

A COMBINED DENSITY FUNCTIONAL THEORY FRAMEWORK FOR MODELING MULTIFACETED ECOLOGIES ACROSS SPATIAL AND TEMPORAL SCALES

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ABSTRACT

It is made problematic for ecosystem to model singularities across numerous timeframes and spatial scales by the intricacy of systems with many interrelating mechanisms. It is made tougher for complex ecologies and the significances of human actions like reaping, deforestation, and environmental change to be realized by us. In order to overcome this, we have established a new context for ecosystem modelling using density functional theory, a physics-based computational practice for many-body problems. Our technique can forecast fallouts for new data and fits experimental and artificial data from multi-species groups across numerous spatial scales with high accurateness. An authenticated cost function that measures the trade-offs between bionetworks mechanisms is a significant innovation. This method allowed DFTE to recover realistic species distributions despite the problem's significant dimensionality and offered insightful information about the relative significance of resource limitation, dispersal, environmental filtering, and interspecific interactions in structuring tropical forest communities. This combined framework offers a promising means of advancing environmental understanding by accomplishment as well as dedicated models for a diversity of systems, such as tropical honey bees.

Keywords: Density Functional Theory, Ecosystem, Spatial and Temporal Scales, Tropical Honeybees.

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1. INTRODUCTION

A small number of species' communications at fine spatial and temporal scales are explicated by extremely thorough automatus theories found in ecology [1-3]. Though, deprived of focussed on the exchanges between specific species, more inclusive combined models can elucidate significant ecological arrangements, such as species area relationships [4-7]. Though, since limited theories efficiently link ecological processes across numerous scales, there is still a noteworthy gap between these two attitudes. Environmental models should preferably be able to precisely forecast patterns at larger scales, such as groups and landscapes, after being parameterized at one level of group, such as discrete creatures or species. By doing this, predictions and better considerations of the dynamics of more complex ecosystems would be allowed by scientists using partial field and experimental data. Ground-breaking measureable methods are required to address these challenges [8-12].

Density Functional Theory (DFT) [13-16], a computational outline usually used in physics/chemistry to examine many-body systems, from atoms to planetary cores, is reformed by us in order to address this problem. The impression that the properties of a system can be determined from the density distributions of its essential parts is regarded as the basis of DFT. An energy, or cost, functional that characterizes the system is considered essential to the theory; equilibrium states are found by minimizing this functional. One of the key benefits of DFT is recognized as its capability to efficiently capture interactions, trade-offs, and constraints among various system components.

The application of DFT to ecological systems is implemented by us, motivated by its success in physics [17-20]. While DFT has been commonly used in molecular natural science, its application in macro-ecology has been comparatively small. It was shown by previous research [21] that fruit fly spatial

distributions in experimental settings could be reliably predicted using statistical techniques inspired by DFT. Building on this concept, Density Functional Theory for Ecology (DFTE) is implemented by us, a more inclusive framework. Energy functions precisely for ecosystems are formed by DFTE by combining DFT ideas with environmental ethics. DFTE does not include quantum mechanics into ecology, notwithstanding prejudiced by physical models like the Thomas-Fermi context [22-23]. Somewhat, by freely parameterizing system subcomponents and integrating them for prediction of the behaviour of more complex ecosystems, it offers a combined approach for connecting ecological processes across scales. We describe this general context and show how it can be applied to a diversity of ecological systems. Here, Tropical Honey Bees spatial distributions in experimental sceneries could be reliably prophesied using numerical techniques inspired by DFT.

2. METHODOLOGY

The energy functional (E), which is constructed as a grouping of several ecological components in accordance with Eq. (1), is the foundation of Density Functional Theory for Ecology (DFTE).

By creating a cost function and an energy functional, we have applied the DFT narrative and methodology to ecology.

$$E[\mathbf{n}] = E_{\text{dis}}[\mathbf{n}] + E_{\text{env}}[\mathbf{n}] + E_{\text{int}}[\mathbf{n}], \quad (1)$$

Where $E[\mathbf{n}]$ - The total energy of the system, E_{dis} - Dispersal energy, E_{env} - Environmental energy, E_{int} - Species interaction energy

The best way to comprehend the underlying methodology is to start by looking at the dispersal and environmental energy terms that are defined in Equations 2 and 3, ignoring species interactions for the time being.

$$E_{\text{dis}}[n_s] = \frac{\tau_s}{2} \int_A n_s(\mathbf{r})^2 d\mathbf{r} \quad (2)$$

Where $E_{\text{dis}}[n_s]$: Dispersal energy of species s , τ_s : Dispersal strength of species s , A : The spatial domain (Study region), $d\mathbf{r}$: Differential area/volume element over the spatial domain, $n_s(\mathbf{r})$: Density of species s at location $\mathbf{r}$.

$$E_{\text{env}}[n_s] = \int_A V_s^{\text{env}}(\mathbf{r}) n_s(\mathbf{r}) d\mathbf{r} \quad (3)$$

Where $E_{\text{env}}[n_s]$: Environmental energy of species s , A : The spatial domain or study area, $d\mathbf{r}$: Differential spatial element, $n_s(\mathbf{r})$: Density or abundance of species s at location, $V_s^{\text{env}}(\mathbf{r})$: Environmental potential (or habitat suitability function) experienced by species s at location $\mathbf{r}$ [24]

The interaction energy term permits the assimilation of further ecological progressions that amend the symmetry between dispersal and environmental favourites. For instance, a bi-functional energy component that amends the ecological potential experienced by species can be used to exemplify responses between organisms and their environs. In these situations, the operative environment changes into an animatedly altering quantity that is reliant on both species densities and environmental circumstances.

