Ecosphere

Appendix S1

Drought Legacies Mediated by Trait Tradeoffs in Soil Microbiomes

Bin Wang [1*], Steven D. Allison [1,2]

[1] Department of Ecology and Evolutionary Biology, University of California, Irvine, CA

[2] Department of Earth System Science, University of California, Irvine, CA

*Correspondence: wbwenwu@gmail.com

1 DEMENTpy

DEMENTpy is a trait-based modelling framework with spatially-explicit representation of individual populations in microbial communities. The model version reported here updates the physiological mechanisms (see **Fig. S1** for conceptual structure) and programming approach (see **Fig. S7** for programming structure) to the DEMENT model that was initially developed in 2012 (**Allison 2012**). The source code in Python is accessible at https://github.com/bioatmosphere/DEMENTpy. Processes simulated in DEMENTpy are described below.

1.1 Microbial community initialization

Using a trait-based approach, DEMENTpy initiates a microbial pool with a large number of hypothetical taxa by randomly drawing values from distributions of physiological traits (**Table S1**) and assigning them to different taxa. These hypothetical taxa in the microbial pool with differing combinations of trait values are randomly placed on the spatial grid to form a spatially structured microbial community. Illustrative animations are available at https://bioatmosphere.github.io/DEMENTpy/, and see **Wang and Allison (2019)** for an application of model spatial resolution for scaling up enzymatic heterogeneity. Trait distributions are all assumed to follow uniform distributions, except that for simplicity, some trait values are assumed to be constant, and values of some traits are derived from established correlations with other traits. These distributions and assumptions are largely informed by field- and lab-based empirical studies (**Allison 2012; Allison and Goulden 2017**).

The key traits determining mass balance in drought simulations are constitutive and inducible rates of enzyme and osmolyte production. The richness of genes encoding different enzymes and osmolytes is determined randomly for each taxon during model initialization.

Therefore, gene richness and production rate together determine the amounts of enzyme and osmolyte a cell can produce. The rate of inducible osmolyte production is then normalized to a value from 0 to 1, which is regarded as drought tolerance. This parameterization of drought tolerance is an update to the previous DEMENT version which instead directly introduced a drought tolerance parameter and imposed a penalty on carbon use efficiency (**Allison and Goulden 2017**). Linking osmolyte production directly to drought tolerance is intended to be more biologically realistic (**Schimel et al. 2007**). Additionally, kinetic traits including *Vmax* and *Km* are assigned to explicitly parameterize a certain number of different enzymes and transporters in the model system.

1.2 Metabolic production of enzyme and osmolyte

Different individuals (hypothetical taxa) comprising the microbial community undergo demographic processes of growth, mortality, and reproduction while degrading substrates and assimilating monomers at rates dependent on temperature and water potential. From these underlying processes emerge dynamics and functioning at both the microbial cell level and the whole system level.

Substrate degradation rates are calculated based on the activities of enzymes with different kinetic properties. Every enzyme degrades at least one substrate, and every substrate is degraded by at least one enzyme. Monomer uptake is calculated based on transporter abundance and kinetic traits which are specific to each taxon. The governing equation for both substrate degradation and monomer uptake follows the Michaelis-Menten equation, which is constrained by temperature (accounting for temperature impacts on enzymatic kinetics) and water potential (accounting for moisture constraints on enzymatic kinetics and diffusion; **Allison and Goulden 2017**):

$$V = \frac{V_{max} f(T)[S][E]}{K_m + [S]} f(\psi)$$

$$f(T) = e^{\left(-\frac{\boldsymbol{\varepsilon}}{R}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right)}$$

$$f(\psi) = e^{k\psi}$$

where *E* and *S* are matrices containing enzyme and substrate concentrations, respectively, *Vmax* represents the enzyme catalytic constant, K_m denotes the concentration of *S* at which *V* is one half V_{max}, $\boldsymbol{\varepsilon}$ is enzymatic activation energy, *R* is universal gas constant, and *k* is a coefficient controlling water potential sensitivity that differs between degradation and uptake.

Cellular metabolism balances carbon upon uptake from degraded substrates and carbon loss through constitutive and inducible metabolite production (**Fig. S1C**). After growth respiration (constrained by a constant), assimilated carbon is directed to enzyme and osmolyte production along with their associated maintenance respiration rates, all of which are treated simultaneously in the model without prescribing an order. The carbon remaining after these processes accumulates toward biomass. We assume the constitutive osmolyte production rate (*Osmo_Con*) varies across taxa independent of water potential, accounting for microbial allocation to maintain water potential balance across the cell wall (**Csonka 1989; Potts 1994**). In contrast, taxon-specific inducible production of osmolytes (O_{ind}) depends on water potential as follows:

