Role of Modelling

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What is a Model ?

- Typically it is a simplification of reality
- Intended to be useful for a specific purpose at a specific scale (spatial and temporal) ".. it is inappropriate to be concerned about mice when there are tigers abroad"
- Often there are many different models of the same or similar phenomena.
- Differ in
  - what processes are included
  - what processes are excluded
  - what scales are required/useful
  - "All models are wrong, but some are useful"

The landscape is heterogeneous

Purposes of Modelling

- Basis of management tools for policy formulation (including online control)
- Predict future behaviour
- Design of monitoring systems (compliance)
- Help interpret experimental data
- Help explore and understand complex scientific, dynamic relationships
- Determine sensitivities to input data, parameter values and spatial scales

Modelling Approaches - 1

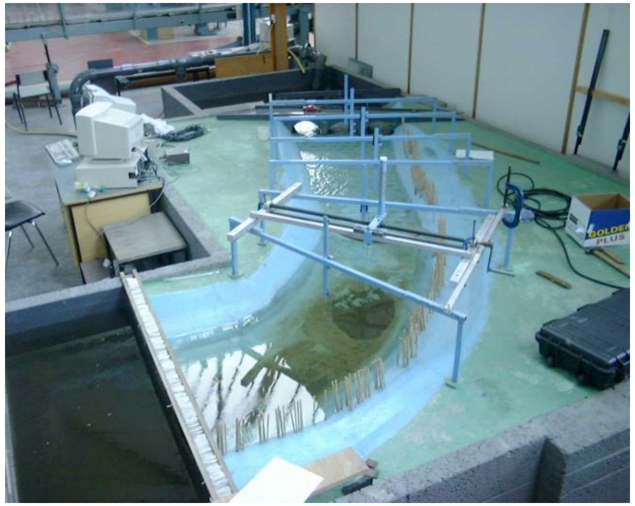
(i) Physical (scale)

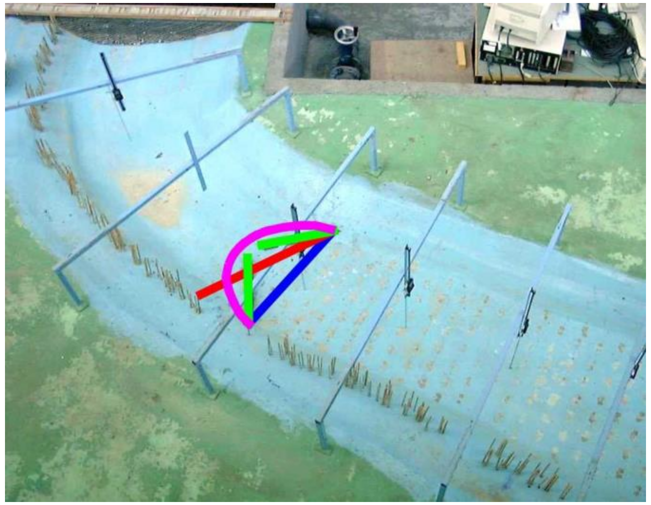
- Laboratory, or
- In the field

Physical Models

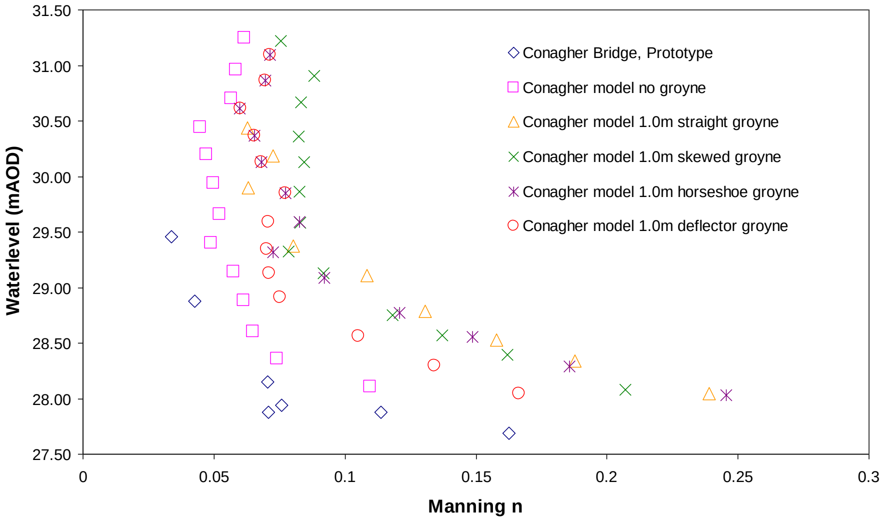
- Field

Physical Modelling of River Features





Laboratory



Physical Modelling of Rain effects

Constructed wetland for treating agricultural waste water – small scale

Modelling Approaches - 2

(ii) Mathematical / Numerical

- Mathematical (from principles/ laws)
- Numerical - Empirical (typically from analysing data)
- Numerical - Conceptual Model
- Numerical – Physically-based (or Process-based)

Steps in Modelling - I

- Define Purpose of modelling
- Determine Scope and accuracy requirements
- Determine information availability
- Resources available
- Choose modelling approach
- Choose existing model or develop new model

Modelling Issues – Commissioning or checking

- Fitness for purpose
- Spatial Scale
- Process detail / complexity
- Parameter estimation / ill-conditioning / equifinality / uncertainty / Fuzzy methods
- Validation (independent data)
- Flexibility / Robustness
- Models for management $\Rightarrow$ more physically-based ?
- Understanding and communicating limitations - credibility

Modelling Brief – technical - 1

- Define purpose and scope of project
- Define ultimate users (and their range of skill sets) of project output
- Define required information
- Define accuracy requirements
- Define ownership and copyright (if appropriate) of project data and outputs, including any software produced.
- Address compatibility issues (programming language, operating system, GIS and database support structure, data formats and storage

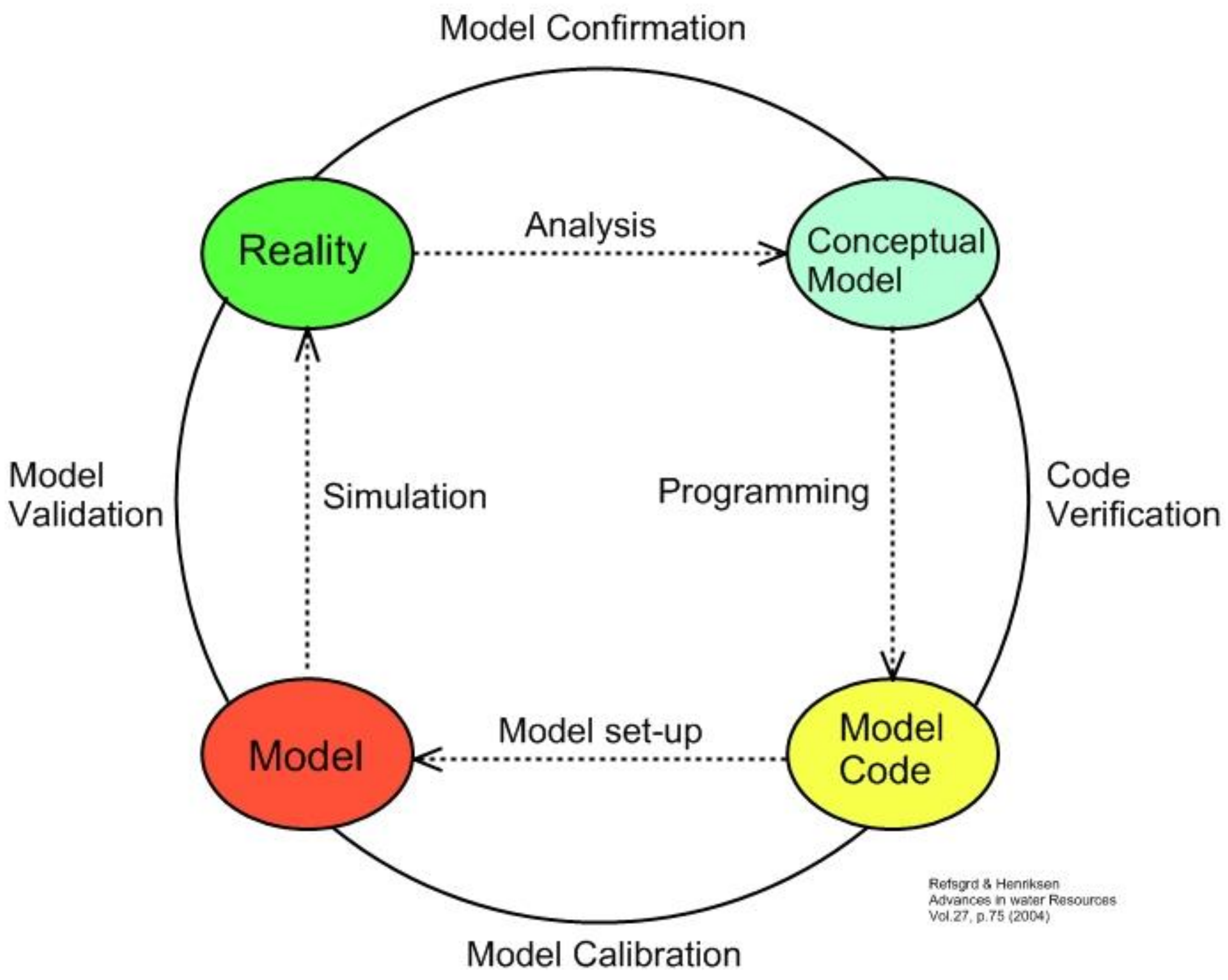
Modelling Brief – technical - 2

- Project may be commissioned in two or three phases, e.g.
  - (i) initial model scoping and data collection;
  - (ii) preliminary analysis – proof of concept;
  - (iii) model development.

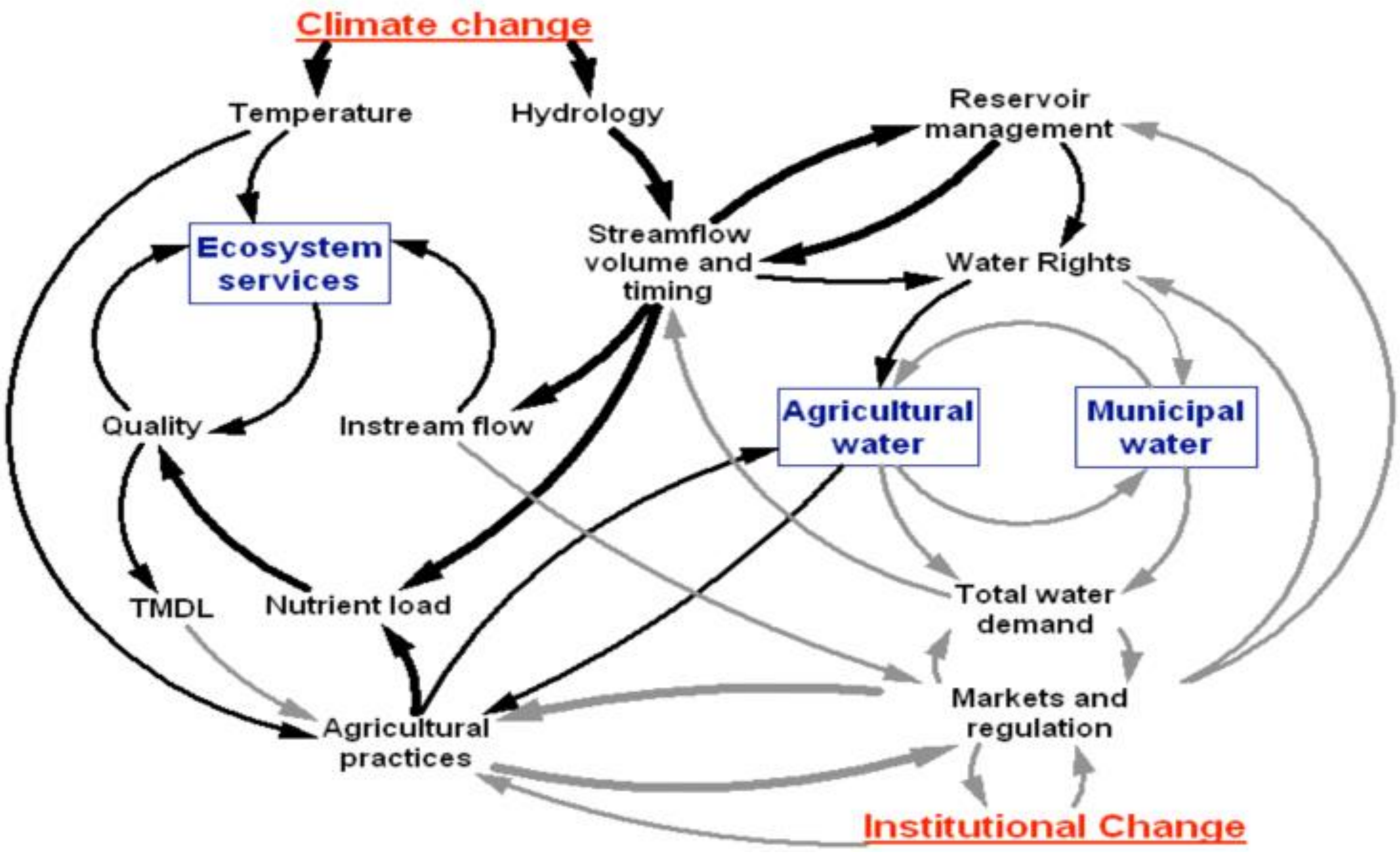
- Provide for internal and external review

- Specify projected time lines, milestones and deadlines.

Model development



Model Conceptualisation



Source: http://wisdm.wsu.edu/

Empirical Methods

- Data Mining: Focus on producing a relationship (e.g. equations or decision table) between the variables to be predicted (LHS) and the factors to be used to predict them (RHS) in the tool,

- Artificial intelligence algorithms

- Regression-type models (linear and nonlinear)

- Many packages available, plus easily used libraries in R and Python

Empirical Method – how it works

- Define quantities to be predicted by tool
- Decide on the factors (which influence them) to be included in equations or decision table
- Decide number and location of catchments required and assemble a data-base of the factors and the quantities to be predicted
- Study database to determine form of prediction relationship (equation or decision table) – incl. Cluster analysis for general patterns; threshold effects
- Calibrate equation or populate decision table
- Validate result
- Link with GIS user interface to form tool

Numerical - Equations

Lotka-Volerrra equations (prey – predator relationship)

x is population of prey

y is population of predators

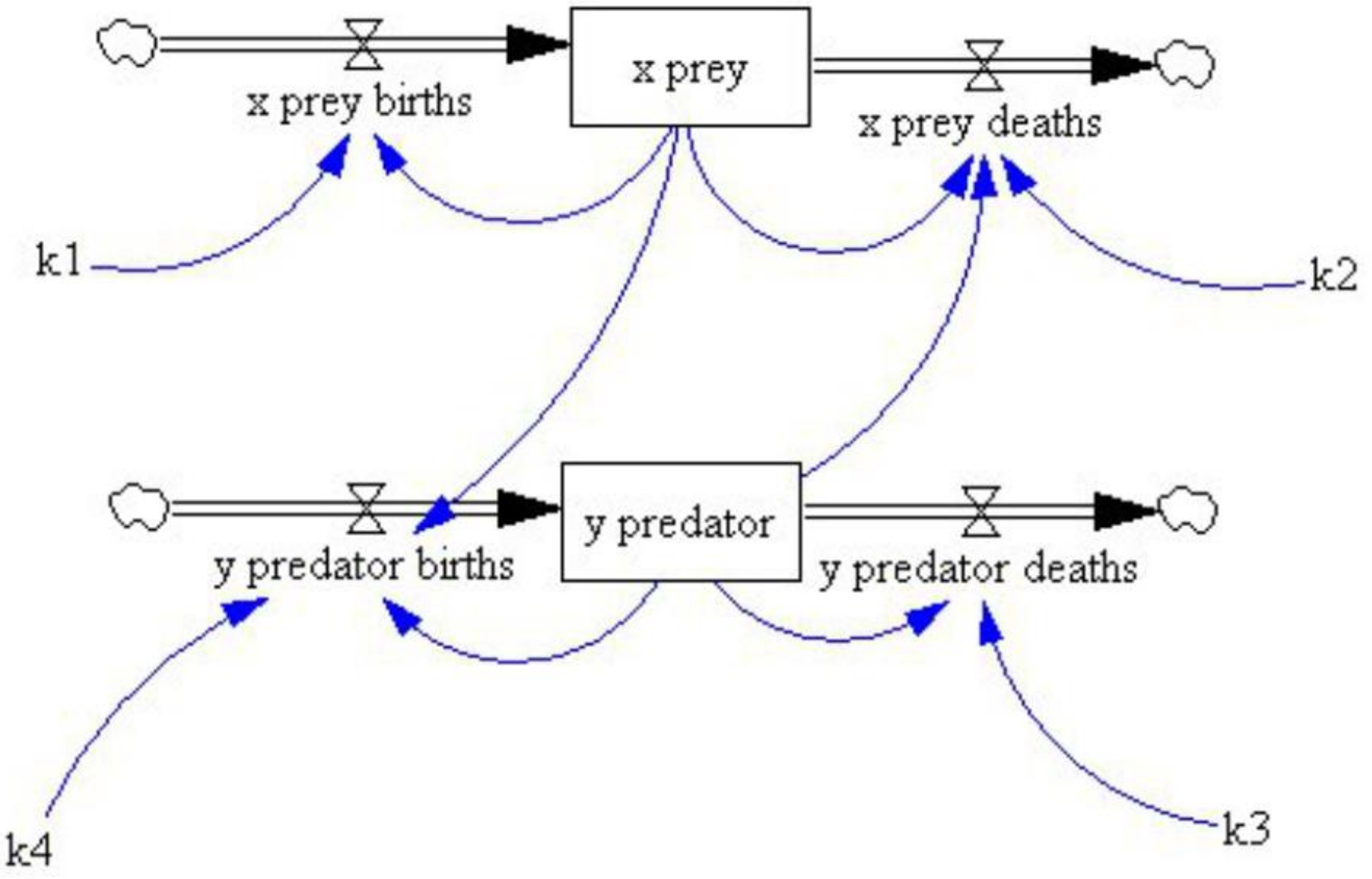
$$\frac{dx}{dt} = x\left(k_1 - k_2 y\right)$$

