IMACS/ISGG WORKSHOP

MASCOT 2018

15[th] MEETING ON APPLIED SCIENTIFIC COMPUTING AND TOOLS

GRID GENERATION,

APPROXIMATION

AND VISUALIZATION

Book of Abstracts

MASCOT 2018 Book of Abstracts IMACS

Edited by

Sandra Carillo
Costanza Conti
Daniela Mansutti
Francesca Pitolli
Rosa Maria Spitaleri

IMACS
International Association for Mathematics and Computers in Simulation

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OCTOBER 2-5, 2018

University *La Sapienza*
Civil and Industrial Engineering Faculty
Via Eudossiana 18, Roma

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ABOUT MASCOT2018

MASCOT 2018 is the 15th edition of the IMACS/ISGG workshop focused on methods and tools for the complete cycle of numerical modelling and simulation, from the development of theoretically well based models and methods to the deep investigation of crucial applications, from geometry and model construction to its implementation, from data analysis and powerful design of computational tools, with advanced capabilities. Aim of the workshop is the presentation and discussion of innovative technologies dealing with all aspects of computational processes. We recall, but without limiting to them, methodologies for effective grid generation, advanced approximation methods, identification and application of efficient PDE numerical solution algorithms, the development of powerful tools for image processing and scientific visualization.

The workshop would bring together developers and users of computational methods and software tools to go deeper into advantages of new methodologies, discuss applications and results, illustrate educational approaches, identify new needs and innovative development directions in a growing variety of problems in applied mathematics.

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MASCOT2018 *Foreword*

IMACS is pleased to publish this Book of Abstracts of MASCOT2018, the volume 21 of the Series in Computational an Applied Mathematics, edited by Sandra Carillo, Costanza Conti, Daniela Mansutti, Francesca Pitolli and Rosa Maria Spitaleri. The eighteenth edition in the series of the IMACS/ISGG International Workshops, MASCOT2018, is organized by the Istituto per le Applicazioni del Calcolo (IAC) of the Consiglio Nazionale delle Ricerche (CNR), along with and hosted by La Sapienza, the Rome1 University, Italy, at the Civil and Industrial Engineering Faculty. This series of meetings has been held to have an updated picture, about year by year, of the broad subject of scientific computing and its applications and refereed reports on relevant achieved results.

In all respects, the meeting aims at giving the opportunity to a large number of researchers and scientists to meet again in Rome, and discuss scientific computing results and future trends. Attendees, mostly authors and speakers, have been getting to know well each other, creating a larger and larger MASCOT Community combining expertise for powerful simulations in classical and new application fields.

The ongoing globalization of the world, in particular in the past decades, has brought about a whole range of new problems, not only those traditionally linked to the hard sciences and industry, but also those attached to the social sciences, to climate change impacts, urban pollution, crowd dynamics, transportation and so on. In line with the general philosophy of IMACS, this MASCOT Series opens mind on several aspects of multidisciplinary problems coming from the real world as well as on the development of new theoretical and computational tools.

The scientific program, as in the past, welcomes its international participants coming not only from Italy, the hosting country, but also from Universities and Research Centers in Australia, Austria, Belgium, Czech Republic, Iran, Spain, France, Germany, Canada, South Corea, USA, Mexico, and others countries.

IMACS is pleased to sponsor this series of high quality meetings, in collaboration with the International Society of Grid Generation, duly represented by Prof. Bharat Soni. We thank gratefully Dr. Rosa Maria Spitaleri for her generous efforts, and being the main contributor to the success of this series.

Robert Vichnevetsky
IMACS Honorary President

INVITED LECTURES

How to Get Molecular Dynamics and Continuum Mechanics to Steer Each Other by Molecularly-based Stress

Giovanni Ciccotti

Continuum Mechanics and Molecular Dynamics have complementary strengths and weaknesses. Both of them are deterministic, predictive theories, quite successful in their respective field of application. Molecular Dynamics enjoys a fundamental atomistic foundation, firmly grounded on Quantum Mechanics via the Born-Oppenheimer approximation. As a counterpoint, it is either impossible or desperately inefficient to apply to large, macroscopic objects for a macroscopic stretch of time. Continuum Mechanics, on the contrary, is basically scale-independent. However, its predictive value is severely curbed by its essential need for ad hoc constitutive prescriptions for the stress, largely based on phenomenological grounds.