$$O_{ind}(i) = \begin{cases} O_{ind}(i), & \psi \geq \psi_{th} \\ O_{ind}(i)\ (1\ -\ \alpha\psi), & \psi < \psi_{th} \end{cases}$$

where O_{ind}, is the i^{th} taxon's inducible osmolyte production rate, ψ is the daily water potential, α is a coefficient determining water potential sensitivity, and ψ_{th} is a system water potential constant, below which inducible osmolyte production is activated. Osmolyte stoichiometry is assumed to be constant at C/N = 3, which governs consumption of N in intracellular metabolism. This ratio is

based on an average of the three most common osmotic compounds in bacteria (**Csonka 1989; Potts 1994**): proline ($C_5H_9NO_2$), glycine betaine ($C_5H_{11}NO_2$), and glutamine ($C_5H_{10}N_2O_3$).

Mortality of microbial cells is simulated both deterministically by accounting for mass balance relative to a threshold, and stochastically based on a death probability constrained by drought tolerance and water potential. Here the taxon-specific mortality probability (*Mort*) is calculated as:

$$Mort_i = Death\_basal_i[1 - Death\_rate_i(1 - Tol_i)(\psi - \psi_{th})\ ]$$

where *Death_basal* is the i[th] taxon's basal mortality probability, *Death_rate* is a death probability coefficient controlling water potential sensitivity, *Tol* is the *i*[th] taxon's drought tolerance, and ψ_{th} is a system water potential constant. Microbial cells that fall below the biomass threshold or that die randomly are removed from the microbial community and added into the substrate pools as dead microbes. Microbial reproduction is calculated by splitting microbes into two equal halves, followed by local dispersal to surrounding grid boxes on the spatial grid (**Allison 2012**).

2. Calculation of community-level traits

Community-level enzyme investment (E_{com}) and drought tolerance (D_{com}) weighted by biomass are calculated as:

$$E_{com} = \sum_{i}^{n} EiMi$$

$$D_{com} = \sum_{i}^{n} DiMi$$

respectively, where *Ei* and *Di* refer to the ith taxon's enzyme production rate and drought tolerance, respectively, and *Mi* is the relative biomass of the *ith* taxon in the community.

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Table S1 Microbial and enzyme parameters and their values

Parameter	Value	Unit	Note
max_size_b	2	mg cm^{-3}	C quota threshold for bacterial cell division
Cfrac_b	0.825	mg mg^{-1}	Bacterial C fraction
Nfrac_b	0.16	mg mg^{-1}	Bacterial N fraction
Pfrac_b	0.015	mg mg^{-1}	Bacterial P fraction
Crange	0.09	mg mg^{-1}	Tolerance on C fraction
Nrange	0.04	mg mg^{-1}	Tolerance on N fraction
Prange	0.005	mg mg^{-1}	Tolerance on P fraction
C_min	0.086	mg cm^{-3}	Threshold C concentration for cell death
N_min	0.012	mg cm^{-3}	Threshold P concentration for cell death
P_min	0.002	mg cm^{-3}	Threshold C concentration for cell death
Uptake_C_cost_min	0.01	transporter mg^{-1} biomass C	Minimum per enzyme C cost as a fraction of uptake
Uptake_C_cost_max	0.1	transporter mg^{-1} biomass C	Maximum per enzyme C cost as a fraction of uptake
Uptake_Maint_cost	0.01	mg C $transporter^{-1}$ day^{-1}	Respiration cost of uptake transporters
Enz_per_taxon_min	0		Minimum number of enzymes a taxon can produce
Enz_per_taxon_max	40		Maximum number of enzymes a taxon can produce
Enz_Prod_min	0.00001	mg C mg^{-1} day^{-1}	Minimum per enzyme production cost as a fraction of C uptake rate
Enz_Prod_max	0.0001	mg C mg^{-1} day^{-1}	Maximum per enzyme production cost as a fraction of C uptake rate
Constit_Prod_min	0.00001	mg C mg^{-1} day^{-1}	Minimum per enzyme production cost as a fraction of biomass C
Constit_Prod_max	0.0001	mg C mg^{-1} day^{-1}	Maximum per enzyme production cost as a fraction of biomass C
Osmo_per_taxon_min	1		Minimum number of osmolyte a taxon can produce
Osmo_per_taxon_max	1		Maximum number of osmolyte a taxon can produce
Osmo_Consti_Prod_min	0.0000001	mg C mg^{-1} day^{-1}	Minimum per osmolyte production cost as a fraction of biomass C
Osmo_Consti_Prod_max	0.000001	mg C mg^{-1} day^{-1}	Maximum per osmolyte production cost as a fraction of biomass C
Osmo_Induci_Prod_min	0.01	mg C mg^{-1} day^{-1}	Minimum per osmolyte production cost as a fraction of C uptake rate
Osmo_Induci_Prod_max	0.1	mg C mg^{-1} day^{-1}	Maximum per osmolyte production cost as a fraction of C uptake rate
CUE_ref	0.5	mg mg^{-1}	Growth efficiency at the reference temperature
CUE_temp	-0.005	mg mg^{-1}	Growth efficiency change with enzyme investment
death_rate_bac	0.001		Bacterial death rate
basal_bac	10		Bacterial basal death probability
wp_th	-2.00	MPa	Water potential threshold at which osmolyte is induced
alpha	0.01	mg C mg^{-1} day^{-1}	Osmolyte production change with water potential
Vmax0_min	5	mg substrate mg^{-1} enzyme day^{-1}	Minimum Vmax for enzyme
Vmax0_max	50	mg substrate mg^{-1} enzyme day^{-1}	Maximum Vmax for enzyme