$$\frac{dy}{dt} = -y\left(k_3 - k_4 x\right)$$

Numerical - Equations

prey–predator relationship

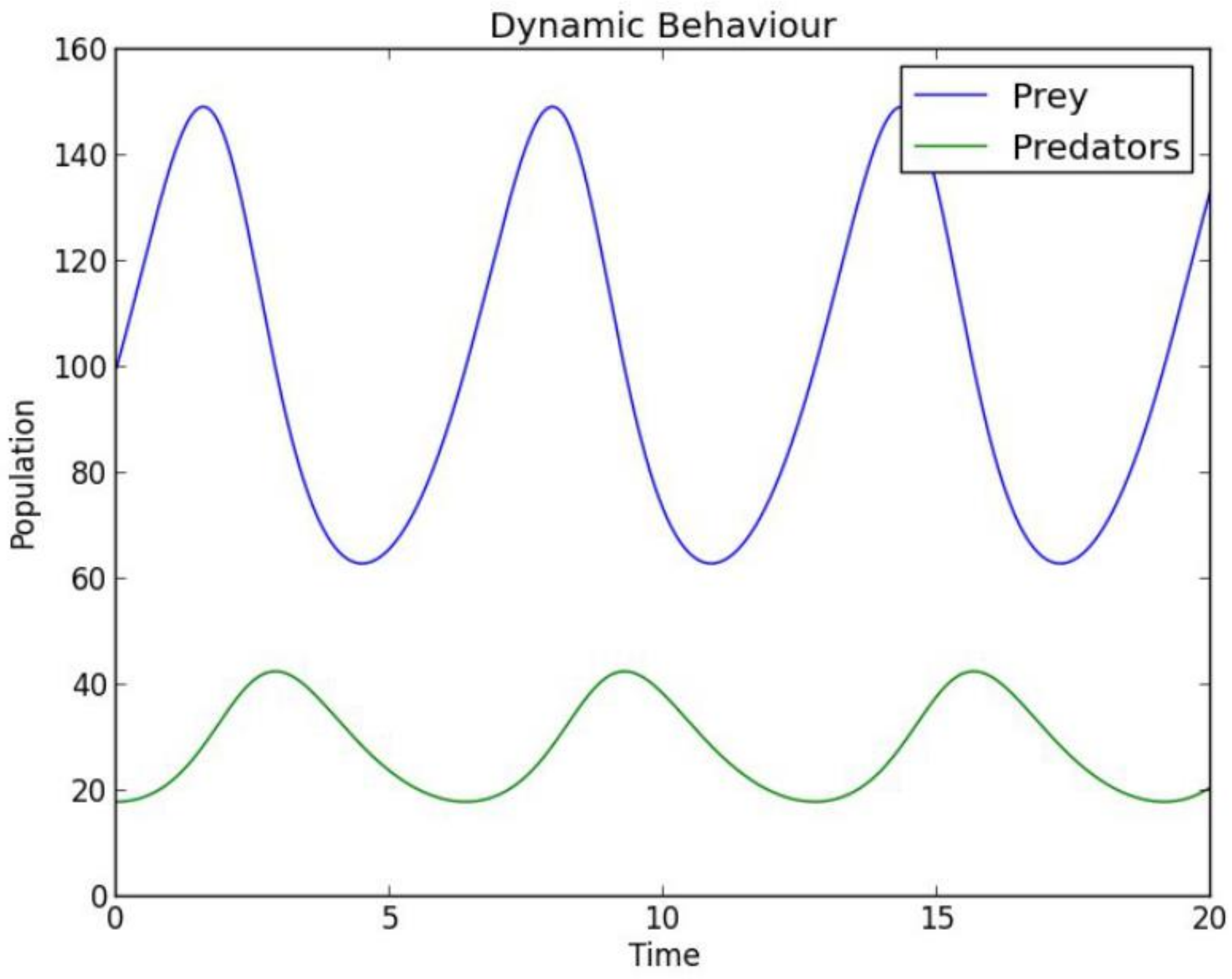
Model Conceptualisation



Numerical - Equations

Lotka-Volerrra equations (prey – predator relationship)

Simulation over time



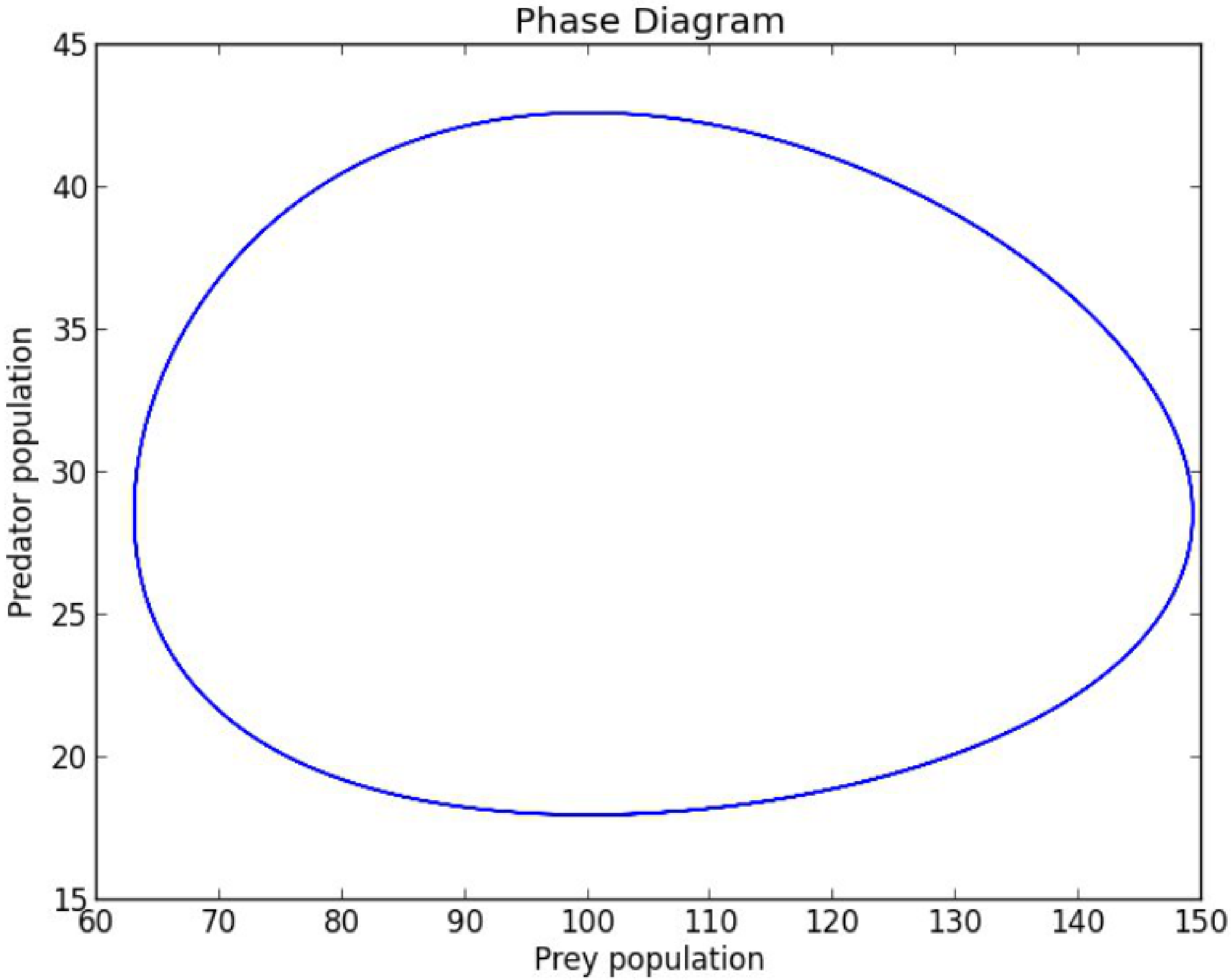
Numerical - Equations

Lotka-Volerrra equations
(prey – predator relationship)

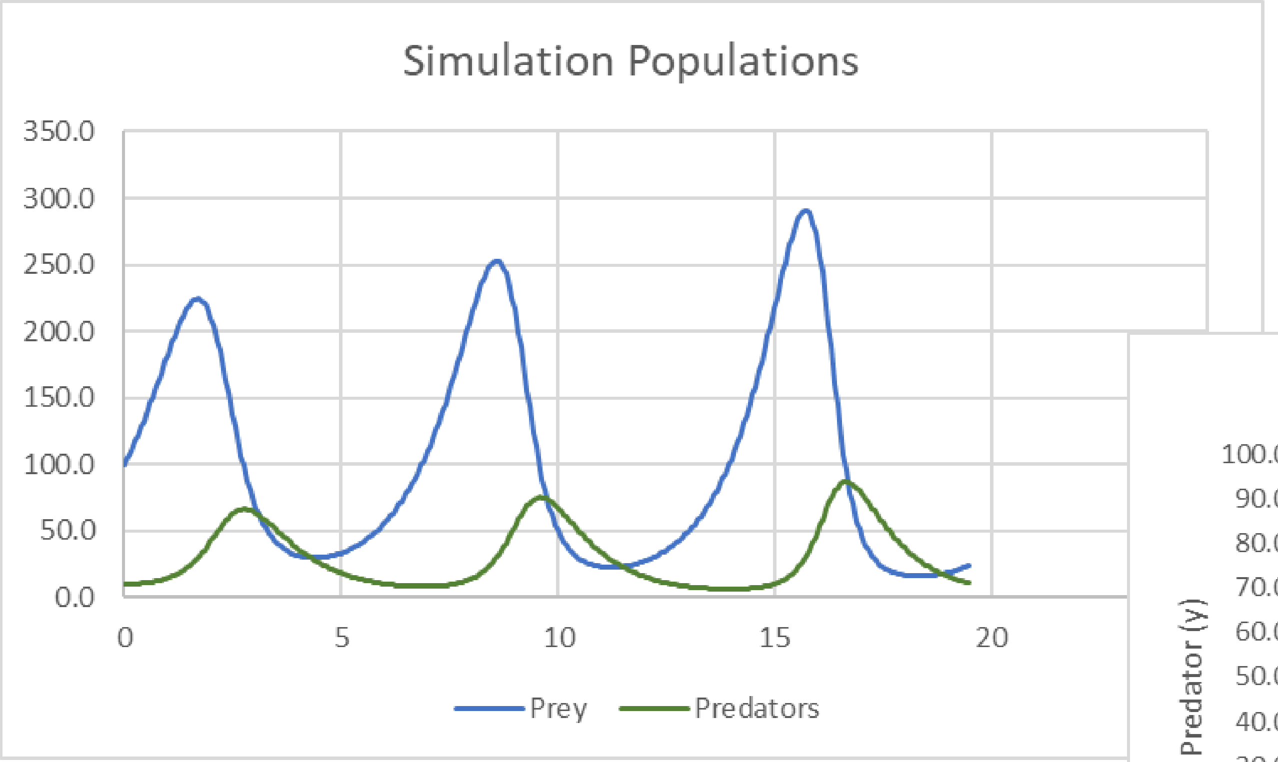
Examples:

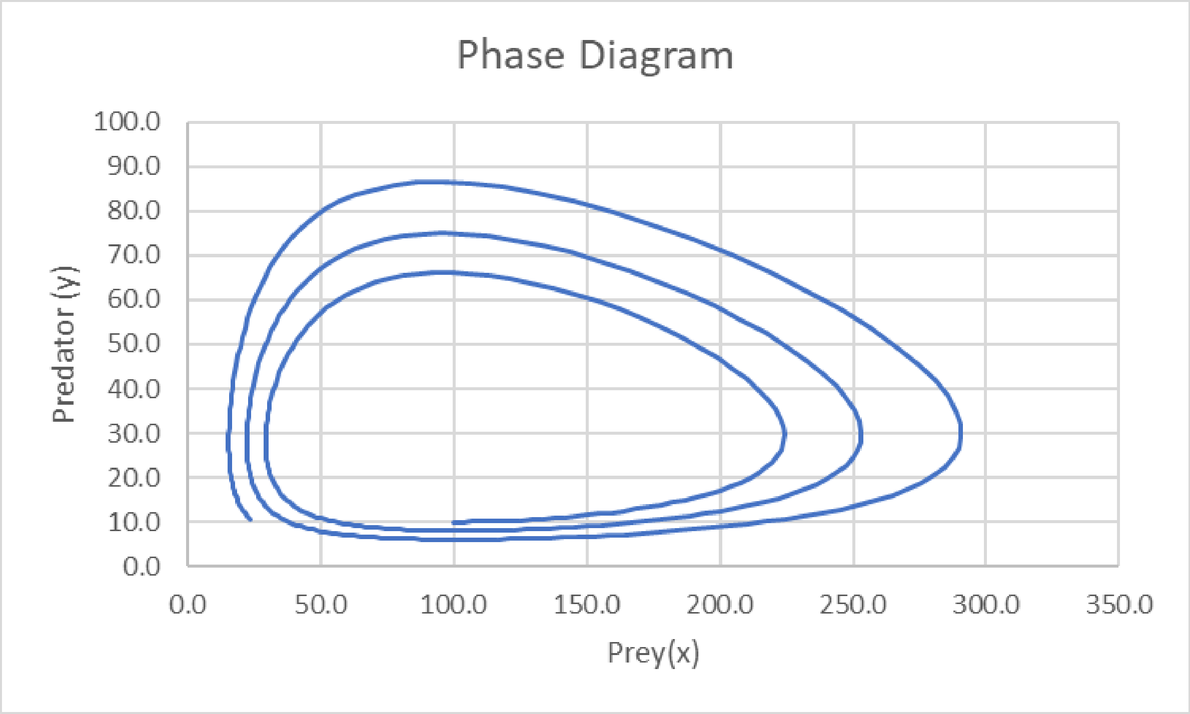
Wolves – Deer

Phytoplankton - Zooplankton



Maths ok, but still things can go wrong !





