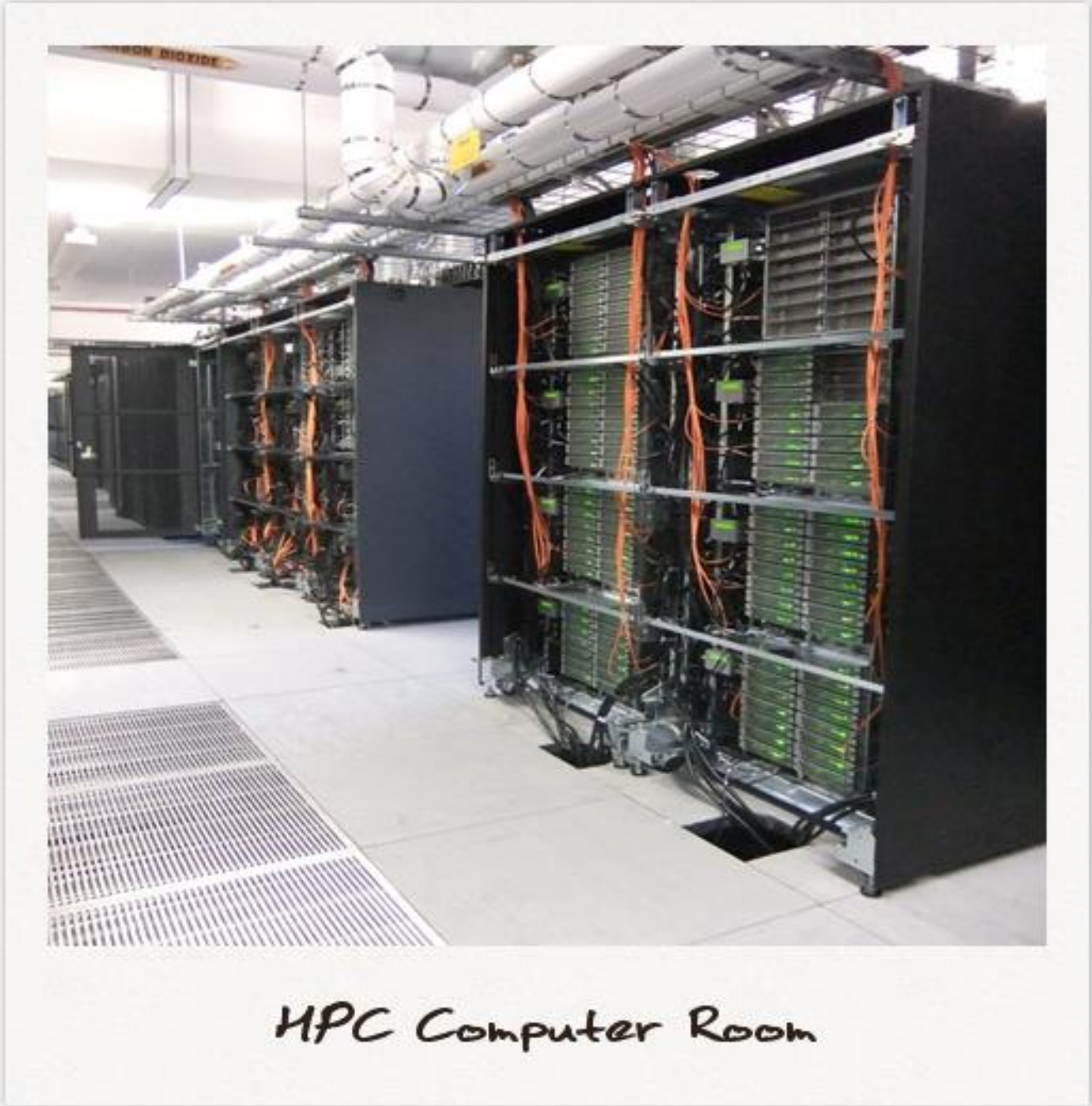
High Performance Computational Methods for Ecology and Evolution

Lauren Attfield

Course objectives

By the end of this course you should be able to:

- Describe different types of high performance computing
- Demonstrate good programming practice
- Identify problems which could benefit from parallel computing
- Run code in parallel on a cluster
- Optimise your code
- Process large amounts of data produced by the cluster



https://www.imperial.ac.uk/admin-services/ict/self-service/research-support/hpc/hpc-service-support/service/

Course objectives

You should also have learned about:

- Ecological neutral theory
- Stochastic and event-based models
- Matrix population models
- Stochastic stage-based population modelling
- Comparing deterministic and stochastic models

Course delivery

- A few short lectures
- Lots of time for practicals
- Developing meaningful code to run simulations on the cluster
- Worksheet to hand in for credit
  - Ecological neutral theory example
  - Demographic population modelling example
- If you get stuck – try Google, StackExchange, ask your peers, ask a GTA or lecturer
- Post Git issues and share them on Teams – either lecturer or a GTA will respond to your Git issues – and help others with their Git issues!
















Ecological Neutral Theory:

Assumes all individuals are ecologically equivalent

(Caswell 1976)
(Hubbell 1979)
Hubbell 1997)
(Bell 2000)
(Bell 2001)
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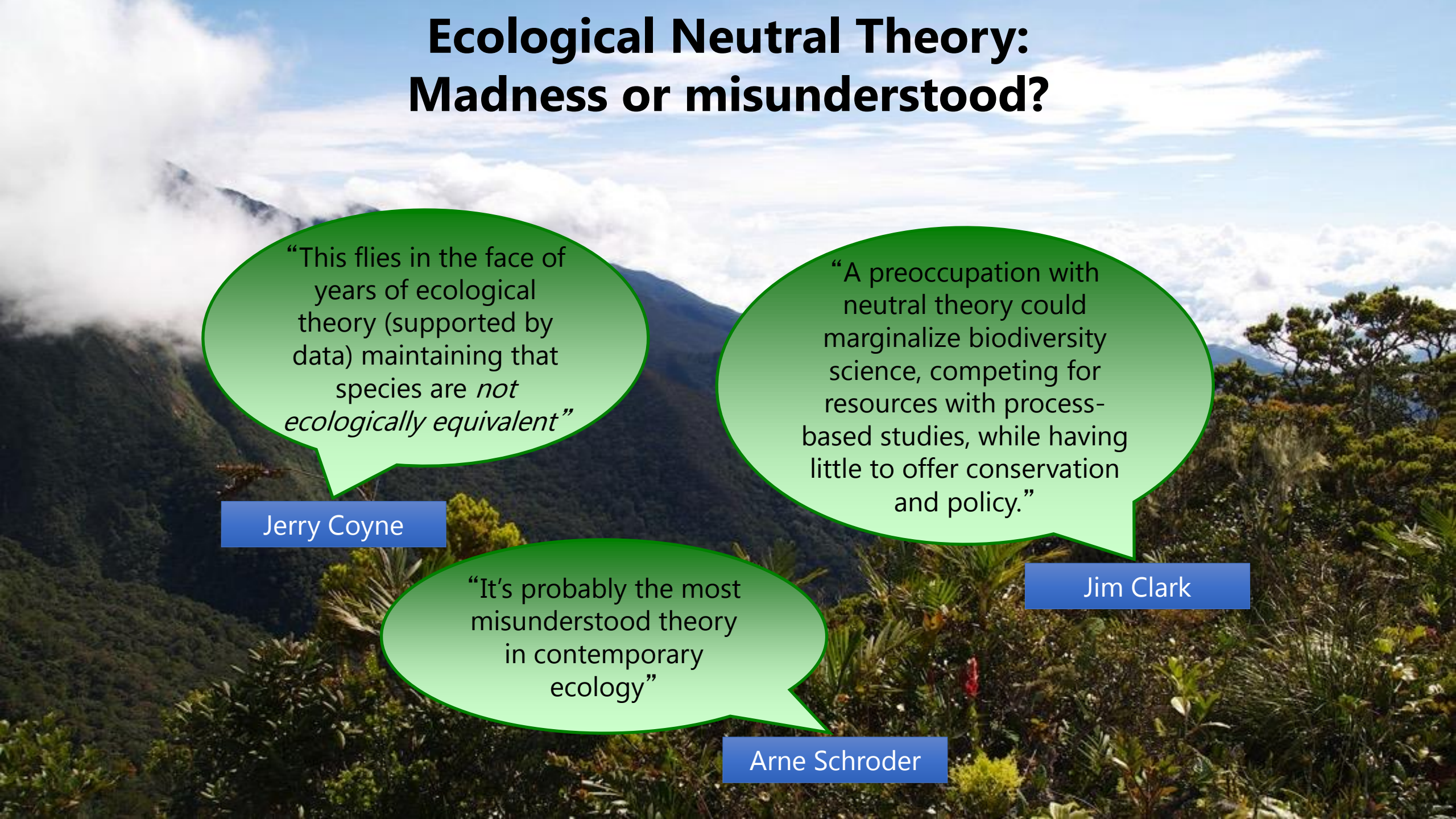
Ecological Neutral Theory: Madness or misunderstood?



Ecological Neutral Theory

1. What is neutral theory?

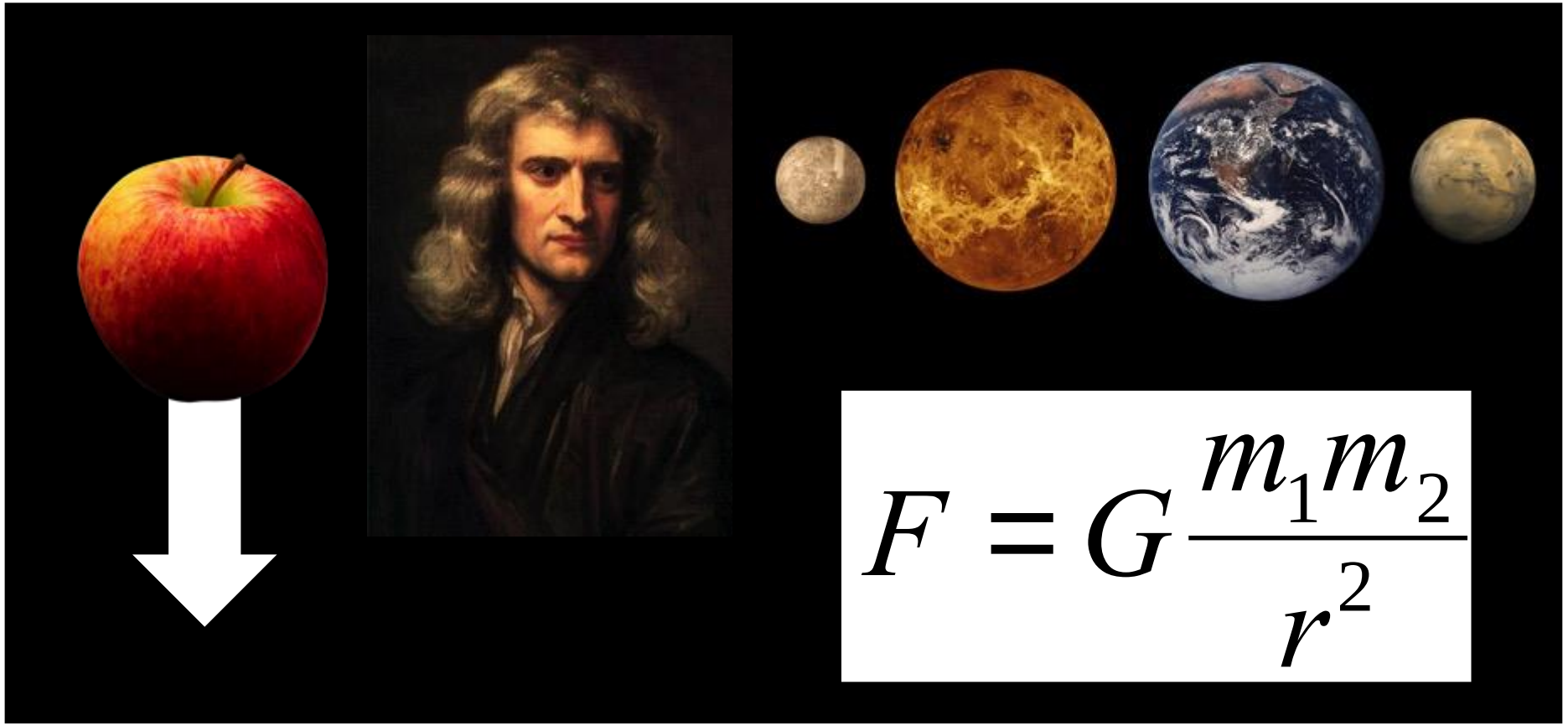
2. Example neutral models

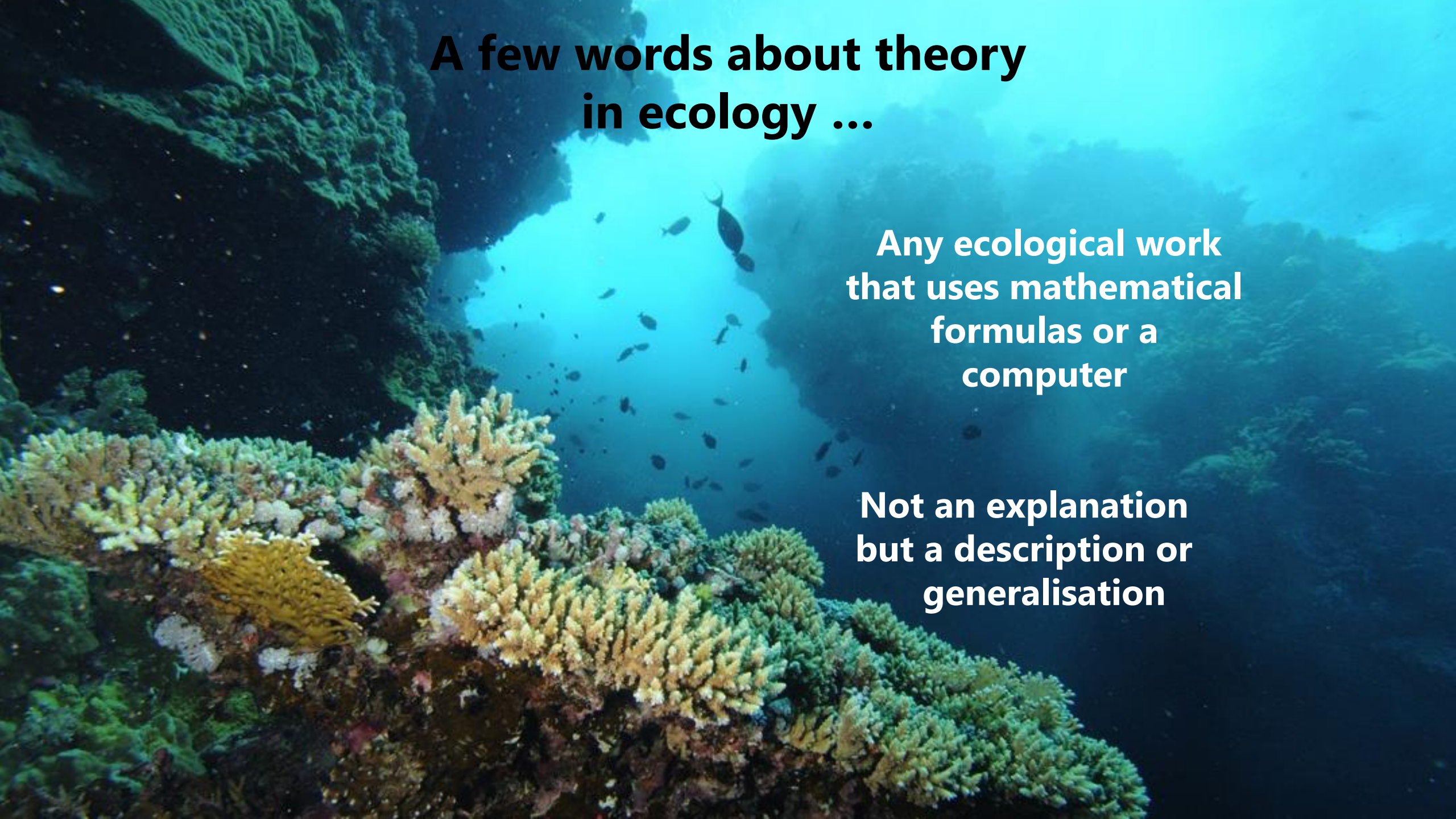
3. Uses of neutral theory

4. Applications in island biogeography

A few words about theory in physics …

- Scientific theory conforms with empirical data and puts forward an ‘explanation’ for observed phenomena





A few words about theory in ecology …

Any ecological work that uses mathematical formulas or a computer

Not an explanation but a description or generalisation

Ecological Neutral Theory

Assumes all individuals are ecologically equivalent

Is not a claim that all individuals are ecologically equivalent

Is about making some assumptions and seeing where they get us

(Caswell 1976)
(Hubbell 1979)
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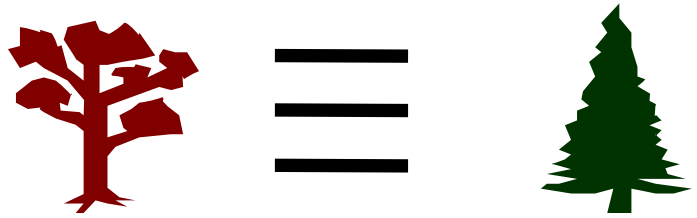
Common misconceptions about what neutral theory is …

The term ‘neutral model’ can be used interchangeably with ‘null model’

‘neutral models’ assume all species are the same



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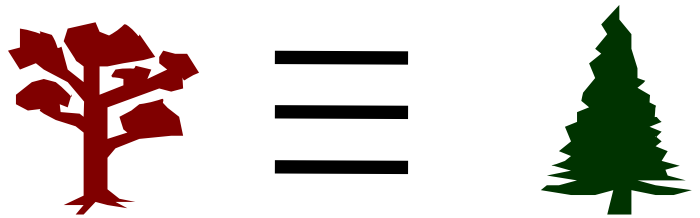
The demographic properties of an individual are independent of its species identity



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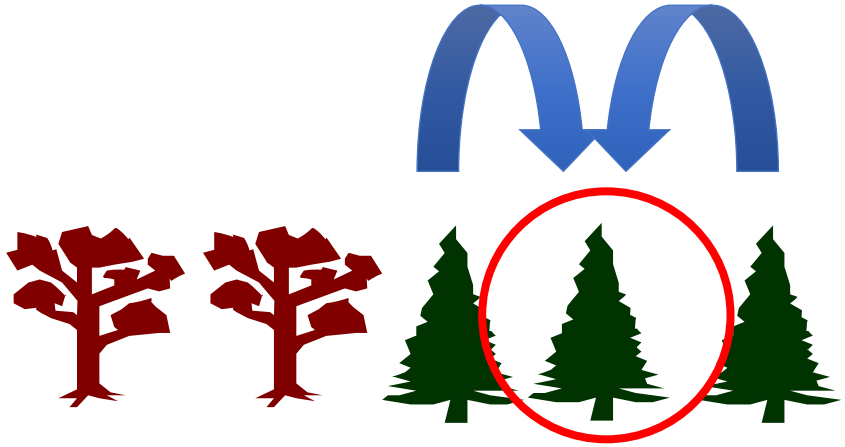

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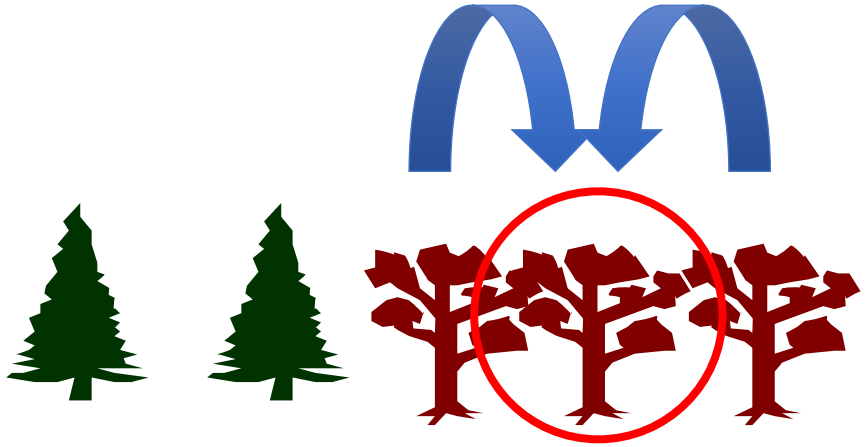

