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Software notes

NicheMapR – an R package for biophysical modelling: the endotherm model

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Endothermic organisms typically maintain high and relatively constant body temperatures in the face of environmental variation by regulating their metabolic and water loss rates in conjunction with behavioural and postural adjustments. A mechanistic understanding of these processes provides a perspective of the fundamental niches of endotherms by quantifying their energy and water requirements, restrictions on habitat use and survival limits.

Here we introduce and document the endotherm model of NicheMapR, an R package that includes a suite of programs for the mechanistic modelling of energy and mass exchange between organisms and their environments. The NicheMapR endotherm model is based on a Fortran program that simultaneously solves for the metabolic rate, water loss rate, fur/feather temperature and skin temperature required to balance the heat budget in a given microclimate. These calculations are a function of traits relating to insulation, shape, physiological and behavioural responses. The program contains algorithms for computing heat transfer through a porous insulative layer (fur/feathers), including solar and infrared radiation fluxes as well as convective and conductive exchange, and can handle differing dorsal and ventral traits and environments.

Here we configure the program to be called from R as part of the NicheMapR package and describe the model in detail. We break the program into a set of modules that can be run in isolation, or jointly, and combined in different ways to capture species-specific thermoregulatory responses. We explain the theory and underlying subroutines, and the default thermoregulatory settings. We discuss how the model can be adapted to incorporate species-specific behaviours and extended to incorporate multiple body parts. We also compare the endotherm modelling setup with the ectotherm model of the NicheMapR package and discuss how the different modelling strategies they require reflect fundamental biological issues.

Keywords: endotherm, heat budget, biophysical model, mechanistic niche model, thermoregulation, water budget

Introduction

The fundamental niche represents the set of environmental conditions that allow an organism to complete its lifecycle in the absence of competitive interactions, predators

or diseases (Hutchinson 1957, Kearney 2019). The heat budget of an organism is one of the most basic aspects of the fundamental niche. For most terrestrial organisms, this budget is dominated by the energy exchanges at their surfaces through the processes of convection, conduction, radiation and evaporation. As a result, the body temperature of these 'ectothermic' organisms fluctuates with the net external heat flux. However, in endothermic organisms the heat produced by their metabolism is sufficient to raise body temperature substantially above 'ambient' temperature. This enables an endothermic organism to operate under much lower ambient temperatures, but also imposes higher energy costs, thermoregulatory trade-offs and greater sensitivity to overheating (Scholander et al. 1950, Angilletta et al. 2010).

Thermoregulatory processes and constraints can be understood mechanistically using the principles of biophysical ecology, which integrate models of microclimate, heat budgets and thermoregulatory behaviour (Porter et al. 1973, Gates 1980, Porter 2016). This allows the fundamental niche to be computed and mapped to real environments through space and time (Kearney and Porter 2009). The NicheMapR package is a suite of open-source programs for mechanistic niche modelling on the basis of biophysical principles <https://github.com/mrke/NicheMapR>. The NicheMapR microclimate modelling routines were described in Kearney and Porter (2017) and the ectotherm modelling routines were described in Kearney and Porter (2020). These previous papers give a general context of the overall mechanistic niche modelling approach (Kearney and Porter 2009). Here, we provide an overview of the endotherm subroutines in the NicheMapR package. In addition to the information provided here, the NicheMapR package includes vignettes relevant to the endotherm model that provide greater detail on model inputs and outputs (Supporting information).

Overview and history of development

The aim of the endotherm model is to compute the metabolic rate, water loss rate, fur/feather temperature and skin temperature required for an organism to maintain a specified core temperature in a given microclimate based on the organism's morphological and physiological functional traits (Kearney et al. 2021). This is achieved by solving a steady-state (i.e. no storage term) heat budget whereby the net heat generated by the body $Q_{\text{gen,net}}$ less the heat lost from the skin by evaporation Q_{evap} is equal to that passing through the fur Q_{fur} and out to the environment Q_{env}:

$$Q_{\text{gen,net}} - Q_{\text{evap}} = Q_{\text{fur}} = Q_{\text{env}}$$

where

$$Q_{\text{gen,net}} = Q_{\text{gen}} - Q_{\text{resp}}$$

and

$$Q_{\text{env}} = Q_{\text{rad}} + Q_{\text{conv}} + Q_{\text{cond}} + Q_{\text{evap,fur}} - Q_{\text{sol}}$$

so, overall,

$$Q_{\text{gen}} - Q_{\text{resp}} - Q_{\text{evap}} = Q_{\text{fur}} = Q_{\text{rad}} + Q_{\text{conv}} + Q_{\text{cond}} + Q_{\text{evap,fur}} - Q_{\text{sol}}$$

Thus, the heat generated by the body Q_{gen} less the heat escaping from the body via respiration Q_{resp} and via cutaneous evaporation Q_{evap} must be balanced by the net exchange of heat via thermal infrared radiation Q_{rad}, convection Q_{conv}, conduction Q_{cond}, evaporation from the fur $Q_{\text{evap,fur}}$, and heat gained via solar radiation Q_{sol} (Supporting information).

The heat budget calculations assume that the organism comprises a mass of heat generating flesh, potentially surrounded by a fat layer and then a fur (or feather) layer (note we will refer to 'fur' from here onward but the model can be applied to feathers). Three important temperatures in the model are the 'core temperature' T_{C}, characterising the central region of the flesh layer, the 'skin temperature' T_{S}, which is at the interface of the fat and fur layers, and the 'fur–air interface temperature' T_{FA}.

The earliest version of the endotherm model assumed that the temperature gradients between core, skin and the fur–air interface were linear and that fur had a constant thermal conductivity (Porter and Gates 1969). Later versions included distributed heat generation, and hence nonlinear gradients (Porter and Kearney 2009), as well as porous fur and hence fur and radiant thermal conductance values that vary with environment, size, shape (posture) and fur properties (Conley and Porter 1986, summarised in Porter et al. 1994, 2000).

Much of the challenge of modelling endotherm energetics relates to the dynamics of heat movement through the fur, which involves parallel processes of conduction and radiative transport both in and out of the fur layer (Porter et al. 1994). This challenge is enhanced when solar radiation is present and a solution to this problem was not published until relatively recently (Mathewson and Porter 2013), whereby both T_{S} and T_{FA} are simultaneously solved for, given a target core temperature, environment and the set of functional traits required by the model. The derivation of this model was provided in the latter publication and is included here as Supporting information with the inclusion of conductive heat exchange. Supporting information also includes all symbols used in this manuscript, the derivation in Supporting information, and in the code.