Modelling Interfaces

- River / aquifer
- River / floodplain
- Soil / Vegetation / Atmosphere
- Hydrosystem / Ecosystem
- Model / user / stakeholder behaviour

Equations / River Hydraulics

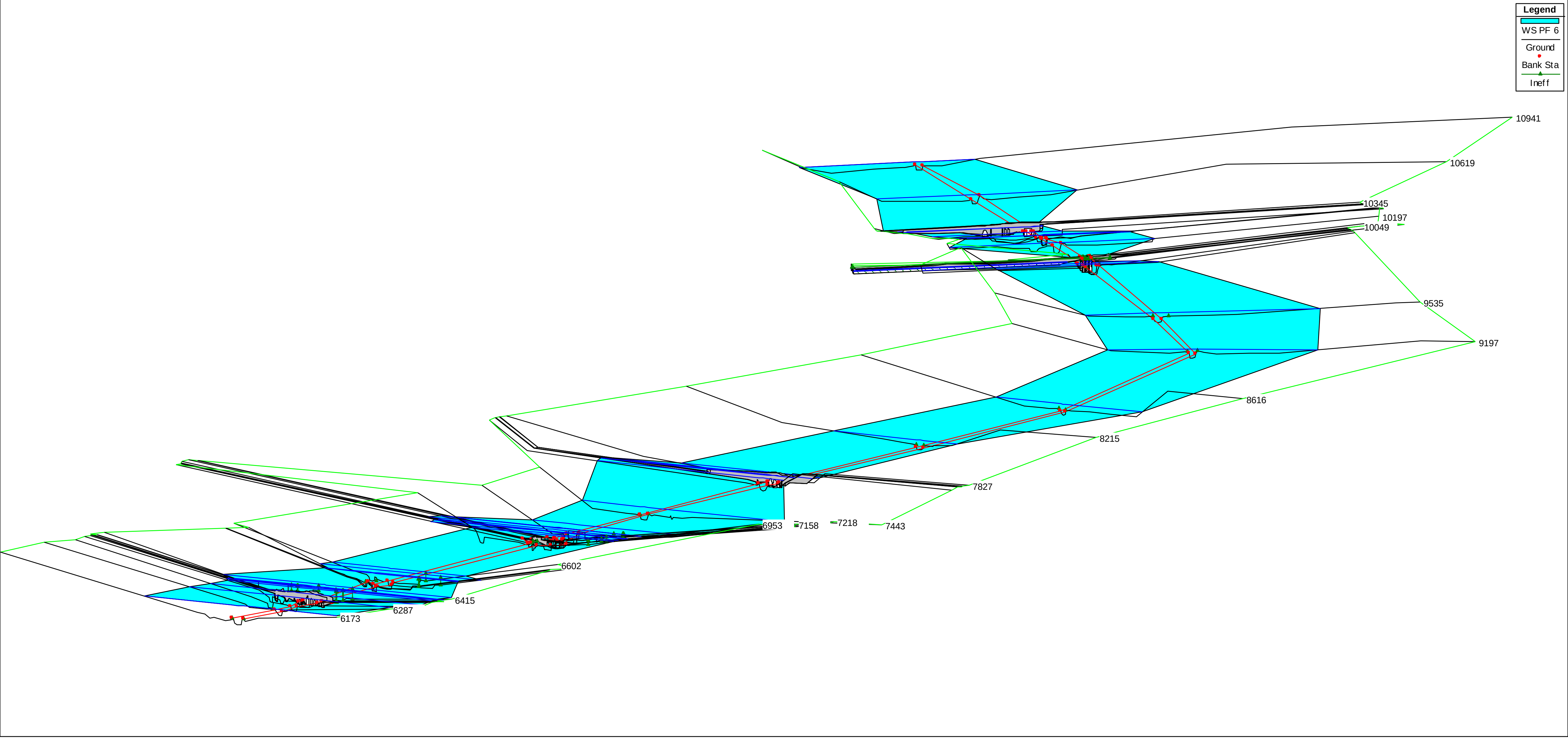
De Saint Venant Equations (1D)

$$\frac{\partial A}{\partial t} + \frac{\partial (Av)}{\partial x} = 0$$

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} + g\frac{\partial h}{\partial x} = -fn(h)$$

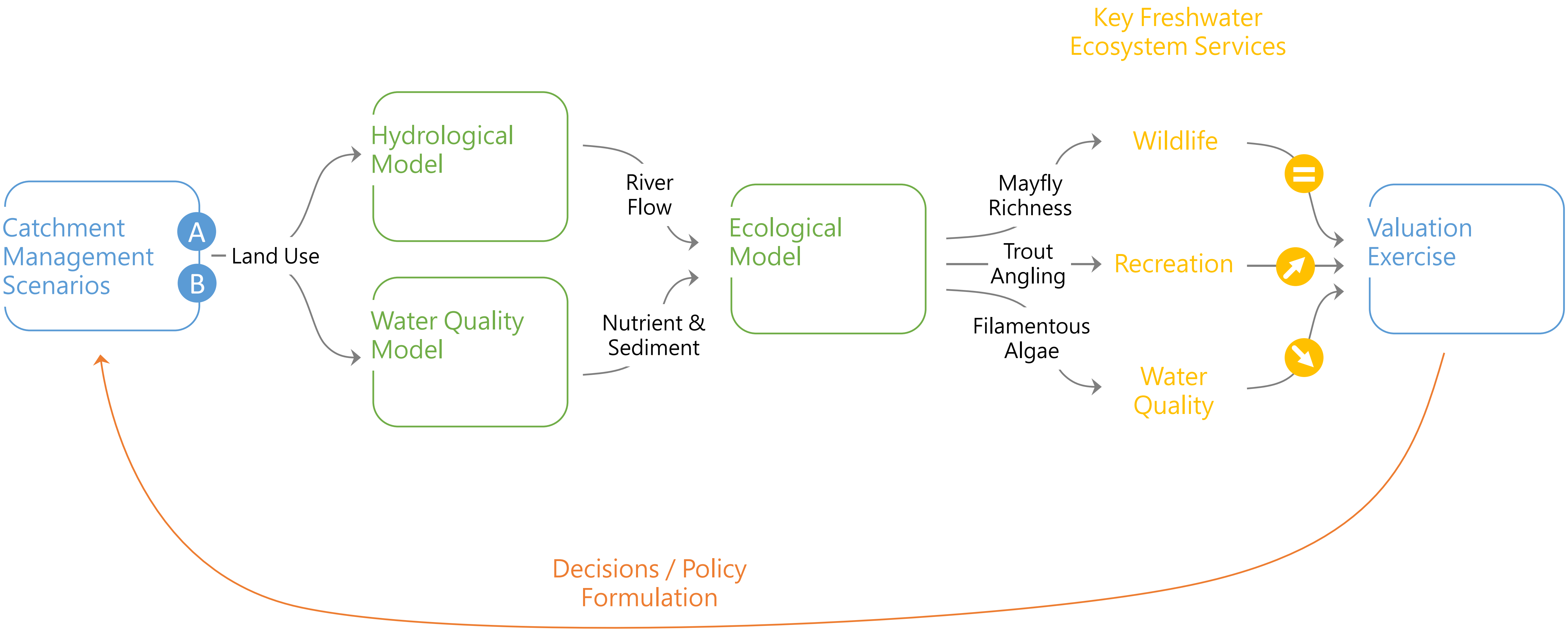
can be extended to 3 dimensions

Duleek Final d/s leg only   Plan: Plan 06   13/11/2014



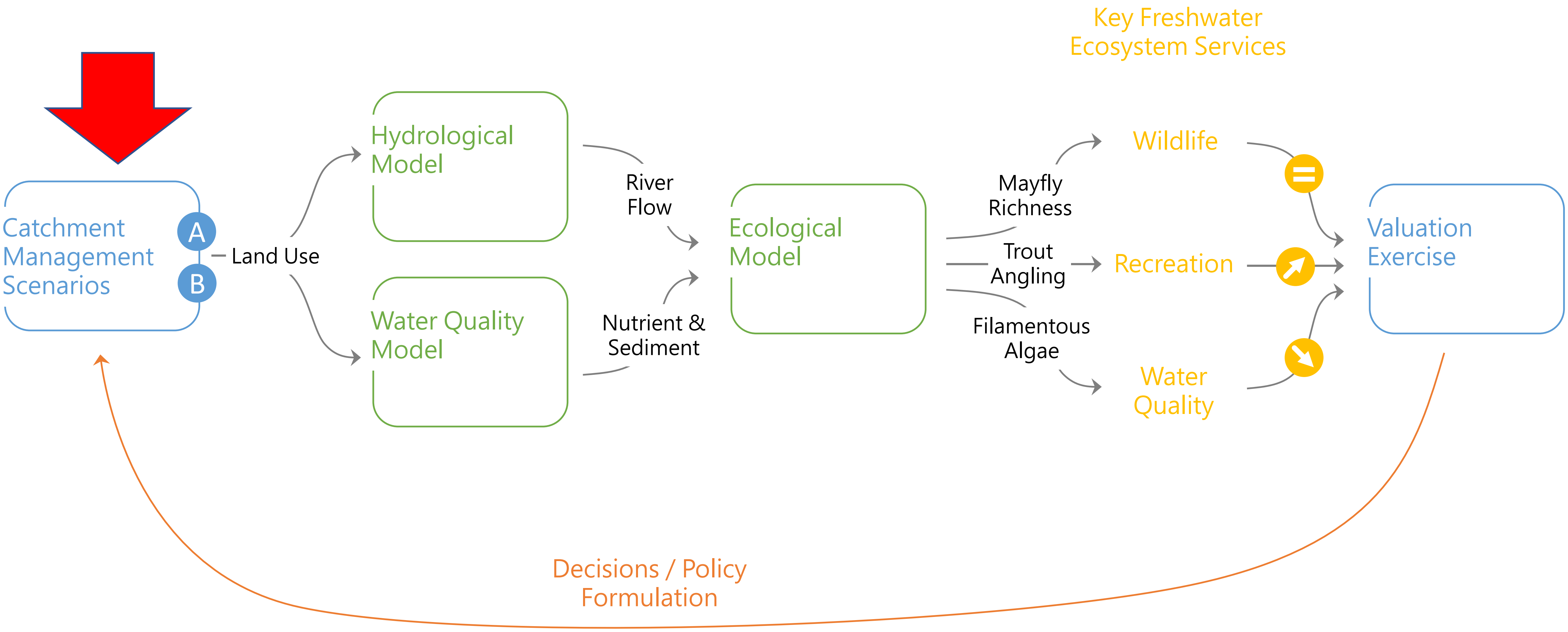
THE ESMANAGE PROJECT

(SOURCE: HALLOUIN , T.)



The ESManage Project

(Source: Hallouin , T.)



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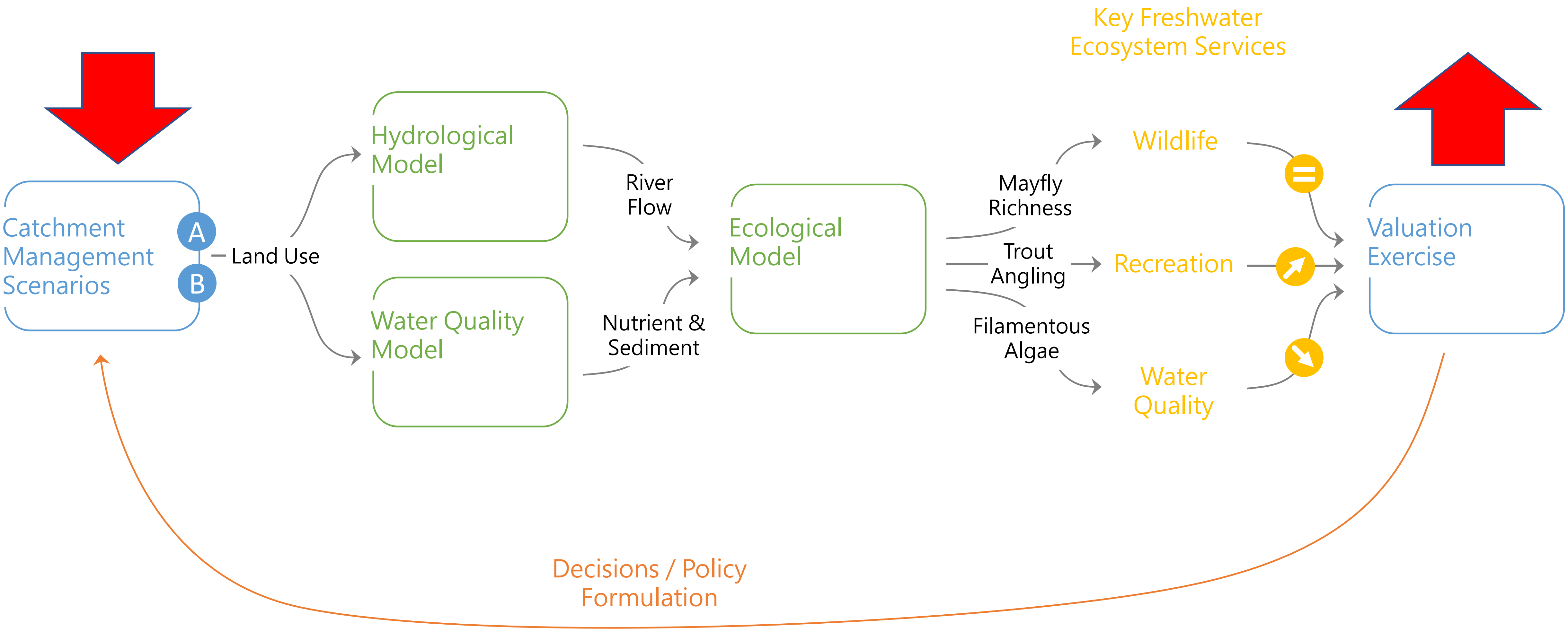

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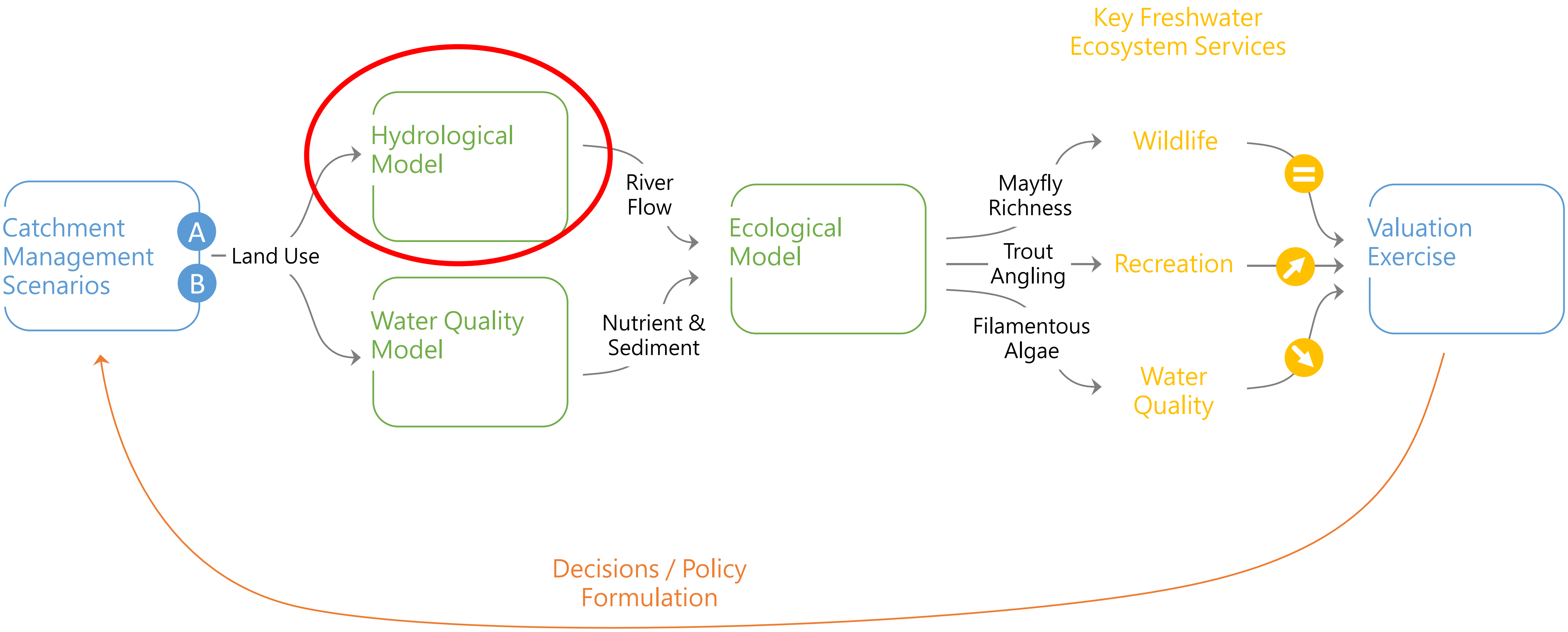
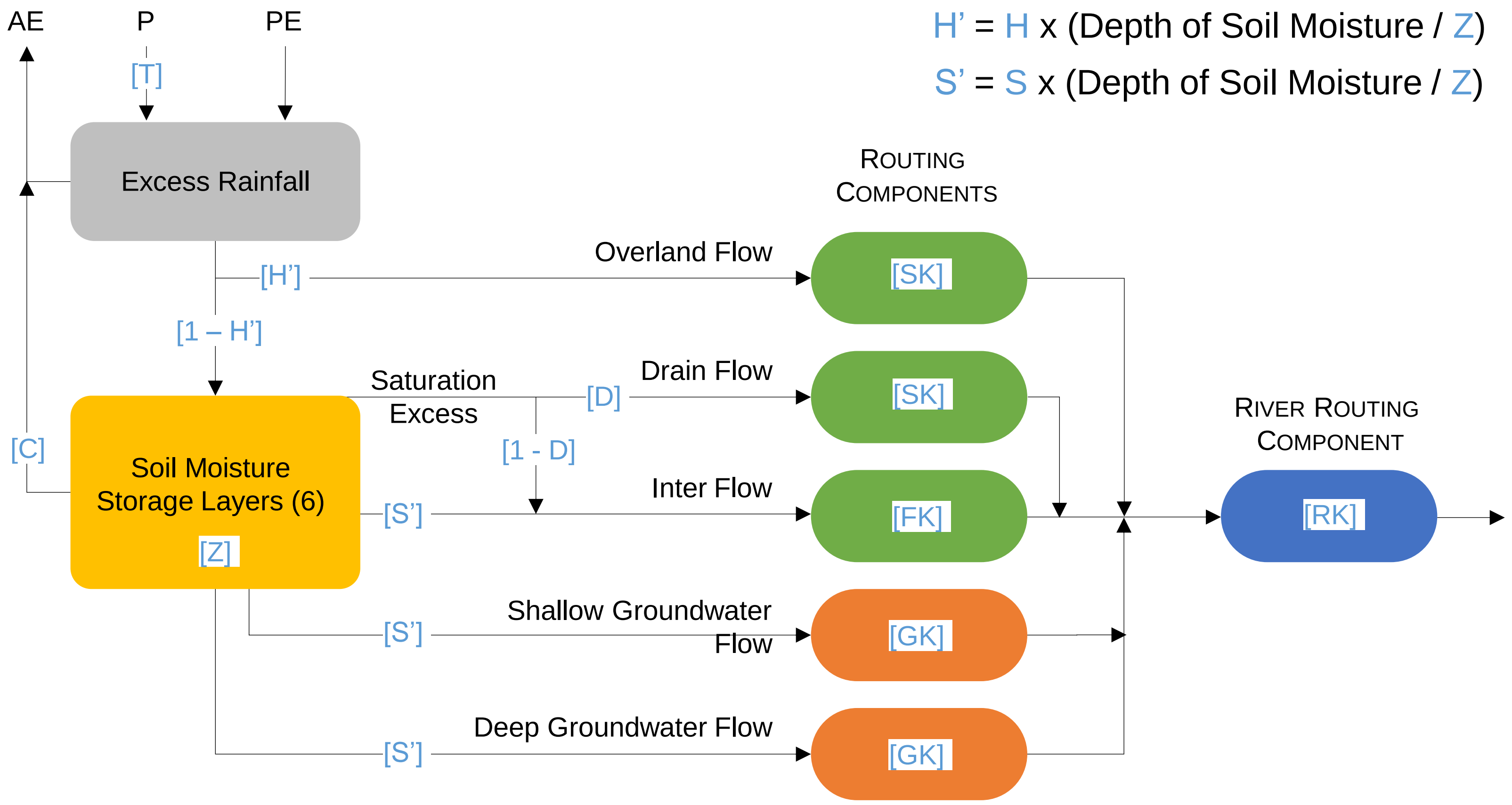