The strength of these interactions is firmed by species-specific scaling limits, and ecological data such as fitness metrics, resource-use traits, or experimentally determined interaction strengths can be used for the parameterization of the interaction kernels themselves. A very pliable context is presented by this formulation, which can illustrate natural interactions that are both locally and spatially extended.

Higher-order interactions concerning three or more species can also be accommodated by the DFTe context. A grouping of pairwise effects or ecological processes that are truly multifarious and cannot be wrecked down into distinct pairwise relations can result in these interactions. Abridged ecological subsystems can be scrutinised under meticulous situations, and the inferred constraints can then be applied to more complex ecological settings, allowing model parameterization to proceed in systems where higher-order interactions are substantial. Similar constructions in physics are used as inspiration for the mathematical form of the interaction energy. For instance, local interactions can be portrayed using contact-type kernels, while long-range interactions can be described using kernels that decay with distance. DFTe does not integrate any quantum-mechanical norms into ecological modelling, despite the mathematical context being taken from Density Functional Theory and related fields of physics. Instead, it takes mathematical methods that work well for exemplifying interacting many-body systems and amends them for ecological settings.

The consequential resource-energy functional is used to measure the disparity between local resource obtainability and community resource consumption. The equilibrium density of a species is made inversely proportional to its resource requirements and directly proportional to the availability of local resources when this term acts alone.

This straightforward equilibrium is then altered by the addition of extra energy components due to species interactions, dispersal pressures, and environmental effects.

The same framework naturally accommodates predator-prey relationships, which views prey abundance as a resource that can be used by predators. According to this formulation, prey dynamics are still controlled by their own ecological limitations, but predator distributions are typically coincided with prey distributions. Because of this directional dependence, trophic interactions can be included in the larger framework of resource consumption.

The focus of the resource-energy formulation on areas with high resource densities is recognized as a key component. Greater impacts on equilibrium outcomes are seen from resource-rich regions than from resource-poor ones because variations between availability and consumption are penalized quadratically. Resource-specific weighting factors are introduced to ensure ecological realism, meaning that all resources, regardless of their absolute abundance, are given the potential to limit population growth. For instance, constraints on species abundances may be experienced as strongly by a rare but necessary mineral as they are by a far more plentiful resource like water. Therefore, rather than focusing only on absolute quantity, it is guaranteed by the weighting scheme that ecological limitation reflects biological importance.

A modular energy-functional framework that can represent a variety of ecological processes is formed by the terms dispersal, environmental, interaction, and resource-energy. The trade-offs between resource availability, environmental suitability, species interactions, and dispersal constraints that collectively determine the structure and dynamics of ecological communities are captured by DFTe.

3. RESULT AND DISCUSSION

Determining constrained equilibrium states is a key component of many basic ecological questions, such as how species abundances redistribute in response to environmental change. This goal is very similar to Density Functional Theory (DFT) in physics. The energy functional, a cost function that describes the system, is the key quantity in DFT. The equilibrium (ground-state) density distributions for a system of (S) interacting species with abundances are obtained by minimizing the energy functional (E) after the constituent components have been defined. A comprehensive picture of the system at equilibrium is provided by these densities, and the spatial distribution of each species is characterized by them.

Building on this framework, an ecological cost function known as the energy functional is created in order for the DFT methodology and principles to be applied to ecology. As stated in equation 1, a unified framework for forecasting equilibrium community structure under particular environmental and biological constraints is offered by this functional by expressing ecological dynamics in terms of species-density distributions and their interactions.

The ecological energy functional is designed to minimize costs specific to species resulting from resource consumption, biotic interactions, environmental factors, and dispersal. The three terms that appear on the right side of Equation 1 correspond to these contributions. Square brackets in expressions like $(f[n])$ indicate that (f) is a functional of the density distribution (n) throughout this framework.

We establish a way to compare different system configurations $[(n', N')]$ by defining energy (E) for a given realization $((n, N))$ of an ecological system. The idea that a system tends to occupy the configuration with the lowest possible energy often referred to as the ground state is a fundamental tenet of physics. Using this idea, we create the DFTe energy functional $(E(N))$ so that the equilibrium state of the ecosystem with abundances is represented by its global minimum.

The energy functional defines a (S) -dimensional energy landscape whose geometry controls system behaviour, even though the current work focuses on establishing the equilibrium properties of DFTe as a basis for future dynamical applications. Specifically, the shape of this landscape can determine both non-equilibrium dynamics, where external drivers like environmental stochasticity may prevent the system from reaching equilibrium, and steady-state dynamics, which are comparable to the trajectories of celestial bodies in a gravitational potential. One way to think of energy is as a gauge of a system's ability to change another system. Since energy is additive, this capacity doubles when the energy is doubled. This characteristic does not, however, imply that the energy functional always breaks down into a straightforward sum of independent contributions. Rather, physical intuition about how various processes contribute to a system's total energy drives the additive decomposition used in Equation (1). In keeping with this viewpoint, we build the ecological energy functional from discrete elements that symbolize important ecological processes and whose mathematical structures are modelled after analogous energy terms in physics. To describe the dispersal behaviour of species (s) , for instance, the dispersal energy is created by modifying the Thomas-Fermi kinetic-energy expression.

