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Preface

This volume is a collection of 39 papers presented at the *Third International Workshop on Scientific Computing and Applications* held in January 2003 at City University of Hong Kong (http://math.cityu.edu.hk/sca03). The first and the second workshops of the series were held at City University of Hong Kong in December 1998 and Banff, Alberta, Canada in May 2000, respectively. The aim of the workshop is to bring together mathematicians, scientists and engineers working in the field of scientific computing and its applications and to provide a forum for the participants to meet and exchange ideas in an informal atmosphere.

This year, more than one hundred people from fifteen different countries attended the four day event. The workshop includes 12 plenary talks, 7 organized mini-symposiums and many contributed talks. The papers presented at the workshop cover a wide range of topics in the field of scientific computing and its applications.

The workshop was supported by the Department of Mathematics and the Liu Bie Ju Center for Mathematical Sciences at City University of Hong Kong. The Editors wish to thank Prof. Roderick Wong, Prof. Jianzhong Zhang and Prof. Qiang Zhang for their contributions to the success of the workshop. We also received significant help from members of the scientific committee and organizers of the mini-symposiums. Special thanks must go to the K. C. Wong Education Foundation which provided financial support for participants from the mainland China. We are also grateful to the authors for their contributions and to the referees for reviewing the papers efficiently.

Hong Kong, October 2003

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Contents

PERIODIC SOLUTIONS AND SIMULATION FOR A LAGOON MODEL*

WALTER ALLEGRETTO†, CHIARA MOCENNI‡, AND ANTONIO VICINO§

Abstract A mathematical model for phytoplankton-zooplankton-oxygen-nutrient dynamics for Italian lagoon ecosystems is proposed. Firstly, an analysis of the model is performed, proving the existence of periodic solutions driven by the seasonal evolution of environmental exogenous inputs. A further numerical comparison between simulation and real measurements (via two subsequent coefficient determination procedures) allows the validation of the model and to derive subsequent scenario analysis. Dystrophic phenomena, like excessive nutrient loading coming from surrounding areas, are finally suggested.

Key words Lagoon ecology, phytoplankton, zooplankton, mathematical model, periodic solutions, parameter estimation

1. Introduction. European coastal lagoons are complex ecosystems balancing human activities and ecological processes. In fact lagoons are located at the interface between sea, farmlands and built-up areas. The environmental impact of urban discharge, agricultural catchments, industrial pollution has produced a large supply of nutrients, organic matter and sediments into the water. What's more, the limited water circulation, the poor exchanges with the sea and the intensive fish production create problems for the maintenance and health of the quality of the water (eutrophication).

In this paper two quite different lagoons are considered. The first one is the Lagoon of Caprolace (located in the National Park of Circeo, 100 km south Rome). It covers an area of about 2.26 km^2 and is of 1.7 m average depth. It is characterized by a modest eutrophication, although the nutrient loading is quite high. The microalgae biomass (phytoplankton and zooplankton) seems to govern the main biochemical and ecological processes. The second one is the Lagoon of Orbetello (Province of Grosseto, 90 km west Siena). It covers an area of about 27 km^2 and is of 1 m average depth. It is characterized by very high eutrophication and it is periodically affected by anoxic crises and by abnormal proliferation of macroalgae that damage the tourism and fishery based economy.

Mathematical models describing ecological activities in the lagoons involve interactions between various species of phytoplankton, zooplankton (hereafter

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denoted by v_1, v_2 respectively), nutrients and oxygen [1, 2, 4, 6, 7]. Intensive human farming activities and high population density in the surrounding areas imply that the lagoons are often in the high nutrients regime, [3, 5], i.e. the only limiting factors in the phytoplankton (and thus zooplankton) growth are the exogenous growth inputs of light and temperature. We present here only results for this situation, and direct the interested reader to [8], where the full system as well as other factors such as: species diffusion; spatial variations of the variables; water current flow and/or zooplankton drift; hostile environment at the lagoon boundary, are considered.