The algorithms presented here as part of the `endoR` (and `endoR_devel`) function of the NicheMapR package represent the amalgamation of all these developments, with additional changes to simplify the code and allow flexible implementation. The function therefore permits a calculation of the energy or water costs required to maintain a constant core temperature of specified value in a given environment as a function of air temperature, wind speed, relative humidity, solar and longwave radiation, with the radiation environment and fur/surface area properties potentially varying dorsally and ventrally.

The NicheMapR endotherm model example and structure

The endotherm model is run with the R functions `endoR_devel` and `endoR`. The former is an R script acting as the 'SOLVENDO' subroutine in Fig. 1, which makes separate calls to all the other Fortran subroutines depicted in Fig. 1. The `endoR` function is simply a wrapper for the Fortran equivalent of `endoR_devel` which runs approximately 5–10 times faster because of reduced computational overheads of frequent interfacing between R and Fortran that occur in `endoR_devel`. The utility of the `endoR_devel` function is to allow more rapid coding of the physiological and behavioural configuration of the model in a more accessible language. Once a satisfactory version of `endoR_devel` has been constructed for an organism of interest, the user can modify the `SOLVENDO` Fortran function accordingly if faster performance is required, as described in more detail below.

First, we illustrate and explain the `endoR_devel` function, which represents one of the many possible configurations of the modelling scheme in terms of the thermoregulatory sequence. We then briefly describe what each of the subroutines in Fig. 1 do (see the Supporting information for greater detail). Finally, we provide further examples of the model's application and discuss how the scheme can be modified to accommodate multiple body parts and different physiological and behavioural thermoregulatory responses. For simplicity, we refer to user-defined parameters by name (i.e. as they are defined in the R program), however names, symbols, units and descriptions for all variables, can be found in the Supporting information (XVII Symbols Table).

The simplest operation of `endoR_devel`, with all default settings, at 0°C air temperature is:

```
> library(NicheMapR)
> endo.out <- endoR_devel(TA=0)
> enbal <- as.data.frame(endo.out$enbal)
> treg <- as.data.frame(endo.out$treg)
> masbal <- as.data.frame(endo.out$masbal)
> morph <- as.data.frame(endo.out$morph)
```

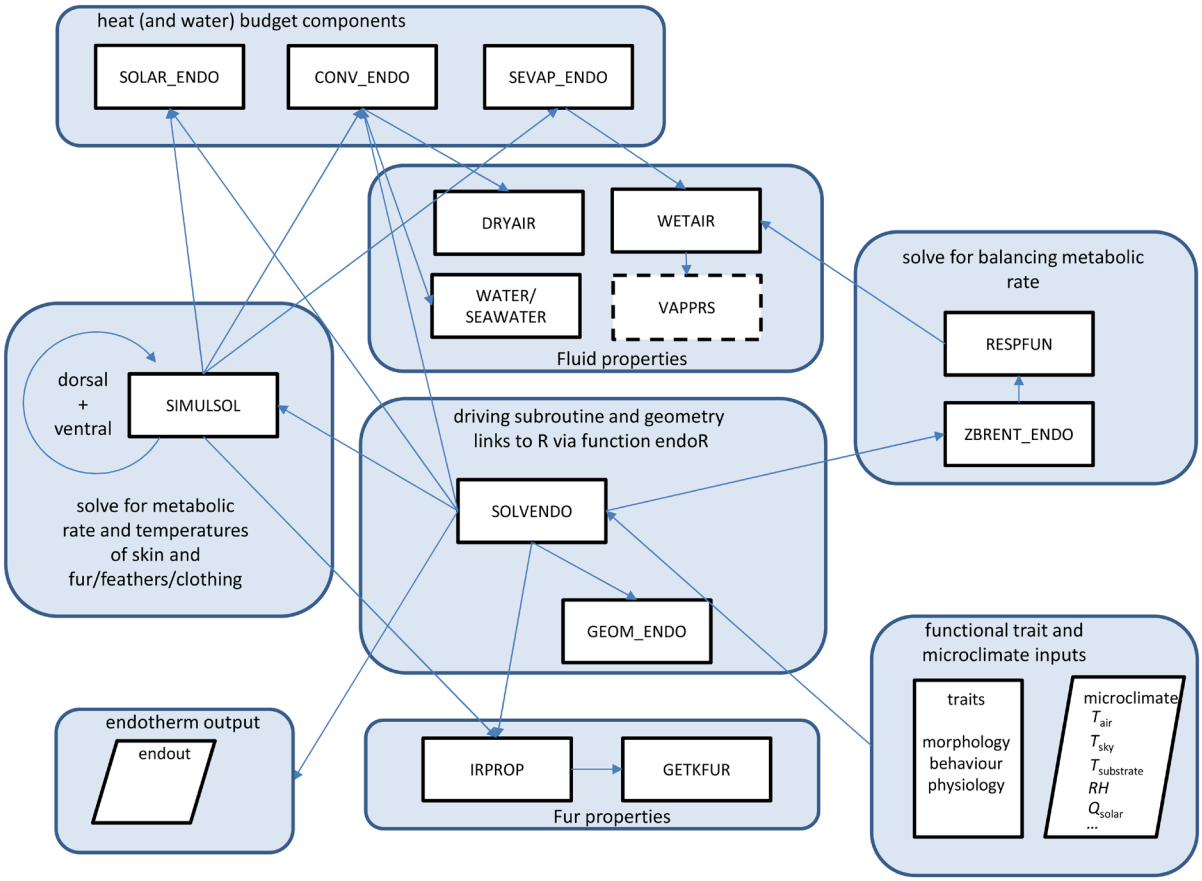

Figure 1. Structure of the Fortran library of the NicheMapR endotherm model and its connection to the R environment. Solid boxes represent Fortran subroutines and dashed boxes represent Fortran functions. Arrows point to routines or functions called by a particular subroutine. The subroutine SOLVENDO is the main driving program, receiving the input data from the `endoR` function via the `SOLVENDO` wrapper, and calling all other subroutines directly or indirectly, and returning the output to R. See main text for further explanation of each subroutine.

These default settings are for a 65 kg ellipsoid-shaped endotherm with a pelt 2 mm in depth and no fat layer, regulating a T_C of 37°C, with ground and sky temperature equal to air temperature, and very low (0.1 m s^{-1}) wind speed and relative humidity (5%) and no solar radiation. That is, it roughly approximates a typical-sized, lightly clothed, resting human in an indoor environment.

The 'enbal' output gives the energy balance components in watts (J s^{-1}) where, in this case, $Q_{sol}=0$, $Q_{cond}=0$, $Q_{ir,in}=272.8$, $Q_{ir,out}=325.1$, $Q_{conv}=42.8$, $Q_{evap}=6.7$ and the metabolic rate $Q_{gen}=101.9$. By default, the minimum possible metabolic rate is based on Kleiber's (1947) general allometric equation for basal metabolic rate of mammals, $Q_{gen}=3.39\ M^{0.75}$, which gives 77.6 W for a 65 kg animal. Thus, the required Q_{gen} to maintain a T_c of 37°C is roughly 1.3 times basal in this case.