RAINFALL-RUNOFF MODEL

Soil Moisture Accounting for Routing and Transport (SMART)

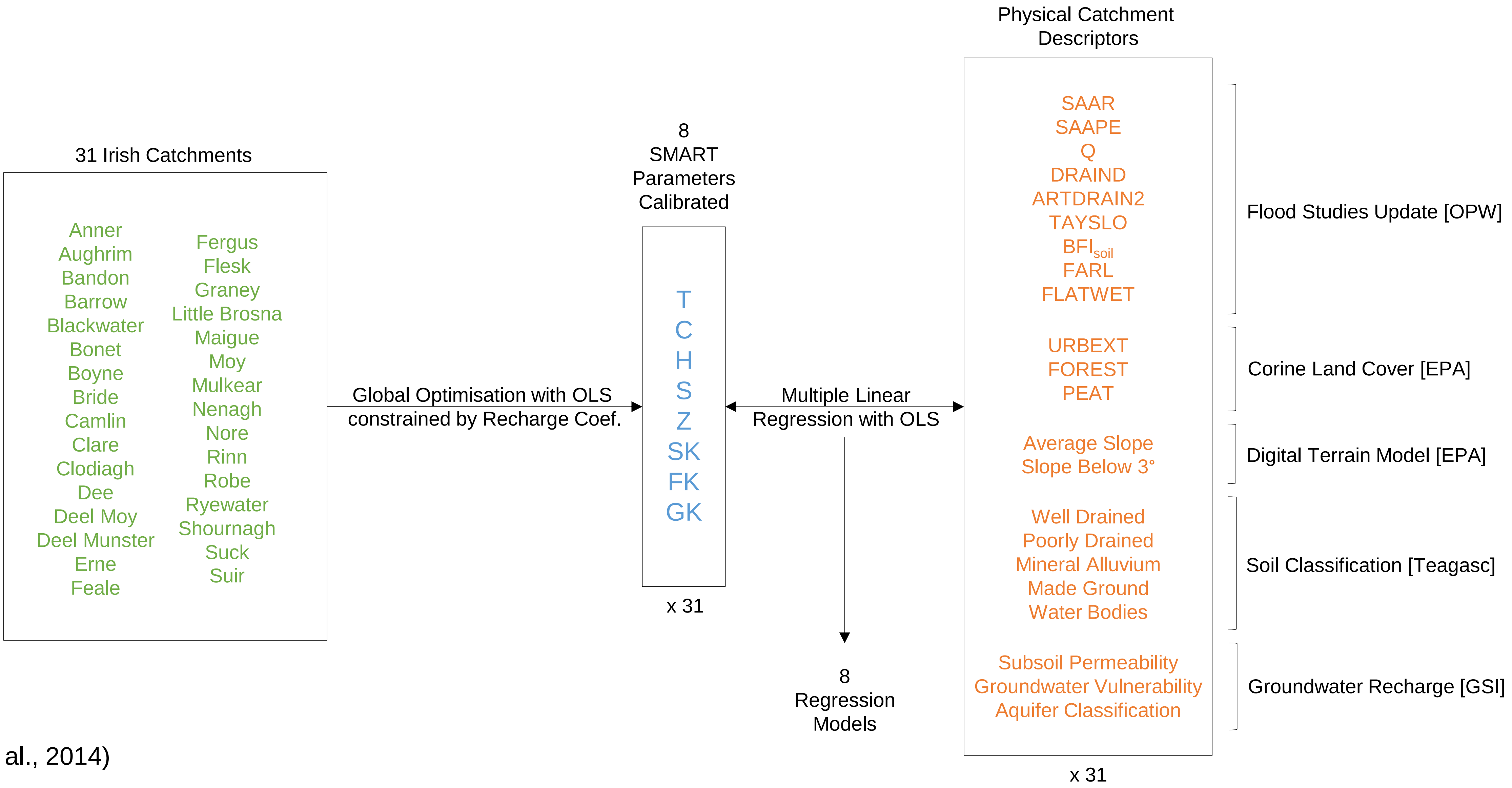
(Mockler et al., 2016)



T	rainfall aerial correction coefficient
C	evaporation decay parameter
H	quick runoff coefficient
D	fraction of sat. excess diverted to drain flow
S	soil outflow coefficient
Z	effective soil depth

SK	surface routing parameter
FK	interflow routing parameter
GK	groundwater routing parameter
RK	channel routing parameter

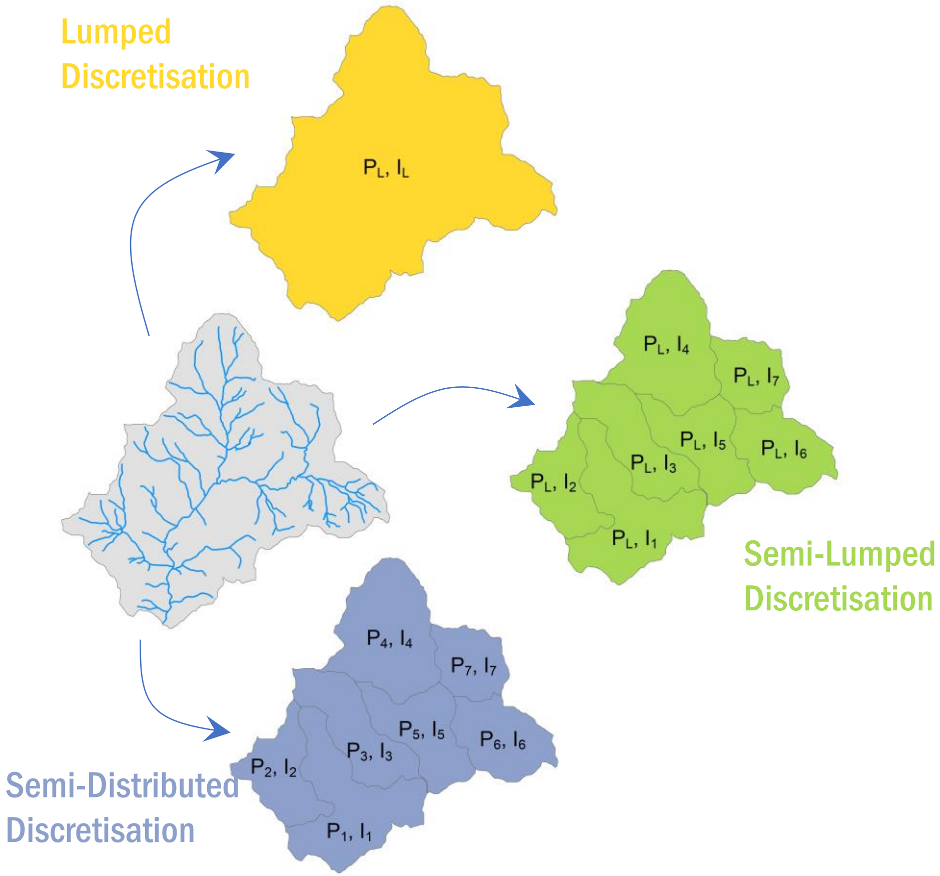
REGIONAL PARAMETER TRANSFER METHOD (*DEVELOPMENT*)



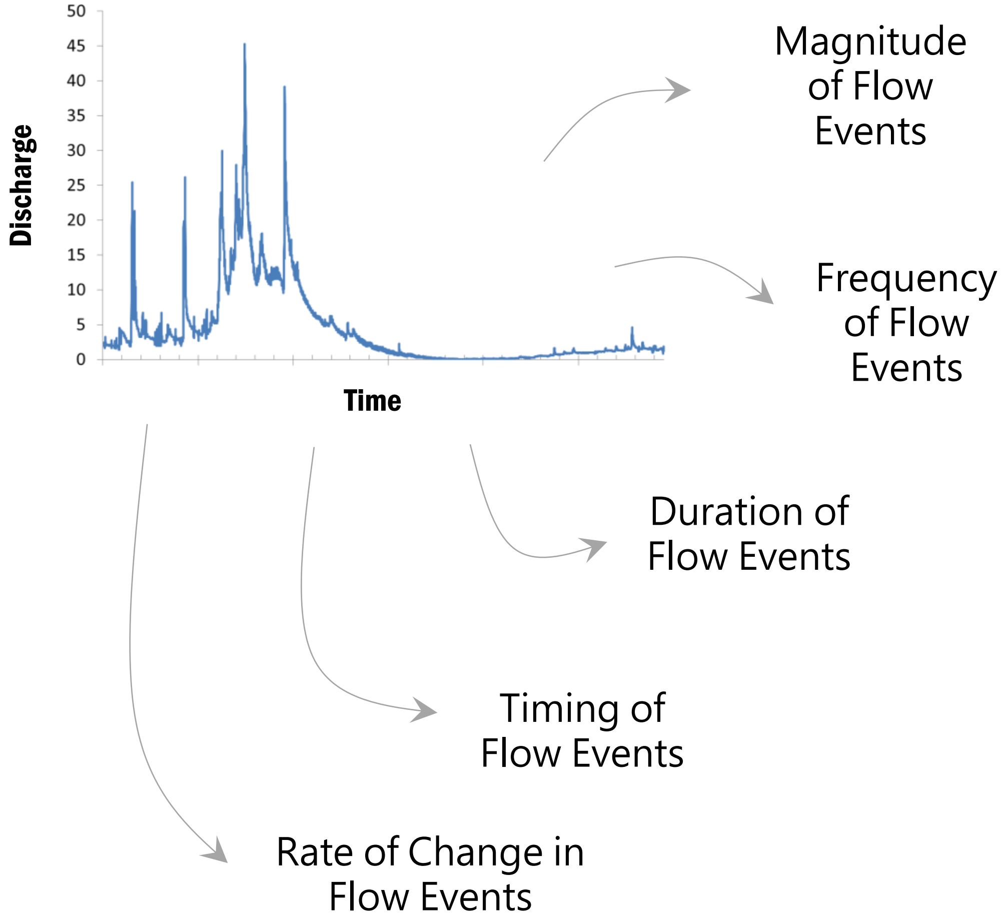
(Mockler et al., 2014)

Catchment Hydrological Modelling [2]

Predictions at different Spatial Scales



Predictions of Streamflow Characteristics (SFCs)



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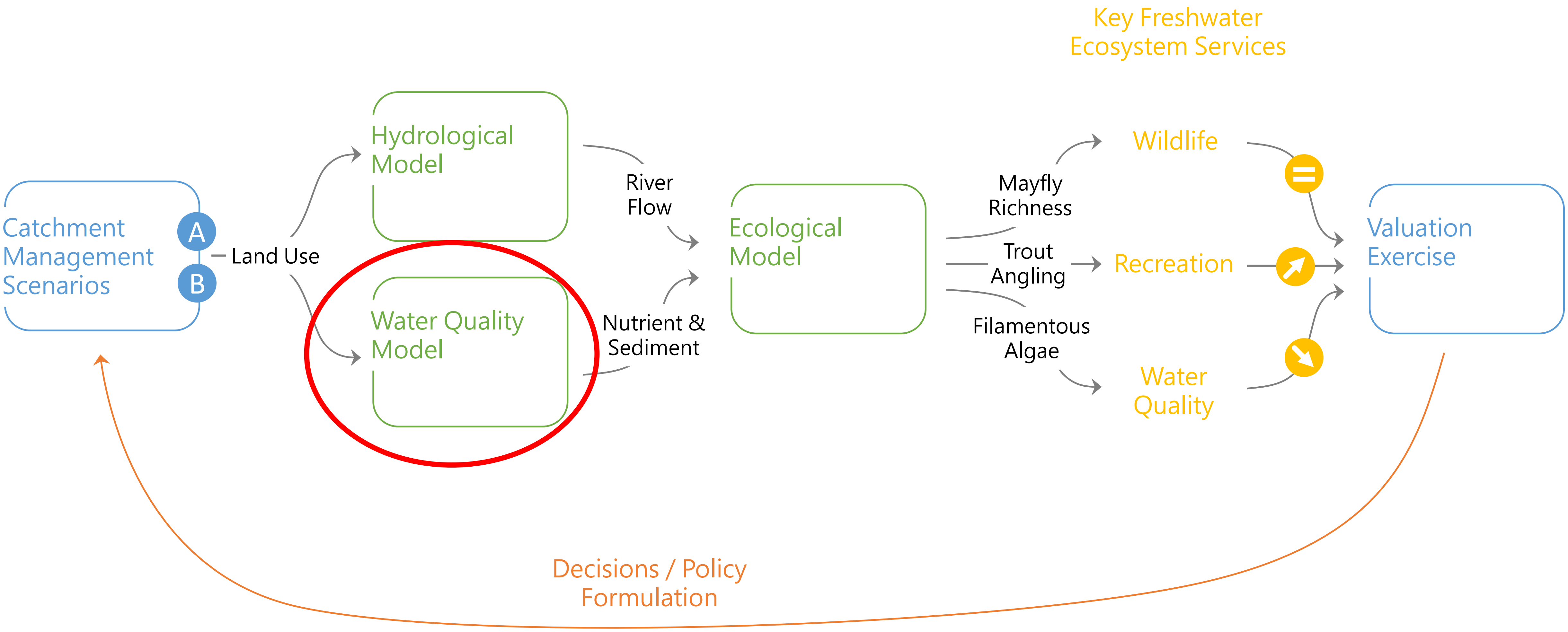


Water Quality Modelling

Agricultural Input

Fertilizer
Manure

Land Phase

N cycle

Plant Fixation / Plant Uptake / Plan Decay
Immobilisation / Mineralisation
Nitrification / Denitrification
Attenuation

P cycle

Plant Uptake
Immobilisation / Mineralisation
Attenuation

Transport of N, P and Sediment

Overland Flow
Tile Drain Flow
Inter Flow
Shallow Groundwater Flow
Deep Groundwater Flow