The integration is carried out across all spatial locations within the focal area (A) , and a species-specific dispersal pressure parameter is represented by (τ) in Eq. (2). A mechanism by which conspecifics may be repelled is represented by this formulation, such as through territorial behaviour, and an intraspecific dispersal pressure for species (s) is captured. In this context, positive energy densities are represented by repulsive interactions, while negative energy densities are represented by attractive interactions.

Unlike other energy components whose integrands exhibit sub-quadratic scaling with density, a type of negative density dependence among conspecifics is suggested by the dispersal energy's quadratic dependence on species density. Crucially, representation by Eq. (2) is not intended for all potential dispersal mechanisms. Additionally, inclusion of this equation is not required by all ecological applications because dispersal processes can also be captured by other elements of the energy

functional. The quadratic density dependence is understood as an emergent consequence of underlying individual-level processes that do not need to be explicitly identified, whereas the parameter (τ) gives rise to the species-specific nature of this term.

The environmental energy is represented as the second part of the total energy functional in Equation (1). This phrase is described by how environmental factors affect each species equilibrium abundance and spatial distribution, much like the function of external potentials in physics. The effects of resource availability, habitat suitability, and other abiotic factors that influence ecological patterns across space are captured by the environmental energy through the integration of species-specific responses to environmental heterogeneity.

The environmental potential experienced by species (s) at a spatial location is represented by V_s^{env} in Equation (3). This term, which is comparable to the external potential energy used in Density Functional Theory, is established by how environmental factors contribute to species energy. Both habitat preferences and external environmental influences, such as resource availability, anthropogenic disturbances like deforestation, and spatial variation in climate, are captured by the environmental energy. This is similar to the formulation suggested in earlier studies.

An amphibian species can be used to demonstrate the ecological interpretation of Eq. (3). Minimizing the total energy functional will favour higher species densities in the lake and lower densities in the desert if locations corresponding to a lake are assigned negative values of V_s^{env} while the surrounding desert is assigned positive values. In this sense, the environmental energy term penalizes occupancy of inappropriate areas while directing species distributions toward habitats that are favourable to the environment. The corresponding contributions to the total energy functional shown in Eq. (1) are obtained by adding Equations 2 and 3 for every species.

It is crucial to stress that the intricate chemical mechanisms underlying ecological processes are not the goal of DFTe. The complexity of ecological systems makes such a strategy unfeasible. Rather, DFTe uses an energy functional that is guided by ecological principles and inspired by the conceptual framework of Density Functional Theory. This functional goal is to give important ecological processes a mathematically tractable representation so that individual system components can be parameterized and then combined to produce predictions at higher ecological organization levels.

Furthermore, observable quantities like species abundances, resource distributions, and associated ecosystem characteristics—rather than energy itself—are focused on by ecology. Energy is functioned as a theoretical construct in the DFTe framework that connects these observable variables via a shared optimization principle. Therefore, the predictive accuracy of the framework is determined by whether the suggested mathematical structure of the energy functional is effectively capturing the ecological processes governing the system rather than whether energy is actually minimized by ecological systems. Accurate predictions of

species distributions, abundances, and ecosystem dynamics can be made by DFTE to the extent that this representation holds true.

Density-Potential Functional Theory (DPFT) [25-30], one of the different forms of Density Functional Theory, is considered especially appropriate for DFTEs goals. An explicit expression for the equilibrium density distribution of species (s) is provided by DPFT when combined with the dispersal energy functional given in Equation 4.

$$n_s[V_s - \mu_s](\mathbf{r}) = \frac{1}{\tau_s} [\mu_s - V_s[\mathbf{n}](\mathbf{r})]_+ \quad (4)$$

Where $\mathbf{n}_s(\mathbf{r})$: Density of species s at location r, $V_s[\mathbf{n}](\mathbf{r})$: Effective potential experienced by species s, which depends on the community configuration n, μ_s : Chemical potential (or Lagrange multiplier) for species s, controlling the total abundance of the species, τ_s : Dispersal strength parameter of species s, $[x]_+$: Positive-part function.

Zero is substituted for negative values by the operator $[]_+$ to guarantee non-negative densities. The abundance constraint within the focal area (A) is enforced by the parameter (μ_s), which is regarded as a species-specific Lagrange multiplier. As $V_s[\mathbf{n}](\mathbf{r})$ is given as in equation 5-

$$V_s[\mathbf{n}](\mathbf{r}) = V_s^{\text{env}}(\mathbf{r}) + V_s^{\text{int}}[\mathbf{n}](\mathbf{r}) \quad (5)$$

Where $V_s[\mathbf{n}](\mathbf{r})$: Total (effective) potential experienced by species s at location r, $V_s^{\text{env}}(\mathbf{r})$: Environmental potential, representing habitat suitability determined by abiotic factors, $V_s^{\text{int}}[\mathbf{n}](\mathbf{r})$: Interaction potential, representing the effects of interactions with other species and depending on the entire community distribution n.

The amount is a representation of the species' (s) effective potential. This potential combines the interaction potential ($V_s^{\text{int}}[\mathbf{n}]$), which is derived from the functional derivative of the interaction energy ($E_{\text{int}}[\mathbf{n}]$), with the environmental contribution (V_s^{env}), which captures the impact of external habitat conditions. The densities of every other species in the community are linked to the distribution of species (s) through this term.