This state of affairs prompts a new approach to combine Continuum Mechanics and Molecular Dynamics, in such a way to take advantage of their strengths, while minimising their limitations. Since all macroscopic fields — stress included — are assumed to vary slowly both in space and time (with respect to molecular space and time scales), a mesoscopically coarse — hence, microscopically very coarse — space-time sampling of the underlying molecular evolution may suffice to obtain a satisfactory reconstruction of the stress field, based on an array of local Molecular Dynamics simulations. The function of the continuum-mechanical field theory — freed of any phenomenological constitutive prescription — is to specify the macroscopic conditions of these scattered molecular samples. In return, the local Molecular Dynamics simulations provide the continuum theory with molecularly-based stress values.

As an illustrative application, we consider a loading test on a rod. At the continuum level, we have a model of the rod, completed by a macroscopic stress-strain law whose solution determines the deformation field. As a microscopic replacement to this phenomenological constitutive prescription, we get the stress, wherever needed, by computing it on-the-fly from suitable microscopic Molecular Dynamics cells. In turn, the Molecular Dynamics simulations are driven by the macroscopic deformation field, determined by the Continuum Mechanics calculation.

In cooperation with Antonio Di Carlo, Mauro Ferrario, Sara Bonella

Beyond Classical Exponential Analysis: Generalizations, Connections and Applications

Annie Cuyt

In classical exponential analysis the objective is to recover the values of the linear coefficients and the mutually distinct nonlinear parameters in the argument of each exponential term through sparse interpolation. When the exponential model contains n terms, then the above inverse problem can be solved from $2n$ samples. If the sparsity n is not known, then theoretically at least one more sample is required. Of course in a noisy setting, both for the recovery of the unknowns and to determine the correct n, a larger number $N > 2n + 1$ of samples is used.

The problem dates back to the real-valued exponential fitting problem of de Prony from the 18-th century. In the past decades several popular numerical methods for its solution were formulated, mostly based on some generalized eigenvalue reformulation. When dealing with complex-valued input data, all algorithms collect their samples following the Shannon-Nyquist rate which guarantees that the solution for the nonlinear parameters is unique and does not suffer from periodicity issues.

We present a technique that allows to break the traditional Shannon-Nyquist sampling condition. While solving the aliasing effect that is a result from not adhering to it, we are also able to recondition the numerical problem statement. The latter proofs to be very useful in the case of clustered frequencies.
We also reformulate the exponential analysis as a tensor decomposition and a rational approximation problem, thereby offering the possibility to use facts and techniques from other domains, such as the coupling of tensor decompositions and the Froissart doublet theory.

Last but not least, we point out that the toolbox of methods put together with these new generalizations and connections, has great potential in several engineering applications, such as DOA or direction of arrival problems, ISAR or inverse synthetic aperture radar imaging, automotive radar, peak fitting in analytical chemistry, seismic data processing, and other application problems.

In cooperation with Prof Wen-shin Lee, wen-shin.lee@stir.ac.uk

Keywords: exponential analysis, sparse interpolation, inverse problems

Foundational Methods of Model Structure Evaluation

Anthony John Jakeman

Before embarking on formal methods of uncertainty analysis that may entail unnecessarily restrictive assumptions and sophisticated treatment, prudence dictates exploring one's data, model candidates and applicable objective functions with a mixture of methods as a first step. It seems that there are several foundational methods that warrant more attention in practice and that there is scope for the development of new ones. Ensuing results from a selection of foundational methods may well inform the choice of formal methods and assumptions, or suffice in themselves as an effective appreciation of uncertainty.

Through the case of four lumped rainfall-runoff models of varying complexity from several watersheds we illustrate that there are valuable methods, many of them already in open source software, others we have recently developed, which can be invoked to yield valuable insights into model veracity and uncertainty.

