

Virtual Ecology Workbench

VEW3 Handbook

Special edition for VEW Workshop, July 2006

Editors

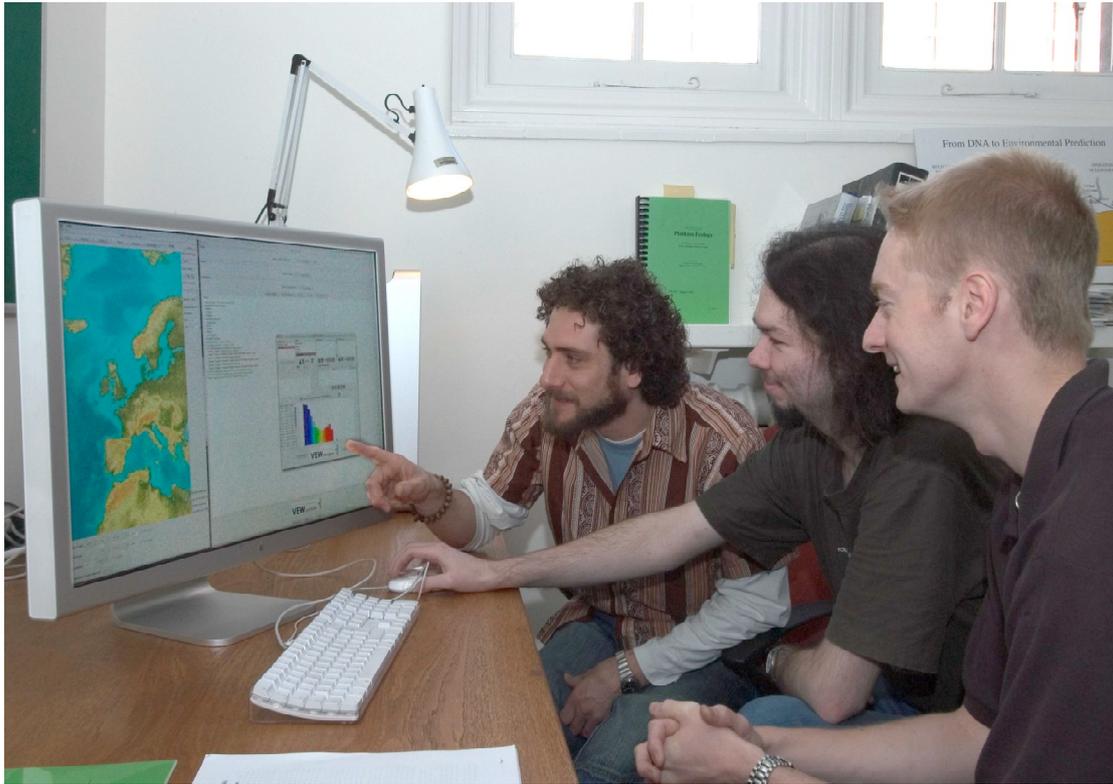
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Young members of the Virtual Ecology research group using VEW³.
From left to right: Matteo Sinerchia, Adrian Rogers and Dr.Wes Hinsley.

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We acknowledge the contributions of the many scientists and engineers who have been members of the Virtual Ecology research group over the past 25 years in Kiel, Southampton and London. They have all contributed to the successful completion of the VEW³.

Wolfgang Barkmann, Alan Brice, Tony Field, Lucas Partridge, Angelo Perilli, Mohammad Raza, Sarah Talbot, Silvana Vallerga, and Roger Wiley.

Preface

This handbook introduces and describes how to use the Virtual Ecology Workbench (VEW), a software tool for creating and analysing Virtual Ecosystems. The VEW eliminates the need for computer programming by the user.

Virtual Ecosystem

A Virtual Ecosystems is a one-dimensional mathematical simulation of the plankton ecosystem in a mesocosm drifting around the ocean. It is created with the Lagrangian Ensemble metamodel, which uses biological equations to describe the physiology and behaviour of individual organisms.

The emergent properties of a virtual ecosystem comprise the three kinds of time series:

1. the life history of each plankter.
2. The demographic properties of each population.
3. the environment as fields of physical, chemical and demographic variables.

The properties depend on the user's specifications for the model equations and the exogenous properties that control trophic closure, and the initial and boundary conditions.

The Virtual Ecology Workbench

VEW provides tools for building and analysing virtual ecosystems without the need for computer programming.

The graphical user interface makes it easy to enter the specifications for a plankton community in terms of functional groups and species. These are defined respectively by the biological equations and values of the parameters in those equations.

The workbench automatically manages the budgeting of chemicals, taking account of their flow between dissolved and particulate forms. It also computes the demography of each plankton population from the record of simulated births and deaths occurring in individual plankters.

VEW Handbook

The VEW handbook is still under development. The comprehensive edition, to be published in 2007, will provide a comprehensive single volume with, we hope, all the information needed by users of the Virtual Ecology Workbench (VEW³).

This Workshop edition introduces VEW³. It outlines a programme of exercises to help new users gain familiarity with its various functions. In the next edition, these exercises will be accompanied by step-by-step instructions with illustrations of the appearance of the graphical user interface at each stage.

We look forward to receiving feedback from readers.

*John Woods & Silvana Vallerga
London 2006*

A brief history

The Lagrangian Ensemble metamodel is an extension of individual-based modelling that predicts demography and biofeedback in simulations of the plankton ecosystem. It was conceived by John Woods in 1980 when he was professor of oceanography in the University of Kiel, Germany. He was motivated by the need to take account of optical biofeedback by plankton on sea surface temperature in climate models. The Institut für Meereskunde and the German Research Council (DFG) supported the research in Kiel.

The first LE model, incorporating the classical food chain of nutrients, diatoms, copepods and top predators, grew from student research projects at Kiel by Reiner Onken, Uli Wolf and Wolfgang Barkmann. After 1986 the work was continued by Wolfgang Barkmann as a postdoc research assistant at Southampton University with support from the UK Natural Environment Research Council. This led to the Woods-Barkmann (WB) model, which was a Lagrangian Ensemble version of the NPZD model used extensively by plankton modellers in the 1980s. The WB model was used to investigate a number of phenomena in biological oceanography.

The LE metamodel was adopted by a number of researchers overseas, including François Carlotti (who added staged growth to the copepods) and Niall Broekuisen (who modelled dinoflagellates in the deep chlorophyll maximum). But an attempt by Lucas Partridge at Southampton to build a food web model proved to be premature. It became clear that the computational complexity of the LE metamodel was a barrier to its uptake by the biological oceanography community. The method demanded a major commitment of skilled computer programmers who were in short supply.

In 1990 John Woods proposed a strategic solution to that problem. He argued that it would be cost-effective to invest substantial effort by highly skilled software engineers to create a tool that would automate programming of LE models. This up-front investment in a Virtual Ecology Workbench (VEW) would lead to much greater cost savings in modelling groups by eliminating the need to fund programmers to build and maintain computer codes. That was the economic case for VEW.

The UK Natural Environment Research Council (NERC) funded the first two versions (VEW¹ and VEW²). VEW¹ was designed by Alan Brice at Southampton University following a conceptual design by Dr. Fred Hopper of the NERC computing service. It was built using VSF* a commercial CASE environment. Our first attempt to build a workbench from scratch produced VEW². It was designed and built at Imperial College by software engineers led by Dr Tony Field of the Department of Computing. VEW³ was also based on his ideas. Planktonica, the innovative kernel of VEW³, was created by Wes Hinsley for his PhD project co-supervised by Tony Field and John Woods. Many features of VEW² & VEW³ were prototyped by computing undergraduates working in their summer vacations. Dr Wes Hinsley was responsible for the final integration and testing of VEW³. He is now the chief software engineer for the VEW development programme. In January 2006 VEW³ was released for testing by independent experts in UK and abroad. The saving in programming costs will soon exceed the up-front investment of about €1M. The next stage will be to expand the international community of VEW users.

* Virtual Software Foundry Ltd., a spinout company from Plessey.

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1 Virtual Ecology

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1.1 Introduction

This chapter provides a brief introduction to the science of Virtual Ecology, which applies the methods of individual-based modelling to the population ecology of plankton.

A Virtual Ecosystem is a mathematical simulation that describes how the model ecosystem responds to exogenous forcing. The emergent properties of the virtual ecosystem include time series of the physical and chemical environment, and of the demography of each plankton population. It also contains audit trails for the life history of every plankter in the virtual ecosystem.

Thus the emergent properties of a virtual ecosystem include all the features of both individual-based modelling and population-based modelling. The features are inter-dependent. Demography and biofeedback are computed from the properties and actions of individual plankters. That makes the virtual ecosystem globally stable.¹

The emergent properties can be divided into two classes: those that can (in principle) be observed, and those that cannot. The latter provide all the information needed for fine-grained diagnosis of the former.

Those are the unique features that make virtual ecology useful in research and teaching.

The Lagrangian Ensemble (LE) metamodel makes that possible. However, simulating the plankton ecosystem with LE involves complex computer codes. Creating and maintaining them by traditional computer programming is labour intense and time consuming. The Virtual Ecology Workbench (VEW) automates that process. It uses a graphical user interface to guide you through the steps needed to create a new virtual ecosystem by specifying the model, exogenous forcing, quality control, output logging and job control. The VEW then automatically compiles the specification into an executable code in Java, which you can run on your personal computer regardless of its operating system.

The Lagrangian Ensemble metamodel uses phenotypic equations that describe the physiological processes and behaviour of an individual plankter. Demography and biofeedback, the core of theoretical ecology, are emergent properties of the simulation. You are not permitted to write equations featuring demographic state variables, such as the biomass of a plankton population. That makes the design of LE model equations look quite different from those used in traditional population-based modelling with Eulerian integration. It takes some time to get used to this way of modelling. The pay-off comes from the purity of the model equations, and their roots in reproducible laboratory experiments. That gives the simulation scientific integrity and useful predictability. Learning how to build LE models and using them to create virtual ecosystems has a steep learning curve, but the results are well worth the effort.

¹ Globally stable means that no property of the virtual ecosystem exhibits artificial oscillation or chaos. The virtual ecosystem has a stable attractor (not a strange attractor). Globally means that this is true over all realistic values of the model parameters, and over the range of exogenous forcing (including resource levels) found in the ocean. (See Woods, Perilli and Barkmann 2005.)

The VEW Handbook will help you learn Lagrangian Ensemble modelling. It approaches the problem in two stages: familiarization and applications.

- Part I (chapters 1 to 5) is designed to familiarize you with Virtual Ecology and the Workbench. Chapter 4 provides a set of exercises.
- Part II is concerned with using VEW³ for scientific research and teaching.
- Part III supports Parts I and II. It provides worked examples, that take you step-by-step through each of the exercises.

VEW³ is supplied with a sample virtual ecosystem and the model and scenario used to create it. These are documented in chapter 9. You can easily extend the VEW³ archive to include new virtual ecosystems featuring additional biological equations, species, functional groups, and chemicals. And you can add new data sets for exogenous forcing.

VEW³ provides a flexible platform for the practice of Virtual Ecology, the science of plankton ecosystem modelling with the Lagrangian Ensemble metamodel.

1.2 Individual-based modelling

Individual-based modelling has long been attractive to marine biologists. They use it to simulate the development of an individual plankter², whose physiology and behaviour³ are described by phenotypic equations.

Phenotypic equations can be derived from reproducible laboratory experiments. Looking to the future, it should become possible to relate the equations to the organism's genotype. When that has been achieved it will become feasible to extrapolate the results of experiments on one species to others that share the same genes. That offers the prospect of establishing phenotypic equations for the thousands of species found in the ocean without performing separate experiments on cultures of every one.

The changing location and biological state of a plankter is computed by integrating its equations. Integration follows the plankter's track as it moves through the water. That biologically-lagrangian integration differs significantly from the eulerian integration used in classical population-based modelling. It avoids the numerical problems associated with the advection terms of eulerian modelling. Phenotypic equations are not contaminated by demographic factors, which is a weakness of eulerian modelling. Demography is a concept of theoretical ecology; it is properly an emergent property of the simulation, not an input of the model.

Attracted by these advantages, biological oceanographers have sought to use individual-based modelling to simulate the observable properties of an ecosystem with its large number of plankters. The challenge is to relate the growth and behaviour of individual plankters to changes in whole populations, and their impact on the environment through physical and chemical biofeedback. The direct approach is impossible because no computer can integrate an individual-based model for an ecosystem with billions of plankters per litre. We need a computationally-affordable method that can derive demography and biofeedback from the changing state of each plankter and its interaction with the environment and other plankters. The Lagrangian Ensemble (LE) metamodel (Woods 2005) provided the first practical solution to that problem.

² We use the names *plankter* for an individual organisms and *plankton* as a collective noun for many plankters. The plankters in one species present in the simulation are collectively called a population, while the plankters in all species are called a community.

³ We define a plankter's *behaviour* as its motion through the water. That displacement is in addition to the advection caused by fluid motion (ocean circulation, upwelling and turbulence).

1.3 Lagrangian Ensemble integration

The Lagrangian Ensemble method uses agent-based computing. Each agent represents one plankter, as in pure individual-based modelling. However, each agent also represents a dynamic sub-population of the same plankters.

This is the method used to scale up from individuals to whole populations when the number of computer agents is much fewer than the number of plankters in the ecosystem. It permits computation of demography and biofeedback while retaining all the advantages of individual-based modelling.

The biological state of every plankter in one sub-population is identical. They all follow the same trajectory, and therefore they all experience the same history of ambient environment. The ambient environment is defined as the set of values that the environmental fields (temperature, light, chemical concentrations, prey concentration, etc.) have at the plankter's location in the sea. So at any instant they have the same state of transient adaptation to their shared history of ambient environment.

For more details see

J.D.Woods (2005) "The Lagrangian Ensemble metamodel for simulating plankton ecosystems" *Progress in Oceanography*, **67**: 84-159.

1.4 Biological equations

The LE method follows individual-based modelling in using phenotypic equations for the physiology and behaviour of each plankter in the sub-population associated with one computer agent. The equations may be diagnostic (computing a biological variable in terms of others) or prognostic (describing the rate of change of a biological variable), or they may be rules (such as “if this then do that”).

Each equation computes the value that one of the biological state variables will have at the end of the current time step. It is applied sequentially to each agent. This resulting values will be used in the next time step. The equation computes the new value for each agent as a function of the following factors:

- The current biological state of the plankters in the agent’s sub-population
 1. One or more of the variables in the ambient environment.

1.4.1 Computing predation

Predation is computed in the same way, with the ambient prey concentration being treated as a component of the biological environment.

This avoids the need to compute the interaction between a predator agent and each of the prey agents in its vicinity. Computing such agent-agent interaction would be expensive; it is avoided in the LE modelling. Indeed using ambient prey concentration to compute the number of prey ingested by a predator in one time step is one of the hallmark features of Lagrangian Ensemble modelling. The same approach is used to compute the uptake of infectious bacteria and viruses for epidemiological prediction.

1.4.2 Depletion of prey

The LE method includes rules for computing the depletion of the prey plankters in each sub-population. And the depletion of infectious viruses and bacteria in the water when some are taken up by the plankton that become their hosts. The rules prevent over depletion. They do this by first computing the total demand for all the plankton, by polling all the agents. If the total demand exceeds the available resource, the actual consumption by each agent is scaled back to avoid leaving a negative resource. This is done automatically by the VEW: you do not need to take account of it in your biological equations.

1.5 Time step

You start by composing your biological equations for VEW³ in MKS (metre-kilogramme-second) units. So you express the rate of a biochemical process as the change in a biochemical variable occurring per second.

1.5.1 Euler integration

The biological equations are expressed in finite difference form. They describe the change that will occur in one biological variable from one time step to the next. In other words VEW³ uses simple Euler integration.

1.5.2 Choosing the time step

Later you will specify the time step to be used when the model is integrated. It is specified in seconds. The time step used in LE modelling normally lies in the range one minute to one hour (60 to 3600 seconds).

1.5.3 Resolving changes in a plankter

The time step must be short enough to avoid error when using Euler integration of the biochemical processes in an individual plankter that you feature in your model.

1.5.4 Resolving changes in the environment

The time step must also be short enough to resolve changes in the environment that are significant for your numerical experiments. Normally your model will include diel migration of the zooplankton, then the time step must be short enough to resolve the rapid changes in solar irradiance profile at dawn and dusk. And the associated rapid changes in the depth of the turbocline, which marks the transition from turbulent flow in the surface mixing layer, and laminar flow in the underlying diurnal thermocline. A half-hour time step usually suffices for diel migration.

1.5.5 Response to changes in ambient irradiance caused by turbulence

A plankter in the surface mixing layer is displaced vertically by turbulence, giving it an erratic variation of depth. That track is computed by a turbulence routine. The form of the routine is related to the choice of time step. For example, if you choose a time step that is longer than the overturning time of the largest eddies, it is reasonable to assume that there is no correlation between the depths of the plankter in successive time steps. The routine can then use a random number generator to compute the new depth at the end of each time step. That is the default routine provided by the VEW. It assumes that you are using a time step of 30 minutes or longer. For shorter time steps it becomes necessary to use a more complicated turbulence routine. For example, the particles depth may follow a random walk, with the statistics related to the power input to the turbulence (a physical state variable of the virtual ecosystem) and the thickness of the mixing layer.

The irradiance profiles for each waveband in the solar spectrum vary strongly with depth. Half the solar energy is absorbed in the top one metre of the ocean. So the plankter's erratic variation of depth is accompanied by corresponding variations in ambient irradiances. A phytoplankter's energy uptake by photosynthesis is affected by this "flickering effect". In order to compute photosynthesis accurately you need to adopt a time step that is short enough to about error due to the flickering effect.

Barkmann and Woods (1996) used a five-minute time step, with a random walk routine for the turbulence.

1.6 Audit trails

An audit trail describes the life history of one computer agent in terms of time series for:

- Its location (latitude, longitude and depth in a one-dimensional simulation),
- The biological state of its plankters (their state of biological adaptation, and the contents of each of their pools⁴),
- Its ambient environment (the value of each environmental field at its location),
- The number of plankters in the agent's sub-population.

1.6.1 Applications

Audit trails are used to clarify the causes of observable emergent features of the virtual ecosystem. Usually an environmental variable, or a demographic property of a plankton population. You select the plankton agents that are present at the event, by space-time windowing. Then you examine the audit trails of those agents to see how their plankters are contributing to the event.

An audit trail shows the depletion of an agent's sub-population when it is subject to predation. And it shows how each of its pools rises or falls as the individual plankter performs biological functions, including:

- uptake of nutrients, or excretion/egestion of waste products,
- internal biochemical reactions,
- digestion in a zooplankter's gut (which makes space for further ingestion),
- growing eggs,
- responding to infection.

1.6.2 Debugging

Examining audit trails of individual agents is particularly useful when you are checking a new biological model. VEW³ provides a debug tool called *LiveSim* that allows you to work step-by step in creating a virtual ecosystem and monitoring the state variables.

1.6.3 Lineages

The VEW contains a tool that extends the computation of an audit trail from one agent to the family of related agents. That permits lineage analysis following the life history of successive generations in the same family.

Over many years, some plankton lineages become extinct, while others survive to provide the members of their population. The *Lifespan* tool takes account of these extinctions in computing a plankter's life expectancy. Using audit trails you can investigate the causes of unexpected features in a life expectancy time series.

⁴ The primary pools contain for chemicals; they are like Droop pools. In modelling epidemics we also use pools to hold the dynamic "population" of viruses contained in an infected plankter.

1.7 Emergent demography and biofeedback

The audit trail is the *Lagrangian* part of the Lagrangian Ensemble method. The *Ensemble* part is the demography of each plankton population and the impact that it has on the environment (i.e. biofeedback).

1.7.1 Strictly phenotypic equations

The LE method prohibits equations that contain variables with demographic content, such as the biomass of a prey population. That ensures a pure separation between: (a) the phenotypic equations for an individual plankter, which are used in the model; and

(b) the demography and biofeedback of populations, which are emergent properties of the virtual ecosystem.

It is important to bear that in mind when you design the biological equations for a new LE model. Your equations must not include information that is not available to an individual plankter. For example, a plankter cannot know the number of plankters in its population or the biological condition of the others, or what they are doing.

1.7.2 Computing emergent demography and biofeedback

The computation of demography and biofeedback requires that all the plankters in the simulated ecosystem are represented by the set of computer agents. In practice, the number of agents that can be used in the computation is limited to about one million per processor on your computer. If you want to simulate the ecosystem in, say, a thousand cubic metre mesocosm (e.g. one kilometre vertically and one square metre in horizontal area) drifting in the ocean, the plankton will be numbered in trillions. It is not possible to allocate one computer agent to each of these vast number of plankters. Nevertheless every one of them *must* be accounted for in the computation of demography and biofeedback. The LE method solves that problem by ensuring that every plankter in the mesocosm is present in one or other of the set of sub-populations.