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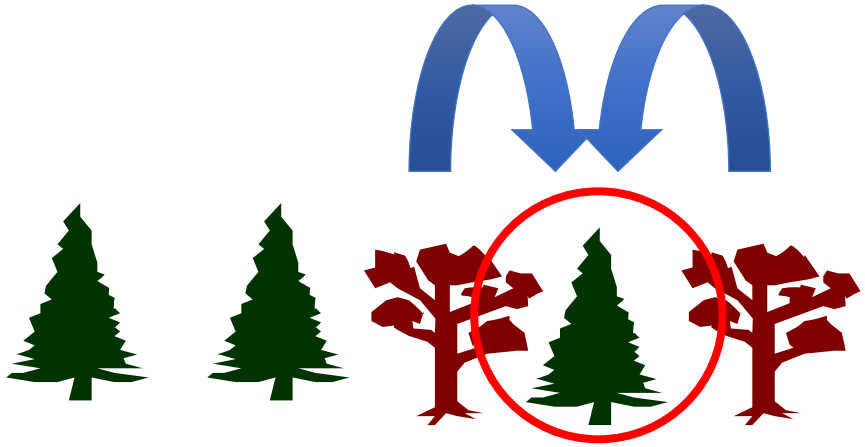

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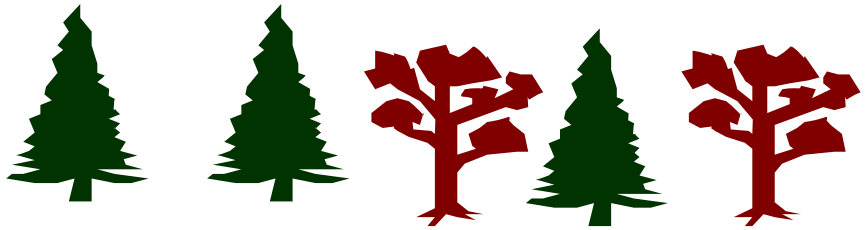

Ecological Neutral Theory

1. What is neutral theory?

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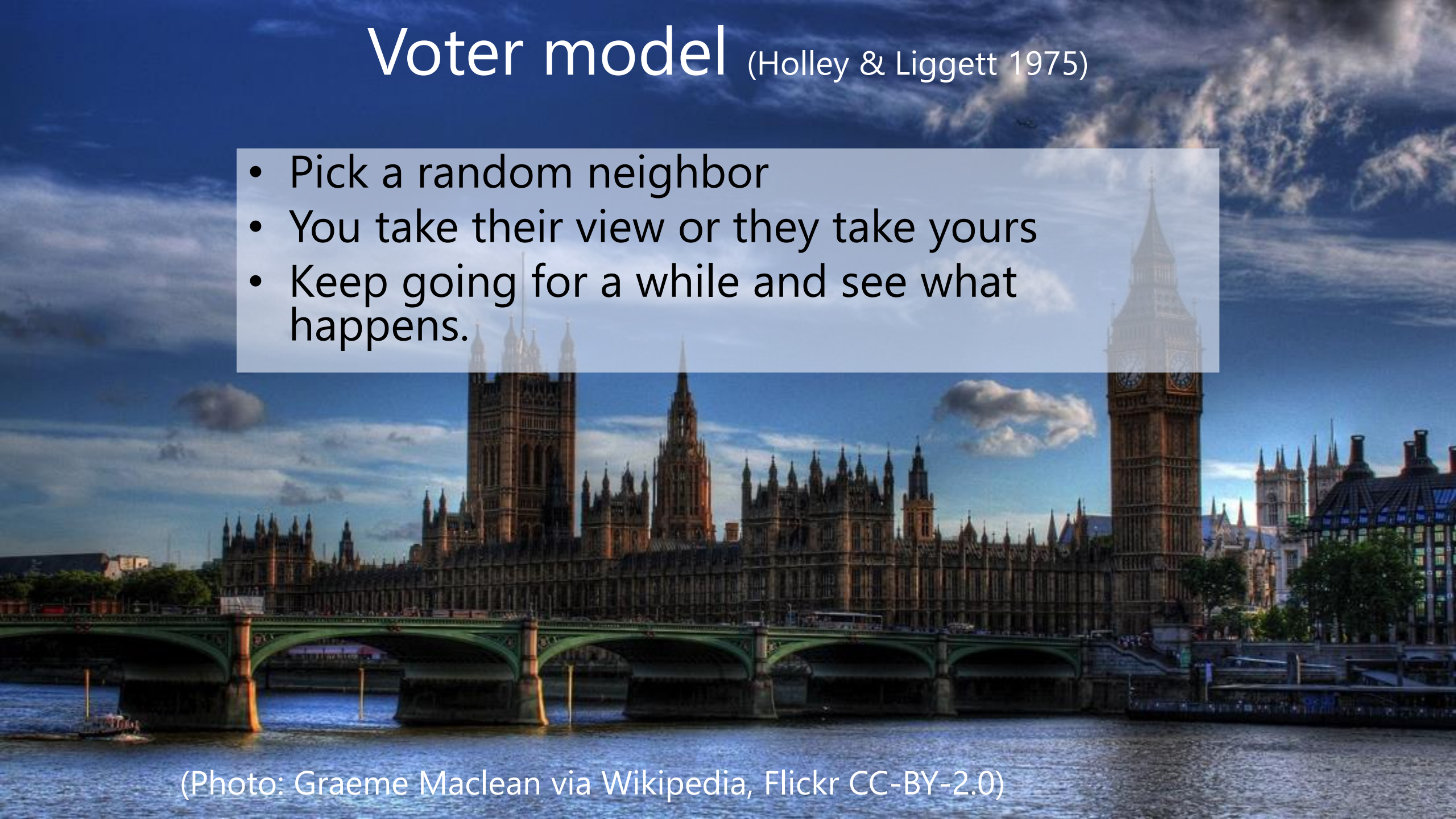
Voter model (Holley & Liggett 1975)

- Pick a random neighbor
- You take their view or they take yours
- Keep going for a while and see what happens.



(Photo: Graeme Maclean via Wikipedia, Flickr CC-BY-2.0)

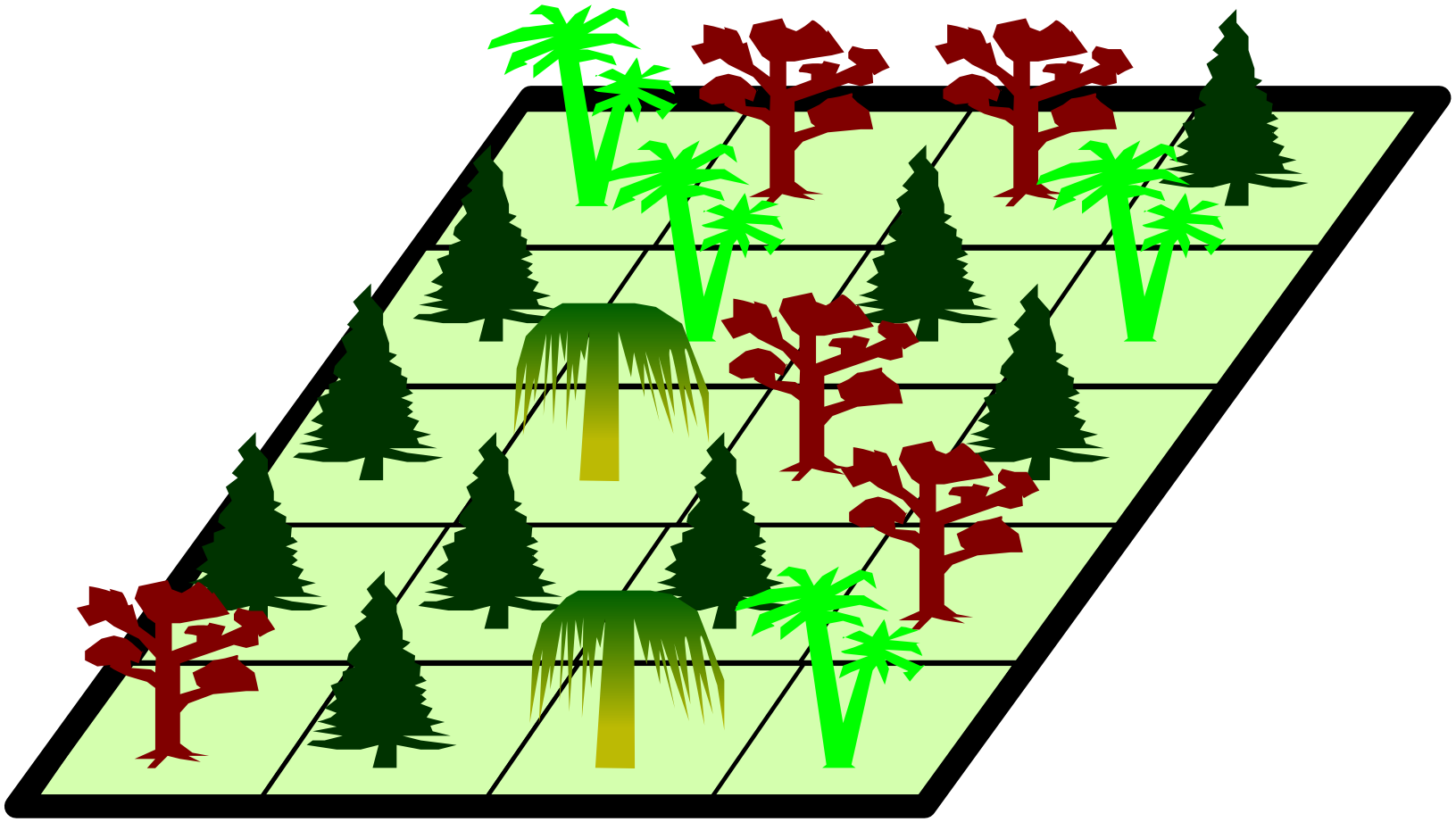
Voter model – relating to biology

- Political view becomes species identity
- People become places in space where an individual could live
- Dispersal is over very short distances

Voter model – what we found

- Found some impenetrable clumps forming
- There are edge effects
- Eventually everyone in each connected group holds the same view
- Hence we introduced mutation

The model rules in brief



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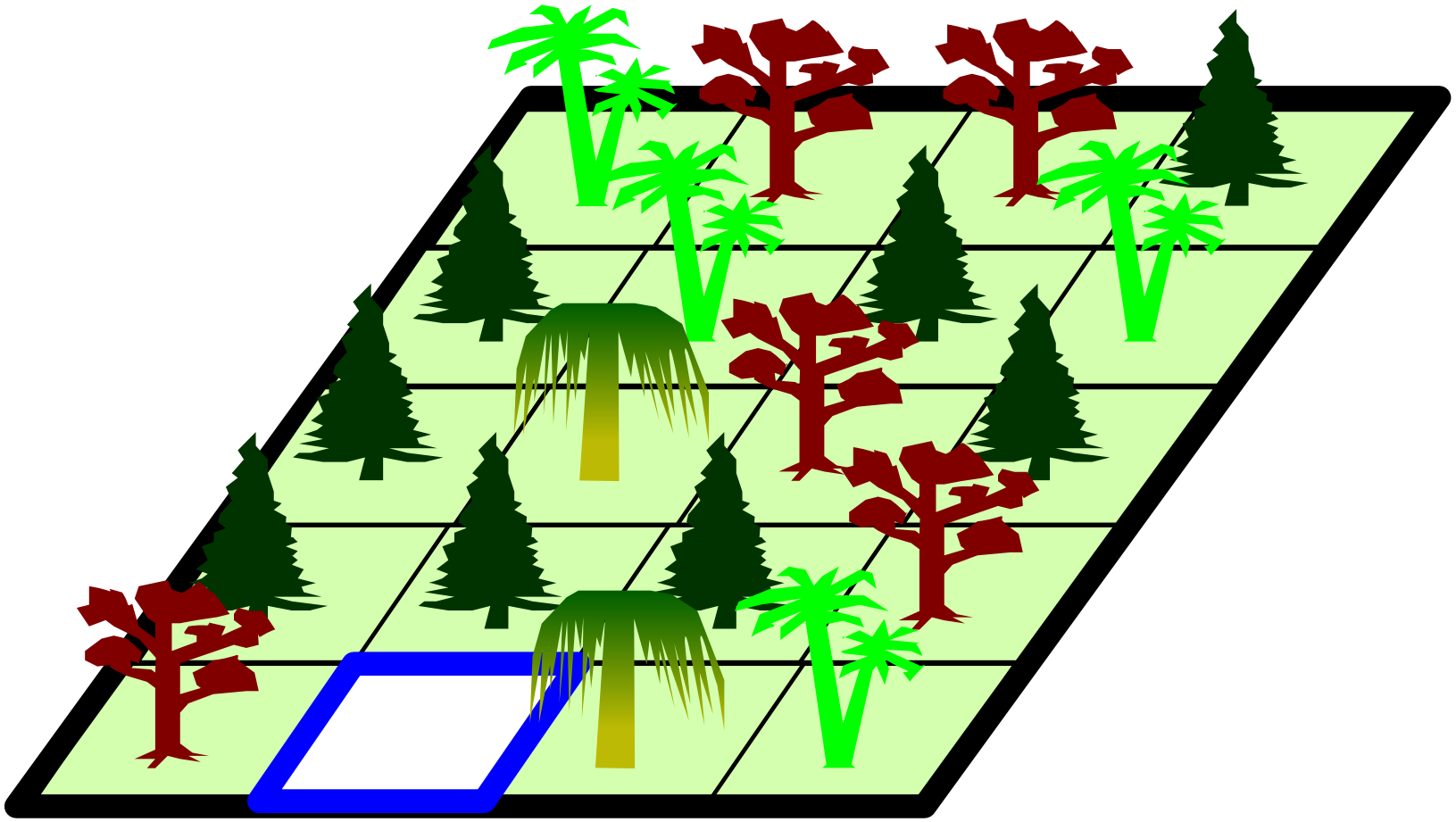

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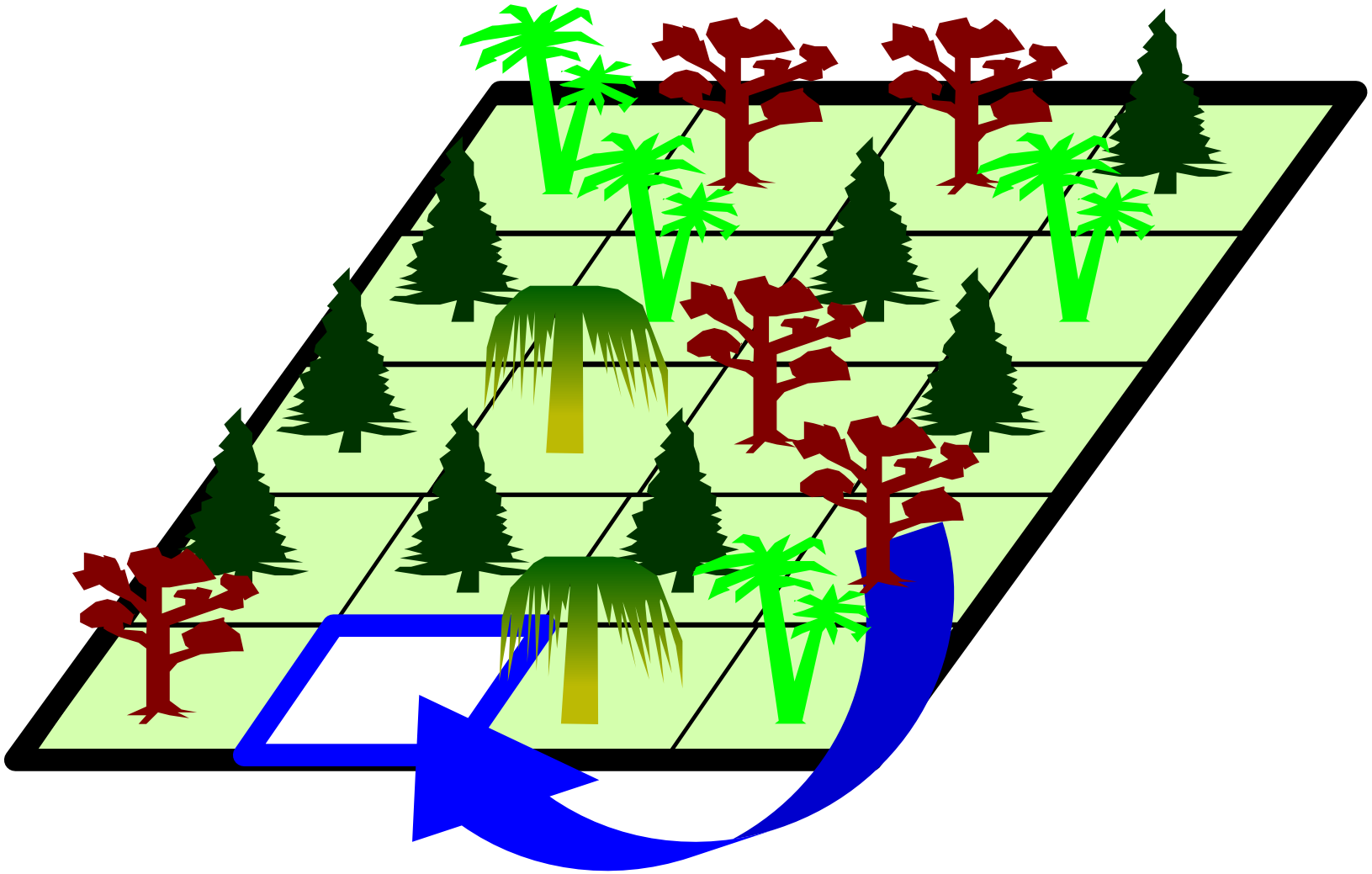

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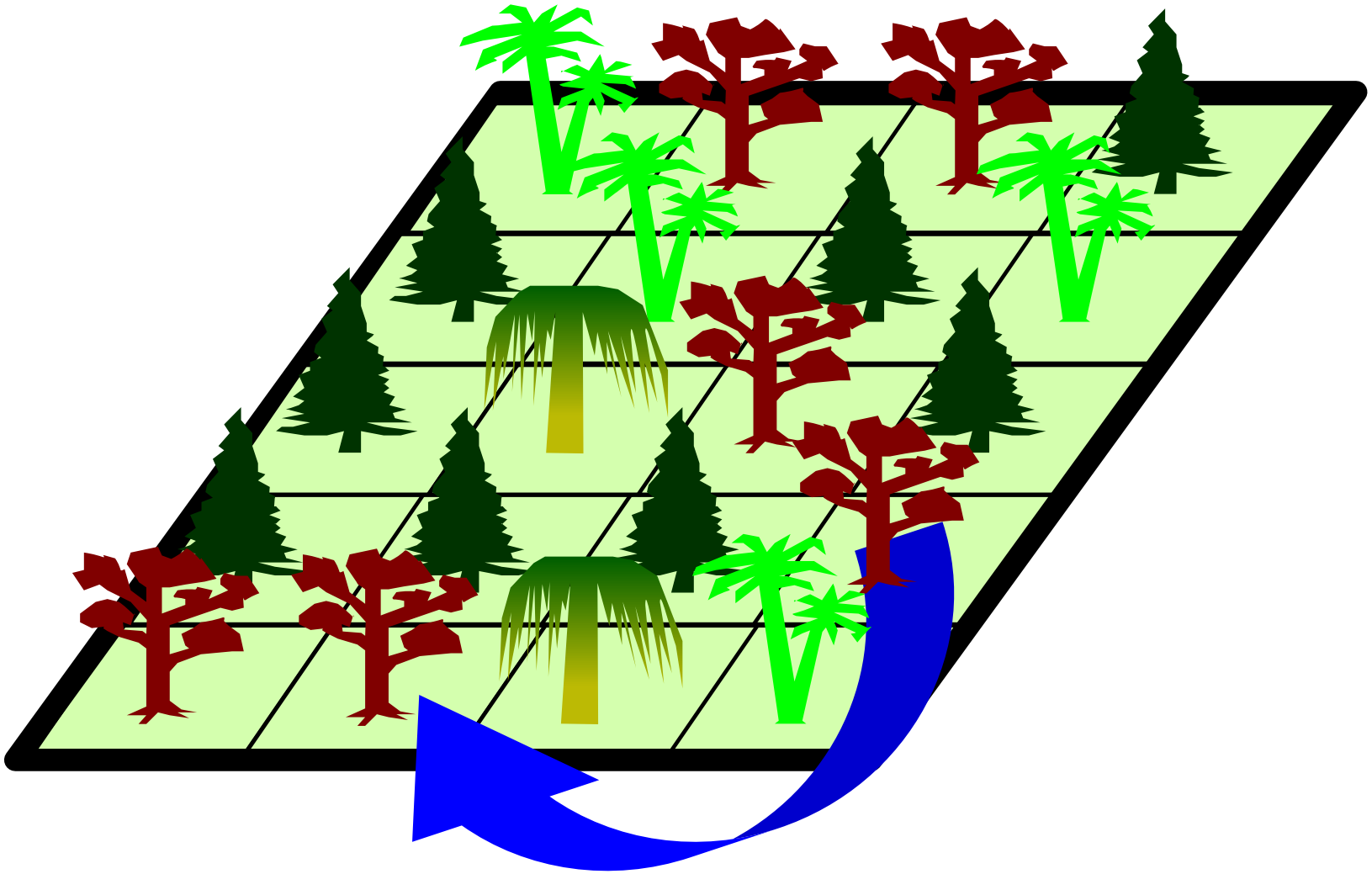