We show results of using methods of global sensitivity analysis that help: determine whether insensitive parameters impact on predictions and therefore cannot be fixed; and identify which combinations of objective function, dataset and model structure allow insensitive parameters to be estimated. We apply response surface and polynomial chaos methods to yield knowledge of the models' response surfaces and parameter interactions, thereby informing model redesign. A new approach to model structure discrimination is presented based on Pareto methods and cross-validation. It reveals which model structures are acceptable in the sense that they are non-dominated by other structures across calibration and validation periods and across catchments according to specified performance criteria

Keywords: Identification; sensitivity analysis; response surface; Pareto

Rate Equations and Memory Properties in Models of Heat Conductors

Angelo Morro

The paper addresses the formulation of rate equations, via objective time derivatives, within continuum physics. First objective time derivatives are defined to leave the tensor character of the appropriate field invariant within the set of Euclidean frames. The general structure of objective time derivatives is then established and the known derivatives of the physical literature are shown to be particular cases.

Next, for definiteness, objective time derivatives are considered for the heat flux and the analysis of thermodynamic restrictions is performed. It follows that thermodynamic consistency requires the occurrence of stress terms induced by the heat flux thus providing a way to investigate experimentally which time derivative the material is undergoing. Finally it is pointed out that, for some derivatives, a corresponding memory functional for the heat flux arises which is independent of the reference configuration.

Revolutionary 21st Century Technology Advances – Transforming Education & Research

Bharat K. Soni

In the 20th Century, the World has observed greatest achievements from electricity and electronics, automobile and airplane, a paradigm shift in communication and high performance computing among others. Innovation associated with these accomplishments has brought major technological advances and improvements via evolutionary incremental changes. Now, in the early decades of the 21st century, the technology advances appear to be on the cusp of revolutionary change—with potential to dramatically reshaping our World and associated industry. For example, in automotive sector, this revolution will be engendered by the advent of autonomous or "self-driving" vehicles. In this respect, rapid transformational improvements in high performance computing and communication (HPCC), robust and efficient numerical and graphics algorithms, visualization and virtual environments, big data and associated analytics, artificial intelligence and expert systems and sensors, robotics and 3D printing with novel materials have great potential to make disruptive advances in applications of scientific computing.

In response to these rapidly changing disruptive advances, several academic and research institutions have undertaken strategic initiatives to reform education and research programs with innovation and entrepreneurship drive.

The progress realized in this endeavor of education and research transformations will be presented. In particular, emphasis will be placed on i^3(Imagine, Inspire and Innovate), IMakerSpace and Innovation and Entrepreneurship program accomplishments in multidisciplinary applications involving interdisciplinary groups of faculty and students. Specific case studies and applications will be described with future directions.

Computational Modelling of Soft Flowing Crystals

Sauro Succi

We present the main ideas behind the computational modelling of soft-flowing crystals, with special attention to the micro-fluidic design of novel families of mesoscale porous materials for medical engineering applications.

IST Numerical Schemes for Solving NonLinear Evolution Equations (and their possible applications for solving time Fractional Differential Equations)

Thiab R Taha

In this talk a survey and a method of derivation of certain class of numerical schemes and an implementation of these schemes will be presented. These schemes are constructed by methods related to the Inverse Scattering Transform (IST) and can be used as numerical schemes for

their associated nonlinear evolution equations. They maintain many of the important properties of their original partial differential equations such as infinite numbers of conservation laws and solvability by IST. Numerical experiments have shown that these schemes compare very favorably with other known numerical methods. In this talk, we will explore the possibility of using these schemes for solving time Fractional Differential Equations.

GENERAL PAPERS

Numerical Investigation on the Acoustic Band Structure of Tensegrity Chains

Ada Amendola, Anastasiia Krushynska, Chiara Daraio, Nicola M. Pugno, Fernando Fraternali

The research field of linear and weakly nonlinear wave dynamics of acoustic metamaterials is devoting considerable attention to so-called "*phononic band gap*" theory (refer, e.g., to [1-4] and references therein). It is well known that composite materials with periodic variations of the density and/or wave velocity can display band gaps where the propagation of mechanical waves is forbidden [1].
The present work aims to reveal band gaps in tensegrity-based metamaterials and to exploit the possibility of their tuning for the design and test of novel bandgap devices. Attention is focused on the optimal design of 1-D chains of tensegrity units and lumped masses, which are tunable by varying the unit's parameters and initial static precompression of the constituent units (internal self-stress) and the whole structure (external prestress) [5-6].
The bandgap response of such metamaterials is investigated through analytic and numerical studies. By suitably designing the topological arrangements of soft and hard tensegrity units, the given results highlight that the analysed systems can be effectively employed as novel wave steering devices, sound proof layers and/or vibration isolation devices [7-8].