1.7.3 The mesocosm as a sample of the broader ecosystem

We find it convenient to design our numerical experiments as though they occur in a virtual mesocosm with well-defined dimensions and implicit side walls. It often has a horizontal area of one square metre and a vertical extent from the sea surface to a maximum depth of one kilometre. In that virtual ecosystem, the number of plankters in each population must be an integer. And the number of plankters in each sub-population must be an integer.

A more flexible approach is to treat the virtual mesocosm as representing the broader (virtual) ecosystem at its location. The demographic properties are then samples of that broader ecosystem. We stop thinking of a number of plankters in the mesocosm, thinking instead of the number of plankters per square metre at that location in the broader ecosystem. One consequence of this change of thinking is that the demographic variables no longer have the units “plankters per mesocosm” but “plankters per square metre”. In the former case the values must be integers: in the latter case they do not. Provided the virtual mesocosm has a horizontal area of one square metre the numbers are the same.

1.7.4 Dynamic sub-populations

The sub-populations are dynamic. The number of plankters in a sub-population changes from one time step to the next. The number increases when the plankters in the sub-population reproduce. They are all identical, so they all reproduce together and each produces the same number of offspring.

The number of plankters in the sub-population decreases when a predator eats some of them. As we noted above, the number eaten in one time step does not have to be an integer.

Every sub-population has its own demographic history defined by these gains and losses each time step. The sub-population's demographic history is controlled by its history of ambient environment, which is determined by its trajectory through the changing environmental fields. Remember that the biological environment comprises demographic variables for its prey and predators.

The trajectory is affected by turbulence. Turbulent dispersion (effected by using a random number generator`) leads the sub-populations to follow different trajectories. As the result, each sub-population develops a unique demographic history as the simulation proceeds.

1.8 Intra-population variability

If the computation uses a sufficiently large number of computer agents (each with its sub-population), the statistics of demographic variation between the sub-populations provides a good representation of the intra-population variability that would occur in a hypothetical simulation with one agent per plankter. There is inevitably a sampling error in a computation based on fewer computer agents than there are plankters. The success of the LE method depends on using a sufficiently large number of agents to keep the sampling errors within acceptable bounds. That is ensured by the procedure called “particle management” (see Woods, Perilli and Barkmann 2005). VEW³ provides tools to control particle management and to measure the LE sampling error by ensemble computation.

1.9 Demography

VEW³ computes the demography of the each plankton population by summing over all its sub-populations. Demographic variables include:

- the *birth rate*, computed from the number of new plankters born in each time step.
- the *death rate* due to each cause of death, computed from the number lost to predators, to natural mortality, and to disease.
- the *total number* of plankters in each population.
- The *biomass* in each population, computed by summing the biomass in each sub-population. That sub-population biomass is defined by its number of plankters multiplied by the weight of one of the plankters. (All members of the sub-population are identical).

These demographic variables are defined for each time step and each layer of the virtual mesocosm. You can choose to log them at this full resolution, or averaged over specified ranges of depth and time.

1.10 Biofeedback

The same ensemble approach is also used to compute biofeedback, defined as the change in the environment wrought by the plankton in each layer used to define the environmental fields in the virtual mesocosm. In the example of a thousand cubic metre mesocosm, each environmental field is defined by values in a thousand cells, each of one cubic metre. (We can think of them as a vertical stack of cells each one metre thick.) Each plankter can change the environment in the cell where it lies. For example, a plankter may extract or release chemicals, or influence the optical properties of the water. The LE method computes the change in the environment in each cell by summing the changes wrought by each of the plankters residing there in that time step. As in the computation of demography, the secret of success (defined by controlling sampling errors) is to ensure that there is a sufficient number of sub-populations of each species in the cell.

Migrating plankters often pass through several one-metre-thick layers in one time step. VEW³ automatically allocates biofeedback pro-rata to those layers.

1.11 Summary

To summarize, the Lagrangian Ensemble method has the following core features:

- a. agent-based computation,
- b. each agent behaves like a single plankton controlled by phenotypic equations,
- c. for each agent the LE method computes audit trails, comprising the location and life history of the plankter, and the history of its ambient environment,
- d. an audit trail can describe a lineage extending over many generations,
- e. every agent carries information about a dynamic sub-population of plankters,
- f. each sub-population has a unique demographic history governed by its trajectory through the changing environmental fields,
- g. the demography of each plankton population is computed by summing over all its sub-populations,
- h. the biofeedback of the plankton to the environment is computed by the contributions of the plankters residing in (or passing through) each cell used to define the environmental fields,
- i. the success of LE computation of demography and biofeedback is measured by controlling the sampling errors arising from using a computationally-affordable number of agents that is much smaller than the number of plankters in the ecosystem being simulated,
- j. the sampling errors are controlled by ensuring that the number of agents in each cell does not fall too low,
- k. that is achieved by particle management, which will be described later .

This list includes only the main features of the LE method. The VEW includes all necessary features, many of which are concerned with budgeting all the state variables in a way consistent with changes in the individual plankters controlled by their phenotypic equations.

1.12 Postscript

One final point. The Lagrangian Ensemble method works because it computes the behaviour of every plankter in the simulated ecosystem. That is made computationally affordable by grouping the plankters into a limited set of sub-populations, each following a unique trajectory through the changing environment. So all plankters are present in the simulation, but they do not all have independent trajectories. The LE method is successful because it uses sophisticated particle management to control the number and distribution of agents used to compute the demography and biofeedback of each species. That particle management is designed to limit the sampling errors in the computation. It is one example of the complex technology used to guarantee the integrity of a LE simulation. We shall see later that the VEW hides that technology from the user, while exposing the scientific processes used to simulate the ecosystem.

1.13 Virtual Ecosystems

Lagrangian Ensemble simulations of the plankton ecosystem are called Virtual Ecosystems. The simulations are much more comprehensive and realistic than can be achieved by observations at sea, or by traditional Eulerian simulation with population-based models. Virtual Ecosystems are Lagrangian Ensemble plankton simulations that combine the scientific integrity of phenotypic equations with the realism found in agent-based computing.

Virtual ecosystems meet the needs of biological oceanographers by presenting the plankton ecosystem from three perspectives:

- the environmental fields
- the demography of each population
- the life history of every plankter.

These are the emergent properties of the ecosystem. By diagnosing those data, the virtual ecologist can discover how the ecosystem responds to different assumptions that are contained in his/her specification for the model and scenario used to create the virtual ecosystem. The simulation is so rich and the processes occurring in it so complex that the emergent properties are often unexpected. They may seem to be counter-intuitive to an oceanographer whose experience has been honed on the products of simple models or skimpy field observations.

The virtual ecosystem contains all the information needed to explain its emergent properties in terms of the biological equations used to create the simulation. When those equations are derived from reproducible experiments on plankton cultures, the explanation is as scientifically robust as any in physics. This opens a new era in biological oceanography. It fosters the transition from exploration to experimentation.

Observable and non-observable properties It is convenient to divide the emergent properties of a virtual ecosystem into three parts. The first comprises properties that can in principle be observed at sea. This category will grow as new instruments and methods are introduced into sea-going biological oceanography. The second part comprises bulk observations that cannot be observed at sea, at least not yet. The third comprises the audit trails of individual plankters.

Analysis The practice of virtual ecology starts with the observable emergent properties. The aim is to document a target feature in the virtual ecosystem, then to show how it arose by studying related finer-grain structures and processes that cannot be observed. This investigation normally has two stages. The first concentrates on the bulk properties: environment and demography. The hypotheses generated from that stage are then tested by examining the audit trails of plankters who were on the scene at the time, and so could have influenced the key features of the bulk properties. The behaviour of each of these plankters is directly controlled by its phenotypic equations. So scientific explanation is complete when the detective has shown how the actions of individual plankters influenced the observable phenomenon that was the target of the investigation.

Experimentation Scientific experimentation involves diagnosing the target phenomenon as it appears in each of a sequence of virtual ecosystems created with slightly different specifications for the biological equations, or with different species. The result is a comprehensive scientific understanding of the target phenomenon; understanding that is rooted in reproducible laboratory experiments.

1.14 One-dimensional Virtual Ecosystems

VEW³ supports the simulation of one-dimensional virtual ecosystems. The formal definition of one-dimensional is that no property of the virtual ecosystem is affected by horizontal flux divergence at any depth. This can occur in the ocean if every property of the ecosystem has a negligible horizontal gradient in the upstream direction. Alternatively it occurs where the horizontal flow is negligible at the site of the simulation. One-dimensional simulation allows individual plankters to move up and down, but not horizontally (or at least they must not move horizontally beyond the scope of the simulation).

This restriction to one dimension is not as severe a constraint as it may at first seem. That is justified by two facts.

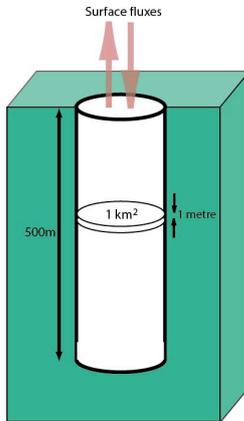
The first concerns the physical environment, which has the character of a turbulent boundary layer in which the structure is controlled by the fluxes of physical properties (light, heat, salinity) directed orthogonal to the boundary, i.e. down from the sea surface. The horizontal gradients of those physical properties are much weaker, typically in the 1: (f/N), where f is the Coriolis frequency and N is the stability (or Brunt-Vaisala) frequency. This ratio is order 1:1000 for the gyre-scale circulation of the ocean.⁵

That leads to the second fact, which concerns the behaviour of plankton. Many species of plankton have evolved locomotion that allows them to change their ambient environment usefully by swimming vertically, but (unlike fish) they cannot move fast enough to change their environment by swimming horizontally. That fact provides the best way to discriminate between fish and plankton. It allows us to include fish larvae in our models of the plankton ecosystem.

⁵However, the ratio may approach 1:10 at mesoscale fronts where the plankton ecosystem must be simulated by a three-dimensional model. See M.K.MacVean & J.D.Woods (1980) "Redistribution of scalars during upper ocean frontogenesis." *Q.J.Roy.Met.Soc.* **106**, 293-311.

1.15 Virtual mesocosm

The virtual mesocosm is defined as a tube with a vertical axis extending down from the sea surface to an open lower boundary that lies well above the ocean floor. The upper boundary is open to air-sea fluxes of radiation, heat, gases and dust. The water flows freely through the sidewall, but produces no horizontal flux divergence at any depth. The axis of the mesosm remains vertical as it drifts with the ocean circulation.



Geographically-lagrangian integration

The large-scale circulation of the ocean can significantly change the geographical location and therefore the ambient environment during one year. VEW³ supports an extension of one-dimensional modelling that takes account of ocean circulation to first order. It does so by simulating the ecosystem in a virtual mesocosm that drifts around the ocean with the large-scale circulation. We call this geographically-lagrangian integration. The ocean velocity field is an exogenous property derived from a general circulation model. A global velocity field derived from OCCAM is bundled with VEW³.

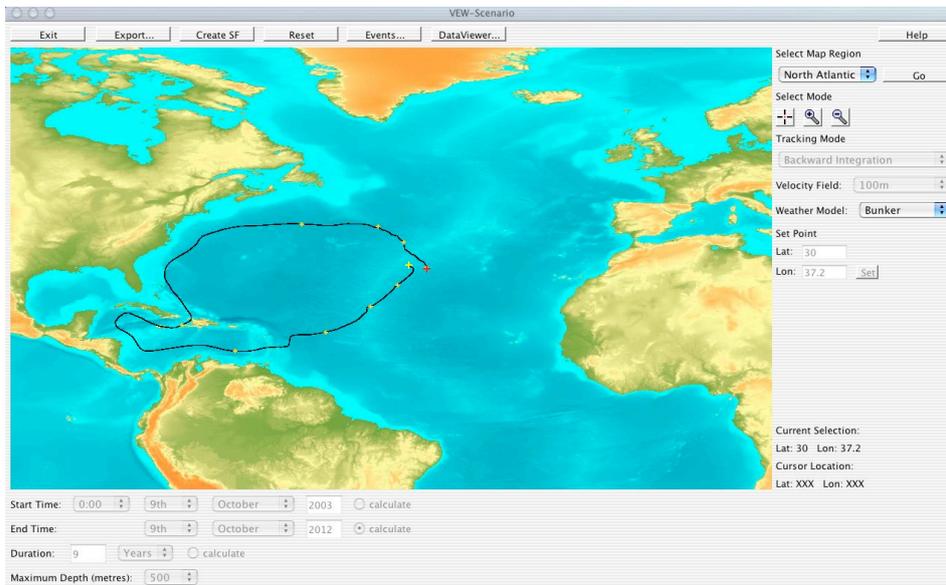


Fig.x The track of a virtual mesocosm simulated over nine years. The large yellow dot marks the start of the track on 9th October 2003 at 30°N 37.2°W. The smaller yellow darts mark the location of the mesocosm each 1st January. The red cross marks the termination of the track on 9th October 2012 close to the starting point.

1.4 Verification

A virtual ecosystem owes its credibility to the use of biological equations that are derived from reproducible experiments performed in the laboratory under controlled conditions. The Lagrangian Ensemble method is used to create a virtual ecosystem by integrating those equations under the influence of scenario for exogenous forcing. The LE method controls sampling errors. The residual uncertainty in the virtual ecosystem due to LE sampling can be computed from an Ensemble (a set of virtual ecosystems differing only in the seed value used to initialize the random number generator used to compute turbulent displacement of each plankton agent). The other sources of uncertainty in the simulation are attributable to the data used to construct the biological equations and the scenario.

Tuning This approach to simulating the plankton ecosystem does not depend on tuning model parameters to observations. Their values are controlled by the experiments that were used to construct the biological equations.

However we do not really expect the observable properties of our virtual ecosystem accurately to simulate observations of the same properties made at sea. Let us suppose for the moment that the observations do not contain significant errors. (We shall return to that point shortly.) In that case the difference between observation and simulation must be attributable to shortcomings of the virtual ecosystem. These might be attributable to the errors in either the scenario or the model.

Errors in the scenario We start by considering the scenario. Obviously it should accurately represent the corresponding conditions occurring during the observations, in particular the air-sea fluxes of radiation, heat, gases and particles. Less obviously, it must accurately represent those fluxes during the previous few years. That is because the ecosystem takes several years to adjust to a balanced state (an attractor) after the simulation started at some distant location upstream.⁶ It is not a trivial matter to ensure that the simulation was forced by atmospheric conditions that match those controlling the observed natural ecosystem. Similar considerations apply to other aspects of the scenario, including the ocean circulation and initial hydrography (notably the nutrient profile).

Errors in the biological model Now we consider the design of the biological model. The main concern lies with the simplified plankton community represented in the virtual ecosystem. The thousands of species present at the site of the observations are represented in the model by a small number of explicit species, or more commonly by a few functional groups (Anderson 2005). The model's truncated biodiversity makes it a vulnerable cartoon of nature.

The modeller seeking realism must reduce the shortcomings of his/her virtual ecosystem by designing more realistic scenarios and plankton communities. The success of this endeavour is judged by comparing the observable emergent properties of the virtual ecosystem with observations. That process of verification is successful if the comparison reveals a difference that is statistically significant, given the known noise in the virtual ecosystem (as measure by ensembles) and in the observations. This process is formalized in the Ecological Turing test (Woods 2005).

⁶ See Woods, Perilli & Barkmann (2005)

1.16 The Virtual Ecology Workbench, VEW

The Virtual Ecology Workbench is a software tool that automates computer programming. It was conceived as an efficiency tool for those simulating the plankton ecosystem by the Lagrangian Ensemble method. It is designed to be used by biological oceanographers with no more computing skill than is needed to use a spreadsheet such as Microsoft Excel.

We originally used Fortran and then C codes for our virtual ecology research. The computer codes were complex and required skilled programmers to build, debug and maintain. Even quite small modifications to an existing code required a substantial effort. Fifteen years ago we decided to invest in a high level tool that would automate the writing of codes according to a user specification entered through a friendly graphical user interface. The assumption was that the downstream savings from eliminating user programming would justify the substantial initial investment in software engineering.

After investing over €1M we now have an operational third version of the workbench (VEW³) that fully satisfies our original dream. Indeed the requirement has been substantially extended to take account of experience gained in virtual ecology research during the last decade at Imperial College. VEW³ generates Java code that can be executed on any personal computer to create a virtual ecosystem with a plankton community specified by the user. It allows the user to introduce new biological equations, design new functional groups and species with staged growth. Other tools simplify the building of initial and boundary conditions.

To summarize, VEW³ offers two main benefits for ecologists seeking to use the Lagrangian Ensemble metamodel to simulate the plankton ecosystem.

- The first is that eliminates the need to employ a computer programmer: bug-free code is generated automatically.
- The second is that it offers a rapid turn-round, making it possible to change the specification of a model/scenario and analyse the resulting virtual ecosystem in a few hours.

A detailed description of VEW³ is given in Chapter 2 of this handbook. Comprehensive user instructions are presented in Chapters 3 and 4. Worked examples are featured in Chapter 7.

1.17 The VEW Handbook

The Virtual Ecology Workbench (VEW³) is a powerful tool that eliminates the need for user programming in virtual ecology. Its graphical interface is designed to be user-friendly. However, it is not trivial to master this powerful and flexible tool. The newcomer must be prepared to climb a fairly steep learning curve before becoming familiar with the procedures used to creating a new virtual ecosystem. This VEW Handbook has been written as a guide for the newcomer. The first draft will be reviewed by biological oceanographers in the UK and abroad who are testing VEW³. It will be presented in the VEW Workshop. After revision it will be published on the web at <http://www.virtualecology.org>.

The learning curve has four stages. The first is adopting the conventions of the Lagrangian Ensemble metamodel. If you have experience in population-based modelling you may find it difficult to switch to the new way of thinking. In particular the experienced modeller must learn to write pure phenotypic equations that describe exactly how an individual plankter responds to its ambient environment without any reference to the state of the population. The Handbook addresses that challenge in Chapter 1.

The second stage in the learning curve involves understanding how VEW³ works. It makes a clear separation between LE science and LE technology. They are separated by a metaphorical curtain, which allows the user to see the science while hiding the technology. The VEW³ graphical user interface makes it easy to specify the science of a new virtual ecosystem (i.e. its biology and scenario). Behind the curtain, VEW³ takes responsibility for budgeting chemicals and plankters, and managing the sub-populations to control sampling errors. The experienced population-based modeller may find it strange to trust VEW³ to handle budgeting that normally has to be written into his/her equations. Chapter 2 introduces the design of VEW³ and documents its various tools and functions.

After learning the strategy behind VEW³ the third learning stage is concerns the tactics of using it to build a new virtual ecosystem. The strategy is based on creating a comprehensive specification, which will be compiled to create the executable code. The tactics involve building that total specification piece by piece in the right order. This involves some fifty tasks, each of which is guided by the VEW³ user interface. The procedure is described in Chapter 3.

The fourth stage is more straightforward. It involves learning how to use VEW³ *Analyser* to select data from a virtual ecosystem and display them graphically. You can think of VEW³ *Analyser* as a quick-look tool. It allows you to search rapidly through the massive data set that is a virtual ecosystem (several gigabytes per simulated year). It contains many of the graphical tools needed to reveal emergent properties of the virtual ecosystem. It is often possible to explain them without leaving VEW³ *Analyser*. But when that is impossible you can easily export selected data to a third party package, such as MS Excel or Matlab for detailed analysis. This diagnosis stage is described in Chapter 4.