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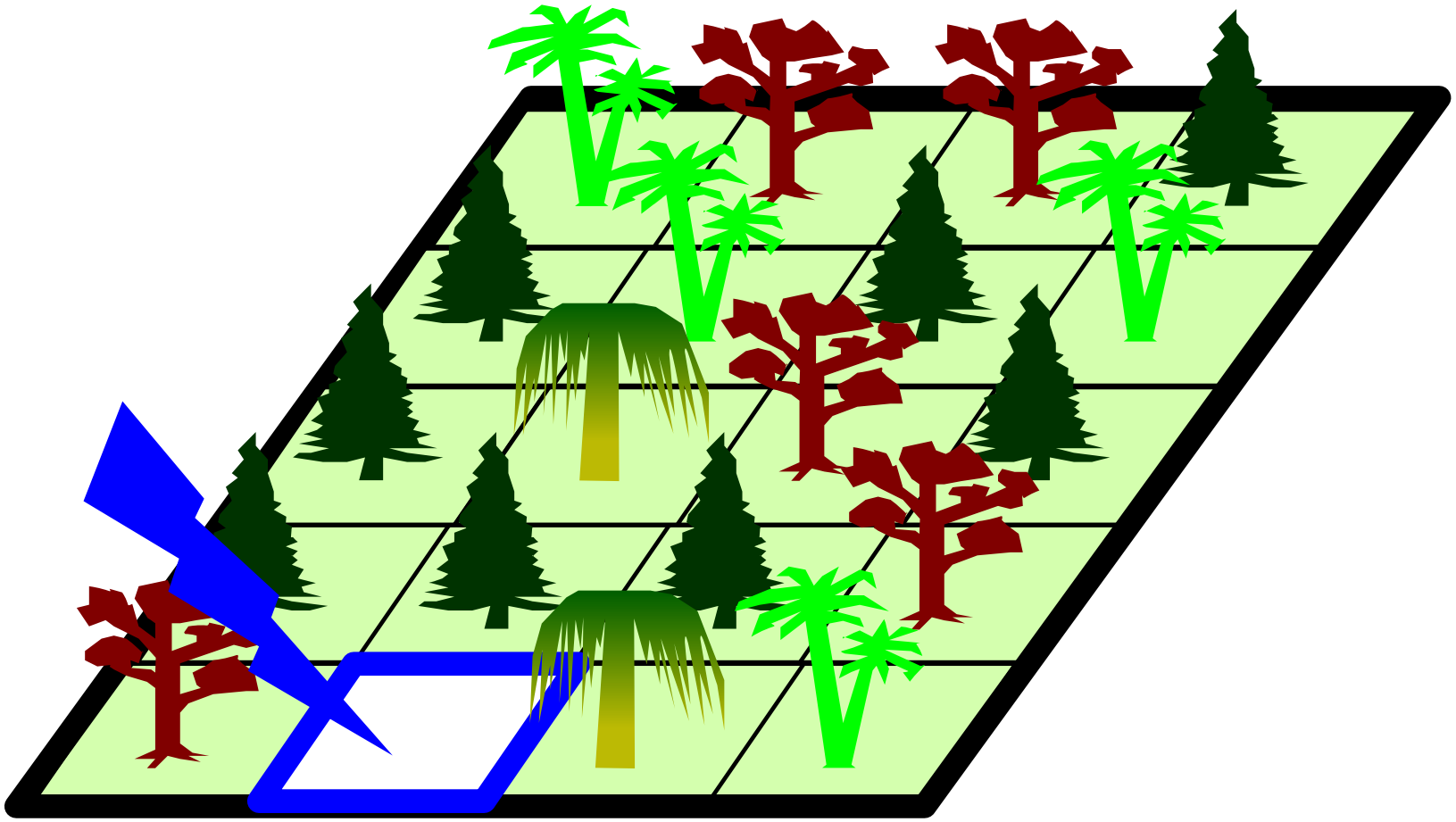

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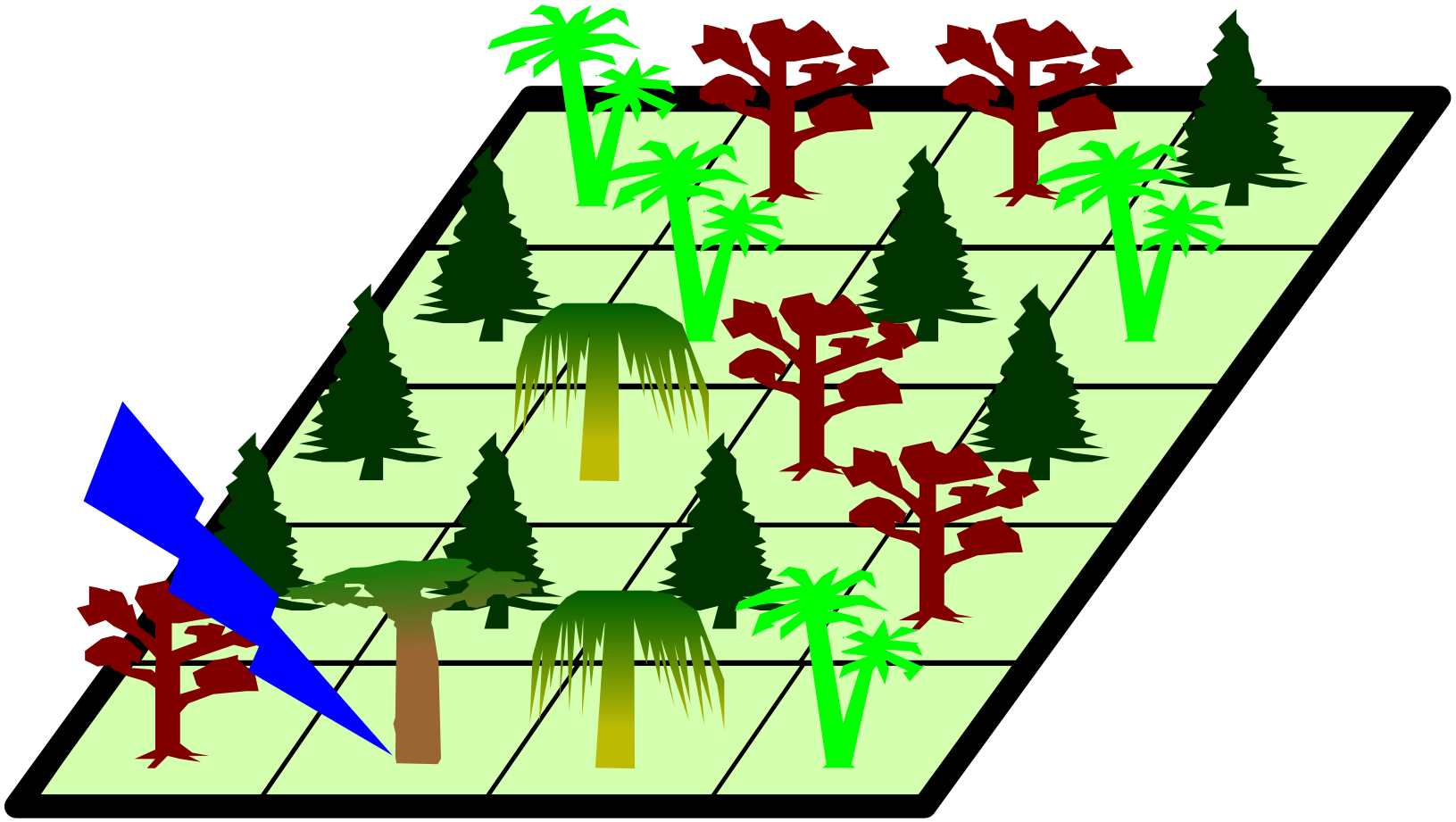
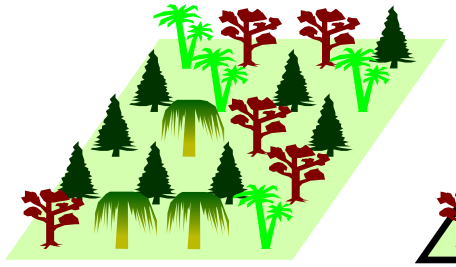
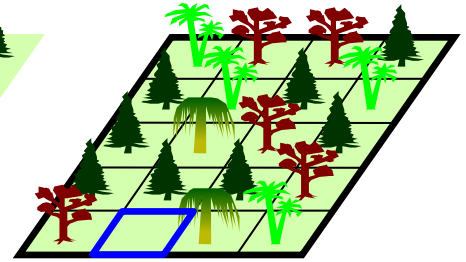


Variations on the theme

- The zero sum assumption





- Speciation mode (none)

(Caswell 1976)
(Bell 2000)
(Bell 2001)

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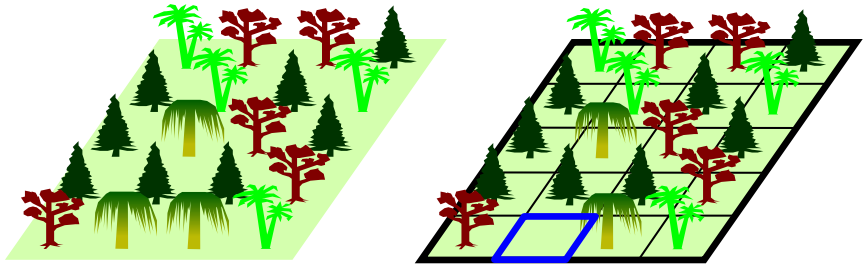
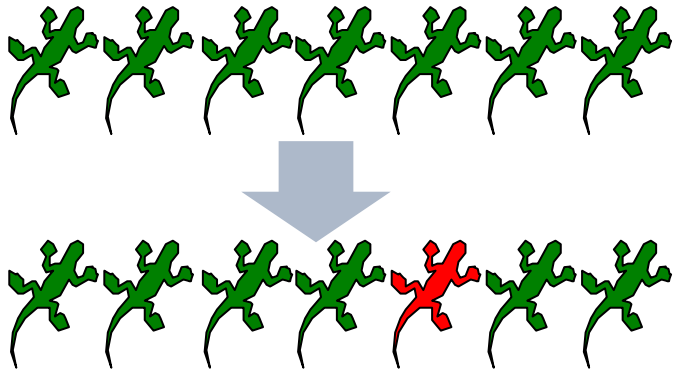


- Speciation mode (point mutation)



(Hubbell 1997)
(Hubbell 2001)

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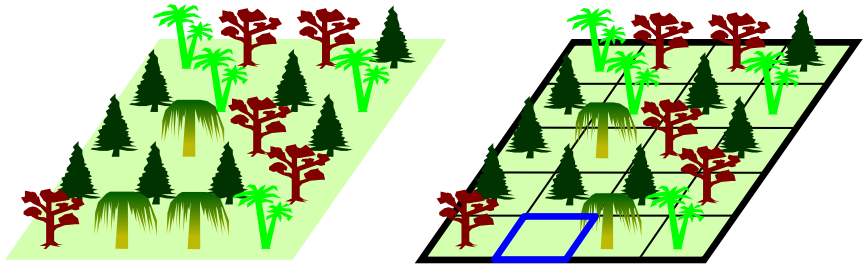
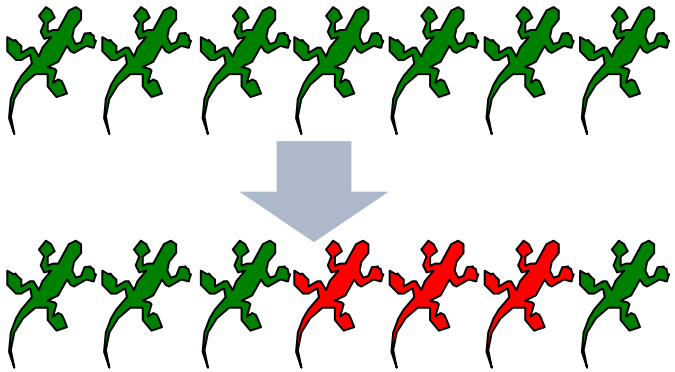


- Speciation mode (random fission)



(Hubbell 2001)
(Hubbell & Lake 2002)

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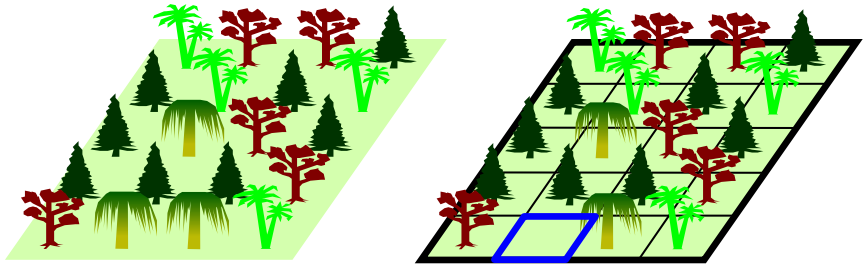
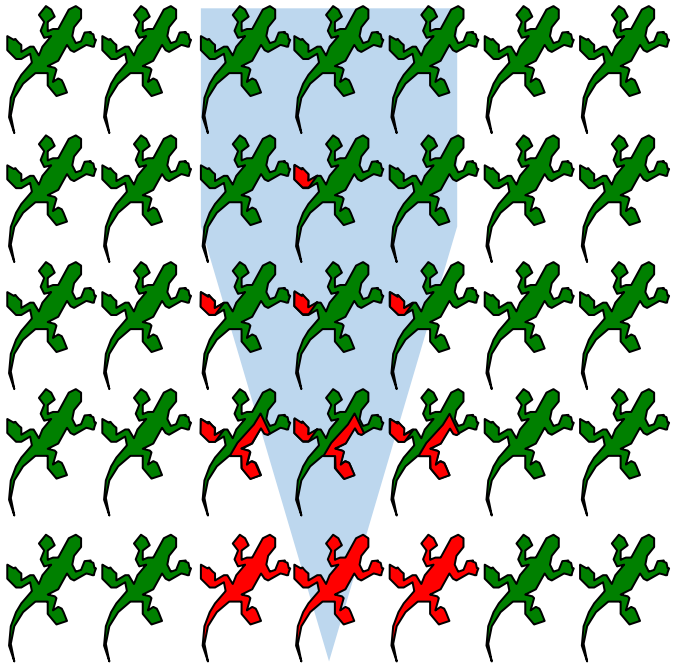


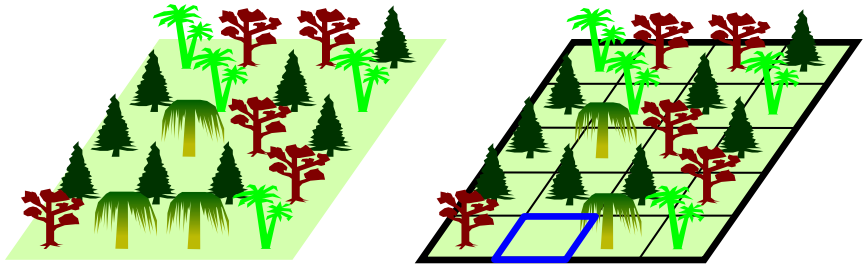
- Speciation mode (protracted)



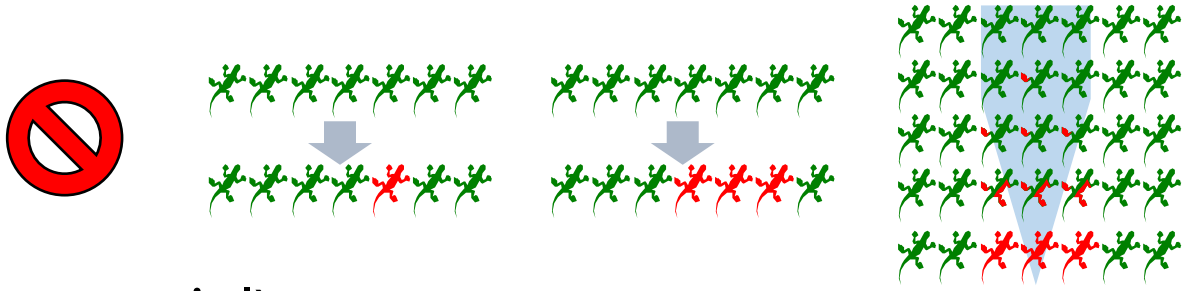
(Rosindell *et al.* 2010)

Variations on the theme

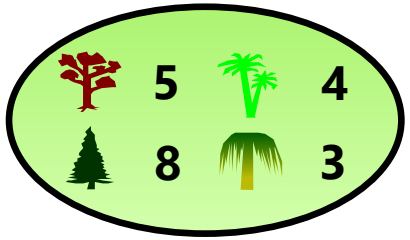
- The zero sum assumption



- Speciation mode



- Spatial structure (non-spatial)



(Caswell 1976)

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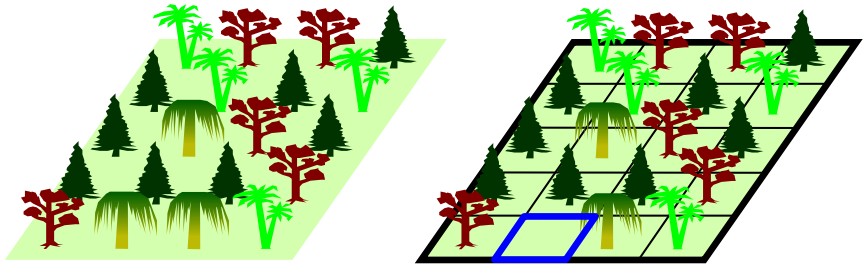

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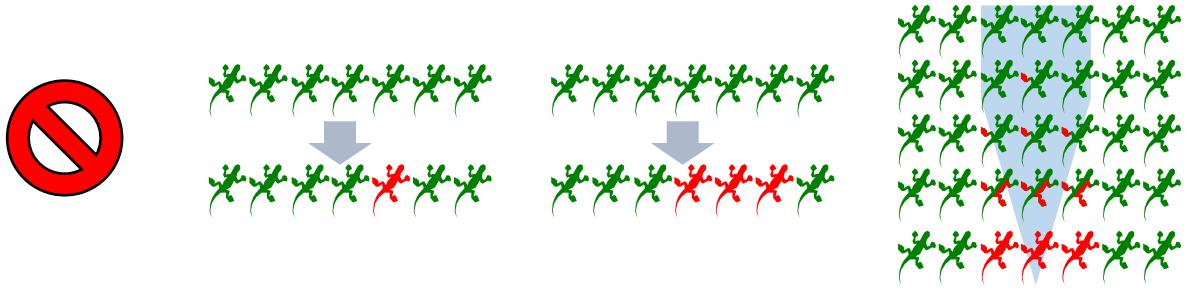
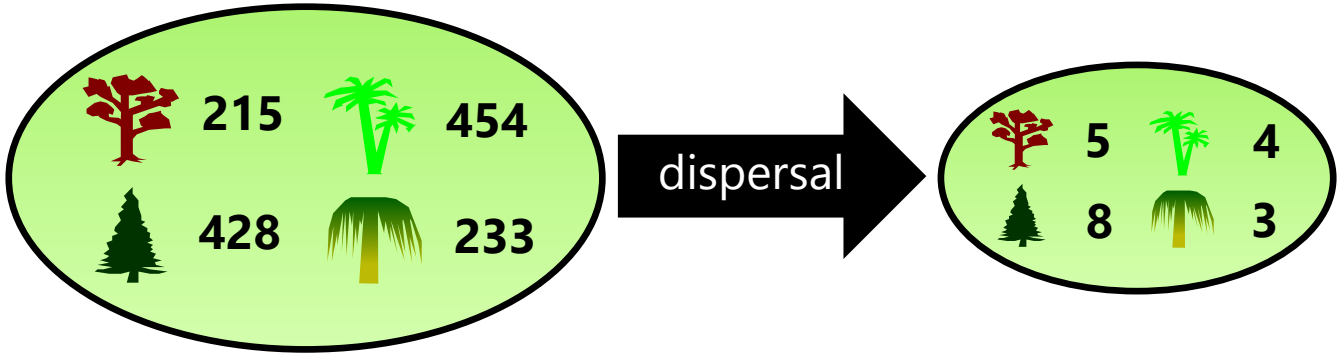