The 'treg' output provides computed values of core and lung temperature (the average of core and skin), dorsal and ventral skin and fur/feather–air interface temperatures, posture of the animal (i.e. shape), the level of panting or skin wetness (e.g. sweating/licking), as well as the flesh and fur conductivities. In the example, skin temperature is predicted to be 20.1°C and fur temperature to be 13.4°C.

The 'masbal' output provides computed aspects of the mass balance including the volumes of air and oxygen flowing through the lungs, masses of water lost from the skin and from breathing, and the molar flows of oxygen, nitrogen and air entering and leaving the lungs. In the above example simulation, the animal is predicted to lose 2.1 g H_2O h^{-1} from respiration and 0.75 g H_2O h^{-1} from the skin (i.e. cutaneous water loss).

Finally, the 'morph' output gives various computed lengths, masses, areas and volumes of the organism, including skin and fur/feather surface area, silhouette areas for solar radiation exchange, and the thickness of any fat layer present.

Running the model as above but across a sequence of air temperatures from 0 to 50°C:

```
> TAs <- seq(0, 50)
> endo.out <- lapply(1:length(TAs), function(x){endoR_devel(TA=TAs[x])})
> endo.out.TAs <- do.call("rbind", lapply(endo.out, data.frame))
> enbal <- endo.out.TAs[, grep(pattern="enbal", colnames(endo.out.TAs))]
colnames(enbal)<-gsub(colnames(enbal), pattern="enbal.", replacement="")
> masbal <- endo.out.TAs[, grep(pattern="masbal", colnames(endo.out.TAs))]
colnames(masbal) <- gsub(colnames(masbal), pattern="masbal.", replacement="")
```

and plotting the metabolic rate and total water loss rate we obtained the results of Fig. 2.

The results in Fig. 2 are the outcome of the particular thermoregulatory configuration encoded in the `endoR_devel` function. The logic of this configuration is depicted in Fig. 3a–b, whereby an initial solution of the heat budget is found in terms of the heat generation required to satisfy the energy conservation law given the starting traits and environment. If this solution is found to be greater than the specified minimum possible metabolic rate (which may be basal or resting if the organism is inactive, or above basal if moving, digesting etc.), then the simulation completes. However, if the required metabolic rate is lower than the minimum (and it may even be negative if the heat load is sufficiently high), physiological and/or behavioural changes are required to increase heat loss so that a biologically (and physically) feasible solution can be found. Note that this default sequence starts in a heat-loss minimising posture but does not include

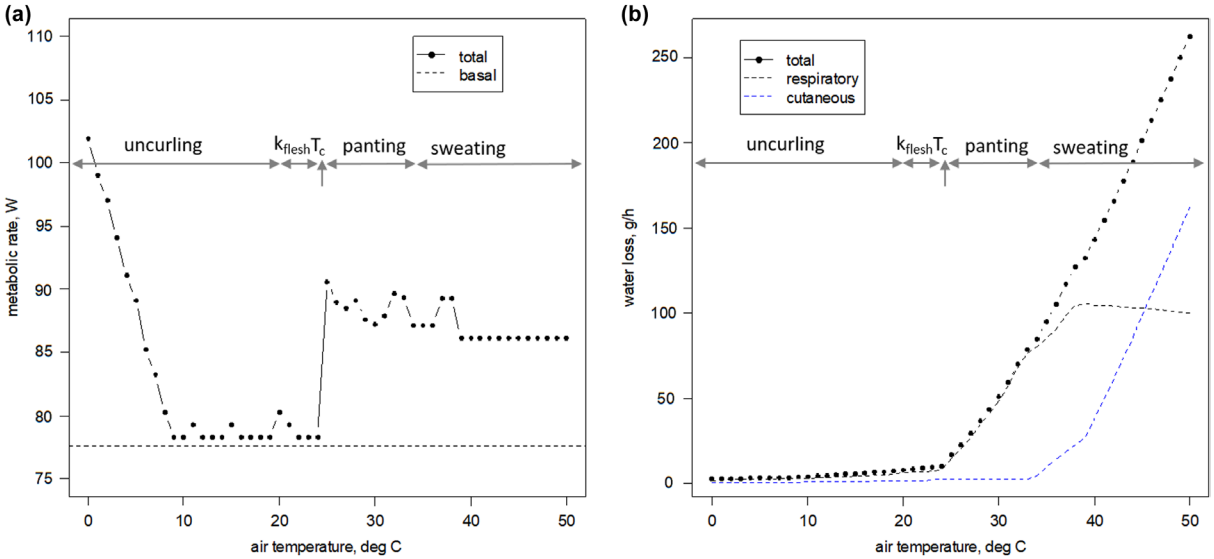

Figure 2. Output of a simulation of the `endoR_devel` function using default settings (65 kg ellipsoid, 2 mm fur) for a sequence of air temperatures from 0 to 50°C under low wind and humidity, showing (a) the metabolic rate and (b) the water loss rate. Annotations indicate the different thermoregulatory responses occurring during the simulation, as explained further in the main text.