1.18 Further reading

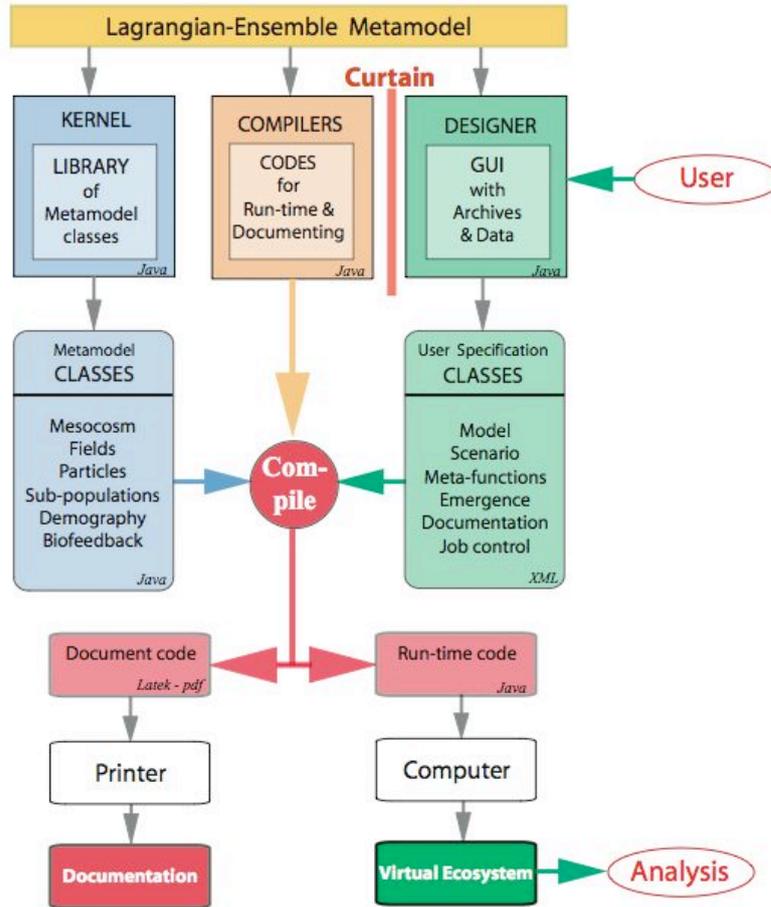
This introduction to virtual ecology is designed to provide the essential information needed to get you started. More detailed information can be found in the publications listed in the bibliography.

2 The Virtual Ecology Workbench (VEW³)

Contents

Design concept
The curtain
Biology
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Chemistry
Biochemical processes in a plankter
Physics
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Turbulence
Air-sea interaction
Hindcasting
Events

Virtual Ecology Workbench VIEW3



JDW 23 October 2004

2.1 Design concept

The Virtual Ecology Workbench is a software tool for simulating the plankton ecosystem using individual-based equations that are integrated by the biologically-lagrangian method. With a few exceptions, you can proceed as though you are creating a pure individual-based simulation with every plankter represented separately by its own computer agent. That is the appropriate mindset to adopt when using VEW³.

In reality VEW³ creates virtual ecosystems by Lagrangian Ensemble integration. All the plankters in a mesocosm are represented, but they are grouped into sub-populations, each associated with one computer agent, which behaves like one of the plankters in its sub-population.

The number of agents is small compared with the total number of plankters in the mesocosm. Managing LE integration requires some complex software engineering. However, VEW³ was designed to hide that technology from the user who can forget about the LE concept of sub-populations when he/she is designing a biological model.

In fact there are only two occasions on which you need to be aware of sub-populations. The first is in specifying how they will be managed to control sampling noise. The second is in analysis of audit trails which present sub-population demography to aid diagnosis.

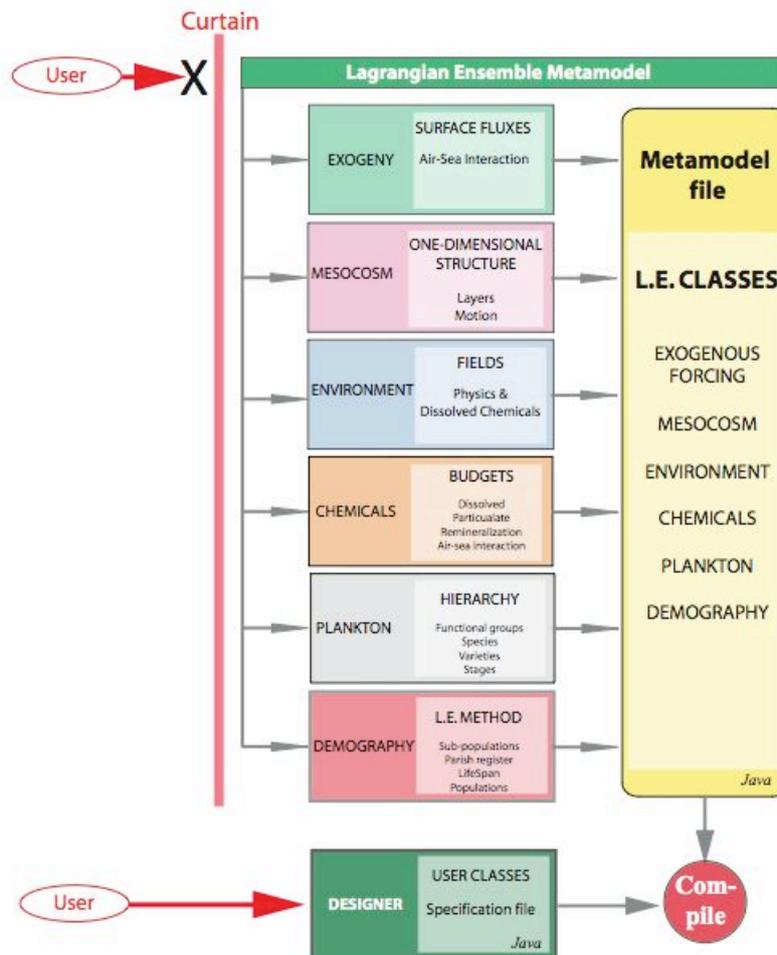
The graphical user interface achieves this separation of science and technology by a metaphorical curtain. The graphical interface presents the science in front of the curtain as though you are creating a pure individual-based model. With the two exceptions mentioned above, you can proceed without taking account of sub-populations.

2.2 The curtain

Behind the curtain, VEW³ takes care of the functions of LE technology, including the management of sub-populations, the budgeting of chemicals and the computation of demography. The goal was to hide behind the curtain every action that does not need user intervention. These hidden functions include many aspects of modelling that are traditionally represented explicitly in the equations written by the programmer in traditional eulerian modelling. The hidden functions are shown in fig.x.

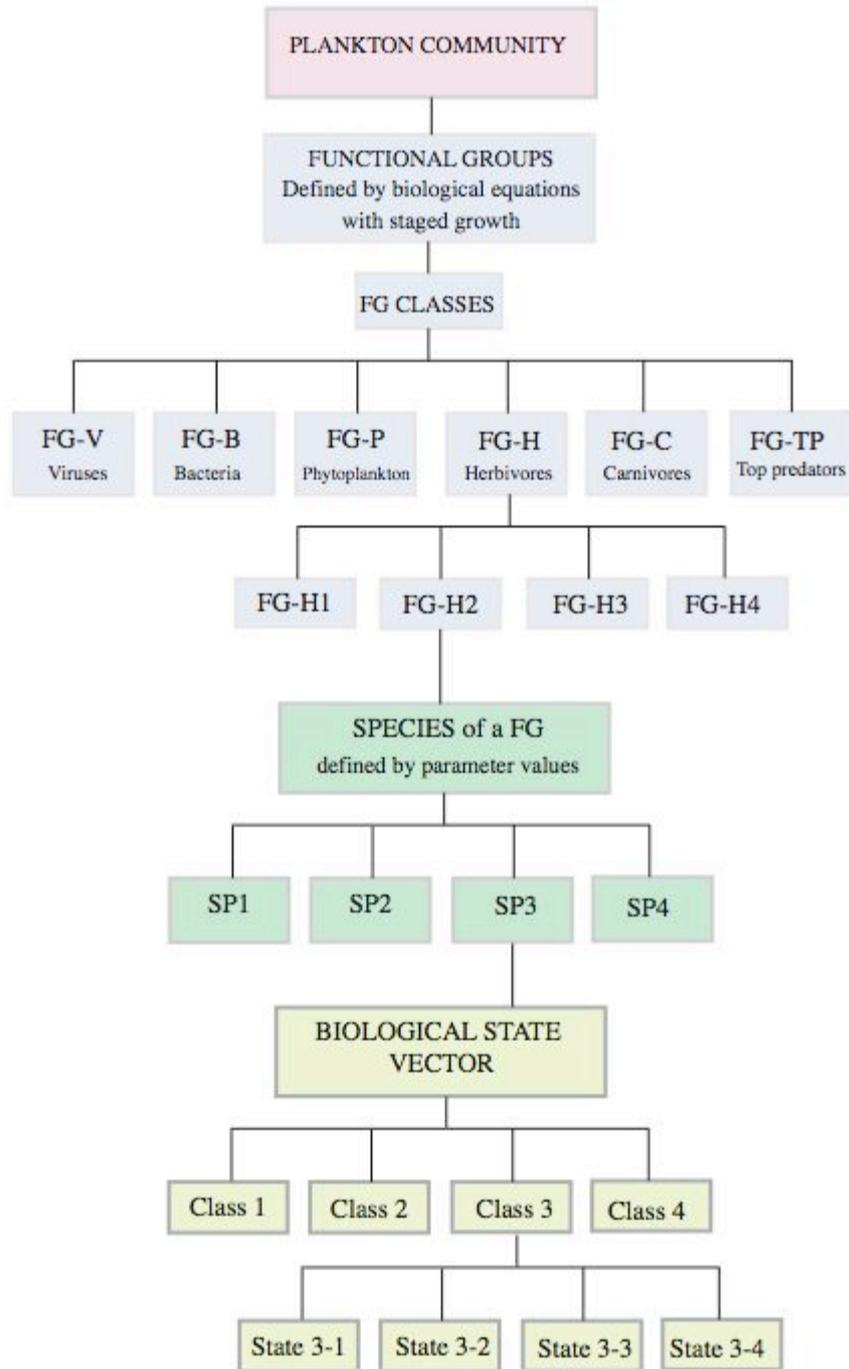
Before writing the equations for a new model you need to know which LE functions are performed automatically behind the curtain, and which functions need to be represented in model equations that operate in front of the curtain. The latter feature in the specification for a virtual ecosystem. Learning what goes on behind the curtain is a pre-requisite for writing biological equations on VEW³.

Virtual Ecology Workbench VEW3 Kernel



JDW 23 October 2004

2.3 Biology



J.D. Woods, March 2006

2.3.1 The plankton hierarchy

The plankton in a virtual ecosystem are classified hierarchically (fig.1).

The top level in the hierarchy is the **community**, which embraces all organisms, living and dead and associated detritus (i.e. the corpses of dead plankters, their faecal pellets, fragments of messy eating, etc.).

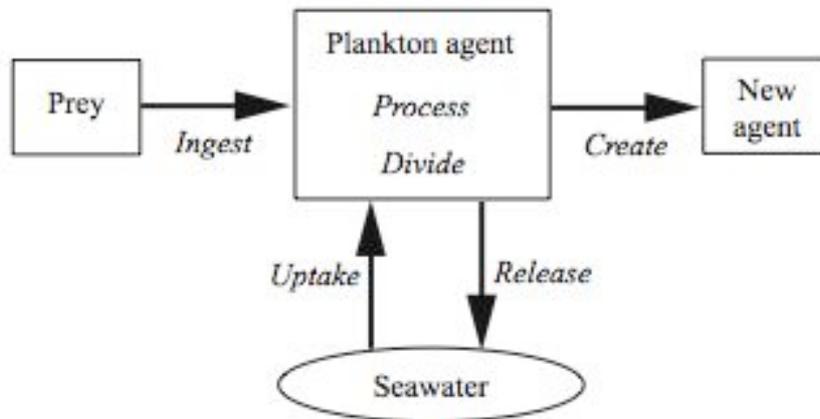
The second level comprises **functional groups**. All the plankton in a functional group share the same phenotypic equations.

The third level comprises **species** of a functional group. The plankton in a species share the same set of values for the parameters in the equations that define their functional group.

The fourth level comprises **states** of a plankter of one species. The biological state of every plankter is identified by its Biological State Vector. The equations for its functional group includes rules that specify when and how that vector changes.

2.4 VEW³ functional calls

The biological equations used to create a virtual ecosystem must comply with the design rules used to create VEW³. This ensures that the equation you write triggers the correct actions behind the curtain, in particular for demography and biofeedback. They also manage depletion of resources (in solution, or in prey), and ensure that the demand by the plankters cannot over-deplete those resources. The rules relate to way that a plankter interacts with its environment and other plankters, and how it reproduces.



The rules are expressed through eight VEW³ *Function calls*.

- Uptake
- Ingest
- Process
- Cell division
- Create
- Release
- Change State
- Probabilistic Stage Change
- Integration by depth over a trajectory

2.4.1 Uptake function call

Many species of plankton filter seawater and take up nutrients and other chemicals. When you declare a new chemical in your virtual ecosystem, VEW³ automatically creates Droop pools of that chemical in every plankter, and in solution. Furthermore, it creates an ‘incoming chemical’ pool, representing the amount of chemical that has been gained from both the solution, by uptake, and from other particles via ingestion.

The VEW³ Uptake function call manages the transfer of a chemical between solution and the incoming chemical pool when you write an equation for the plankter to take up that chemical from solution.

When the user writes a rule containing the uptake function, they specify that an individual plankton should attempt to uptake a specified amount of a named chemical. Behind the curtain, a request for the chemical is created in the layer in which the plankton is situated, and the amount of chemical requested is scaled up by the sub-population size of the agent. If the plankton passes through a number of layers, or parts of a layer, requests will be issued in each layer visited, with the amounts scaled correspondingly to the proportion of the timestep the plankton spent in each layer.

The requests are buffered until all particles have been updated – that is, all plankton have made their requests for chemical. At this point, which is effectively between timesteps, the requests for chemical in each layer are summed. If for any layer, the total of the requests is greater than the available chemical, then the requests are proportionally scaled down, such that the sum of the corrected requests is equal to the available chemical.

Then all the requests are processed, and for each the amount, (potentially corrected), is removed from the chemical in solution, and added to the ‘incoming’ pool for the individual that made the request. Note that this value will have been scaled back down from sub-population, to per-individual.

Note also that it is the user’s responsibility in VEW³ to specify what should be done with the chemical that has been gained. Usually, (but not always), the chemical gained should be added to the droop pools with a rule of the form: $A_{\text{pool}} = A_{\text{pool}} + \text{Again}$. In other cases, it may be necessary to process the chemical in some way, and then add it into a number of different pools. For the moment, this can be done by the user with rules of their own, which offers full flexibility, at the cost of requiring the user to ensure their chemical budgeting is correct. Later we discuss the *process* function, a candidate for providing flexible transfer of chemicals between pools, while providing automatic chemical budgeting.

2.4.2 Ingest function call

Zooplankton prey on other plankton. This ingestion is specified using the *Ingest* function call, in which the user specifies a list of potential food sources (specified by species and state), and for each source an ideal ingestion rate, measured in individuals per second.

The user must also give a minimum threshold for each source. Ingestion will not be permitted to cause the concentration of a food source to drop below this threshold. If at the end of the timestep the total of all ingestions exceed the available food, then all the requested ingestion rates are scaled down proportionally. This is identical in principle to the depletion protection for the uptake call.

Having checked for depletion problems, the sub-populations of the prey are reduced, and the chemicals for those ingested prey are added to the incoming chemical pool.

Furthermore, a special variable called *Ingestion* is available to the user, which gives the number of individuals eaten by the predator in the previous timestep, categorised by species and state of the prey.

2.4.3 Process function call⁷

VEW³ automatically allocates to every plankter a set of Droop pools, one for each chemical in the virtual ecosystem.

You may want to express in the biological model a biochemical process that increases the level in one pool at the expense of others. When you do this with the *Process* function call VEW³ automatically manages the chemical pools in all the plankters in which that biochemical process occurs.

If you choose not to write source/sink equations for exchange between these pools (using *Ingest/Create*) or between a pool and solution (using *Uptake/Release*) then the level in that pool (or solution) will retain the value used to initialize the computation, which may well be zero. For example, you may wish to include chlorophyll as a chemical, with equations for its mass to change in an individual phytoplankter, at the expense of other chemicals in that plankter. However, you may choose to ignore chlorophyll in solution, leaving at zero concentration throughout the simulation.

2.4.4 Divide function call

Two types of reproduction are provided in VEW³. The first is *division*, where an individual splits into two (or more) identical parts, and the second is *creation*, which describes the production of new individuals, which may be of the same functional group as the parent, but of any specified stage. Therefore, *create* may be used for birth, or for pellet production.

The reason these two methods exist is for memory efficiency; diatom cell divisions happen very frequently, and creation of new computer agents to represent the divided particles would be burdensome in terms of memory and performance. For this reason, supported by the rationale that cell division and reproduction (or excretion) are separate biological processes, we have chosen to treat them distinctly.

The *divide* function causes the sub-population size of a Lagrangian Ensemble agent to be multiplied by a number the user has specified. This number will often be '2', meaning the individuals on that LE agent each split into two, but in principle, the user may put any number here, including fractional numbers, and numbers below 1.

Note that when division occurs, the chemical pools need to be reduced, since the available chemical is shared between the newly divided individuals. However, the *divide* function does not automatically perform these adjustments, but the user needs to write these equations. There are technical reasons for this, which may be resolved indirectly by introduction of the *process* function in VEW⁴ – see earlier.

⁷ This function call will be implemented in VEW⁴. Users of VEW³ must write chemical budgeting equations that in future will be handled automatically behind the curtain. For example, you must write an equation for the depletion of the pools that contribute to the rise in the product pool.

2.4.5 Create function call

As mentioned, the *create* function is the second way of modelling reproduction. The user specifies how many new individuals to create, and the state that these new individuals should begin their lives in. Additionally, all biological properties of the new individuals may be initialised here, using the properties of the parent and its ambient environment.

Since *create* allows particles of the same functional group, but different state to be created, this also provides convenient way of modelling some other processes such as the production of faecal pellets, or releasing viruses from an individual, provided that the pellets or viruses can be represented as a 'state' of the functional group.

The number of individuals created will be the product of the number of 'offspring' the user specified, and the sub-population size of the parent, and a new agent is created with a sub-population size that represents this product.

2.4.6 Release function call

The *release* function is used to transfer chemical from an individual's internal pool into solution in the individual's ambient environment. The user specifies the chemical, and the amount to be released. The amount that is added to the water is multiplied by the sub-population size of the agent that performed the release.

2.4.7 Change State function call

The *change* function simply causes an individual to change from one state to another at the end of the timestep. This can be used, for example, to change a diatoms into a cyst state in winter, and back again in early Spring.

2.4.8 Probabilistic (Proportional) State change function call

The *pchange* function can be used to specify that there is a probability that some event should happen, and the result is that an individual should change state. This is typically used for events such as infant mortality, where for instance, 90% of the infants may die at birth.

The user specifies a probability, between 0 and 1, and the state that affected particles should be moved into. However, it is important to note that no random factor is in fact incorporated here. Rather, what the user specifies as a probability, the system interprets as a proportion of the sub-population that should be split off from the agent, and put into the specified state. Note that since chemical pools are per individual, there is no need for the pools to be altered when using a *pchange*; it is simply a rearrangement of individuals into two agents of different state.

2.4.9 Integrating over depth

The *integrate* functional call differs from all the others in that it returns a numerical value. It is used for plankton that can swim a number of metres in a timestep, and a calculation is required concerning some depth-dependent property, throughout the journey that the plankton made in the previous timestep.

The depth-dependent properties that may be used are the field properties in the system: physical properties, (light, temperature, salinity, density), chemical concentrations (both particulate and in solution) for each chemical, and biological concentrations of the particles, categorised by species and state.

The *integrate* function takes an expression that contains one or more of these depth-dependent properties, and sums the result of that expression for each layer, and each fraction of layer that the plankton passed through during the last timestep.

Some example applications of this function are: to calculate the average irradiance over a particle's journey, or to calculate the number of virus particles encountered during the particle'

2.5 Plankton states

The plankton state is a powerful concept that you can use in many different ways. For example it can be used to represent the growth stages in a functional group. A diatom may have only three growth stages alive, cyst or dead. A copepod has many growth stages, starting with egg, then hatchling, a dozen or so juvenile stages separated by moulting, a mature stage that includes the rules for reproduction, and a senile stage, leading to death which is the transition to the final stage, a corpse.

States can also be used to distinguish between the biological state of plankters in the same growth stage. For example, in epidemiological modelling the infected plankters can be identified by a separate state tag. The model equations will specify the conditions under which a plankter becomes infected, and how it responds to that infection, including the generation of an immune response. Equally, the bacteria or viruses causing the infection will themselves be treated as individual plankters, with different states when they are in the water and in a host plankter.

Another application of the concept of a plankton states is to define when material is egested from a plankter and what it contains. The egested material is carried by a separate agent because it follows a different trajectory. But it is convenient to represent the new agent as a state of the source species. Examples are a faecal pellet, and (in epidemiological models) a “sneeze” comprising a bundle of viruses. The advantage of treating these as a state of the source plankter is that it allows you to discriminate between such egested particles on the basis of their species.