The quadratic form selected for the dispersal energy in Equation 2 directly leads to the straightforward linear relationship between the equilibrium density (n_s) and the effective potential (V_s). Equation 6 illustrates alternative dispersal functional those are equally feasible and might be more suitable for particular ecological systems, even though this formulation is adequate for the proof-of-concept applications discussed here. In the discussion that follows, explicit functional arguments are omitted for notational simplicity whenever doing so does not impair clarity.

$$E_\gamma[\mathbf{n}] = \sum_{s,s'=1,S \atop s \neq s'} \int_A \int_A d\mathbf{r} d\mathbf{r}' n_s(\mathbf{r})^{\alpha_s} \gamma_{ss'}(\mathbf{r}, \mathbf{r}') n_{s'}(\mathbf{r}')^{\beta_{s'}} \quad (6)$$

Which include mutualism, amensalism, commensalism, and so on.

Where $E_\gamma[\mathbf{n}]$ - The total energy functional depending on the set of densities $\mathbf{n} = \{n_1, n_2, \dots, n_S\}$, A - A double integral over the spatial domain A (surface area or volume), α_s, β_s - Power-law exponents that scale the density, often used to account for non-linear correlation or exchange effects, $\gamma_{ss'}(\mathbf{r}, \mathbf{r}')$ - An interaction kernel describing how

species s at position r interacts with species s' at position r', $n_s(\mathbf{r})$ and the density of species s at position r. Equations 4 and 5 together form the foundation of DPFT and its ecological extension, DFTE. In this case, fitness proxies of species s and s' are used to assemble $\alpha_s, \beta_s \geq 0$ and the interaction kernels $\gamma_{ss'}$. The distribution of species and the biotic and environmental factors influencing them are directly linked by these coupled equations. The balance between a species' abundance constraint (μ_s) and its effective potential (V_s), which takes into account both environmental factors and species interactions, determines the species' local density, according to Eq. (4). By using this method, DFTE offers a unified framework for forecasting equilibrium spatial distributions from a limited number of cost-function components that are ecologically understandable.

Equation 4 states that individuals of species (s) preferentially occupy areas with the lowest effective cost (V_s) resulting from biotic interactions and environmental conditions. Local density increases when (V_s) decreases, suggesting that more advantageous habitats for the species are associated with lower effective potential values. The spatial distribution of (V_s) is determined by the self-consistent solution of Equations 4 and 5, which link species densities and ecological conditions in a mutually dependent framework. The trade-off between habitat suitability and dispersal is naturally captured by this formulation. On the one hand, as local density increases, intraspecific dispersal pressure rises and additional aggregation is considered costly. Conversely, advantageous areas are drawn to by people due to the confining force of the effective potential (V_s). Significantly, the underlying environmental conditions represented by (V_s^{env}) in this effective potential are altered by species interactions, which can be understood as a modified environmental landscape.

Significant flexibility in the specification of species-interaction functionals ($E_{\text{int}}[\mathbf{n}]$) is provided by this framework, despite being only one potential application of Density Functional Theory for Ecology (DFTE). A reliable and accurate description of empirical ecological patterns and distributions is offered by this method, as will be shown by the analyses that follow.

This biological system is used as a representative case study in order to develop and validate the Density Functional Theory for Ecology (DFTE) framework. By using this example, it is hoped that:

- i. DFTE predictions are shown to agree with both empirical observations and well-established ecological modelling techniques
- ii. The advantages and disadvantages of DFTE are assessed in comparison to other approaches.
- iii. The fundamental elements of the framework can be applied practically.
- iv. Customized DFTE models can be derived from the general energy functional to study modified or extended ecological systems.

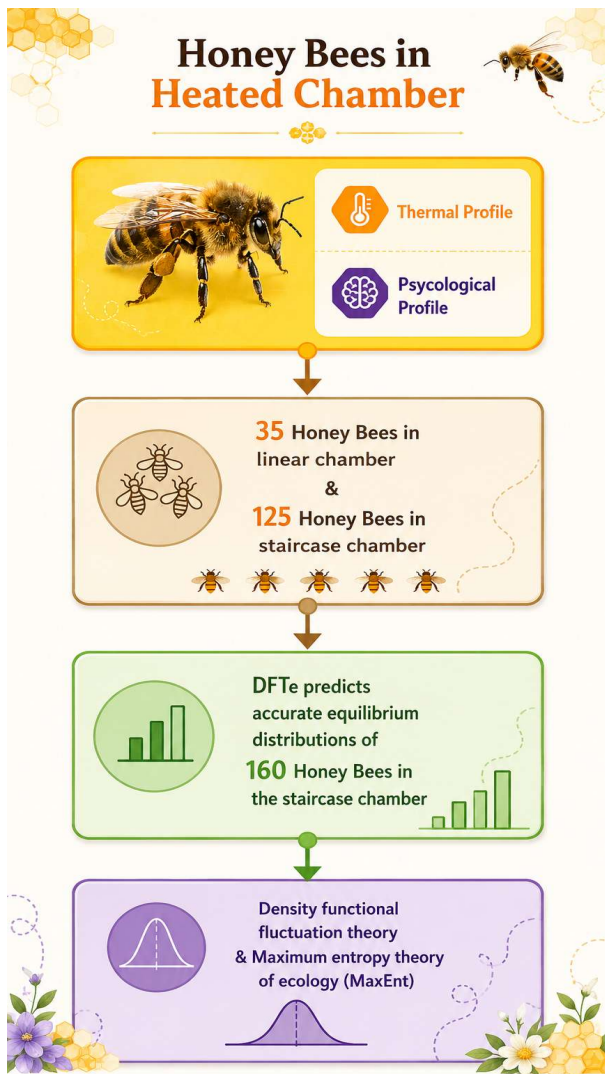


Figure 1: Our DFTe framework is the first step towards a universal density functional theory for ecology as a whole, and the successful modelling of these diverse setups offers hope that it can handle a far wider range of ecological systems

An outline of this agenda is given in Figure 1, which summarizes the main components and conclusions drawn from the DFTe analyses of this case study.