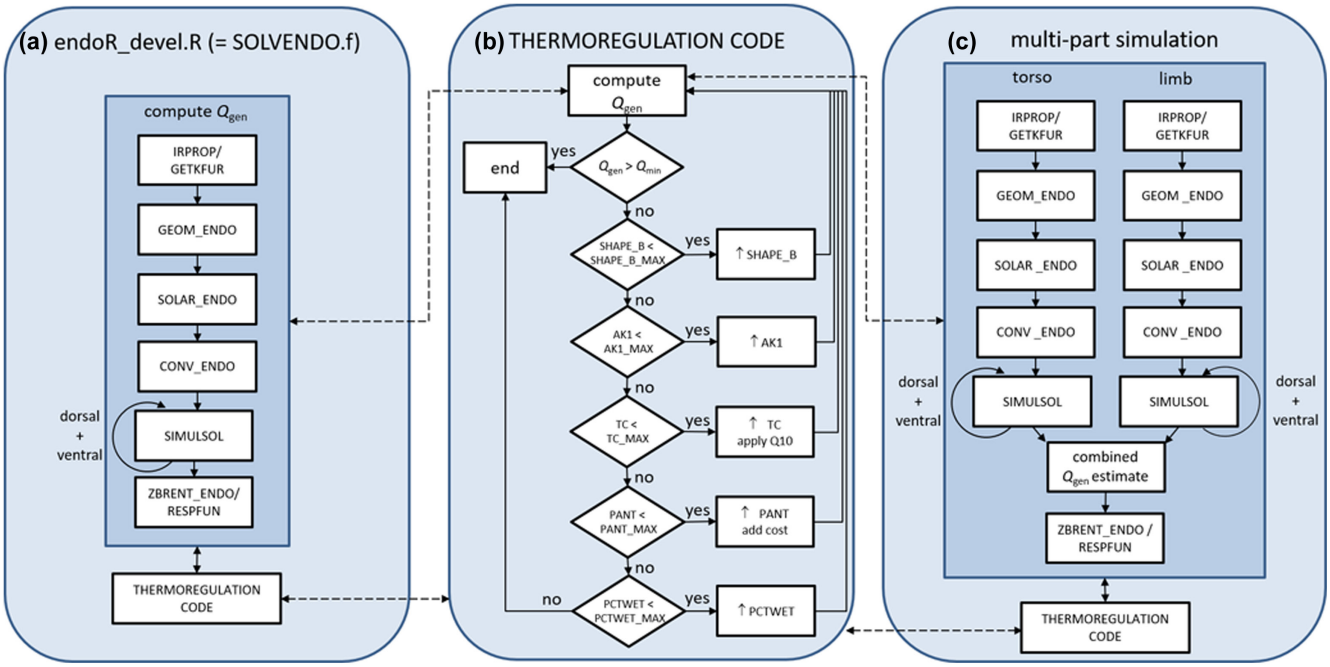

Figure 3. The thermoregulatory scheme of the endoR_devel function showing (a) the overall configuration, (b) the specific thermoregulatory response it assumes (which can be modified by the user) and (c) an example of how the scheme can be modified to including multiple body parts.

possible thermoregulatory responses to cold such as reduced flesh conductivity or piloerection.

In the `endoR_devel` function, the sequence is depicted in Fig. 3 is described in more detail below.

1) *Change posture:* By default, the parameter controlling posture, 'SHAPE_B', is set to 1.1, which means that the long axis of the animal is 1.1 times longer than its short axis. This means the animal starts in a more heat-conserving, 'curled-up' posture; in the example case of an ellipsoid shape it is near spherical. The natural activity posture will often be different to this and, if the SHAPE_B parameter was set to a value of 4, the required metabolic rate for the example above at 0°C would be 142.3 W, i.e. 2× basal. The animal may alter posture as a thermoregulatory response such that surface area is increased relative to volume (e.g. by uncurling). This happened gradually in the above simulation as a first response to heat stress, with the step-size of the change set by the parameter 'UNCURL', the value of which is the amount SHAPE_B is increased each iteration. The maximum ratio allowed is set by the parameter SHAPE_B_MAX which, by default, is set at 5. In the example of Fig. 2, SHAPE_B remained at 1.1 until an air temperature of 9°C, and gradually uncurled from there to the maximum value at 20°C. In Fig. 2, the lower critical temperature (LCT), i.e. the temperature at which the thermoneutral zone (TNZ, i.e. the zone where metabolic rate is near basal and no evaporative water loss is required) starts, is 10°C corresponding to when postural changes are initiated. This LCT would shift to 20°C if SHAPE_B were set to 5.
2) *Increase flesh thermal conductivity:* By default the flesh thermal conductivity, parameter 'AK1', is set to the typical value of 0.9 W m^{-1} $°C^{-1}$ but it is allowed to reach a maximum value 'AK1_MAX' of 2.8 W m^{-1} $°C^{-1}$, with a step-size 'AK1_INC' of 0.1. Increases in flesh conductivity represent changes in peripheral tissue blood flow. This occurred in the simulation of Fig. 2 at an air temperature of 20°C and reached the maximum at 24°C.
3) *Allow core temperature to rise:* As a third response, the target core temperature, set by parameter 'TC' (default 37°C), is allowed to rise to the value of parameter 'TC_MAX' (default 39°C) with a step size set by 'TC_INC' (default, 0.1°C). In Fig. 2 this occurred between 24 and 25°C air temperature. The 'Q10' (default is 2) parameter determines how the change in core temperature affects metabolic rate.
4) *Increase respiratory water loss (pant):* After the sensible ('dry') heat exchange options above are exhausted, the next thermoregulatory step is to use evaporative water loss. The first option in the `endoR_devel` function is to increase respiratory water loss. As described below, the model computes the required air flow through the lungs, given the estimated metabolic rate, atmospheric oxygen levels and oxygen extraction efficiency, to compute respiratory water loss. However, this base level can be increased, via the 'PANT' parameter (default value 1), up to the maximum possible level set by 'PANT_MAX' (default value 10) at a step size set by 'PANT_INC' (default value 0.1). This started at an air temperature of 25°C in Fig. 2 and reached the maximum rate by 34°C air temperature.

A metabolic cost to panting is imposed by the parameter 'PANT_MULT' (default value 1.05) which is a multiplier on the basal metabolic rate which the user should choose to match the metabolic rate at maximum panting level.

5) *Increase cutaneous water loss (sweat/salivate):* Finally, heat may be lost by increasing the cutaneous water loss through changes in the parameter 'PCTWET' (default value 0.5%) which is the percentage of the skin surface area acting like a free-water surface up to the maximum value 'PCTWET_MAX' (default value 100%) at a step size set by 'PCTWET_INC' (default value 0.1%). This started in Fig. 3 at 34°C air temperature and reached 29% by 50°C air temperature.

Underlying subroutines

The sequence of one iteration for the heat budget solution first calls IRPROP, then GEOM_ENDO, SOLAR_ENDO and CONV_ENDO. The SIMULSOL function is then called for the dorsal and ventral sides of the body, followed by a call to RESPFUN via the ZBRENT_ENDO function. We will now provide an abridged explanation for what each of these functions and their dependencies do, with the full details and equations described in the Supporting information.

IRPROP

IRPROP is called by SOLVENDO and SIMULSOL. This subroutine tests for the presence of fur and coordinates the computation of the fur properties needed for computing conduction and longwave radiation through the fur layer. It calls function GETKFUR which holds the governing equations for determining the parameter k_{eff}, the effective conductivity of the fur, from which the overall fur conductivity k_{fur} is later determined. It also returns the average absorption coefficient β. The IRPROP subroutine obtains these properties for the dorsal and ventral sides of the organism, as well as their weighted average based on the user input of the maximum percentage ventral fur. Note that the actual fraction of ventral fur may change as the organism changes from a curled to an uncurled posture, so the user may wish to alter the percentage of ventral fur as part of the thermoregulation code. The IRPROP subroutine also computes the conductivity of compressed fur for computing conduction to the substrate.