The concept of a state provides you with great flexibility in designing a biological model. As usual you have to learn what needs to be specified in front of the curtain, and what VEW3 will do automatically behind the curtain. The solution is to focus on how to specify when a change of state will occur, and what are the physiological (and behavioural) consequences for the host plankter, and in the case of egestion, what depletion occurs in the host plankter and what the egested particle contains, how it behaves (e.g. sinks through the water) and how it interacts with other plankters (e.g. with bacteria which remineralize its chemicals, releasing them to solution). You can then trust VEW³ to look after the budgeting and other actions hidden behind the curtain.

2.6 Predation

The LE metamodel handles predation in a particular way that is designed for computational efficiency. The predation equation includes terms for the biological state of the predator, treated as an individual, the ambient environment (e.g. temperature, light intensity, etc.), and the ambient concentration of prey. This procedure deliberately violates the concept of writing biological equations for a pure individual-based model.

The advantage of this approach is that you do not need to write equations for the interaction between an individual predator and an individual prey. The disadvantage is that you need a state variable that is the predator's ambient concentration of prey. VEW3 has been designed to resolve that problem. It has a special function called `Ingest` which makes available the prey concentration as a demographic variable which you can use in writing your equation for predation.

2.7 Depletion

In the LE metamodel, predation reduces the number of plankters in the sub-populations of all the prey agents that contributed to the computation of ambient prey concentration. The management of this process of depletion is quite complicated. It must ensure that there is enough food to satisfy the demand expressed in the predators equation for ingestion. If not it reduces the intake. These processes are managed automatically behind the curtain. You do not need to take account of depletion in your ingestion equation.

2.8 Reproduction

Your equations for reproduction must specify the conditions under which reproduction will occur in one plankter, and the number of offspring and their state. Planktonica automatically manages the consequent depletion of resources in the mother, and its change of state. And VEW³ automatically allocates the offspring to the mother's sub-populations (for phytoplankton) or to a new agent that follows an independent trajectory (for zooplankton).

2.9 Trophic closure

Every biological model must include a special functional group of top predators. The plankton in this group have explicit ingestion equations (i.e. in front of the curtain). But the number of top predators in the virtual ecosystem, and their biological condition and their depth distribution are specified by exogenous equations. You must write those exogenous equations for the top predators.

2.10 Chemistry

VEW³ has a universal way of treating chemicals that are present in the virtual ecosystem. It contains a tool to allow you to introduce a new chemical at any time while you are building a biological model. Each chemical is expressed as a distinct chemical molecule or ion, with molar units for the primary chemical element. For example, ammonia will be expressed in molN.

2.10.1 Chemical elements

One of the limitations of VEW³ is that it does not budget chemical elements automatically behind the curtain.⁸ So it cannot budget separately the nitrogen and the oxygen in ammonia. If you need to do that, you must write explicit chemical equations in your model to budget each element in a chemical compound. That applies both to chemicals in solution and in plankton.

2.10.2 Chemical budgeting

VEW³ includes powerful functions for automatically budgeting chemicals behind the curtain. When a new chemical is introduced into the model, Planktonica introduces that chemical into solution as an environmental field with values in each cell defining the environment. It also creates a Droop pool for the chemical in every plankter (for all states, including detritus). If you add a new functional group at any stage in building a model, VEW³ will then allocate a Droop pool to every plankter in that species. (Of course the plankters are grouped into sub-populations, associated with agents, so there is one Droop pool per agent, with its content scaled for the number of plankters in its sub-population. VEW³ handles all that automatically.)

Behind the curtain, VEW³ takes care of budgeting each chemical, allowing for conversion from solution to particulate form when a phytoplankter takes up a nutrient, or vice versa, when a living plankter releases chemicals to solution, or bacteria release chemicals from a detritus particle (remineralisation). At each time step, VEW³ updates the mass of dissolved chemical in every cell of the environment, and in the Droop pools of every plankter. It also manages depletion of chemicals in solution, to ensure that plankton demand cannot cause local over-depletion.

⁸ We plan to introduce budgeting of chemical elements in VEW⁴.

2.11 Biochemical processes in a plankter

A plankter can take up chemicals from solution or ingests chemicals contained in the Droop pools from its prey. The rates are specified in your biological equations. Chemicals taken up are allocated to the plankter's pre-existing Droop pool for that chemical species. For example, if a diatoms takes in ammonia from solution, it is stored in the diatoms ammonia pool. (Remember that Planktonica automatically created such pools for every chemical declared in the model.) You are free to write equations that describe the subsequent conversion of that chemical into another chemical form. For example, carbon digested by a copepod when it eats a diatom may be converted to a variety of chemical forms, including lipids, protein, ketone. Etc. When you write an equation for such a chemical process, Planktonica automatically creates Droop pools for the new chemicals in every plankter regardless of species, and in solution. That is done behind the curtain. You only need to write equations for those chemical processes that you need in your model. A plankter that contains chemicals created by such biochemical processes may become the prey of another plankter. If so the chemicals are transferred to the pools of the prey plankter. They will remain in that chemical form in the predator unless you write equations for further biochemical processing in it.

2.12 Physics

VEW³ has a prescribed model for physical processes. The model is held behind the curtain, so you cannot change it.⁹ However the physical state variables that are used in the physical model (temperature, salinity, light in 24 wavebands) can be used in your biological equations.

You can find a detailed description of the physical model in Woods (2005). Here we sketch out its main features.

⁹ We plan to bring the physics in front of the curtain in VEW⁴.

2.13 Light

The optical model in VEW³ divides the solar spectrum into 24 wavebands including both UV and IR. Nine of the wavebands lie in the range 400-700nm; they make up the photo-synthetically-active waveband (PAR). The solar spectrum is fixed at the sea surface, with the downward irradiance in all wavebands being modulated by the solar elevation and cloud cover. An astronomical equation is used to compute solar elevation as a function of geographical location, time of day and day of the year. Cloud cover is derived from the exogenous meteorological data (see Ch.10).

The attenuation with depth of the light in each waveband is computed using Morel's bulk parametrization, which depends on the profile of chlorophyll concentration in the phytoplankton.¹⁰ The emergent spectrum of downward irradiance is available for your biological equations, which can specify action spectra for the various pigments in the plankton. VEW³ supports pigments with action spectra as a type of chemical.

¹⁰ We plan to introduce C.C.Liu's RTE and Monte Carlo optics as two options in VEW⁴.

2.14 Turbulence

VEW³ assumes that turbulence exists only in the surface mixing layer of the ocean. This is bound above by the sea surface and below by a turbocline. The Woods-Barkmann mixed layer model is used to compute the depth of the turbocline at the end of each time step.

The flow is laminar below the thermocline.¹¹ Vertical turbulent diffusivity is therefore zero in the diurnal, seasonal and permanent thermoclines. In the mixing layer it is so vigorous that each property of the seawater is homogenized by the end of every time step. Temperature and chemical concentrations are therefore uniform in the mixing layer, but they change from one time step to the next.

¹¹ See J.D.Woods (2001) "Laminar flow in the Ekman layer." In: R.Pearce (Ed.) *Meteorology at the Millennium*, Academic Press.

2.15 Air-sea interaction

The virtual ecosystem is forced by the vertical fluxes of radiation, heat, gases and particles between the atmosphere and ocean at the top of the mesocosm. These provide the boundary conditions for integration of the model. They are a key feature of the scenario used to create a virtual ecosystem.

The fluxes are computed from equations that depend on two factors: emergent properties of the virtual ecosystem, and exogenous data for the state of the atmosphere (see Ch.9).

The fluxes change with the time of day, and day of the year. They also depend on the geographical location of the virtual mesocosm, which may be held at a fixed location, or allowed to drift around the ocean.

VEW³ creates a scenario for the boundary conditions, which comprise time series of the surface fluxes with values every time step of the virtual ecosystem.

2.16 Hindcasting

It is normal practice to create this scenario from meteorological data collected in past years. VEW³ includes the ERA40 time series of the global state of the weather every six hours with a geographic resolution of one degree of latitude and longitude. The ambient weather every half-hour time step at the location of the mesocosm is computed by interpolation from the ERA40 data. The time series extends over a range of dates selected from the 40 year scope of the ERA40 data. A virtual ecosystem forced by these historic data is a hindcast of the state of the modelled ecosystem as it evolved during that range of dates.

2.17 Events

Starting with such a historic weather sequence, you can perturb the boundary conditions according to your own specification. For example, you can add a solar eclipse, or a hurricane. These alterations represent one aspect of the events procedure supported by VEW^{3,12}. This can be used to investigate the sensitivity of the virtual ecosystem to anomalous forcing.

¹² Other kinds of events include changing the exogenous data for top predators, or introducing chemicals (e.g. fertilizer run-off from the land) or adding alien species (as occurs when ballast water is released).

3 VEW³ tools

Contents

Creating a new virtual ecosystem
Graphical user interfaces
VEW Biology controller
VEW Ecology controller
VEW Analyser

Introduction

VEW³ provides a set of tools that are designed to make it easy to create and analyse a virtual ecosystem. There are three primary tools:

- (1) *VEW Biology*, which you use to design a biological community,
- (2) *VEW Ecology*, which you use to design a virtual ecosystem that incorporates a plankton community that you designed earlier,
- (3) *VEW Analyser*, which you use to explore the emergent properties of a virtual ecosystem.

3.1 Creating a new Virtual ecosystem

You perform the following tasks with VEW³

- Create a new community (set of functional groups)
- Build each functional group (states, equations)
- Create a set of species in each FG (allometry)
- Set biological initial conditions
- Specify the scenario for forcing by exogenous factors
- Specify rules for particle and memory management
- Logging emergent properties to feature in the VE
- Batches of VEs with different specifications
- Ensembles of VEs with different RNG seed values
- Compile
- Document
- Export to Archive
- Run (with LiveSIM switched on or off. Set it on for debugging.)
- Go to VEW Analyser

3.2 Graphical user interfaces

VEW Controller uses a Graphical User Interface (GUI) to guide you through each of these tasks. Clicking on the icon for each task opens a new GUI with detailed instructions. These may be to select an option from a list, or to enter numbers into a table.

3.3 VEW Biology controller

The GUI for VEW Biology guides you through the sequence of actions needed to design and test a new plankton community. Although this is normally performed step-by-step through the biological hierarchy, the GUI also allows you to modify any feature at any stage.

You can design a new plankton community by editing an existing one stored in the archive. VEW³ provides a number of sample communities that you can use as a starting point. One is the WB food chain model which has three functional groups (diatoms, copepods and top predators) and one species in each functional group. Another is the LERM model with four functional groups (diatoms, copepods, squid larvae and top predators), featuring staged growth. You can select one from the list, or you can start with a blank sheet of paper and introduce functional groups *ab initio*. You then proceed step by step to specify:

- the community (set of functional groups);
- the properties of each functional group, including states; and
- the species in each functional group.

That completes your design for the plankton community.

When you specify a new element of the plankton community, or edit one you specified earlier, VEW³ performs a number tasks “behind of the curtain”. These tasks ensure the integrity of the model. It manages state variables and parameters, and the chemistry (see §2.4). This integrity checking may identify secondary changes that are needed elsewhere in the model. VEW³ can often handle these secondary changes behind the curtain without any need for user intervention. In that case the Controller signals the changes that have been made automatically. Sometimes, VEW³ requires a decision by the user. In that case the GUI signals where you need to make a decision.

When a plankton community has been fully specified, it can be exported to the VEW Archive. It can then be imported into VEW Ecology and embedded in the specification of a Virtual Ecosystem. Analysing the emergent properties can indicate whether the community you have created meets the needs of your research or teaching. If not, you can return to VEW Biology to modify the specification of the plankton community. You may find it necessary to iterate through this cycle several times before your plankton model meets you needs. The sequence of trial models produced during the development phase are stored in the Archive as versions of a named plankton community.

The controller points you to VEW Documenter, which can generates a html file with detailed documenting of any model stored in the archive.

3.3 VEW Ecology controller

The GUI for VEW Ecology guides you through the sequence of actions needed to create a virtual ecosystem that contains a plankton community imported from the VEW Archive.

It starts by providing access to the Archive, so that you can create a new VE based on one you made earlier, possibly with a modified plankton community.

VEW Controller offers to connect you to VEW Biology (see below) so that you can create a new plankton community with the missing equations and export it to the archive. Once the archive contains the plankton community needed for the new virtual ecosystem VEW Controller connects you to VEW Scenario (see below), which allows you to specify the initial and boundary conditions.

When that is complete, VEW Controller opens VEW Quality, which allows you to specify the number of agents to be used to represent each plankton population. This tool allows you to control LE sampling errors in the LE.

The next step is to specify what should be included in the Virtual Ecosystem. Options include:

- surface forcing,
- water column properties, such as the depth of the turbocline at the base of the mixing layer,
- fields of all the environmental variables,
- demography of each plankton population, either in each layer or averaged over specified depth ranges, or the whole mesocosm
- audit trails of all or selected plankton agents (including the demography of each sub-populations).

The penultimate step is to instruct VEW³ to create a comprehensive documentation of the specifications for the new virtual ecosystem. Finally, VEW³ Controller invites you to specify details of the job that will integrate the model. Options include batch and ensemble integrations. It is necessary to specify which computer will be used and where the output will be stored.

Finally, you push the RUN button to compile and integrate.

3.4 VEW Analyser

The next step is to explore the emergent properties of the Virtual Ecosystem you have just created. You do this with VEW *Analyser*.

VEW Analyser allows you to select data from a Virtual Ecosystem and plot the results. It also allows you to export the selected data for more sophisticated analysis and plotting with third party statistics/graphics packages.

4 Getting started

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- 4.2 The sample virtual ecosystem and its model & scenario
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4.1 Introduction

The best way to become familiar with VEW³ is to start by exploring an existing virtual ecosystem, and then to see how it changes when you modify the model and scenario used to create it. In this way you can learn all the functions of the workbench, and gain familiarity with the novel products of virtual ecology.

The first step is to learn how to extract information from a virtual ecosystem. The information is contained in its emergent properties. VEW³ *Analyser* makes it easy for you to plot selected emergent properties in a space-time window. Learning how to use VEW³ is the first step into virtual ecology.

That is followed by a carefully graduated series of exercises. In each exercise you will create a new virtual ecosystem after editing one feature of an existing model/scenario. You will import the modified virtual ecosystem into VEW³ *Analyser*, which you use to discover how the emergent properties of your new virtual ecosystem differ from those in the reference one that you analysed in the first step.

You will find worked examples for each exercise, with step-by-step screen images, on the accompanying CD.

The exercises are carefully staged to help you move smoothly up the learning curve. They will prepare you for using VEW³ in your own research. That will be the subject of Part II of the Handbook.

4.2.1 Exercise 1 - Emergent properties

Your first exercise in this self-training course is designed to familiarize you with using VEW³ *Analyser* to select and plot emergent properties of a virtual ecosystem.

You will pay special attention to the three classes of emergent properties that are the quintessence of all virtual ecology: environment, demography and audit trails.

You will later apply the skill acquired in this exercise to explore the emergent properties of virtual ecosystems created in all the other exercises.

Only when you have mastered VEW³ *Analyser*, will you be ready for the next exercise in which you create a new virtual ecosystem, with your own specifications for the biological model and scenario.

The figures in Woods (2005) illustrate the kind of plots you should aim to produce.

For this exercise you will explore the emergent properties of the Azores (WB) virtual ecosystem that come bundled with VEW³. This is an updated version of the virtual ecosystem used to produce the illustrations in Woods (2005). The only changes were those needed to use the function calls of VEW³ (described in §2.4) and the new trophic closure (§2.9).

We recommend that you start by using VEW³ *Analyser* to reproduce those illustrations. Then you can make additional plots that reveal aspects of the virtual ecosystem relating to your own research.

Start by opening VEW³ *Analyser* and selecting the “Azores (WB)” from the pick-list of virtual ecosystem. Then use the functions listed below (§4.2.1.1).

4.2.1.1 VEW³ Analyser

VEW³ Analyser makes it easy to perform the following tasks:

- Select a virtual ecosystem from the VEW³ archive.
- Choose the class of data:
 - Water column
 - Environment
 - Demography
 - Audit trail
- Choose a variable in that class,
- Window the selected data in depth and time.
- Plot the select variable (or its logarithm) in one of three forms
 - Synoptic profile at one time step,
 - Time series at one depth,
 - D e p t h - t i m e c o n t o u r
 - (environment or demography, at a time resolution of your choice).
- Label the axes, colour the lines, etc.
- Superimpose one or more line graphs on a contour plot (or plain background).
- Print the plot.
- Save the plot as a graphics file.
- S a v e t h e d a t a
- (in csv format for import into a third party statistics program like MS Excel).

When you have completed the specification for data selection and plot, you press the *Plot* button. A progress bar is displayed while the data are being retrieved and the plot prepared.

You will find that some plots take longer than others. Often you can save time by specifying that a plot be based on a reduced time resolution (e.g. only one sample per day, rather than at full resolution with all 48 time steps per day).

When a plot meets your needs you can save the data used to prepare it. Those saved data can be imported into a third-party application (e.g. Microsoft Excel, MatLab, or a specialist graphing package) for further processing and high-quality plotting.

You will quickly learn to use VEW³ Analyser. It provides easy access to the emergent properties contained in the virtual ecosystem. You will soon get a feeling for the great depth of information contained in a virtual ecosystem.

Exploring the emergent properties of the Azores (WB) virtual ecosystem bundled with VEW³ will stimulate your thoughts about how Virtual Ecology might be applied to your research. To do so you will need to create a new own virtual ecosystem based on your own biological model and scenario. That takes us to Exercise 2.

4.2.2 Exercise 2 - Creating a new virtual ecosystem

Having become adept at using VEW³ Analyser to plot emergent properties of an existing virtual ecosystem, your next step is to learn how to build a new virtual ecosystem based on your own specification.

It is import you become familiar with this procedure at the outset, because you will use in all the exercises that follow.

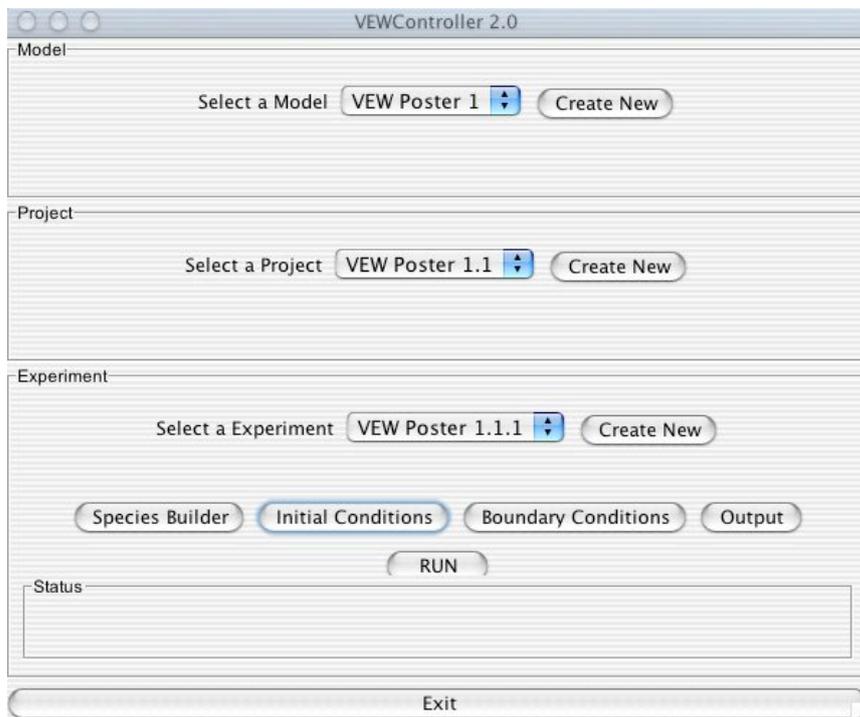
The next exercise takes you through the sequence of actions needed to create a new virtual ecosystem.

Reproducing the default virtual ecosystem

In Exercise 2 you will replicate the Azores-WB virtual ecosystem analysed in exercise 1 .

To do so you will have to open all the GUIs in sequence. You may examine the contents of each GUI to become familiar with its role in generating the complete specification for the virtual ecosystem. But in this exercise you will not manipulate any of them to change the specification for the virtual ecosystem.

You start by opening VEW³ Controller.



4.2.2.1 VEW³ Controller

VEW³ Controller invites you to base your new virtual ecosystem on one that was made earlier. The specifications of all previous virtual ecosystems are stored automatically in the VEW³ Archive.

