

## Towards quantitative ecology: Newton's principia revisited

Pertti Hari<sup>1)</sup>, Jaana Bäck<sup>1)</sup>, Kari Heliövaara<sup>1)</sup>, Veli-Matti Kerminen<sup>2)</sup>,  
Liisa Kulmala<sup>3)</sup>, Annikki Mäkelä<sup>1)</sup>, Eero Nikinmaa<sup>1)</sup>, Tuukka Petäjä<sup>2)</sup> and  
Markku Kulmala<sup>2)</sup>

<sup>1)</sup> Department of Forest Sciences, P.O. Box 27, FI-00014 University of Helsinki, Finland (\*corresponding author's e-mail: pertti.hari@helsinki.fi)

<sup>2)</sup> Department of Physics, P.O. Box 64, FI-00014 University of Helsinki, Finland

<sup>3)</sup> Finnish Forest Research Institute, P.O. Box 18, FI-01301 Vantaa, Finland

Received 27 Jan. 2013, final version received 6 June 2014, accepted 6 June 2014

Hari, P., Bäck, J., Heliövaara, K., Kerminen, V.-M., Kulmala, L., Mäkelä, A., Nikinmaa, E., Petäjä, T. & Kulmala, M. 2014: Towards quantitative ecology: Newton's principia revisited. *Boreal Env. Res.* 19 (suppl. B): 142–152.

Qualitative argumentation dominates the research in ecology, whereas quantitative approaches characterize the physical and chemical studies. Further development of powerful quantitative methods is needed in ecology to improve the utilization of ecological knowledge in the research of present changes on the globe and to enhance the utilization of physical knowledge in ecology. Here, we (1) define new concepts that enable the quantitative formulation of the most essential features of photosynthesis, and (2) derive exact predictions of the relationship between photosynthesis and light together with the action of stomata. We predicted 300 daily patterns of photosynthesis of a pine shoot from 50 000 measurements of light, temperature and water-vapor concentration in the field. Our theory predicted 95%–97% of the variance of measured photosynthesis. Our example indicates that the theory-formation approach can successfully be applied in ecology to describe photosynthesis, a phenomenon fundamental to life on Earth.

### Introduction

The discrepancy between qualitative and quantitative theories and applied methods is striking among different disciplines of current science. Much of this discrepancy originates from the history of each discipline and their choices underlying the theories. Isaac Newton introduced already in 1687 theory-driven quantitative thinking to physics where quantitative approach has dominated since then, whereas qualitative approaches still characterize many disciplines, including ecology, although quantitative methods gained attention during the last decades. The

qualitative approaches not only slow down the development in ecology but they also clearly hinder the knowledge flow from ecology to physics and from physics to ecology.

*Principia Mathematica* by Isaac Newton (Newton 1687) was the corner stone of the classical physics, as it opened an era of rapid development of theory formation dealing with the circulation of planets around the sun and with the movement of particles. In *Principia Mathematica* (Newton 1687, Suntola 2012), the theory development is characterized by four phases. First, the book begins with the definitions of concepts, after which axioms are intro-

duced to characterize the connections between the concepts. The third phase, the mathematical analysis of systems defined by the concepts and axioms, dominates the book. Finally, Newton rather briefly treats the testing of the obtained predictions with measurements, and such tests play an important role in the conclusions.

The Newtonian approach to construct theories has provided classical physics and other natural science an effective way to find regularities in nature: since identical material objects in similar conditions behave in a similar way, their behavior can be predicted from the definitions and axioms within the measurement accuracy and precision. The application of physical knowledge and generalization into real-world problems faced, however, the problem of variability. The insufficient understanding of variability has been particularly evident in atmospheric sciences in the subject areas such as weather forecast (Kerr 2012) and climate change prediction (Sanderson and Knutti 2012), and in atmospheric phenomena such as initiation of precipitation (Ren *et al.* 2013) and secondary aerosol particle formation (Kulmala *et al.* 2013).

The diversity and variability are typical features of living systems, which, especially in ecology, manifest the differences between individuals. Ever since the work by Locke (Anstey 2003) and Linné (Linne 1758, Cajander 1913, Basset *et al.* 2012) over two centuries ago, ecological research has therefore focused on the diversity in nature and on qualitative systems to describe nature. The resulting qualitative argumentation has effectively hindered the utilization of powerful and quantitative mathematical tools in the development of ecological theories and their applications.

Despite their variability, regularities in the structure and metabolism govern the living organisms. For example, two pine needles are very similar to each other in their shapes and many other properties, and the metabolism of plants is based on the actions of the same chains of enzymes, membrane pumps, and pigments (Priestley 1772, Ingen-Housz 1779, Li *et al.* 2000). The behavior of the living systems reflects the regularities in the basic structure and metabolism and thus, we can expect regularities in the resulting material fluxes and in the devel-

opment of the vegetation structure. On the other hand, since variability is a characteristic feature in ecological phenomena in natural conditions, we should be able to identify the regular and random components in the behavior of ecological objects.

## Construction and testing the theory of photosynthesis according to Newtonian approach

Is the Newtonian approach only valid for theory formation in the classical physics, or can it also be applied to ecology for detecting regularities in the metabolism and in the development of structure of vegetation? Here we investigate the applicability of the Newtonian approach to theory formation in ecology using an example dealing with photosynthesis (Fig. 1).

