015). The same assumption can be used between flux data and *in situ* spectral
- 20 measurements. However, a number of factors related to footprint variability, pixel heterogeneity,
- 21 the BRDF properties of the surface, and the geometry of the measurements can momentarily or
- 22 systematically decouple optical and flux data adding noise or bias to their relationship.
- 23 Despite of efforts to orientate the FOV of *in situ* spectral measurements to cover the dominant
- 24 footprint of EC measurements (e.g. using footprint modelling techniques), the flux footprint will
- 25 still differ from that of optical measurements most of the time due to footprint variability. Most flux
- sites are located in places with homogeneous vegetation where footprint variability is not expected
- 27 to decouple flux and optical data. For example, accurate modelling of the flux footprint did not
- improve the predictive power of optical data to estimate GPP in a Mediterranean savanna (Pacheco-
- Labrador et al. 2015) or in a subalpine grassland (Vescovo et al. 2015). However, the mismatch can
- 30 be relevant in sites with heterogeneous vegetation like agricultural land, ecotones, or sites with
- 31 adjacent patches of vegetation. In these sites, characterization of the area of interest and footprint
- modelling will be critical for the successful implementation of data driven models, e.g. the light use

efficiency model introduced in Eqn. 1. For example, when estimating GPP in an agricultural area using MODIS data and a footprint model, Gelybó et al (2013) were able to reduce the RMS error by 28% compared to non-footprint weighted values. Dealing with the effect of optical vs flux footprint mismatch is challenging from a point of view of tower based measurements. One of the conclusions from EUROSPEC was that new tools are needed to characterize these scale issues more precisely. One of them is the use of small and relatively affordable UAVs or remotely piloted aircrafts (RPAs) on which light weight spectrometers, both multi and hyperspectral, and cameras can be deployed. Hyperspectral imaging systems onboard of aircraft or unmanned aerial vehicles (UAV) can for example provide high spatial resolution imagery enabling the identification of pure species pixels within the flux footprint (Zarco-Tejada et al., 2013a). The flexibility, maneuverability, and capacity to view the same target from different heights allows to study the impact of footprint variability and to bridge in situ spectral measurements with coarser satellite or airborne data, facilitating their interpretation and un-mixing (Fig. 6). For example, the availability of pure pixels can be used to investigate the effect of aggregating different species or land-cover classes on the resulting hyperspectral signal (Zarco-tejada et al., 2013b). As reported in Gamon et al. (2015) or Whitehead K. and Hugenholtz (2014), the cost effectiveness of UAV platforms make them a valid solution to address footprint variability. Two UAV-based statistical sampling approaches are possible to systematically address footprint variability: i) with no previous knowledge a regular grid might be recommended, whereas ii) if the spatial patterns of vegetation are already known, a stratified sampling for different vegetation types might be more efficient. Overall, the systematic optical sampling of the footprint/pixel area can serve to characterize the different sources of error when upscaling from in situ spectral measurements to the satellite pixel level. These topics have just started to be addressed as low cost UAVs and proper instrumentation are becoming available. The technology is relatively under-explored in the context of flux scaling studies, but there are a growing number of papers that comment on the utility of UAVs for fine-scale sensing of landscape ecology and vegetation parameters (e.g. Dandois and Ellis, 2013).

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Data from *in situ* and remote sensing measurements are also affected by the structure of the canopy and the geometry of the observation and illumination *per se* (Jones and Vaughan, 2010). The reason is that photons hitting a surface are preferentially scattered (or reflected) in given directions depending on the properties of the surface. This can be characterized by the BRDF of the surface (Nicodemus et al., 1977; Roberts, 2001). In other words, if we would measure an ideal plant canopy with constant fAPAR and LUE, our sensors would still register diurnal and seasonal variations in vegetation parameters due to variations in solar elevation and azimuth. This is particularly relevant