GETKFUR

GETKFUR is called by IRPROP. This subroutine takes as input the depth and density of the fur, hair length, diameter and thermal conductivity, and computes k_{eff} and β based on the theory presented in Conley and Porter (1986) as modified from Kowalski and Mitchell (1976). The thermal conductivity of the fur is computed along the horizontal and vertical directions as a weighted mean of air and hair conductivity, the former varying with air temperature in the fur. The longwave radiation absorption coefficient β is computed as a function of the effective hair density.

GEOM_ENDO

GEOM_ENDO is called by SOLVENDO. This subroutine computes various lengths, areas, masses and volumes given the shape chosen, which presently includes a cylinder, sphere, plate or ellipsoid. The relative dimensions for each shape are determined by the input parameters 'SHAPE_B' and 'SHAPE_C' which are ratios between axes of a given shape. These ratios, together with the specified mass and density, and hence body volume, can then be converted by GEOM_ENDO into absolute dimensions for each axis. The user can also specify the percentage of the mass that is fat and then GEOM_ENDO will determine the implied thickness of the subcutaneous fat layer.

For all shapes, the characteristic dimension for convection is assumed to be the cube root of the volume following Mitchell (1976). Also, for all shapes, once skin area is computed, if fur is present the area for evaporative water loss is computed by subtracting the hair area using the weighted average hair properties between the dorsal and ventral sides. Similarly, the area for convection is corrected for the proportion of the area conducting to the substrate.

In addition to using standard geometric formulae to compute surface areas, for the ellipsoid shape one can use empirical functions of surface area. Specifically, if the user parameter 'SAMODE' (default value 0) is set to 1, the skin and feather–air interface surface areas are computed according to empirical formulations for birds (Walsberg and King 1978) that capture the fact that birds have a greater skin surface than feather–air interface surface. Or, if 'SAMODE' is set to 2, the skin surface area is computed according to an empirical relationship for mammals (Stahl 1967).

SOLAR_ENDO

SOLAR_ENDO is called by SOLVENDO and SIMULSOL. This subroutine computes absorbed solar radiation, Q_{sol}, for both the direct (point source) and diffuse (scattered) components reaching the dorsal and ventral halves of the organism. To do this, the solar absorptivities of the dorsal and ventral areas and the associated silhouette and total surface areas are required as input, as well as the direct and diffuse components of solar radiation and the solar absorptivity of the substrate.

CONV_ENDO

CONV_ENDO is called by SOLVENDO and SIMULSOL. This subroutine computes the heat exchange by convection, Q_{conv}, as the sum of the free (driven by surface-free stream temperature difference) and forced (driven by wind speed) components. This requires calculation of the heat transfer coefficient given the characteristic dimension of the organism (computed in GEOM_ENDO) and a set of dimensionless numbers (Nusselt, Reynolds, Schmidt, Prandtl, Grashof) as well as the thermal properties of the fluid. The heat transfer coefficient is determined from different Nusselt–Reynolds correlations for the forced and free components, which are then combined in the final calculation.

This subroutine allows the fluid to be air, fresh water or sea water. The thermal properties of dry air (which depend on temperature and pressure), including thermal conductivity, are computed by a call to the function DRYAIR which is part of the NicheMapR package and is fully described in Tracy et al. (2016). The thermal properties of fresh water and sea water (which depend on temperature) are obtained from the functions WATER and SEAWATER, which hold regressions for how density and thermal conductivity vary with water temperature.

The mass transfer coefficient, for determining cutaneous water loss in subroutine SEVAP_ENDO, is also computed in CONV_ENDO, using the Chilton–Colburn analogy (involving the Schmidt and Sherwood numbers).

SEVAP_ENDO

SEVAP_ENDO is called by SOLVENDO and SIMULSOL. This subroutine computes aspects of evaporative heat loss including the term Q_{evap}, from Eq. 1 above. It takes as input the relative humidity, barometric pressure, air temperature and wind speed, as well as the mass transfer coefficient computed in CONV_ENDO and the skin surface area computed in GEOM_ENDO. The WETAIR subroutine and its sub-function VAPPRS, described in Tracy et al. (2016), is used to compute the skin (saturation) and air vapour densities.

Evaporation may occur from the skin but also from the eyes, if they are assumed to be open, and from the fur or feathers, if wet from rain, licking or other sources. Evaporation from furred/feathered skin can occur via free convection-driven mass transport only, whereas both forced and free convection will drive evaporation from bare skin or from the fur/feather surface. Overall, the percentage of the skin surface area acting as a free water surface is set by the parameter 'PCTWET'. The user input 'PCTBAREVAP' determines the percentage of the free-water surface (not total skin surface) that is bare skin. Thus, the effective area of the skin for evaporation will vary for these different scenarios. For example, with the default settings of endoR_devel, the total skin surface area is 0.7830 m^2 but, after subtracting the area taken up by the hairs, the potential area for cutaneous evaporation is 0.7664 m^2. With the default value for PCTWET of 0.5%, the actual area for cutaneous evaporation is 0.0038 m^2. PCTBAREVAP controls what percentage of the latter area has both forced and free convection-driven mass transport. If the organism is in a state of flight (bird/bat), set by parameter 'FLYHR', it is assumed that forced and free mass transport drive all cutaneous evaporation (i.e. effectively PCTBAREVAP = 100%).

If the eyes are open, an additional amount contributes to non-respiratory evaporation driven by the parameter 'PCTEYES' which is the percent of the surface area taken up by the eyes when open. Finally, the percentage of the fur/feather surface area that is wet is determined by the input 'FURWET' and could be set by the user to a non-zero value e.g. when rain occurs.

The subroutine reports the separate mass losses of water as well as the heat lost by evaporation from the skin/eyes and the fur.

SIMULSOL

SIMULSOL is called by SOLVENDO. This subroutine simultaneously solves for the skin and fur–air interface temperature that balances the heat budget for a non-respiring part of the body, accounting for dorsal and ventral differences and evaporation from the skin. It is the core algorithm of the endotherm model.

There are two sections to this subroutine, one for the case that fur/feathers are present, and one for when the skin is bare. The most complex solution is for when fur is present, as there are three unknowns to solve for (skin and fur–air-interface temperature as well as metabolic rate), as explained in Supporting information. The approach taken in SIMULSOL is as follows (we do not describe the bare skin approach in detail here as it is a simpler version of the approach below):

Step 1. Guess an initial fur–air interface temperature. The first guess is air temperature at animal height.

Step 2. Guess an initial skin temperature. The first guess is core temperature.

Step 3. With the skin and fur–air interface temperature guesses, compute the longwave thermal conductivity of the fur which is used with the effective conductivity of the fur computed by IRPROP to determine the overall fur thermal conductivity.

Step 4. Calculate the fur–air interface temperature from the Eq. 23 in the Supporting information. The fur–air interface temperature guess is used to calculate the convective and radiative heat transfer coefficients needed in Eq. 23, and skin temperature guess is used to estimate Q_{evap}, via calls to CONV_ENDO and SEVAP_ENDO.