Uptake_Vmax0_min	1	mg substrate mg^{-1} substrate day^{-1}	Minimum uptake Vmax
Uptake_Vmax0_max	10	mg substrate mg^{-1} substrate day^{-1}	Maximum uptake Vmax
Uptake_Ea_min	35	kj mol^{-1}	Minimum activation energy for uptake
Uptake_Ea_max	35	kj mol^{-1}	Maximum activation energy for uptake
Km_min	0.01	mg cm^{-3}	Minimum Km
Uptake_Km_min	0.001	mg cm^{-3}	Minimum uptake Km
Vmax_Km	1	mg enzyme day cm^{-3}	Slope for Km-Vmax relationship
Vmax_Km_int	0	mg cm^{-3}	Intercept for Km-Vmax relationship
Uptake_Vmax_Km	0.2	mg biomass day cm^{-3}	Slope for uptake Km-Vmax relationship
Uptake_Vmax_Km_int	0	mg cm^{-3}	Intercept for uptake Km-Vmax relationship
Specif_factor	1		Enzyme efficiency-specificity

Table S2 Substrate concentrations initialized in DEMENT simulations (mg cm^{-3}).

Substrate	C	N	P
DeadMic	0	0	0
DeadEnz	0	0	0
Cellulose	146.89	0	0
Hemicellulose	85.855	0	0
Starch	12.21	0	0
Chitin	4.9952	0.83254	0
Lignin	48.51	0.40425	0
Protein1	10.6	2.09704	0
Protein2	10.6	2.09704	0
Protein3	10.6	2.09704	0
OrgP1	12.48	0	0.478469
OrgP2	1.8182	0.79745	0.478469