The usual practice is to edit the specification of one of these existing virtual ecosystems. For the purposes of this exercise you will choose the default Azores Virtual Ecosystem, and will proceed through all the steps needed to edit it, but without changing anything.

Before you can initiate the run you must have addressed each of the steps listed in Table X.

As you complete each step, VEW³ stores that piece of the specification in an XML file.

When you finally push the RUN button, VEW³ will compile that XML file into an executable Java code, and run it to create the virtual ecosystem.

Creating the new virtual ecosystem will probably take a few hours on your personal computer.

When it is ready you can import the new virtual ecosystem into VEW³ Analyser and explore its emergent properties, as you did in the previous exercise.

4.2.2.2 Documenting a virtual ecosystem

VEW³ makes it easy to document a VE: you merely have to click on the appropriate button. The specification file (stored in XML) is then compiled into a html file that can be displayed and searched using your web browser. This is illustrated on p.36.

It is good practice to document every virtual ecosystem as soon as you have created it. We recommend you do this even if the VE is one of a sequence differing only in some small respect from its predecessor.

For the exercise, create the document file and check that the biological equations and parameter values match your expectations.

4.2.2.3 Archiving your virtual ecosystem

You will have specified the file name and location of your new virtual ecosystem. It is then archived there for later investigation using VEW Analyser (as in exercise 1). The archived VE is self-documenting. It contains information (in XML files) needed to configure VEW Analyser with, for example, the appropriate names of variables in the full-down menus to select data for plotting. That configuration is performed automatically when you import a VE from the archive.

Table 4.2.1 Steps in building a new Virtual Ecosystem (VE)	
Select an existing VE as a template	Name your new VE
	Name Directory for storing the VE
Build the biological model	Create each functional group (FG) (Add new FG to the list and name it)
	Define biological states for each FG Enter rules for a plankter to: change from one state to another, create a new agent of a particular state
	Enter the phenotypic equations for each FG
	Specify the species in each FG (Add a new species to the list and name it)
	Define each species by entering A values for the every parameter
	If the species are members of an allometric set, define the base parameter (surrogate for size) Enter the number of species in the set and their "sizes". Enter the B values for each parameter.
Specify the scenario for exogenous forcing	Press reset button
	Start and end dates and times
	Start geographical location
	Choose 4D velocity field for ocean circulation
	Choose atmospheric forcing (e.g. ERA40 synoptic or mean climate)
	Plot maps of selected atmospheric and oceanic (exogenous) data using VEW ³ Data
	Display mesocosm track on map of ocean
	Press RUN to create XML files for: hydrographic initial conditions, and atmospheric boundary conditions
	Press STORE to create optional CSV files of these initial and boundary conditions
Specify the vertical extent of the mesocosm	Default value is 500m with one metre layers

<p>Specify exogenous data for top predators (They provide the trophic closure for the virtual ecosystem.)</p>	<p>(1) Demography (number in the mesocosm) (2) Depth distribution (3) Biological condition of TP plankters</p>
<p>Specify the time step in seconds</p>	<p>Default value is 1800s (half an hour)</p>
<p>Set biological initial conditions</p>	<p>Number and biological condition of plankters in each species Also their initial vertical distribution</p>
<p>Specify particle management rules</p>	<p>Thresholds for particle splitting and combination</p>
<p>Specify memory management rules</p>	<p>Intervals between Restart files</p>
<p>Specify batches of VEs (for sensitivity testing)</p>	<p>Enter number of VEs in batch, and values of parameters differing between them</p>
<p>Specify ensemble of VEs (for computing LE sampling noise)</p>	<p>Enter the number of VEs in the ensemble and the seed value of the RNG to be used for each</p>
<p>Specify data logging Specify which emergent properties are to be logged so they will feature in the VE</p>	<p>(1) Field variables Enter start and end date for logging and the sampling interval Mark each variable on the list to be logged or not</p>
	<p>(2) Demography Tick box for the creation of a “Parish register” of demographic events in each plankton agent (To be used later by VEW³ LiveSpan)</p>
	<p>(3) Audit trails Specify criteria for selecting plankton agents to be logged for audit trail plots</p>
<p>Compile</p>	<p>Converts XML specification file to executable Java code</p>
<p>Export specification file to VEW³ Archive</p>	<p>This is done automatically when the code is compiled</p>
<p>Document the Virtual Ecosystem</p>	<p>Press button to generate a comprehensive documentation of the VE based on the specification file.</p>
<p>Run</p>	<p>(1) with LiveSim turned on, for debugging</p>
	<p>(2) with LifeSim turned off for faster integration</p>
<p>Close</p>	

4.3 Modifying the virtual ecosystem

In the remaining exercises you will create a series of virtual ecosystems, each of which differs from the bundled (WB-Azores) virtual ecosystem in one respect. The aim is to discover how the emergent properties change when you alter the specification for the model and scenario.

The staged approach is summarized in Table 4.3.

Table 4.3 Exercises that create a modified Virtual Ecosystem			
Exercise	Model	Scenario	Comment
1	Default	Default	Use VEW Analyser to plot emergent properties in the Azores (WB) VE
2	Default	Default	Create a copy of the Azores (WB) VE using VEW Controller. Investigate each function of VEW Controller without making and changes to the specification of the model or scenario.
3	Default	New track	Make a new track for the mesocosm
4	Default	New event	Original track Add an event
5	Default	Trophic closure	Parameter in top predator demography
6	Modified species	Default	Change one biological parameter
7	Allometric set	Default	Create an allometric set of diatoms Then add three species with different sizes
8	Modified biological equation	Default	Modify one of the biological equations in the default model
9	Modify a biological state	Default	Change the list of biological equations
10	Add a new chemical	Default	Add a new nutrient (e.g. phosphate)
11	Change a pigment	Default	Photosynthetic pigment
12	New functional group	Default	Add a new functional group Enter its biological equations Populate the new FG with species

The default virtual ecosystem describes changes occurring in a mesocosm that is anchored at a site near the Azores.

This exercise familiarizes you with the way that VEW³ simulates the influence of ocean circulation. It does so by computing the track followed by the mesocosm when it is allowed to drift freely with the currents.

For this exercise you leave the default model unchanged.

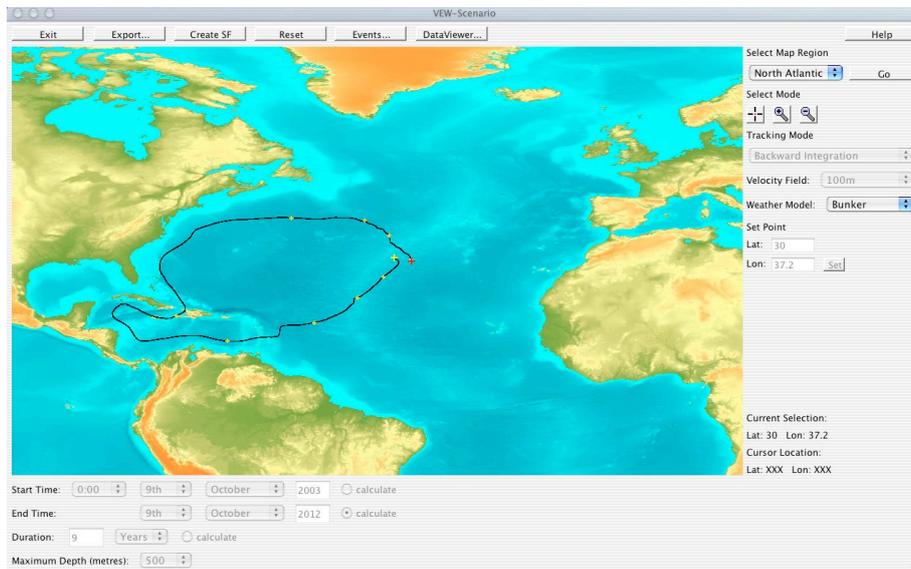
4.3.1 Exercise 3 - Ocean circulation and the mesocosm track

In Exercise 3 you use VEW³ *Scenario* to specify the track followed by the mesocosm as it drifts in the ocean circulation. Doing so automatically creates files for the hydrographic initial conditions and the atmospheric boundary conditions. This is a basic part of the scenario for exogenous forcing that controls the way that the virtual ecosystem evolves.

This exercise is designed to familiarize you with the use of exogenous data sets for ocean hydrography and the weather.

VEW Scenario

You start at the VEW Controller and use the button marked “Boundary conditions” to open VEW Scenario.



The Graphical User Interface for building the scenario is shown above. The buttons appear in clusters on the screen.

Buttons on the right

- Help* Open contextual help
- Map region* Pull down menu with choice of maps, including the whole world, or the GOOS regions
- Zoom* Zoom in or out within the selected map
- Select mode*
- Tracking mode* Choose a mesocosm that is anchored at one location, or Drifts downstream with the ocean circulation, or Drifts upstream against the ocean circulation.
- Velocity field* Pull down menu for choosing version of ocean circulation
- Weather model* Pull down menu offering a selection of exogenous meteorological data sets, including:
 - Bunker monthly mean
 - ERA40 six-hourly synoptic
 - ERA40 six-hourly mean over 40 years

<i>Set point</i>	Fix the initial location of the virtual mesocosm at the current position of the cursor on the map.
<i>Lat & Long</i>	Type in the latitude and longitude of the initial location (as an alternative to using the map cursor).
<i>Set</i>	Freeze the starting point of the track.

The Buttons at bottom right provide a reminder of the current status of the specified initial location and the current location of the map cursor.

Buttons at bottom left

Start time	Type in Time (GMT) and date (day-month-year)
End time	Type in Time (GMT) and date (day-month-year)
Duration	Appear automatically if you specify in the end time Alternatively you can specify the duration and the end time will appear automatically
Maximum depth	The depth of the bottom of the vertical mesocosm (500m in the bundled scenario) <i>VEW3 is designed to simulate the plankton ecosystem in the open ocean where there is always water between the bottom of the mesocosm and the ocean floor. When you have made track, check that the mesocosm has not grounded in shallow water.</i>

Buttons along the top

<i>Exit</i>	Terminate the session.
<i>Export</i>	Create a computer file with the data for the track, initial and boundary conditions.
<i>Create SF</i>	Create the scenario file for this virtual ecosystem. The track of the mesocosm will now be computed. It will gradually appear the map.
<i>Reset</i>	Start the procedure for specifying a new track for the mesocosm.
<i>Events</i>	Open the tool for creating events.
<i>Data viewer</i>	Open the tool for displaying maps of the exogenous data.

4.3.2 Forcing

VEW³ supports five kinds of forcing:

- *Ocean hydrography.* Used for initial conditions, especially nutrients.
- *Meteorology.* Used for boundary conditions (fluxes through the air-sea interface).
- *Ocean circulation* For computing advection of virtual mesocosms.
- *Top predator demography.* From observations at sea.
- *Events.* Your choice of deviations from the above data.

Exogenous data sets

VEW³ is supplied with the following default data sets:

- Hydrography NOAA world ocean climatology
- Meteorology ERA40 – 6-hourly synoptic state of the global atmosphere
 ERA40 – 6-hourly mean state of the global atmosphere
 Bunker monthly mean climatology
 IPCC history and scenario for atmospheric pCO₂.
- Circulation OCCAM world ocean monthly velocity fields for 1999.
- Demography Squid demography at Azores.

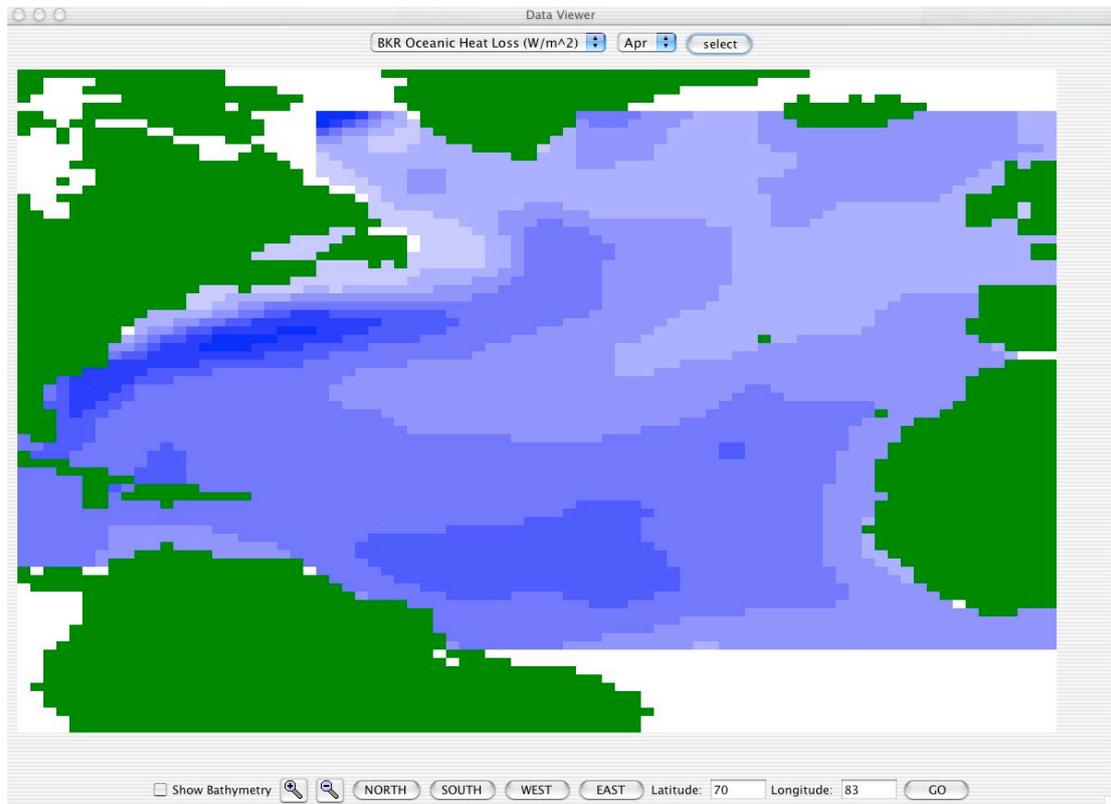
You can examine maps and profiles of these exogenous data using *VEW³ Data viewer*.

You can add new exogenous data sets to the *VEW³ Archive*. They must be pre-formatted according to the specification in Appendix x. For example you may wish to use a description of ocean circulation derived from a different model. Or you may choose to base trophic closure on data for a different set of top predators.

Exogenous data are used by *VEW Ecology* to create to create the initial and boundary conditions and trophic closure, which are all features of the Scenario.

VEW Data viewer

You can use VEW3 Data viewer to map and variable in the exogenous data sets.



Procedure

Exercise 3 involves the following steps.

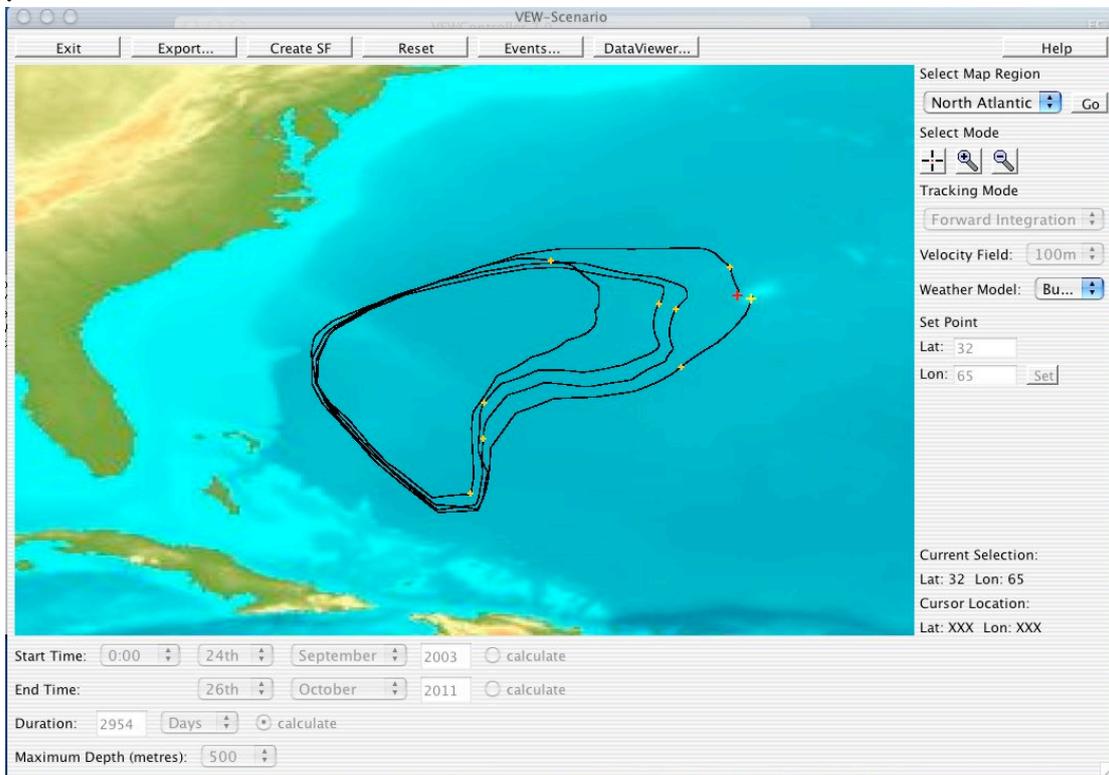
- Specify the start and end dates and times for the simulation. The times must be expressed in GMT
It is good practice to start an integration at the end of winter, just before the start of the growing season. And it is usually convenient to start simulation at the end of night, just before solar heating causes the turbocline to rise. The duration of the simulation must be sufficient to allow the virtual ecosystem to adjust to the attractor, in which the plankton community are in balance with the simulated environment, under the control of exogenous forcing. The pace of adjustment is largely determined by the annual reproduction of plankton. So you will probably need to run the simulation for several years. Once the virtual ecosystem has adjusted to its attractor, it has lost the memory of any imbalances in the initial conditions. In other words the purpose of the balancing process is to allow the virtual ecosystem to shed any anomalies due to inconsistencies in the initial conditions. The period of adjustment is not needed if the virtual ecosystem is initialized in perfect balance. This can be achieved by starting with a balanced state derived from a previous simulation that had the same model and scenario. VEW3 makes it easy for you to create such "Restart" files (see below). It is good experimental practice to create such a Restart file and then use it to initialize a series of simulations.
- The second step is to specify the geographical location of the virtual mesocosm at the start of the simulation. You do this by typing in its latitude and longitude, or by clicking on the location in the map provided in the Scenario builder GUI.
- Next you must decide whether the virtual mesocosm will remain anchored at the initial location, or whether it will drift with the ocean circulation. For the latter case, you must select the velocity field that best describes the ocean circulation for your numerical experiment.
- You now choose the atmospheric data set that will be used to compute the air-sea fluxes of heat, water and carbon-dioxide (i.e. the upper boundary condition) during the simulation.
- You now press a button to compute the track that the virtual mesocosm will be follow during the simulation. The track is displayed on the map of the ocean. You can pan and zoom to get a better picture. The track specifies the geographical location of the virtual mesocosm at every time step of the simulation.
- VEW³ then automatically computes the hydrographic profiles at the start location (critically the nutrient profiles) by interpolation of the archived NOAA climatology.
- It is not possible to derive useful initial biological conditions from the NOAA climatology (or any other: for example SAHFOS), because the observations on which they are based are unlikely to map easily onto the plankton community you have designed for your
 So, in practice, it is better to specify the biomass in each species of your model

on the basis of other evidence. Most likely this will be experience gained in previous experiments

A better choice is to initialize the biology with “Restart” data.

However you choose the initial plankton biomasses, it is likely that they will not be in balance with the other features of the virtual ecosystem at that time. However, that is not too worrying, because the correct values for that time of year will emerge as the simulation adjusts to its attractor. Within a few years, any errors in your choice of biological initial conditions will have evaporated.

- VEW³ then computes the atmospheric boundary conditions that apply at each time step along the track. These will be used during the integration to compute the air-sea fluxes of solar radiation, sensible and latent heat, thermal (IR) radiation and carbon dioxide. (The computation combines exogenous atmospheric data with emergent data from the simulation using air-sea flux formulae that you can change.)



4.3.3 Exercise 4 - Introducing an event

One of the most powerful features of scenario-builder is the tool that allows you to create initial or boundary conditions that differ in some way from the standard climatologies supplied with VEW³.

For example, you might be interested to discover how a virtual ecosystem changes when you initialize it with resources (e.g. nutrient concentration) that are higher or lower than the climatological value. You will find an example of such a sensitivity study in Woods (2005).