- 1 when comparing seasonal time series of optical data which may have been acquired with
- 2 significantly different sun elevations (e.g. in boreal latitudes). Accordingly, knowledge on the
- 3 BRDF properties of the surface under examination becomes essential to correct for these geometry
- 4 effects.
- 5 The BRDF can be quantified and investigated by mounting sensors on pan-tilt heads (e.g. Huber et
- al., 2014), by deploying a number of (low-cost) sensors with different fixed off-nadir positions, or
- by using the UAV systems discussed above. Hilker et al. (2007, 2010), presented a hyperspectral
- 8 system capable of quantifying and measuring these effects, the AMSPEC and AMSPEC II systems
- 9 (Automated Multiangular Spectro-radiometer for Estimation of Canopy reflectance). The AMSPEC
- system (see previous chapter) is a DFOV system that samples hemispherical-conical reflectance
- 11 factors at different observation angles from the canopy surrounding the tower. Multiangular
- measurements are used to retrieve the BRDF and can be used to normalize observations to the same
- viewing and illumination conditions. Data acquired by AMSPEC system over forest stands in North
- America showed how optical indices, such as the PRI, can be influenced by view angle and shadow
- fractions (Hilker et al., 2008b). Moreover, retrieved BRDF estimates allows mimicking off-nadir
- observations of remote sensors and provides a top-of-canopy reference for atmospheric corrections
- 17 (Hilker et al., 2009).

#### 4. Future challenges and opportunities

- 19 Quantifying and modelling the spatiotemporal dynamics of the carbon cycle remains a key goal in
- 20 climate change and global biogeochemistry research. Global questions call for global initiatives to
- 21 provide sensible data at the global scale. Flux tower networks such as FluxNet
- 22 (http://fluxnet.ornl.gov/) and other long-term monitoring infrastructures such as ICOS
- 23 (https://www.icos-ri.eu/) or NEON (http://www.neoninc.org/) are responding to these needs by
- 24 ensuring a long-term and an increasing flow of global carbon flux and ecological data.
- 25 Simultaneously, the increasing number of current and planned satellite missions warranties an
- equally increasing flow of remotely sensed data (e.g. Venus, Sentinel-2 and 3; OCO-2, FLEX),
- offering improved geographical coverage, as well as temporal, spatial, and spectral resolutions.
- However, our capacity to capitalize on these space developments depends very much on how well
- 29 we can relate the resulting satellite data to ground observations of ecosystem processes, such as
- 30 photosynthetic carbon assimilation.
- 31 EC measurements provide good temporal resolution of carbon fluxes at the ecosystem level but they
- are limited by spatial resolution and coverage. In contrast, remote sensing data provides good to

- moderate spatial resolution and coverage but are limited by temporal resolution. The 1 complementarity and synergy between these two sources of data is clear but their integration 2 remains a challenge due to scale mismatch. We need a Rosetta stone to help us translate and link the 3 information from these two sources of data: something that can be done only via in situ spectral 4 measurements. On one hand, in situ spectral measurements can provide the same optical indices 5 than satellites, serving as a landmark to interpret, calibrate and validate remotely sensed data 6 7 products (i.e. we can establish a link between satellite data and ground optical data). On the other hand, because data from in situ spectral measurements has comparable temporal resolution and 8 9 relatively similar biological footprint to that of EC measurements, they can be used to develop 10 quantitative models that associate the two signals.
- Overall, there is a clear need to establish a global network of sites with standardized and coordinated *in situ* spectral measurements to facilitate the integration of remotely sensed data and EC data towards improving the global monitoring of the carbon cycle. In addition, such network is also needed to calibrate and validate satellite data products, and to resolve and avoid problems that appear when inferring ecosystem properties directly from satellite data, such as the "spurious amazon green-up" (Morton et al., 2014; Soudani et al., 2014); or the controversy around the remote sensing of foliar-nitrogen (Knyazikhin et al., 2013; Townsend et al., 2013).
- 18 The EUROSPEC Cost Action was a starting point for the organization of the European community of scientists working with in situ spectral measurements. We identified many areas that still need 19 20 further work and perhaps the main conclusion of EUROSPEC was to realize that we need more projects such as EUROSPEC. As a continuation, a new COST Action (ES1309) "Innovative optical 21 22 tools proximal sensing of ecophysiological processes (OPTIMISE) (http://optimise.dcs.aber.ac.uk/) was recently begun that expands the work of EUROSPEC to 23 24 include UAVs, "smart" spectral data storage systems and to go in-depth into the measurement and 25 interpretation of multi-scale chlorophyll fluorescence data.
- 26 Despite that regional level networking projects such as the EUROSPEC and OPTIMISE COST AusCover (http://www.auscover.org.au/), **EcoSIS** 27 Actions, or (http://labs.russell.wisc.edu/townsend/tag/ecosis/) are important, we need also activities and 28 networking at the global level. SpecNet is an excellent platform that could be used to accomplish 29 this coordination goal and liaise with national and regional projects. SpecNet could be also used to 30 31 share information, know-how, data, general guidelines on measurement and calibration protocols, 32 and challenges between scientists, but also including industry stakeholders. This is perhaps the