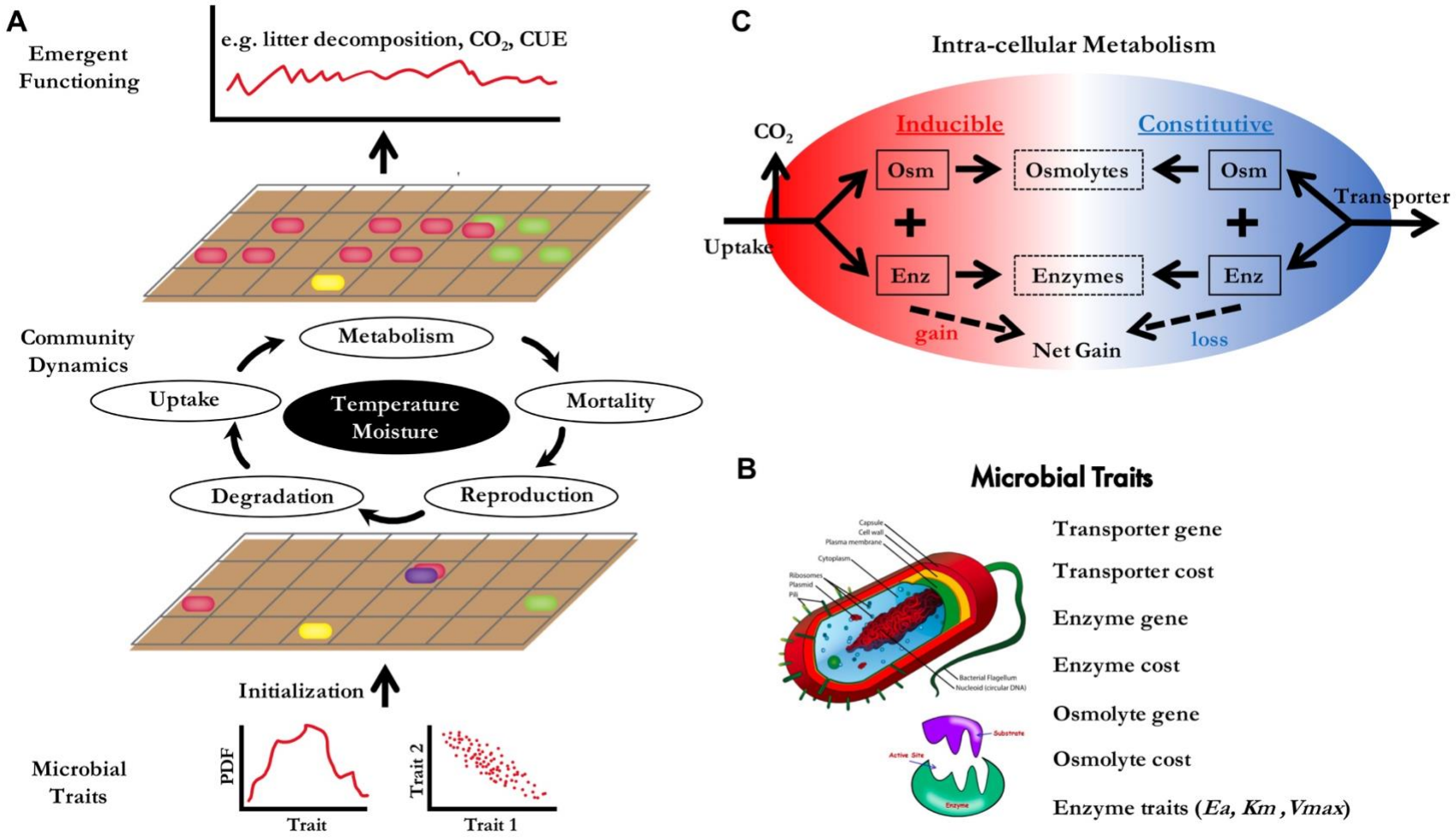

Fig. S1 DEMENTpy conceptual structure (A), microbial traits (B), and intra-cellular metabolism (C).