Step 5. Adjust the fur–air interface temperature guess, given the new fur thermal conductivity estimate, until it matches up with the fur–air interface temperature calculated by step 4. This is done by first adjusting the starting guess to match the previously calculated value, and calculating another estimate using Eq. 23 in the Supporting information. If that procedure fails to produce convergence within acceptable error bounds, a new iterative guessing procedure is implemented where the new guess is set to the average of the previous and current fur–air interface temperatures calculated in step 4. The final approach is to adjust the guessed value incrementally in the direction of the fur–air interface temperature calculated in step 4 to avoid large jumps, particularly when dealing with evaporation at high temperature.

Step 6. Using the fur–air interface temperature calculation from step 5, calculate $Q_{env} = Q_{rad} + Q_{conv} - Q_{sol} = Q_{gen,net} = Q_{evap}$. This involves also calculating skin temperature using Eq. 14 and 16 in Supporting information to see how it matches the initial skin temperature. If the guess matches the calculated skin temperature values, move on to step 7. If not, adjust the skin temperature guess to match the calculated values and return to step 3. This is done by adjusting the starting guess to match

the previously calculated one and calculating another skin temperature, as in the first step above for the fur–air interface temperature. There is typically convergence on skin temperature within 5–10 guesses and subsequent adjustments on the starting guess.

Step 7. At this point, the fur–air interface temperature guess used to calculate convective and radiative heat transfer coefficient values in the fur–air interface temperature equation, and the skin temperature guess used to calculate Q_{evap}, each match the calculated fur–air interface and skin temperature values at steady state. We can thus calculate the $Q_{gen,net}$, Q_{fur} and Q_{env} for an animal in steady state.

Step 8. Check that 1) the two skin temperature calculations match, within specified tolerance and 2) that $Q_{gen,net} - Q_{evap} = Q_{fur} = Q_{env}$.

RESPFUN and *ZBRENT_ENDO*

`RESPFUN` is called by `ZBRENT_ENDO`, which is called by `SOLVENDO`. `RESPFUN` is a molar balance for computing water loss from breathing, Q_{resp}. It uses the oxygen demand for maintaining a core temperature to compute the amount of air flowing in and out of the lungs and hence the heat lost by evaporation. The user can specify the ambient gas levels so that, for instance, conditions in a burrow can be simulated. The required oxygen consumption rate at standard temperature and pressure is determined from the value of Q_{gen} passed to the function via the `ZBRENT_ENDO` subroutine (below). That value is not permitted to be lower than the user-specified minimum metabolic rate. The actual airflow computed can be modified by the user-specified parameter 'PANT' to allow for enhanced respiratory heat loss via panting as part of the thermoregulatory response.

`ZBRENT_ENDO` is a root finding function (Brent 2002, p. 200) that passes the weighted mean guess of $Q_{gen,net}$ from the `SIMULSOL` calls to `RESPFUN` via the root finding function `ZBRENT` to calculate Q_{resp}. This is done by guessing for a value of Q_{gen} that balances the relationship $Q_{gen,net} = Q_{gen} - Q_{resp}$. This guessing process is needed because Q_{resp} is dependent on total Q_{gen}, not simply $Q_{gen,net}$. Once a suitable value for Q_{resp} is found, it can be added to the value of $Q_{gen,net}$ to determine Q_{gen} and the value of $Q_{gen,net}$ can be checked against the user-provided minimum value to see whether the while-loop can be terminated.

Installation and extensions

The following code will install the NicheMapR package from github:

```
> install.packages('devtools')
> devtools::install_github('mrke/NicheMapR')
>library(NicheMapR)#loadtheNicheMapR package
> get.global.climate() # this will download and unzip a 0.5 GB global monthly climate data
```

All Fortran source code is now included with the package and can thus be compiled locally, producing a shared object 'NicheMapR.dll' (Windows) or 'NicheMapR.so' (OSX or Linux), which contains the microclimate, ectotherm, endotherm and global aerosol database subprograms. A Fortran compiler must be available for R. Rtools <https://cran.r-project.org/bin/windows/Rtools/> will achieve this for Windows, and OSX gfortran must be installed, e.g. via <https://github.com/fxcoudert/gfortran-for-macOS/releases>.

An example of how to run the model as a function of the output of the NicheMapR microclimate model (Kearney and Porter 2017) is as follows, using the default settings that produced Fig. 2, with the results plotted in Fig. 4:

```
> library(NicheMapR)
> loc <- c(131.04, -25.34) # location in decimal degrees, here Uluru, central desert of Australia
> Usrhyt <- 0.5 # height above ground of midpoint of animal, in metres
> maxshade <- 100 # maximum % shade for microclimate simulation
>micro<-micro_global(loc=loc,Usrhyt=Usrhyt, maxshade=maxshade) # get microclimate
>
>metout<-as.data.frame(micro$metout) # unshaded above-ground conditions
> soil <- as.data.frame(micro$soil) # unshaded below-ground soil temperatures
> shadmet <- as.data.frame(micro$shadmet) # shaded above-ground conditions
> shadsoil <- as.data.frame(micro$shadsoil) # shaded below-ground soil temperatures
> dates <- micro$dates
>
> # set environment for simulation
> TAs <- metout$TALOC # air temperatures at height of animal (°C)
> TAREFs <- metout$TAREF # air temperatures at reference height (°C)
> TSKYs <- metout$TSKYC # sky temperatures (°C)
> TGRDs <- soil$D0cm # surface temperatures (°C)
> VELs <- metout$VLOC # wind speeds at animal height (m/s)
> RHs <- metout$RHLOC # relative humidity at animal height (%)
> QSOLRs <- metout$SOLR # solar radiation (W/m2)
> Zs <- metout$ZEN # zenith angle of the sun (degrees)
```

```
> ELEV <- micro$elev # elevation (m)
> ABSSB <- 1 - micro$REFL # substrate solar absorptivity (%)
>
> # run the model
> endo.out <- lapply(1:length(TAs), function(x){endoR(TA=TAs[x], TAREF=TAREFs[x], TSKY=TSKYs[x], TGRD=TGRDs[x], VEL=VELs[x], RH=RHs[x], QSOLR=QSOLRs[x], Z=Zs[x], ELEV=ELEV, ABSSB=ABSSB, SHADE=0)})
```

Further details, code and additional examples are provided in the vignettes 'endotherm model components' (Supporting information) and 'endotherm model tutorial' (Supporting information) included in the package.

