Research Statement: Towards a Computational Plant Science

Dr. Alexander Bucksch

Research summary:

An increasing human population faces the growing demand for agricultural products and accurate global climate models that account for individual plant morphologies to sustain human life (Lynch, 2007; Stringer, 2009; Godfray et al., 2010). Both demands are ultimately rooted in an improved understanding of the mechanistic origins of plant development and their resulting phenotypes (Evans, 1998; Tilman et al., 2011). Such understanding requires geometric and topological descriptors to characterize plant phenotypes and to link phenotypes to genotypes (Araus and Cairns, 2014; Granier and Vile, 2014). However, the current plant phenotyping framework relies on simple length and diameter measurements, which fail to capture the exquisite architecture of plants. My research aims to set new frontiers in combining plant phenotyping with recent results from mathematical shape theory at the interface of geometry and topology. The core technical method I will use is to expand and apply the mathematical concept of a "shape descriptor" to the plant sciences. Shape descriptors describe the current state and growth of complex structures, including the rich geometric and topological characteristics of plants. More generally, understanding adaptation of plants to their environments is best observed within imaging data capturing the spatial arrangement of plant organs forming the plant phenotype. Spatial arrangements appear in leafs, branches, roots etc. on all biological scales. A full understanding the formation of morphological phenotypes requires analysis of the interplay with the underlying formation processes on cellular and genetic scales.

Applying and extending shape theory for plants is the centerpiece of my current work towards unravelling the formation of plant phenotypes. In doing so, I utilize data collected with various imaging instruments from which shape descriptors are extracted. I have developed robust shape descriptors, embedded them as part of software and computing products to characterize tens to thousands of plant phenotypes in a high-throughput fashion. These methods include SkelTre for analyzing 3D laser-scanner derived tree crown data (Bucksch, Lindenbergh, and Menenti, 2010), extending 3D algorithms for phenotyping rice roots grown in the lab (Topp et al., 2013), and leading the development of automated trait extraction algorithms for analyzing crop root phenotypes measured in the field (Bucksch et al., 2014b). As a high-risk/high-reward part of my research, I am also developing new simulation concepts to link shape with development (Bucksch, Turk, and Weitz, 2014), e.g., asking "How does the morphometric shape of plant roots feedback to influence the growth process.

In response, my future research plans will include an analysis of plant shapes across developmental stages and between different biological scales, such as organismal and morphogenetic scales with cellular and genetic scales. Future community activities focus on fostering computational mathematics within the plant sciences with an emphasis on supporting developments that reach out into field conditions. In particular, I organized (w/Dan Chitwood, Danforth Center for Plant Science) a NIMBioS workshop on "Morphological Plant Modelling" to foster the unity between mathematics, computational scientists and plant biologists. The workshop included 40+ scientists and is the basis for an upcoming Frontiers in Plant Science Research Topic for which I am serving as lead editor.

My strongly interdisciplinary and collaborative approach reflects my interests and multi-disciplinary training. The novelty of my research is my ability to tackle foundational plant science problems with rigorous research. Both my PhD training and postdoctoral research experiences have included extensive, long-term collaborations with plant biologists and forest ecologists to resolve challenges in the context of *in situ* and *in vitro* studies. Overall, my scientific mission is to unite mathematical and computational approaches with the experimental plant sciences, enabled by technological advancements embedded in software tools.

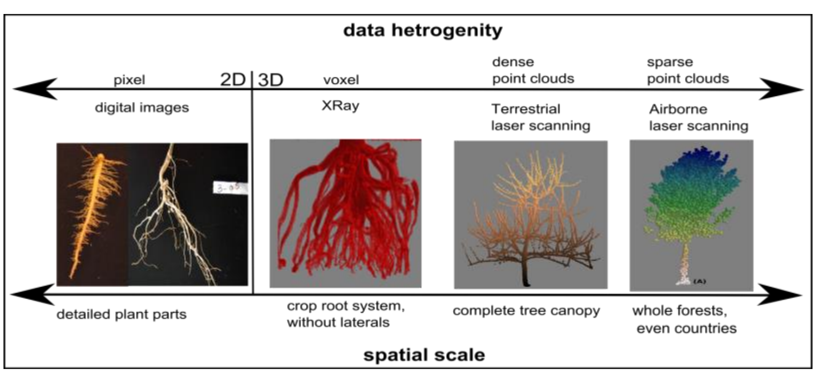

Figure 1: Examples of different 2D and 3D data sources and scales in my research. From left to right a 2D digital image of a cowpea root and an excised maize root with high detail and color information (Bucksch et al., 2014b). A root reconstructed from preliminary X-Ray data, an apple tree scanned with a terrestrial laser scanner (Bucksch, 2011) and a single tree scanned with an airborne laser from a helicopter (Bucksch et al., 2014a).