- 1 fastest and most effective way, in terms of costs and results, to promote standardization. As long as
- 2 the information remains disperse and the global network links remain weak, independent groups
- 3 will continue to adopt different solutions for *in situ* spectral measurements without following a set
- 4 of general guidelines. This is perhaps the main risk behind in situ spectral measurements in the near
- 5 future.
- 6 The following challenges and opportunities were identified during EUROSPEC:
- 7 1) Need to compile information on best-practices for *in situ* spectral measurements. Information on
- 8 what to purchase, how to install, maintain, calibrate, analyze, and store the data from *in situ* spectral
- 9 measurements is to some extent available from a number of studies conducted as part of
- EUROSPEC or by other groups (see e.g. Anderson et al., 2011; Balzarolo et al., 2011; Gamon et al.,
- 2015; Harris et al., 2014; Jin and Eklundh, 2015). These types of studies will most likely continue
- to appear in the near-future. However, a major up-to-date synthesis effort is urgently needed to
- provide a comprehensive treatise on such measurements. This would facilitate the different phases
- of decision-making by site PIs and promote standardization within relevant networks such as ICOS
- and FLUXNET.
- 16 2) Quantifying and dealing with uncertainty. Measurement uncertainty is instrument- and
- 17 environment-specific. Accordingly, characterization of sensor performance and quantification of
- measurement uncertainty is crucial to produce accurate data (Anderson et al., 2011; Castro-Esau et
- al., 2006; Jung et al., 2012). Anderson et al (2011) have demonstrated that laboratory-derived
- 20 measurement uncertainties do not present a useful means of quantifying all uncertainties in field
- 21 spectroscopy. Laboratory measurements can serve to define features such as signal-to-noise ratio,
- 22 noise equivalent radiance and linearity, but these uncertainties are added to by complexities of the
- 23 hemispherical illumination environment experienced in the field. Clearly, the optimal way to
- 24 characterize measurement uncertainty is to do so in the conditions that typify the measurement
- scenario. Protocols for systematic measurement uncertainty characterizations in the field should be
- adopted in the future.
- 27 3) Need for characterization and calibration. Networks of research sites engaged in optical sampling
- 28 should follow an instrument characterisation and calibration scheme to ensure direct result inter-
- comparison (Anderson et al., 2013; Balzarolo et al., 2011). Optical sensors could for instance be
- 30 characterized and calibrated against a common standard in a central laboratory prior to field
- 31 deployment then tested annually to monitor change or degradation. In addition, portable
- 32 calibration/verification standards could be rotated periodically around sites to conduct validation

1 measurements across space and time. Cross calibration of sensors in DFOV systems is also critical

and should be accomplished regularly. Calibration frequency will depend on signal drift rate which

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3 may be instrument- and climate-dependent. Accordingly, it would seem logical to characterize and

adjust calibration demands to each site and instrument, for example by calibrating at high

5 frequencies during the first measuring season and adjusting later on depending on signal drift rate.

6 4) Need for a 'smart' data repository and information access portal. Spectral data are time intensive 7 to collect but their analysis is even more time consuming. In turn, most spectral data collections remain poorly documented which greatly reduces their use for data sharing, if not nullifying it. 8 There is an urgent need for a spectral information system that: (a) establishes a data pool that can 9 hold spectral data collected from various instruments, providing them in an easily accessible and 10 11 generic form, and (b) includes metadata that is standardised to a degree that allows data selections 12 to answer new science questions. Such databases have been developed (Bojinski et al., 2003; Ferwerda, 2006; Hueni and Tuohy, 2006), but their adoption by the spectroscopy community has 13 been slow. Currently, there are only a few available and persisting spectral information systems, the 14 most prominent one being the open source SPECCHIO (Hueni et al., 2009). SPECCHIO has seen 15 16 many upgrades over time with a large contribution by the Australian National Data Service (Hueni et al., 2012) and support from EUROSPEC. The challenges for the future are numerous, but most 17