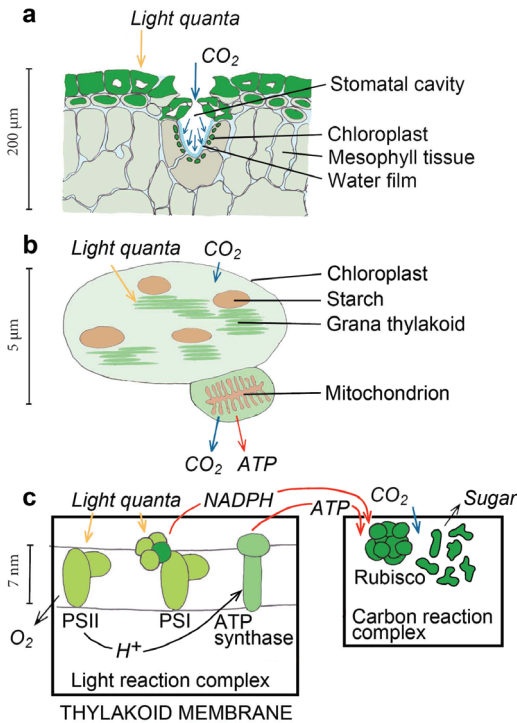
In traditional ecology, theoretical ideas are typically introduced as assumptions in the model development, often appearing only as small technical details. This contrasts the Newtonian approach which stresses the role of connections between the concepts and the theoretical basis of these connections. Below we apply the Newtonian approach to photosynthesis in two steps: First we consider simple case when we form a theory considering only the effects of CO<sub>2</sub> and photosynthetically active radiation on photosynthesis. In the second phase, we include the stomatal action into our theory formation.

### Effects of radiation and CO<sub>2</sub> concentration on photosynthesis

#### Theory formation

First, we consider only the effects of CO<sub>2</sub> and photosynthetically active radiation on photosynthesis. Following the steps in the Newtonian theory formation, we define five concepts:

C1: Photosynthesis at a point in space and time is the amount of formed sugars in a small space element during a short time interval divided by the product of the leaf area in the space element and the length of the time element.



**Fig. 1.** A schematic illustration of photosynthesis. **(A)** Leaf element: diffusion transports  $\text{CO}_2$  via stomatal pores from the atmosphere into the stomatal cavity, where it is dissolved into water film surrounding mesophyll cells, and eventually moving into chloroplasts according to the concentration gradient (Leuning 1983, Evans and von Caemmerer 1996). Photosynthesis generates the flux by drawing  $\text{CO}_2$  out from the stomatal cavity into chloroplasts. **(B)** Subcellular elements: light is absorbed in chloroplast grana thylakoids, converted into chemical energy, and used for binding up the  $\text{CO}_2$ . The cell metabolism is consuming energy, and thus the carbohydrates are broken down in respiration, liberating energy as ATP and forming carbon dioxide in mitochondrion (Penning de Vries *et al.* 1974, James 1953, Farrar 1995). **(C)** Reaction complexes in chloroplasts: The solar energy is captured in the chlorophyll antenna systems (PSI and PSII) of chloroplast thylakoid membranes (Hill and Bendall 1960, Duysens *et al.* 1961, Anderson and Chow 2002, Nelson and Ben Shem 2004) and converted to chemical energy (ATP and NADPH) (Elston *et al.* 1998, Kurisu *et al.* 2001). Simultaneously, water is split into oxygen and hydrogen atoms (Hill 1939, Renger and Renger 2008). In the chain of carbon reactions in the chloroplast stroma, i.e., Calvin cycle,  $\text{CO}_2$  is bound into sugar phosphates with the help of Rubisco and several other enzymes, and chemical energy from light reactions (Calvin and Benson 1948, Calvin and Bassham 1962). Photosynthesis becomes saturated with high light intensities.

C2: Photosynthetically active radiation at a point in space and time is the number of visible

light quanta arriving on a small area element during a short time element divided by the product of the area in the surface element and the length of the time element.

C3: Respiration at a point in space and time is the amount of consumed sugars in a small space element during a short time interval divided by the product of the leaf area in the space element and the length of the time element.

C4: The  $\text{CO}_2$  flux into the stomatal cavity at a point in space and time is the amount of  $\text{CO}_2$  flowing into the stomatal cavities in the space element during a short time element divided by the product of the leaf area in the space element and the length of the time element.

C5:  $\text{CO}_2$  concentration in a space element is the mass of  $\text{CO}_2$  in the element divided by the volume of the space element.

As the second step, we postulate four axioms that concern the photosynthetic process (carbon fixation), diffusion and  $\text{CO}_2$  concentration in the stomatal cavity.

A1: The product of the saturating response to the photosynthetically active radiation at a point in space and time and  $\text{CO}_2$  concentration in the stomatal cavity determines the photosynthesis at a point in space and time.

A2: The  $\text{CO}_2$  flux into the stomatal cavity at a point in space and time is proportional to the  $\text{CO}_2$  concentration difference between the stomatal cavity and ambient air.

A3: The mass of carbon needs to be conserved regardless of how it is transported or chemically processed.

A4: The  $\text{CO}_2$  concentration in the stomatal cavity is stable over the time scales of photosynthesis.

We derive from the definitions of the theoretical concepts new mathematical concepts that enable strict mathematical formulation of the axioms resulting in the density of photosynthetic and respiration rates, density of photosynthetically active radiation flux and density of leaf area. The analogous mathematical formalism to treat spatially and temporally nonhomogeneous phenomena is commonly used in physics, for example in the treatment of rotating bodies.

The axioms obtain more exact form with the above mathematical concepts. The first axiom (A1) concerns the density of photosynthetic rate,  $p(x,t)$  in point  $x$  at time  $t$ . We obtain

$$p(x,t) = bf[I(x,t)]C_s(x,t) \quad (1)$$

where  $b$  is the efficiency of photosynthesis,  $C_s$  the  $\text{CO}_2$  concentration in the stomatal cavity, and  $f$  is a saturating function

$$f(I) = \frac{I}{I + \gamma}, \quad (2)$$

where  $I$  is the density of photosynthetically active radiation flux and  $\gamma$  is a parameter to be estimated.

The second axiom (A2) concerns the  $\text{CO}_2$  flux density between the stomatal cavity and the atmosphere

$$f_{\text{CO}_2}(x,t) = g[C_a - C_s(x,t)], \quad (3)$$

where  $g$  is the stomatal conductance and  $C_a$  is the ambient  $\text{CO}_2$  concentration.