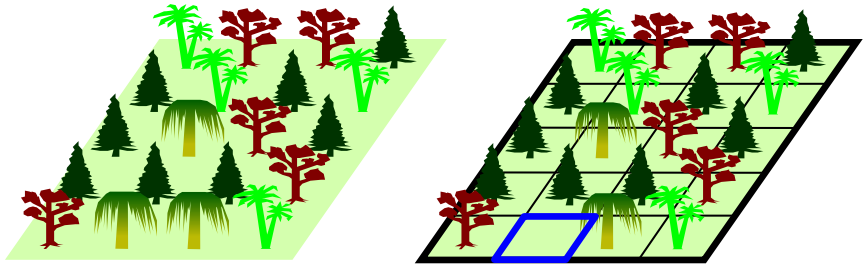
- Spatial structure (spatially implicit)



(MacArthur and Wilson 1963)
(Hubbell 2001)

Variations on the theme

- The zero sum assumption



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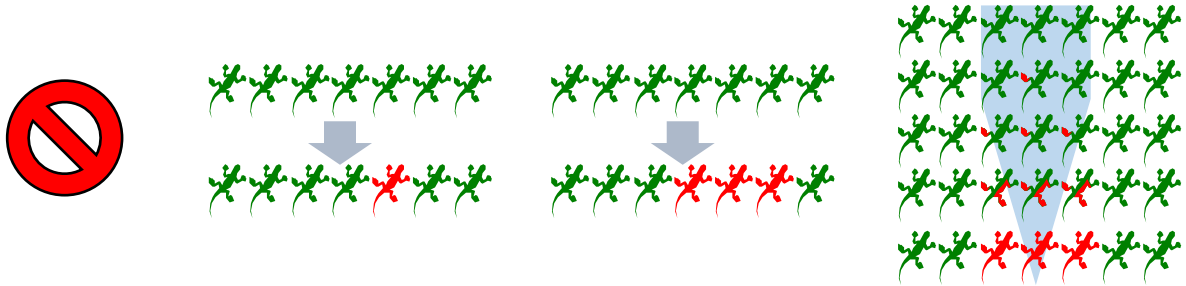
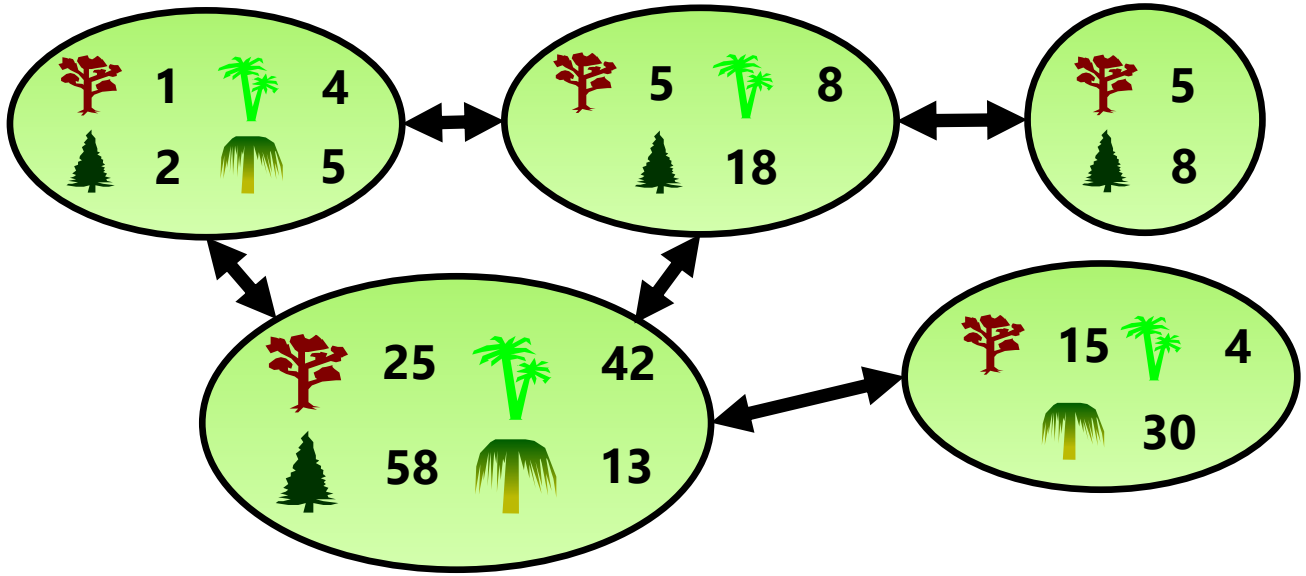


- Spatial structure (spatially explicit network)



(Economo & keitt 2008)
(Warren 2010)
(Vanpeteghem & Haegeman 2010)
(Muneepeerakul *et al.* 2008)

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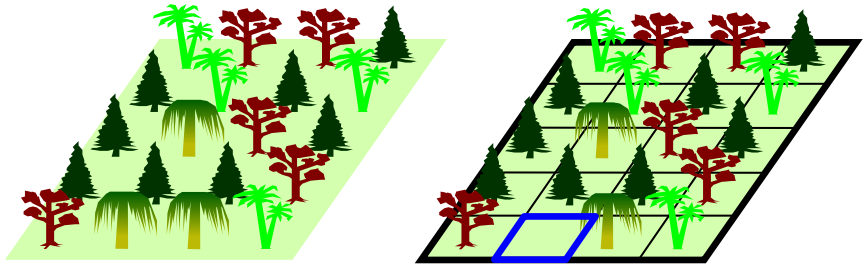
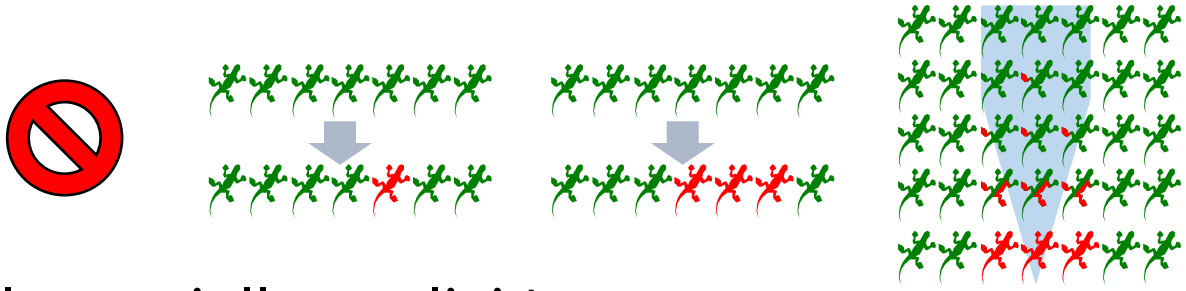
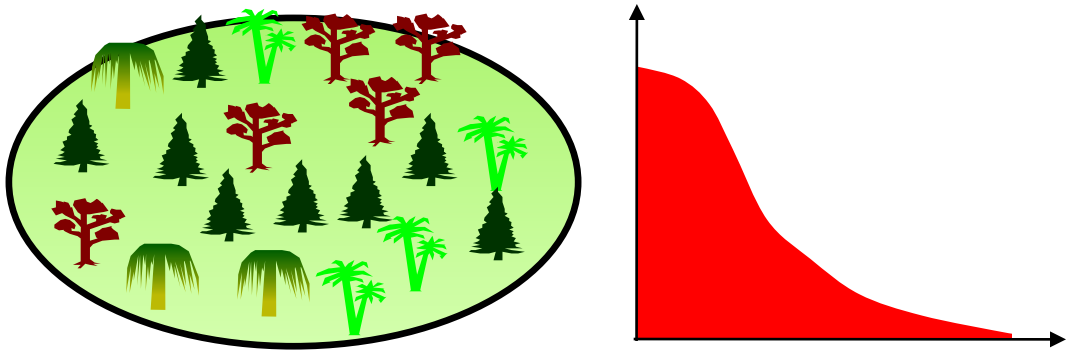
- The zero sum assumption



- Speciation mode



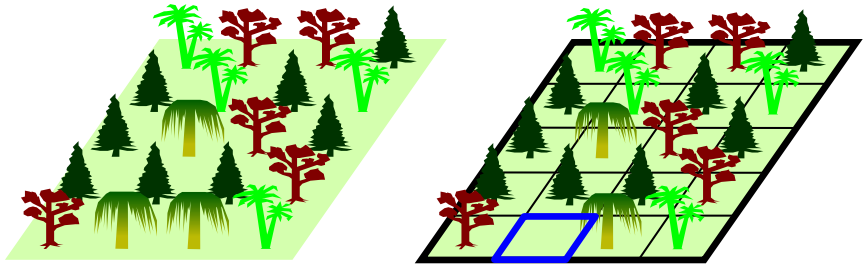
- Spatial structure (fully spatially explicit)



(Holley & Liggett 1975)
(Bramson et al. 1998)
(Durett & Levin 1996)
(Hubbell 2001)
(Chave et al. 2002)
(Chave & Leigh 2002)
(Zillio et al. 2005)
(Rosindell & Cornell 2007,2009)
(Pigolotti & Cencini 2009)
(O'Dwyer & Green 2010)
(Etienne & Rosindell 2011)

Variations on the theme

- The zero sum assumption



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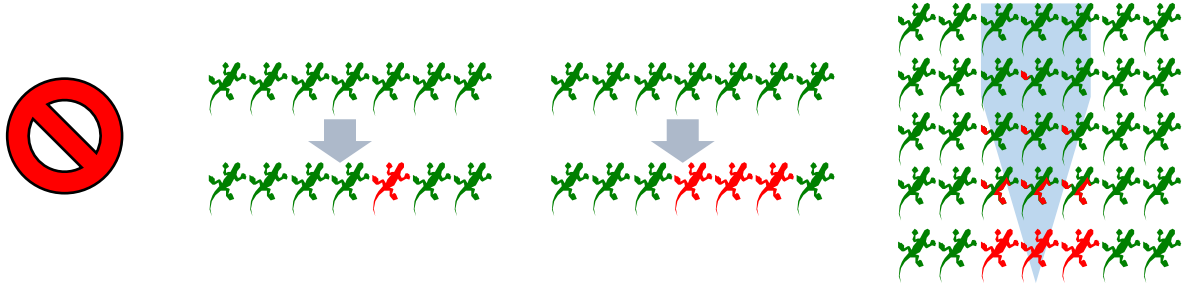
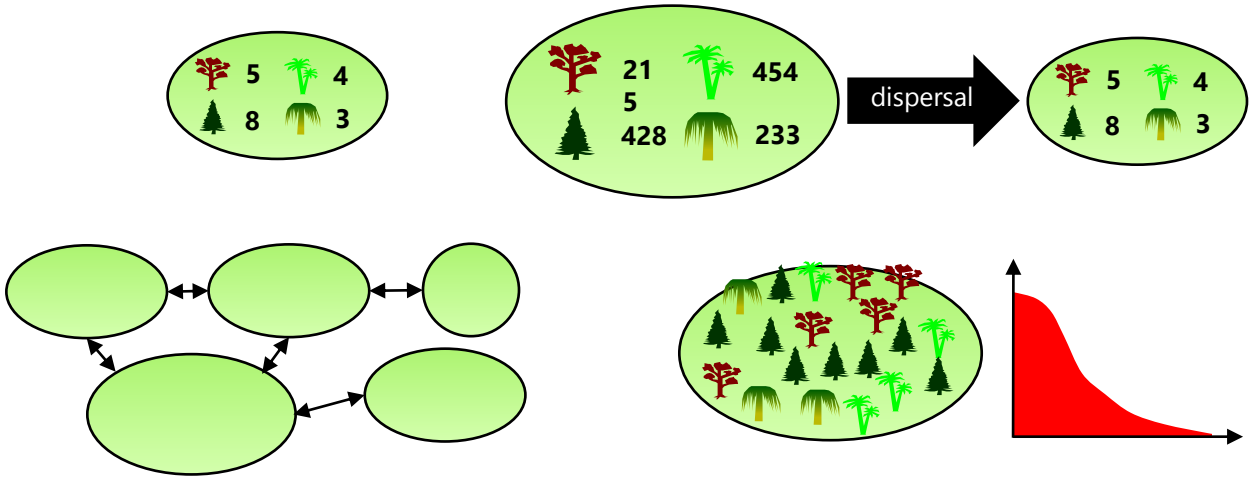
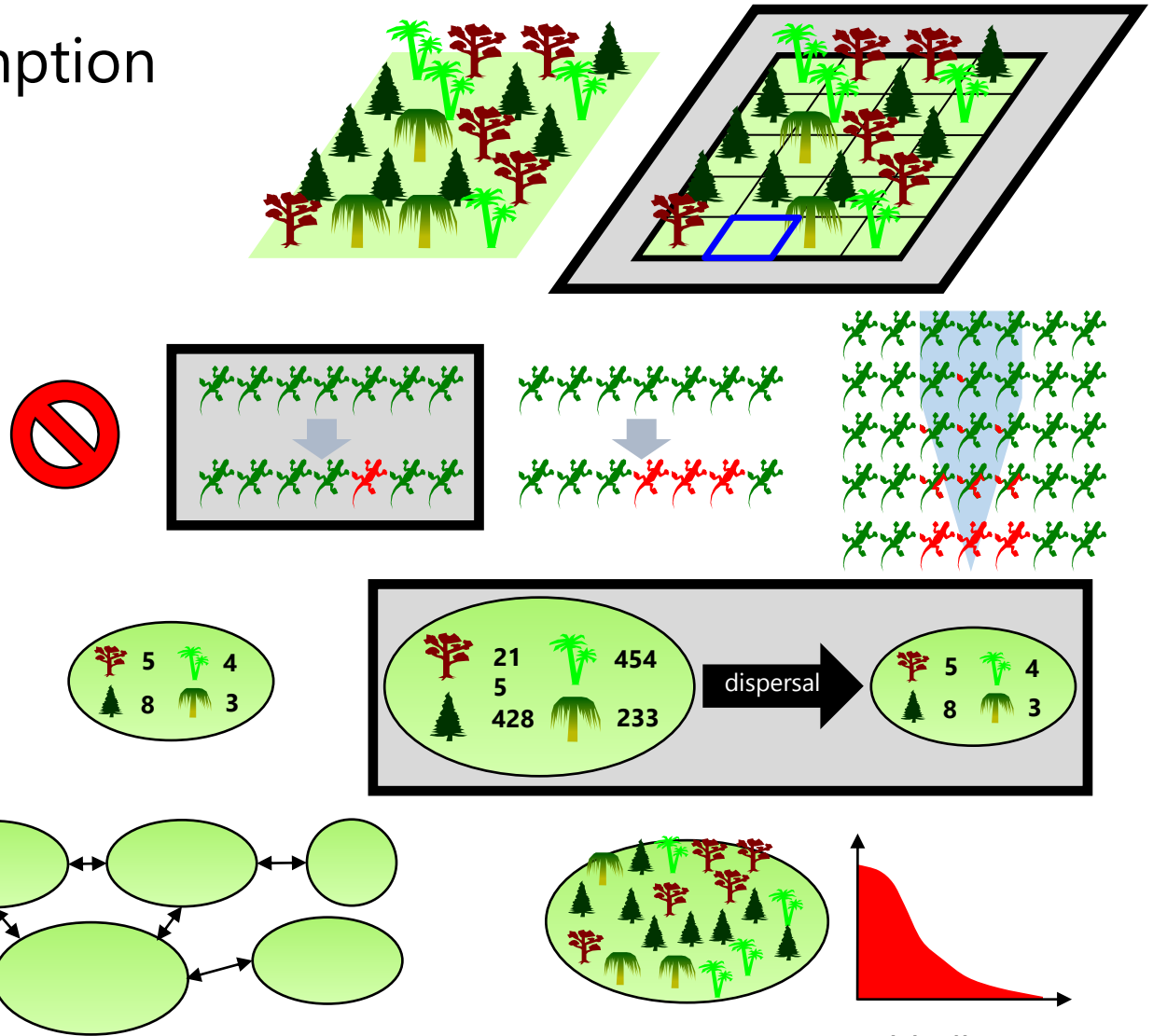


- Spatial structure



Variations on the theme

- The zero sum assumption
- Speciation mode
- Spatial structure



(Hubbell 2001)
(Leigh 2007)
(Leigh *et al.* 2010)

Variations on the theme

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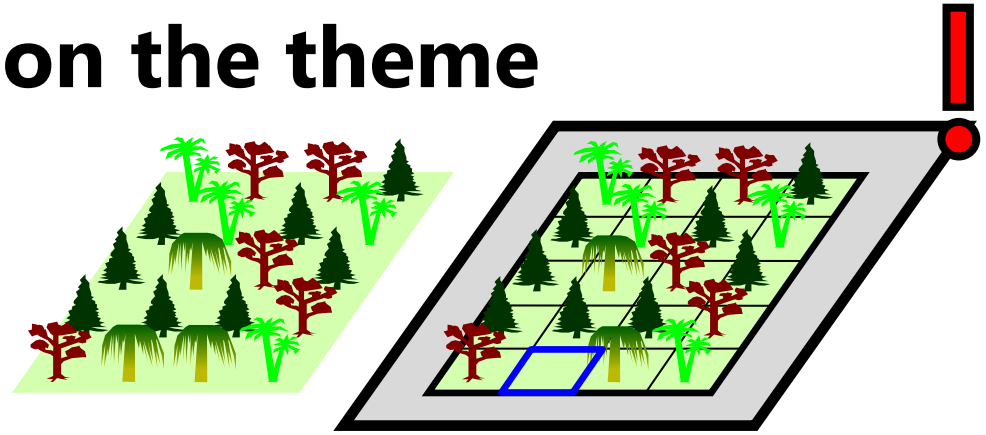

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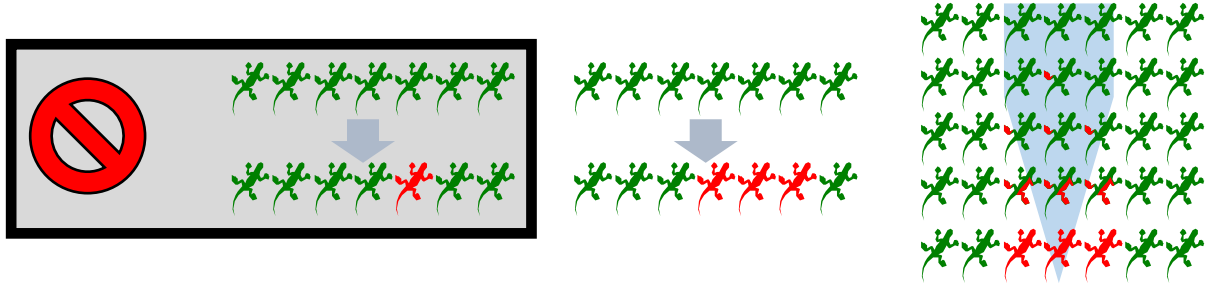

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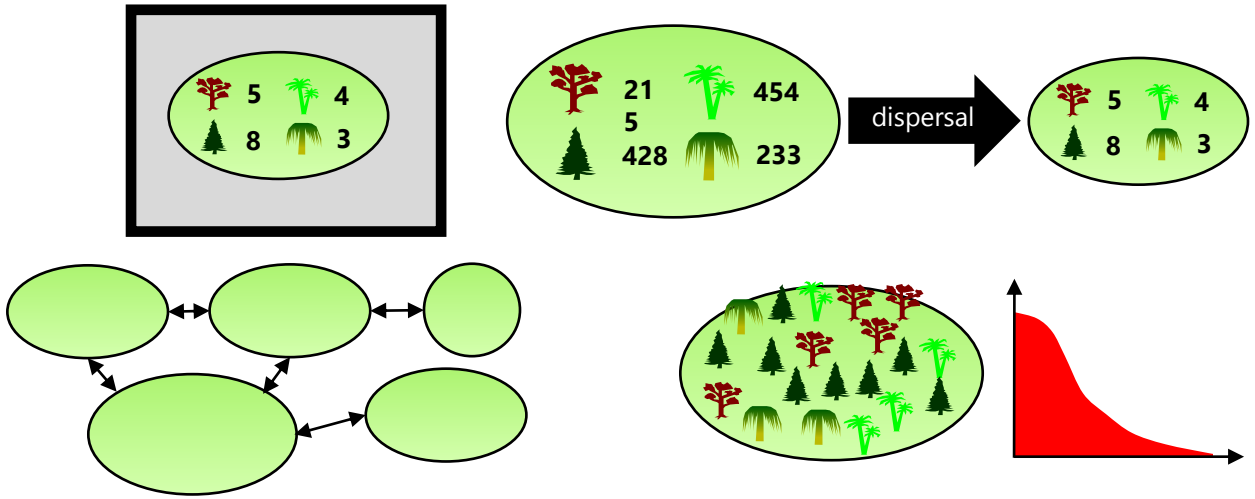