2. Mathematical analysis. Since the lagoons of interest here are extremely shallow ($\lesssim 1$ m), we also ignore diurnal depth effects. The equations we consider thus reduce to

$$\frac{\partial v_1}{\partial t} - \varepsilon_1 \, \Delta v_1 = \left[k_1 M(x,t) - k_2 v_1 - \frac{k_3 v_2}{k_p + v_1} \right] v_1 \tag{2.1}$$

$$\frac{\partial v_2}{\partial t} - \varepsilon_2 \, \Delta v_2 = \left[\frac{k_4 v_1}{k_p + v_1} - k_5 \right] v_2 \tag{2.2}$$

in a domain $\Omega \subset \mathbb{R}^3$ which represents the lagoon. On $\partial\Omega$, the natural boundary conditions: $\frac{\partial v_1}{\partial \vec{n}} = \frac{\partial v_2}{\partial \vec{n}} = 0$ are assumed. In equations (2.1) and (2.2), $0 \leq M(x,t)$ represents the exogenous inputs mentioned earlier, periodic of period T, while $0 < \varepsilon_1, \varepsilon_2$ represent the (small) diffusions and $k_1, \cdots, k_5$ represent positive constants. The interpretation of the other terms of the right hand sides of equations (2.1) and (2.2) is as follows: the terms of equation (2.1) represent growth, natural mortality and predation (according to [9]); the terms of equation (2.2) represent growth by predation and natural mortality.

While there have been many ecological studies on various lagoon models, to the best of our knowledge the analysis and quantitative simulation of the proposed model are the first such. Related results may be found in [12, 15, 16] and [13, 14], concerning qualitative and quantitative aspects respectively.

Our first results are theoretical and deal with the existence of positive periodic solutions. This is the situation we expect to occur under "normal" ecological conditions in the lagoon.

THEOREM 2.1. *If*

$$k_4 \left(\int_\Omega \int_0^T \sqrt{M} \right)^2 > \left(k_2 k_5 |\Omega| T \right) \left[k_1 |\Omega| T + \frac{(|\Omega| T)^{1/2}}{k_2} \left(\int_\Omega \int_0^T M^2 \right)^{1/2} \right], \tag{2.3}$$

then there exists a T-periodic solution $v_1, v_2 > 0$ of system (2.1)-(2.2).

We remark that if $M = M(t)$ and we seek v_1, v_2 purely functions of time, then (2.3) can be replaced by the following better condition:

$$k_4 \left(\int_0^T \sqrt{M} \right)^2 > k_2 k_5 T \left[k_1 T + \frac{1}{k_2} \int_0^T M \right]. \tag{2.4}$$

The proofs of these results are based on topological methods as well as principal eigenvalue estimates and, as mentioned earlier, can be found together with other such results in [8].

3. Numerical Examples. We now pass to a discussion of the validation of the model (2.1)–(2.2) by means of parameter estimation-comparison with experiment. We select data from the lagoon of Caprolace, [11], and estimate coefficients $(k_1, \cdots, k_5)$ by parameter fitting, with the small diffusivities $\varepsilon_1, \varepsilon_2$ set equal to zero. This process is simplified by the fact that the homogeneous nature of this lagoon enables us to set $M(x,t)$, v_1 and v_2 as purely functions of time.

This process is briefly described as follows: we divide by v_1 and integrate both sides of equation (2.1), obtaining

$$ln\left[\frac{v_1(t_I)}{v_1(t_0)}\right] = \int_{t_0}^{t_I}\left[k_1\ M(t) - k_2\ v_1 - \frac{k_3\ v_2}{k_p + v_1}\right] dt. \tag{3.1}$$

Since k_p is known from the biological processes [9], we integrate the right hand side numerically, as well as replacing $v_1(t_I)$ by the experimental measurements at time t_I, for $I = 1, \cdots, D-1$ where D is the number of experimental results. This produces a system of $D \times 3$ linear equations in k_1, k_2, k_3 which enables us to estimate the above parameters by least square fitting. Exactly the same process is followed for equation (2.2) and k_4, k_5 are estimated. We emphasize that no periodicity condition is imposed a priori in the constant determination process. Next, system (2.1)–(2.2) is solved numerically in one and two dimensions, using a backward Euler method in time together with exponential fitting for the second equation. For the 2-d case, the diffusivities are reintroduced and the simulations employ a control volume (finite box) discretization in space. The constants $k_1, \cdots, k_5$ are then readjusted by scale changes to improve the comparison of the critical values of the measured and computed v_1 and v_2.

Further details of this procedure are given in [10], from which we select also the following examples of results obtained by the process.

We solved the initial value problem (with fairly arbitrary initial data) for equations (2.1)–(2.2) with the constants determined earlier. We found that a periodic solution is approached, typically within a couple of simulation years. Fig. 3.1 shows the comparison between this periodic solution and the data after about 10 simulation years for the phytoplankton density v_1.

Fig. 3.2 is the equivalent result for the zooplankton density (v_2).

Fig. 3.3 shows the simulation of the 2D model for the lagoon of Caprolace, modelling a very high nutrient spill at a point of the lagoon boundary, after the homogeneous periodic solution regime has been established. The seasonal spatial distributions of zooplankton biomasses are calculated in winter and spring.