Stream Phase

N cycle

Nitrification / Denitrification
Attenuation

P cycle

Attenuation

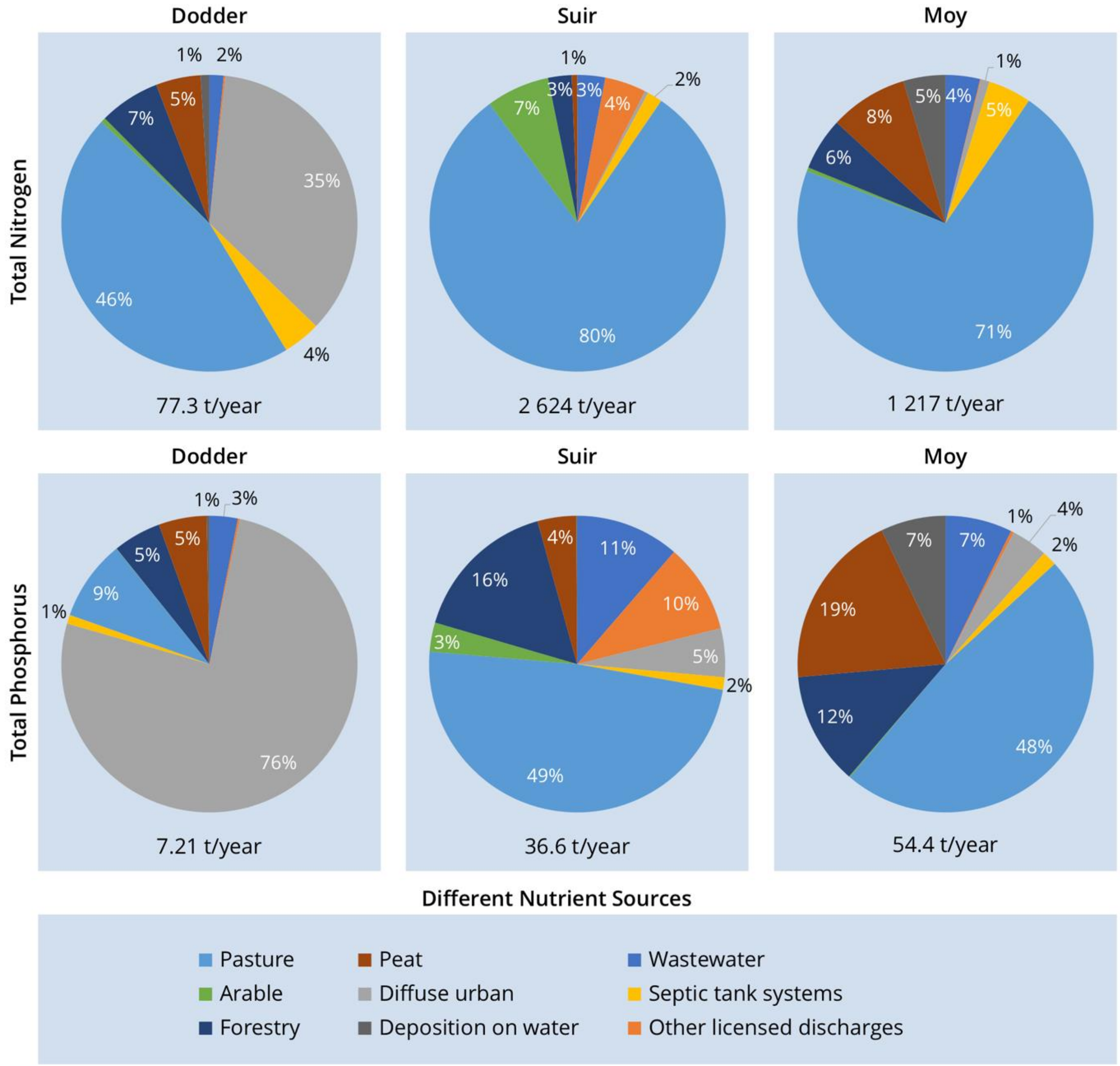
Transport of N, P and Sediment

River Flow

Nutrient
And
Sediment
Export

SLAM
(source load apportionment tool)

based on Pathways CCT (catchment characterisation tool)



Other Widely-used Models

SWAT (USA)

HYPE (SMHI, based on HBV model)

AnnAGNPS

HSPF (used in BASINS)

INCA (INCA-N, INCA-P, INCA-Sed and SimplyP)

Wellen, C., Kamran-Disfani, A.-R., & Arhonditsis, G.B. (2015), **Evaluation of the Current State of Distributed Watershed Nutrient Water Quality Modeling.** *Environmental Science & Technology* **2015** *49* (6), 3278-3290 DOI: 10.1021/es5049557

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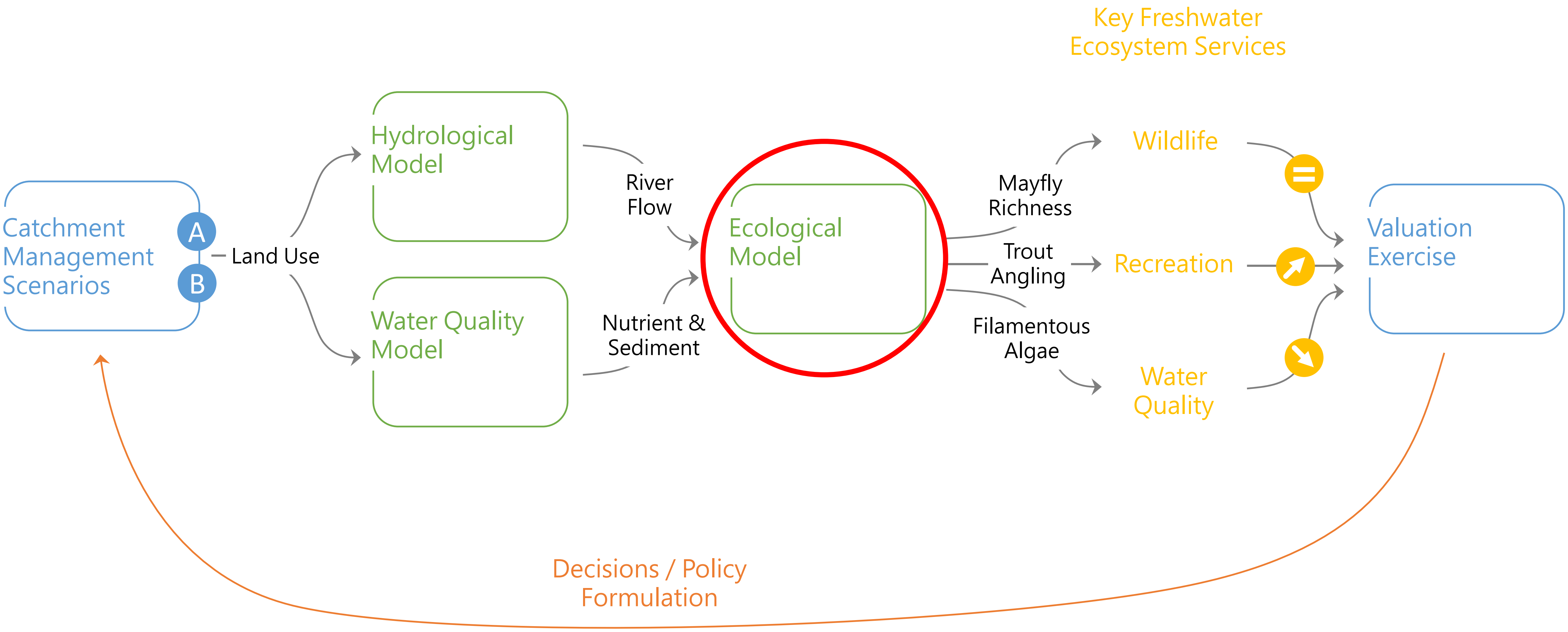
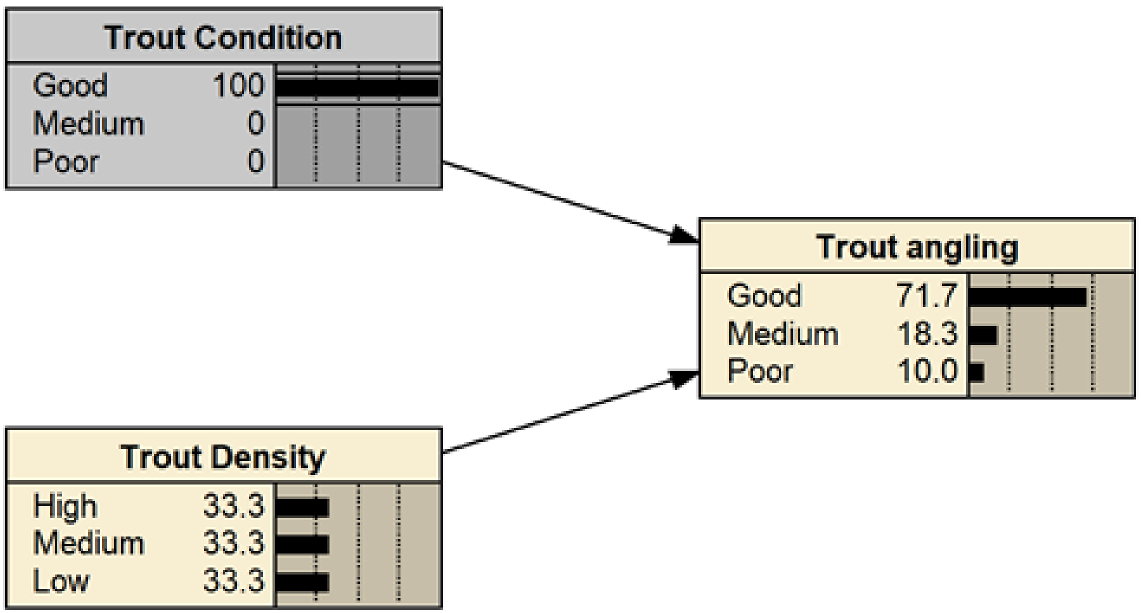


BAYESIAN BELIEF NETWORKS – NODES AND LINKS



Bayesian Belief Networks – Conditional Probabilities

			Trout Angling		
Scenarios	Trout Condition	Trout Density	Good	Medium	Poor
1 *	**Good**	**High**	100	0	0
2	Good	Medium	65	25	10
3	Good	Low	50	30	20
4	Medium	High	50	30	20
5	Medium	Medium	25	50	25
6	Medium	Low	20	30	50
7	Poor	High	20	30	50
8	Poor	Medium	10	25	65
9 **	Poor	Low	0	0	100

** perceived best case and ** worst case scenarios influencing trout angling*

Bayesian Belief Networks – Calculations

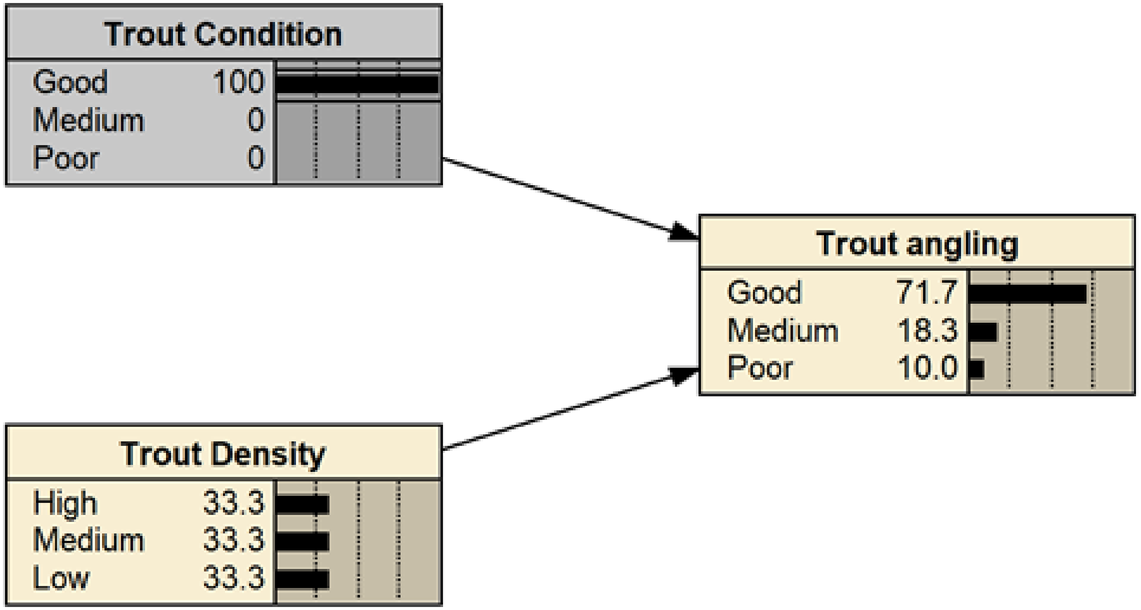
Bayes' rule : $P(A|B) = \frac{P(B|A)P(A)}{P(B)}$

Two factors:

$$P(A|B \cap C) = \frac{P(B|A \cap C)P(A|C)}{P(B|C)}$$

Similarly for more factors:

BAYESIAN BELIEF NETWORKS – CONDITIONAL PROBABILITIES



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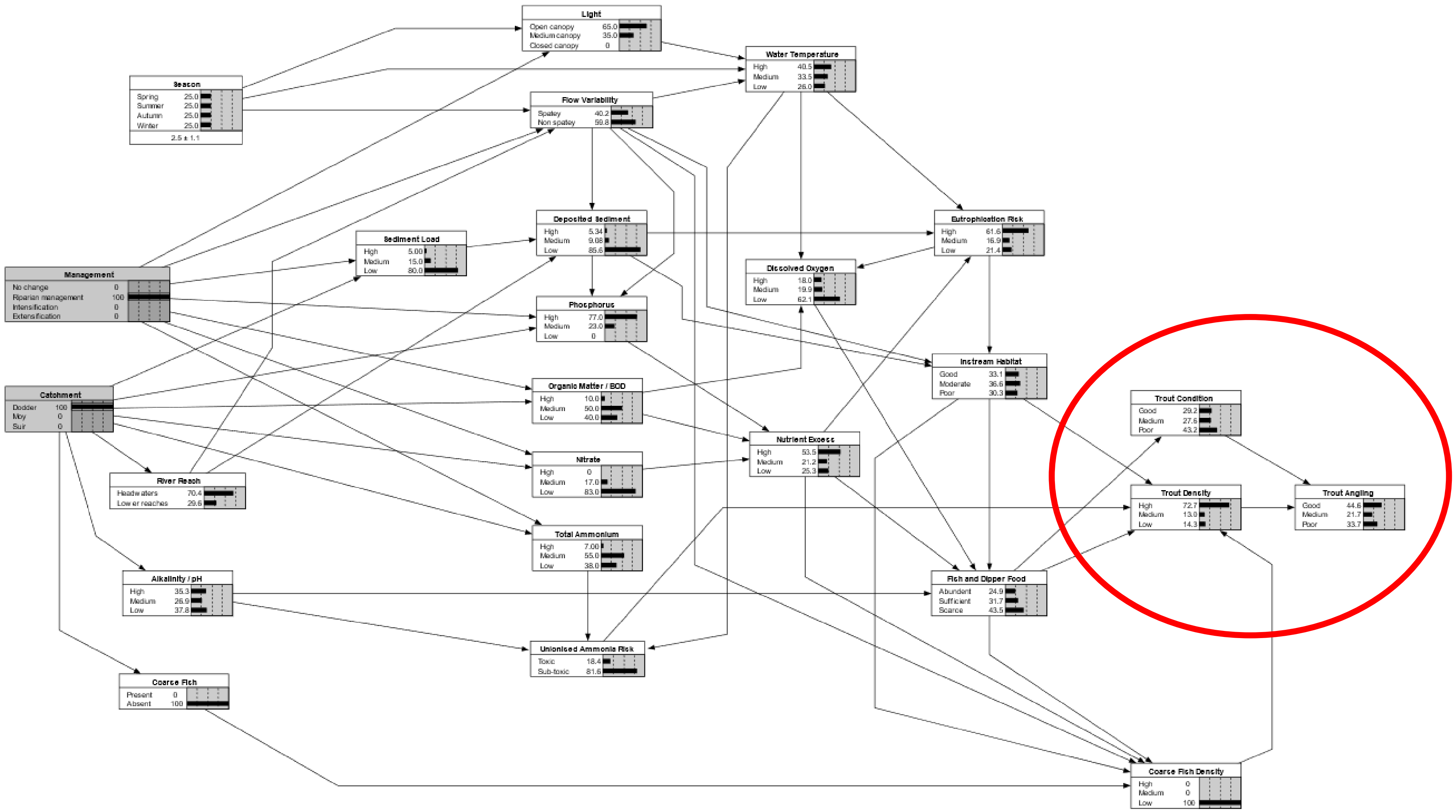