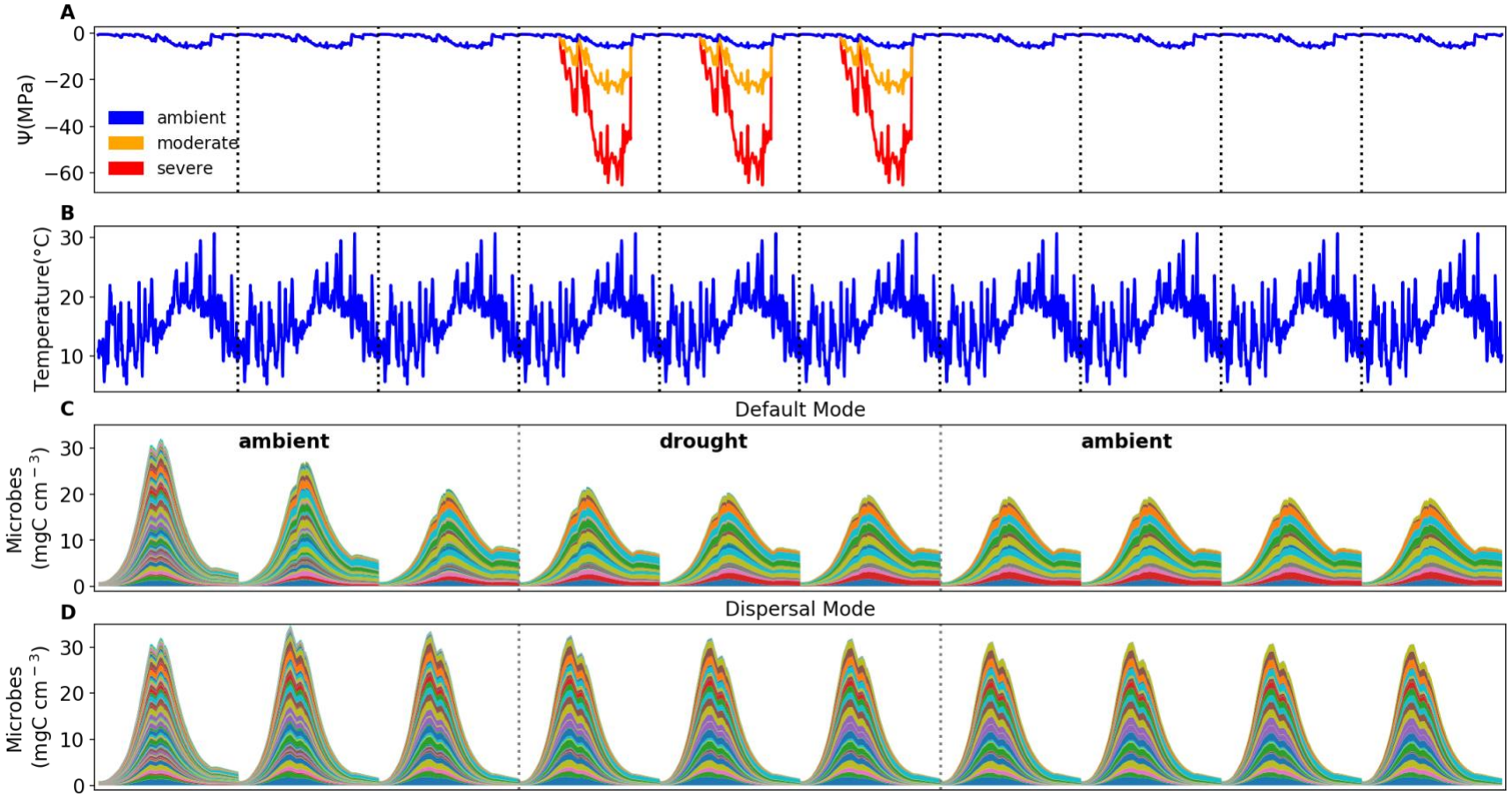

Fig. S2 Environmental forcing and microbial community dynamics. (**A**) Ambient daily water potential for 2011, with the orange and red lines denoting the moderate and severe drought scenarios, respectively. Drought forcing was obtained by multiplying the ambient water potential across the dry season (from April through September) by 4 and 10, respectively. (**B**) The corresponding daily temperature in 2011. (**C, D**) Microbial community dynamics of the default vs. dispersal mode over 10 years under the ambient scenario. The

simulation comprises three phases as separated by the dashed grey lines: a spin-up phase of three years to realize a relatively stable community; a disturbance phase imposing different drought scenarios for three years; and a final recovery phase after drought disturbance for four years. Colored bands represent biomasses of hypothetical taxa.

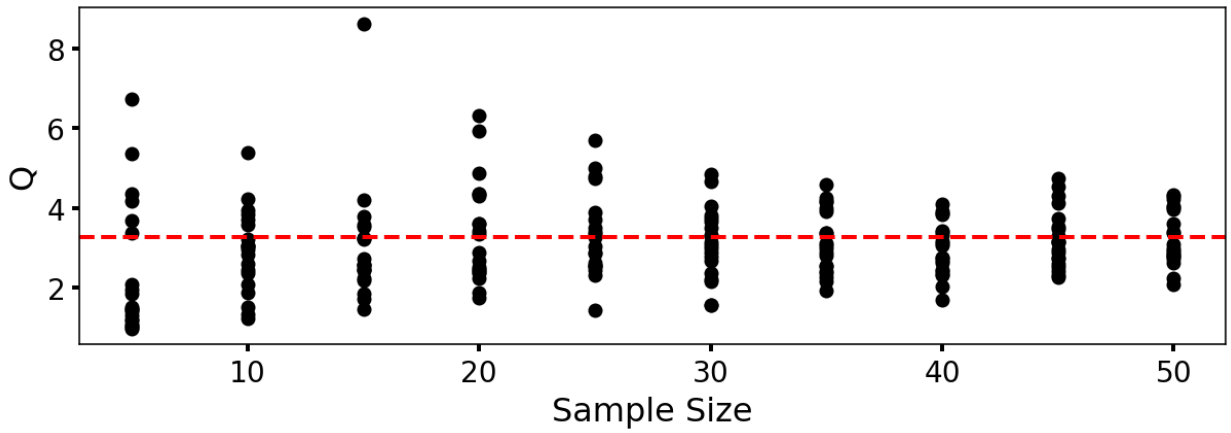

Fig. S3 DEMENTpy stochasticity convergence analysis. Q (quotient) is calculated as (90% percentile -10% percentile)/median substrate degradation following Bugmann et al. (1996). Each sample size has 20 replicates that were randomly drawn from a sample pool of 112 runs. This analysis illustrates that a sample size (i.e., ensemble of simulations) of 40 displays relatively stable, convergent variation that balances the tradeoff between precision and consumption of computing resources.