The conservation of mass (A3) results in a differential equation describing the behavior of  $\text{CO}_2$  in a small leaf element

$$\begin{aligned} & \frac{d[\Delta VC_s(x,t)]}{dt} \\ &= A(\Delta V)[f_{\text{CO}_2}(x,t) - p(x,t) + r(x,t)] \quad (4) \\ &= A(\Delta V) \left\{ \begin{array}{l} g[C_a - C_s(x,t)] \\ -bf[I(x,t)] + r(x,t) \end{array} \right\}, \end{aligned}$$

where  $\Delta V$  is the volume of the leaf element,  $A(\Delta V)$  its surface area in the volume element and  $r(x,t)$  is the density respiration rate.

The fourth axiom (A4) states that the  $\text{CO}_2$  concentration is stable in the volume element, thus its time derivative is zero and we obtain

$$g[C_a - C_s(x,t)] - bf[I(x,t)]C_s(x,t) + r(x,t) = 0. \quad (5)$$

When we solve the  $\text{CO}_2$  concentration in the volume element from Eq. 5 and insert the obtained solution into Eq. 1, we can predict the dependence of the density of photosynthetic rate on the density of the photosynthetically active radiation

$$p[I(x,t)] = \frac{[gC_a + r(x,t)]bf(I)}{g + bf[I(x,t)]}. \quad (6)$$

When we take in consideration that the density of photosynthetically active radiation flux varies we obtain

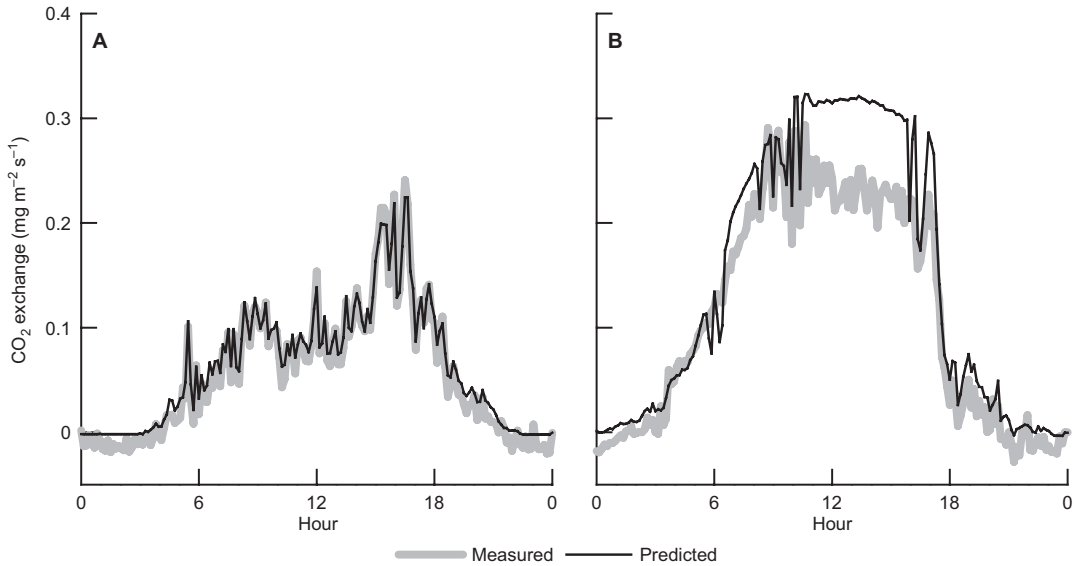
$$p(x,t) = \frac{[gC_a + r(x,t)]bf[I(x,t)]}{g + bf[I(x,t)]}. \quad (7)$$

## Testing the theory

The Newtonian approach to construct theories resulted in clear equations and a prediction that we can test with field data. We can accurately measure the  $\text{CO}_2$  exchange of leaves (Hari *et al.* 2013), i.e. photosynthetic minus respiratory flux, which reflects photosynthesis at a point in space and time enabling the testing of the theory with field data. We utilized measurements from the SMEAR I measurement station (Hari *et al.* 1994) in northern Finland during several years. A branch chamber in the upper branches of Scots pine is closed during a measurement for 70 seconds and open otherwise (Hari *et al.* 2013). When the chamber is closed the flux between leaves and the air in the chamber changes the  $\text{CO}_2$  concentration inside the chamber and we obtain the  $\text{CO}_2$  exchange from the  $\text{CO}_2$  mass balance equation.

If the photosynthetically active radiation at a point in space and time is spatially constant within the measured leaves, then we obtain the amount of  $\text{CO}_2$  exchange of the leaves by multiplying the photosynthesis minus respiration at point in space and time with the leaf area in a chamber. In this way, we can convert the predictions dealing with the photosynthesis at a point level in space and time into the leaf level that we can measure.

Equation 7 can be interpreted as predictions of the daily patterns of the photosynthesis at point in space and time generated by the variation in the photosynthetically active radiation. We determined the parameters  $b$ ,  $g$ ,  $r$ , i.e., the efficiency of photosynthesis, the stomatal conductance and respiration, respectively, as well as the parameter  $\gamma$  in the saturation of light reactions (Eq. 2) from measurements during a cloudy day (20 June 2012). Using these values, we predicted the daily pattern of the  $\text{CO}_2$  exchange for a cloudy day 28 July (Fig. 2A) and a sunny day 13 July 2010



**Fig. 2.** Comparison of daily patterns of measured and predicted (Eq. 7)  $\text{CO}_2$  exchange on (A) a cloudy (26 June 2010), and (B) a sunny day (13 July 2010). Parameter values:  $b = 0.00098 \text{ m s}^{-1}$ ,  $\gamma = 0.9 \text{ mmol m}^{-2} \text{ s}^{-1}$ ,  $g = 0.002 \text{ m s}^{-1}$ ,  $r = 0.000001 \text{ g m}^{-2} \text{ s}^{-1}$ .

