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An explicit and computationally efficient method to initialise first-order-based soil organic matter models – the Geometric Series Solution (GSS)

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Abstract

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This paper derives an algebraic solution (the Geometric Series Solution; GSS) to replace iterative runs of soil organic matter (SOM) models for initialisation of SOM pools. The method requires steady-state / long-term-average series of plant input and soil climate driving data. It calculates the values of SOM pools as if SOM models are iterated for a large number of cycles. The method has a high computational efficiency because it is an explicit solution to the calculations used to initialise the model and so requires a single iteration of the SOM model. Under the premise that the iterative pool inputs can be derived analytically, the GSS equations are applicable for other first-order-based SOM models. To illustrate applicability the method is applied to the coupled JULES-ECOSSE model.

10 Keywords: Algebraic method, Model initialisation, Soil organic matter (SOM), Spin-up,

the ECOSSE model, the JULES model

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2 1. Introduction

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Process-oriented, multi-compartment models of soil organic matter (SOM) are useful tools for studying the impact of global change on SOM. The majority of SOM models, including the CENTURY (Parton et al., 1988), ECOSSE (Smith et al., 2010a), RothC (Jenkinson, 1990) and Yasso (Liski et al., 2005) models, are based on model compartments (pools) with first-order decomposition kinetics. The defining characteristic of these is that the rate of decomposition of each SOM pool is described as a first order reaction:

$$dS/dt = -kS \tag{1}$$

in which S represents the amount of organic matter in the pool (kg m⁻²) and k is a decomposition rate constant (s⁻¹). Integrating over a time-step of length Δt , the pool size is updated as:

$$S(t + \Delta t) = [I + S(t)] \exp(-k_0 \Delta t \prod_i f_i(X_i))$$
(2)

in which I is the material input to the pool over the time-step (kg m⁻²) and the rate constant is expressed as a standard value k_0 which is adjusted by dimensionless functions f_i of time-or space-varying environmental variables X_i (e.g. soil temperature and moisture).

Initialisation of the SOM pools is an important step in any modelling study and is a non-trivial process. Incorrect initialisation can result in spurious trends when the model is run forward from the initial state. Early papers describing SOM models (Liski et al. (2005), Jenkinson (1990), Parton et al. (1988)) did not focus on spin-up techniques. Only recently have studies suggested numerical methods to address the issue (e.g. Thornton and Rosenbloom (2005), Lardy et al. (2011), Xia et al. (2012)). There are two important issues that users of SOM models need to be aware of. Firstly, the pools in most SOM models are conceptual. Although it is possible to relate the initial states of the pools to physical

measurements, as illustrated by Zimmermann et al. (2007), such data are often not available,
particularly for large-scale studies (Yeluripati et al., 2009). Secondly, first-order based SOM
models have an in-built tendency to establish an equilibrium state in which inputs to each
pool balance losses. When the pools are not at equilibrium they will tend to move towards
equilibrium despite constant driving data (e.g. climate). Such transient changes can be difficult to interpret and may obscure the underlying behaviour in studies of the response of
SOM to environmental change and so the assumption that the initial state is in equilibrium
is commonly used. Despite this, the steady-state assumption can be challenged (e.g. Wutzler
and Reichstein (2007)) since soils experience legacy effects for decades or even centuries after
an external change.

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In practical terms, the most common approaches used to bring C and N pools to steady 36 state are to use a long run of the model so as to allow the pools to approach equilibrium 37 (Lardy et al., 2011) or to fit the model pool sizes iteratively. The first approach requires a model simulation of hundreds to thousands of years for recalcitrant SOM pools (Wutzler and Reichstein, 2007) due to the slow rate constant. Because reliable driving data (e.g. meteorology) are rarely if ever available for hundreds of years, modelers commonly cycle repeatedly through a shorter time series of driving data (e.g. a single year of long-term average climate data). Increasingly, SOM models are being coupled with climate and land surface models 43 to explore environmental changes in the coupled land-atmosphere system. These models are often run on high temporal resolutions (e.g. sub-daily time-steps) and, for land surface models, high spatial resolution (e.g. 1km²). This is computationally demanding, even with modern computer technology, making it all the more important to identify computationally efficient methods for model initialisation.