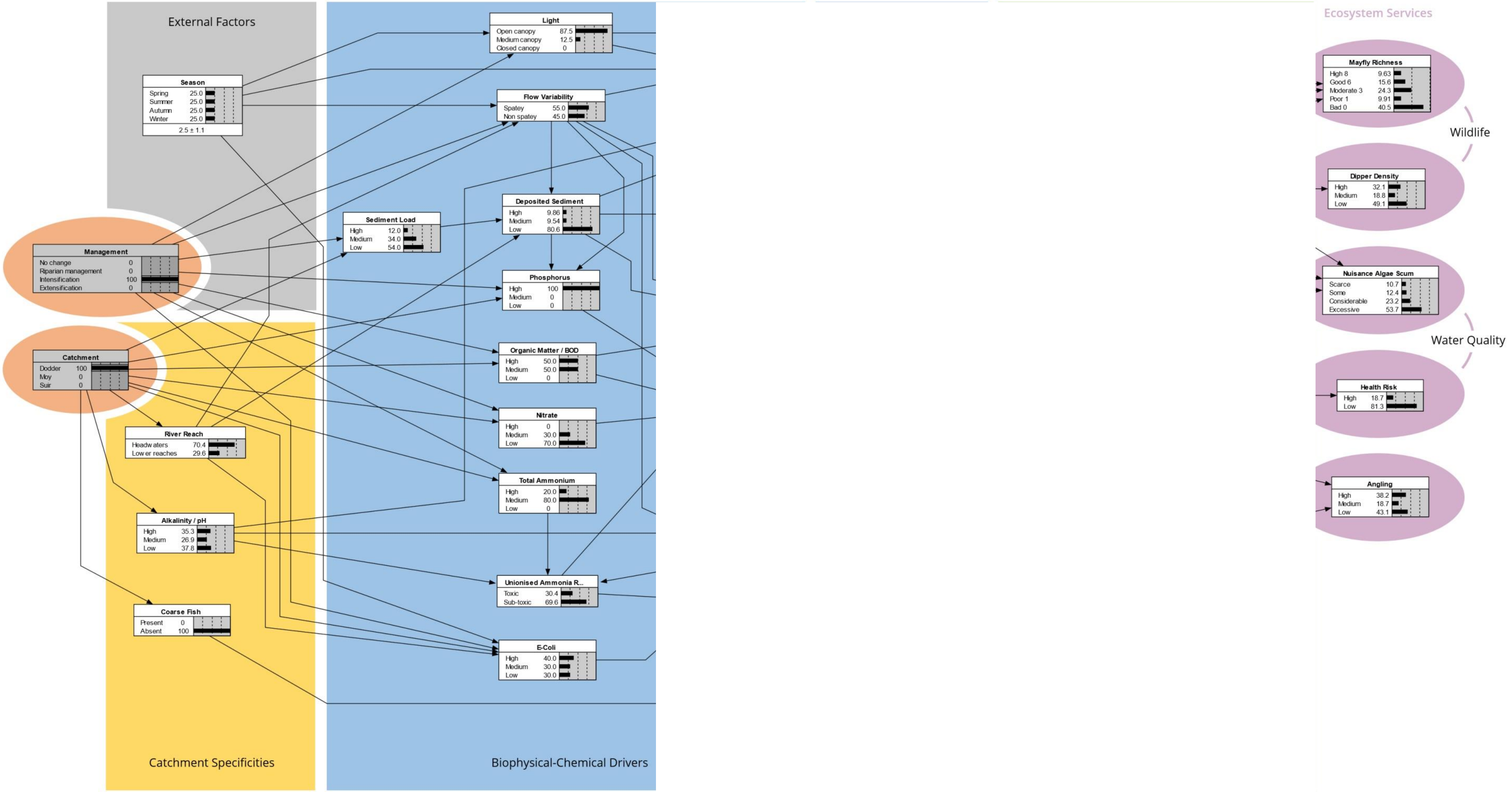

External Factors
Season
Spring 25.0
Summer 25.0
Autumn 25.0
Winter 25.0
2.5 ± 1.1
Management
No change 0
Riparian management 0
Intensification 100
Extensification 0
Catchment
Dodder 100
Moy 0
Suir 0
River Reach
Headwaters 70.4
Lower reaches 29.6
Alkalinity / pH
High 35.3
Medium 26.9
Low 37.8
Coarse Fish
Present 0
Absent 100
Catchment Specificities
Light
Open canopy 87.5
Medium canopy 12.5
Closed canopy 0
Flow Variability
Spatey 55.0
Non spatey 45.0
Sediment Load
High 12.0
Medium 34.0
Low 54.0
Deposited Sediment
High 9.86
Medium 9.54
Low 80.6
Phosphorus
High 100
Medium 0
Low 0
Organic Matter / BOD
High 50.0
Medium 50.0
Low 0
Nitrate
High 0
Medium 30.0
Low 70.0
Total Ammonium
High 20.0
Medium 80.0
Low 0
Unionised Ammonia R...
Toxic 30.4
Sub-toxic 69.6
E-Coli
High 40.0
Medium 30.0
Low 30.0
Biophysical-Chemical Drivers
Ecosystem Services
Mayfly Richness
High 8 9.63
Good 6 15.6
Moderate 3 24.3
Poor 1 9.91
Bad 0 40.5
Wildlife
Dipper Density
High 32.1
Medium 18.8
Low 49.1
Nuisance Algae Scum
Scarce 10.7
Some 12.4
Considerable 23.2
Excessive 53.7
Water Quality
Health Risk
High 18.7
Low 81.3
Angling
High 38.2
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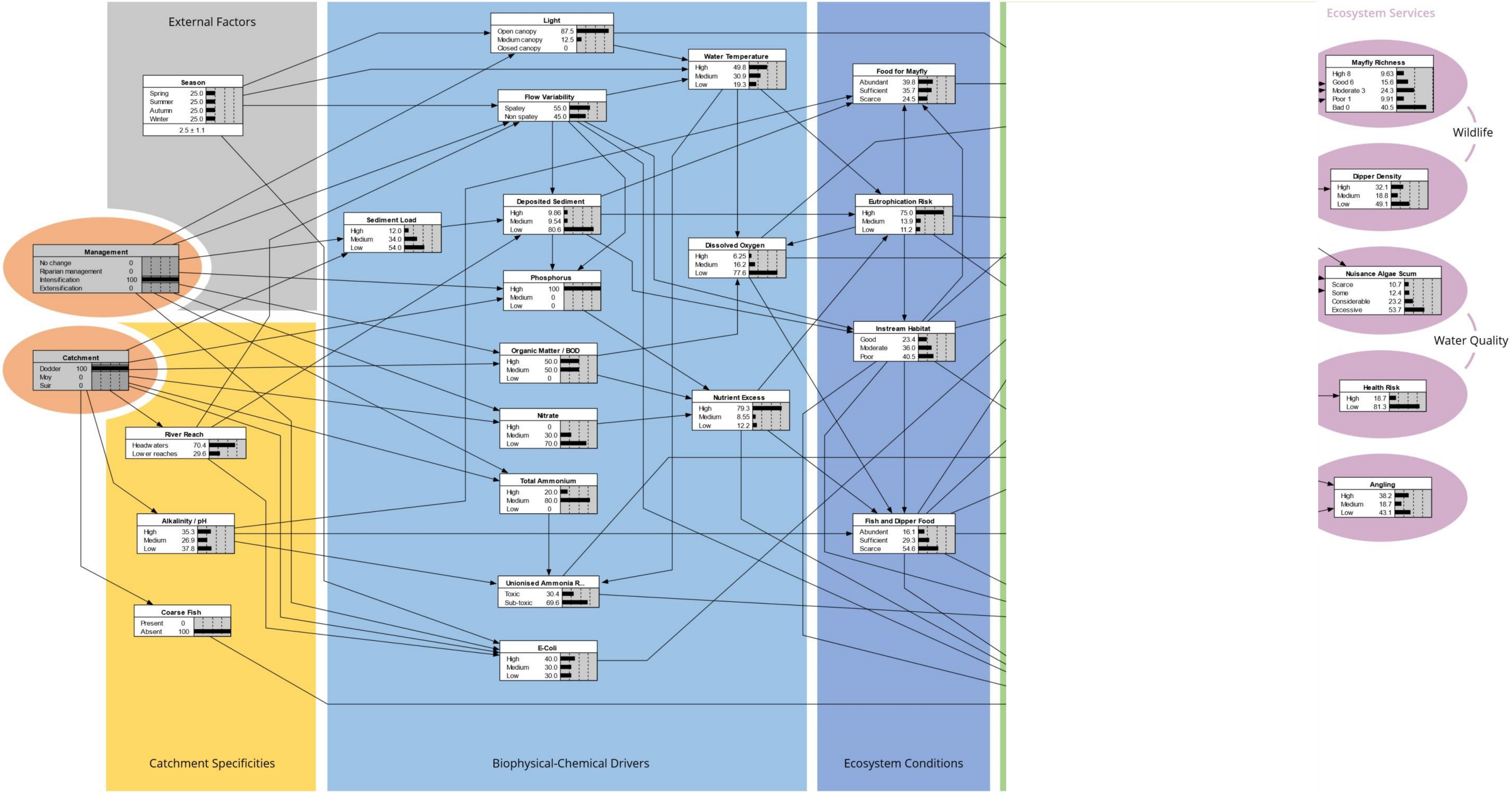

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Water Temperature
High 49.8
Medium 30.9
Low 19.3
Dissolved Oxygen
High 6.25
Medium 16.2
Low 77.6
Nutrient Excess
High 79.3
Medium 8.55
Low 12.2
Food for Mayfly
Abundant 39.8
Sufficient 35.7
Scarce 24.5
Eutrophication Risk
High 75.0
Medium 13.9
Low 11.2
Instream Habitat
Good 23.4
Moderate 36.0
Poor 40.5
Fish and Dipper Food
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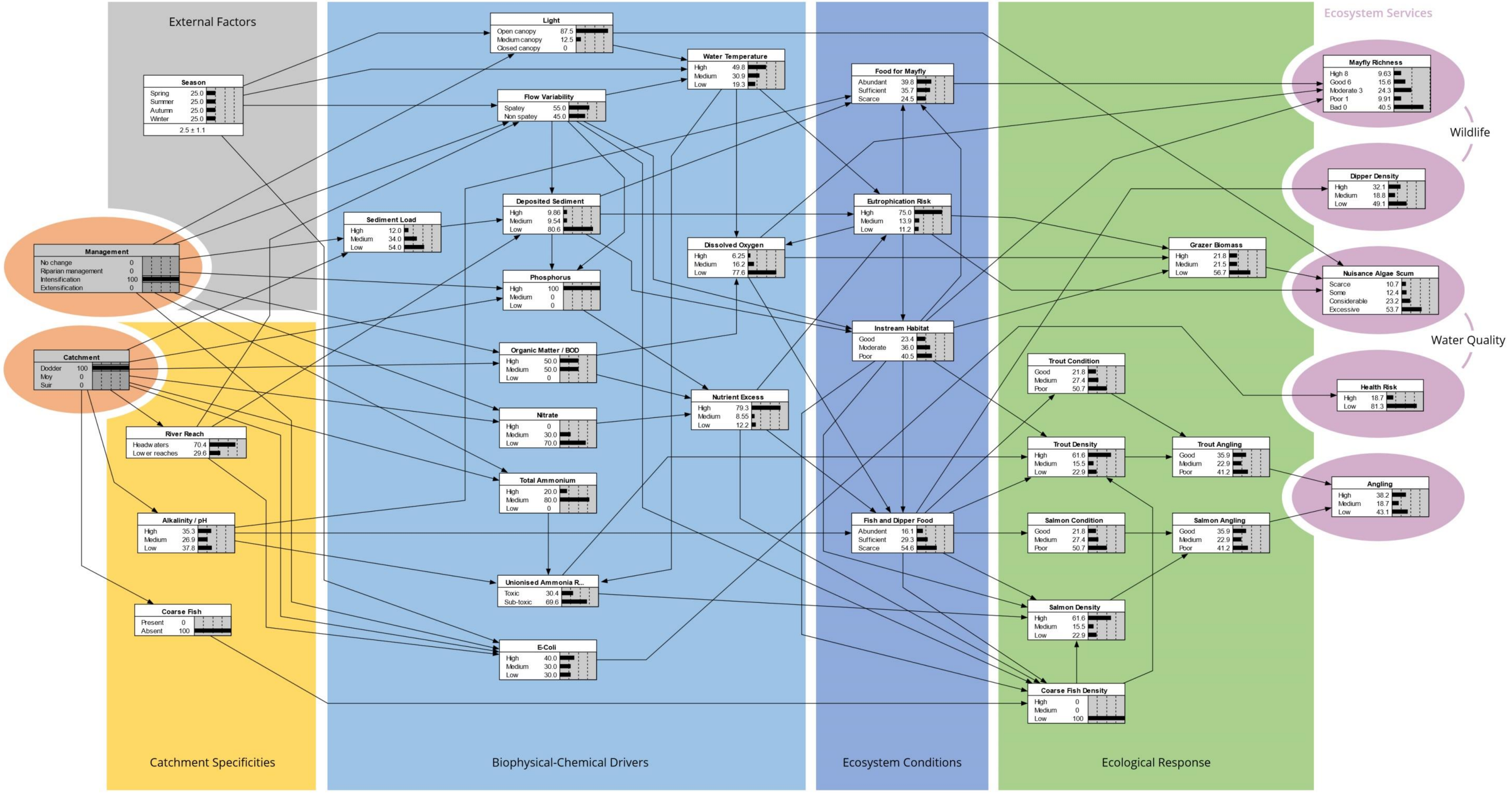


Kelly-Quinn, M., Bruen, M., Christie, M., Bullock, C., Feeley, H., Hannigan, E., Hallouin, T., Kelly, F., Matson, R. & Siwicka, E. (2020)
Incorporation of Ecosystem Services Values in the Integrated Management of Irish Freshwater Resources: ESManage. EPA Research Report, Dublin, pps.54

Sample of Results: Effects of management options

Kelly-Quinn, M., Bruen, M., Christie, M., Bullock, C., Feeley, H., Hannigan, E., Hallouin, T., Kelly, F., Matson, R. & Siwicka, E. (2020)

Incorporation of Ecosystem Services Values in the Integrated Management of Irish Freshwater Resources: ESManage.

EPA Research Report, Dublin, pps.54

		Angling (nos. catchable fish)					
Catchment Management		High 5	Medium 2	Low 1	Score	Absolute change	Re (% ch
Dodder	No change	41.8	18.5	39.8	2.86		
	Riparian management	46.5	17.9	35.6	3.04	0.18	6
	More livestock	38.7	18.7	42.6	2.74	-0.12	-4
	Fewer livestock	43.2	18.2	38.6	2.91	0.05	2
Moy	No change	40.6	18.1	41.2	2.80		
	Riparian management	47.8	17.9	34.3	3.09	0.29	10
	More livestock	37.6	18	44.4	2.68	-0.12	-4
	Fewer livestock	43.7	18.1	38.1	2.93	0.12	4
Suir	No change	38.4	18.1	43.5	2.72		
	Riparian management	45.6	17.9	36.5	3.00	0.29	11
	More livestock	34.9	17.9	47.2	2.58	-0.14	-5
	Fewer livestock	40.9	18.1	40.9	2.82	0.10	4

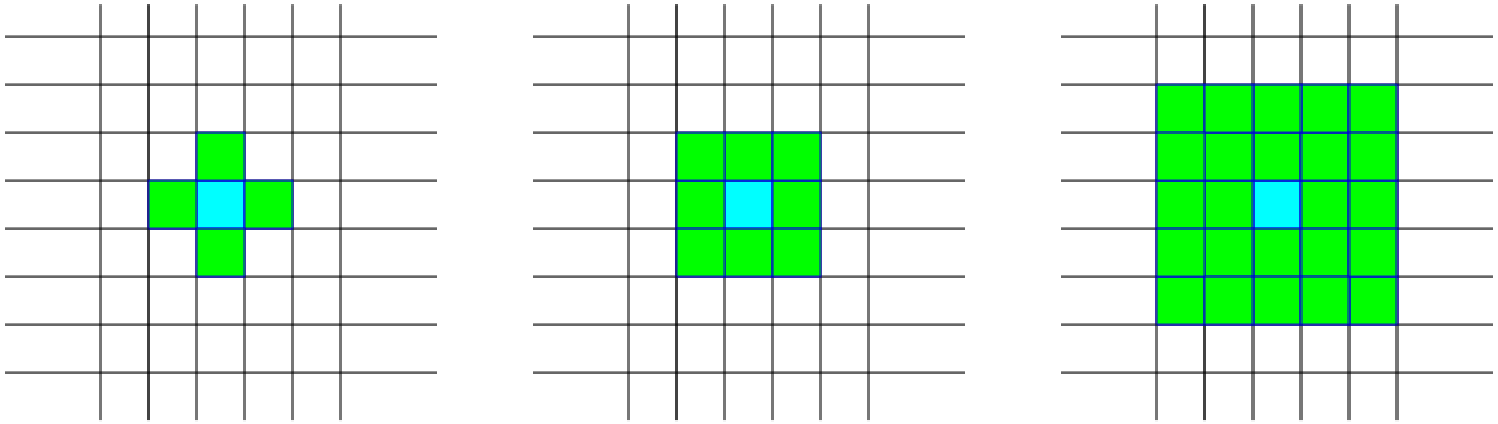
Cellular Automata

First ideas from S. Ulam and J. Von Neumann (1940s)

- Fixed Spatial grid structure (checkerboard) each square (cell) represents place
- Local interactions (Von Neumann neighbourhood – 4 neighbours
  Moore neighbourhood – 8 neighbours
  5 x 5 Moore neighbourhood)
- Agents in the cell have a state represented by numbers
- States can change depending on their original state and those of its neighbour. (time moves in discrete steps – all step together – or cells may change in sequence)
- Influence dynamics (agents don’t change location)
- Migration dynamics (agents may move to other locations)

https://youtu.be/C2vgICfQawE Conway’s Game of Life

Cellular Automata (for spatial simulation)