Research Theme I: Deciphering Heterogeneity of Below-ground Plant Structure

Accomplishments

A starting point to recognize the scientific challenges when working with below ground plant structures is the huge diversity of root system architectures and associated morphologies. This morphologic diversity can be thought of as the result of evolutionary adaptation given biophysical and geometric constraints. Plant root structure varies amongst species and varieties, among individuals of the same species or variety, and across the development of a given individual. In part, these transformations are driven by mutualistic and competitive interactions of nearby individuals. The study of root-root interactions, i.e., neighborhood relations in a geometric sense, is under-exploited mathematically. Hence, they are key examples of ways in which theories and tools from computational geometry can be leveraged to analyze the plasticity of plant shapes spatially.

Therefore, my research, and indeed first-hand experience at field sites in the USA, Europe, and Africa, led to the design of a unique *in situ* experiment in which 3 common bean genotypes were sampled 5000 times. This experimental effort should reveal their root phenotypes and their spatial interactions under terminal drought conditions. Over the last 3 years I developed the technological and computational basis for such large scale experiments by rigorously translating subjective visual scores into quantitative values, developing field-ready shape algorithms and imaging set-ups. As a consequence, enhanced reproducibility and statistical significance led to a broader impact of these field studies (Bucksch et al., 2014b). Within the Weitz group, I also directed a PhD candidate in Bioinformatics to develop high-throughput computing tools to enhance the large-scale analysis of field data utilizing supercomputing platforms and cyberinfrastructures. Together we developed DIRT, as an open source grid-computing platform that is accessible via a web application (http://dirt.iplantcollaborative.org/) to quantify root architecture (Das et al., 2015). Overall, altmetric ranks my root research as the Plant Physiology article receiving the most public attention ever.

Key Collaborators: James Burridge and Jonathan Lynch (Penn State, USA), Tobias Wojciechowski (FZ Jülich, Germany), Nirav Merchant (U of Arizona, USA), Chris Topp (Danforth Center for Plant Science, St. Louis, USA), Patompong Saengwilai (Mahidol U, Thailand), Joseph Chimungu (Lilongwe U of Agriculture and Natural Resources, Malawi)

Future Work

As a next step, I am excited to face the mathematical challenge to (1) quantify the transitions between root morphologies during the developmental process, (2) relate root structure directly to root function, and (3) elucidate the spatial interrelations in agro-ecological contexts. As a consequence, there is plenty of room for experimentalists to collaborate in sample acquisition and validation. In addition to the current manually driven possibilities, I actively participate in multi-disciplinary funding activities with optical scientists, engineers and plant scientists to enable the direct observation of root development in the field. I am Co-PI on a software development grant to extend DIRT to the analysis of root hairs and I applied as PI for a transformative grant within the NSF BREAD program (Co-PIs: Lynch, Chimungu, and Saengwilai).

Research Theme II: Linking above ground plant structure with plant and ecosystem functioning

Accomplishments

Detailed phenotype description opens up the question of how much environmental, developmental and genetic history is encoded in the shape of the plant phenotype (Bucksch, 2011). Plant history is encoded in the hierarchy of branches, distances between internodes or curvature and roughness of the surface on various scales. The above ground structure is accessible through a variety of imaging systems ranging from 2D digital photography to 3D laser scanning in field settings. Thus, the shape of the plant phenotype can be assessed in detail such that shape features can be directly related to environmental, developmental and genetic functions. Yet, questions emerging from the individual plant history are intrinsically coupled to methodological questions: for example, how much information about plant shape can be captured in an image with different imaging technologies? This question poses significant methodological problems because of the (i) amount, (ii) heterogeneity and (iii) spatial scale of available data (Figure 1). Hence, new biological insights about developmental features, environmental deformations and morphological patterns of plant phenotype shape can be found through combined mathematical and biological research.

So far I tackled examples of this problem in my graduate and postdoc work on the above ground structure of trees, and applied my methods to data obtained with 3D imaging systems such as laser scanning (Figure 1). I have collaborated with a diverse range of plant biologists and environmental scientists on projects including: the influence of soil dynamics on the resulting tree shape for early landslide prediction (Razak et al., 2011; Razak et al., 2013) and the estimation of biophysical parameters to model canopy-light interactions (Bucksch and Fleck, 2011; Bucksch and

Khoshelham, 2013). The methods developed during my graduate research are already widely used and even further developed across many disciplines ranging from gene discovery projects (Schöler and Steinhage, 2012) to graphics research (Livny et al., 2010).