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To reduce the demand for computational resources, Thornton and Rosenbloom (2005) suggest the Accelerated Decomposition method in which decomposition rate constants can

be linearly scaled to allow a faster turnover of SOM pools. Lardy et al. (2011) and Xia et al. (2012) analytically derive a set of equations and apply matrix-based formulation to accelerate iteration of SOM models. It is reported that these methods can reduce the computational time to 63%-96% dependent on the model set-ups and levels of acceptable errors. Despite the reduction in computational time, there is still a demand for continuing research because (1) the published methods are mainly approximation schemes that either require extra error analysis or require some more iterations to close the difference between the approximate results and the exact steady-state; (2) the published methods are implicit methods and the form of relationship between the inputs (e.g. plant inputs, soil climate data) and the outputs (i.e. steady-state SOM pool sizes) is not revealed. To derive an explicit solution to initialisation, this paper uses two assumptions (listed below) and applies algebra to derive the Geometric Series Solution (GSS) method. The GSS method has a high computational efficiency because it requires only a single iteration of the SOM models to solve the steadystate pool sizes without approximation. To illustrate the application of the method, results from a particular model are provided, but we emphasise that the method can be more widely applicable. The two assumptions are: 67

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Assumption 1 Other parts of the model (e.g. plant inputs to the soil) are prescribed as fixed series so as to avoid the extra complications introduced if those inputs are themselves a function of SOM. This assumption implies that the GSS method is not yet applicable for studies of combined initialisation of SOM and vegetation (see Hashimoto et al. (2011)).

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Assumption 2 When SOM models achieve steady-state (i.e. flows between pools become a fixed series), the model architecture allows derivation of input series to each pool from plant inputs.

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78 2. Methods

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2.1. Model description and analytical derivation of pool inputs

processes provide the key inputs required by the SOM models.

In this paper we develop and illustrate the method using the JULES-ECOSSE model,
which couples a land surface model (JULES) with a model of SOM (ECOSSE). The land
surface model simulates the temperature and water state of the soil and vegetation and provides the SOM model with estimates of the inputs of C and N to the soil. The SOM model
then simulates the turnover of C and N in the soil, and the emissions of greenhouse gases
(including carbon dioxide, nitrous oxide and methane) from the soil. Brief details of both
models are provided here.

The Joint UK Land Environment Simulator [JULES, Best et al. (2011), Clark et al. (2011)] is a process-based model that simulates the fluxes of carbon, water and energy between the land surface and the atmosphere, and also describes subsurface fluxes of heat and moisture in the soil. JULES represents the land surface as nine land cover types, including five plant functional types, and applies a multi-layer canopy scheme for light interception, a coupled scheme of leaf photosynthesis and stomatal conductance, and growth and population dynamics among the plant functional types. The process-based descriptions of key ecological

The Estimation of Carbon in Organic Soils - Sequestration and Emissions model (ECOSSE) is based on the four-pool scheme of the RothC model (Jenkinson, 1990) and adds nitrogen components, simulation of methane, dissolved organic carbon (DOC) and dissolved organic nitrogen (DON), and more detailed representations of SOM dynamics in organic soils. Detailed descriptions of ECOSSE can be found in Smith et al. (2010a,b).

The four-pool scheme includes pools of decomposable and resistant plant materials (DPM and RPM), biomass (BIO) and humus (HUM). Each pool has both carbon and nitrogen com-

ponents which are linked by parameterized carbon-nitrogen ratios. The defining characteristic 105 of each pool is its specific decomposition rate constant in Table 1. The decomposition at 106 each time-step is a first-order process (Equations (1) and (2)) with the amount of decom-107 position depending on the decomposition rate constant and environmental rate-modifying 108 factors including soil temperature, soil moisture, soil oxygen level and soil pH. All decompos-109 ing fractions of the pools become decomposing materials (D). For carbon components, the decomposing materials are partitioned into respired soil CO₂ and CH₄ fluxes, leached DOC 111 or immobilized to BIO and HUM pools. The simplified four-pool scheme are illustrated in 112 Fig. 1. As the organic carbon and nitrogen components of each SOM pool are linked by 113 parameterized carbon-nitrogen ratios in the model, the nitrogen pools can be initialised from 114 the initial carbon pools.

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Table 1: Default values of pool-specific decomposition rate constants of SOM pools. The pools are decomposable and resistant plant material (DPM, RPM), biomass(BIO) and humus(HUM).