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Keywords: Tensegrity, prestress, frequency bandgaps

Splines of clothoids and related computational algorithms

Enrico Bertolazzi

Aim of this work is to present a technique to build a spline of clothoid curves that interpolates a sequence of points with associated angles and curvatures. This is a Hermite interpolation up to the second derivative (G2 data) and exhibits curvature continuity, a desirable property in many industrial applications. The use of clothoid curves instead of polynomials is motivated by the fact that they easily model the trajectory of wheeled non-holonomic robots (for instance, the car-like vehicles). They have a piecewise linear curvature, which is useful for limiting the lateral accelerations and hence improving the quality of the trajectory. Finally, clothoids are naturally parametrised by arc length. The price to pay for such good properties is a (relatively) higher computational burden compared to the polynomial approach. Another limitation is that clothoids are planar curves and it is not possible to directly extend them to higher dimension, e.g.in 3D.

Clothoids have been studied intensively for a couple of decades, and numerical algorithms that allow an easy handling of many base subproblems have been proposed only recently, e.g.: efficient clothoid evaluation, interpolation problems (G1 and G2), spline construction, efficient point-curve distance.

In this paper we present some clothoid-related algorithms that address some practical problems that appear in the application of clothoids to industrial problems, e.g. in robotics and machining.

More in detail we discuss how to find the intersection of two clothoids, a problem that arises for instance if two robots have colliding trajectories. A closely related issue is the study of curves that are parallel to a reference clothoid (offset curves), and their intersections with a given clothoid (-spline). A typical example can be found when a vehicle tracks a path and has to stay on a road or lane, or when a milling machine has to stay inside the tolerance band aroundthe nominal trajectory.

We will show how to organise the clothoid spline into an efficient structure (AABB trees) with bounding boxes that allow us to easily find intersections between two splines of clothoids.

Iterative Methods for Linear and Nonlinear Poromechanics

Radim Blaheta

The flow in porous material (matrix) including a possible deformation of the solid matrix appears in many applications in geomechanics and biomechanics. The contribution firstly concerns iterative solvers for the solution of problems of poroelasticity (linear poromechanics) formulated by using three basic variables – displacements, (Darcy) velocities and pore pressures. The contribution assumes a discretization with either conforming or nonconforming P1 elements for displacements, lowest order Raviart-Thomas elements for velocities and piecewise constant P0 elements for pressures combined with a fully implicit discretization in time. (Nonconforming P1 elements for elasticity are used in the case if the conforming discretization suffers by a locking effect.) The MINRES method with block diagonal SPD preconditioners is suggested for solving the systems arising in each time step. A way how to analyse the efficiency and robustness of such preconditioners is shown as well as some illustration by numerical experiments is provided. The contribution also describes efficient inner solvers for individual blocks within the preconditioner. Finally, it is discussed how to extend the obtained results to nonlinear poromechanics e.g. when the flow concerns variably saturated porous material.

Keywords: poromechanics; iterative solvers; preconditioners

Sportello Matematico: Mathematical Technologies for Innovation

Maurizio Ceseri, Anna Melchiori, Antonino Sgalambro, Silvia Vermicelli

Mathematical Technologies are the fundamental tool to strengthen the innovation capacity of Enterprises. In order to fully exploit their innovative potential, it is mandatory a proactive activity to promote Mathematical Research towards Italian Enterprises.

This is the aim of Sportello Matematico per l'Industria Italiana, a project devoted to strengthen Industry/Research cooperation in the field of Mathematical Technologies.

Solution of Richards' Equation Using Generalized Differences and Adaptive Time Integration

Francisco J. Domínguez-Mota, Carlos Chávez-Negrete, Daniel Santana-Quinteros, Cuauhtémoc Rivera-Loaiza, Gerardo Tinoco-Guerrero

In this talk, we address some details of an adaptive time integration method, which was designed to calculate the numerical solution of nonlinear Richards' equation using generalized finite differences solution in general grids. Some examples show some effective ways to avoid numerical oscillations near the infiltration front that appear in some applications using other spatial discretizations.