(Fig. 2B). The agreement between predictions and measurements was very good during the cloudy weather, but during sunshine there was a clear discrepancy between the prediction and the measurement. When expanding the calculation into days of intermittent cloudiness, the predictions were successful during mornings but in the afternoon the predicted  $\text{CO}_2$  flux was clearly higher than measured (Fig. 2B). This discrepancy is evidently caused by the action of stomata, whose partial closure reduces the  $\text{CO}_2$  flux into the cavity further reducing photosynthesis.

### The effect of stomatal action, radiation and $\text{CO}_2$ concentration on photosynthesis

#### Theory formation

Plants are known to close their stomata to restrict transpiration to prevent damages due to drying since also the flow of water vapor takes place via the stomatal pores. The proper action of stomata has been essential during evolution and a very good action principle has developed to reduce transpiration and to simultaneously avoid loss in photosynthesis (Cowan and Farquhar 1977, Hari

and Mäkelä 2003). Thus, we have to expand our theory to involve transpiration and the partial closure of stomata to manage the reduction of photosynthesis during the sunny afternoons.

The stomatal action caused evidently the discrepancy between predicted and measured photosynthesis. Therefore, we have to include the stomatal closure in our theory development. The application of the Newtonian approach to the action of stomata begins with the definition of new concepts:

- C6: The transpiration at a point in space and time is the amount of transpired water from a small space element during a short time interval divided by the product of the leaf area in the space element and the length of the time element.
- C7: Water saturated air contains the maximal amount of water vapor in conditions of the air.
- C8: The amount of photosynthesis at a point in space during a time interval is the amount of formed sugars in a small space element during the time period divided by the leaf area in the space element.
- C9: The amount of transpiration at a point in space during a time interval is the amount of

water transpired from a small space element during the time period divided by the leaf area in the space element.

We need two additional concepts for the stomatal action:

C10: The degree of stomatal opening is the actual area of the stomatal pore divided by its maximal area.

C11: The cost of transpiration is the amount of sugars used to construct the water uptake and water and carbon transport systems in roots, stem and branches.

This last concept is different from the previous ones: so far we have considered the leaf being autonomous but this concept takes into consideration that the water and carbon fluxes at the leaf–atmosphere boundary must be matched by the water and carbon fluxes at the leaf boundary with the rest of the tree.

We need additional axioms for transpiration and for the stomata action:

A5: The outflow of water vapor through stomatal pores is proportional to the product of the degree of stomatal opening and the water-vapor concentration difference between the stomatal cavity and ambient air.

A6: The air in the stomatal cavities is water-vapor saturated.

A7: The water-vapor concentration in saturated air depends on temperature.

A8: The transpiration cost is proportional to the amount of transpiration during a time period.

A9: The action principle of the stomata is to maximize the photosynthetic production minus transpiration cost in a point.

The concepts concerning transpiration at a point in space and time as well as the amount of photosynthesis and transpiration at a point in space enable the mathematical treatment of the axioms.

The densities of photosynthetic rate,  $p_A$ , and photosynthetic production,  $p_p$ , are connected with each other

$$p_p(x, t_1, t_2) = \int_{t_1}^{t_2} p_A(x, t) dt. \quad (8)$$

A similar equation also holds between densities of transpiration rate,  $h_A$ , and amount of transpiration,  $h_p$ ,

$$h_p(x, t_1, t_2) = \int_{t_1}^{t_2} h_A(x, t) dt. \quad (9)$$

Our analysis of the system defined by concepts C1–C5 and axioms A1–A4 assumes that diffusivity from the atmosphere through stomatal pores into the stomatal cavity does not change. The stomatal action that reduces diffusion is, however, evident during high evaporative demand.

Stomatal closure reduces the diffusion of  $\text{CO}_2$  and water vapor into and out from a leaf. The partial closure of stomata, introduced with the concept C10, reduces the diffusion of water vapor out from the stomatal cavity. Let  $u$  denote the degree of stomatal opening. Then, according to axiom A5 is

$$h_A(x, t) = ag_{\max} u(x, t) D(x, t), \quad (10)$$

where  $g$  is the stomatal conductance for  $\text{CO}_2$  when the stomata are fully open, the parameter  $a$  introduces the difference in diffusivity between water vapor and  $\text{CO}_2$  ( $a = 1.6$ ) and  $D$  is the water-vapor concentration difference between stomatal cavity and ambient air. The degree of stomatal opening can take values only between 0 and 1. When  $u$  is introduced into Eq. 7, we get

$$p_A(x, t) = \frac{[u(x, t) g_{\max} C_a + r] bf [I(x, t)]}{u(x, t) g_{\max} + bf [I(x, t)]}. \quad (11)$$

According to axiom A8, the transpiration cost is proportional to the amount of transpiration during a time period:

$$\text{transpiration cost} = \lambda h_p(x, t_1, t_2), \quad (12)$$

where  $\lambda$ , ( $\text{g}(\text{CO}_2)/\text{g}(\text{H}_2\text{O})$ ), is a parameter.

Axiom A9 states that the action principle of the stomata is to maximize the photosynthetic production minus transpiration cost in a point. This results in the following optimization problem (Hari *et al.* 1986, 2009):

$$\text{Max}_u \{ p_p(x, t_1, t_2) - \lambda h_p(x, t_1, t_2) \}. \quad (13)$$

The above optimization problem can be solved with the Lagrange method, which is rather commonly used in system analysis and economics. As the first step, the Lagrange function,  $L$ , is formed:

$$L = bf[I(x,t)] \frac{u(x,t)g_{\max}C_a + r(x,t)}{u(x,t)g_{\max} + bf[I(x,t)]} - \lambda u(x,t)g_{\max}D(x,t). \quad (14)$$

The next step is to differentiate the Lagrange function with respect to  $u$ . The optimal stomatal opening during the interval from  $t_1$  to  $t_2$  is obtained as a zero point of the derivative of the Lagrange function. The derivative of the Lagrange function with respect to  $u$  includes  $u$  as first and second power. Thus it can be solved resulting in

$$u^*(x,t) = \left( \sqrt{\frac{C_a - r(x,t)/\{bf[I(x,t)]\}}{\lambda aD(x,t)} - 1} \right) \times \frac{bf[I(x,t)]}{g_{\max}}. \quad (15)$$