Alternatively, you might be interested to see how the virtual ecosystem responds to the injection of a mass of nutrient after it has settled to the attractor consistent with the initial conditions. In this case you will need to specify the magnitude of the nutrient injection, the depth range, and the time window.

A third possibility is that you may want to specify an event that injects a chemical pollutant that was not present in the initial conditions. In order to do so you must first declare the pollutant as a chemical in the virtual ecosystem. You will recall (§2.10) that VEW³ automatically creates a profile of that new chemical in solution and pools for it in every plankton, dead or alive, and in every faecal pellet. Your pollution event will produce non-zero values of the new chemical for the first time into solution. It will then spread through the plankton as it is taken up first by phytoplankton, then by zooplankton grazing on them. You might specify that this chemical produces a biological response in the plankton (as in ecotoxicology). In which case you will have written the appropriate biological equations into your model. Or you might be interested in using the polluting chemical as a passive tracer to explore how it spreads through the water column (i.e. bio-transport by migrating zooplankton as in Arrese, 2002).

Another application of the Events tool involves introducing an anomaly in the boundary condition file. For example, you might specify a hurricane, or a solar eclipse, or the progressive change in the atmospheric concentration of carbon dioxide.

There is no limit to the range of disturbances that can be created with the Events tool in VEW³. The aim of this exercise is to familiarize you with the GUI used to create an event. As usual to specify the change that you want to make, then complete the specification for the virtual ecosystem, run the job and analyse the results on VEW Analyser.

Now that you have become familiar with creating and analyzing virtual ecosystems, we leave you to decide what event you will use for this exercise.

VEW Handbook - First draft

X	Event	Start	Occurrences	Depths	
<input type="checkbox"/>	Initial	October 09 2003	1	All	Modify
<input checked="" type="checkbox"/>	Climate change	December 09 2003	1	0m - 0m	Modify
<input checked="" type="checkbox"/>	Nitrate run-off	December 09 2003	100	0m - 50m	Modify

Remove All Exit Create Event From...

Remove Selected Nitrate run-off

4.3.4 Exercise 5 Changing the top predator

The virtual ecosystem's attractor is sensitive to the specification of the top predator used for trophic closure. Biological oceanographers often call this phenomenon the trophic cascade. This exercise is designed to familiarize you with the procedure for changing the top predator, and with checking the impact those changes in forcing have on the emergent properties of the virtual ecosystem

The exogenous demography of the top predator

Virtual ecology bases trophic closure on one or more top predators that ingest their prey according to the standard kind of biological equations (function of biological condition of the predator, ambient concentration of the prey, ambient environment). The demography, biological condition and vertical distribution of the top predators are all exogenous properties. They are therefore elements of the scenario.

Ideally, these properties of the top predators are derived from observations of the dominant species at that trophic level. For example, when Sinerchia designed LERM(PS) with squid larvae as the top predators, he used published data on the most common species observed at the Azores.

VEW³ supports the use of exogenous equations to compute the values of these properties of the top predator at each time step of the virtual ecosystem. That avoids the need to populate large files with exogenous data before the job is run.

These top predator equations contain TP parameters, which are by definition exogenous. You can change the properties of the top predator population by varying the values of these TP parameters. By doing so you are changing the trophic closure applied to the model. The resulting trophic cascade causes the virtual ecosystem to adjust to a new attractor.

You can either change the value of a TP parameter in such a way that the new closure specification remains constant throughout the simulation. Or you can use the Events controller to introduce a TP parameter change for a period of time.

Finally, you can specify more than one top predator, each designed to prey on a particular species of plankton (or perhaps only when the prey species are in a particular state). Each top predator has its own set of exogenous TP equations and parameters.

The exercise

The aim of this exercise is to learn how to use VEW³ to change a TP parameter, and then to plot the resulting change in the emergent properties of the modified virtual ecosystem. The default model bundled with VEW³ has one top predator, which preys visually on juvenile and adult copepods. You can inspect the ingestion equation, and the exogenous equations for demography, biological condition and vertical distribution.

The exogenous equation for demography has three TP parameters. The first specifies the date when the predators arrive each year. The second specifies their initial concentration (number per cubic metre), and the third specifies the e-folding time of the exponential decline in numbers as the year progresses.

The exercise is to change the value of one of those three demographic TP parameters. The worked example in Part III shows how to halve the initial concentration of top

predators. However, you may want to change one of the others. Having made the change, you proceed to run the job, creating the virtual ecosystem with its modified trophic closure.

4.4 Changing the model

Having learnt how to specify a new scenario, and seen how it changes the virtual ecosystem, your next step is to use VEW³ to modify the biological model.

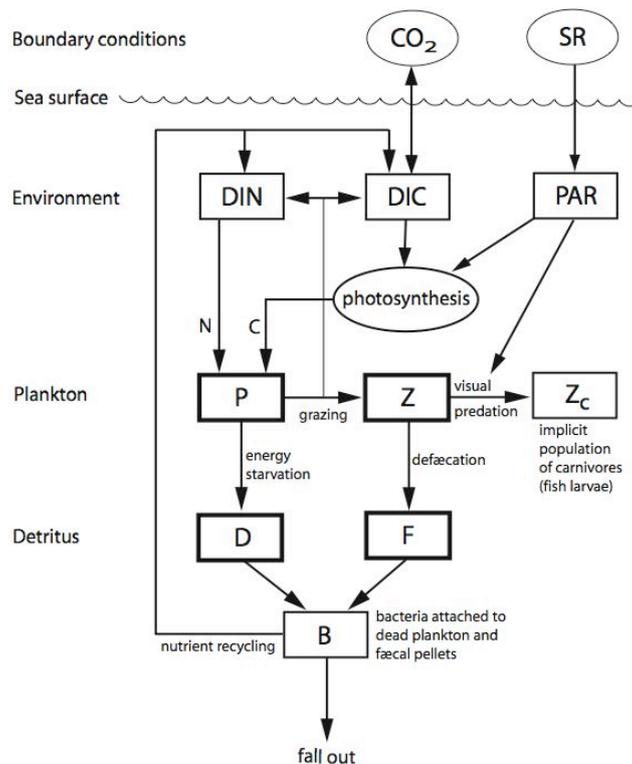
In the next set of exercises you learn how to change the model in the following ways:

- Exercise 6 modify one of the species,
- Exercise 7 introduce an allometric set of species,
- Exercise 8 modify one of the biological equations,
- Exercise 9 modify one of the biological states
- Exercise 10 add a new chemical
- Exercise 11 change a pigment
- Exercise 12 add a new functional group

The plankton model used to create the Azores virtual ecosystem

The model supplied with VEW³ is based on the WB model described in Woods (2005). It comprises the classical food chain of diatom, copepod and top predator (for trophic closure). The single nutrient is nitrogen, which comes in two forms: nitrate and ammonium. An implicit population of bacteria remineralize the nitrogen and carbon in dead plankton and faecal pellets.

The WB food chain model



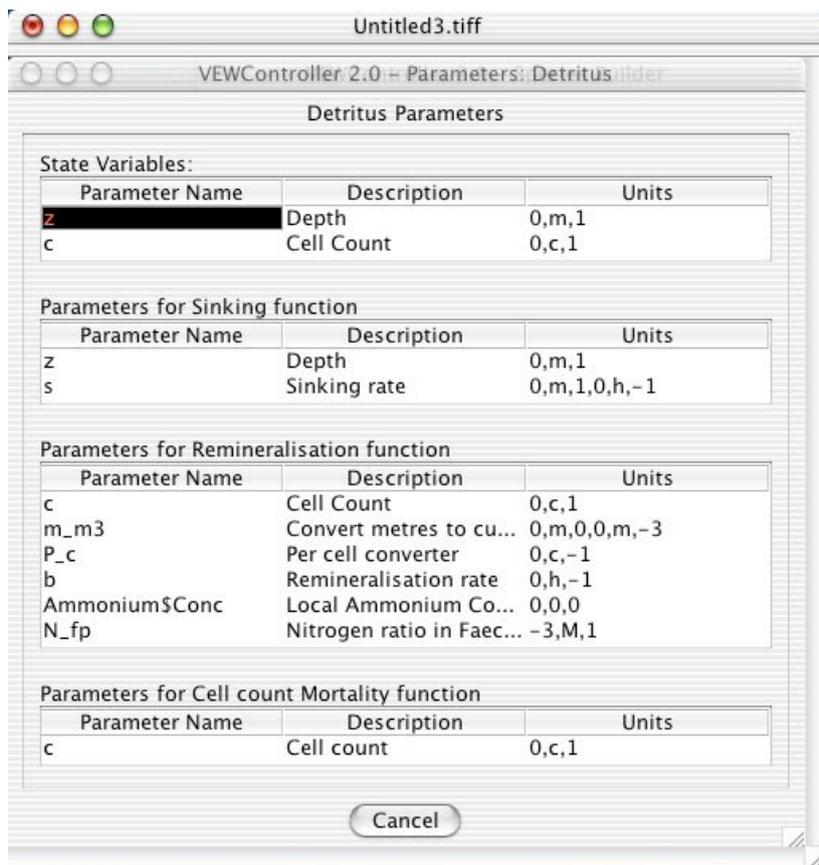
John Woods, Imperial College, 19 April 2001

4.4.1 Exercise 6 - Modifying a species

It will be helpful to refer to the plankton hierarchy illustrated in fig.1 (page 26). The community comprises functional groups, each of which is defined by a set of biological equations. A species in one of the functional groups is defined by the values of the parameters in that the biological equations.

The default model has three functional groups (diatoms, copepods and top predators) with one species in each. The species builder GUI provides you with a list of the parameters and values of two allometric parameters for each, A and B, respectively. The default model has no allometric sets of species, so all the B values are zero. The set of A values defines the species.

In this exercise you change the value of one of the parameters. You are free to choose which species and what parameter. The worked example in Part III describes the procedure when you increase the respiration parameter for the diatoms from the default value (...) to double that value. We would expect that to have a significant effect on the diatoms' birth rate and death rate by energy starvation (natural mortality). You can explore those and other changes by creating a virtual ecosystem with the revised parameter value.



4.4.2 Exercise 7 - Creating an allometric set of species

The VEW³ species builder supports the creation of allometric sets of species. Each biological parameter in the functional group is allocated an allometric equation of the following generic form:

$$[\text{Value of parameter } P_n \text{ for species } m] = A_n \cdot [\text{size of species } m]^{B_n}$$

where A_n and B_n are the allometric coefficients for parameter P_n

and the size of species m is defined by one of its biological parameters (or by a function of several biological parameters). For example, the size may be defined by the total mass of carbon in the plankton, summed over all its carbon-containing pools.

4.4.3 Exercise 8 - Modifying a biological equation

Modify one of the biological equations in the default model

4.4.4 Exercise 9 - Modifying one of the biological states

Change the selection of biological equations that will be active in this state.

Specify the conditions for the plankter to change from one state to another

Add a new nutrient (e.g. phosphate)

4.4.5 Exercise 10 - Adding a new chemical

4.4.6 Exercise 11 - Changing a pigment

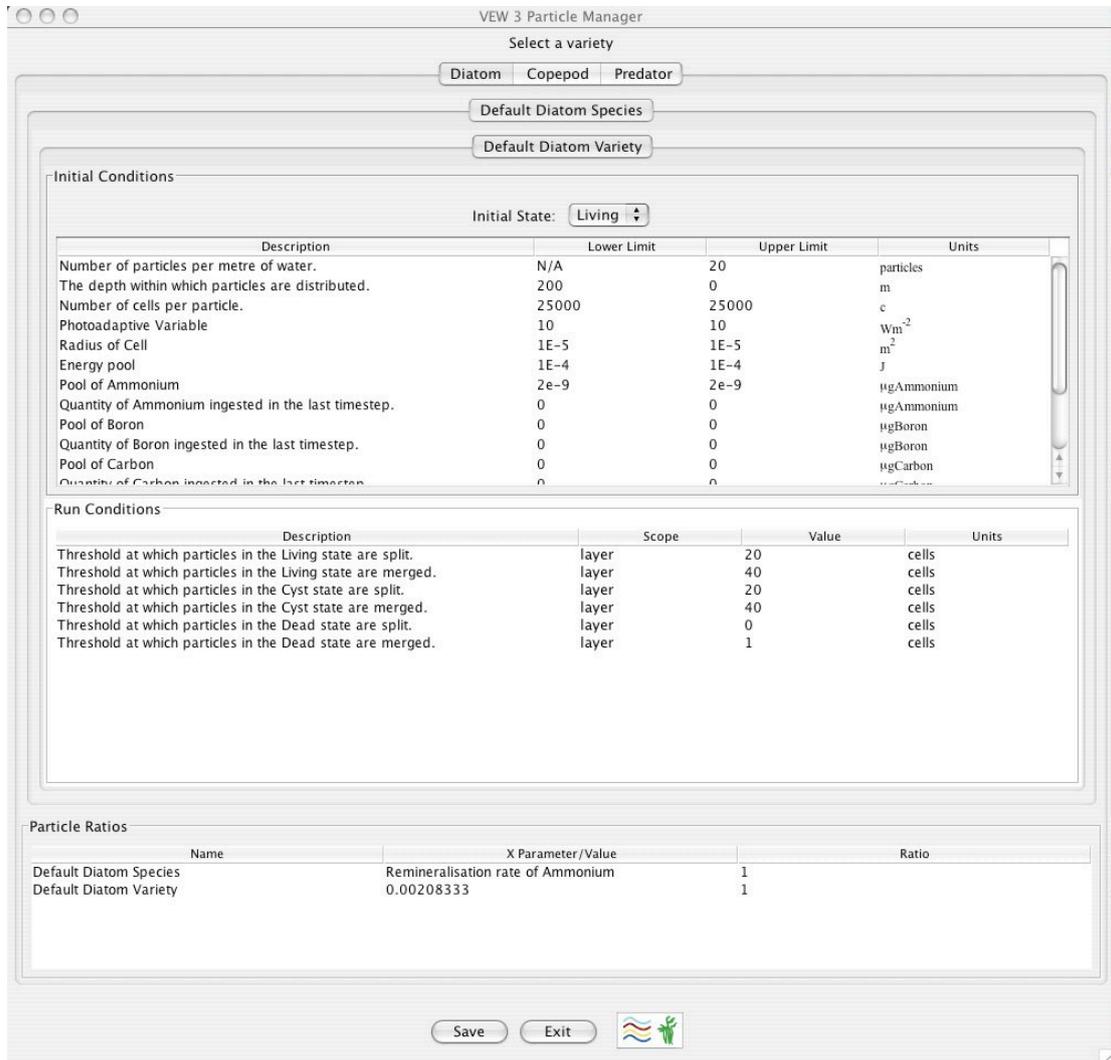
The screenshot shows the VEW 3 Designer interface. At the top, there are four panels: 'Categories' (with 'Chemicals' selected), 'Items' (with 'Chlorophyll' selected), 'Functions', and 'Sub-Functions'. Below these are various control buttons like 'Mark as Top Predator', 'Edit Var', and 'Stage Management'. A central area contains a checkmark for 'Chemical has pigmentation?' and a dropdown menu set to 'Heat Response'. At the bottom left, a table displays wavelength ranges and values. To the right of the table is a spectral graph with a rainbow color gradient. At the bottom, there are 'Save Changes' and 'Close' buttons, and the VEW designer logo.

Min w	Max w	Value
300.0	357.5	0.0
357.5	387.5	0.0
387.5	412.5	0.112
412.5	437.5	0.109
437.5	462.5	0.095
462.5	487.5	0.077
487.5	512.5	0.061
512.5	537.5	0.047
537.5	562.5	0.041
562.5	587.5	0.035
587.5	612.5	0.035
612.5	637.5	0.041
637.5	662.5	0.045
662.5	687.5	0.049
687.5	712.5	0.034

4.4.7 Exercise 12 - Adding a new functional group

4.5 Technical matters

4.5.1 Exercise 13 - Particle management



For each exercise you created a virtual ecosystem in which the specification deviated from that of the default model in the scenario of in one of the features of the model. To do so you followed the procedure that you practiced in §

4.5.2 Exercise 14 - Batches for sensitivity testing

4.5.3 Exercise 15 - Ensembles for computing LE sampling noise

4.6 Documenting a virtual ecosystem

5 Planning your work

- 5.1 Introduction**
- 5.2 Goals**
 - 5.2.1 Marine biology
 - 5.2.2 Biological oceanography
 - 5.2.3 Coastal oceanography
 - 5.2.4 Limnology
 - 5.2.5 Verification
 - 5.2.6 Numerical experiments
- 5.3 Creating a new Virtual Ecosystem**
- 5.4 The virtual ecosystem**
- 5.5 The attractor**
 - 5.5.1 Initial conditions
 - 5.5.2 Adjustment to a balanced state
 - 5.5.3 The attractor
 - 5.5.4 A moored mesocosm
 - 5.5.5 A drifting mesocosm
- 5.6 Competition**
 - 5.6.1 Introduction
 - 5.6.2 Competitive advantage
 - 5.6.3 Extinction
 - 5.6.4 Well-fitted species
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 - 5.6.6 Stability
- 5.7 Endogenous tuning**
 - 5.7.1 Introduction
 - 5.7.2 Goal
 - 5.7.3 Theory
 - 5.7.4 Method
 - 5.7.5 Outcome
 - 5.7.6 Example
- 5.8 Analysis**
 - 5.8.1 Introduction
 - 5.8.2 Balance
 - 5.8.3 Transient state
 - 5.8.4 The attractor
 - 5.8.5 Demographic noise
 - 5.8.6 Annual cycle of the environment
 - 5.8.7 Annual cycle of the plankton populations
 - 5.8.8 Diurnal variation of environment and demography
 - 5.8.9 Features
 - 6.8.10 Audit trails

5.1 Introduction

As in all science, success in virtual ecology depends on meticulous planning. Before sitting down in front of the VEW you should have a fully worked up design for the numerical experiment you want to perform. Your design will lead to the specification for a virtual ecosystem to be used in the experiment. It will specify every detail of the biological model and scenario.

This design phase is best done on paper. Only when it is complete should you use it to convert your design into code, which can be compiled and executed on a computer to create the virtual ecosystem. It is not good practice to design a virtual experiment while working at the VEW. It does not work in virtual ecology, because the value of each biological function can only be judged in the context of a complete ecosystem. VEW³ has been designed to permit you to code a new plankton community step-by-step; it even allows you to unwind and redo earlier steps that have already been coded. However we do not recommend that way of building a new model of the plankton community. Better to design it thoroughly on paper first.

In this chapter we summarize the main steps that must be taken to design a virtual ecosystem.

5.2 Goals

The first step is to write down what you are trying to do. It is convenient to consider seven options:

- marine biology modelling data from laboratory experiments
- biological oceanography simulating observations in the deep ocean
- coastal oceanography simulating observations in shallow water
- limnology simulating observations in lakes
- patchiness simulating the mesoscale turbulence
- verification finding the limits of your simulation
- numerical experiments. testing hypotheses

5.2.1 Marine biology

Scientific explanation of observable properties discovered in virtual ecosystems depends on the veracity of the equations used to represent biological functions of the species represented in your model. When those equations are derived from reproducible experiments on plankton cultures under controlled conditions in the laboratory, they have the same status as the physical equations in your model: the equations for motion, turbulence, thermodynamics and radiation; or the equations for chemical reactions. Meteorologists call these “primitive” equations because they touch the bedrock of science. Ideally our models of the plankton community should be based on biological primitive equations that are equally trustworthy.

In practice, marine biologists are still working to improve the equations that accurately describe the biological functions of plankton. Many of the equations we find in the scientific literature are best described as “provisional”. Sometimes there exist alternative equations of comparable provenance. One of the goals of virtual ecology is to reveal the ecological consequences of switching between rival equations for the same biological function. It goes without saying that the difference between the same emergent property featured in virtual ecosystems based on rival biological equations must not be masked by LE sampling errors. You can achieve that by specifying appropriate particle management rules in your design.

Laboratory mesocosm

VEW³ is primarily designed to reveal the ecological consequences of basing a model on particular biological equations. However, it can also play a role in extracting those equations from experimental data collected from laboratory experiments with plankton cultures. To do so, we replace the open ocean (virtual) mesocosm by one that describes the laboratory apparatus, in short a “laboratory mesocosm”. The main difference between the oceanic and laboratory mesocosms lies in the method used to control the environment. In the former it is done indirectly by fluxes through the sea surface, which are under the control of exogenous data for the weather, ocean circulation and hydrography. In the latter the environment is controlled directly as in the laboratory. For example, the temperature or ambient spectrum of irradiance is specified directly for the virtual laboratory mesocosm.