Your exercise questions

Ecological Neutral Theory

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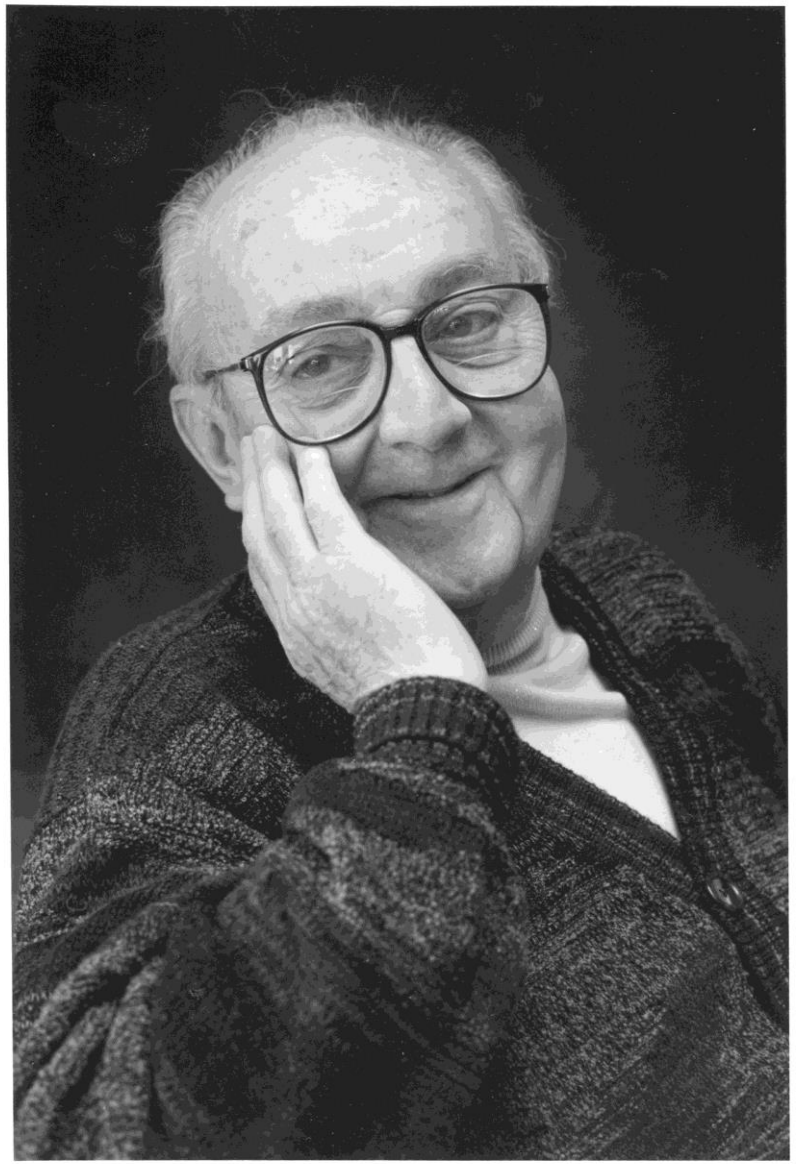
2. Example neutral models

3. Uses of neutral theory

4. Applications in island biogeography



© David McEddy

George E P Box (Box & Draper 1987)

Essentially, all models are wrong,

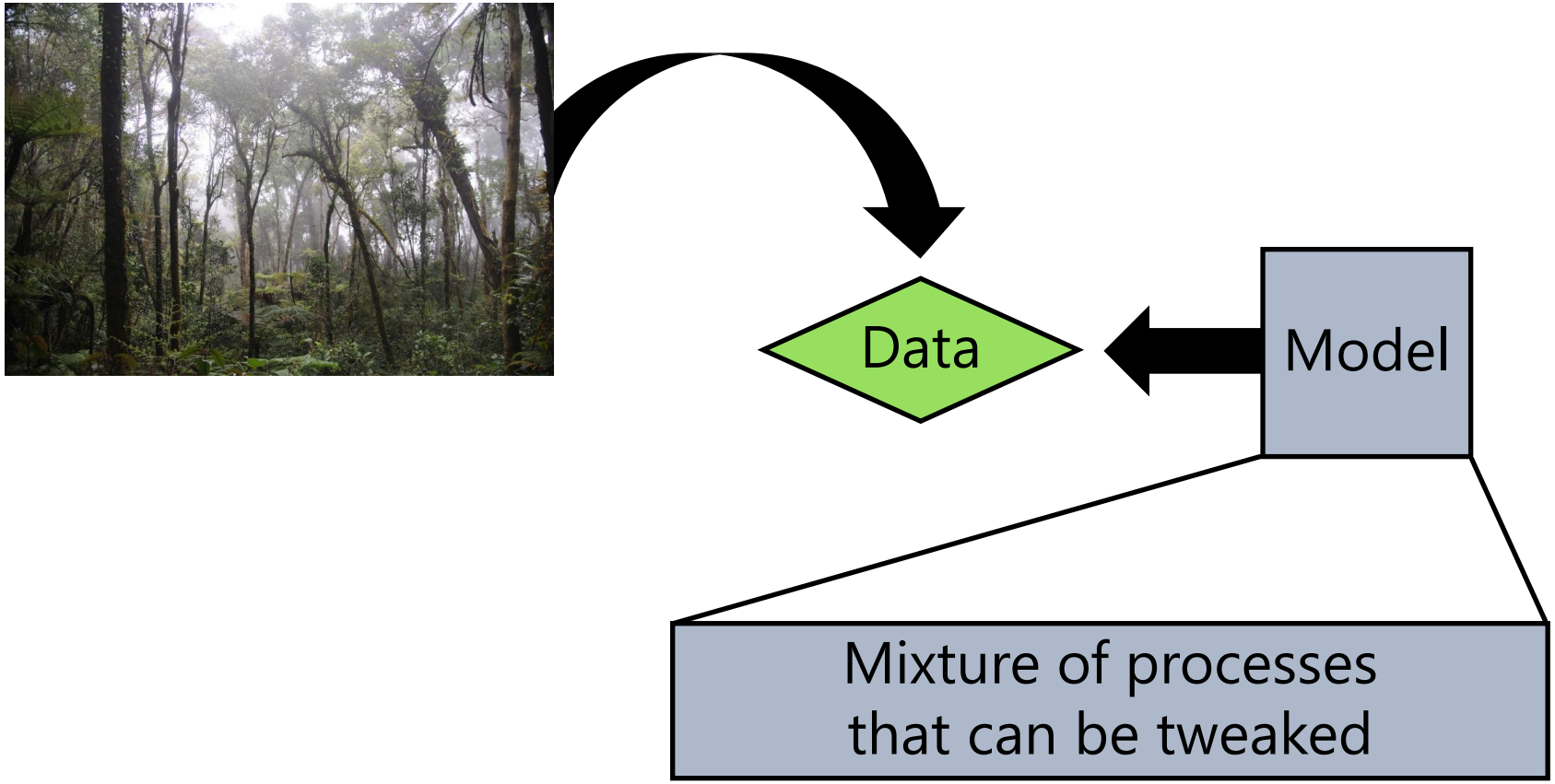
All models can fail upon being challenged with data

That's OK!

but some are useful

1. Helping to understand
2. Helping to predict

Ecological Neutral Theory:
How is it useful for understanding?



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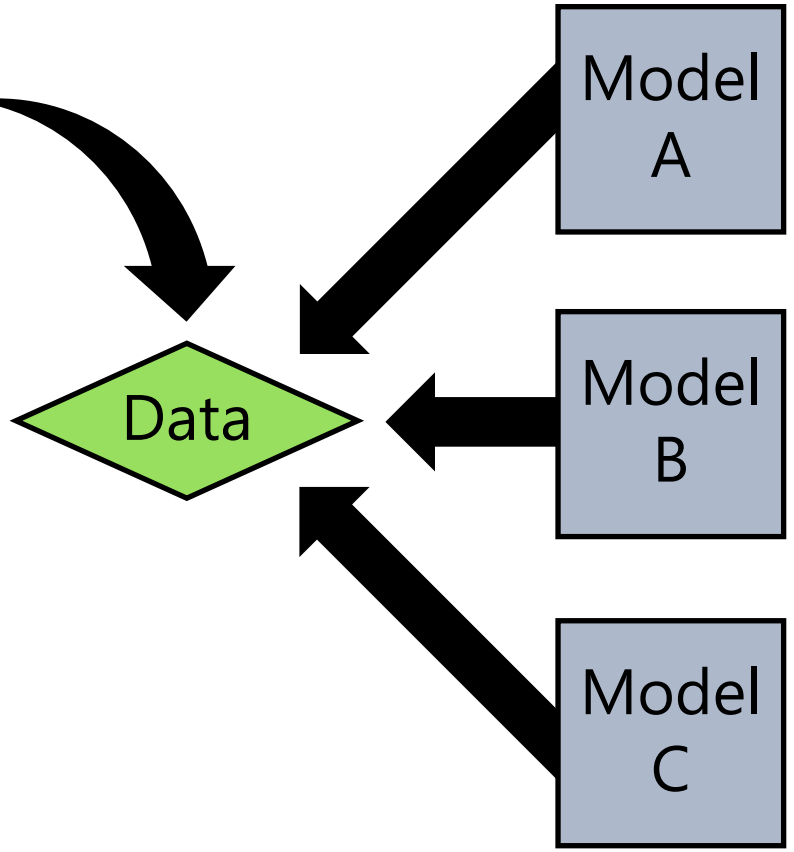


Ecological Neutral Theory: How is it useful for understanding?

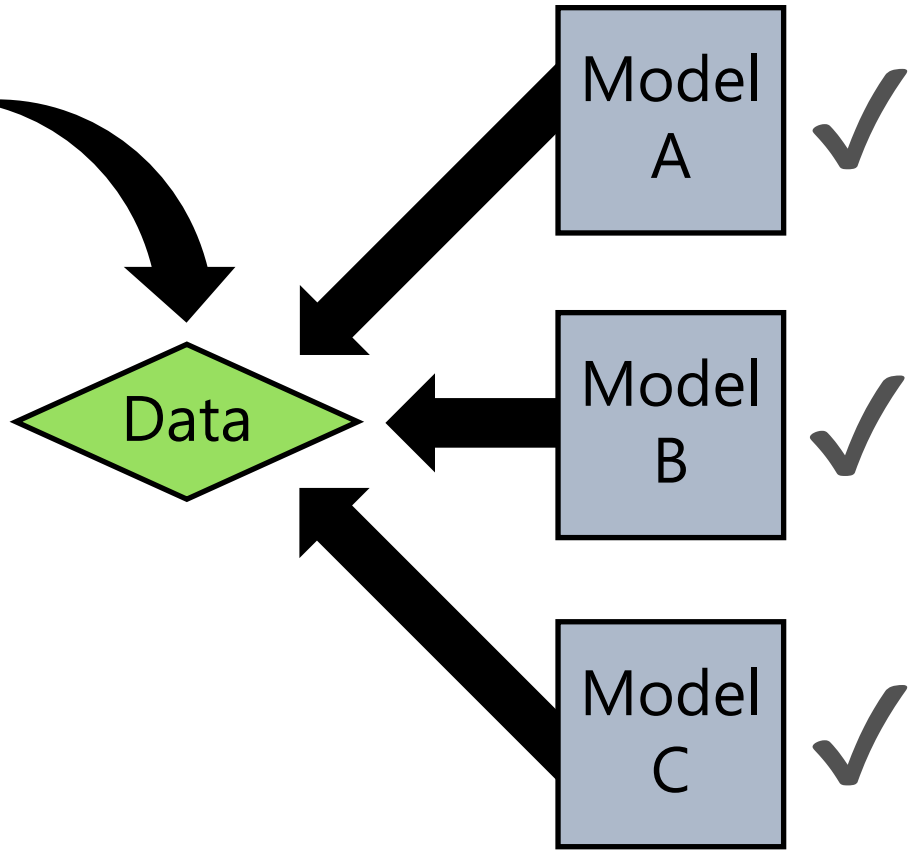
Data

Model A ✗

Model B ✓

Model C ✗

Ecological Neutral Theory:
How is it useful for understanding?



Ecological Neutral Theory: How is it useful for understanding?

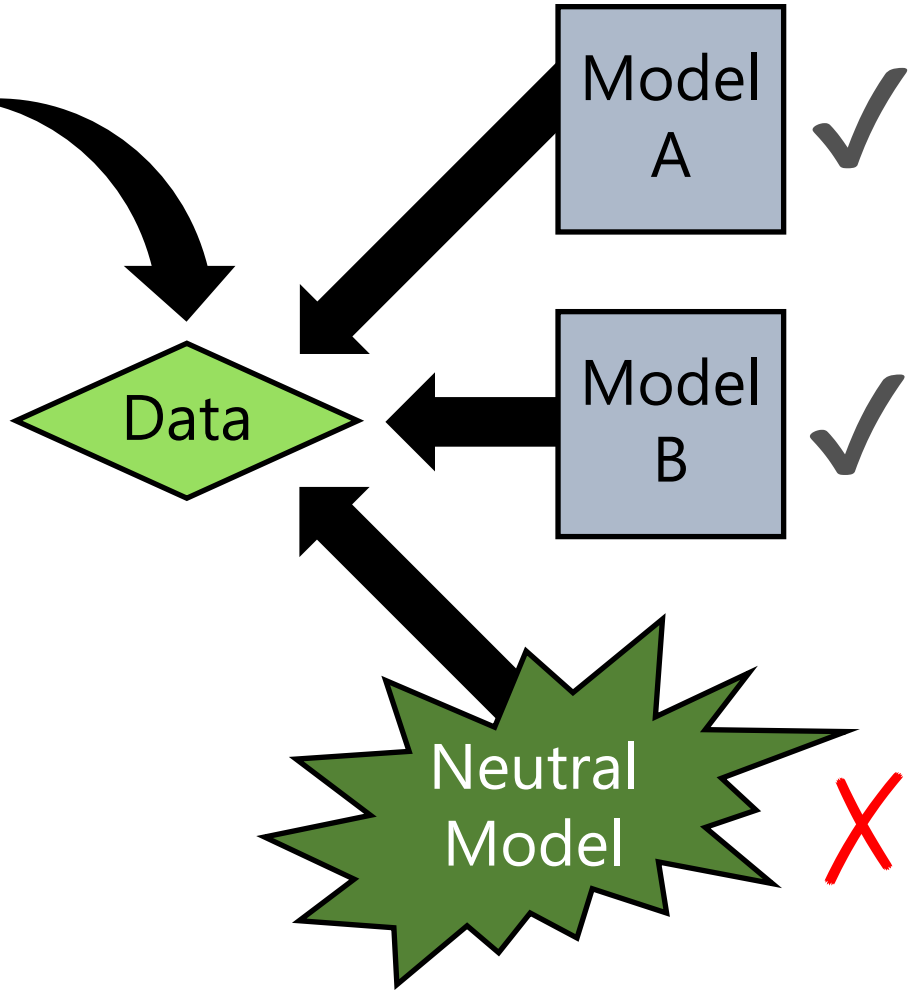
Data

Model A ✓

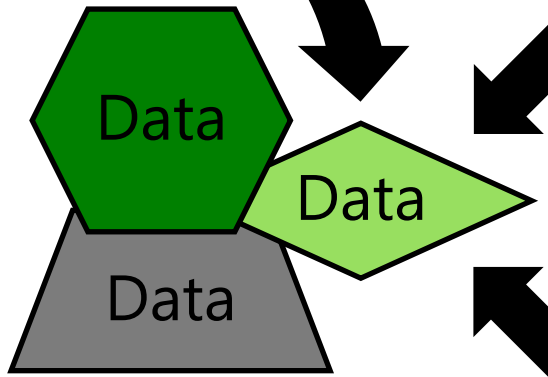
Model B ✓

Neutral Model ✓

Ecological Neutral Theory: How is it useful for understanding?



Ecological Neutral Theory: How is it useful for understanding?

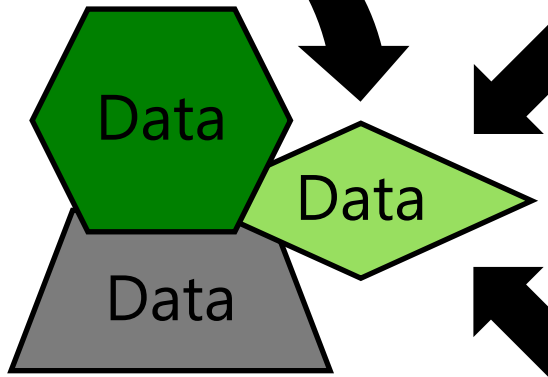


Model A ✗

Model B ✓

Neutral Model ✗

Ecological Neutral Theory:
How is it useful for understanding?

