Institut national de la recherche scientifique

PLAN DE COURS

Nom du cours :

Applied mathematics and numerical modeling for environmental science

Sigle du cours :

ETE406

Offert au trimestre :

(Fall session)

Nombre de crédits :

3

Heure :		Date :		Local :	

PROFESSEUR RESPONSABLE ET COORDONNÉES

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AUTRES PROFESSEURS PARTICIPANTS AU COURS, LE CAS ÉCHÉANT

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DESCRIPTION DU COURS

The course will present fundamental mathematical principles from calculus, linear algebra, and functional analysis. Building on these, we will study powerful transform methods, analytical solution techniques, and numerical discretization approaches. The course places a particular emphasis on ordinary and partial differential equations, on understanding the physical processes that these equations represent, and on illustrating model applications in the water, Earth, and environmental sciences that are based on the principles, methods, and equations introduced.

Students taking this course should have some prior exposure to undergraduate mathematics (from a science or engineering programme, for instance). Interested students not wishing to take the course for credit (*auditeurs libres*) are welcome. The course is organized into 12 themed modules, as described below.

OBJECTIFS DU COURS

- Gain skills in a broad range of mathematical techniques, together with insights into the physical underpinnings of the methods presented;
- Learn the fundamental principles of modeling (conservation of mass, governing and constitutive equations, dimensional consistency, initial and boundary conditions, numerical performance measures, discretization errors, etc);

- Through examples from ecology, water resources management, hydrogeology, and other fields, see how complex models can be built up (from uni- to multi-dimensional systems, from linear to nonlinear phenomena, from single processes or components to coupled systems with interacting species, etc).

CONTENU DU COURS

Module 1. Some preliminaries
We begin with a review of some basic calculus that will provide a foundation for the rest of the course. The review will include: trigonometry; coordinate system transformations; logarithmic and exponential functions; complex numbers and complex-valued functions; the mean value theorem; Taylor series and power series expansions; the gradient and divergence operators for multidimensional spaces; the Riemann sum; and integration. We will present both analytical and numerical methods of integration (the analytical/numerical dichotomy will be a constant theme in the course). The connections between the trapezoidal rule, Simpson’s rule, and higher order or more robust quadrature rules for numerical integration will be discussed. We will also introduce the important divergence theorem and Green's lemma, and show their connection, in the case of one-dimensional spaces, to integration by parts.

Module 2. Logistic and other models of population and ecosystem dynamics
Many dynamical systems exhibit exponential growth or decay behavior. We will examine some simple yet powerful models of such systems, ranging from first order kinetics (e.g., radioactive decay) to the Lotka-Volterra predator–prey model. Particular attention will be devoted to the logistic model of population growth, and to its many variants in the fields of finance, epidemiology, thermal engineering, etc.

Module 3. Conservation of mass principle and the continuity equation of fluid dynamics
In the previous module we presented various model equations, and then we proceeded to analyze the models from different perspectives. In this module we will, in a sense, do the reverse. We will first stipulate in detail the problem to be solved, and then we will carefully build, or derive, the equations that allow us to address the problem at hand. In a first illustration of this model-building process, we will see how a logistic-type model, such as those from the previous module, also emerges when we use the principle of conservation of mass to derive a model for lake pollution (the so-called mixing model). Next, applying this principle more rigorously to an infinitesimally small volume of fluid will lead us to the continuity equation of fluid dynamics and a first look at a partial differential equation. On the basis of this equation and some necessary constitutive relations, two important examples of a mass conservation equation in the field of hydrogeology will be derived, and connections will be drawn to the water balance concept that is the basis for most hydrological models.

Module 4. Differential equations and differential geometry
In the previous two modules we have seen how ordinary and partial differential equations (“odes” and “pdes”) arise naturally when formulating a physical problem (for population growth, for example) in mathematical terms. Before more formally considering odes and pdes in the next two modules, respectively, we present here some of the important elements and frameworks needed to interpret and solve these equations: classifications of differential equations; boundary and initial conditions; the method of images for Dirichlet and Neumann conditions; parametric equations; and normal vectors and tangent planes. We will also present a general solution to a certain class of linear (first order) and nonlinear (Bernoulli) odes, and we will examine an application of a coordinate transformation to solve a classic (inverse) problem in hydrogeology.

Module 5. Ordinary differential equations ("odes")
Our focus in this module on ordinary differential equations is on a variety of techniques for solving, analytically, some general classes of these equations as well as some special cases (e.g., Euler equations). In doing so, we will introduce concepts, terminology, definitions, and results that extend or apply also to partial differential equations: homogeneous differential equations; quadratic equations; linearity and nonlinearity; linear independence of two functions and the Wronskian; the method of reduction of order; the principle of superposition; and partial fraction expansions.

Module 6. Partial differential equations ("pdes")
We will develop a classification scheme for second order linear partial differential equations that has important implications for the practical application of these pdes and for the numerical algorithms used to solve them. The Cauchy data problem that we will analyze to derive the canonical forms of the classification scheme provides insights into the behavior of boundary conditions and characteristic curves on the surface representing a pde's solution, as well as on the use of coordinate system transformations and their associated Jacobians. The three canonical forms (and their corresponding archetype equations) will be summarized: hyperbolic (wave equation); parabolic (diffusion equation); and elliptic (Poisson and Laplace equations). An example of the procedure for transforming a pde to its canonical form will be presented for the Tricomi equation. In a second example, we will illustrate an analytical solution technique (the method of separation of variables) that can be used when a pde's solution is of a particular form.