DFTe performs similarly to establish modelling approaches created specifically for the corresponding ecological problems across all systems analysed. Climate-envelope models, Lotka-Volterra models, R^* theory, density-functional fluctuation theory, the Maximum Entropy Theory of Ecology, and various statistical techniques are among them. One of the main benefits of DFTe is its generality, which is highlighted by the requirement for such a wide range of alternative models to handle the various case studies. DFTe offers a unified theoretical structure that can handle a wide range of ecological phenomena, as opposed to depending on a separate modelling framework for every ecological application.

However, it is not always appropriate to view models built within the DFTe framework as precise depictions of fine-scale causal mechanisms. Rather, they frequently serve as

useful explanations of ecological processes in which observed patterns might not be directly related to particular elements of the energy functional. The consistent relations avowed in Table 1 are consequently prototypical slightly than difficult. For instance, as illustrated in figure 1, the psychological profile of honey bees in this case study may be represented by nonlocal repulsive interactions, local dispersal pressure, or a combination of both mechanisms.

Table 1: Links between ecological concepts/phenomena and DFTe parameters

Intra-specific Interaction	τ_s	Interpretation
Spreading/ Dispersal	> 0	Avoidance of conspecifics
Aggregation	< 0	Beneficial proximity of conspecifics
Environment	V_s^{env}	Interpretation
Attraction	Small	Favourable region
Repulsion	Large	Hostile region
Bipartite Interactions	$\gamma_{ss'}$ (α_s, β_s)	Impact on s, s'
Amensalism	> 0 (0, 1)	(0, -)
Repulsion	> 0 (1, 1)	(-, -)
Parasitism	> 0 (1, 2)	(+, -)
Commensalism	< 0 (0, 1)	(0, +)
Mutualism	< 0 (1, 1)	(+, +)

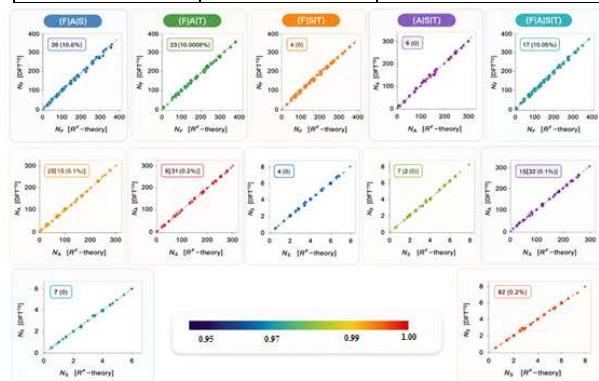


Figure 2: DFTe's capacity to manage resource limitations is demonstrated through an

application to Tilman's algae competition experiments

Spatial Distribution (Contour Heatmap)

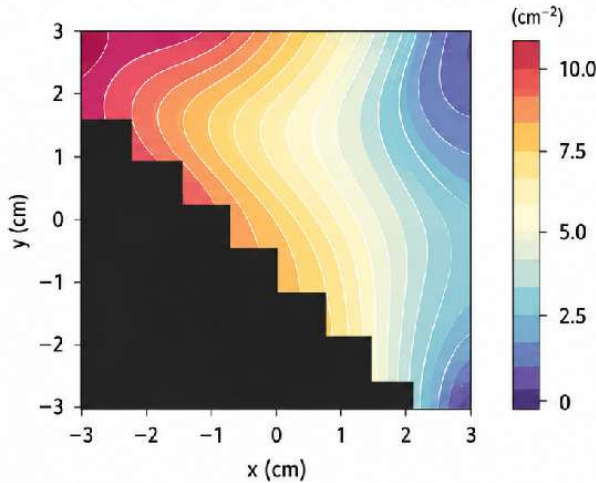


Figure 3: DFTe's ability to forecast a population's spatial distribution given a fixed total abundance is demonstrated through an application to confined honey bees

To demonstrate the fundamental computational procedure of DFTe namely, the minimization of the energy functional (E) subject to fixed species abundances (N), we first consider the honey bee experiment reported by Dhruva Naug et al. [31]. We find that DFTe accurately predicts the spatial distributions of honey bees under novel environmental conditions, achieving performance comparable to state-of-the-art modelling approaches (Figure 3).

Fitting a two-parameter energy functional (E) to two experimental datasets that describe the spatial distributions of bees is the first step in the DFTe workflow (Figure1).

Applications of the Maximum Entropy Theory of Ecology would be similarly limited if the constraints were limited to low-density observations. Maximum-entropy approaches must assume that individuals are independent of each other in the absence of additional system-specific information. In contrast, density-dependent dispersal and interaction processes are explicitly included in DFTe, allowing for more accurate predictions under shifting population and environmental conditions.

Overall, this case study illustrates how DFTe combines biotic interactions, environmental heterogeneity, and dispersal effects into a single theoretical framework, showcasing both its predictive ability and its potential for mechanistic ecological inference.

We looked into DFTe's capacity to include resource constraints controlling species coexistence in order to further highlight its adaptability. In a series of seminal experiments, D. Tilman examined competition between four algal species to test the predictions of R^* theory [32]. He demonstrated that a dynamic model parameterized from single-species experiments could be used to predict the results of pairwise competition. Predictions for multispecies competition were also produced by these

fitted models, though they have not yet undergone experimental verification.

