Coarse graining of an individual-based plant model

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Abstract: The evolution and structuring of plant communities is governed by local plant-to-plant interaction. It has been shown that the individual variability of the organisms and the spatial neighbor constellation is essential for plant system dynamics. Therefore, several spatially explicit individual-based model approaches for plant communities have been developed in the last decades. Among these the *field of neighborhood* approach is promising as it describes the system at an intermediate level of complexity. A present limitation of this approach, and many other individual-based models, is that it can only be studied by simulation. In general simulations of large individual-based models are computational demanding and reveal only limited information on the long-term dynamics of the system. Here, we report ongoing work that aims to investigate the dynamics of field of neighborhood by a numerical coarse-graining technique. This so-called "equation-free" method, uses short burst of individual-based simulation to extract information that is necessary to investigate the system on the level of plant distributions. This approach allows us to investigate the individual-based model as if macroscopic equations of motion were available, providing more information in shorter time. We emphasize that our approach is well suited for implementation on CELL or GPU systems, as it can be parallelized with high efficiency and most time-critical operations can be performed on the rendering pipeline.

1 Introduction

The history of ecological modeling started long before the invention of modern computers. Therefore, the early models needed to be simple enough for analytical investigation. Such models models were composed of a small number of equations describing the system on a macroscopic level. With the emergence of computers, more complex models appeared. These described the system on a more detailed level, but were still based on coupled systems of equations and could therefore take advantage of the powerful tools of dynamical systems theory. Only later the steady increase in computing power led to the formulation of individual-based models. These models are no longer based on equations but rather on a set of explicit rules that govern the individuals. This *microscopic* view allows for a more realistic description of the system at hand. In particular individual-based models can

describe important macroscopic patterns observed in nature and, therefore, have attracted keen scientific interest [GLR96, Gri99, Lev94, BH00, MWL$^+$07, NXLF08].

Compared to equation-based models describing the system on an emergent *macroscopic* level, a major drawback of individual-based models is that they can not be analyzed directly by the tools of dynamical systems theory and are therefore almost exclusively studied by simulation. In comparison to more advanced mathematical tools simulation reveals less information on the long-term dynamics of the system at a significantly higher computational cost. In particular the simulation of large individual-based models tends to be computationally demanding and difficult to parallelize.

In order to close the gap between a macroscopic equation-based models, which can be analyzed quick and comprehensively, and a microscopic individual-based model, which allow for a detailed description the so-called "equation-free" coarse-graining approach was proposed [KGH$^+$03]. This approach makes use of the fact that the state of most systems can be described faithfully by a small number macroscopic variables. Additional microscopic degrees of freedom change much faster than the slow macroscopic variables. In the long term behavior they therefore equilibrate and become enslaved to the macroscopic variables. Much effort in physics focuses on the identification of such slow variables in a variety of systems and subsequently on the formulation of closed equations of motion in terms of these variables. However, for ecological systems of realistic complexity the formulation of closed analytic equations is prohibitively difficult.

The "equation-free" approach is based on the insight that coarse-graining does not have to be performed analytically in order to analyze the system with the tools of dynamical systems theory. The established numerical tools do not use information on the functional form of the equations of motion, but only evaluate them in a finite number of points. If we can identify a set of slow variables and are able to evaluate the change of these variables over time for a given system, we can thus extract all information that is needed by the numerical methods. Note, that in an individual based model the change of the slow macroscopic variables can be extracted from a short burst of microscopic simulation. The numerical tools of dynamical systems theory can therefore be used to investigate the dynamics of equations of motion, which are not available but can be evaluated by running properly-initialized bursts of microscopic simulations on-demand. In the past this approach has been successfully applied in many areas including chemical reaction systems, synchronization, chemotaxis and epidemic spreading [KGH04, MGK06, EKO06, GK08]. The coarse-graining of ecological interaction, however, is complicated by the enormous range of different time-scales in the system: The individual behavior takes place on the scale of hour and days, while behavioral adaptation requires weeks or month, and population dynamical consequences take years or decades to manifest.

Here, we report ongoing work on the implementation of the "equation-free" approach to ecological models of plant communities. Plant growth is the source of nearly all biomass on earth, and local plant-to-plant interactions (such as competition or facilitation) are key processes in driving and structuring ecological communities. For the understanding and prediction of the effects of such local interactions on the higher hierarchical level, a multitude of modeling approaches have been developed. They range from aggregated models, considering only averaged plants characteristics and macroscopic variables

like abundance or biomass at the population level, to spatially explicit individual-based models, describing both the individual variability of the organisms and the local neighbor constellation[BPSG08]. While basic models may not be able to explain certain observed patterns of interest, detailed models are computationally demanding and may be hard to calibrate and analyze as they contain many, often unknown, parameters. A compromise between necessary simplicity and sufficient complexity is achieved by the so-called field of neighborhood (FON) approach [BH00], which models the interaction between neighboring plants using a heuristic formula.