Keywords: Richards' equation; generalized finite differences; adaptime time integration

A Mathematical Model to Infer Underground Thermal Parameters for Designing of Borehole Heat Exchangers

Nadaniela Egidi, Josephin Giacomini, Maria Chiara Invernizzi, Pierluigi Maponi, Massimo Verdoya

Low-temperature geothermal applications, based on borehole heat exchangers coupled with ground-source heat pumps, are one of the most promising applications in the frame of renewable and sustainable energies. Such applications are almost independent of seasonal variations, can be used in nearly all geological environments and the system setting up is relatively simple. However, design and installation must consider numerous influencing factors, with particular reference to the underground thermal regime and the borehole properties. In this paper, we focus on the inference of underground thermal properties, i.e. the thermal conductivity and diffusivity, and the thermal resistance of the borehole. Such parameters can be considered constant only in a rough approximation and, in addition, their estimation often requires expensive and time-demanding in-situ analyses.

The technique we propose is based on a best-fit problem. In more detail, we describe the heat transfer inside the exchanger by means of the classical cylindrical source model, then a best-fit problem between the measured and computed temperatures is solved and the thermal parameters are obtained. The cylindrical source model is quite accurate in absence of significant groundwater flow, and at present works under simplifying assumptions on the spatial domain, i.e. the depth coordinate is neglected. We want to test the approach on a set of temperature time series, which have been collected during the thermal recovery after a thermal stimulation made on a pilot geothermal plant that is implemented at the University of Camerino (Italy). The computed values of thermal conductivity and diffusivity will be compared with the values obtained from direct analyses on ground samples. A future improvement of this study could be the refinement of the model describing the exchanger. This means the implementation of a model that gives the temperature of the fluid inside the device when the depth increases, avoiding the hypothesis of constant fluid and soil temperatures. A further improvement could be to investigate how relevant is the interaction between the surrounding soil and the exchanger, by implementing a coupled model where the soil and fluid temperatures mutually influence.

Keywords: thermal conductivity and diffusivity; borehole resistance; geothermal mathematical model

Strong stability preserving general linear methods for differential systems

Zdzislaw Jackiewicz

We investigate strong stability preserving (SSP) general linear methods (GLMs) for systems of ordinary differential equations (ODEs). Such methods are obtained by the solution of the minimization problems with nonlinear inequality constrains, corresponding to the SSP property of these methods, and equality constrains, corresponding to order and stage order conditions. These minimization problems were solved by the sequential quadratic programming algorithm implemented in MATLAB subroutine \texttt{fmincon.m}, starting with many random guesses. Examples of transformed SSP GLMs of order p=1, 2, 3, and 4, and stage order $q=p$ have been determined, and suitable starting and finishing procedures have been constructed. The numerical experiments performed on a set of test problems have shown that transformed SSP GLMs discussed in this talk are more accurate than transformed SSP DIMSIMs and SSP Runge-Kutta methods of the same order.

(This is a joint work with Giovanna Califano from University of Salerno, and Giuseppe Izzo from University of Naples).

Keywords: General linear methods, strong stability preserving

Iterative Solution of Horizontal Linear Complementarity Problems in Hydrodynamic Lubrication

Francesco Mezzadri, Emanuele Galligani

Horizontal linear complementarity problems, often abbreviated as HLCPs, are a popular generalization of the well-known linear complementarity problems (LCPs). These problems have several applications in many different fields, including in structural mechanics, in engineering and in transportation science.

In the literature, it is possible to find a variety of methods to solve HLCPs, including interior point methods and reduction to LCP. These procedures, however, can be quite complex and computationally onerous.

Here, on the other hand, we aim at solving HLCPs by simpler and efficient iterative techniques. In particular, we focus on methods based on generalizations of projected and of modulus-based methods which are currently used to solve LCPs.

We do so by considering a famous problem that can be modeled as a horizontal linear complementarity problem: the analysis of cavitation in lubricated contacts. This phenomenon consists in the formation of gaseous bubbles in fluid films and is particularly important in lubrication processes in mechanical engineering.