By calibrating DFTe to the pairwise competitive outcomes predicted by R^* theory, we created an alternative framework for forecasting the results of multispecies competition. Crucially, rather than using Tilman's experimental pairwise results, some of which represented transient dynamics rather than equilibrium states the calibration was based on the theoretical pairwise predictions of R^* theory. As seen in Figure 2, the resulting DFTe model demonstrated exceptionally good agreement with the R^* theory predictions in every competitive scenario investigated.

Our method makes the assumption that two important ecological characteristics the inverse of the minimum resource requirement ((R^*)) and the nutrient requirement per cell determine species-specific competitive abilities. Fitness proxies from Tilman's monoculture experiments and species-specific resource demands were used to parameterize the energy functional used in this analysis. Only two free parameters needed to be estimated after this parameterization, and these were fitted collectively to all pairwise competition outcomes produced by R^* theory.

The case study is demonstrated by DFTe to show how data can be converted from comparatively simple ecological systems into forecasts for more intricate community assemblages. The results of an established resource-competition theory are successfully replicated by the framework, while a cohesive mathematical structure is preserved, despite its extremely general formulation. Thus, it is shown by the findings that DFTe has the potential to be a scalable method for connecting ecological processes at different biological complexity levels, ranging from pairwise interactions to multispecies community dynamics.

More specialized ecological theories, such as R^* theory and the recently proposed community assembly rule, which holds that species that can coexist in multispecies communities are those that can coexist in all pairwise interactions, are compared to DFTe's predictive performance. It is shown by this agreement that, while a cohesive mathematical structure is retained, the results of theories created especially for specific ecological processes can be replicated by a general framework like DFTe.

However, R^* theory is deviated from by DFTe in a number of significant ways. One drawback is that pairwise competition results, not data from single-species experiments, were used to parameterize the DFTe model. Data from a higher level of ecological organization is depended upon by this method, but the need for specific mechanistic information is also lessened. However, the difficulty of creating highly parameterized, fine-scale descriptions of multispecies systems is circumvented by this approach, which frequently become more complicated and challenging to calibrate as the number of interacting species increases.

Furthermore, parameters that are essential to R^* theory, like resource supply rates ((F)) and maximum species growth rates, are not explicitly included in our DFTe formulation. Therefore, predictions for alternative

resource-flow regimes cannot be directly generated by the DFTE energy functional calibrated for a specific value of (F) without additional parameterization, even though equilibrium community composition across a range of resource-supply conditions can easily be predicted by R^* theory [33-34].

In a broader sense, a potentially fruitful method for researching intricate ecological systems is offered by this application. To gain a thorough grasp of systems with comparatively few interacting components, detailed mechanistic theories, like R^* theory, can first be used. Predictions can then be scaled up to larger and more complex ecological communities by incorporating the patterns and insights from these well-characterized systems into the DFTE framework. In this way, DFTE acts as a link between predictive modelling at larger levels of ecological organization and mechanistic understanding at smaller scales (Figure 2).

The emergence of zonation, which is defined by sudden shifts between species distributions even in the presence of a continuous environmental gradient, was a noteworthy result of these simulations. According to the DFTE framework, zonation is caused to emerge as a fleeting phenomenon by species interactions rather than sudden changes in the environment. If full equilibrium is consistently prevented from being achieved in the system by environmental disruptions, long stretches of time may be endured by such patterns in natural ecosystems and even developed into long-lived dynamic steady states.

It is shown by this case study that intricate and ecologically significant predictions can be produced by DFTE from comparatively small datasets. The framework is recognized as a potent tool for examining both the static and dynamic characteristics of ecological communities since information about transient ecological processes and the formation of spatial patterns can be revealed in addition to equilibrium distributions being reproduced.

The wider applicability of DFTE beyond static ecological predictions is demonstrated by these results. A promising way to comprehend and forecast ecological systems that show cyclic behaviour, persistent fluctuations, and other types of non-equilibrium dynamics is provided by the framework through the connection of equilibrium theory with dynamic population processes.

When combined, it is shown by these findings that DFTE is still useful in species-rich environments with high levels of uncertainty and scant ecological data. Large-scale spatial patterns are successfully replicated by the framework, which also produces insights that align with more specialized ecological methodologies.

The wide range of applications of DFTE is recognized as one of its unique features. To the best of our knowledge, no ecological framework currently in use has been demonstrated to effectively model such a wide range of ecological systems within a single theoretical framework. Although these findings are encouraging, they should not be interpreted as conclusive proof of universal applicability. Instead, attention is drawn to the need for on-going assessment of the framework across a wider range of ecological systems, environmental circumstances, and organizational scales.

Therefore, the empirical testing of DFTE should be increased by future studies, the performance in systems with higher ecological complexity and uncertainty should be investigated, and alternative formulations of its energy components should be examined. The elucidation of the frameworks advantages and disadvantages will be aided by these initiatives while the creation of a more cohesive and predictive theory of ecology will be advanced.

All things considered, DFTE is represented as a promising step toward combining statistical and mechanistic methods into a single theoretical framework. A fresh approach to long-standing issues about species coexistence, community assembly, ecosystem dynamics, and biodiversity maintenance is offered by it through a scalable framework that can connect ecological processes across levels of organization.