In this paper, we illustrate the application of the "equation-free" approach to the FON approach. In particular we show how the coarse graining procedure can be used to extract information that is not directly accessible in simulations. We further show that the approach can be used to parallelize the system efficiently and can thus yield a considerable speed up on multi-core systems. Finally we emphasize that the computation of plant interactions can take advantage of the rendering power of GPUs and is therefore very well suited for implementation on such systems.

2 The FON approach

Plants are competing with their local neighborhood for several resources like sunlight, water and nutrients. In the zone-of-influence (ZOI) approach, for each plant a circular domain with age-dependent radius R represents the area where a plant exploits resources. Plants with overlapping ZOI are assumed to be neighbors and the size of the overlapping area defines the intensity of competition. An more realistic description of a spatial competition is achieved by the field-of-neighborhood (FON) approach. Here, again for each plant a circular ZOI is assumed, but furthermore the competitive impact on other plants is modeled by a scalar field $FON(r)$ which decreases from its center to its boundary (Fig. 1). For all points outside the ZOI the $FON(r)$ is set to 0. The overall influence F_k on a plant k with a ZOI of size A interacting with several neighbors is assumed to depend on the aggregated field $F_k(\vec{r})$, which corresponds to the total field $F(\vec{r}) = \sum_n FON_n(\vec{r})$ without the contribution of plant k, such that

$$\begin{aligned} F_k &= \frac{1}{A}\int_A F(\vec{r})\mathrm{d}\vec{r} = \frac{1}{A}\int_A \sum_{n\neq k} FON_n(|\vec{r}-\vec{r}_n|)\mathrm{d}\vec{\mathrm{r}} \\ &= \frac{1}{A}\sum_{n\neq k}\int_{A'} FON_n(|\vec{r}-\vec{r}_n|)\mathrm{d}\vec{\mathrm{r}}, \end{aligned}$$

with A' the overlapping area of the ZOI of plants k and n. The factor $1/A$ scales the influence of neighbors on the focal plant to the size of it's ZOI, so that for instance competition is weak if only a small fraction of the focal plant's ZOI overlap with other ZOI. An example of the competition field in a forrest is shown in Fig. 2. In general large values of F decrease the growth rates and may increase mortality. However, the relation between F, growth rate and size of the ZOI depend on the specific plants under consideration and are

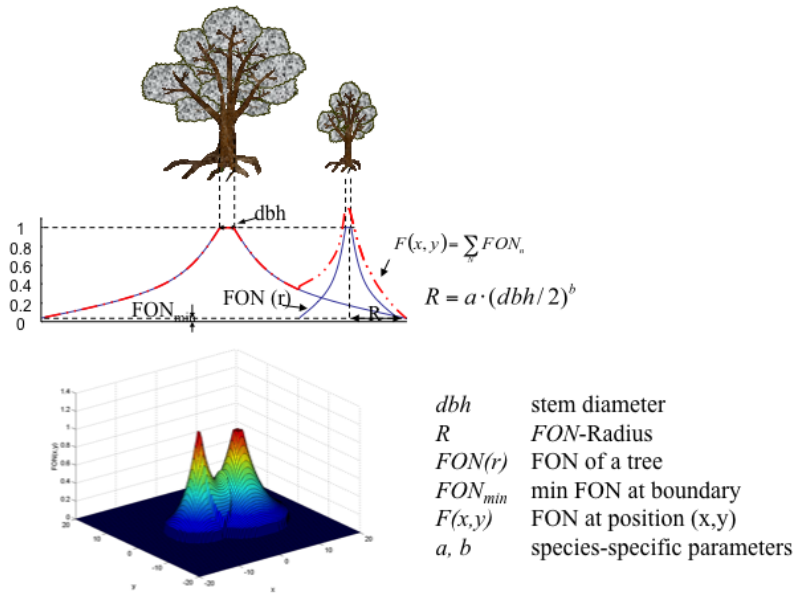

Figure 1: FON as used in the KiWi model [BH00] for mangrove forests. Fields of neighbors are assumed to be additive.

hence not considered here. For an example we refer to the application of ZOI approach to mangrove forests described in [BH00].

3 Numerical coarse-graining

The idea of "equation-free" modeling is to identify a few macroscopic variables which are sufficient to describe the macroscopic state of the system under consideration and to determine the derivatives of these variables through short burst of properly initialized microscopic simulation. Therefore, the implementation of this approach involves three key challenges: Identification of suitable slow variables (the state variables); extraction of the change of these state variables from microscopic simulations; and perhaps most importantly formulation of an algorithm for the efficient and consistent initialization of microscopic simulations.