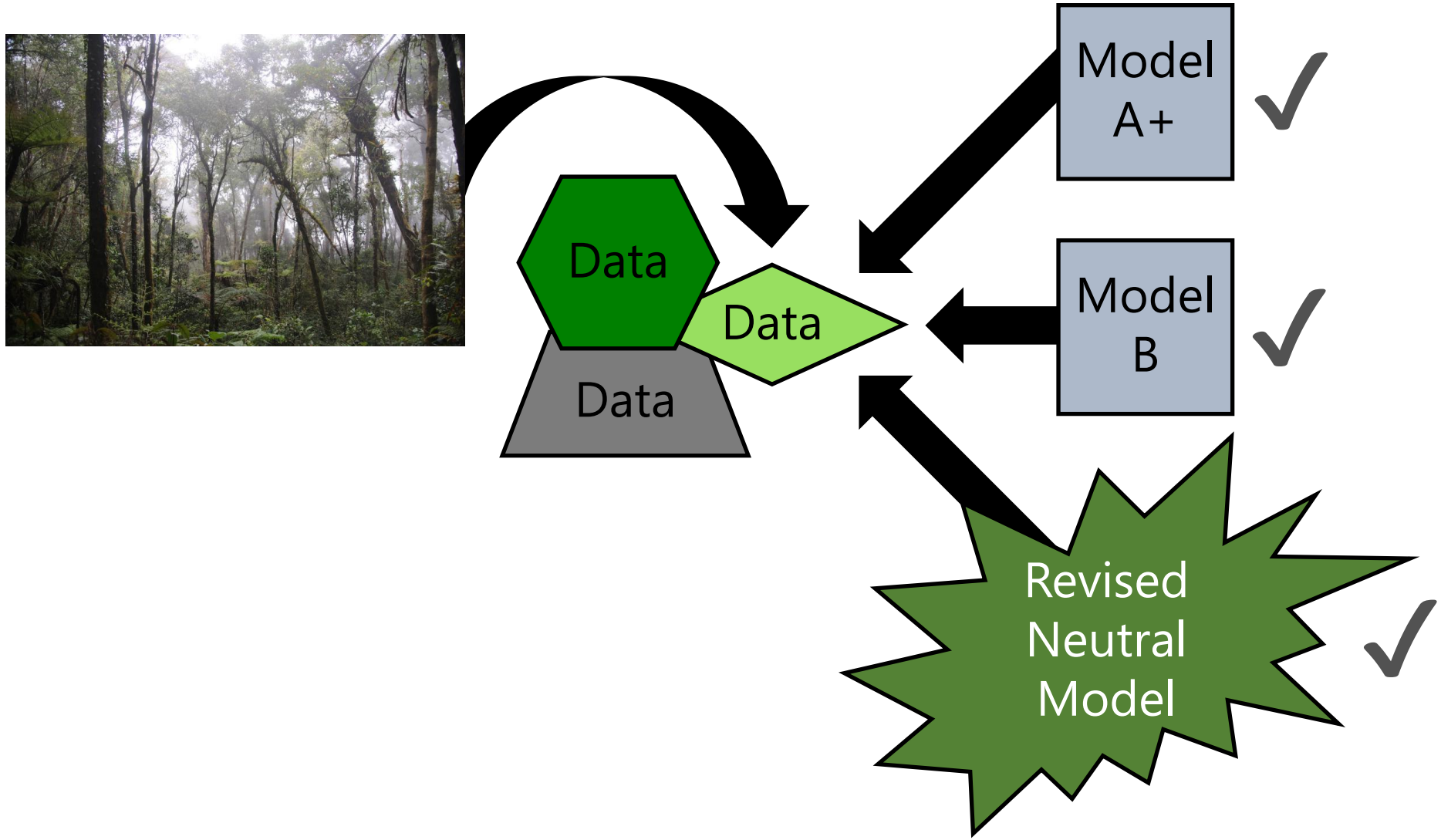


Model A+ ✓

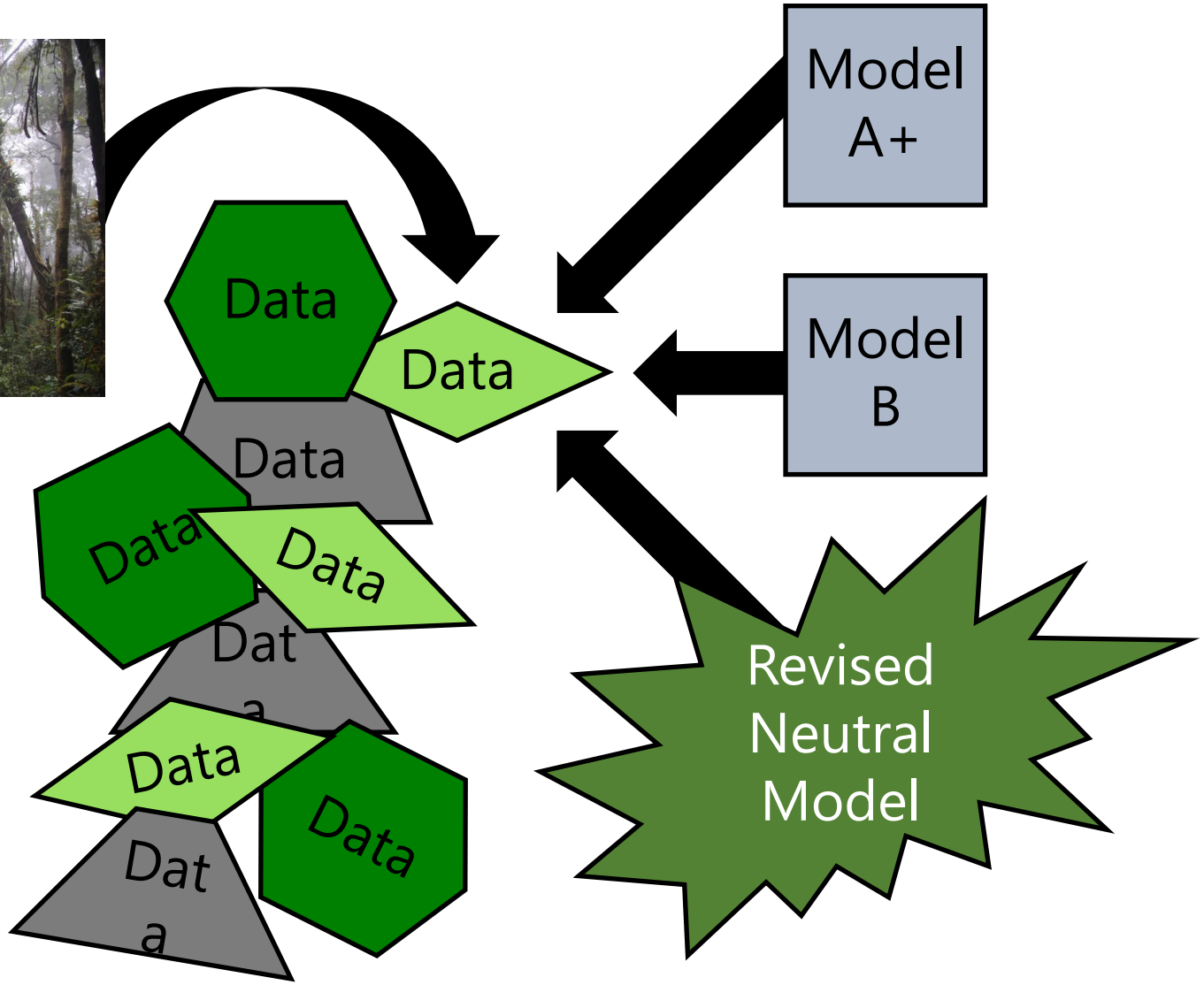
Model B ✓

Neutral Model ✗

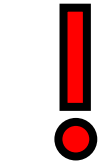
Ecological Neutral Theory: How is it useful for understanding?



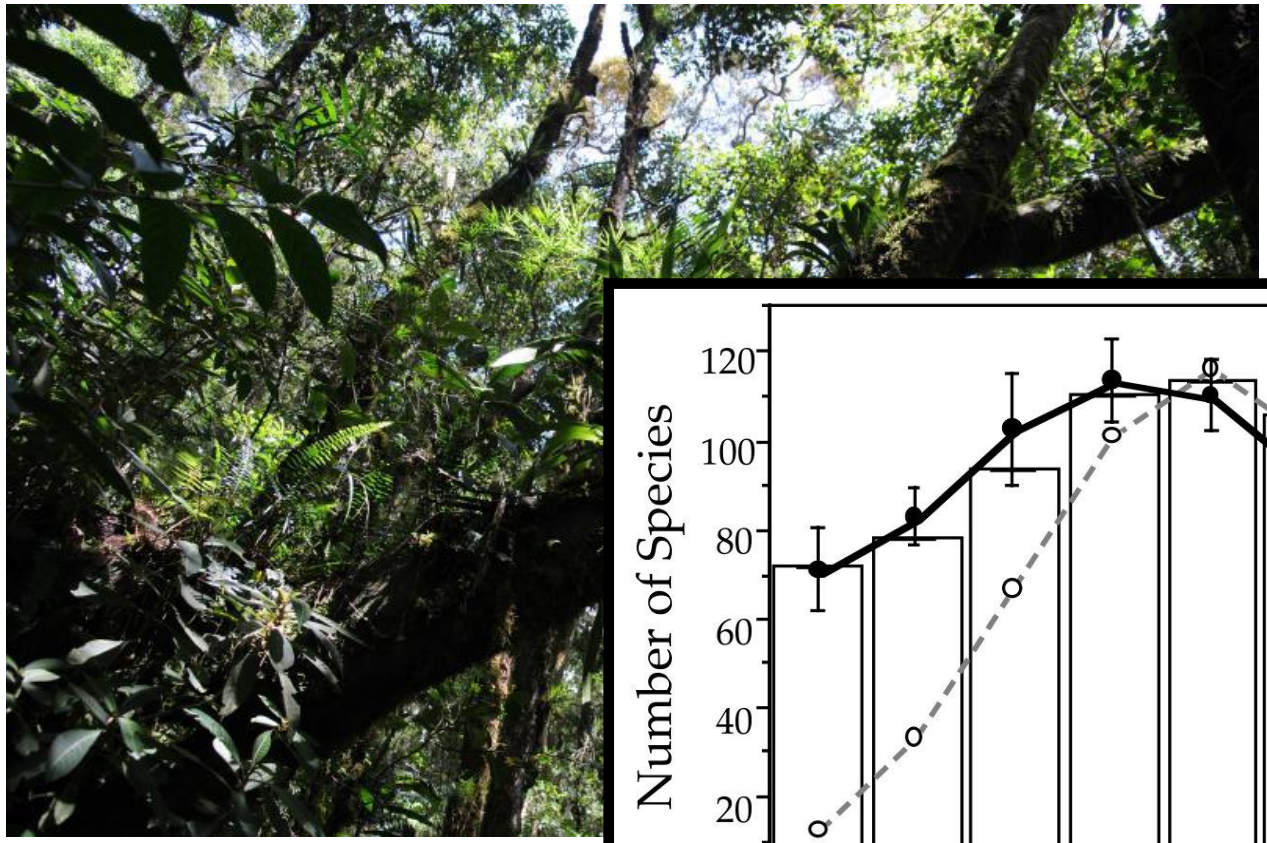
Ecological Neutral Theory: How is it useful for understanding?



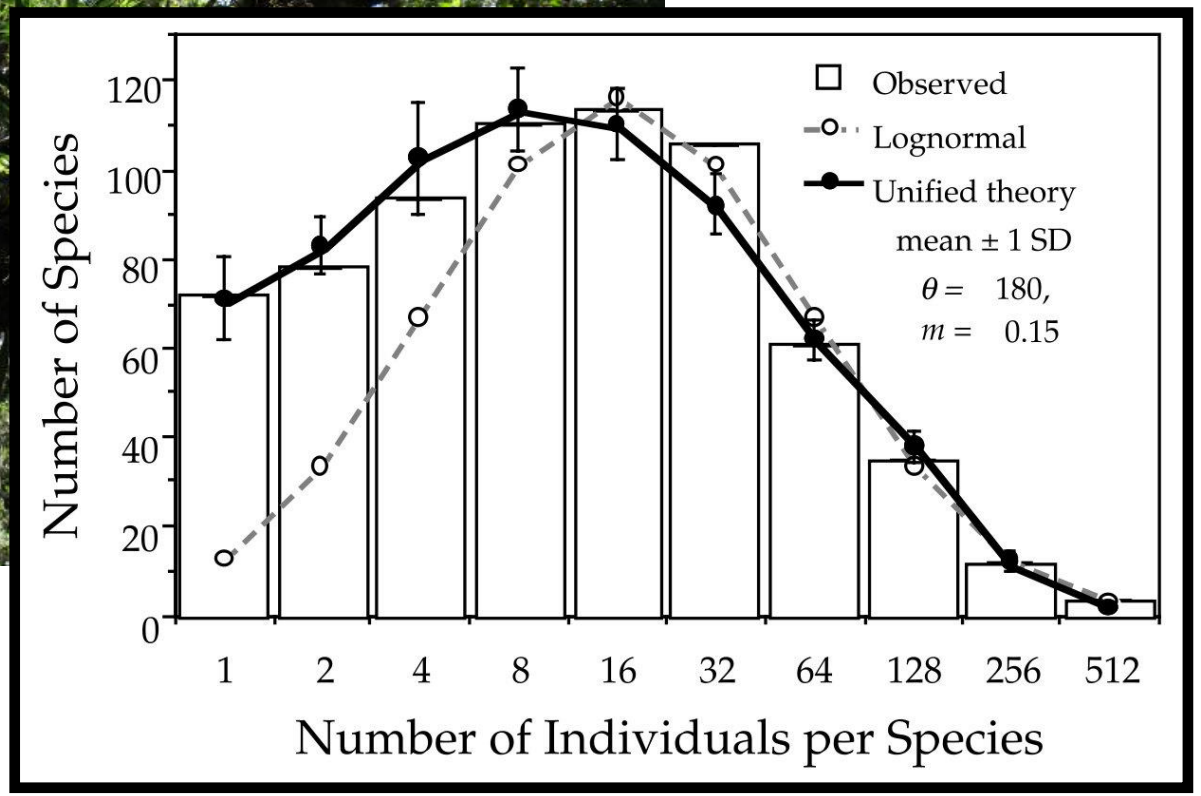
Example data comparison



Species abundance distributions



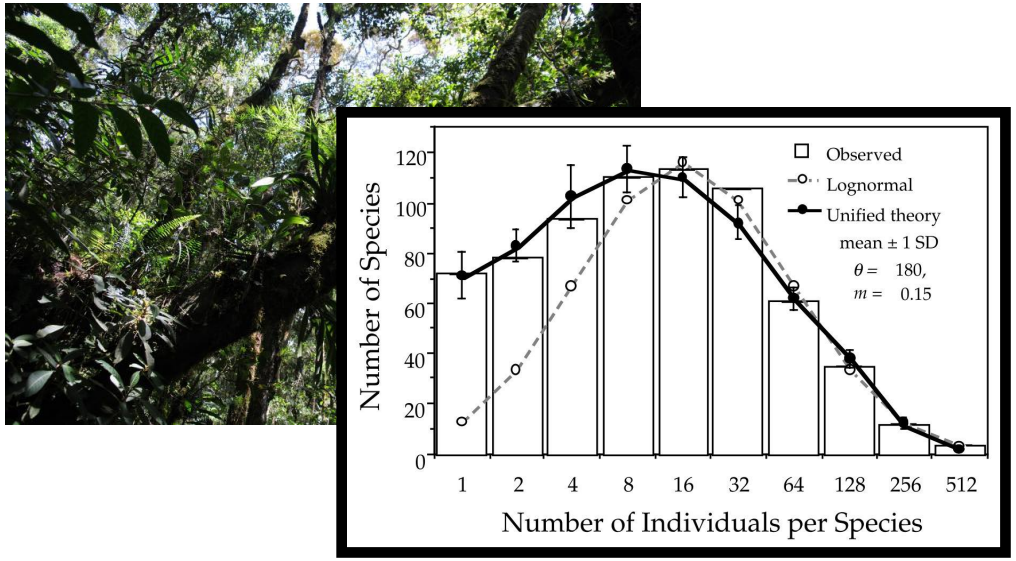
(Hubbell 2001)



Example data comparison

Mean species lifetimes are too short

(Ricklefs 2003, Nee 2005, Ricklefs 2006)

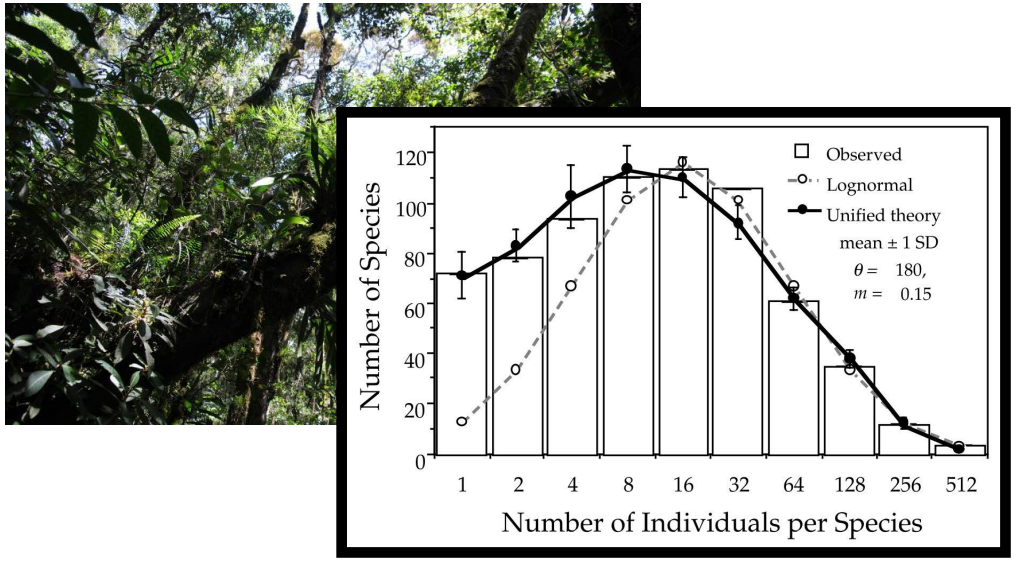


Example data comparison

Mean species lifetimes are too short

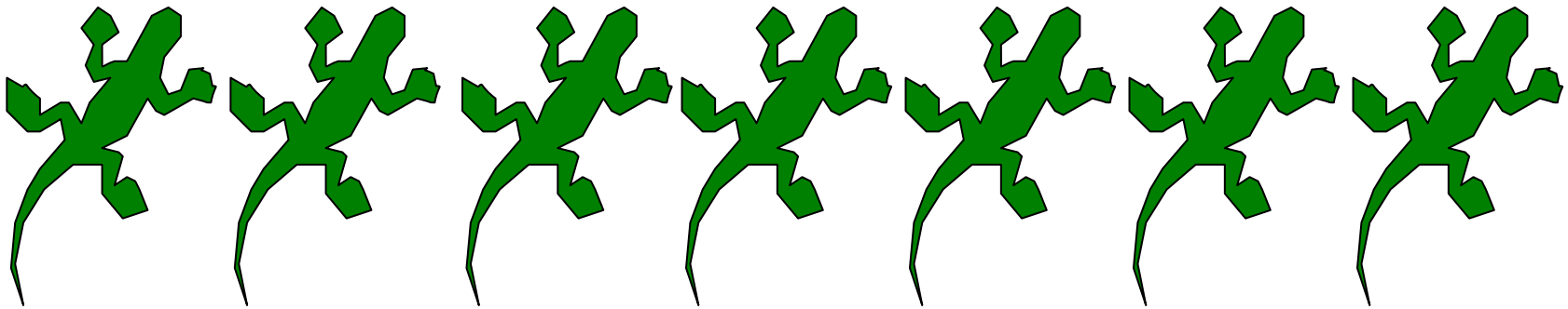
(Ricklefs 2003, Nee 2005, Ricklefs 2006)

but that was for point mutation speciation



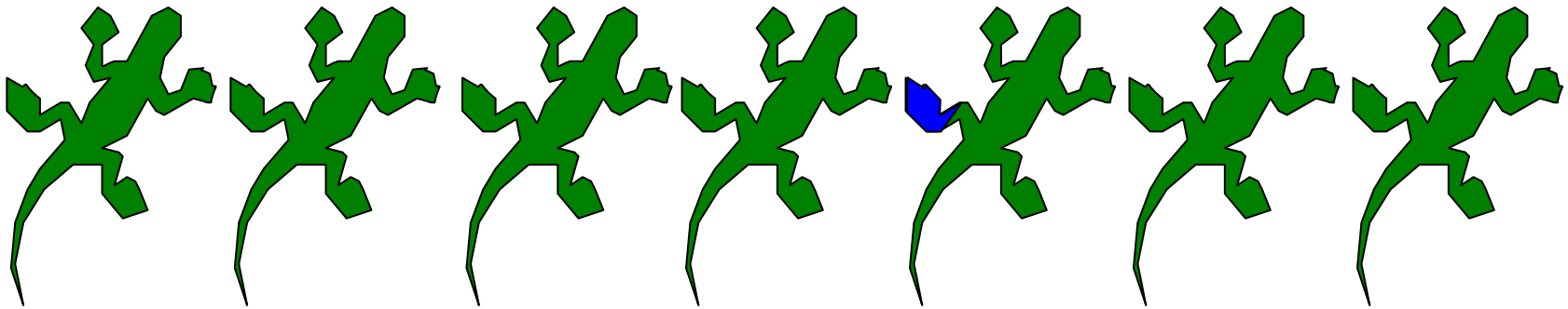
Protracted speciation

Not an instantaneous event



Protracted speciation

Not an instantaneous event



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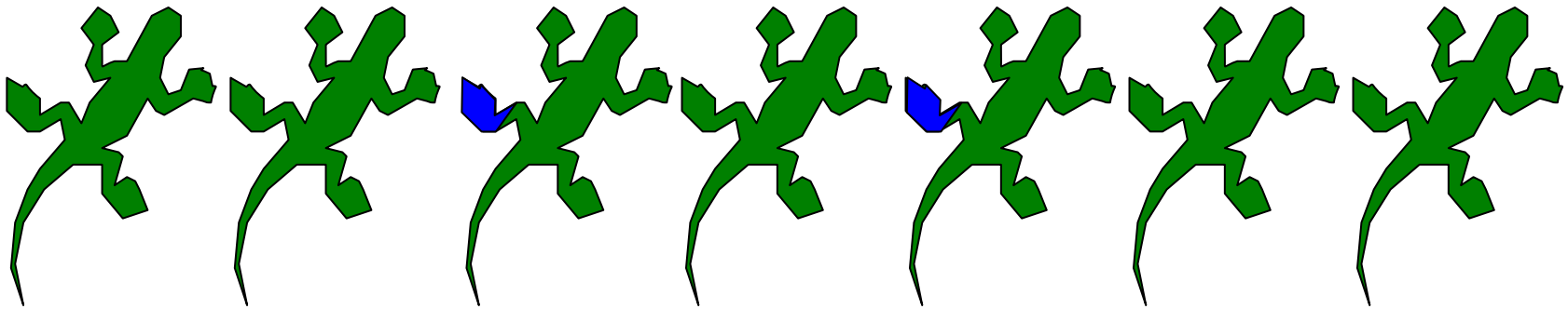