The above solution yields values that are greater than 1 or negative which are outside the range of degree of a stomatal opening. In these cases, the optimal degree of stomatal opening,  $u_{\text{opt}}$  takes value 1 or 0. The final solution for the optimal degree of stomatal opening (Hari et al. 1986) is

$$u_{\text{opt}}(x,t) = \begin{cases} 0, & \text{if } u^*(x,t) \leq 0 \\ u^*(x,t), & \text{if } 0 < u^* < 1. \\ 1, & \text{if } u^*(x,t) \geq 1 \end{cases} \quad (16)$$

The light intensity and water-vapor concentration difference between the stomatal cavity and surrounding air vary during a day and the degree of stomatal opening,  $u$ , responds to this variation as well as to light intensity. Since the water-vapor concentration difference is low in the mornings, the stomata are usually fully open after sunrise and they partially close if the day is sunny and the water-vapor concentration difference is large. These variations in the light and water-vapor concentration difference generate strong daily patterns in photosynthesis.

By taking into account the new axioms (A5–9), we obtain a revised version of Eq. 7

(Hari et al. 1986, Hari et al. 2009):

$$p(I) = \frac{(u_{\text{opt}}g_{\max}C_a + r)bf(I)}{u_{\text{opt}}g_{\max} + bf(I)}. \quad (17)$$

Here,  $g_{\max}$  is the stomatal conductance when stomata are fully open, and  $u_{\text{opt}}$  is the optimal degree of stomatal opening obtained as the solution of the maximization problem. Equation 17 differs from Eq. 7 in that the optimality principle (A9) introduces the stomatal action into the prediction.

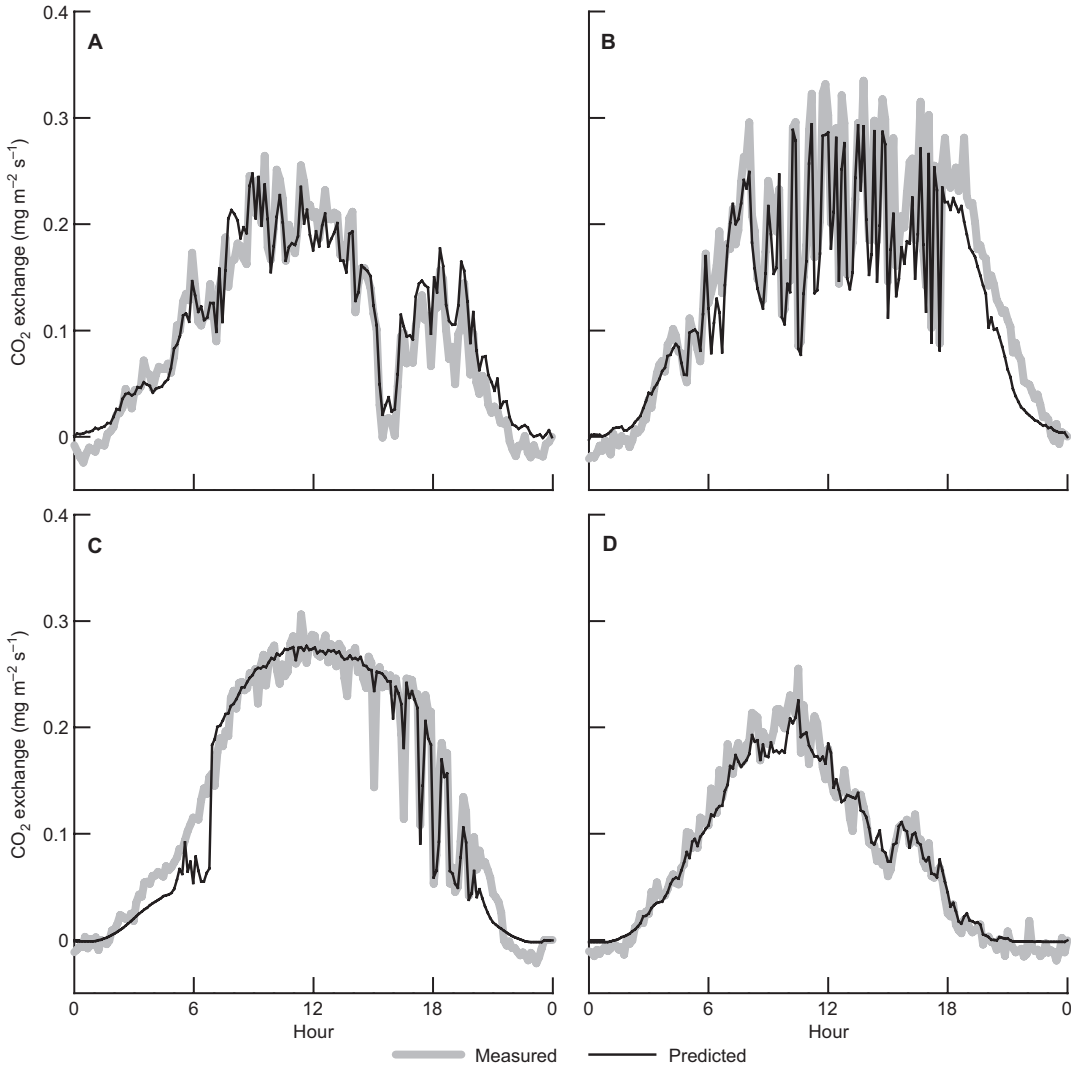
## Tests of the predictions

Next, we test these predictions with field data, following the Newtonian approach. We selected measurements obtained during July in the years 2010, 2011 and 2012 for testing our revised theory. The number of measurements of photosynthesis, light, temperature and water-vapor concentration used in this testing was over 50 000. Our model, based on the concepts and axioms, includes five parameters which we estimated using five days of measurements each summer, including both sunny and cloudy days. These days were rejected from the further analysis.