In order to properly initialize a microscopic simulation we need to create a microscopic state that is consistent with a given set of state variables. This process is called *lifting*. Since the state variables do not completely determine the microscopic degrees of freedom,

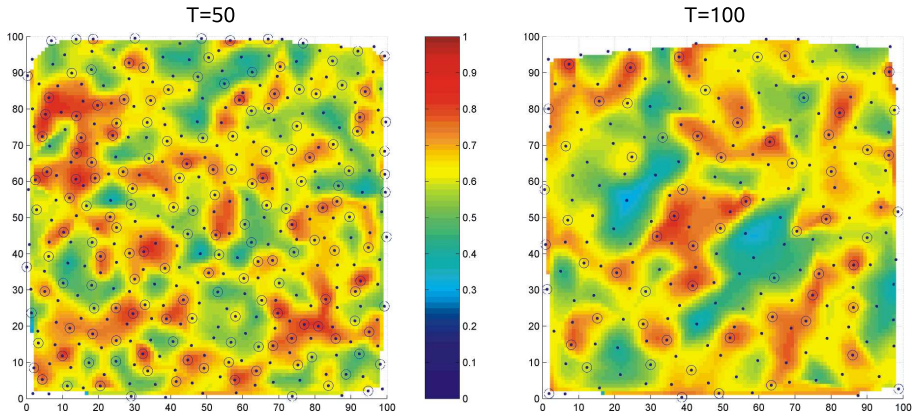

Figure 2: Competition between trees in a forest after 50 respectively 100 years. Dots mark position of trees. Strength of competition is color coded.

there is in general a multitude of micro states that are consistent with a given set of state variables. Not all of these micro states are suitable for our purposes as not all of them occur in naturally in the long-term behavior of the system. We therefore demand that the lifted state is consistent, meaning that one could reasonably expect it to be encountered in the long term behavior of the system with high probability. Several algorithms for constructing consistent lifted states have been proposed in the literature. If the state variables are chosen well a consistent state can be reached by initially lifting the system into a potentially non-consistent state and then simulating the time evolution of the system for a few steps. During this simulation the microscopic degrees of freedom should quickly relax back to a consistent value. If the state variables are well chosen they should change only little during this time. Thus the desired state is approximately obtained.

An example for the application of the "equation-free" approach is the coarse projective integrate (CPI)[KGH$^+$03]. In this scheme a standard numerical integrator is used to simulate the system on the macroscopic emergent level. Starting with some initial values of the state variables, we lift the system constructing a consistent micro state. Then we run a short simulation and estimate the derivative of the state variables from the resulting time series. By doing so we have obtained the information that is necessary to perform one integration step on the macroscopic level. We now discard the microscopic simulation and compute the value of the state variables at a later time by extrapolation. Repeating these steps, yields an approximation to the trajectory of the macroscopic variables over time. This process is illustrated in Fig. 3. For systems were the extrapolation step size can be chosen much larger than the microscopic simulation step needed to estimate the derivatives, this method can decrease the time needed for the simulation by several orders of magnitude.

In order to take large steps in the coarse projective integration the derivatives of the state variables need to be determined precisely. For this purpose it is advantageous to determine them not only from one burst of microscopic simulation, but average over several of

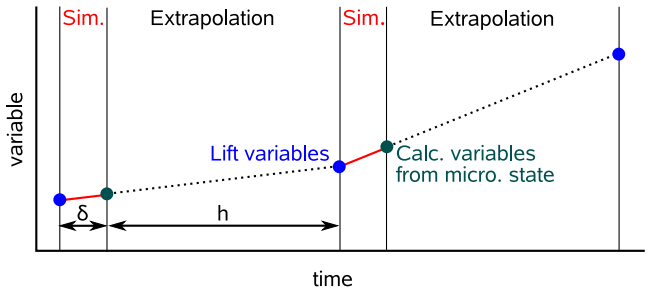

Figure 3: Sketch of coarse projective integration (CPI). Starting from initial values of variables $\vec{v}_0$, an according microscopic state is lifted and evolved for a time δ by microscopic simulation. During simulation variable values change by $\Delta\vec{v}$. This change is extrapolated for a time step h: $\vec{v}_1 = \vec{v}_0 + \Delta\vec{v}/\delta h$. Therefore, the speedup compared to microscopic simulation is about h/δ in this simple scheme.

such bursts. Let us point out that these microscopic simulations are completely independent and can thus be parallelized with high efficiency. In particular the total area under consideration, e.g., the forrest does not need to be kept in memory at the same time.

In many applications we are not interested in the trajectories but rather in the stationary states of a system. In this case simulation on the macroscopic level is not necessary. The "equation-free" approach can provide all information that is necessary to drive specialized fixed-point algorithms such as Newton's method. In contrast to simulation which often takes millions of steps to arrive close to a steady state, Newton's method can often locate a steady state in only 20 steps up to numerical precision. In contrast to simulations it also finds saddle points which are interesting, as they can mark the basin boundaries between different types of long-term behavior. Just like fixed-point algorithms other powerful tools of dynamical systems theory can be applied. These include continuation of solution branches, bifurcation detection, computation of Lyapunov exponents and numerical normal form analysis.