		DPM	RPM	BIO	HUM
pool-specific decomposition rate constant (year ⁻¹)	(k_0)	10.00	0.30	0.67	0.02

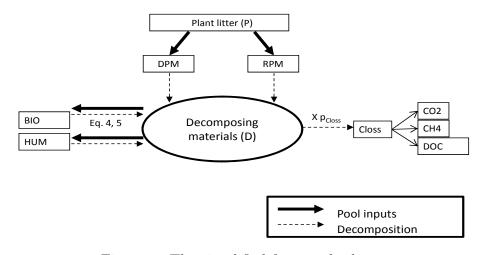


Figure 1: The simplified four-pool scheme

In a steady state, the inputs to each pool can be derived analytically from the (steady-

state) inputs of plant material. The DPM and RPM pools are augmented directly by the incoming plant materials (P). The partition of P between the DPM and RPM pools is described by a constant parameter which only depends on plant functional type (and hence is constant for steady-state plants).

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It takes more analytical steps to find the steady-state inputs to BIO and HUM pools 125 because, as well as been augmented by decomposition of DPM and RPM, decaying BIO and HUM creates fresh BIO and HUM. More SOM in the BIO and HUM pools results 127 in greater amounts of decomposing materials, which in turn cause higher inputs to these 128 pools. To derive the final steady-state inputs to these pools we note that the ECOSSE 129 model is structured so as to partition decomposing materials into carbon lost (C_{loss}) to the 130 environment as CO_2 , CH_4 or DOC and carbon immobilized ($C_{immobilized}$) to the BIO and 131 HUM pools. The partition ratio (E) between C_{loss} and $C_{immobilized}$ is a function of soil clay 132 percentage (clay) which is an input to the model and generally is assumed to be constant in 133 time. 134

$$E = \frac{C_{loss}}{C_{immobilized}} = 1.67 \times (1.85 + 1.6 \times e^{-0.000786 \times clay})$$
 (3)

We define the ratios of C_{loss} and $C_{immobilized}$ with respect to decomposing materials (D) as

$$p_{Closs} = \frac{C_{loss}}{D} = \frac{E}{1 + E} \tag{4}$$

$$p_{C_{immobilized}} = \frac{C_{immobilized}}{D} = 1.0 - p_{Closs} = 1.0 - \frac{E}{1 + E}$$

$$(5)$$

Based on empirical work, a constant ratio (X) is used to partition the immobilized carbon that goes into the BIO $(C_{immobilized_{BIO}})$ and HUM pools $(C_{immobilized_{HUM}})$:

$$X = \frac{C_{immobilized_{BIO}}}{C_{immobilized_{HUM}}} = 0.85 \tag{6}$$

We now make use of the definition of a steady state, namely that the input of plant materials (P) balances C_{loss} , so that Eq. 4 can be rearranged to find D in terms of the known P and P_{Closs} . The time series of $C_{immobilized}$ can then be calculated by rearranging Eq. 5 and finally the time series of inputs to the BIO and HUM pools can be derived by partitioning $C_{immobilized}$ using X.

In summary, the structure of the JULES-ECOSSE model allows steady-state series of pool inputs analytically derived from plant inputs. This allows the derivation of the GSS method in Section 2.2.

48 2.2. The Geometric Series Solution Method

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As discussed previously, the iterative method for initialisation requires the SOM model to be run for a large number of cycles with a given set of input data. This procedure is illustrated on the left of Fig. 2. The proposed GSS method (on the right of Fig. 2) replaces the iteration by first calculating the steady-state pool inputs and then applying the GSS equations (described below).

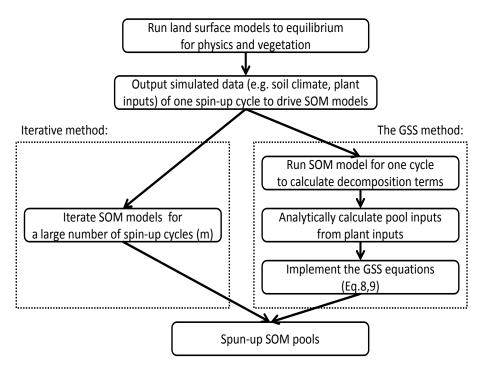


Figure 2: The comparison of steps between the iterative method and the GSS method