In this context, we present and analyze projected and modulus-based methods to solve HLCPs. We then demonstrate their capabilities by several numerical experiments. Finally, we compare the proposed methods to existing interior point methods for solving HLCPs in hydrodynamic lubrication.

Another division of a cube into six tetrahedral with three similarity classes

Miguel Angel Padron

In this work a new triangulation of a cube is obtained by subdividing the cube into six tetrahedra. For this division, two regular right-type tetrahedra similar to each other, two regular trirectangular tetrahedra similar to each other, and finally two quasi-right-type tetrahedral similar to each other, are generated.

We focus in this paper on the 8-tetrahedra longest-edge partition (8T-LE) of these tetrahedra. The study of the partition of these tetrahedral is of interest because the conversion from a octree-based hexaedral mesh to a tetrahedral mesh is straightforward.

For any kind of initial tetrahedra *t* cited before, we prove that the iterative 8T-LE partition of *t* yields into a sequence of tetrahedra where the number of dissimilar classes are bounded, and hence the non-degeneracy of the meshes is simply proved. For right-type tetrahedra, the number of dissimilar classes has already been studied.

These meshes are also of acute type and then satisfy trivially the maximum angle condition. All these properties are highly favourable in finite element analysis.

Keywords: Similarity classes; Non-degeneracy; 8-tetrahedra longest-edge partition; Trirectangular tetrahedron; Right-typetetrahedron;Quasi-right-typetetrahedron

A Quantile-based Approach for the Robust Optimization of a Supersonic ORC Turbine Cascade

Nassim Razaaly, Giacomo Persico, Giulio Gori, Pietro Marco Congedo

Organic Rankine Cycle (ORC) power systems have become very attractive for the exploitation of low-temperature heat sources, such as waste heat recovery, biomass, geothermal, and solar energy, generally featuring variable heat load. ORC turbines usually operate in thermodynamic regions characterized by high-pressure ratios and strong non-ideal gas effects in the flow expansion, complicating significantly their aerodynamic design. Systematic optimization methods accounting for multiple uncertainties due to variable operating conditions,referred to as Robust Optimization may benefit to ORC turbines aerodynamic design.This study presents an original robust shape optimization approach to overcome the limitation of a deterministic optimization that neglects operating conditions variability, applied on a typical 2D ORC turbine cascade. Flow around the blade is solved by means of inviscid simulation using the open-source SU2 code, from which a Quantity of Interest (QoI) is recovered. Non-ideal gas effects are modeled through the use of the Peng-Robinson-Stryjek-Vera equation of state. Starting from a baseline blade parametrized using B-splines, wesearch for a shape optimizing the QoI, which is a random function.A classic Robust Optimization strategy consists of minimizing a cost function reflecting some statistical property of the random QoI. Classical cost functions are the mean or a linear combination of mean and standard deviation. This latter has the advantage, w.r.t. the mean, to take into account the variability of the QoI, but it suffers from the strong dependence on the selected linear weights.The popular multi-objective Taguchi's formulation attempts to tackle this issue. Unfortunately, its drawback consists of a higher cost, by several orders, of the number of CFD evaluations. The mentioned formulations suffer from a lack of interpretation in the control of variability. We propose here a mono-objective formulation consisting in minimizing the α-quantile of the QoI, at a low computational cost. For example, selecting α to 95%, this formulation can be interpreted as minimizing the threshold below which 95% of the QoI realizations lie. The goal of the paper is to propose an efficient and physically sound robust optimization approach, based on a state-of-the-art quantile estimation and on an advanced Bayesian optimization method. The robustly optimized ORC turbine shape is finally compared to the baseline configuration and to the deterministic optimal shape. The impact of the quantile level is also explored, minimizing the α-quantile of the QoI for values of α equal to 90%, 95%, and 99%, respectively.