The estimation of the parameter values is based on the normal statistical principle, i.e. minimization of the residual sum of squares. The compensating effects of the parameters hamper the finding of the solution with numeric methods and we have to do stepwise iterations.

We determined the respiration term from the midnight measurements during the last day of July since our measuring station is about 200 km north of the Polar Circle and the nighttime photosynthetically-active radiation is too high in early July. The parameter  $g_{\max}$  was set to  $0.1 \text{ m s}^{-1}$  (Hari et al. 2013). We selected five days during each July containing sunny and cloudy days to estimate the values of the parameters  $b$ ,  $\lambda$  and  $\gamma$  in three steps:

Step 1: Estimation of  $\gamma$ . First, we fix the value of  $\lambda$ . Thereafter we estimated the daily values of the parameter  $b$  and the value of  $\gamma$  for the five days using the obtained daily values of  $b$ .



**Fig. 3.** Comparison of daily patterns of measured and predicted (Eq. 17) daily patterns of  $\text{CO}_2$  exchange on four days in July 2010 (Chamber 4). (A) the 4th (varying cloudiness), (B) the 11th (varying cloudiness), (C) the 24th (sunny day), and (D) the 25th (cloudy day). Parameter values:  $b = 0.00098 \text{ m s}^{-1}$ ,  $\gamma = 0.9 \text{ mmol m}^{-2} \text{ s}^{-1}$ ,  $\lambda = 0.004 \text{ g (CO}_2\text{)/g (H}_2\text{O)}$ ,  $g = 0.002 \text{ m s}^{-1}$ ,  $r = 0.000001 \text{ g m}^{-2} \text{ s}^{-1}$ .

Step 2: Estimation of  $\lambda$ . First, we fix the value of  $\gamma$ . Thereafter we estimated the daily values of the parameter  $b$  and the value of  $\lambda$  for the five days using the obtained daily values of  $b$ .

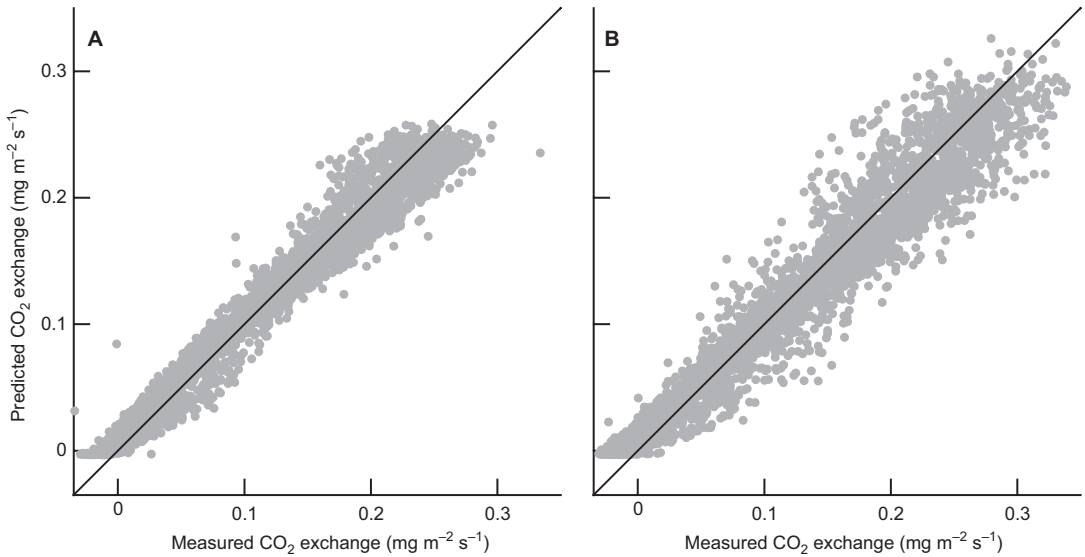
We repeated the iteration procedure steps 1 and 2 sequentially utilizing previously obtained values for the parameters  $\lambda$  and  $\gamma$  until the solution of the minimization was sufficiently stable.

Step 3: Finally, we estimated the daily values

of the parameter  $b$  using the obtained values of  $\lambda$  and  $\gamma$ . We applied the mean of the daily values in the test of the predictions.

The daily patterns of photosynthesis varied according to the weather, with sunny, cloudy and intermittent-cloudiness days looking very different from each other (Fig. 3). Our theory was able to predict this great variability as the predicted  $\text{CO}_2$  exchange followed closely the measured one. Changes in the photosynthetically-active radiation





**Fig. 4.** Comparison of measured and predicted CO<sub>2</sub> exchange in two chambers (**A** and **B**) in July 2010. Parameter values are  $b = 0.00059 \text{ m s}^{-1}$ ,  $\gamma = 0.4 \text{ mmol m}^{-2} \text{ s}^{-1}$ ,  $\lambda = 0.0018 \text{ g (CO}_2\text{/g (H}_2\text{O))}$ ,  $g = 0.002 \text{ m s}^{-1}$ ,  $r = 0.000001 \text{ g m}^{-2} \text{ s}^{-1}$  for chamber **A**, whereas for chamber **B**, the values are the same as in Fig. 2.

explained the rapid variation during days and the partial closure of the stomata explained the slow decline of CO<sub>2</sub> exchange in sunny afternoons.

We compared the predictions with measurements utilizing extensive data sets (Fig. 4). The predictions explained 95%–97% of the variance in the measured CO<sub>2</sub> exchange during July in the years 2010, 2011, and 2012. Only 3%–5% of the variance was attributed to measurement noise and shortcomings in the model structure used in the prediction. Thus, regularities generated by the metabolism, diffusion and evolution play a dominant role in the photosynthesis according to our data and our ecological theory of photosynthesis gained a strong corroborative support in the test with the field data.