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As the aim of the GSS method is to reproduce the results of the iterative method with less computational expense, the derivation of the GSS equation takes the results of an iterative run as the starting point. The derivation below is for any one pool and we will consider mcycles each of n time-steps. A value for time-step j in cycle i is indicated by subscripts i,j. Considering the fate of the incoming material that is input during the first time-step of the first cycle $(I_{1,1})$, the part of the inputs that remains undecomposed after the first time-step is $I_{1,1} \exp(-k_{1,1})$, where $k_{1,1}$ is the decay coefficient given the environmental conditions for that time-step. Each time-step adds a further exponential term, so that by the end of the first cy-163 cle (after n time-steps) the part of $I_{1,1}$ that remains undecomposed is $I_{1,1}e^{-k_{1,1}}e^{-k_{1,2}}\dots e^{-k_{1,n}}$.

At the end of the first cycle, the inputs from any time-step j which have not decomposed 166 are $I_{1,j}e^{-k_{1,j}}e^{-k_{1,j+1}}\dots e^{-k_{1,n}}$. Table 2 illustrates the terms across m cycles. 167

Table 2: Undecomposed pool inputs at the completion of an iterative run. Rows denote the spin-up cycles i = 1, m while columns describe the time-steps j = 1, n within a cycle. Further details are in the text.

In Table 2, rows (and the first subscript on terms) represent the i^{th} spin-up cycle, while columns (and the second subscript) represent time-steps within a cycle. Each entry can be broken down into a head and a tail. The head $(I_{i,j})$ represents the input to the pool during a given time-step, while the tail $(e^{-k_{i,j}}e^{-k_{i,j+1}}\dots e^{-k_{mn}})$ represents the decomposition terms associated with the input from its entry until the end of the spin-up run.

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For any time-step j, when the spin-up run is complete after m cycles the contribution to the remaining SOM is found by summing the terms in column j. Because the inputs and the environmental conditions that affect decomposition are the same for every cycle (i.e. $I_{i,j} = I_{l,j}$ and $k_{i,j} = k_{l,j} \, \forall i$ and l), the subscript i can be dropped.

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For any time-step (i.e. column in Table 2), the sum of the column (C_i) is

$$C_{j} = I_{j}(e^{-k_{j}}e^{-k_{(j+1)}}\dots e^{-k_{n}})(1 + e^{-k_{a}} + e^{-2k_{a}} + \dots + e^{-(m-1)k_{a}})$$

$$(7)$$

where $e^{-k_a} = e^{-k_1}e^{-k_2}\dots e^{-k_n}$ represents the decomposition across a full cycle.

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The sum of exponential terms in the final bracketed term in Eq. 7 is an exponential series

$$e^{-k_a} + e^{-2k_a} + \dots + e^{-(m-1)k_a} = \frac{(1 - e^{-mk_a})}{(1 - e^{-k_a})} - 1$$
(8)

, as proved in Appendix A. Substituting into Eq. 7 gives

$$C_j = I_j(e^{-k_j}e^{-k_{(j+1)}}\dots e^{-k_n})(1 - e^{-mk_a})/(1 - e^{-k_a})$$
(9)

To recap, C_j is the amount of material input during the j^{th} time-step of each spin-up cycle that remains in the pool after m cycles.

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The sum of all columns represents the SOM in the pool at the end of the spin-up run:

$$S_{\text{final}} = \sum_{j=1}^{n} C_j \tag{10}$$

In summary, to calculate the final SOM in a pool the GSS method requires an array of the inputs to the pool at each time-step in a cycle $(I_1, I_2, ..., I_n)$ and the associated decomposition terms $(e^{k_1}, e^{k_2}, ..., e^{k_n})$. For each time-step j = 1, n, Eq. 9 is used to sum all undecomposed pool inputs across all spin-up cycles, then Eq. 10 gives the final value of the pool at the end of the spin up run. The m cycles each of n time-steps required by the 'brute force' iterative method is replaced in the GSS method by a single cycle from which the input and decomposition terms are saved and then used in Eq. 10.