5) Upscaling issues: BRDF and footprint analysis. Scaling up *in situ* spectral measurements to those acquired from airborne and satellite platforms and linking this optical data to that of EC measurements remains an issue (Ju et al., 2005; Simic et al., 2004; Wu and Li, 2009). BRDF effects, footprint variability, and scale mismatch are factors that constrain our capacity to link and upscale remotely sensed and EC data. The rapid advances in UAV technology have opened new opportunities to deal with these challenges. Micro-hyperspectral field spectrometers and imaging sensors can now be mounted on UAVs. These measurements can serve to retrieve the BRDF of challenging Earth surfaces, such as forest canopies, to measure footprint optical variability, or to sample the same target at different heights facilitating the treatment of the scale issue. Deployment of specialized instruments on board UAVs with a view to collecting narrowband multispectral or hyperspectral data will constitute a step-change in scientific understanding of the connection between spectral data and multiple ecosystem processes. Investigating this potential is again one of the goals of the new COST Action OPTIMISE.

pressing appears the issue of automated data quality and metadata standards. SPECCHIO is

currently being further developed under the new COST Action OPTIMISE.

- 6) Permanent platform for communication and information dissemination. The need for and the 1
- potential of a permanent channel for cross-talk between research communities as well as between 2
- scientists and industry stakeholders was identified. Such a channel could be for example a 3
- moderated mailing list (e.g. Fluxnet type) or making use of other social media. This platform would 4
- provide the opportunity to share known-how and best-practices between users helping to promote 5
- standardization. In addition, it would also promote collaboration between research groups as well as 6
- 7 between scientists and industry stakeholders, which in turn might foster the development of new
- 8 instruments.

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Table 1. Advantages and disadvantages of different approaches and configurations for *in situ* spectral measurements.

	Advantages	Disadvantages
Method of data acquisition		
SFOV	<ul> <li>Only one instrument, lower cost</li> <li>No need for intercalibration</li> </ul>	<ul> <li>Non-simultaneous up-welling/downwelling measurements.</li> <li>Need to automate the system for target and reference measurements.</li> <li>Either temperature control, or characterization of the temperature sensitivity of the instrument and post-processing, are needed to acquire consistent time series of radiometric measurements</li> </ul>
DFOV	Quasi-simultaneous upwelling/down-welling measurements     No need to automate for target and reference measurements.	<ul> <li>Typically two instruments, higher cost (but see Piccolo and SIF-Sys)</li> <li>Need for regular intercalibration</li> <li>Either temperature control, or characterization of the temperature sensitivity of each of the instruments and post-processing, are needed both for derivation of reflectance factors and to acquire consistent time series of radiometric measurementsMore sensitive to component degradation effects (each unit degrading at different rate)</li> </ul>
Spectral		
Resolution		
Multispectral	<ul><li> Low cost</li><li> Low weight and power consumption</li></ul>	<ul><li>Fixed wavelengths/ no post-purchase flexibility</li><li>Spectral calibration is difficult</li></ul>
Hyperspectral	<ul><li> High versatility</li><li> Possibility to estimate several</li></ul>	<ul><li> Higher cost</li><li> More sensible to spectral shifts and</li></ul>

	indices (including future indices) and	miscalibration
	resample to specific spectral bands.	• Higher power consumption (either due to
	• Increased range of possibilities for	automation or temperature control units)
	the inversion of radiative transfer	
	models	
Configuration		
Hemispherical-	• Easier comparison with airborne or	• Small sampling area (depending on FOV),
conical	satellite measurements	requires taller towers for increased
	• Small sampling area (allows	sampling area.
	studying smaller units: shoots, single	Poor cosine response of cosine receptor
	canopies)	and Spectralon in the SWIR
		• If using Spectralon (SFOV): more
		expensive and delicate than cosine
		receptor.
Bi-hemispherical	Wider sampling area	• More prone to BRDF effects of vegetation
		• Difficult for comparison with airborne or
		satellite measurements if sun zenith angle
		is large
		• Reflectance measurements not
		comparable with nadir observations
		• Poor cosine response of the receptors in
		the SWIR