In order to apply the "equation-free" approach to FON models we need to define slow variables that are able to capture the patterns under consideration and contain all information necessary to determine the long-term dynamics. For instance, if we are interested in the evolution of the ratio of two different plant species which suffer from inter- and intra-species competition, we need at least two variables to store the abundance respectively the biomass of both species. Furthermore we know that the spatial distribution of plants is of importance, therefore this distribution needs to be parameterized as well. For this purpose we will use an expansion of the observed two and three point correlation functions as this results in variables that allow for easy lifting. An important question is whether the age distribution needs also be parameterized. Also detailed investigations of this question are needed. There is reasonable hope that the age distribution equalized sufficiently fast, so it does not need to be captured by a slow variable.

For the implementation of the coarse-graining procedure the use of CELL or GPU proces-

sors is advantageous. The most time-critical step of the individual based simulations is the computation of the overlap of FONs. The individual steps involved in this computation can be significantly accelerated using the specialized functionality provided by the rendering pipeline of modern graphics processors. Our aim is to integrate over the intersections of different ZOI where we weight every point by the focal plant's FON. This can be done by scaling and interpolation of the FON to fill a two dimensional graphic buffer (Fig. 4). Then this buffer is multiplied with another buffer representing the ZOI of a neighboring plant by the numbers 0 and 1. While the power of graphics processing can thus be harnessed to speed up individual-based simulations, an additional speed up can be achieved using the "equation-free"' approach. As described above this approach is based on short bursts of simulations, which can be run in parallel. In particular several such bursts can be run in parallel on the 8 SPEs of a CELL processor or side by side in a large frame buffer of a GPU.

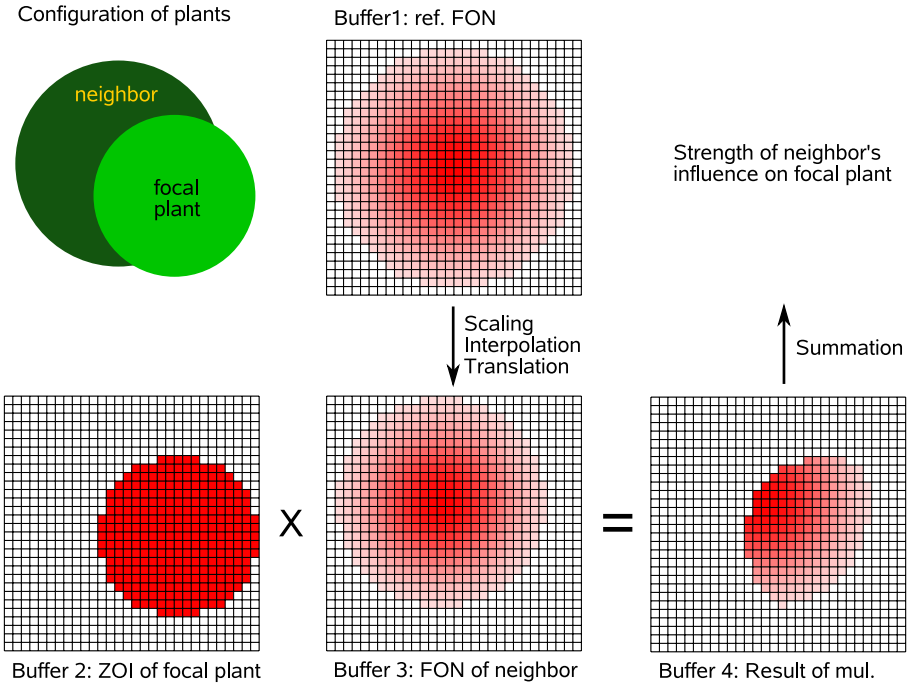

Figure 4: Calculation of interaction strength F. A rasterized reference FON is permanently stored in memory (strength is color-coded). For a given configuration of focal and neighboring plant the reference FON is transformed to the size and position of the neighboring plant and stored to a buffer. The ZOI of the focal plant is represented by ones in another buffer. The interaction strength F is then estimated by summing over the product of both buffers.

4 Conclusions

The simulation of FON-based models is computational demanding and only provides limited information. Here, we described how the "equation-free" approach can be applied to these models. This approach enables us to analyse such models on the emergent level of spatial plant distributions, providing more information at a lower computational cost. Moreover, this approach allows for simple parallelization, which in some cases, can be distributed within a GPU or between the SPE units of a cell processor. Most importantly the most computational intensive step of the FON approach, the integration over the intersecting ZOI, can easily be parallelized on GPUs.

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