Significant attention was given to the development of the SkelTre algorithm (Bucksch, Lindenbergh, and Menenti, 2009; Bucksch, Lindenbergh, and Menenti, 2010) to compute shape describing skeletons from point clouds. I initially published SkelTre as a theoretical algebraic concept at a shape retrieval workshop. Transforming this skeletonization concept into plant science practice in collaboration with forest ecologists and tree physiologists initiated my interest in improving algorithmic and mathematical principles within the wider plant science audience (Bucksch, 2014).

Future Work

My graduate work on tree canopies is exemplary for reconstruction and analysis of above ground plant structures. Yet unprecedented is the high-throughput characterization of above-ground phenotypes over several years. Such observations most likely reveal the map from plant shape features and patterns to underlying drivers of plant competition, environment or development, as well as variation in the overall productivity of a forest, industrial crop field, or orchard. I expect significant long-term impact in contexts of perennial agriculture and with "tree-like crops" such as cassava. However, orchards and forests can serve as a first starting point to overcome technical and mathematical challenges in the 3D reconstruction and segmentation of foliage from the branching structure, e.g. to investigate the amount of sunlight reaching the partly shadowed leave area. Pre-knowledge of tree physiology will feedback into the mathematical segmentation problem to identify leave position. As faculty, I plan to seek funding in the NSF Advances in Biological Informatics program.

Key Collaborators: Khamarul Razak (UT Malaysia, Malaysia), Kourosh Koshelham (U Melbourne, Australia), Stefan Fleck (Northwest German Forest Research Station, Germany)

Research Theme III: Process simulation of plant structure

Accomplishments

In the context of shape formation, the opportunity to study the interplay of distinct shape forming processes on different biological scales is currently missed. Translating this interplay into experimentally observable measures is an open, yet high –risk/high-reward area of my research. To date, typical models assume a locally fixed and symmetric plant shape while the plant grows in size, complexity and volume. It is key to recognize that the growth process of a plant implies lateral growth of a tissue within the surrounding physical space whenever a plant part elongates. As a postdoc, I developed the Fiber Walk model (Figure 2) as a formal model of geometric random growth that describes the effect of simultaneous lateral expansion of randomly growing lines (Bucksch, Turk, and Weitz, 2014). There are many consequences to this explicitly spatial treatment of growth. For example, I have shown that blocked regions are formed that are impossible to occupy by a growth process. Furthermore I showed that an increasing amount of expansion of any thickening process results in a straighter grown shape, thus, creating a spatial constraint to development.

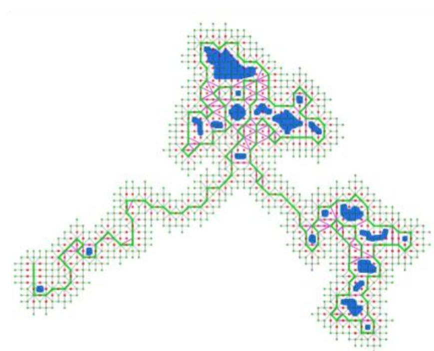

Figure 2: The Fiber Walk model (Bucksch, Turk, and Weitz, 2014) as a 2D example. On the left preliminary computations of blocked regions (blue) created by a 2D Fiber Walk (green) on a square lattice are shown. Purple lines indicate locations where the curvature of the walk was influence by itself and red points indicate the regions occupied by expansion.

Key Collaborator: Jonathan Lynch (Penn State, USA), Greg Turk (Georgia Tech, USA)

Future Work

Which mathematical process characteristics describe the drivers of shape formation? I seek to address the understudied relationship between a shape generating process interplays with internal shape regulating processes. Here, an exemplary long-term goal is the feedback between the curvatures of growing branch surface and the internal plant hormone gradients. The simple interplay to study here is that every newly grown tissue occupies new space, which in turn limits possible curvatures of later grown tissue. However, state-of-the-art experimental research assumes a static relation between curvature and hormone gradient (Grieneisen et al., 2007). The current Fiber Walk model exhibits the mechanisms to simulate the mathematical space of branching structures to investigate the limits of possible spatial branch arrangements. Such limits potentially translate into limits of plant breeding for optimal root structures. I identified cross-scale coupling of internal hormonal scale and external geometric plant growth dynamics as a high-risk/high reward element of my research program. I seek collaborations with experimentalists and theorists to define and describe the shape regulating processes of plants. A potential funding source is the "Studying Complex Systems" program of the James S. McDonnell Foundation.

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