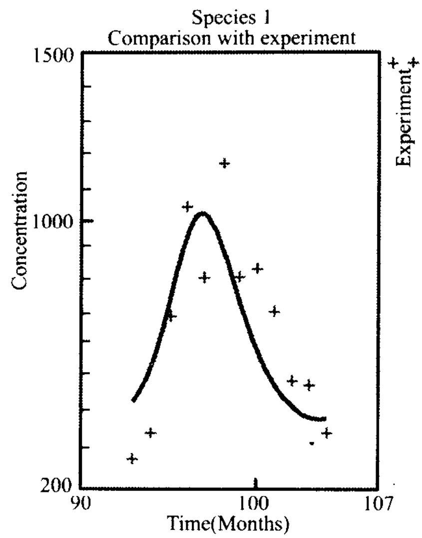

Fig. 3.1. *Phytoplankton density in the Lagoon of Caprolace: simulation compared with experiment, under spatial homogeneous conditions*

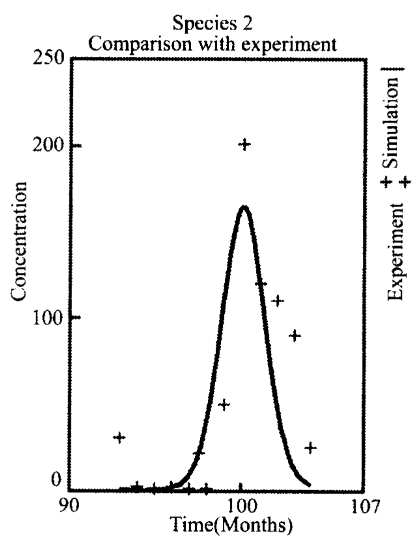

Fig. 3.2. *Zooplankton density in the lagoon of Caprolace: simulation compared with experiment, under spatial homogeneous conditions*

Changes in the ecological conditions corresponding to external nutrients loading are evident: the main effect is the growth of micro algae and zooplankton species. The effects of this fact on oxygen concentration and the feedback on nutrient concentration are not discussed in this paper (for a reference, see

[8, 10]).

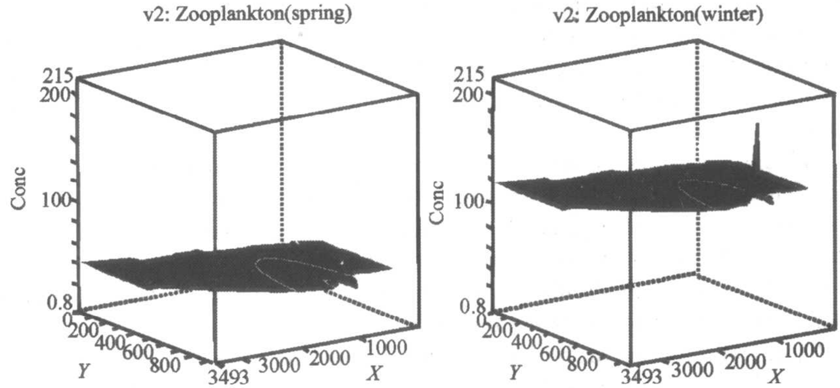

Fig. 3.3. *2D model simulation of zooplankton in the lagoon of Caprolace The figures represent the spatial distribution in spring and winter, illustrating a nutrient inflow at a point on the lagoon border*

Fig. 3.4 shows the 2D model simulation of the phytoplankton biomass in the Lagoon of Orbetello. It is evident the exaggerated growth of v_1 as a consequence of the high nutrient regime "near city"; in fact the city of Orbetello is located in a strip of land in the center of the lagoon.

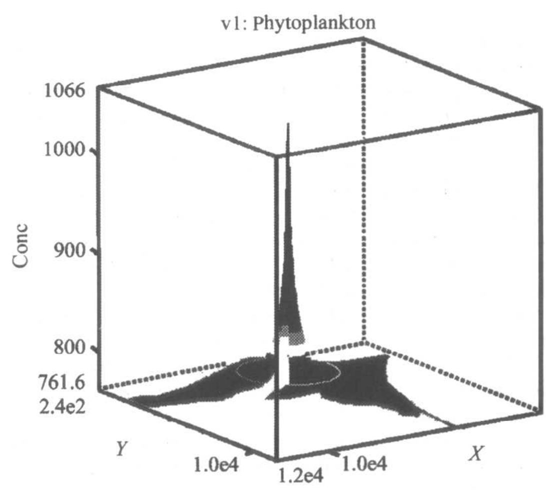

Fig. 3.4. *Phytoplankton density in late fall in the Lagoon of Orbetello: 2D model simulation*

4. Conclusions. The present paper focused on the integration between the mathematical analysis of the distributed model, in order to assess the existence of periodic solutions, and the validation of the model via simulation-measurements comparison. Different situations were investigated and related to the specific nature of the studied ecosystems. In particular, the fitting procedure was applied under the plausible hypothesis of homogeneous conditions to the Lagoon of Caprolace. On the contrary, the spatially distributed model was simulated in the real situation of abundant nutrient sources, corresponding to the location of Orbetello city, and to a canal runoff at the border of Caprolace lagoon.