A version of VEW3 to simulate the ecosystem in a laboratory mesocosm

We have built a new version of VEW³ in which the user specifies the environment in a laboratory mesocosm with the help of a special graphical user interface. We have used this to simulate data collected in laboratory experiments by a leading marine biologist and his research associate (who have asked to remain anonymous in this VEW Handbook).

To test the performance of VEW³ used in this marine biology mode, we have shown that it reproduces exactly the emergent demography and chemical environment measured in the laboratory mesocosm, when we provide it with the corresponding biological primitive equations. The results are available in unpublished reports by W.Hinsley (2006a,b).

Recently, F.Hellweger (*Ecological Modelling*, in press) has extended this approach to take account of intra-population variability in the laboratory mesocosm. He shows how biological primitive equation can be extracted from such noisy data by simulating the published population-mean data with an individual-based model.

5.2.2 Biological oceanography

For more than a hundred years biological oceanographers have concentrated on scientific exploration of the plankton ecosystem. The plankton ecosystem is so complex, with such rich biodiversity, that oceanographers still expect to make fundamental discoveries about its properties. The long-term goal has been to establish the geographical distribution of each species and the diurnal, annual and longer-term variation of those distributions. The task has been complicated by two factors. The first is the biodiversity of plankton, with many thousands of species. The second is the patchy distribution with substantial spatial variance on scales less than one hundred kilometres. Both factors make it very difficult to avoid large sampling errors in data collected at sea. So inferences based on those data are at risk. And the data seldom contain the depth of information needed to test hypotheses about the processes causing the observed distributions.

Virtual ecosystems are based on a tiny fraction of the natural biodiversity. And one-dimensional virtual ecosystems do not contain the processes responsible for generating spatial patchiness; so they may not accurately simulate the spatially-averaged conditions over the, typically, one hundred kilometre resolution of the exogenous data used for the scenario. So the virtual ecosystem is at best a cartoon of the natural ecosystem.

Nevertheless, it is scientifically interesting to analyse a virtual ecosystem in the same way that we would analyse a data set collected at sea. Putting aside constraints arising from limited biodiversity and lack of patchiness dynamics, the virtual ecosystem still contains information that can help us better to understand the natural ecosystem. Indeed, it has two advantages over the observations. The first is that, within its limitations, it is complete; there is no aliasing due to inadequate sampling. The second is that the simulation contains two kinds of emergent properties: those that can be observed (in principle, if not always in practice), and those that cannot be observed (at least not with techniques available today, and perhaps not ever). The latter offer a unique link between observable features and the laws of physics, chemistry and biology that cause them. They provide the information needed for scientific explanation.

So it is worthwhile to explore the observable properties of a virtual ecosystem in the same way that we explore the properties of our observations at sea. The virtual ecosystem always contains the information needed to explain features that you discover in it. The explanation is unambiguous. It is untainted by sampling errors and does not depend on conjectures.

As to the limitations caused by neglecting processes responsible for patchiness, the only solution is to make the major step from one to three dimensions. That lies beyond the scope of this handbook, which deals with the wide range of scientific problems you can address with one-dimensional virtual ecosystems. But see §6.2.5.

As to the limitations caused by truncated biodiversity, your research strategy should follow Okham's razor. You start by modelling a very simple plankton community, like the classical food chain of diatom, copepod and top predator used in the WB model. When you have thoroughly explored and understood the properties of that simple virtual ecosystem, you can study more simulations with more complex biological communities. Added complexity is justified if it leads to greater realism, as

judged by comparison with observations. Verification will be discussed below (§6.2.6).

Predictability

One of the strengths of virtual ecosystems is that they do not suffer from inter-annual variability due to artificial instability of the kind sometimes found in population-based (Eulerian) simulations. Each virtual ecosystem adjusts to a unique attractor for its model and scenario. Once the simulation has settled onto its attractor it has useful predictability.

The attractor is reached after a period of adjustment, during which imbalances in the initial conditions are progressively eliminated. During that period of adjustment, the emergent properties of the virtual ecosystem often exhibit damped oscillations. In planning your numerical experiments, you must allow time for the virtual ecosystem to adjust to its attractor.

When the virtual ecosystem has relaxed to its attractor every emergent property is in balance with the model and scenario. It is not possible for all but one of the emergent properties to be in balance. The ecological processes in the virtual ecosystem bind all its properties to the values in the attractor. If one is artificially perturbed, they all respond. That fact opens the door to practical verification.

5.2.3 Coastal oceanography

VEW³ has been designed to support biological oceanography in the deep ocean, where the ocean floor is much deeper than the bottom of the virtual mesocosm, which is open, allowing particles to sink out into the deep ocean. It is planned to extend future versions of the VEW to support plankton ecology in shallow water. Initially, that extension will retain the simplifying assumption of one-dimensional modelling, with geographically-lagrangian integration. Later we plan to create a new version of the VEW that will support three-dimensional virtual ecosystems, in order to address mesoscale turbulence, both in the open ocean and in coastal waters.

The upgrading of the VEW to support one-dimensional modelling of shallow water ecosystems requires an extension of the physics sub-model to include the turbulent boundary layer on the seabed, and optical influence of the seabed and sediments in suspension. Here is a brief summary of current ideas on how to incorporate these phenomena.

Mesocosm

The shallow-water mesocosm extends from the sea surface to the seabed. The latter depth may be defined as lying deep enough into the sediments to avoid being exposed by re-suspension. Thus, the lowest few layers of the mesocosm may lie inside the sediments on the seafloor.

Turbulence

There are two tasks. The first is to compute the thickness of the mixing layer on the seabed. This is defined by a turbocline, above which the flow is normally laminar.¹⁴ One option is to use the bulk, energy-balance method used as a default in VEW³ for computing the turbocline at the base of the upper mixing layer. We assume that there is no contribution from buoyant convection. So the energy input to the turbulence on the mixing layer is proportional to the cube of the current speed measured at some standard height above the seabed. Data are needed for the drag coefficient, which will depend on the nature of the bottom. The turbocline depth is then computed from a model of the turbulent energy balance, taking account of the above source plus two sinks, viscous dissipation and work done against gravity in mixing the water uniformly between the sea bed and the turbocline..

The second task is to compute the turbulent displacement of particles in the mixing layer. This can follow the method used to compute plankton movement in the surface mixing layer. In this case we are concerned not only with plankton, but also with sediment.

Sediments

The non-living sediments will be modelled by the same agent-based method used in VEW³ to model the plankton. Each sediment agent will behave like a single grain of sand, mud, or whatever. And each such agent will carry information about a dynamic sub-population of identical grains.

¹⁴ In some cases this turbocline will be diagnosed to lie inside the mixing layer at the sea surface, in which case the water column is mixed from top to bottom.

Rules will be needed for various sediment processes, including:

- Collision between sediment grains of the same or different sizes;
- aggregation of sediment grains carried by separate agents;
- re-suspension into the water column of grains that have previously settled onto the sea floor.

Ante Munjiza and John-Paul Latham have developed such rules for their Virtual Geoscience Workbench (VGW), which uses agent-based methods to simulate the generation of sedimentary rocks.

The sediments may be divided into a number of “populations” for different classes of grain, e.g. mud, fine and coarse sand, gravel, and pebbles.

Optics

It will also be necessary to introduce data for the optical properties of the seabed.

The contribution that suspended sediments make to the optical properties of the seawater can be computed in the same way that is done in VEW³ for plankton.

It may be desirable to replace the Morel optical model used in VEW³ by the more accurate models developed by C.-C.Liu for LE modelling. These are based on either the Monte Carlo or Radiative Transfer Equation.

Status

VEW3 cannot be used to simulate the plankton ecosystem in shallow water where seabed processes are important. However, we have seen from the above discussion, that it should be straightforward to extend it to do so. That will permit applications in coastal waters. We are seeking partners, who are expert in shallow water modelling, to work with us towards that goal.

5.2.4 Limnology

The LE metamodel is as valid for ecosystems in lakes as it is in the ocean. VEW³ can be used without change to simulate the plankton ecosystem in very large, deep lakes. There are two approaches for smaller bodies of water. The simplest is to follow the practice of many limnologists, who treat the lake a set of interconnected boxes, with appropriate inflow and outflow by rivers and streams. This solution is to create a lake mesocosm that starts rather like that used for marine biology experiments. It is then modified to take account of vertical structure and exogenous forcing by introducing aspects of the virtual mesocosm used for biological oceanography. Once the geometry of the lake mesocosm is established the fluxes that control its environment can be specified using the VEW³ *Events* tool.

The alternative to that box-model approach is to go all the way to the three-dimensional simulation described in the next section (§6.2.5).

Status

We would welcome the opportunity to collaborate with limnologists with a view to developing versions of the VEW that can apply the LE metamodel to simulating the plankton ecosystem in lakes, initially with a box model and later in three-dimensions.

5.2.5 Plankton patchiness

Mesoscale turbulence

The observed universal patchiness in plankton biomass is caused by mesoscale turbulence. The dynamics of mesoscale turbulence are well understood. They are governed by conservation of isopycnic potential vorticity. That control prevents overturning, which is the predominant phenomenon in three-dimensionally isotropic (3D) turbulence found in the surface mixing layer. Mesoscale turbulence is a chaotic motion found primarily in thermoclines, whether permanent, seasonal or diurnal. (However, its influence outcrops through the mixing layer to the sea surface.)

Mesoscale jets

Most of the kinetic energy of 3D turbulence occurs in overturning eddies that fill the space between the sea surface and the turbocline. They decay largely through a cascade of smaller eddies which are well described by theories of chaotic flow that are statistically homogeneous and isotropic.

By contrast the kinetic energy of mesoscale turbulence occurs in transient jets, which do not overturn. The generation of these jets involves significant vertical motion, called mesoscale upwelling and downwelling. Later as the jets become unstable and develop meanders, there is further mesoscale up- and down-welling along them. Mapping this mesoscale vertical motion gives the jets the appearance of a speckled band.

Fronts

The mesoscale jets are coupled to the density field in a semi-geostrophic balance. The spatial variation of density (or rather isopycnic potential vorticity) is a dynamically-active scalar field. It acts like a brake that resists the tendency of the jets to become ever narrower and swifter. The challenge is to model that process accurately so that the three-dimensional velocity field can be used to compute the advection of particles and passive scalar fields embedded in it.

The most familiar feature of a mesoscale jet is the associated front in passive scalars, such as nutrient concentration. The jet and the front develop together as two aspects of the same feature. However the jet is very much broader than the front. That is best understood by mapping the various scalar fields on isopycnic surfaces (surfaces of constant density). The shape of the density surface is revealed by isobars. They are dynamically active and resist being advected. But others, like temperature, salinity and nutrient concentrations are dynamically passive. They are advected freely by the mesoscale velocity field. As the jet develops these passive contours become concentrated into a sharp front, unlike the isobars.¹⁵

¹⁵ See for example M.K.MacVean & J.D.Woods 1980 "Redistribution of scalars during upper ocean frontogenesis" *Q.J.Roy.Met.Soc.* **106**, 293-311

Response of the ecosystem

Plankton patchiness develops in the combination of the relatively broad jet (with its associated vertical circulation) and the sharp front in passive scalars, like temperature and nutrient concentrations. Together they affect the mean biological production averaged for example over one degree of latitude and longitude. The neglect of mesoscale turbulence on one-dimensional models of the plankton ecosystem is a significant source of error, which can jeopardise comparison between observations and simulation.

Vertical diffusivity in the thermocline

Modellers often seek to parametrize the impact of mesoscale upwelling by introducing a vertical diffusivity in the thermocline. However is far too crude to represent the complex processes involved in the plankton response to meoscale turbulence. The results can be misleading. It is better to avoid such security blankets.

Mesoscale modelling

The solution is to use a mesoscale model to simulate the changing three-dimensional velocity field. This can be treated as exogenous, because changes in the plankton ecosystem cannot affect it. The latter is simulated with the LE metamodel applied in three-dimensions. The plankton agents follow three-dimensional trajectories in response to a combination of advection by the mesoscale velocity field and their own motion relative to the water (sinking or swimming).

The mesoscale model must satisfy two criteria. First it must accurately simulate changes in the coupled three-dimensional fields of velocity and potential vorticity field. The mesoscale jets must be predicted to high accuracy. Even small errors, produce large errors in the patterns of passive scalars (such as nutrient concentration) generated by mesoscale advection.

The second criterion is that the mesoscale model must accurately compute advection of passive scalars. That is far from trivial. It is much more difficult than the lagrangian computation of plankton trajectories. In fact, some modellers prefer to avoid the problems of computing eulerian advection; they decompose the passive scalar fields into a cloud of particles and use lagrangian advection instead.

Status

Various attempts have been made to simulate the plankton ecosystem under the influence of mesoscale turbulence. So far, none has captured the subtle relationship between the jet and its embedded front. The range of scales presents a major challenge for modellers. We believe that this might be solved by the relatively new technique of adaptive mesh modelling. This is used in the Imperial College Ocean Model (ICOM). A.Maggiore (unpublished report) combined LE ecology to an ICOM model of a mesoscale jet/front. We aim to continue this research in collaboration with Professor Chris Pain (who leads the ICOM group). The goal is to develop a three-dimensional version of the VEW within the next few years.

5.2.6 Verification

The credibility of a virtual ecosystem depends on how closely it predicts features that are diagnosed on observations collected at sea. One of the motivations for numerical experiments is to compare the feature in the two data sets derived from observation and simulation respectively. In principle it does not matter which feature you choose for this comparison, provided the simulation is on its attractor. If you detect a significant difference in one feature, then have shown that all features of your virtual ecosystem are unrealistic. The goal of verification is to detect differences between simulation and observation.

There are two pre-requisites for successful verification. The first is that the virtual ecosystem should be on its attractor. There is no point in comparing a simulation that is still wobbling as it sheds errors inherited from the initial conditions. The second pre-requisite is that the difference must be statistically significant. It must not be masked by uncertainties in either the observations or the simulation or both. Your experimental design must ensure that the LE sampling errors in your virtual ecosystem do not prevent you from detecting a significant difference between observation and simulation. That is achieved by appropriate criteria in particle management.

The Ecological Turning Test (ETT, see Woods 2003) provides the basis for statistically-significant comparison of observed and simulated features of the ecosystem, taking account of their associated errors. The first application was by C.-C.Liu (1997), who compared the annual cycle of ocean colour observed near the Azores (27°W 41°N) by SeaWIFS, with ocean colour computed by a Monte Carlo optical model (billions of photons per waveband) applied to our WB virtual ecosystem. There was a statistically-significant difference in the spring bloom. The difference was eliminated by two improvements to the specification for the virtual ecosystem: (1) the cloud routine used to compute surface irradiance was upgraded, and (2) the plankton community was enhanced by using an allometric set of diatoms, (following Nogueira et al 2006). After making these two improvements, the difference was no longer statistically significant. The information in the SeaWIFS ocean colour data has then been exhausted. It could make no further contribution to verifying the Azores virtual ecosystem.

5.2.7 Numerical experiments

Biological oceanography began with scientific exploration. The observed patterns on geographical and temporal variation were explained in terms of ecological processes. The most famous example explains the light-limited phase of the spring bloom in terms of turbulent mixing of phytoplankton that have equations for photosynthesis and respiration. Early simulations of the plankton ecosystem illustrated such theories with models in which contained equations only for the processes directly featured in the theory. Sverdrup's (1953) model is a classical example. The weakness of such "process" models is that they filter out all other processes that may affect the phenomenon. And, as we noted above, all processes do affect every emergent property in a tightly-bound virtual ecosystem.

Virtual ecology follows a different strategy. It identifies the phenomenon of interest (e.g. the spring bloom) in a comprehensive simulation, the virtual ecosystem, and explains it in terms of all the emergent properties, including the fine-grained processes that cannot be observed. For example Woods & Barkmann (1993) showed that in a virtual ecosystem with diurnal variation in the depth of turbulence the growing season began three months earlier than was predicted by the Sverdrup model. This result, which resolved previously mysterious observations in the continuous plankton recorder data, was explained in terms of phytoplankton subducted into the laminar flow diurnal thermocline.

One motivation for numerical experiments in virtual ecology is to revisit the classical paradigms of biological oceanography, with a view to testing the underlying hypotheses against the rich seam of information contained in a virtual ecosystem. The ethos is that of physics, in which you seek to disprove a conjecture by showing that it leads to predictions that are inconsistent with reliable experimental data, or in this case reliable observations collected at sea. The criteria for model design are similar to those described above for *Verification*.

5.3 Creating a new Virtual Ecosystem

Having decided what you want to achieve in your next numerical experiment, the next step is to specify the virtual ecosystem. This involves a number of topics.

First you need to list the emergent properties needed for your investigation; and the level of uncertainty that is acceptable in each properties.

Then you need to design a biological model that will deliver these emergent properties, and contain the biological functions you believe are appropriate for your investigation.

Having fixed the model the next step is to design the scenario for initial and boundary conditions.

Then you need to specify the number of agents that will be used in your calculation, and the particle management rules that maintain that number throughout the simulation. This will control the level of LE sampling errors.

Finally you specify how the model will be computed to create the virtual ecosystem.

5.4 The virtual ecosystem

The virtual ecosystem is a large data set. For a simple food chain model it will typically be several gigabytes per simulated year. You can economize on data storage (and on the time take by VEW Analyser to search through the data for each plot) by choosing to log only a subset of all the emergent properties that are potentially available. The risk is that you may find that you need some emergent property that you chose not to log. In which case you will have to repeat the computation with the new specification for data logging. It is often good practice to break an investigation into stages, logging a different subset of the emergent properties for each stage. As you gain experience you will find the best balance between data storage, on the one hand, and repeated computation on the other.

You can save computation time by using the VEW³ Restart facility. This allows you to make one long integration to get the virtual ecosystem onto attractor. You then use the restart facility to store the complete state of the ecosystem. That is used as the balanced initial condition for each of a set of identical integrations in which you log different emergent properties. You can follow a similar strategy for making an ensemble of instances of the same virtual ecosystem with different values of the random number seed, or a batch of virtual ecosystems that differ in the specification of some small property for sensitivity analysis).

5.5 The attractor

It is important that the virtual ecosystem has relaxed to its attractor before you start to log emergent properties for analysis. In practice this means you must design the duration of the simulation to be long enough to lose any imbalance in the initial conditions. This is specified in the *Scenario* (see below).

The attractor for a virtual ecosystem is determined by a balance three factors: (1) the model, (2) the exogenous forcing, and (3) the resources (i.e. nutrients).

5.5.1 Initial conditions

We distinguish between the initial conditions for nutrients, on the one hand, and for all other state variables, whether environmental or biological, on the other.

Nutrients

The initial profiles of nutrients determine the resource levels of the virtual ecosystem. They are a controlling factor for the attractor. VEW³ uses, as default, nutrient profiles derived from the NOAA World Ocean Climatology. It offers you the opportunity to modify these profiles.

Other state variables

The initial profiles of all other state variables play no part in determining the attractor. The virtual ecosystem adjusts towards that attractor over a period of years. The period of adjustment would be zero if the initial conditions were in balance with the three determining factors (model, forcing, resources). But that is seldom possible in practice. Normally, your choice of initial conditions is likely to deviate from that perfect balance. The deviation is the initialization error for each state variable.

5.5.2 Adjustment to a balanced state

Virtual ecosystems based on the LE metamodel are globally stable. They progressively shed any imbalance in the state variables until they are all “on attractor”. That is the case for initialization errors. Over a period of years the legacy of those errors declines until it is lost in the inherent demographic noise of the virtual ecosystem (which is caused by turbulence, and therefore real).

The period of adjustment is governed by the slowest component of the ecosystem. Normally this is the annual reproduction cycle in the zooplankton. The shortest period for adjustment is three years, with secondary production overshooting in the first year, undershooting in the second, then hitting the attractor in the third; or vice versa, depending on the sign of the initialization error.

Some state variables shed their initialization error much faster than that. For example, the depth of the mixed layer settles close to the attractor in the first day, then slowly drifts towards the final balanced state as biofeedback errors decline.

5.5.3 The attractor

When a virtual ecosystem is “on attractor” every state variable is in balance with the determining factors (model, forcing and resources). It is not possible for some to be in balance and others not. The virtual ecosystem is a total system to which all state variables are connected.

When on attractor the state variables follow diurnal and annual cycles under the influence of the exogenous forcing. And if the forcing features multi-year cycles or secular change, the attractor will do so too.