Thermoregulatory behaviours can be simulated by incorporating them directly into a customised version of `endoR_devel` and this may include gradual increases in shade levels as implemented with the ectotherm model of NicheMapR. Alternatively, one can run hourly simulations under a range of shade values and then select the optimum level each hour based on predicted energy or water costs. For situations where it is important to be explicit about body parts, the `endoR_devel` function can be reconfigured to separately model each type of body part once and then sum the estimated heat generation before computing the final balance via `ZBRENT_ENDO/RESPFUN`, as illustrated in Fig. 3.

A customised setup of the `endoR_devel` code can be compiled into a stand-alone Fortran library by editing the SOLVENDO.f code accordingly, then compiled with the following code:

```
> cmnd<-"rcmd SHLIB SOLVENDO.f GEOM_ENDO.f CONV_ENDO.f WATER.f WETAIR.f DRYAIR.f SEAWATER.f VAPPRS.f SEVAP_ENDO.f IRPROP.f GETKFUR.f SOLAR_ENDO.f ZBRENT_ENDO.f RESPFUN.f SIMULSOL.f"
> system(cmnd) # run the compilation on windows
> cmnd<-"R CMD SHLIB SOLVENDO.f GEOM_ENDO.f CONV_ENDO.f WATER.f WETAIR.f DRYAIR.f SEAWATER.f VAPPRS.f SEVAP_ENDO.f IRPROP.f GETKFUR.f SOLAR_ENDO.f ZBRENT_ENDO.f RESPFUN.f SIMULSOL.f"
> system(cmnd) # run the compilation on linux
```

and then called within R by modified versions of the `endoR` and `SOLVENDO` functions (this will require the relevant Fortran compilers to be installed for R).

Discussion

The integration of the endotherm model into NicheMapR means that most types of terrestrial animal can now be captured by the package. The ectotherm model of NicheMapR (Kearney and Porter 2020) could be constructed to be generally applicable to a wide range of functionally different species using the same general behavioural algorithm. However, in using the endotherm model we found that it usually required substantial structural changes to accommodate different species, hence our presentation of the model in a modular set up. This pragmatic coding feature also reflects something important about the biological differences between endotherms and ectotherms that ultimately come about because of the greater energetic intensity at which endotherms operate. This is most evident under heat stress, where the strongly non-linear consequences of changes in body temperature on metabolic rate, and any additional heat production associated with panting, cause rapidly escalating positive feedback cycles on heat load. This high sensitivity calls for careful parameterisation in terms of the order and step-size of the behavioural and physiological responses on the part of the programmer, and similarly requires sophisticated neurological control systems on the part of the organism in reality (Tan and Knight 2018). In addition, the greater pace of living in endotherms means that changes in surface areas associated with posture, the particular shapes of limbs, ears and other appendages, orientation and the effects of partial shading of the body, can have substantial consequences.

Specialised configurations of the `endoR` model components will thus not only facilitate its application to a diverse range of taxa but will also help with the interpretation of subtle behavioural and physiological thermoregulatory adaptations via sensitivity analyses. We hope that by providing the `endoR` code in a modular setup, the scientific community that uses it will collectively develop a library of configurations to capture endothermic thermoregulatory diversity. This will require repositories not only for the relevant functional traits (Kearney et al. 2021) but also for the different model configurations.

The endotherm model can readily be connected to energy and water budgets to determine potential for growth and reproduction, as has been done via 'static energy budgets' (Porter et al. 2000, 2006, Kearney et al. 2010, 2016, Briscoe et al. 2016, Lovelace et al. 2020). Future work must also link the endotherm model with the dynamic energy budget (DEB) theory (Kooijman 2010), as has been done with the ectotherm model (Kearney and Porter 2020). This linkage to DEB theory will give a thermodynamically formalised framework for assessing nutritional, life cycle and life history consequences of the heat (and water) budget. The complete integration of microclimate endotherm heat exchange and energy budget models will allow strong inferences to be made about the consequences of past, present and future climatic changes on mammals, birds and other endotherms.

Online resources

The NicheMapR R package source is currently available at <https://github.com/mrke/NicheMapR>, with the latest release at <https://github.com/mrke/NicheMapR/releases> and a website with general information at <https://mrke.github.io/>. For help and discussion, join the Google Group <https://groups.google.com/forum/#!forum/nichemapr>.

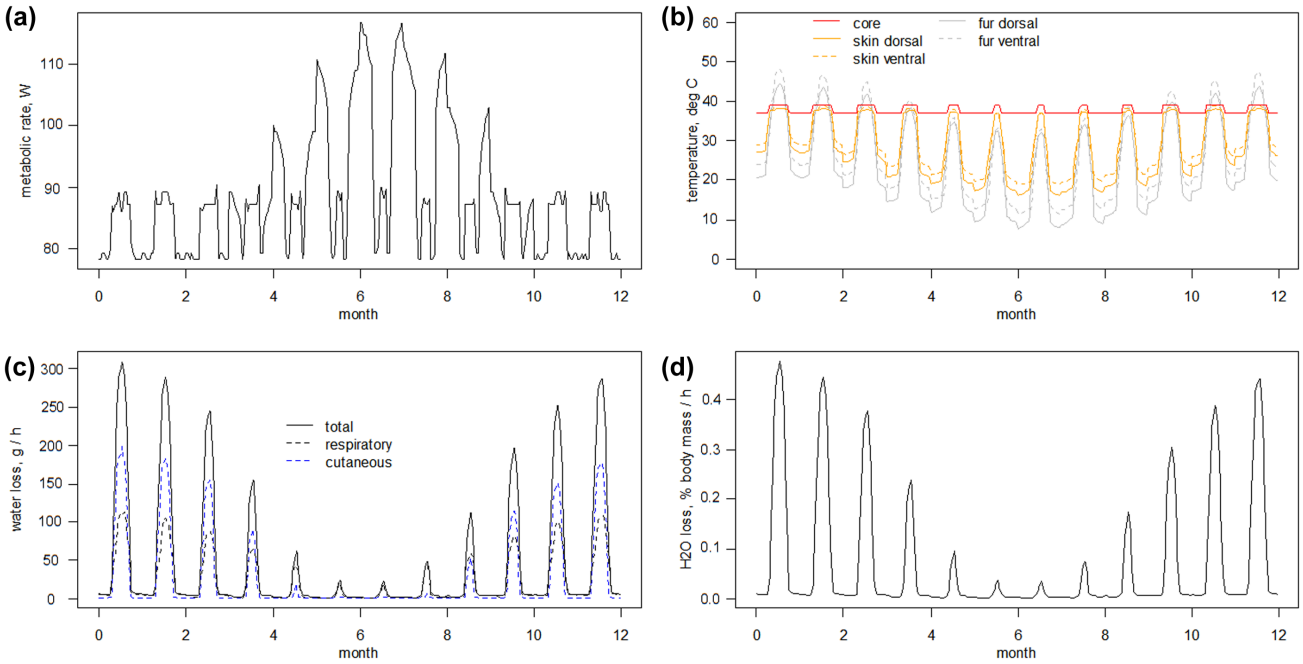

Figure 4. Microclimate model-driven hourly calculations for the typical day of each month (e.g. 0–1 is a typical day in January) of (a) metabolic rate, (b) core, skin and fur temperature, (c) absolute water loss and (d) relative (to body mass) water loss, for a site in central Australia (Uluru). These calculations are for the default animal settings of a 65 kg ellipsoid-shaped animal with 2 mm fur, and are for unshaded conditions. Cold stress is apparent in the winter months (especially May–August) and water requirements reach up to 300 g h^{-1} (~0.5% body mass) in the summer month of January.