The main results of the work concern the identification of a parameter-dependent condition for the existence of periodic solutions capable of reproducing the qualitative ecological conditions of the aquatic system as well as the quantitative information contained in real data.

In addition, some simulation experiments of spatially distributed models under high nutrient local inflow regime are carried out.

There remain the problems of determining the long time behaviour and stability of the periodic solution found, as well as the practically very important question of determining beforehand when anoxic crises are about to occur.

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ARTIFICIAL BOUNDARY CONDITIONS FOR SCHRÖDINGER-TYPE EQUATIONS AND THEIR NUMERICAL APPROXIMATION

X. ANTOINE* AND C. BESSE

Abstract The construction of a hierarchy of high-frequency microlocal artificial boundary conditions for the two-dimensional linear Schrödinger equation is proposed. These conditions are derived for a circular boundary and are next extended to a general arbitrarily-shaped boundary. They present the features of being differential in space and non-local in time since their definition involves some temporal fractional derivative operators. The well-posedness of the continuous truncated initial boundary value problem is provided. A semi-discrete Crank-Nicolson-type scheme for the bounded problem is introduced and a stability result is given. Next, the full discretization is realized by the way of a standard finite-element method to preserve the stability of the scheme. Numerical simulations are given to illustrate the effectiveness and flexibility of the method.

Key words Schrödinger equations, artificial boundary conditions, Crank-Nicolson schemes, stability, numerical simulation

AMS subject classifications 65M12, 35Q40, 58J40, 26A33, 58J47

1. Introduction.

We investigate the numerical computation of the solution u to the two-dimensional linear Schrödinger equation with constant coefficients

$$\begin{cases} (i\partial_t + \Delta)u(x,t) = 0, & \forall (x,t) \in \mathbb{R}^2 \times \mathbb{R}^{*+}, \\ u(x,0) = u_0(x), & \forall x \in \mathbb{R}^2, \end{cases} \tag{1.1}$$

where u_0 designates the initial datum, Δ is the Laplace operator defined by $\Delta = \partial_{x_1}^2 + \partial_{x_2}^2$ and $x = (x_1, x_2)$ stands for the space variable. This kind of equation has many technological applications as for instance in quantum mechanics (modeling of quantum devices [6]), in electromagnetic wave propagation [24], in underwater acoustics (paraxial approximations of the wave equation [31]) or also in optic (Fresnel equation [21]). It can be used to model some problems arising in plasmas or relativistic physics but also for beam propagation in non-linear Kerr media [11] if a non-linear perturbation is added to the model. For all these reasons, the construction of efficient numerical schemes for solving (1.1) represents an important issue.

A standard discretization for system (1.1) is given by the well-known implicit Crank-Nicolson scheme. To bound the computational domain Ω, one usually imposes a boundary condition of Dirichlet or Neumann-type. However, when the wave u impinges the fictive boundary on which this boundary condition is set, some visible spurious reflections occur [14] and are prejudicial to

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the numerical observation of the propagation phenomenon. Then, one must consider a larger computational domain which can be difficult to numerically handle especially for multidimensional calculations. Therefore, a usual adopted solution consists in imposing a more suitable boundary condition on the fictive boundary which does not affect the solution in the interior domain by not generating some undesirable parasistic reflected waves. Numerous works have been devoted to this problem in the one-dimensional case. The ideal boundary condition, also often called artificial, may be simply designed by the Laplace or Fourier transform [4, 7, 9, 10, 13, 18]. The resulting condition is then non-local in time and involves a time fractional derivative operator of order $1/2$. The time discretization of this convolution operator is then delicate to achieve since an unsuitable discretization may destroy the underlying stability of the interior Crank-Nicolson scheme [27] and lead to an ill-posed problem. Several solutions have been considered to remedy to this problem [1, 4, 7, 8, 9, 13, 17, 18, 29, 30].