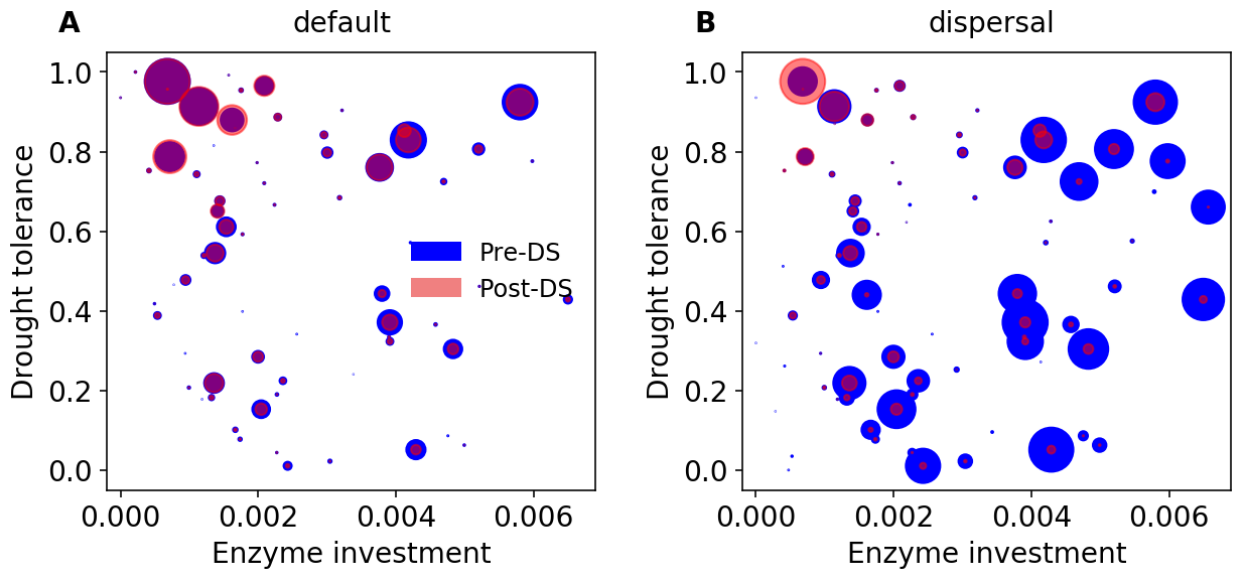

Fig. S4 Taxonomic changes in traits across the dry season. (A) Taxon-specific traits of drought tolerance and enzyme investment of a microbial community without dispersal before (blue) and after the dry season (red) under the ambient scenario. (**B**) The same for a microbial community with dispersal. Each point corresponds to a different taxon, and the size is proportional to its biomass.