## Discussion and conclusions

Descriptive statistical analysis dominates the field studies of photosynthesis, while theory-driven studies are quite few. Farquhar *et al.* (1980), Farquhar and von Caemmerer (1982), Laik and Oja (1998) and Kirschbaum *et al.* (1997) utilize physiological knowledge in the derivation of the model structures of light and carbon reactions. However, the action of stomata

has often been described with a phenomenological approach (Ball *et al.* 1987). The unique feature of our theory is that it treats the action of stomata in connection with a rough treatment of light and carbon reactions. Here axiom 10, derived from the evolutionary argumentation, states that maximizing the surplus carbon after considering the cost required for providing the leaf with water transport capacity should be beneficial for the plant. However, we have recently shown that explicit description of material flows within the tree and leaf when sugar supply from the leaves to the rest of the plant is maximized results in similar behavior as in Eq. 17 (Nikinmaa *et al.* 2013).

The Newtonian approach to construct theories provides a clear skeleton for scientific thinking, stressing the most important aspects of theory formation. The starting point is the definition of concepts. This requirement is problematic in ecology where one needs to address the great variability of living phenomena. Our solution is to start the considerations from elements with so small spatial and temporal dimensions that the metabolism can be considered homogenous within the element. Thereafter, we can apply physiological, physical and evolutionary knowledge to formulate the axioms characterizing the

most important phenomena for the photosynthesis. The axioms enable the utilization of powerful mathematical tools for deriving predictions.

The concepts in our theory concern mass and energy flows that H.T. Odum (1983) considered playing a key role in ecosystems. We can evidently expand the applications of the Newtonian approach to Odum's proposal and develop it further. We can utilize physiological and physical knowledge to formulate the axioms since metabolism and physical phenomena generate concentration, temperature and pressure differences that give rise to the mass and energy flows (Hari *et al.* 2013). We can base the mathematical analysis of the systems defined by concepts and axioms in ecology on the conservation of mass and energy to obtain differential equations, similarly as in physics. Modern instrumentation provides a wide range of measurements to obtain the necessary test data. The Newtonian approach to construct theories can apparently be widely applied to ecological phenomena.

Newton's ideas have already received some attention in ecology (Ulanowicz 1999, Murray 2001), where the Newtonian approach to construct theories provides clear advantages: it forces to formulate the ideas precisely, it enables the utilization of physiological and physical knowledge, it allows the use of effective mathematical tools in the development of the theory, and it allows to separate the regular and random components in the behavior of the research object.

By applying the principles of Newtonian theory formation on the effects of environment on photosynthesis we were able to formulate a novel theory that successfully passed the tests with large sets of field data. These principles can evidently be successfully applied to several ecological phenomena where material and energy flows play an important role whereas the definitions of the concepts and formulation of the axioms will be more challenging in certain subareas, e.g. biodiversity. Following the steps of Newtonian theory formation, we can proceed towards quantitative ecological theories and improve the information exchange between ecology and physics.

*Acknowledgments:* We thank the Academy of Finland Centre of Excellence program (grant no. 1118615) and the European

Research Council Project (grant no. 227463-ATMNUCLE) for financial support, and Riitta Hari for discussions and critical reading of the manuscript. The data is archived and available on request from the authors.

## References

- Anderson J.M. & Chow W.S. 2002. Structural and functional dynamics of plant photosystem II. *Phil. Trans. Roy. Soc. B* 357: 1421–1430.
- Anstey P.R. 2003. Locke on method in natural philosophy. In: Anstey P.R. (ed.), *The philosophy of John Locke: new perspectives*, Routledge, London, pp. 26–42.
- Ball J.T., Woodrow I.E. & Berry J.A. 1987. A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions. In: Biggins J. (ed.), *Progress in photosynthesis research*, vol. IV, Martinus Nijhoff, Dordrecht, pp. 221–224.
- Basset Y., Cizek L., Cuénoud P., Didham R.K., Guilhaumon F., Missa O., Novotny V., Ødegaard F., Roslin T., Schmidl J., Tishechkin A.K., Winchester N.N., Roubik D.W., Aberlenc H.-P., Bail J., Barrios H., Bridle J.R., Castaño-Meneses G., Corbara B., Curletti G., Duarte da Rocha W., De Bakker D., Delabie J.H.C., Dejean A., Fagan L.L., Floren A., Kitching R.L., Mediano E., Miller S.E., Gama de Oliveira E., Orivel J., Pollet M., Rapp M., Ribeiro S., Roisin Y., Schmidt J.B., Sørensen L. & Leponce M. 2012. Arthropod diversity in a tropical forest. *Science* 338: 1481–1484.
- Cajander A.K. 1913. Über Waldtypen. *Acta Forestalia Fennica* 1: 1–175.
- Calvin M. & Benson A.A. 1948. The path of carbon in photosynthesis. *Science* 107: 476–480.
- Calvin M. & Bassham J.A. 1962. *The photosynthesis of carbon compounds*. W.A. Benjamin, New York.
- Cowan I.R. & Farquhar G.D. 1977. Stomatal function in relation to leaf metabolism and environment. *Symp. Soc. Exp. Biol.* 31: 471–505.
- Duysens L.N.M., Amez J. & Kamp B.M. 1961. Two photochemical systems in photosynthesis. *Nature* 190: 510–514.
- Elston T., Wang H.Y. & Oster G. 1998. Energy transduction in ATP synthase. *Nature* 391: 510–513.
- Evans J.R. & von Caemmerer S. 1996. Carbon dioxide diffusion inside leaves. *Plant Physiol.* 110: 339–346.
- Farrar J.F. 1995. The respiratory source of CO<sub>2</sub>. *Plant Cell Environ.* 8: 427–438.
- Farquhar G.D., von Caemmerer S. & Berry J.A. 1980. A biochemical model of photosynthetic CO<sub>2</sub> assimilation in leaves of C3 species. *Planta* 149: 78–90.
- Farquhar G.D. & von Caemmerer S. 1982. Modelling of photosynthetic response to environmental conditions. In: Lange O.L., Nobel P.S., Osmond C.B. & Ziegler H. (eds.), *Encyclopedia of plant physiology new series*, Springer-Verlag, Berlin, pp. 549–587.
- Hari P. & Mäkelä A. 2003. Annual pattern of photosynthesis in Scots pine in the boreal zone. *Tree Physiol.* 23:

- 145–155.
- Hari P., Heliövaara K. & Kulmala L. (eds.) 2013. *Physical and physiological forest ecology*. Advances in Global Change Research, Springer Verlag,
- Hari P., Mäkelä A., Korpilahti E. & Holmberg M. 1986. Optimal control of gas exchange. *Tree Physiol.* 2: 169–175.
- Hari P., Hänninen H., Berninger F., Kolari P., Nikinmaa E. & Mäkelä A. 2009. Predicting boreal conifer photosynthesis in field conditions. *Boreal Env. Res.* 14 (suppl. A): 19–28.
- Hari P., Kulmala M., Pohja T., Lahti T., Siivola E., Palva E., Aalto P., Hämeri K., Vesala T., Luoma S. & Pulliainen E. 1994. Air pollution in eastern Lapland: challenge for an environmental measurement station. *Silva Fennica* 28: 29–39.
- Hill R. 1939. Oxygen produced by isolated chloroplasts. *Proc. Roy. Soc. Lond. B* 127: 192–210.
- Hill R. & Bendall F. 1960. Function of two cytochrome components in chloroplast: a working hypothesis. *Nature* 186: 136–137.
- Ingen-Housz J. 1779. *Experiments upon vegetables, discovering their great power of purifying the common air in the sun-shine, and of injuring it in the shade and at night. To which is joined, a new method of examining the accurate degree of salubrity of the atmosphere*. P. Elmsly in the Strand and H Payne in Pall Mall.
- James W.O. 1953. *Plant respiration*. Clarendon Press, Oxford.
- Kerr R.A. 2012. Weather forecasts slowly clearing up. *Science* 338: 734–737.
- Kirschbaum M.U.F., Küppers M., Schneider H., Giersch C. & Noe S. 1997. Modelling photosynthesis in fluctuating light with inclusion of stomatal conductance, biochemical activation and pools of key photosynthetic intermediates. *Planta* 204: 16–26.
- Kulmala M., Kontkanen J., Junninen H., Lehtipalo K., Mannonen H.E., Nieminen T., Petäjä T., Sipilä M., Schobesberger S., Rantala P., Franchin A., Jokinen T., Järvinen E., Äijälä M., Kangasluoma J., Hakala J., Aalto P.P., Paasonen P., Mikkilä J., Vanhanen J., Aalto J., Hakola H., Makkonen U., Ruuskanen T., Mauldin R.L.III, Duplissy J., Vehkamäki H., Bäck J., Kortelainen A., Riipinen I., Kurten T., Johnston M.V., Smith J.N., Ehn M., Mentel T.F., Lehtinen K.E.J., Laaksonen A., Kerminen V.-M. & Worsnop D.R. 2013. Direct observations of atmospheric nucleation. *Science* 339: 943–946.
- Kurisu G., Kusunoki M., Katoh E., Yamazaki T., Teshima K., Onda Y., Kimata-Ariga Y. & Hase T. 2001. Structure of the electron transfer complex between ferredoxin and ferredoxin-NADP(+) reductase. *Nat. Struct. Biol.* 8: 117–121.
- Laisk A. & Oja V. 1998. *Dynamics of leaf photosynthesis: rapid-response measurements and their interpretations*. CSIRO Publishing, Collingwood, Victoria, Australia.
- Leuning R. 1983. Transport of gases into leaves. *Plant Cell Environ.* 6: 181–194.
- Li X.P., Björkman O., Shih C., Grossman A.R., Rosenquist M., Jansson S. & Niyogi K.K. 2000. Pigment-binding protein essential for regulation of photosynthetic light harvesting. *Nature* 403: 391–395.
- Linné C. 1758. *Systema naturae per regna tria naturae: secundum classes, ordines, genera, species, cum characteribus, differentiis, synonymis, locis*. Laurentius Salvius, Stockholm.
- Murray B.G.Jr. 2001. Are ecological and evolutionary theories scientific? *Biol. Rev.* 76: 255–289.
- Nelson N. & Ben-Shem A. 2004. The complex architecture of oxygenic photosynthesis. *Nat. Rev. Mol. Cell Biol.* 5: 1–12.
- Newton I. 1687. *Philosophiae naturalis principia mathematica*. A new translation by I.B. Cohen and A. Whitman, University of California Press, Berkeley.
- Nikinmaa E., Hölttä T., Hari P., Kolari P., Mäkelä A., Sevanto S. & Vesala T. 2013. Assimilate transport in phloem sets conditions for leaf gas exchange. *Plant Cell Environ.* 36: 655–669.
- Odum H.T. 1983. *Systems ecology: an introduction* John Wiley, New York
- Penning de Vries F.W.T., Brunsting A.H.M. & van Laar H.H. 1974. Products, requirements and efficiency of biosynthesis: a quantitative approach. *J. Theor. Biol.* 45: 339–377.
- Priestley J. 1772. Observations on different kinds of air. *Phil. Trans.* 62: 147–264.
- Renger G. & Renger T. 2008. Photosystem II: the machinery of photosynthetic water splitting. *Photosynth. Res.* 98: 53–80.
- Ren L., Arkin P., Smith T.M. & Shen S.S.P. 2013. Global precipitation trends in 1900–2005 from a reconstruction and coupled model simulations. *J. Geophys. Res.* 118: 1679–1689.
- Suntola T. 2012. *Tieteen lyhyt historia — vai pitkät tie luonnonfilosofian ja empirismin kohtaamiseen*. Physics Foundations Society.
- Sanderson B.M. & Knutti R. 2012. On the interpretation of constrained climate model ensembles. *Geophys. Res. Lett.* 39, L16708, doi:10.1029/2012GL052665.
- Ulanowicz R.E. 1999. Life after Newton: an ecological metaphysic. *BioSystems* 50: 127–142.