Studies concerning the construction of the exact boundary condition in two dimensions have received less attention and only a few developments have recently been achieved. To the best of the authors knowledge, the analysis has only been restricted to some canonical geometries such as the half-plane [14, 17, 22, 26] or the circular (and cylindrical) cases [21, 19, 28]. In these situations, the construction can be handled (as in the one-dimensional case) by the classical Fourier or Laplace analysis. Unfortunately, these conditions appear as being non-local both in space and time and hence lead to a prohibitive computational cost even if it can be reduced with the help of a fast evaluation algorithm (see e.g. [26]). A prospected direction has been the design of some fully localized approximate boundary conditions (also called artificial boundary conditions) involving only some differential operators [1, 14, 17, 22]. Even if these conditions are efficient, they may generate some unphysical reflections at the boundary which can be due for instance to the presence of singularities in the geometry of the domain (generally a rectangular domain). Moreover, there is only a few results concerning the well-posedness of the resulting truncated initial boundary value problems. We propose here an alternative construction of a hierarchy of artificial boundary conditions for an arbitrarily-shaped boundary. These conditions are non-local in time but present the interesting feature of being local in space. This issue is essential from a practical point of view since the approximation of the problem by a finite-difference or finite-element method leads to the resolution of a linear system defined by a sparse matrix.

In order to give an idea of the construction of these artificial boundary conditions, we propose in Section 2 an explicit treatment for the disk. The artificial boundary conditions can then be constructed as a high-frequency microlocal approximation of the exact condition by some elementary calculations. We generalize these results to a general domain. The question of the uniqueness of the solution is tackled. We prove a bound of the total energy associated to the system. In the third Section, we investigate the well-posedness of the semi-discrete problem discretized by the Crank-Nicolson scheme. The fractional time operators arising in the definition of the artificial boundary conditions are approximated by some quadrature formulas previously derived for the one-dimensional case [4]. The essential result of this section is that the energy remains bounded at the semi-discrete level and implies hence the stability of the whole scheme. In a fourth Section, we propose a full discretization of the system by a conform finite-element method. Numerical simulations are next performed to show the effectiveness of the approach.

2. The truncated boundary value problem. We present in this section the derivation of a class of absorbing boundary conditions for the two-dimensional Schrödinger equation (1.1). In the case of a general boundary, the technical design of the transparent boundary condition is based on the use of a pseudodifferential calculus [3]. To make the presentation clearer, we rather propose a simpler derivation for a fictive circular boundary. In this case, the construction only requires a Fourier analysis associated to the use of the Hankel's functions. From this point of view, this approach can be interpreted as a generalization of the method of Kopylov *et al.*'s [21] for X-ray diffraction optic simulations.

Let us assume that the computational bounded domain is the disk $\Omega = D(0,R)$ centred at the origin and of radius R. The Schrödinger equation sets in the whole-space can be expressed in polar coordinates (r,θ) as

$$i\partial_t u + \partial_r^2 u + \frac{1}{r}\partial_r u + \frac{1}{r^2}\partial_\theta^2 u = 0,\ (r,\theta,t) \in \mathbb{R}^+ \times [0,2\pi] \times \mathbb{R}^{*+}.$$

In order to use the time Fourier transform, we introduce $\tilde{u}$ as the function equals to u for $t \geq 0$ and extended to $\mathbb{R}$ by 0 for $t < 0$. Let us designate by $\widehat{\tilde{u}}$ the time Fourier transform of $\tilde{u}$ and by τ the associated time covariable. Then, $\widehat{\tilde{u}}$ satisfies the following equation

$$-\tau\widehat{\tilde{u}} + \partial_r^2\widehat{\tilde{u}} + \frac{1}{r}\partial_r\widehat{\tilde{u}} + \frac{1}{r^2}\partial_\theta^2\widehat{\tilde{u}} = \widehat{iu_0\delta_0},\ (r,\theta,\tau) \in \mathbb{R}^+ \times [0,2\pi] \times \mathbb{R}. \tag{2.1}$$

If we assume that the initial datum u_0 is compactly supported in Ω, then there exists $R_0 > 0$ such that

$$\begin{cases} R_0 > R > 0, \\ \mathrm{Supp}(u_0) \cap \{(r,\theta) \in \mathbb{R}^+ \times [0,2\pi],\ r > R_0\} = \emptyset. \end{cases}$$

Restricted to the set $\mathcal{A} = \{(r,\theta) \in \mathbb{R}^+ \times [0,2\pi],\ r > R_0\}$, Eq. (2.1) yields

$$-\tau\widehat{\tilde{u}} + \partial_r^2\widehat{\tilde{u}} + \frac{1}{r}\partial_r\widehat{\tilde{u}} + \frac{1}{r^2}\partial_\theta^2\widehat{\tilde{u}} = 0,\ (r,\theta,\tau) \in \mathcal{A} \times \mathbb{R}. \tag{2.2}$$