Keywords: Robust Optimization ; Turbine Cascade ; Quantile

Uncertainty Quantification Framework for Complex Systems of Solvers

Francois Jacques Sanson, Olivier Le Maitre, Pietro Marco Congedo

As computational power become more and more affordable, industrial solvers seek to simulate ever increasingly complex problems. In some cases, their resolutions are obtained through the coupling of the several individual coupled solvers where each solver solves a specific aspect of the physics.In this context, propagating uncertainties is challenging for mainly two reasons : the composition of several solvers often leads to a very non linear answer for which learning a surrogate model will be a complex task. The second reason stems from the large dimensionality of the system of coupled solvers. Since each solver has its own set of uncertain inputs, the overall number of uncertainties we wish to propagate may be extremely large and classical approaches based on Polynomial Chaos or Kriging may be impractical. Instead, in this work we propose an original and efficient method for building surrogate models and propagating uncertainties in large industrial systems of solvers. The approach relies on the composition of Gaussian Processes (GP) into a System of Gaussian Processes (SoGP) that can accurately reproduce the structure of the system and better capture its non linearities while mitigating the curse of dimensionality. The method also features active learning methods that are able to identify unreliable component of the SoGP and propose suitable additional training points to improve the accuracy of the overall SoGP. This framework is validated on multiple analytical test cases where it outperforms state of the art methods. Furthermore, the framework is applied to an industrial problem of quantifying the uncertainties during a reentry of a space debris.

Keywords: Surrogate models ; uncertainty quantification

An Adaptive Curvature and Gradient Based Grid Generation Method

Bonita Valerie Saunders

In 2010, the National Institute of Standards and Technology (NIST) launched the Digital Library of Mathematical Functions (DLMF) (https://dlmf.nist.gov), an online resource containing definitions, recurrence relations, differential equations and other crucial information about functions useful to researchers working in various application areas in the mathematical and physical sciences. The NIST DLMF graphics team created close to 600 graphical representations of complex mathematical functions with more than 200 rendered as interactive 3D surface visualizations [1]. Our primary goal was to quickly design graphs and visualizations that accurately captured key function features such as zeros, poles and branch cuts.

While the quality of most of the visualizations is quite good, in some cases color maps and surface regions near key features could be enhanced by improving the underlying grids. We designed the original grids using simple structured techniques like transfinite blending function interpolation, or variational methods with tensor product B-splines, but the grids were generated separately from the function data. Ideally, they should be adapted to curvature or gradient information gleaned from the function data.

We have designed a composite mapping of tensor product B-splines to create an adaptive code, but the challenge of obtaining the adaption data is exacerbated by the fact that the most reliable software for computing a given function may only be available in a specific language or package. We will demonstrate the effectiveness of our adaptive method and show our progress in integrating the grid generation code with various external codes and packages.

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Keywords: structured grid generation; adaptive grid generation; tensor product B-splines, 3D web graphics

Study of the Stability of a Generalized Finite Difference Scheme Applied to the Diffusion Equation in Highly Irregular 2D Space Regions Using Convex Grids.

Jose Gerardo Tinoco-Ruiz, Francisco Javier Dominguez-Mota, Gerardo Tinoco-Guerrero, Juan Salvador Lucas-Martinez

Many phenomena are mathematically expressed by using evolution equations, the diffusion equation is one of them. It can model the behavior of the dispersion of pollutants in water bodies such as lakes, rivers and groundwater.

In this work, the analysis of an implementation of a Generalized Finite Difference Scheme applied to approximate the solution of the diffusion equation in highly irregular domains on the plane on structured convex grids is presented, discussing some general stability conditions.

Keywords: diffusion equation; generalized finite differences; stability analysis

MS1

NUMERICAL METHODS IN FUNCTIONS

AND DATA APPROXIMATION

Organizers

Costanza Conti, Lucia Romani

Reconstruction of Discontinuous Functions Using Multiquadric Local Interpolation with Adaptive Parameter Estimation

Francesc Arandiga, Rosa Donat, Lucia Romani, Milvia Rossini

Radial Basis Functions (RBF) have been used as reconstruction techniques in WENO-type finite difference schemes for hyperbolic conservation laws. It has been proposed adaptive finite difference ENO/WENO methods that slightly perturb the polynomial reconstruction coefficients using infinitely smooth radial basis functions (RBFs). It is numerically observed that, by locally optimizing the shape parameters in the RBFs, the accuracy (in smooth regions) of the numerical scheme is somewhat enhanced. On the other hand, around discontinuities in the solution, these RBF-WENO schemes revert to the classical WENO reconstruction.

