**Exemplary model results description: PPA**

In this model, long-lived pioneers (tall stature, average PC1 score, high PC2 score) are the species that achieve highest biomass in monoculture (Fig. 1). The competitively strongest species combine a high PC1 score (slow lifestyle) with a high PC2 score (tall stature) and achieve slightly lower monoculture biomass than long-lived pioneers, but the highest biomass in mixture (Fig. 2). Thus, monoculture biomass and competitive strength are related, but not perfectly (Fig. 3, monoculture biomass versus time to extinction in mixtures of high planted species-diversity).

**Shannon and species richness**

Across planted-species richness treatments: Low-diversity communities show the largest variation in terms of biomass and include the highest-biomass communities (i.e. long-lived pioneers, Figs. 4, 5). The higher the number of species, the higher the chance of including a species with high biomass in mixture (sampling effect), but the smaller the between-community variation.

Within planted-species richness treatments: At low species richness (Ninitial=2-8), there is a negative relationship between diversity and community biomass. This is because at low initial species richness, average fitness differences between species are often large: as competitive strength and biomass in mixture are strongly related, communities including a competitively strong species quickly become dominated by this species (low richness, high biomass). In contrast, communities without competitively dominant species maintain higher richness and lower biomass.

At higher species richness, this negative relationship becomes flatter and even positive (Ninitial=32), especially when isolated from dispersal. This is because at higher species richness, it is more likely that the community includes several species of similar competitive ability that are able to coexist. These species lie on a line (tradeoff) in trait space including long-lived pioneers (high PC2 score) at one end and slow species (high PC1 score) at the other (Fig. 2). Long-lived pioneers maximize biomass in upper canopy layers, while slow species maximize biomass in lower layers. Thus, these species partition light, leading to a positive relationship between realized Shannon diversity and biomass.

**Functional diversity**

Across planted-species richness treatments: Functional dispersion *per se* does not promote overyielding. Specific trait combinations achieve high biomass while others do not (Fig. 6). For example, high diversity along PC1 does not promote community biomass (Fig. 2A)



Figure 1. Monoculture biomass per species at the final simulation year.



Figure 2. A: The average biomass per species within the 32-species planted species-richness treatment. Color represents the natural logarithm of total biomass. During the metacommunity stage, many species are fully maintained by seed addition, and thus have no biomass at the end of the isolation stage. B: Average time to extinction per species within the 32-species planted species-richness treatment.



Figure 3. Time to extinction within 32-species mixtures versus monoculture biomass per species. Color designates species identity. Each point represents a replicate in which that species is present.



Figure 4. The relationship between realized Shannon diversity and total community biomass. Colored lines refer to the fits within-richness treatments, while the black lines refer to the larger trend, inclusive of all planted-species richness treatments. Total biomass is scaled from 0 – 100. The assembly stage is defined as the first 100 iterations of the simulation, in which external seed addition is present. The isolation stage is defined as the following 100 iterations, once external seed addition has been excluded. Ribbons represent the 95%, 80% and 50% credibility intervals of the fits, while estimates with dashed lines include a slope of 0 with their 89% highest density intervals, suggesting that they are not statistically significant.



Figure 5. The relationship between richness total community biomass. Colored lines refer to the fits within-richness treatments, while the black lines refer to the larger trend, inclusive of all planted-species richness treatments. Total biomass is scaled from 0 – 100. The assembly stage is defined as the first 100 iterations of the simulation, in which external seed addition is present. The isolation stage is defined as the following 100 iterations, once external seed addition has been excluded. Ribbons represent the 95%, 80% and 50% credibility intervals of the fits, while estimates with dashed lines include a slope of 0 with their 89% highest density intervals, suggesting that they are not statistically significant.



Figure 6. The relationship between functional dispersion and total community biomass. Colored lines refer to the fits within-richness treatments, while the black lines refer to the larger trend, inclusive of all planted-species richness treatments. Total biomass is scaled from 0 – 100. The assembly stage is defined as the first 100 iterations of the simulation, in which external seed addition is present. The isolation stage is defined as the following 100 iterations, once external seed addition has been excluded. Ribbons represent the 95%, 80% and 50% credibility intervals of the fits, while estimates with dashed lines include a slope of 0 with their 89% highest density intervals, suggesting that they are not statistically significant.