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5 3. Applications and illustrative results

196 3.1. Data

To illustrate the application of the GSS method this paper uses a simulation by the JULES-ECOSSE model forced by an updated version of the WATCH Forcing Data (Weedon et al., 2011) which provides the meteorological data required by JULES. A single year of meteorological data averaged over all cells in the United Kingdom is used. For present purposes JULES and ECOSSE are run with one-way coupling, i.e. JULES calculates the state of the 'physical' environment and passes this information to ECOSSE, with no feedback from ECOSSE. The steps of the process are:

- 1 Spin up the physics and vegetation of JULES to steady state. This defines the time series of steady-state plant inputs (P) to the soil, one value for every timestep in the year.
- ²⁰⁷ 2 Calculate the time series of steady-state inputs to each pool (I). For the DPM and RPM pools these are simple fraction of P. For the BIO and HUM pools the inputs are calculated using Equations (4) to (6).
- 3 Calculate the exponential terms for each timestep, describing how environmental conditions modify the decomposition rate (see Eq. (2))
- 4 Apply Equations (9) and (10) to calculate the SOM in each pool at steady state.

3.2. Results

The fast reaction rate constants allow the DPM and BIO pools to spin up quickly, even in
the iterative run, meaning that relatively little time is saved for those pools by using the GSS
method. The real advantage of the GSS method is for the more slowly-evolving RPM and,
particularly, HUM pools. The HUM pool takes more than 200 years to reach equilibrium, so
the GSS method saves at least 200 repetitions of the model when compared to the iterative
method in this example. The spin-up results by the iterative method and the GSS method

are compared for RPM and HUM pools in Fig. 3. Both pools are assumed to be zero at the beginning of the spin-up process.

In this examples JULES was driven by repeating the single year of meteorological data until the vegetation and soil physical state had reached equilibrium. The data from JULES were then fed into ECOSSE which was spun up using both the iterative and GSS methods. The resulting estimates of the pools are shown in Fig. 3 in which the solid lines represent the amounts of SOM after different numbers of spin-up cycles (each one year long) from the iterative run, while the triangles represent discrete results of the GSS method (with the value of m increasing with time).

For the RPM pool, the results between the two methods match at any point of spin-up cycle (including both equilibrium and non-equilibrium stages). For the HUM pool, the results converge when the number of spin-up cycle increases. The underlying reasons are that the steady-state pool inputs to RPM are simply a part of the constant plant inputs whereas the inputs to the HUM pool need to run for a number of cycles (approximately 250 cycles in this example) to become stable (see Section 2.1). As the GSS method is used to find the equilibrium values of SOM pools, the divergence between the methods at the earlier cycles does not affect the equilibrium results. However, users should be aware of this characteristic and set m to suitably large values (e.g. m = 1000 cycles) when the GSS method is applied.

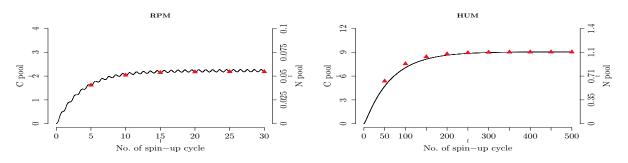


Figure 3: Values of SOM pools (kgC/Nm^{-2}) modeled by the iterative method (solid line) and the GSS method (triangle). Left: RPM pool; Right: HUM pool.

As a further test the pools calculated by the GSS method for m=1000 were used to initialise a further run of the model, which was then analysed using the additive time series model $x_t = m_t + s_t + z_t$ in which m, s and z represent trend, seasonal and random error components respectively and Subscript t is time-step. The seasonal component was found to account for all of the variation of SOM, while there was no trend even for the HUM pool, confirming that the GSS method had correctly spun up the pools to equilibrium.

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4. Discussion & Conclusion

Many papers describing SOM models (e.g. Liski et al. (2005); Jenkinson (1990); Parton 251 et al. (1988)) do not describe initialisation methods in detail. Different methods have been 252 used to initialise the SOM pools and, without explicit proof of the methods and their suitabil-253 ity, errors introduced from the initialisation can eventually interfere with the interpretation of 254 model results. It is only relatively recently that studies have appeared that explicitly address 255 the issue of spin up (e.g. Thornton and Rosenbloom (2005); Lardy et al. (2011); Xia et al. 256 (2012)). Different modelling teams use different techniques because model structures differ 257 and the models are executed under different assumptions and for different purposes. With 258 this background, there is an ongoing need to explore and expand the available methods, and 259 possibly to seek a small set of methods that are generally applicable. 260