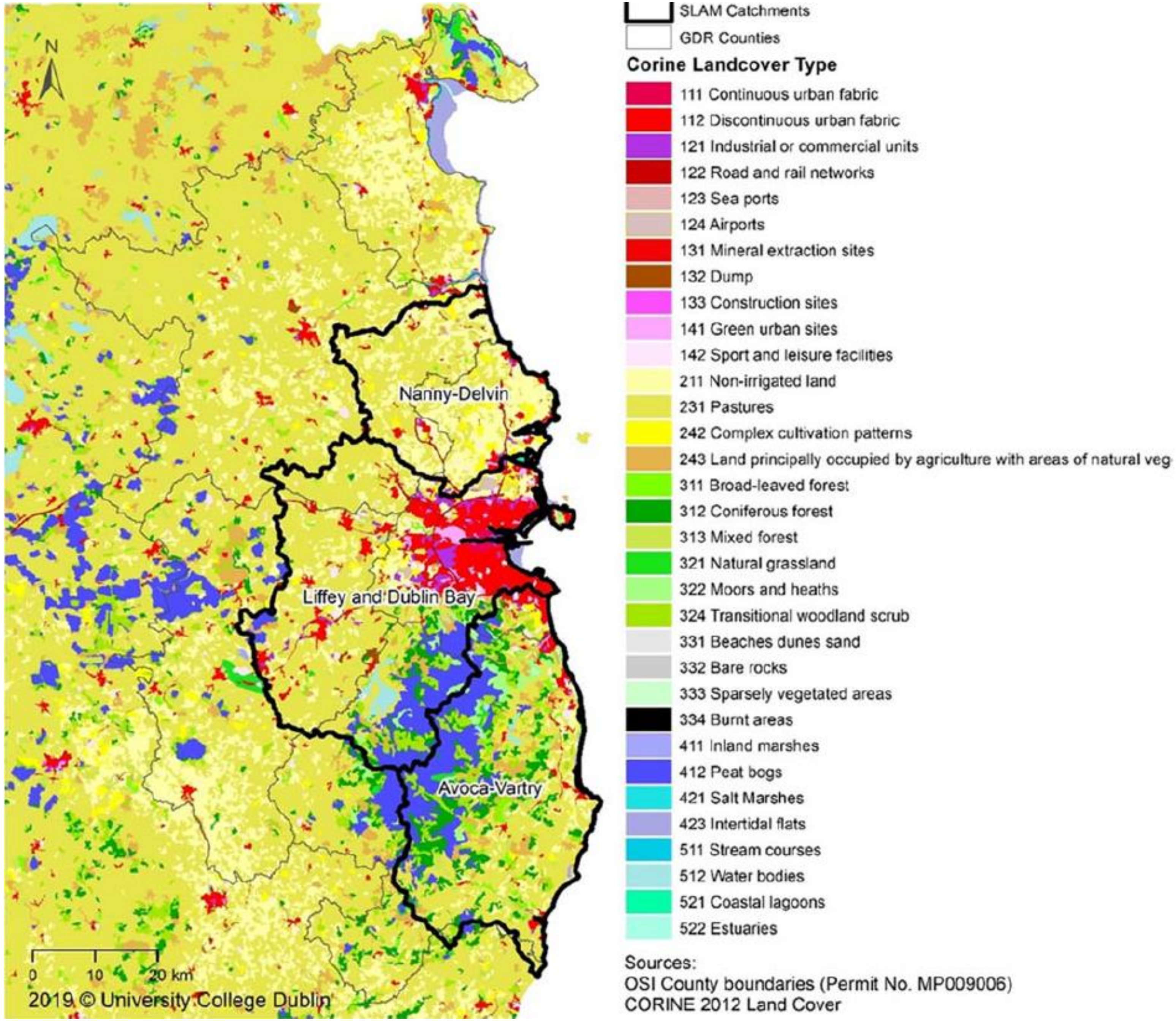


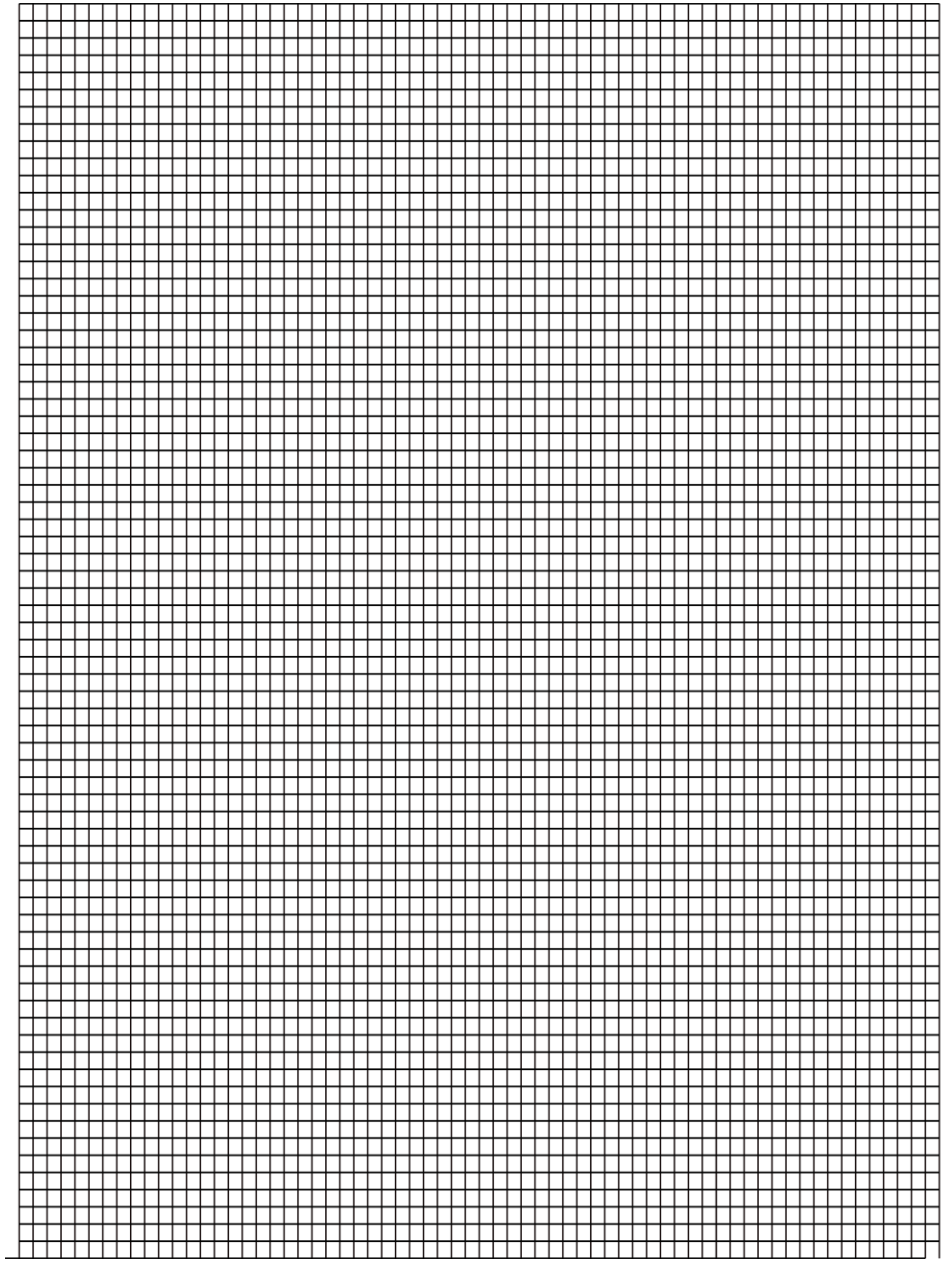
Von Neumann neighbourhood (4) Moore neighbourhood (8) Extended Moore neighbourhood (24)

Land-use around Dublin

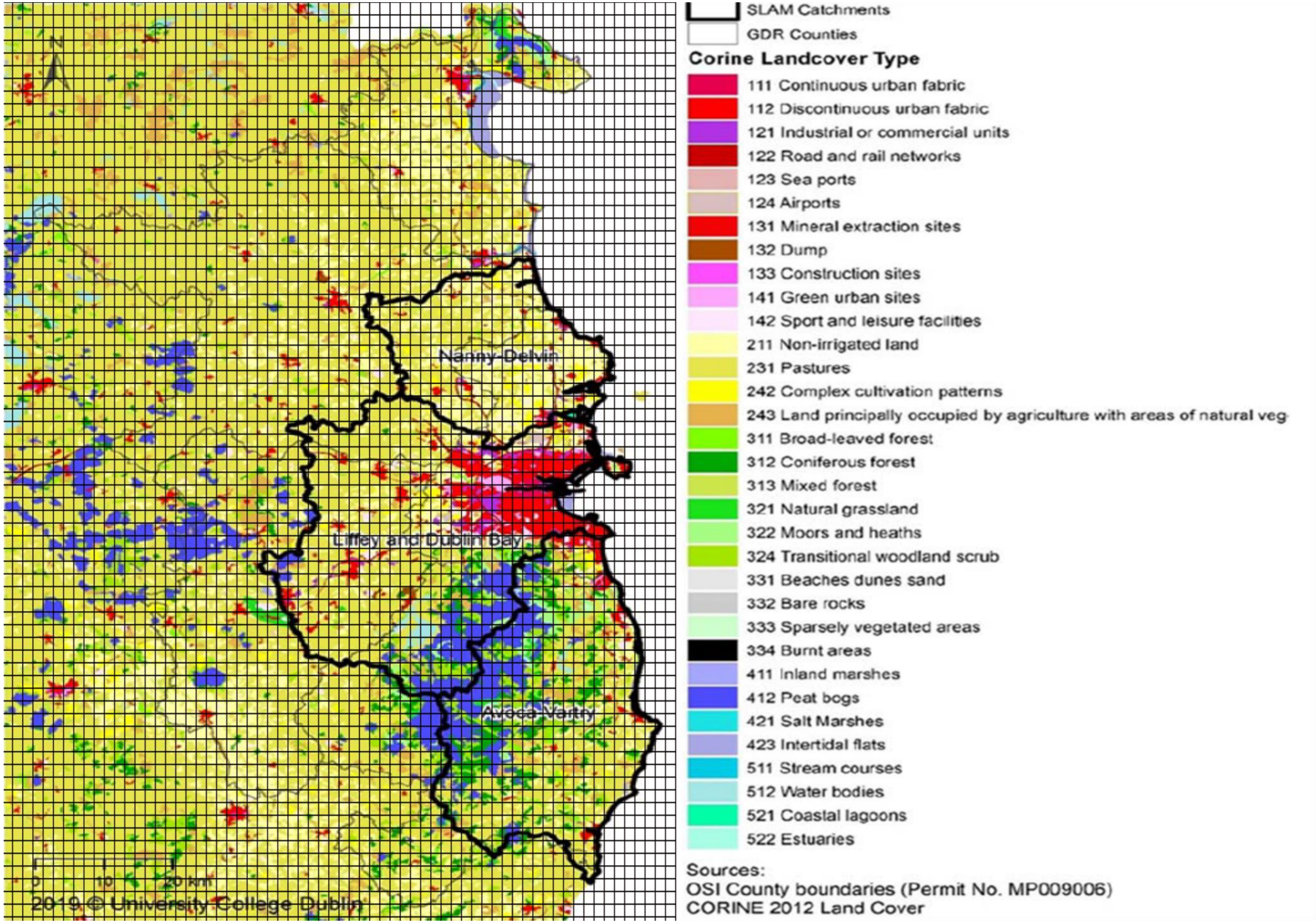
Source:
Mockler, E., Shahumyan, H., Williams, B. & Bruen, M. (2020) **Coupling Land Use and Nutrient Emissions Models to Assess Effects of Regional Development Scenarios on Nutrient Emissions to Water.** *Environmental Modelling & Assessment*.

https://doi.org/10.1007/s10666-020-09711-z





Actual grid used is finer than illustrated


N
Nanny-Delvin
Liffey and Dublin Bay
Avoca-Vartry
0 10 20 km
2019 © University College Dublin
SLAM Catchments
GDR Counties
Corine Landcover Type
111 Continuous urban fabric
112 Discontinuous urban fabric
121 Industrial or commercial units
122 Road and rail networks
123 Sea ports
124 Airports
131 Mineral extraction sites
132 Dump
133 Construction sites
141 Green urban sites
142 Sport and leisure facilities
211 Non-irrigated land
231 Pastures
242 Complex cultivation patterns
243 Land principally occupied by agriculture with areas of natural veg
311 Broad-leaved forest
312 Coniferous forest
313 Mixed forest
321 Natural grassland
322 Moors and heaths
324 Transitional woodland scrub
331 Beaches dunes sand
332 Bare rocks
333 Sparsely vegetated areas
334 Burnt areas
411 Inland marshes
412 Peat bogs
421 Salt Marshes
423 Intertidal flats
511 Stream courses
512 Water bodies
521 Coastal lagoons
522 Estuaries
Sources:
OSI County boundaries (Permit No. MP009006)
CORINE 2012 Land Cover

Land-use around Dublin

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Mockler, E., Shahumyan, H., Williams, B. & Bruen, M. (2020) **Coupling Land Use and Nutrient Emissions Models to Assess Effects of Regional Development Scenarios on Nutrient Emissions to Water.** *Environmental Modelling & Assessment*.

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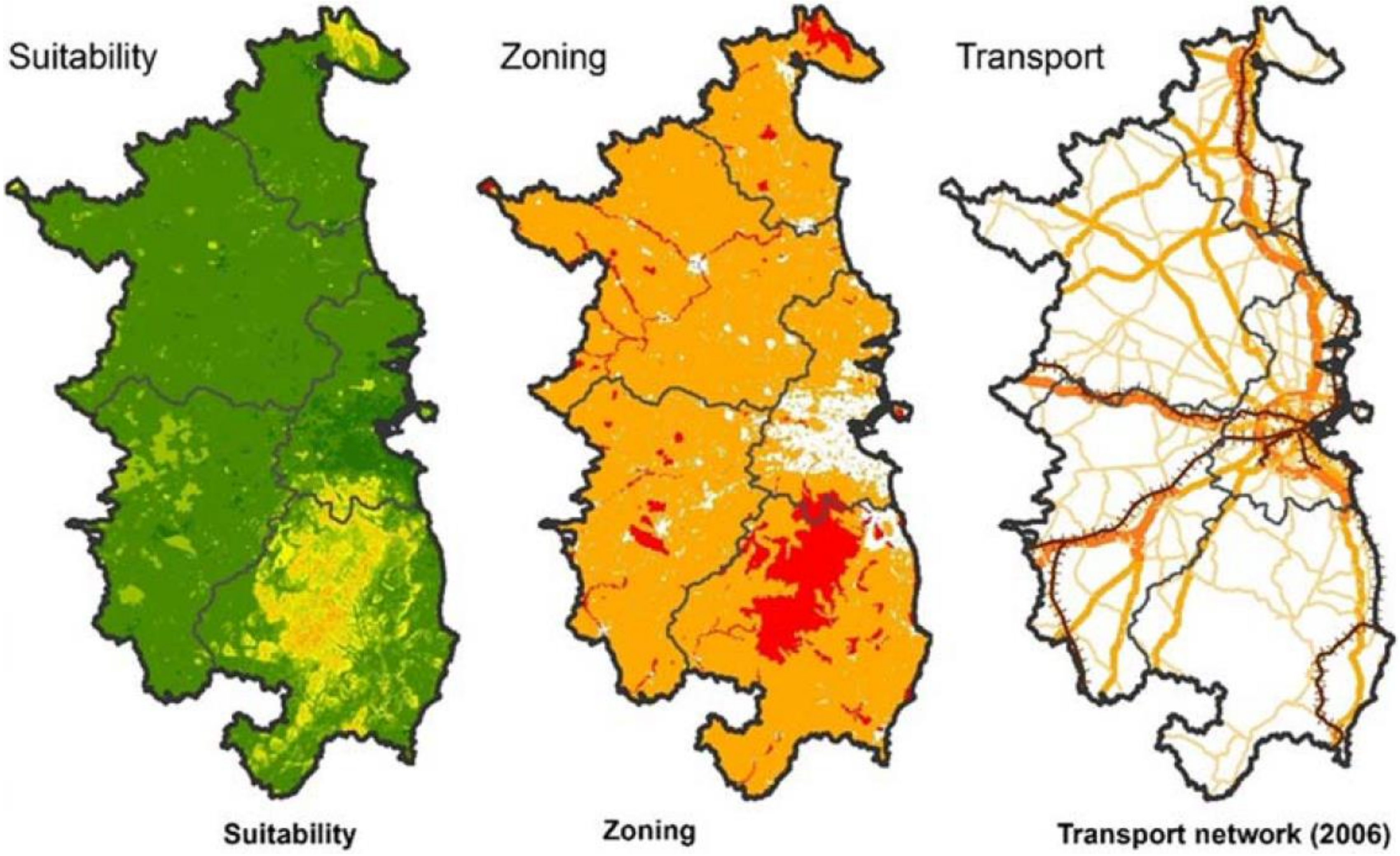

MOLAND-SLAM model coupling

Source:
Mockler, E., Shahumyan, H., Williams, B. & Bruen, M. (2020) **Coupling Land Use and Nutrient Emissions Models to Assess Effects of Regional Development Scenarios on Nutrient Emissions to Water.** *Environmental Modelling & Assessment*.