Module 7. Green's functions
In Module 5 on odes we presented some powerful theoretical results that guarantee existence and uniqueness of solutions to linear second order initial value problems (IVPs – see Module 4), including the concept of a fundamental set of solutions for the homogeneous ode case, and a procedure for finding such solutions. Green's functions, the topic of this module, are in some respects a counterpart to these results for linear boundary value problems (BVPs), be they odes or pdes. We will develop, via an example, the procedure for finding the Green's function for a linear BVP, and we will demonstrate some of the important properties of Green's functions. We will moreover discuss how Green's function characterizes the impulse response of a system (in doing this, we will also introduce the Dirac delta function and the convolution operation). This characterization provides a very useful means of analyzing the impacts of a forcing term in a physical system that is represented by a linear differential equation (the classic example of a vibrating string will be used to illustrate this).

Module 8. Laplace transform method (LTM)
Having focused on BVPs in the last module, we now return to IVPs, and we develop an integral transform method that has some similarities to the Green's function method. LTM transforms a linear differential equation to an algebraic equation, which considerably reduces the complexity of solving the original equation. The Laplace transforms and inverse transforms of several elementary functions will be derived, as well as important results concerning the Laplace transforms of derivatives and the derivatives of Laplace transforms. In the context of LTM, we will also discuss piecewise continuous functions, the convergence of improper integrals, and shifting theorems. The so-called second shifting theorem relies on the unit (or Heaviside) step function, which in turn is related to the Dirac delta function introduced in the previous module. The unit step function has many applications for dynamic systems that are characterized by discrete, intermittent, periodic, or piecewise continuous driving forces.

Module 9. Linear algebra and functional analysis
We will present a concise review of linear algebra and some fundamental concepts and results from functional analysis. We will use simple, small (2 x 2 or 3 x 3) systems for illustration. The techniques we will introduce, or variants of them, can then be applied to solve systems of equations containing hundreds, thousands, millions, ... of variables. Some of the ideas and formalisms introduced in this

module will be important in the presentation of numerical methods in the next three modules. The topics to be covered include: determinants and Cramer’s rule; conditions for existence of a unique solution (nonsingular matrices); sparse, symmetric, and positive definite matrices; quadratic forms and the minimization problem; basis vectors, orthogonal vectors, projection operators, and norm metrics; eigenvalues and eigenvectors; and the link between spectral radius (of a matrix) and convergence (of an iterative scheme).

Module 10. Iterative methods for linear and nonlinear equations
A simple iterative method (Jacobi) arises directly out of our exploration of linear algebraic systems of equations in the previous module. It is a fixed point method, and we will use it to introduce concepts such as convergence and error analysis that are very important in numerical algorithms. We will return to these ideas in the second part, on nonlinear equations. Following our short examination of the Jacobi method, we will present in detail the prototype method for iteratively solving linear systems, namely the conjugate gradient method. In the second part of this module, we will shift our attention to nonlinear equations, where again we will begin with a rudimentary scheme that nonetheless provides some very useful insights. We will then present the prototype iteration technique for nonlinear equations, namely Newton’s method. The concept of ill-conditioned equations and system matrices will also be discussed.

Module 11. Finite element method
The many elegant methods for analytically solving odes and pdes that we have examined in previous modules are unfortunately not always applicable, owing to nonlinearities or variable coefficients in the equation, an irregularly shaped problem domain, complex boundary conditions, and various other factors. Numerical solution techniques are thus often required. We will begin with a very brief presentation of the finite difference method that will also reveal how different discretization choices give rise to different orders of accuracy. This will be followed by a much more detailed presentation of the finite element method (FEM) that will include definitions of trial and basis functions, the Galerkin method, and a variety of numerical performance criteria. An application of FEM to the Richards equation for variably saturated groundwater flow will be provided for reference. To conclude this module, we will again borrow ideas and concepts from linear algebra and functional analysis to show how a given BVP can be formulated in three very different and yet equivalent ways – namely the differential, variational, and minimization formulations – and how the so-called weak formulation can be advantageous.

Module 12. Numerical analysis and coupled systems
In the first part of this module, we will perform a numerical analysis of different discretization techniques applied to the classic advection–diffusion equation. The analysis will introduce difference equations and the grid Péclet number, and it will illustrate important concepts of numerical diffusion, oscillations, and stability. Upwind schemes will then be discussed, and the Courant number will be introduced. We end the module (and the course) with a very quick look at the complexities of modeling in a real-world context. We will use two examples (specifically, an integrated groundwater–surface water model of catchment hydrology and a variable density flow and transport model of seawater intrusion) to illustrate different conceptualizations and representations of coupled systems (interactions between processes, between components, and across interfaces).

MATÉRIEL DIDACTIQUE ET APPROCHES PÉDAGOGIQUES

The course is structured as 13 weekly 3-hour sessions and a 14th session for the final exam. The lecture notes for each module will be made available beforehand.

ÉVALUATION

- Assignments (60%) - Final exam (40%)

Pour plus de détails:
Politique d'intégrité en recherche:
(http://www.inrs.ca/sites/default/files/inrs/politiques_procedures_reglements/Politique_IntegriteRecherche%20_VersionFinale.pdf)
Intégrité en recherche : Guide pour les étudiants:
(http://www.inrs.ca/sites/default/files/etudier_inrs/etudiants_actuels/INRS_Guide_de_letudiant_Integrite_Recherche.pdf)

CONSIGNES RELATIVES AUX RETARDS DES TRAVAUX ET ABSENCE À UN EXAMEN

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INFORMATIONS COMPLÉMENTAIRES

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