The modular structure of DFTE is recognized as one of its main advantages. Each of the various components that make up the energy functional is represented as a unique ecological process with a distinct biological interpretation. Crucially, the parameters related to these components can frequently be estimated from simpler subsystems, which allows for the gradual construction of ecological complexity. Another important benefit is that the determination of species distributions and the identification of trade-offs between competing ecological processes are not significantly complicated by the mathematical complexity of the energy functional, which naturally increases with ecosystem complexity. The long-standing problem of integrating various interacting mechanisms and constraints within species-rich communities living in complex environments is thus addressed by DFTE.

Ecological processes are modelled as separately parameterized energy components connected by a common energy functional in the DFTE framework. Differences between predictions and observations are noted every time, and the model can be easily extended and refined thanks to its modular architecture. New ecological mechanisms can be added without changing the framework as a whole. For instance, the interaction energy term can be extended to introduce higher-order species interactions.

However, compared to extremely detailed mechanistic theories like R^* theory, DFTE is regarded as more phenomenological. For instance, results from R^* theory were used as inputs in the analysis of algal competition to expand predictions to more intricate ecological scenarios. DFTE is not seen as a completely first-principles framework that is directly derived from individual-level interactions, just like all other contemporary ecological theories. Rather, the energy components are based on parsimonious assumptions, empirical observations, and ecological intuition. This intermediate degree of mechanistic detail is undoubtedly recognized as one of the best features of the framework. The use of DFTE in data-constrained environments is regarded as a crucial practical consideration. Once more, the framework is placed somewhere in the middle of conventional mechanistic and statistical methods. Useful predictions can still be produced by DFTE if reasonable ecological assumptions are available, even though poor performance

is frequently exhibited by statistical models when data are scarce. In this context, two challenges are considered especially significant. The first step in keeping the number of fitted parameters and model complexity under control is finding the most important elements of the energy functional. Enough ecological intuition must be developed to create energy-function expressions that correctly integrate the pertinent ecological variables and processes, which is the second challenge.

The case studies in this work show that DFTE models with predictive performance comparable to that of well-established ecological approaches can be built with even a relatively basic understanding of ecosystem functioning. We have shown the potential of DFTE as a unified framework for ecological modelling through tropical honey bee. Although the framework is inspired by physics' Density Functional Theory, it is fundamentally different in that its energy functional cannot be obtained from first principles. Rather, ecological knowledge, empirical data, and parsimonious modelling assumptions must be combined to create ecological energy functionals.

Like any ecological theory, the worth of DFTE is ultimately determined by how well empirical observations are explained and forecasted. A common theoretical foundation is maintained by DFTE while a performance similar to that of specialized ecological models is exhibited across the various systems studied in this study. These results imply that a great deal of potential is held by DFTE to develop into a widely applicable framework for researching ecological systems, encompassing both equilibrium and dynamic phenomena at various temporal and spatial scales. However, methodological advancement and on-going empirical validation will be considered necessary for its long-term usefulness. Many examples in history of physics-based ideas that have developed into significant frameworks in other fields are present. It was started out as a heuristic analogy and, after decades of improvement, evolved into a potent predictive framework. A similar direction might be taken by DFTE, with its development from a fundamental conceptual framework to more robust and all-encompassing ecological applications [35].

More generally, we hope that this work will encourage multidisciplinary research at the nexus of ecology and physics. Density Functional Theory's guiding principles may be useful for a variety of complex phenomena, such as the spread of epidemics, transportation networks, urban dynamics, and financial systems, in addition to ecological systems. It will take persistent interdisciplinary cooperation to overcome such obstacles. By presenting DFTE, we hope to start a more extensive discussion about how one of the most effective theoretical frameworks in physics can be modified to answer important issues in ecology and other fields.

4. CONCLUSION

In this work, we present Density Functional Theory for Ecology (DFTE), a unified modelling framework that draws inspiration from physics' Density Functional Theory (DFT). DFTE offers a common framework that can connect mechanistic descriptions of basic ecological interactions with predictive models of large, complex

communities by adapting the conceptual and mathematical underpinnings of DFT to ecological systems. We show that DFTE effectively replicates observed ecological patterns and produces predictions that are in line with accepted ecological theories and experimental data across a variety of systems through a number of empirical and synthetic case studies.

The species that make up the synthetic ecosystem vary in a number of ecological traits, such as their dispersal strengths (τ_s), habitat preferences (V_s^{env}), interaction types (α_s, β_s), interaction strengths ($\gamma_{ss'}$, α_s & β_s), and the kinds and amounts of resources needed for survival.

A number of ecological quantities, such as individuals per unit area, biomass density, species frequency, fractional land cover, or any other appropriate metric, can be represented by the density (n_s) of each species. Accordingly, the model parameters, like (τ_s), (V_s^{env}), and associated quantities, incorporate units and absolute scales. Within the coarse-grained study area (A), we assume that individuals are only directly impacted by conspecifics and hetero-specifics that occupy the same spatial unit. The honey bee system that was previously experimentally studied, is in good agreement with our computational results by DFTE Theory.

This method allowed DFTE to recover realistic species distributions despite the problem's significant dimensionality and offered insightful information about the relative significance of resource limitation, dispersal, environmental filtering, and interspecific interactions in structuring tropical forest communities.