To cite NicheMapR or acknowledge its use, cite this Software note as follows, substituting the version of the application that you used for 'version 1.0':

Kearney, M. R. et al. 2021. NicheMapR – an R package for biophysical modelling: the endotherm model. – Ecography 44: XX–XX (ver. 1.0).

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Michael R. Kearney: Conceptualization (equal); Methodology (equal); Software (lead); Validation (supporting); Writing – original draft (lead); Writing – review and editing (lead). **Natalie J. Briscoe**: Conceptualization (supporting); Methodology (supporting); Software (supporting); Validation (supporting); Writing – review and editing (supporting). **Paul D. Mathewson**: Conceptualization (supporting); Methodology (supporting); Software (supporting); Validation (supporting); Writing – original draft (supporting); Writing – review and editing (supporting). **Warren P. Porter**: Conceptualization (equal); Formal analysis (lead); Methodology (equal); Software (equal); Validation (lead); Writing – review and editing (supporting).

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Data availability statement

The Zenodo DOI for the package is: <https://doi.org/10.5281/zenodo.5149309>.

References

Angilletta, M. J. et al. 2010. The evolution of thermal physiology in endotherms. – Front. Biosci. E2: 861–881.

Brent, R. 2002. Algorithms for minimization without derivatives. – Dover Publications.

Briscoe, N. J. et al. 2016. Unpacking the mechanisms captured by a correlative species distribution model to improve predictions of climate refugia. – Global Change Biol. 22: 2425–2439.

Conley, K. E. and Porter, W. P. 1986. Heat loss from deer mice *Peromyscus*: evaluation of seasonal limits to thermoregulation. – J. Exp. Biol. 126: 249–269.

Gates, D. M. 1980. Biophysical ecology. – Springer.

Hutchinson, G. E. 1957. Concluding remarks. – Cold Spring Harb. Symp. Quant. Biol. 22: 415–427.

Kearney, M. R. 2019. The fundamental niche concept connects individuals to populations: a comment on Angilletta et al. – Integr. Comp. Biol. 59: 1509–1510.

Kearney, M. R. and Porter, W. P. 2009. Mechanistic niche modelling: combining physiological and spatial data to predict species' ranges. – Ecol. Lett. 12: 334–350.
Kearney, M. R. and Porter, W. P. 2017. NicheMapR – an R package for biophysical modelling: the microclimate model. – Ecography 40: 664–674.
Kearney, M. R. and Porter, W. P. 2020. NicheMapR – an R package for biophysical modelling: the ectotherm and dynamic energy budget models. – Ecography 43: 85–96.
Kearney, M. R. et al. 2010. Correlative and mechanistic models of species distribution provide congruent forecasts under climate change. – Conserv. Lett. 3: 203–213.
Kearney, M. R. et al. 2016. An estimate of the water budget for the endangered night parrot of Australia under recent and future climates. – Clim. Change Responses 3: 14.
Kearney, M. R. et al. 2021. Where do functional traits come from? The role of theory and models. – Funct. Ecol. 35: 1385–1396.
Kleiber, M. 1947. Body size and metabolic rate. – Physiol. Rev. 27: 511–541.
Kooijman, S. A. L. M. 2010. Dynamic energy budget theory for metabolic organisation. – Cambridge Univ. Press.
Kowalski, G. J. and Mitchell, J. W. 1976. Heat transfer from spheres in the naturally turbulent, outdoor environment. – J. Heat Transf. 98: 649–653.
Lovelace, D. M. et al. 2020. Modeling dragons: using linked mechanistic physiological and microclimate models to explore environmental, physiological and morphological constraints on the early evolution of dinosaurs. – PLoS One 15: e0223872.
Mathewson, P. D. and Porter, W. P. 2013. Simulating polar bear energetics during a seasonal fast using a mechanistic model. – PLoS One 8: e72863.
Mitchell, J. W. 1976. Heat transfer from spheres and other animal forms. – Biophys. J. 16: 561–569.
Porter, W. P. 2016. Heat balances in ecological contexts. – In: Johnson, E. A. and Martin, Y. E. (eds), A biogeoscience approach to ecosystems. Cambridge Univ. Press, pp. 49–87.
Porter, W. P. and Gates, D. M. 1969. Thermodynamic equilibria of animals with environment. – Ecol. Monogr. 39: 227–244.
Porter, W. P. and Kearney, M. R. 2009. Size, shape and the thermal niche of endotherms. – Proc. Natl Acad. Sci. USA 106: 19666–19672.
Porter, W. P. et al. 1973. Behavioral implications of mechanistic ecology – thermal and behavioral modeling of desert ectotherms and their microenvironment. – Oecologia 13: 1–54.
Porter, W. P. et al. 1994. Endotherm energetics: from a scalable individual-based model to ecological applications. – Aust. J. Zool. 42: 125–162.
Porter, W. P. et al. 2000. Calculating climate effects on birds and mammals: impacts on biodiversity, conservation, population parameters and global community structure. – Am. Zool. 40: 597–630.
Porter, W. P. et al. 2006. Po'ouli landscape bioinformatics models predict energetics, behavior, diets and distribution on Maui. – Integr. Comp. Biol. 46: 1143–1158.
Scholander, P. F. et al. 1950. Adaptation to cold in arctic and tropical mammals and birds in relation to body temperature, insulation and basal metabolic rate. – Biol. Bull. 99: 259–271.
Stahl, W. R. 1967. Scaling of respiratory variables in mammals. – J. Appl. Physiol. 22: 453–460.
Tan, C. L. and Knight, Z. A. 2018. Regulation of body temperature by the nervous system. – Neuron 98: 31–48.
Tracy, C. R. et al. 2016. Properties of air: a manual for use in biophysical ecology, 5th edn. – <https://mrke.github.io/NicheMapR/inst/doc/properties-of-air>.
Walsberg, G. E. and King, J. E. 1978. The relationship of the external surface area of birds to skin surface area and body mass. – J. Exp. Biol. 76: 185–189.