## Figure Legends

1

- 2 Fig. 1. Main instrument configurations adopted for *in situ* spectral measurements.
- 3 Fig. 2. Different sampling strategies: discrete vs continuous. Spectral resolution denoted by
- 4 bandwidth and sampling intervals. The narrower the bandwidth and the shorter the interval between
- 5 bands the higher will be the resolution at which spectral features can be resolved. Note that sensor
- 6 responses are here represented as Gaussian just for simplicity reasons but typical sensor responses
- 7 may present different shapes.
- 8 Fig. 3. Spectralon® panel refectance before (dotted line) and after cleaning (solid line). The panel
- 9 had been 'lightly' and carefully used in the field for one season. Data provided by C. MacLellan,
- 10 NERC/NCEO Field Spectroscopy Facility, GeoScience, U. of Edinburgh.
- 11 Fig. 4. Hyperspectral systems in use before and during EUROSPEC. The UNIEDI System (A), the
- 12 S-FLUOR/MRI System (B), the HSI System in which both the up- and down-welling
- measurements are hemispherical (C) and the AMSPEC-MED System where the spectrometer
- measuring up-welling radiance can measure at multiple zenithal and azimuthal angles (D). Down-
- welling hemispherical foreoptics (1), Up-welling conical-FOV foreoptics (2) and the box housing
- the spectrometers (3) are marked in the respective panels.
- 17 Fig. 5. Hyperspectral systems developed during EUROSPEC. The Piccolo system (A) and the SIF-
- Sys (B) use a single spectrometer to measure two fields of view by means of a bifurcated fibre
- optics. The White-Ref system (C) uses a sliding white reference panel to measure irradiance. See
- 20 further details in the text.

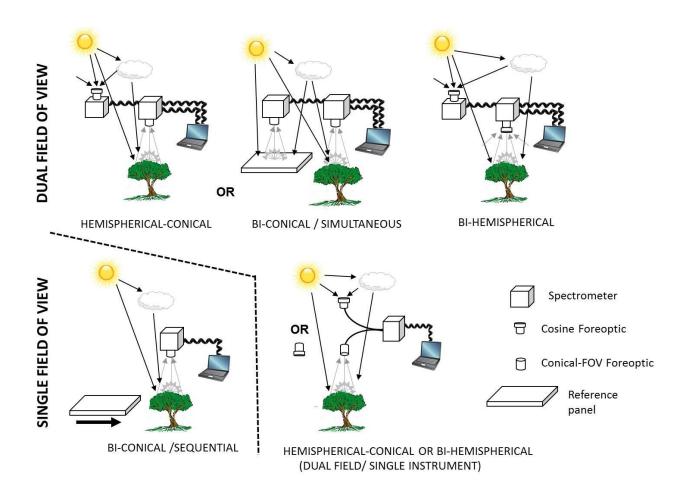
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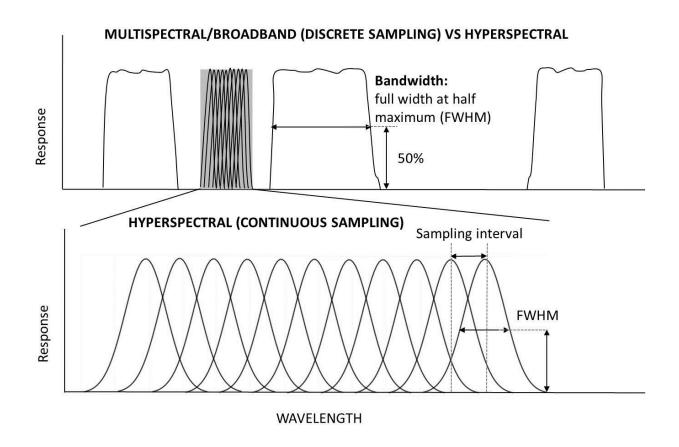
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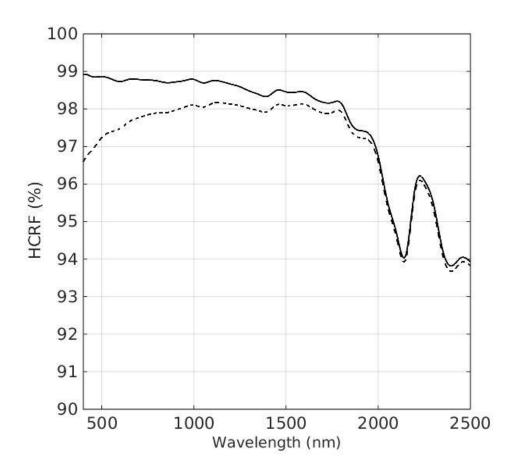
- Fig. 6. Upscaling of optical and flux data across space and time. While long-term in situ spectral
- 23 measurements help us establish a link between optical and flux data across time, new tools like
- 24 UAVs are still needed to facilitate the spatial upscaling from the footprint to the landscape level.