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The main characteristics of the GSS method is the application of the explicit equations (Equations (9) and (10)). This reveals the form of relationship between the values of the spun-up pools and the driving determinants (i.e. series of pool inputs and soil climate). The explicit equations allow high computational efficiency: (1) it does not require alteration of the science encoded in a model; (2) it does not involve complicated numerical methods; (3) it requires only that Equations (9) and (10) are implemented, which can be done in around 50 lines of code; (4) the reduction in computational resource use is probably maximal as

the method requires a single iteration of the SOM model; (5) as the GSS method is not an approximation scheme of the types suggested by Lardy et al. (2011) and Xia et al. (2012), it does not require error analysis. The derivation of the equations (Equations (9) and (10)) is not model-specific and the equations are applicable to first-order-based (Equation (1)) SOM models. The general applicability of this method depends on whether a model structure allows iterative pool inputs to be derived from other known values. In Section 2.1 it is shown that the JULES-ECOSSE model satisfies this requirement. This is mainly a consequence of the use of non-time-varying ratios to partition plant inputs and decomposing SOM in the model, which might also hold for other SOM models.

As described, the GSS method only describes the spin up of SOM pools and assumes that the vegetation (and hence plant inputs) are in a steady state. The simultaneous initialisation of both SOM and vegetation is complicated by the close two-way coupling between those components. The assumption of steady-state plant inputs might not hold in modelling studies that consider the influence of nitrogen limitation on plant growth during the spin-up stage. We recommend further research into how to relax the requirement for steady-state plant inputs and the combined initialisation of SOM and vegetation (see Hashimoto et al. (2011)).

Of course no method for model initialisation can guarantee that the SOM amounts in the spun-up state will closely match those measured at any given site. Amongst other possible sources of error, simplified model representation of the science and the quality of the input data can both affect results. Aside from those, care is also required to ensure that the environmental conditions (e.g. meteorology) assumed during the spin-up are representative of a long term average. For example, if a hotter-than-average year is chosen for the spin-up data this will tend to result in faster SOM turnover and under-estimated values of SOM pools. In most cases a multi-year average of meteorological data should be used to improve 296 representativeness.

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The large reduction of computational time required for spin up allows the resources to be spent instead on research that might otherwise have been too computationally demanding, given that for many studies of SOM evolution over timescales of 10s to 100 years the spin up phase can consume the majority of the computational time. For example, high spatial resolution, ensemble runs and sensitivity analysis using multiple sets of parameters are easier given an efficient initialisation method, such as the GSS method.

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352 6. Acknowledgement

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7. Appendix A – Algebraic proof of Eq. (8)

Proof of exponential series for Eq. (8):

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Let S be Eq. (11), then $e^x S$ be Eq. (12).

$$S = \sum_{n=0}^{N-1} e^{nx} = e^0 + e^x + e^{2x} + \dots + e^{(n-1)x}$$
(11)

$$e^{x}S = e^{x}(e^{0} + e^{x} + e^{2x} + \dots + e^{(n-1)x})$$

$$= e^{x} + e^{2x} + \dots + e^{nx}$$
(12)

 $e^x S - S$ results in Eq. (13)

$$e^{x}S - S = e^{x} + e^{2x} + \dots + e^{nx}$$

$$- (e^{0} + e^{x} + e^{2x} + \dots + e^{(n-1)x})$$

$$= -e^{0} + e^{nx}$$

$$= e^{nx} - 1$$
(13)

Eq. (14) can then be derived from Eq. (13):

$$e^{x}S - S = e^{nx} - 1$$

$$S(e^{x} - 1) = e^{nx} - 1$$

$$S = \frac{e^{nx} - 1}{e^{x} - 1}$$

$$S = \frac{-(1 - e^{nx})}{-(1 - e^{x})}$$

$$S = \frac{(1 - e^{nx})}{(1 - e^{x})} = \sum_{n=0}^{N-1} e^{nx} = e^{0} + e^{x} + e^{2x} + \dots + e^{(n-1)x}$$

$$(14)$$

Starting from n=1 instead of $n=0,\,e^0$ is removed from S in Eq. (14). It results in Eq. (15):

$$\sum_{n=1}^{N-1} e^{nx} = S - e^0 = \frac{(1 - e^{nx})}{(1 - e^x)} - e^0 = \frac{(1 - e^{nx})}{(1 - e^x)} - 1$$
(15)