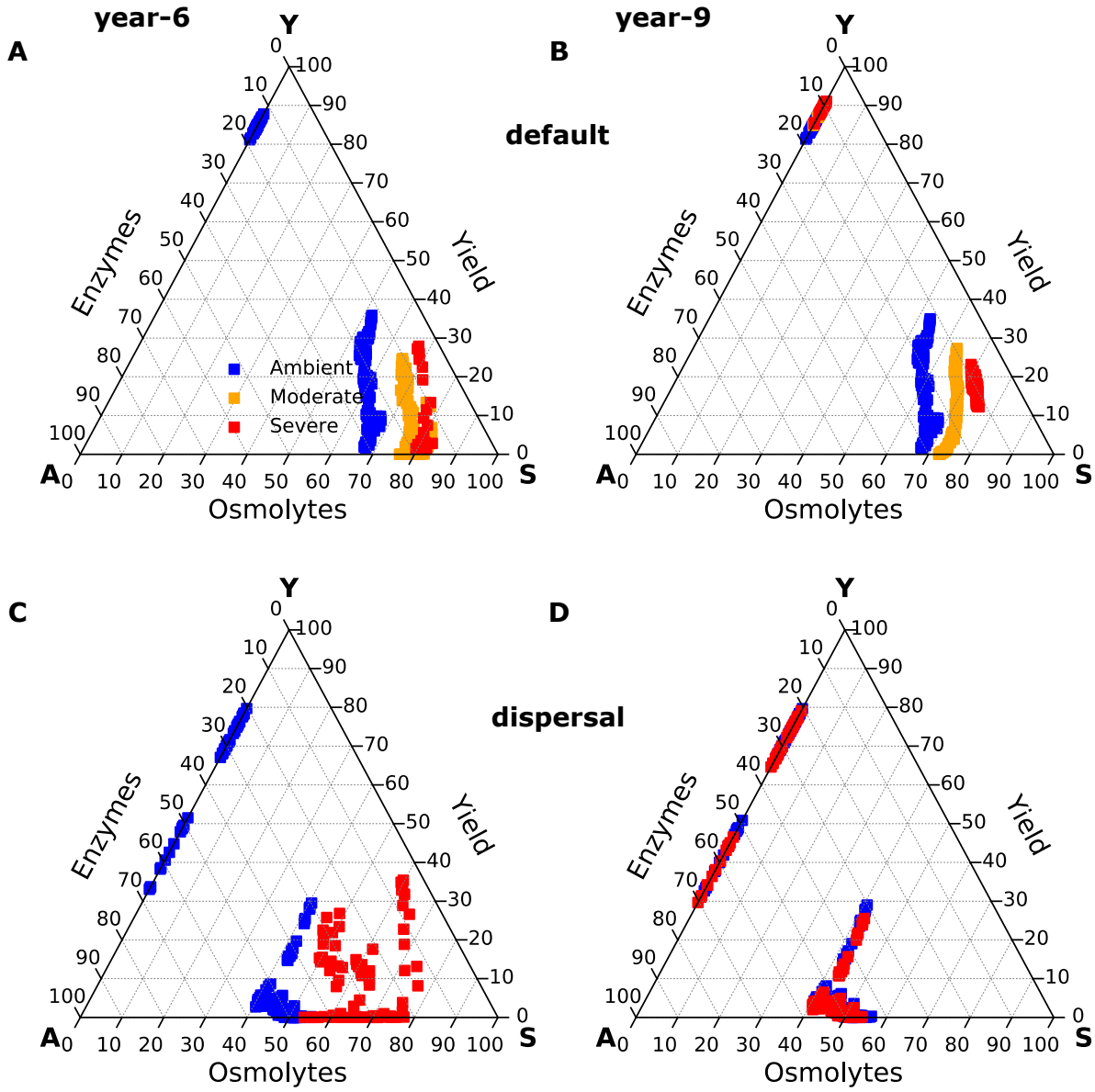

Fig. S5 Ternary plots of community-level allocation of assimilated carbon among enzymes, osmolytes, and yield over time under different drought scenarios. (A, B) Enzyme-Osmolyte-Yield tradeoff of communities during year 6 (3rd year under drought) and year 9 (3rd year after drought), respectively, of the default mode (without dispersal). (**C, D**) The same for the dispersal mode. The Y (Yield), A (Acquisition), and S (Stress tolerance) labels at the vertices correspond to yield, enzymes, and osmolytes, respectively. Points with negative net biomass gain were omitted.