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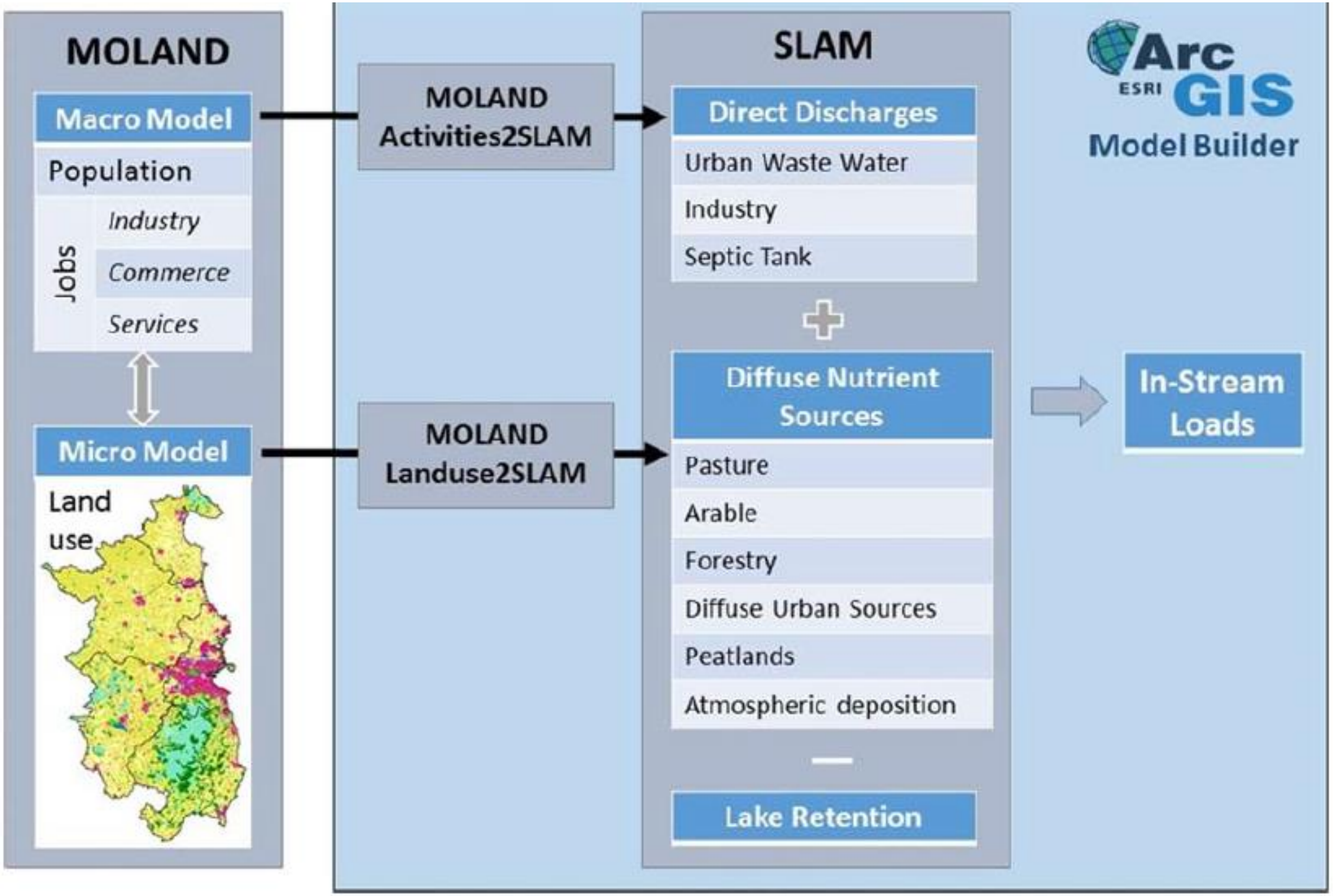
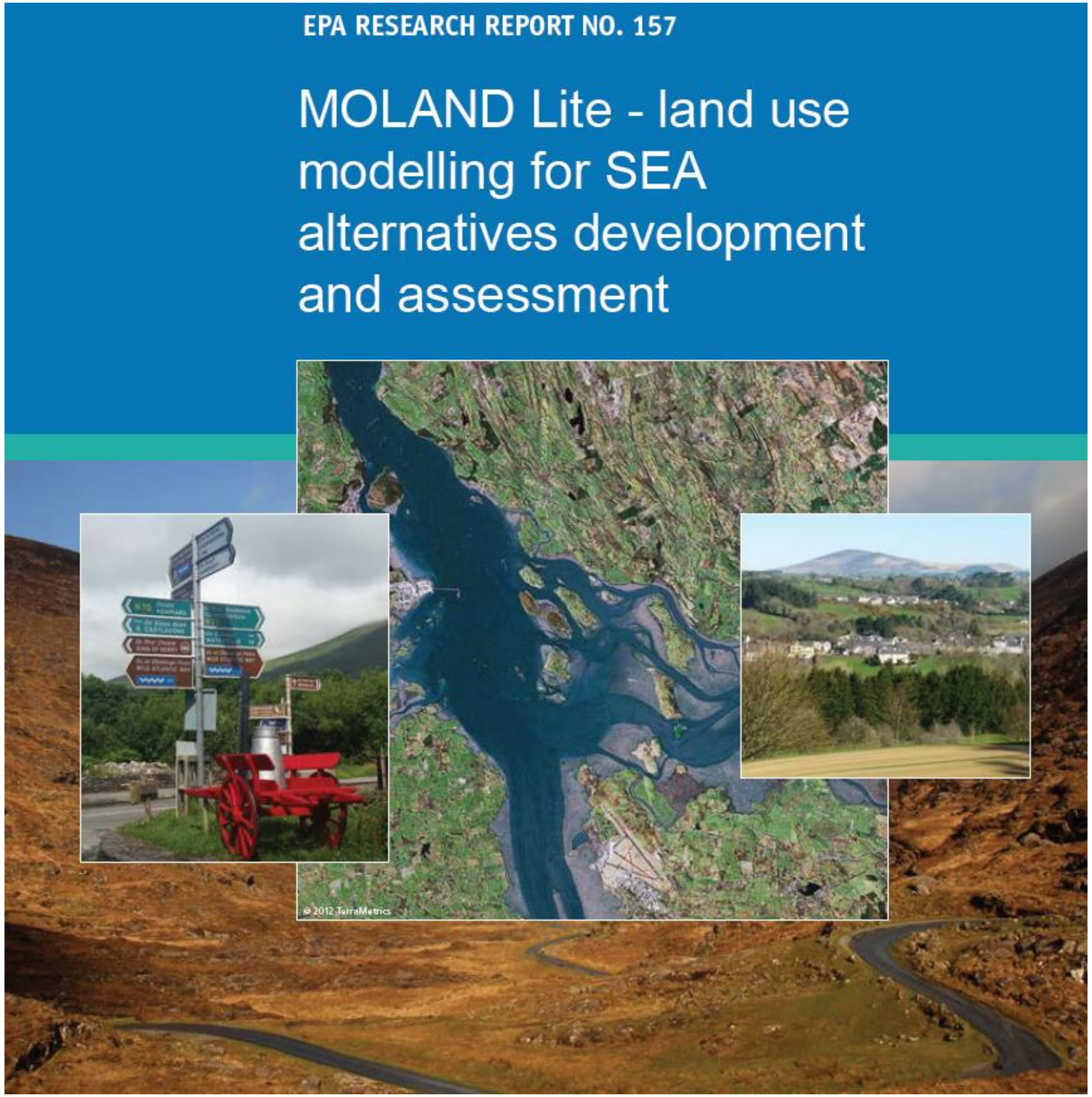


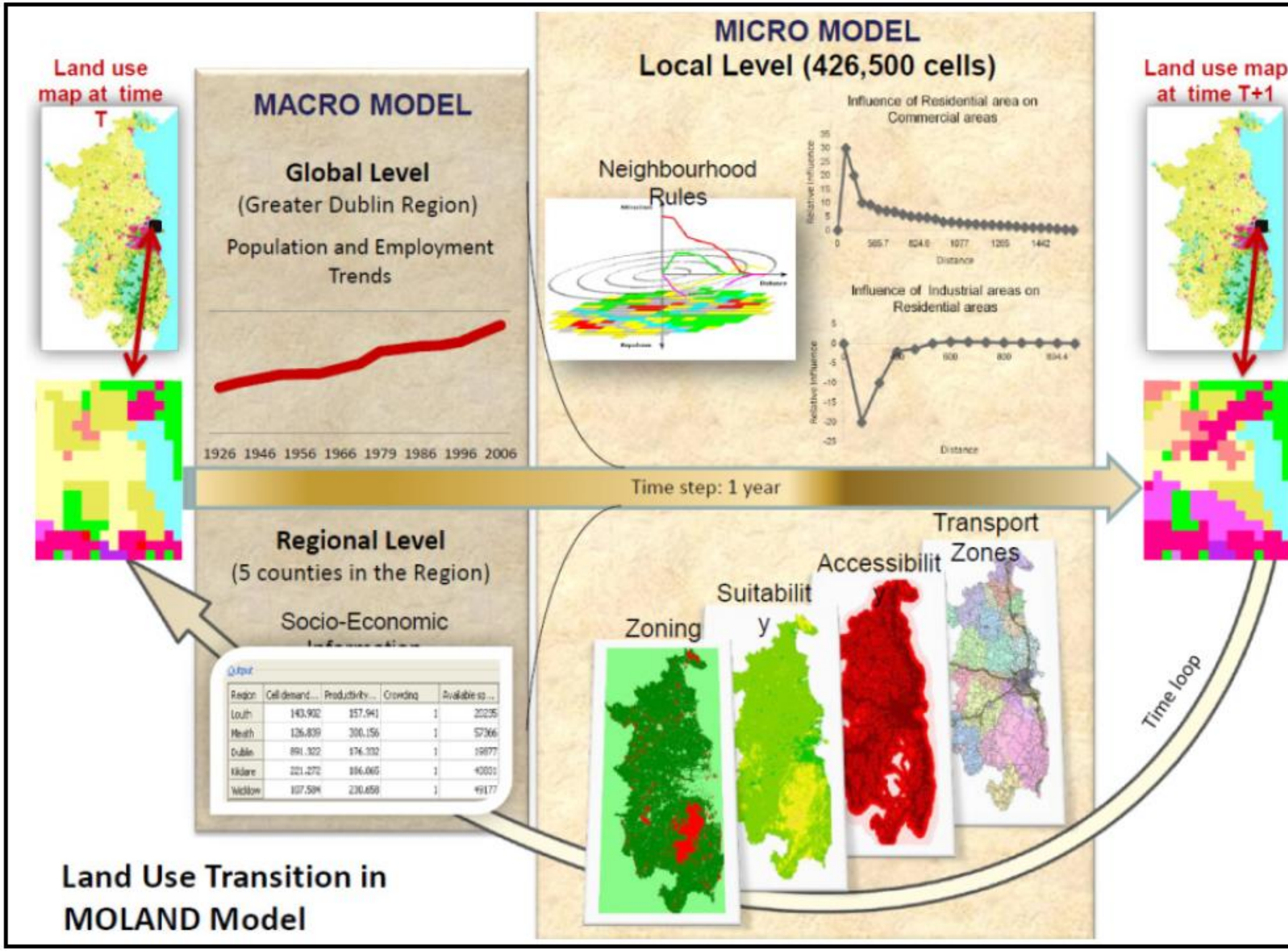
MOLAND

Foley, W., et al. (2015). MOLAND Lite – land use modelling for SEA alternatives development and assessment.
EPA Research Report 2013-SL-DS-1. Dublin, EPA.



MOLAND

Foley, W., et al. (2015). MOLAND Lite – land use modelling for SEA alternatives development and assessment. EPA Research Report 2013-SL-DS-1. Dublin, EPA.



Cellular Automata – other applications

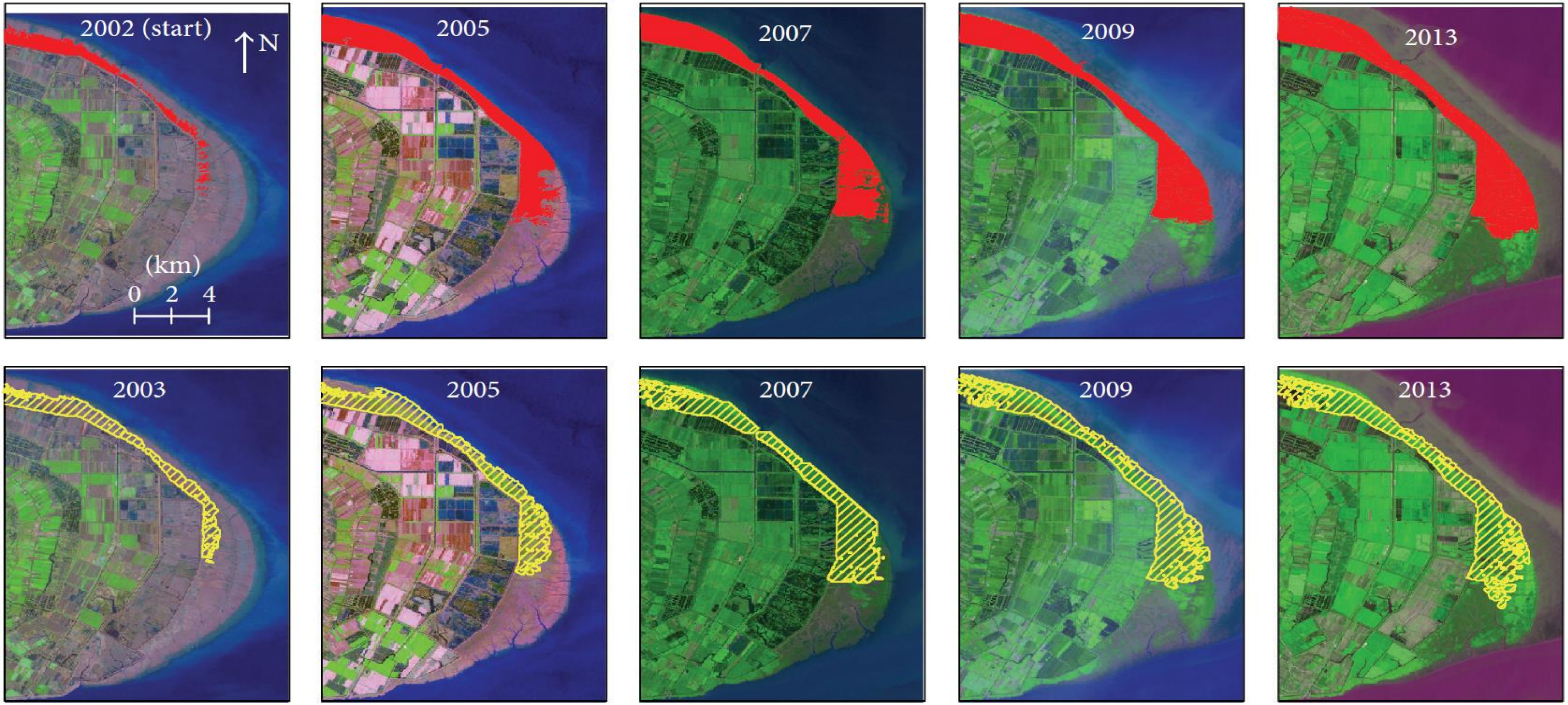
Bird migration [Aurbach, A., et al. (2020). "Simulation of broad front bird migration across Western Europe." Ecological Modelling **415**: 108879.]

Invasive species [Parks, S. C., et al. (2005). Argus invasive species spread model constructed using agent-based modeling approach and cellular automata. Proc. IEEE Winter Simulation Conf. New York.

Range expansion [Zheng, Z. S., et al. (2015). "Simulating the Range Expansion of Spartina alterniflora in Ecological Engineering through Constrained Cellular Automata Model and GIS." Mathematical Problems in Engineering **2015**: 8.]

Cellular Automata model usage: Range expansion of *Spartina alterniflora* -- Chongming Dongtan wetland

Source:Zheng, Z., et al. (2015). "Simulating the Range Expansion of *Spartina alterniflora* in Ecological Engineering through Constrained Cellular Automata Model and GIS." Mathematical Problems in Engineering **2015**: 875817.



Cellular Automata model usage: Lionfish invasion

Source: Johnston, M. W. and S. J. Purkis (2012). "Invasionsoft: A web-enabled tool for invasive species colonization predictions." Aquatic Invasions **7**(3): 405-417.