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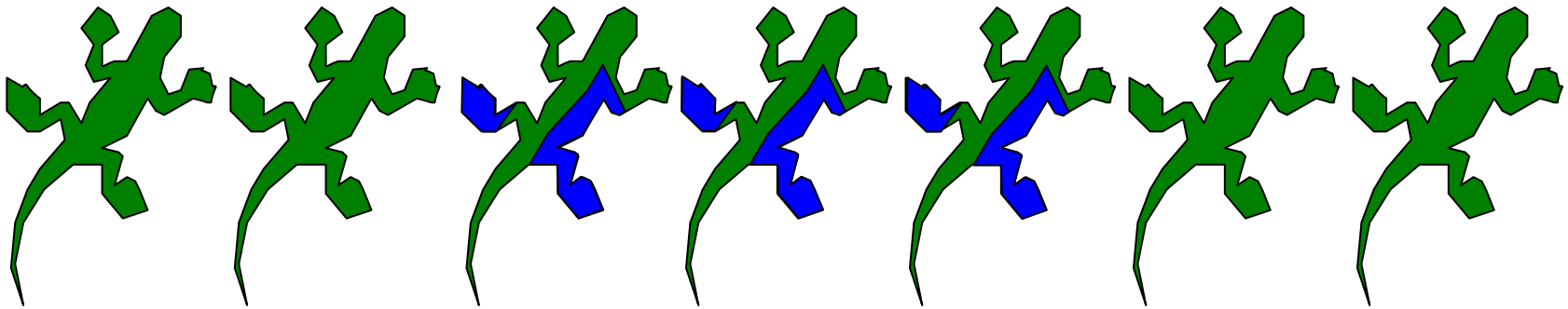

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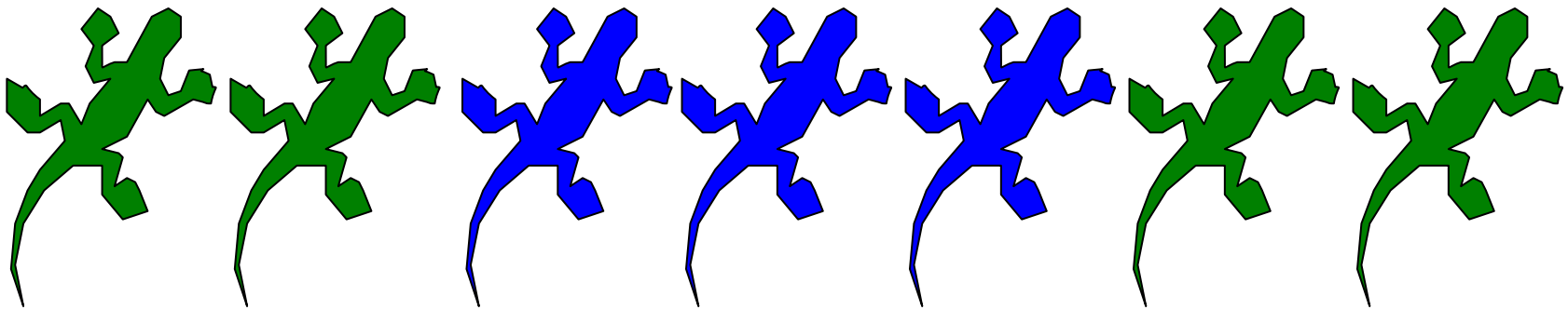
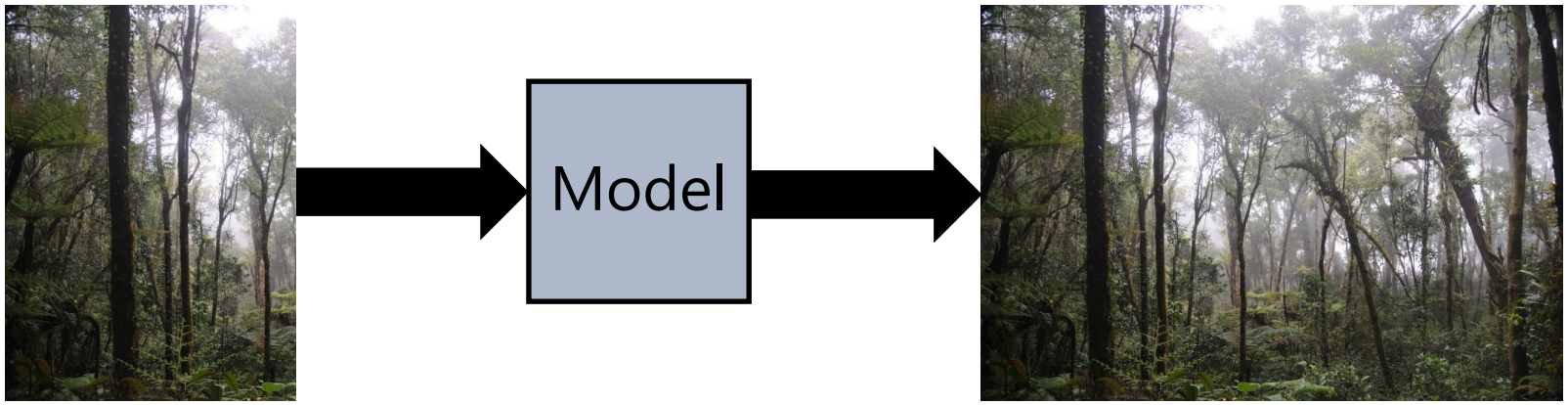


Ecological Neutral Theory: How is it useful for predicting?



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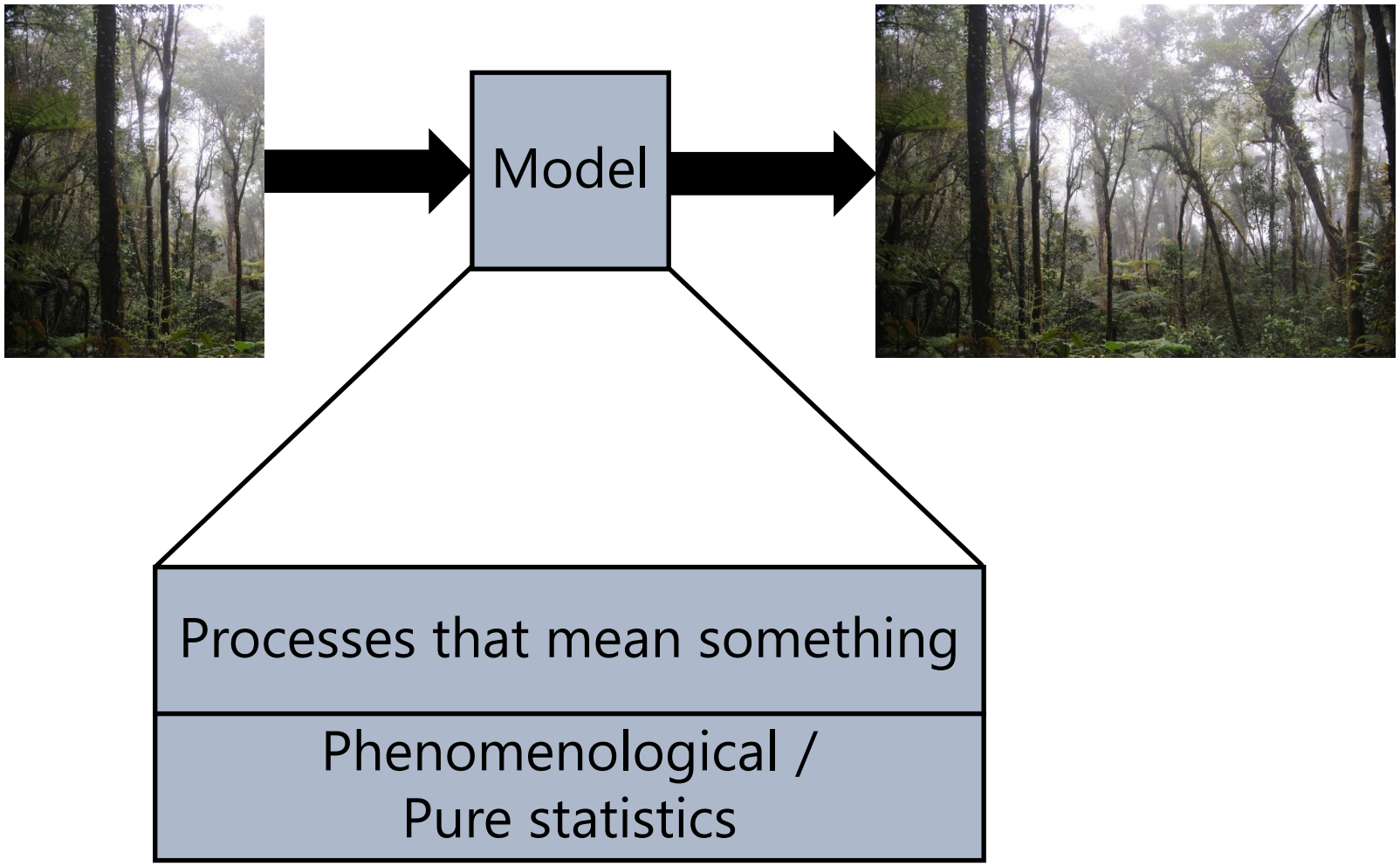

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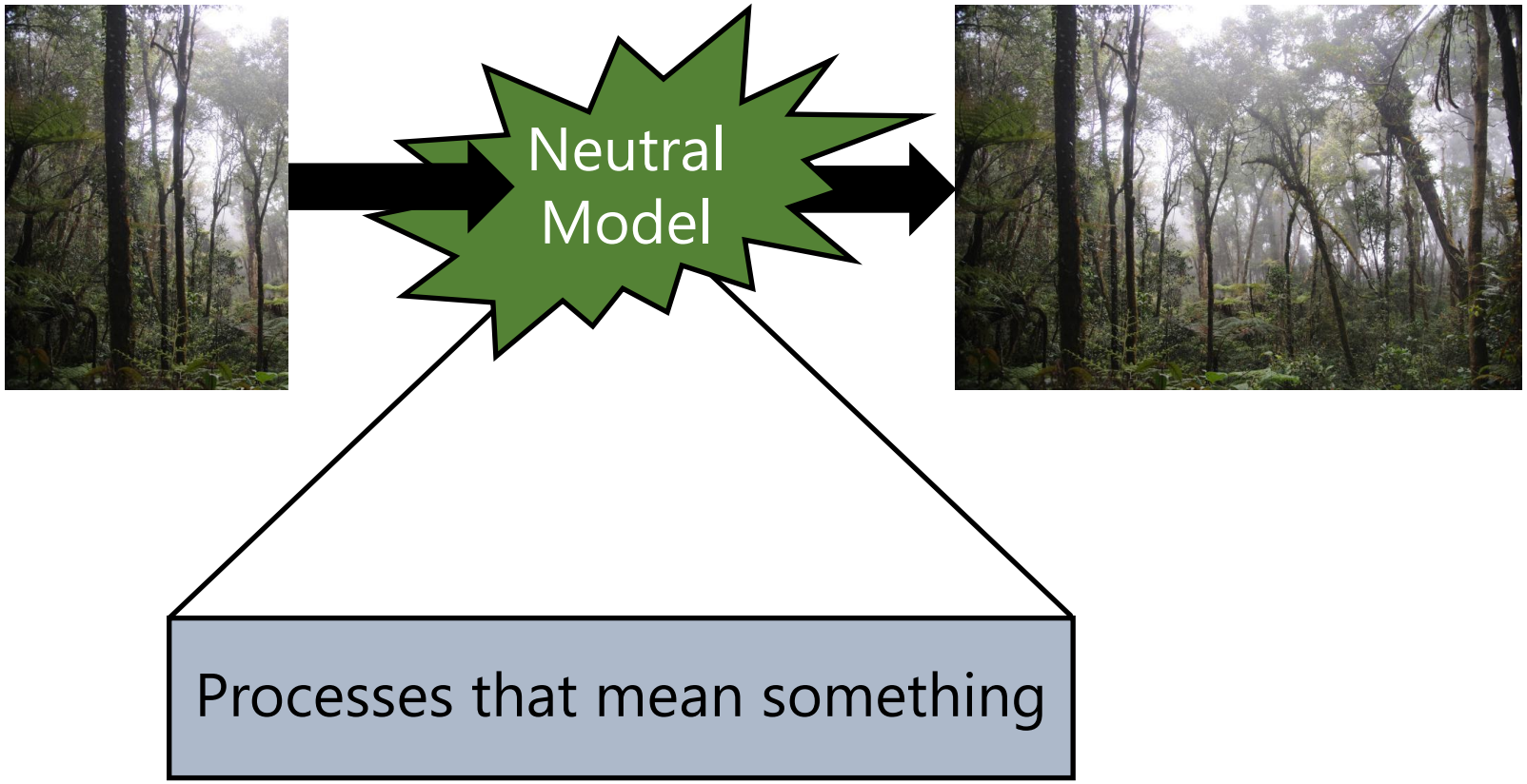
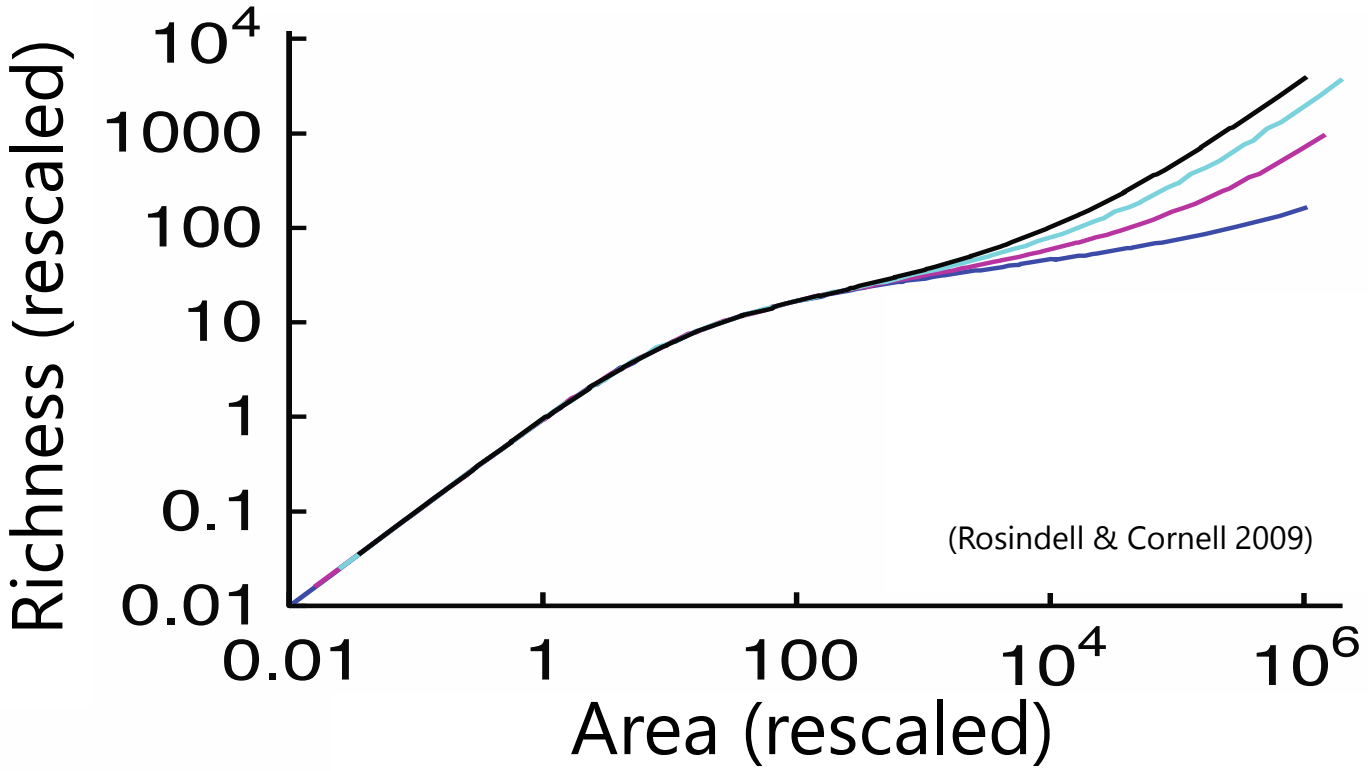
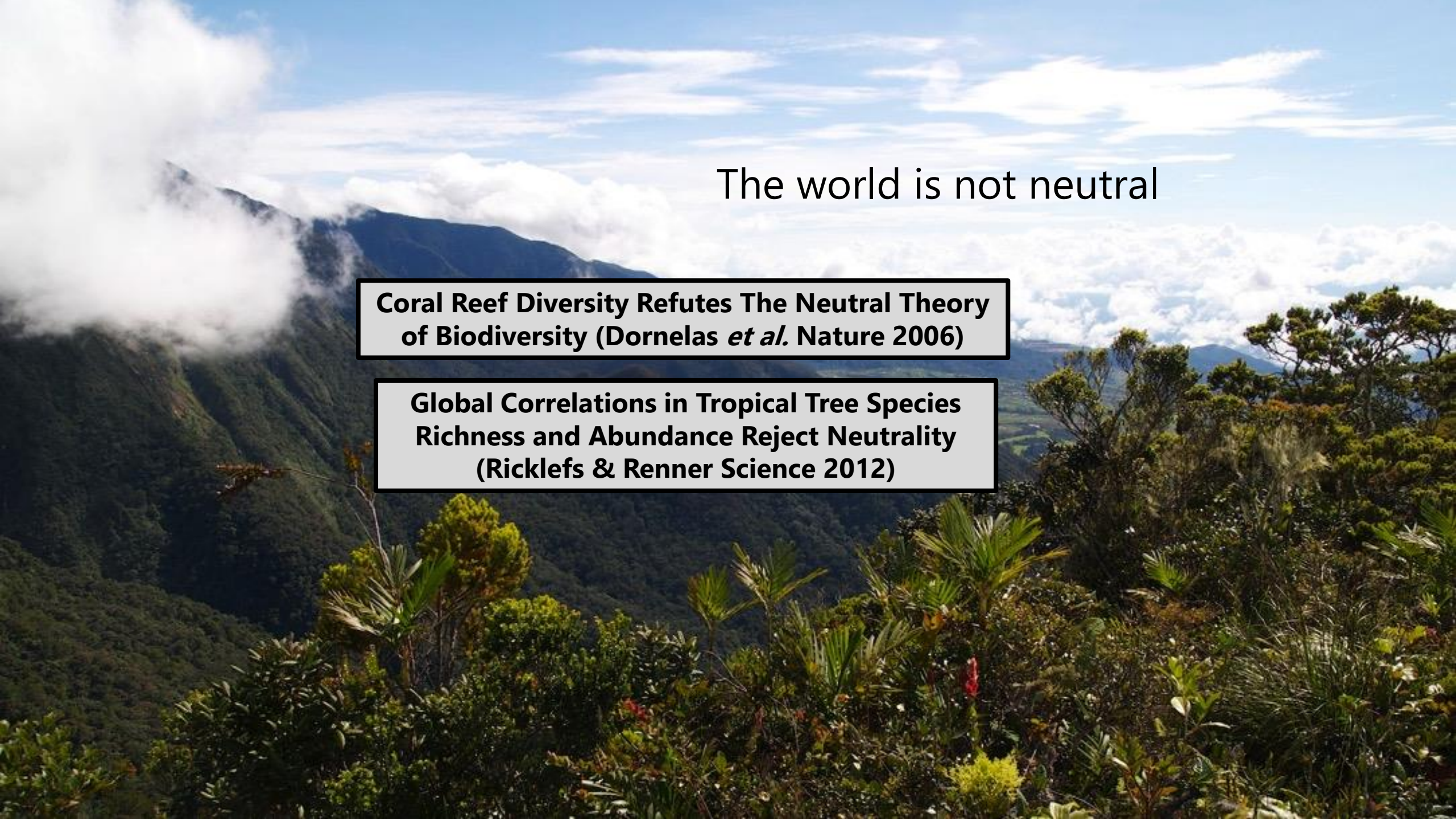