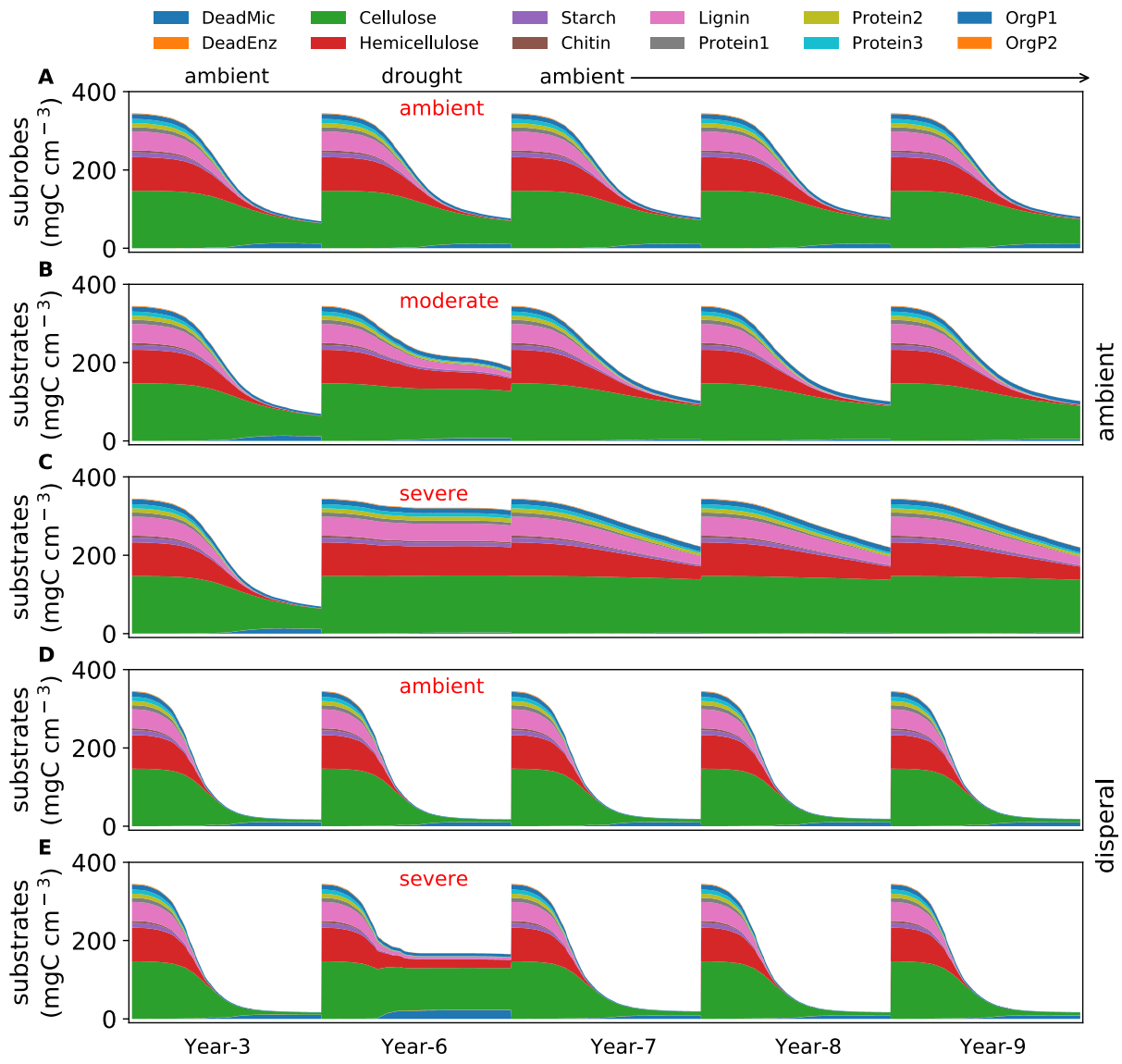

Fig. S6 Substrate-specific dynamics under differing drought scenarios. (A, B, C) Dynamics under ambient, moderate, and severe drought scenarios in default mode for year 3 and year 6 (the 3rd year under drought disturbance) through year 9. (**D, E**) The same for the dispersal mode but with only ambient and severe scenarios. Each color band represents one type of 12 different substrates.

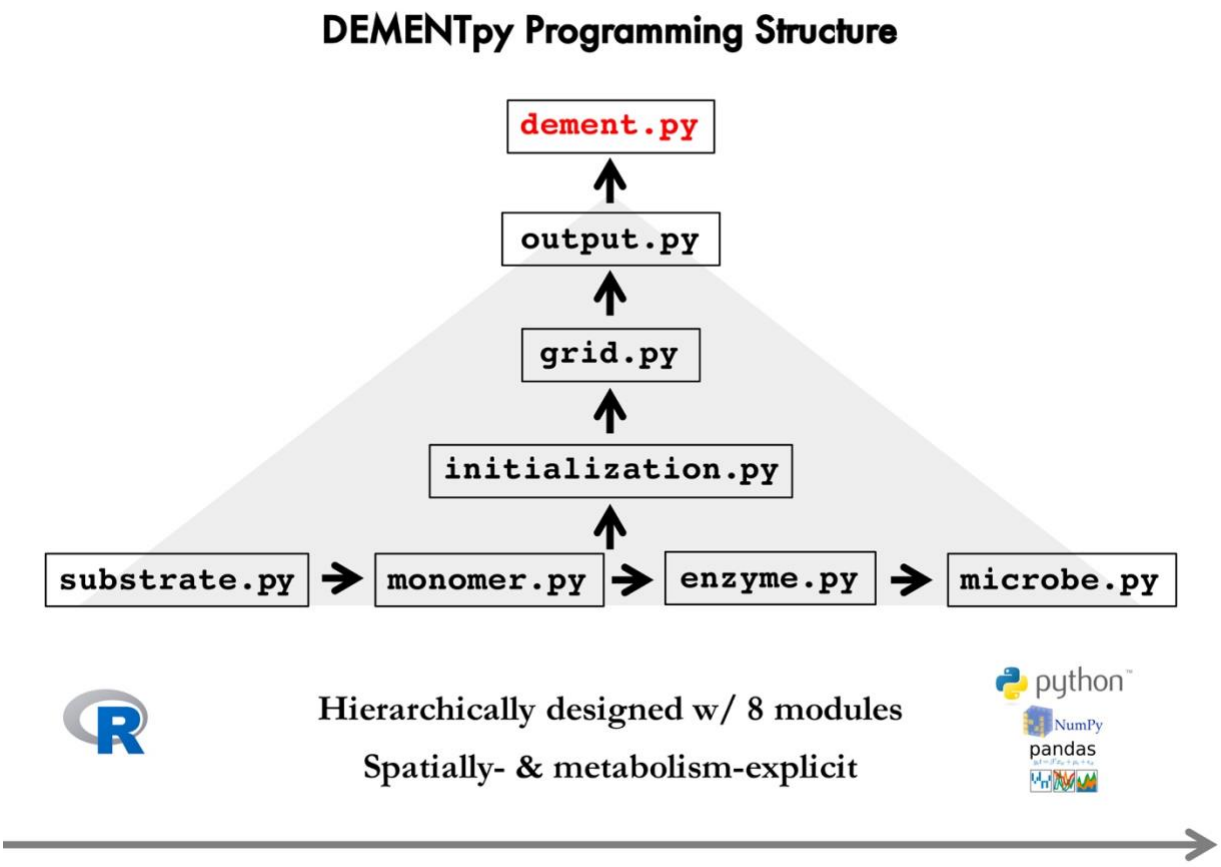

Fig. S7 DEMENTpy programming structure. DEMENTpy emerges from hierarchically restructuring and mechanistically updating DEMENT, which was programmed in R.