5.5.4 A moored mesocosm

Woods, Perilli & Barkmann (2005) considered the simple example of a moored mesocosm with no advective flux divergences and a stationary diurnal-annual cycle of surface fluxes. The (WB) model featured one nutrient (nitrogen), diatoms, copepods and a top predator for trophic closure. The virtual ecosystem adjusted to the attractor in three years. The attractor was independent of large differences in the initial conditions. Changes to the initial nutrient profile led the attractor to occupy a different location in state-variable space. So, too, did changes in the model parameter values.

5.5.5 A drifting mesocosm

The same authors report an extension of that numerical experiment. In this case the virtual mesocosm drifted barotropically with the ocean circulation in the Sargasso sea. For the purposes of the experiment, they arranged for the mesocosm's track to follow a closed circuit that was broadly consistent with the ocean circulation. The circuit was closed in exactly five years, during which period the surface heat flux was in balance (i.e. annual heating in the tropics was balanced by annual cooling in the extr-tropics). In this case the virtual ecosystem took fifteen years (three laps of the circuit) to reach an attractor. Once on attractor the state variables exhibited exactly the same values at each geographic position around the circuit as they passed through every at five-year intervals. This attractor was not in local balance with the surface forcing. It was in balance with the upstream history of surface forcing.

5.5.6 Geographically-lagrangian attractor

We have subsequently investigated the nature of the attractor for a virtual ecosystem in a mesocosm that drifts around the ocean along an arbitrary track determined by the circulation that has a stationary annual cycle. As in the previous case the state variables never attain a local balance with the exogenous forcing. But they do achieve a unique balance with the history of forcing upstream along the track of the mesocosm. We call this the geographically-lagrangian attractor. It is achieved when the legacy of the initialization error has declined to a negligible level (compared with demographic noise). It is not known *a priori* how long that that will take. We must assume it will take several years, but the duration will vary with the history of forcing experienced along the track of the mesocosm. One way to establish that there is no significant legacy of initialization errors is to compare virtual ecosystems that follow the same track, but start at different distances upstream.

5.5.7 Diagnosing a virtual ecosystem

It is obvious that a virtual ecosystem must be “on attractor” before you seek to understand emergent properties by using fine-grained properties, such as audit trails, to diagnose their cause.

5.5.8 Comparison with observations

It is equally important that a virtual ecosystem is “on attractor” before its emergent properties are compared with observations. The comparison should not be contaminated by the legacy of initialization errors.

5.6 Competition

5.6.1 Introduction

The sea contains a rich biodiversity. Many of the co-existing species compete for the same resources. Computer modelling has barely begun to address this complex issue. Available computers do not have sufficient power to simulate more than a tiny fraction of the species collected in plankton nets.

5.6.2 Theoretical ecology

We follow our usual approach of insisting that concepts developed in theoretical ecology should be analysed as emergent properties of virtual ecosystems. We are not concerned with models that assume, for example, that each species has a specified competitive advantage. We expect that to emerge from our primitive equation simulations.

5.6.3 Test model

To develop our ideas we have designed a test model based on the WB model, which has one population of diatoms preyed on by one population of copepods. We now split the diatoms into 8 or 16 populations. These sixteen species all have the same biological equations: they are members of the same functional group. They differ in only one of the parameters of those biological equations. The chosen parameter specifies the energy reserve held in a diatom after it has reproduced (by cell division). If this parameter is zero, a diatom that reproduces just before sundown is likely to die during the coming night due to energy starvation. We call this phenomenon infant mortality; the parameter is called the infant mortality parameter (IMP). Infant mortality can be prevented by making the IMP larger than the respiration during the night. However that has a disadvantage. Reproduction will occur less frequently because the diatom must acquire not only the normal threshold energy for cell division, but also twice the energy specified by the IMP. Diatoms with the optimal value of the IMP will have a long-term demographic advantage with those that have lower or higher values.

In our numerical experiment the sixteen diatom populations compete for the same resources (light and nitrogen) and are grazed equally by the copepods. The aim was to discover what value of the IMP produced diatoms that were best fitted to the conditions of the experiment, which were defined by the model, forcing and resources.

5.6.4 Attractor

The first result is that the virtual ecosystem quickly adjusts to an attractor in which the total number of diatoms and the total number of copepods follow annual cycles that are almost indistinguishable from those in the case where there was only one population of diatoms. However, over the years (or rather the decades) as the best-fitted diatoms drive out the others, the attractor adjusts slightly to one with a different balance of primary and secondary production. The changing relative abundance of the 16 populations of diatom does not affect the stability of the virtual ecosystem.

5.6.5 Extinction

The relative success or otherwise of each diatoms population is revealed by time series of their number in the virtual mesocosm. The best-fitted diatoms, those with the optimal IMP, steadily increase in numbers. The others proceed to extinction at varying rates, depending on the value of their IMP. Plotting a time series of the logarithm of the number of diatoms in each population shows that the decline towards extinction as a straight line. The slope of that line gives the extinction time.

5.6.6 Competitive advantage

The relative competitive advantage of each population is revealed by ranking them by extinction time.

5.6.7 Neutral competition

Diatoms with IMP values close to the optimal value exhibit neutral competition, with one then another becoming the most prolific. The turnover time is many years. This phenomenon arises from the demographic noise in the virtual ecosystem, which causes inter-annual variation of a few percent in the diatom numbers.

5.6.8 Seasonal succession

The extinction time tends to be many years, so the relative abundance of diatoms with different IMP values changes slowly. This suggest that there might be seasonal succession between co-existing species, even though one is more highly ranked than the other in long-term competitive advantage.

Enrique Nogueira (2006) performed a numerical experiment to investigate seasonal succession and short-term co-existence in a WB model with three diatoms populations. In this experiment the diatoms in the three populations differed in size. They had different values of all their biological parameters, the values being were controlled by allometric equations. (VEW³ makes it easy to specify such allometric sets.) Analysis of audit trails revealed how the three populations were able to co-exist despite very different parameter values.

5.6.9 Conclusion

These simple numerical experiments show that natural selection is simulated well in virtual ecosystems based on the LE metamodel. Competition does not affect the stability of the virtual ecosystem. It is easy to measure extinction time and the ranking of competitive advantage as emergent properties of the simulation. Seasonal succession of diatoms of different sizes is explained in terms of different behaviour revealed by audit trails. VEW³ makes it easy to perform such numerical experiments on virtual ecosystems with competing species of plankton.

5.7 Tuning

5.7.1 Introduction

It is common practice to tune model parameters to obtain a better fit between observations and the corresponding emergent properties of simulations. The rationale is pretty straightforward. Models need to represent the complex biodiversity of the ocean with a few functional groups each with a small number of species. Ideally the equations used in the functional groups are based on laboratory experiments; they are biological primitive equations. However, the species in those groups must somehow represent the much greater number of such species in the ocean. So it may not be best practice to base their parameters on laboratory values for declared species. Tuning may lead to the best choice for “representative” species. The best choice depends on your goal, which may be to simulate some observations, or to build an operational model for prediction.

The main objection to tuning in this way is that it cannot target single species in isolation. The emergent properties that are matched to observations are influenced by the whole plankton community.

A second objection is that good observations are a rare commodity, which should be reserved for the scientific process of testing models rather than the engineering process of tuning them. It is more important to improve our understanding of the plankton ecosystem than to produce a model tuned for operational prediction.

5.7.2 Goal

If the prime value of observations lies in testing our models, as a step to finding and correcting their weaknesses, then we should do everything possible to improve the prospects of such testing. One pre-requisite is to ensure that the virtual ecosystem is on attractor. Another is to ensure that the species in the model have best fitted values for their parameters. It would be a mistake to compare observations with the emergent properties of a model that includes species that are not best fitted to the virtual ecosystem. In passing we note that that was the case with the version of the WB model used to illustrate the LE metamodel in Woods (2005): in that model the diatoms has an $IMP = 0$, whereas we know from natural selection experiments described in §6.6 that the best fitted values is about $14 \mu J$.

5.7.3 Method

The method of natural selection can be used to discover the best-fitted value of each parameter in the biological equations used to describe a functional group of plankton in our model. This is an example of optimization.

5.7.4 Summary

Before comparing observations with emergent properties of a virtual ecosystem, its species should be optimized by natural selection within the virtual ecosystem. This method of “endogenous tuning” is preferable to exogenous tuning against observations.

5.8 Analysis

5.8.1 Introduction

Whatever your motivation, every run on VEW³ will produce a virtual ecosystem, which you will import into VEW³ Analyser for study. Here we offer some tips on the best way to investigate a virtual ecosystem. Of course the procedure will be shaped by the particular aims of your investigation. However, there are some generic features of all investigations on VEW³ Analyser. These lay the foundations for best practice, which guides every investigation, regardless of motivation.

You should start by surveying the nature of the new virtual ecosystem before you home in on the particular goal of your investigation. This avoids surprises when you start to analyse features of special interest.

You proceed in stages through this initial survey. The aim is to reassure yourself that the virtual ecosystem has the general features needed for your investigation. You will assess each stage. If it does not meet the requirements of your investigation, you will develop a hypothesis in which you identify some aspect of the specification for model or scenario that should be changed before you proceed.

You then abandon the unsatisfactory virtual ecosystem, change the specification, create a revised virtual ecosystem and start again through the staged initial survey. Eventually you will have created a virtual ecosystem that satisfies the needs of your investigation.

You then proceed to identify the features that characterize your investigation. You will illustrate those features, using the full power of VEW³ Analyser, with which you have previously become familiar (see Chapter 4).

5.8.2 Balance

Your first task is to check that the virtual ecosystem has settled to a balanced state, in which all the emergent properties lie on the attractor for the specified model and scenario for exogenous forcing. You have probably created a virtual ecosystem extending several years from a rather uncertain initial condition that was almost certainly not in balance. The hope is that, after a few years of transition, the virtual ecosystem will settle to the attractor.

- *Plot time series for the multi-year duration of the virtual ecosystem.*
 - *The depth of the mixed layer*
 - *The number of organisms in each population each day.*
 - *The mixed layer environment (temperature, nutrient concentrations)*

5.8.3 Transient state

For some investigations you will want to study the changes occurring in the virtual ecosystem that occur during the transitional stage before it reaches a stable attractor. For example, you may be studying the demographic changes that occur in a set of species that are competing for the same resource. (see §5.6). Or you may be concerned with the transient response of the ecosystem triggered by an event that you have deliberately introduced into the specification for exogenous forcing (§2.17).

In such cases you select a year in the transient state of the virtual ecosystem, and proceed through the remaining stages of documentation. Of course, the annual Poincaré maps (Woods *et al* 2006) will not be closed, as they are when the virtual ecosystem is on attractor.

5.8.4 The attractor

In most investigations you will want to work with a virtual ecosystem that has settled to an attractor. The virtual ecosystem is deemed to have settled to its attractor when the inter-annual variation has declined to small random fluctuations (which will later be related to the LE sampling noise).

This definition applies to the special case of a virtual ecosystem that is subject to a stationary annual cycle of exogenous forcing. That applies, for example, to a mesocosm moored at a geographical location where the annual solar heating balances the annual cooling to the atmosphere. This condition is satisfied in the virtual ecosystem bundled with VEW3 and analysed in Chapter 4.

The definition becomes more complicated when the forcing changes from year to year, as it does in the mesocosm drifting with the ocean circulation. (For an example see Woods, Perilli and Barkmann 2005.) The virtual ecosystem then adjusts to a “geographically-Lagrangian” attractor (§5.5.6). The annual geographically-Lagrangian attractor can be synthesized from a set of 365 virtual ecosystems, one for each day of the year. The resulting data set is then analysed as described below.

In §6.5.2 you documented the process of adjustment to the attractor in multi-year time series. You now choose one year after adjustment has ended, so that the virtual ecosystem is on the attractor. You document the general character of the attractor with Poincaré maps that document the flow of resources through the food chain. For these plots you sample the data once per day for the chosen year.

- $\text{Log}_{10}(\text{concentration of nutrient}) : \text{Log}_{10}(\text{number of phytoplankton})$
- $\text{Log}_{10}(\text{number of predator species}) : \text{Log}_{10}(\text{number of prey species})$

5.8.5 Demographic noise

It is important to know the uncertainty of emergent properties that is attributable to the Lagrangian Ensemble method. This uncertainty, or noise, arises from describing a plankton population in the mesocosm with a number of computer agents that is much fewer than the number of plankters in that population. You can estimate the magnitude of that noise by statistical analysis of an ensemble of instances of the virtual ecosystem. Each instance differs only in the seed value used to initialize the random number generator, which is used to simulate the advection of individual agents by turbulence in the mixing layer. Changing the seed value leads to small differences in the demography of each plankton population. The aim here is to document the standard deviation of that inter-instance variation.

- *Use the ensemble tool in VEW Controller to create a set of instances of the virtual ecosystem*
- *Import the set of instances into VEW³ Analyser.*
- *Use the VEW³ Analyser statistics tool to compute the mean and standard deviation of emergent properties of the virtual ecosystem.*

- *Following the procedure of §6.5.3, plot Poincaré maps of these mean and standard deviations.*

You now embark on a broad reconnaissance of the virtual ecosystem when it on attractor or in a known transient state.

5.8.6 Annual cycle of the environment

The first step is to plot the annual cycle of the environment. You should sub-sample the data at a time resolution of one value per day.

Plots

- *Time series of the depth of the mixed layer (defined by the daily maximum depth of the turbocline).*
- *Time series of environmental variables at selected depths (The physical includes temperature, light and turbulence; the chemical environment includes dissolved nutrients)*
- *Depth-time contour plots extending from the sea surface to the bottom of the seasonal thermocline (defined by the annual maximum depth of the turbocline)*

5.8.7 Annual cycle of the plankton populations

The next step is to plot the annual cycle of demographic properties of the plankton populations represented in the virtual ecosystem. (Remember to include the top predators.) Again the data should be sub-sampled at one variable per day.

The demographic variables comprise:

- Number of plankters
- Number of plankters created by reproduction (organisms per time step)
- Number of plankters lost as the result of starvation
- Number of plankters lost by being eaten
- Number of plankters lost by succumbing to mortal disease
- Number of plankters lost by succumbing to senility
- Life expectancy (in days)

Plots

- *Time series of a demographic variable integrated vertically over the whole mesocosm*
- *Time series of a demographic variable integrated vertically over a specified depth range*
- *Depth-time contour plot of the profile of a demographic variable*

5.8.8 Diurnal variation of environment and demography

The diurnal variation of environmental or demographic variables is best displayed in a time window of three days. You position the time window to suit your particular scientific interests. The data should be sampled at full resolution i.e. with values for every time step of the integration.

5.8.9 Features

Having completed a broad reconnaissance of the annual and diurnal variation in your virtual ecosystem, you will now want to zoom in on a feature that is of special interest for your investigation. For example, you may wish to examine the spring bloom in more detail, or summer oligotrophy, or the autumn bloom, or the winter.

Whatever your target, the procedure is to window the data in time with start and end dates that embrace the feature of interest. This may involve a little “trial and error-correction”.

You will probably also want to window the data in depth. This depth window might embrace

- the mixed layer if you are concerned with the spring bloom,
- the top 100m if you want to explore diel migration of zooplankton
- the seasonal thermocline for the deep chlorophyll maximum.

In order to explore a feature you will probably want to compare the timing and depth of several emergent properties. VEW³ Analyser allows you to start with a base contour plot of a field variable (environmental or demographic variables), and then superimpose a number of time series.

5.8.10 Audit trails

Finally we arrive at the *fons et urbis* of virtual ecology: the audit trail of a plankton agent. The audit trail provides time series of the following properties:

- Depth
- Ambient environment, defined by the value of environmental variables at the agent’s location (i.e. depth in a one-dimensional simulation).
 - Physical environment (temperature, light, turbulence, etc.)
 - Chemical environment (e.g. concentration of each nutrient)
 - Biological environment (concentration of prey plankters)
- Number of plankters in the sub-population associated with the agent.
- Biological state of the plankters (they are by definition all identical)
- Biochemical condition of the plankters.
This is defined by the chemical concentration in each Droop pool.
- Digestive condition of each plankter>
Defined by the number of undigested prey in its gut.
- For zooplankton, the number of eggs accumulated prior to hatching.

The challenge is to select one particle of the many thousands in the virtual ecosystem. Normally the specification for logging will have pre-selected about one thousand agents from each species. It remains to choose a small number for plotting.

You can include in one plot time series of the same variable for several plankton agents. This provides a useful illustration of intra-population variation, which is an important – indeed a unique – feature of LE modelling.

6 Support

6.1 Website

The new VEW website is now in final stages of design and will be available during summer 2006 at <http://www.virtualecology.org>

6.2 Documentation

The earlier series of Virtual Ecology technical reports is now closed. It is replaced by this VEW Handbook, which will be progressively expanded in the future. The current version will be available in pdf format for download from the website

6.3 Training

We plan to offer professional training sessions lasting one or more days at Imperial College London, or at your site. These will be tailored to the needs of each user.

6.4 Workshop

The plan is to hold a VEW Workshop each July in Alpicella, starting in 2006.

6.5 Technical support

Users will receive technical support from Imperial College London through the VEW website. This involves submitting a request for support (or a bug-report) through the web. We aim to respond within one week.

6.6 Forum

The VEW website will support a forum for users.

7 Bibliography

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W.Hinsley Using the VEW to simulate emergent properties from a laboratory mesocosm (a) Phytoplankton (b) Zooplankton

Appendix

Disease modelling in plankton

Jeremy Cope , MSci 4th year project report, June 16, 2006

Abstract

Viruses are well known to take a major role in the marine ecosystem, and their biochemistry is well documented. However, there are currently no models of the plankton ecosystem which make use of this detailed biological and biochemical knowledge. This report describes the biological processes involved in virus infection of plankton and the current state of the art in modelling of this ecosystem. It then makes use of this knowledge to develop a new model, based on the Lagrangian Ensemble method and implemented using the Virtual Ecology Workbench system, and uses this model to draw meaningful conclusions about the role of viruses in the ocean ecosystem.

6.3 Achievements

To demonstrate the applicability of population-based modelling to diseases in plankton, the work of Singh et al has been described. This relatively simple model encompasses the salient features of viral infection in a simple predator-prey system and suggests that virus-mediated mortality may account for the random bloom patterns observed in phytoplankton.

A model of virus infection in diatoms has been built using the VEW, based on the WB model of Woods and Barkmann, with a certain amount of success. The model has been shown to produce a stable ecosystem, at least over the period for which it was run. The advantages of the individual-based approach have been demonstrated by obtaining concrete scientific conclusions through experimentation. In that respect, the project has provided a successful proof-of-concept for disease modelling using the LE method.

However, there are a number of concerns about the LE virus model that has been developed.

Due to time constraints, the new model was only integrated for a year of virtual time. This is unsatisfactory, as the WB model is known to take a number of years to properly settle down to its attractor. Also, conclusions from an individual-based model should be based on an ensemble of runs which was not done, again due to time constraints.

The method chosen to model the state of infection, conditioning on the virus pool v , is of doubtful usefulness. It was chosen in order to demonstrate a scalable approach to disease modelling in the VEW, and due to a need to reduce computational overhead. However the alternative, modelling infection explicitly using states, should be better in spite of the increased computational cost, since it avoids the reduction in natural variation of times-to-infection.

The new model was based on the WB model, and the diatoms in the WB model were chosen as a host population due to their single-celled nature.

Unfortunately it proved difficult to apply experimental results from the literature to this situation as, for whatever reason, most research in this area has been done on protists (a miscellaneous group of single-celled eukaryotes) and bacteria. It would be easier to apply these results directly if a model of virus infection in bacteria was built, for example.

These concerns notwithstanding, there now exists a concrete demonstration which shows that the VEW as it stands can be, in principle, used to model virus infection and similar situations.

The new LE-based model has been used to run some experiments, and it has been shown how it is relatively simple to draw useful conclusions from an individual-based model. The demonstration of use of the model to produce a solid conclusion (regarding the need for a low contact success rate for virus infections) is a pleasant but unexpected benefit.

Considering the application of results from a population-based model to an individual-based one, at least in the case of the models described in this report, the models are just too far apart in their level of abstraction. The Singh et al model, while it does a good job of modelling the situation, is too far away from the basic biology to allow the conclusions drawn regarding its parameters to be applied to an individual-based model.

During the development of the LE-based model, a number of limitations of the VEW were discovered, which have been documented. The suggested solutions to these problems are of course subjective, and may not be appropriate to implementation in the VEW, either in the current iteration or generally. However, it is hoped that they will be helpful.

A major advantage of the Virtual Ecology Workbench is its generality. If the modifications suggested in Section 6.2 were made, it would be possible to model the attachment of *V. cholerae* to zooplankton exuviae and begin testing theories to explain how and why this behaviour occurs.

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