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REFERENCES

- [1] Tilman, D. Tests of resource competition theory using four species of Lake Michigan algae. *Ecology*, 62, 802 (1981).
- [2] Pacala, S.W. et al. Forest models defined by field measurements: estimation, error analysis and dynamics. *Ecological Monographs*, 66, 1 (1996).
- [3] Cabral, J.S., Valente, L., and Hartig, F. Mechanistic simulation models in macroecology and biogeography: state-of-art and prospects. *Ecography*, 40, 267 (2017).
- [4] Levin, S.A. The problem of pattern and scale in ecology: the Robert H. MacArthur award lecture. *Ecology*, 73, 1943 (1992).
- [5] Leibold, M.A. et al. The metacommunity concept: a framework for multi-scale community ecology. *Ecology Letters*, 7, 601 (2004).
- [6] McGill, B.J. Towards a unification of unified theories of biodiversity. *Ecology Letters*, 13, 627 (2010).
- [7] Udy, K. et al. Environmental heterogeneity predicts global species richness patterns better than area. *Global Ecology and Biogeography*, 30, 842 (2021).
- [8] Benton, T.G., Solan, M., Travis, J.M.J., and Sait, S.M. Microcosm experiments can inform global ecological problems. *Trends in Ecology & Evolution*, 22, 516 (2007).
- [9] Evans, M.R. Modelling ecological systems in a changing world. *Philosophical Transactions of the Royal Society B: Biological Sciences*, 367, 181 (2012).
- [10] Stewart, R.I.A. et al. Mesocosm Experiments as a Tool for Ecological Climate-Change Research. In:

- Woodward, G. (Ed.), *Global Change in Multispecies Systems*, Part 3, Chapter 2. Academic Press (2013).
- [11] O'Dwyer, J.P. and Cornell, S.J. Cross-scale neutral ecology and the maintenance of biodiversity. *Scientific Reports*, 8, 1 (2018).
- [12] Kéfi, S. et al. Advancing our understanding of ecological stability. *Ecology Letters*, 22, 1349 (2019).
- [13] Hohenberg, P. and Kohn, W. Inhomogeneous electron gas. *Physical Review*, 136, B864 (1964).
- [14] Kohn, W. and Sham, L.J. Self-consistent equations including exchange and correlation effects. *Physical Review*, 140, A1133 (1965).
- [15] Levy, M. Universal variational functionals of electron densities, first-order density matrices, and natural spin-orbitals and solution of the v -representability problem. *Proceedings of the National Academy of Sciences USA*, 76, 6062 (1979).
- [16] Dreizler, R.M. and Gross, E.K.U. *Density Functional Theory*. Springer (1990).
- [17] Sholl, D.S. and Steckel, J.A. *Density Functional Theory: A Practical Introduction*. Wiley (2009).
- [18] Burke, K. Perspective on density functional theory. *Journal of Chemical Physics*, 136, 150901 (2012).
- [19] Becke, A.D. Perspective: Fifty years of density-functional theory in chemical physics. *Journal of Chemical Physics*, 140, 18A301 (2014).
- [20] Hasnip, P.J. et al. Density functional theory in the solid state. *Philosophical Transactions of the Royal Society A*, 372, 20130270 (2014).
- [21] Martin-I. Trappe & Ryan A. Chisholm, A density functional theory for ecology across scales, *Nature Communications* (2023) 14:1089.
- [22] Fermi, E. Un metodo statistico per la determinazione di alcune proprietà dell'atomo. *Rend. Lincei* 6,602(1927).
- [23] Kalita, B., Li, L., McCarty, R. J. & Burke, K. Learning to approximate density functionals. *Acc. Chem. Res.* 54, 818 (2021).
- [24] Méndez-Valderrama, J. F., Kinkhabwala, Y. A., Silver, J., Cohen, I. & Arias, T. A. Density-functional fluctuation theory of crowds. *Nat. Commun.* 9,3538, (2018).
- [25] Englert, B.-G. & Schwinger, J. Thomas-Fermi revisited: the outer regions of the atom. *Phys.Rev.A*26,2322(1982).
- [26] Englert, B.-G. *Lecture Notes in Physics: Semiclassical Theory of Atoms* (Springer, 1988).
- [27] Trappe,M.-I.,Len,Y.L.,Ng,H.K.,Müller,C.A.&Englert,B.-G. Leading gradient correction to the kinetic energy for two dimensional fermion gases. *Phys.Rev.A*93,042510(2016).
- [28] Trappe,M.-I.,Len,Y.L.,Ng,H.K.&Englert,B.-G. Airy-averaged gradient corrections for two-dimensional fermion gases. *Ann. Phys. (N. Y.)* 385, 136 (2017).
- [29] Trappe, M.-I., Ho, D. Y. H. & Adam, S. First-principles quantum corrections for carrier correlations in double-layer two-dimensional heterostructures. *Phys.Rev.B*99,235415 (2019).
- [30] Englert, B.-G. Julian Schwinger and the Semiclassical Atom, pp. 261–269 in *Proceedings of the Julian Schwinger Centennial Conference*, Englert, B.-G. (Ed.) (WorldScientific, 2019).
- [31] Christopher Mayack, Dhruva Naug, A changing but not an absolute energy budget dictates risk-sensitive behaviour in the honeybee, *Animal Behaviour*, Volume 82, Issue 3, 1 September 2011, Pages 595-600.
- [32] David Tilman, Resource Competition between Plankton Algae: An Experimental and Theoretical Approach, *Ecology*, Vol. 58, No. 2 (Mar., 1977), 338-348.
- [33] Friedman, J. & Higgins, L. M. Community structure follows simple assembly rules in microbial microcosms. *Nat. Ecol. Evol.* 1, 0109 (2017).
- [34] Marquet, P.A. et al. On theory in ecology. *BioScience*, 64,701(2014).
- [35] Jost, C. & Ellner, S. P. Testing for predator dependence in predator prey dynamics: a non-parametric approach. *Proc.R.Soc.Lond.B* 267, 1611 (2000).