2 Figure 1.



2 Figure 2.



2 Figure 3.

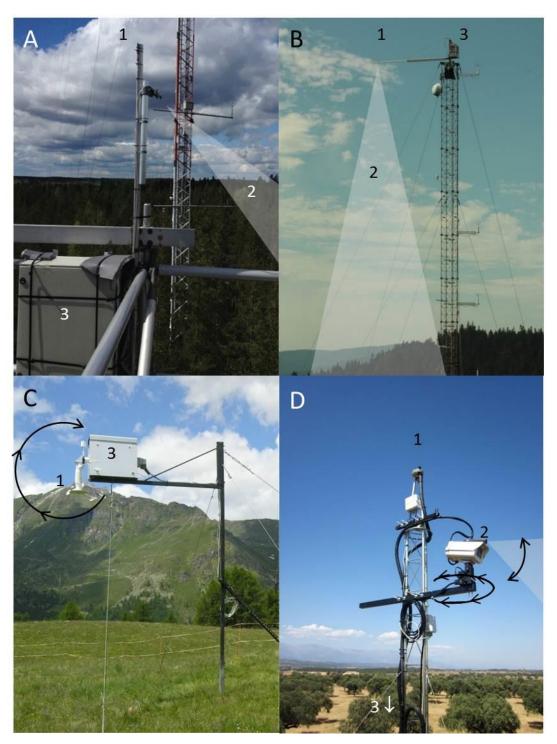
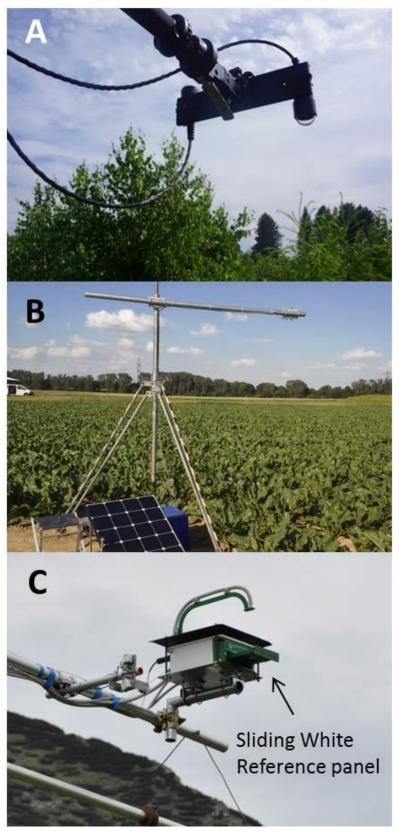


Figure 4.



2 Figure 5.

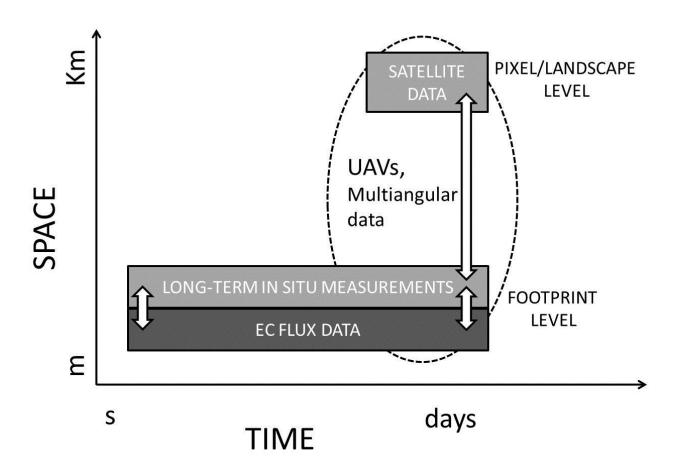


Figure 6.