Species-area relationships

Species-area relationships

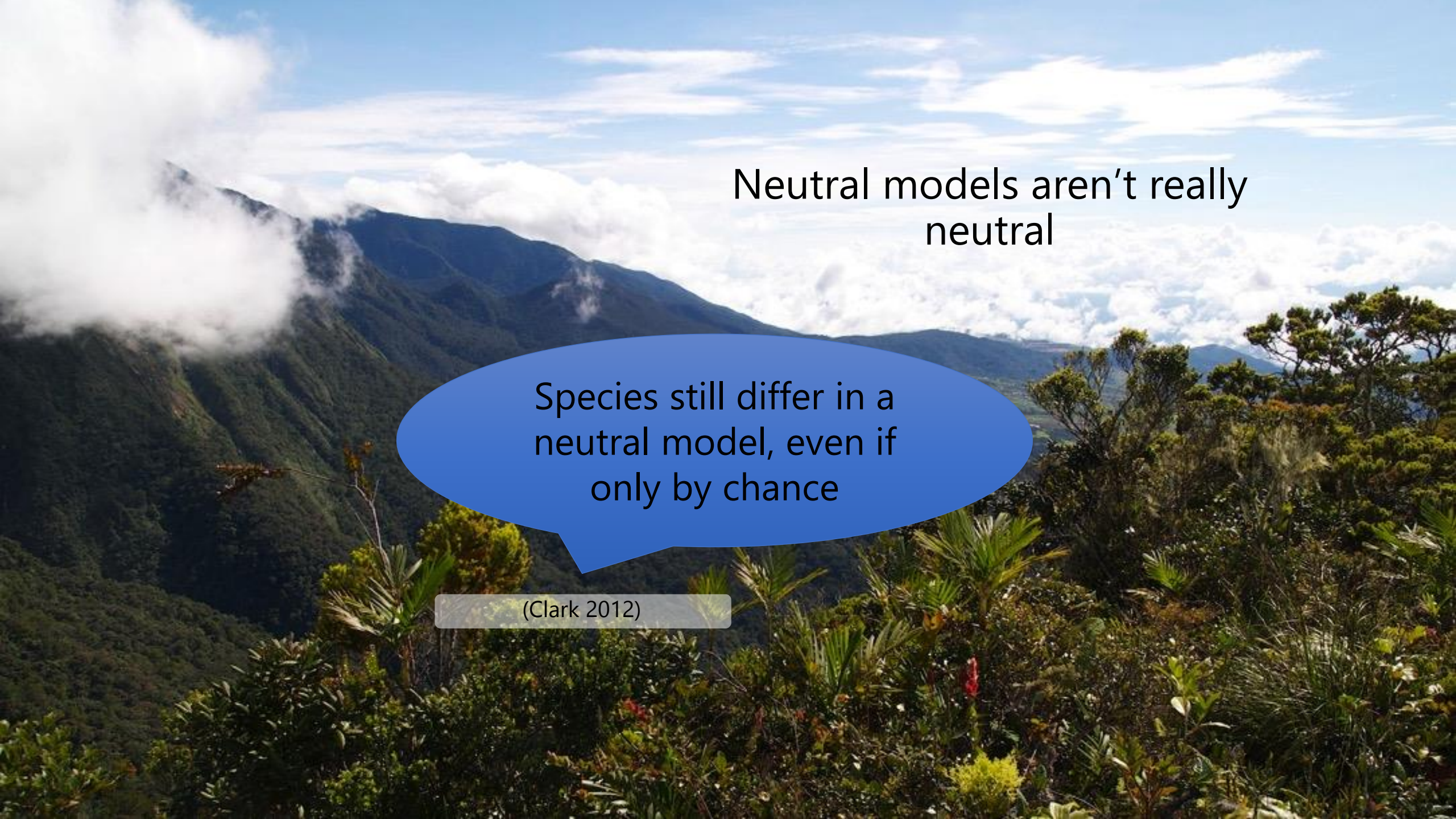




The world is not neutral

Coral Reef Diversity Refutes The Neutral Theory of Biodiversity (Dornelas *et al.* Nature 2006)

Global Correlations in Tropical Tree Species Richness and Abundance Reject Neutrality (Ricklefs & Renner Science 2012)



Neutral models aren’t really neutral

Species still differ in a neutral model, even if only by chance

(Clark 2012)

These are the real issues …

The link between pattern and process

The realism and instrumentalism perspectives

Tradeoff between simplicity and complexity

Ecological Neutral Theory

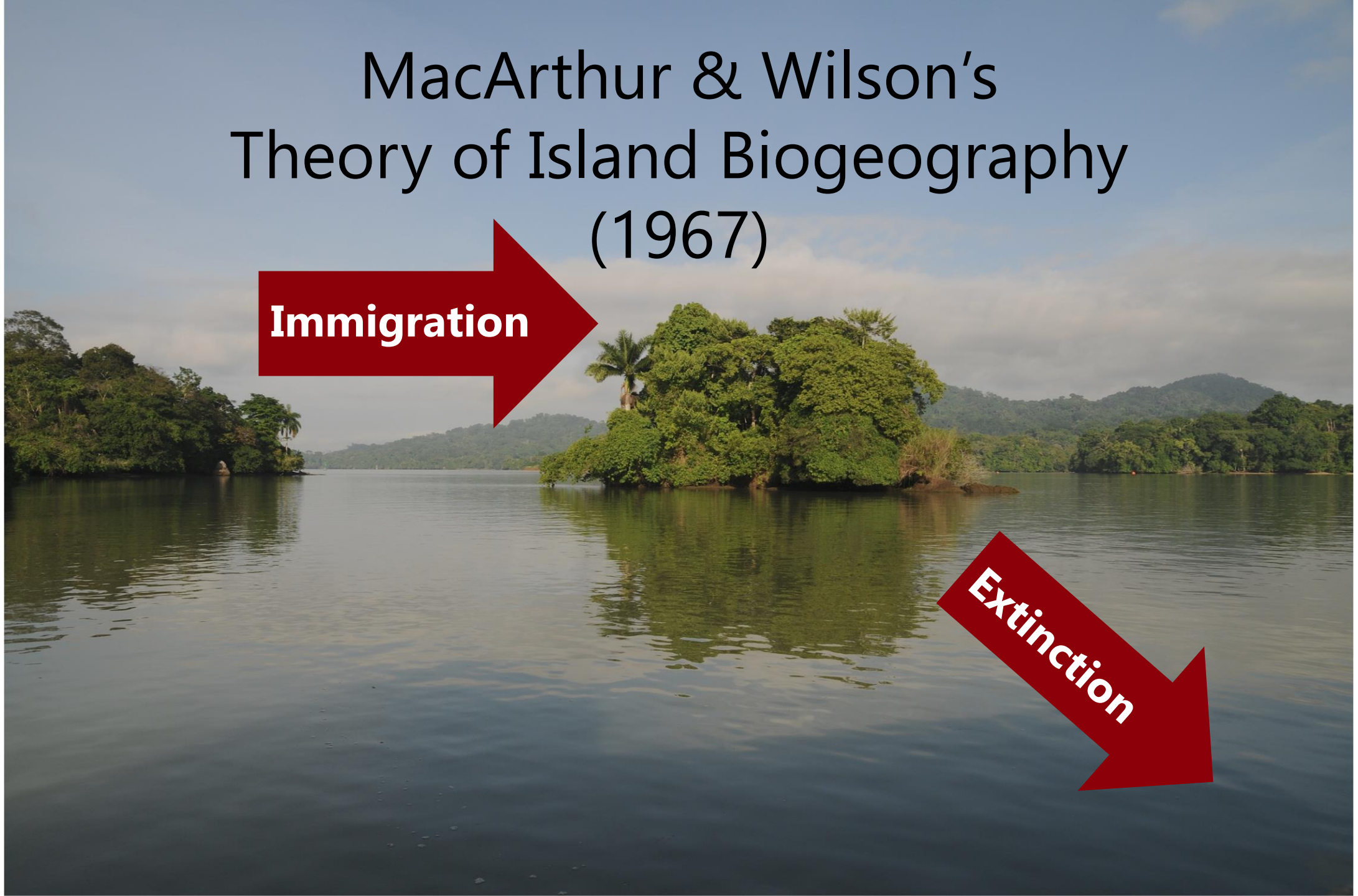
1. What is neutral theory?

2. Example neutral models

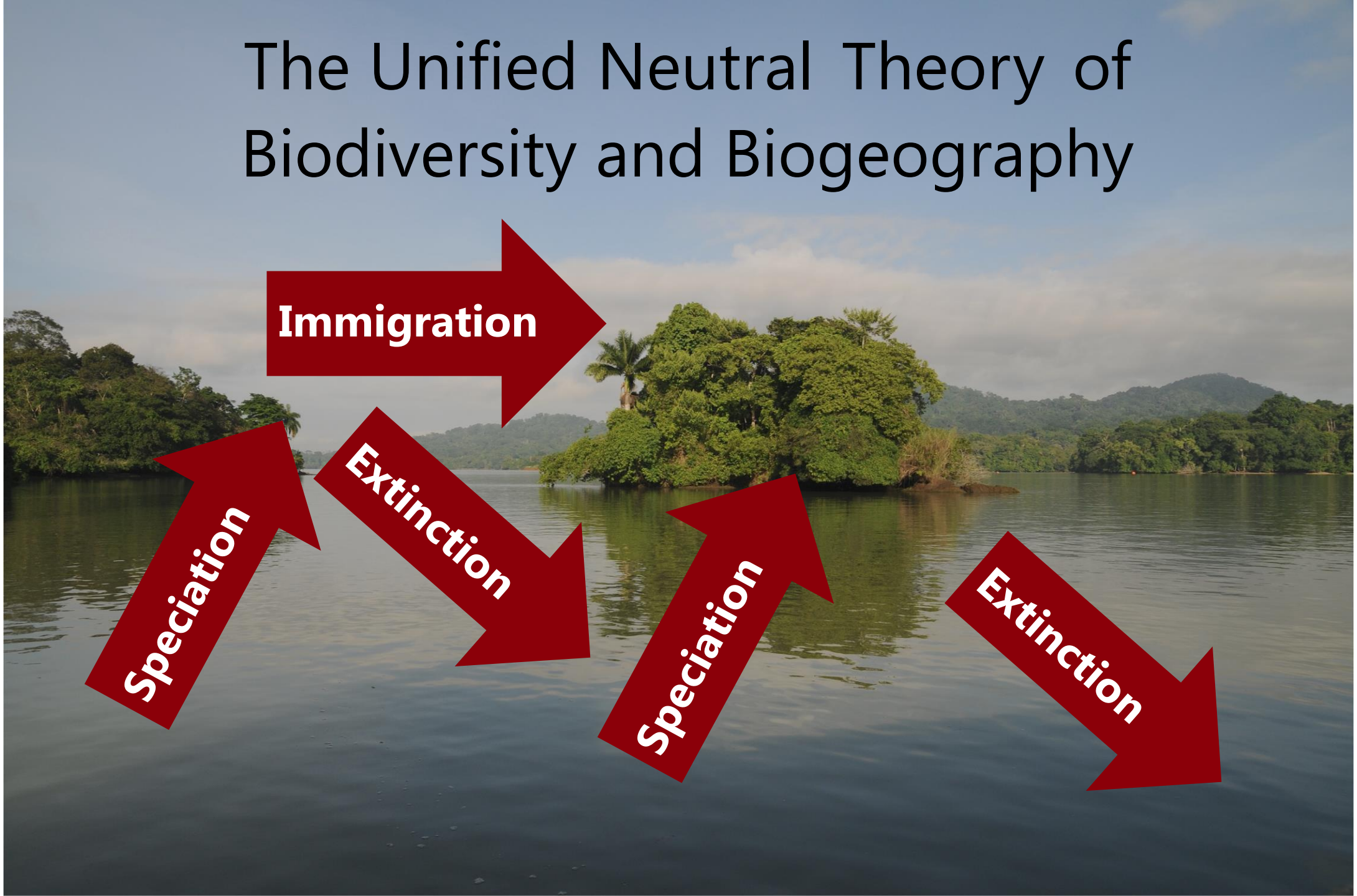
3. Uses of neutral theory

4. Applications in island biogeography

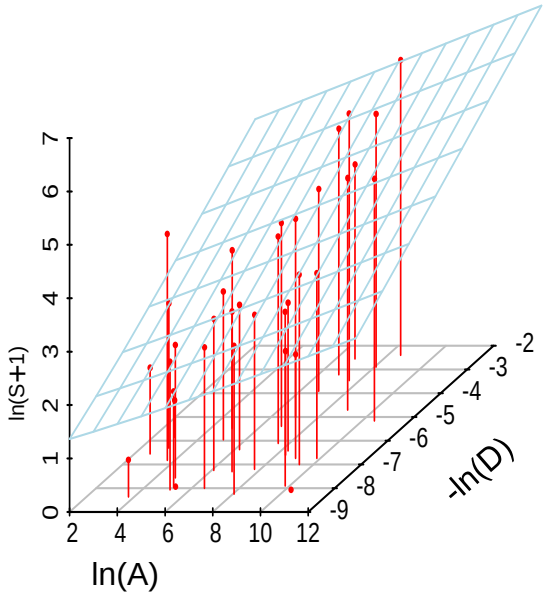
MacArthur & Wilson's Theory of Island Biogeography (1967)



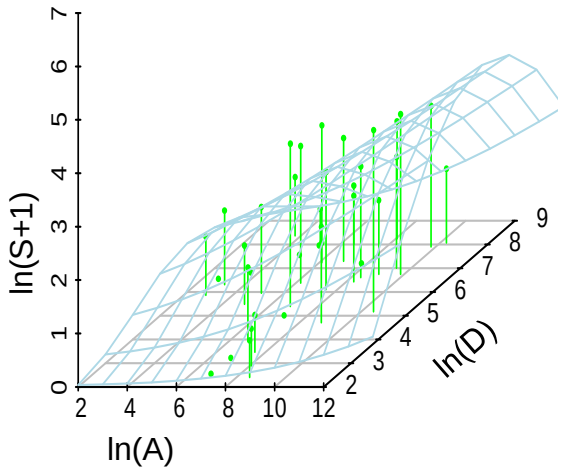
The Unified Neutral Theory of Biodiversity and Biogeography



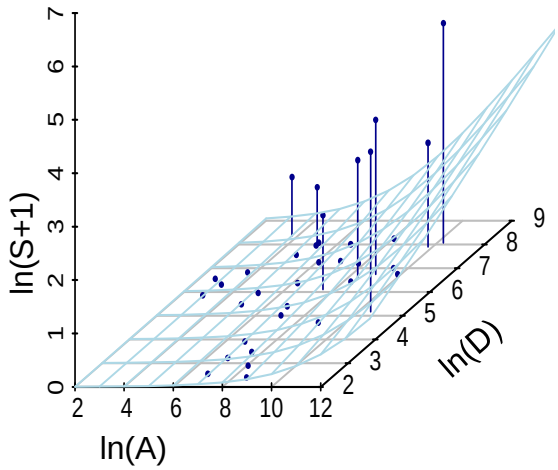
Empirical data: Island avifauna



Immigrant Species

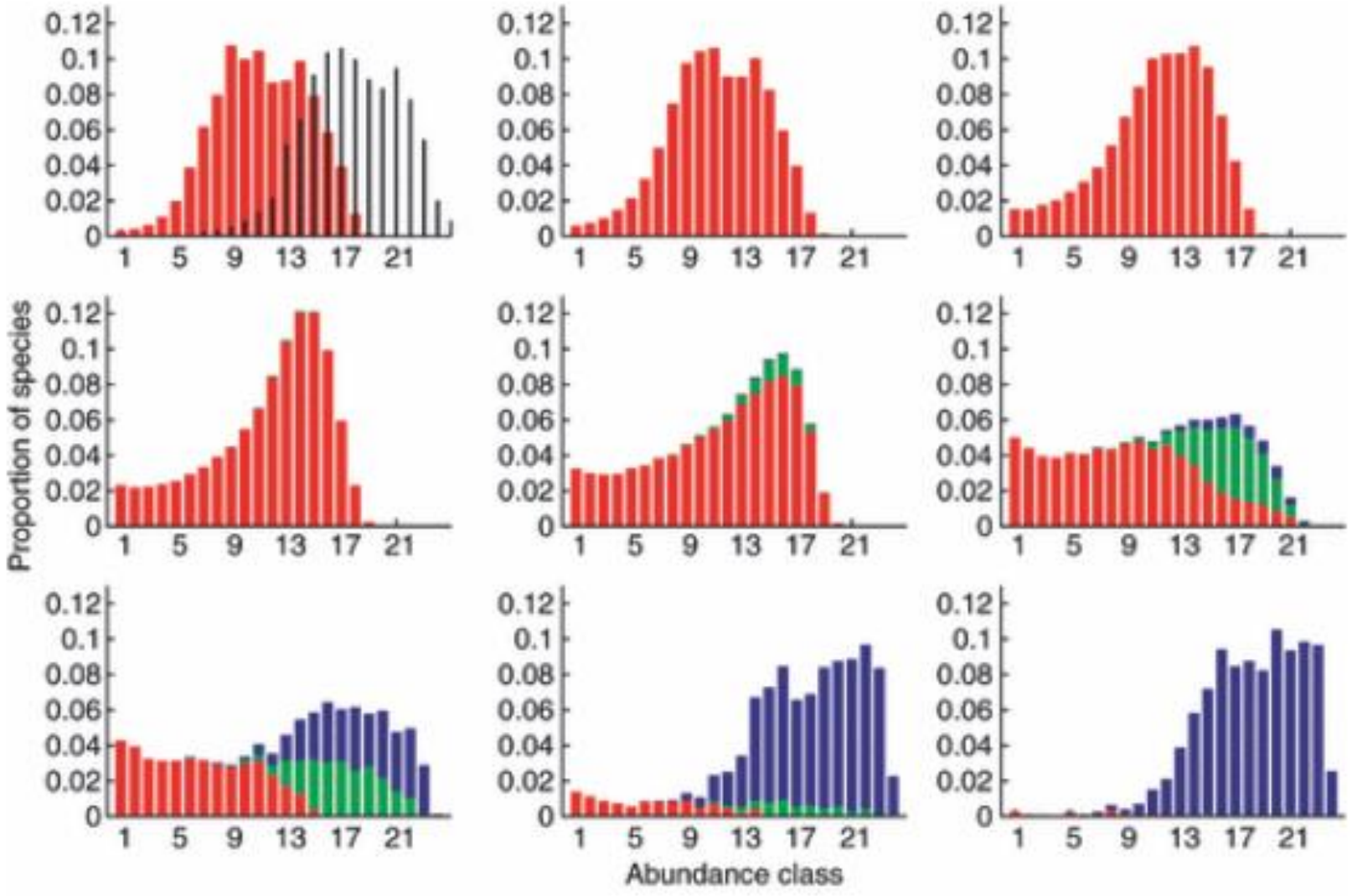


Anagenetic Species



Cladogenetic Species

Unified neutral theory simulations



(Rosindell & Phillimore 2011)

What have we learned about modeling

- John von Neumann “Give me four parameters, and I can fit an elephant. Give me five, and I can wiggle its trunk”.

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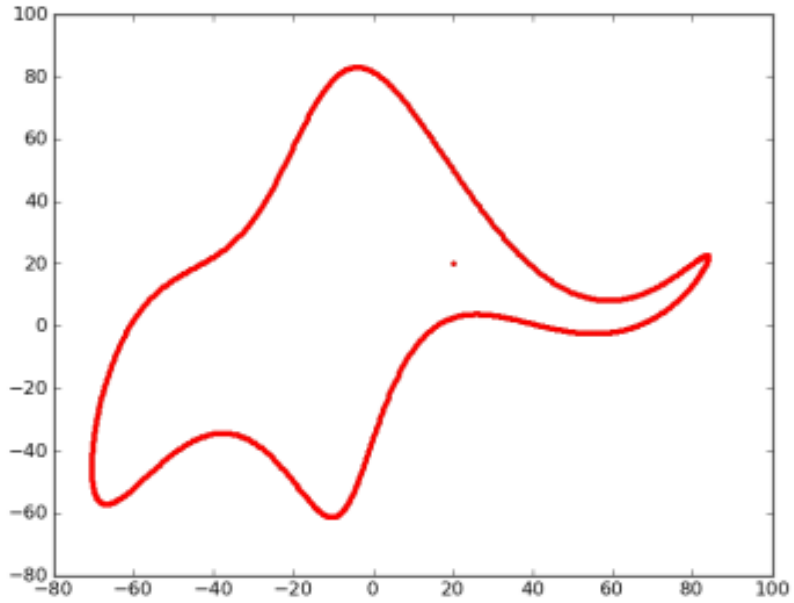

Mayer, Khaled Khairy, and Jonathon Howard (2010). “Drawing an elephant with four complex parameters”, Am. J. Phys. 78, 648, DOI:10.1119/1.3254017.

What we have learned about modelling

- John von Neumann “Give me four parameters, and I can fit an elephant. Give me five, and I can wiggle its trunk”.
- Theories in biology and in physics are very different
- Modelling for making predictions, and for gaining understanding are two different types of exercise
- Not all data are very informative
- Simplicity vs. complexity – only add complexity when it’s needed, use computers when needed
- Start with the end in mind

Neutral theory conclusions

- Neutral theory is a collection of neutral models assuming the demographic properties of an individual are independent of its species identity
- Useful for understanding and predicting but not both at the same time.
- Explains species area relationships and other spatial biodiversity patterns.
- Makes rich predictions about biodiversity and endemicity on islands.
- Neutral theory is one of the many useful tools you have in your tool box.

Today

- Ensure you have everything prepared to access the cluster
  - See the file “HPC starter checklist.pdf”

- Start working on the worksheet problems
  - To start with, these do not require cluster access

Tomorrow:

Learn more about parallel computing and how to run jobs on the cluster so you can attempt the more advanced sections of the worksheet at your pace.