In this talk we propose to incorporate the ENO/WENO techniques in the computation of the shape parameter of the RBF reconstruction. This *adaptive calculation of the shape parameter* leads to more accurate reconstructions and sharper solution profiles even near jump discontinuities. As a result, our RBF-WENO techniques can be applied as reconstruction techniques in finite difference numerical schemes for conservation laws, without having to return to classical WENO techniques near discontinuities. We shall also present numerical evidence of the improved behavior of the proposed RBF-WENO reconstruction technique.

Trivariate Blending Spline Quasi-interpolation

Domingo Barrera, Catterina Dagnino, María José Ibáñez, Sara Remogna

In this talk, we deal with the construction of trivariate spline quasi-interpolation operators (QIOs) by blending univariate and bivariate operators whose linear functionals allow oversampling. The coefficient functionals are obtained by minimizing an objective function constructed from the BB-coefficients of the Lebesgue function of the resulting operator. In this way, we can study the problem by subdividing it into one and two dimensions, instead of addressing the problem directly in the three dimensional set, for example by using trivariate box splines.

In particular, we construct new operators based on univariate B-splines and bivariate box splines, exact on appropriate spaces of polynomials and having small infinity norms. An upper bound of the infinity norm for a general blending trivariate spline QIO is derived from the Bernstein-Bézier coefficients of the fundamental functions associated with the operators involved in the construction. The minimization of the resulting upper bound is proposed and the existence of a solution is proved.
Finally, we present the quadratic and the quartic cases in details.

Path Reconstruction Using Bezier Splines and Clusterization

Enrico Bertolazzi, Marco Frego, Paolo Bevilacqua

A problem often encountered in the inexact sciences is the smoothing of data which is affected by some kind of noise. It is not desirable to directly use the collected data in computer simulations and a treatment must be performed in order to minimize the effect of the inexact sampling phase. There are essentially two approaches to filter and approximate measured data that come from an experiment, the first is straight interpolation, which is feasible if the noise is low enough to be ignored, the second is the smoothing. The difference is that an interpolating spline (or surface) passes through each of the sampled points, while the fitted spline can in general not contain either point of the original data. The advantage of the second method is that a lower degree curve can be used, whereas for interpolation, usually high degree polynomials are involved.
In literature there is a huge amount of techniques for both interpolation and fitting, with many subfields for each method: the motivation depends often on the application and the dimension of the problem. Most of the literature is devoted to the approximation of data made of points in the real plane R^2 or in the real space R^3, and only a minority of articles treat the most general case of points in R^n. This is due to the specific properties of curves in the plane, where the study of the curvature is easier than in the three dimensional space where also the torsion in involved. The general case requires the abstract concept of multi dimensional curvature which does not permit to exploit many simplifications that are possible in the low dimensional cases. Nevertheless there are methods that can be naturally extended from the two dimensional case to higher dimension, whereas there are methods that is not possible to extend from the plane to the three dimensional space (at least without to pay the price of introducing new concepts or new definitions). A typical example of curve that can be used in all dimensions without any essential change in the method is the \bez{} curve, at the contrary, the extension to three dimension of a transcendental curve, like it could be the clothoid, is not possible without a heavy change of the definition and the introduction, for example, of hyperclothoids. On the other side, (cubic) polynomial splines are difficult to handle if conditions on the curvature are posed, while transcendental curves usually permit an easier treatment. The question of the curvature is so important in many applications, that a classification of the methods is performed on the basis of how the curvature and the tangents are considered. In general tangents and curvature are not considered along the whole curve, but attention is focused only at the joints of the various spline segments that forms the curve. If the curve at the joints is only continuous, it is classified as C^0, if the first derivative is continuous, is called C^1, but if the tangents at the joints are only proportional (that is, it is possible to parametrize the curve to made it C^1, it is called G^1, i.e. geometrically differentiable. The same concept of geometric continuity is extended to the case of the curvature (G^2 continuity), and in particular cases also the third derivative is considered, G^3 case. In this paper a quasi-G^2 fitting with cubic Hermite splines is proposed, in order to take advantage

of the possibility to fit multidimensional sampled points while trying to approximate the benefit of a curve with continuous curvature and low degree. The proposed algorithm follows the following steps: we cluster the pointsusing a single cubic and measuring the standard deviation of the fitted data via an almost orthogonal projection of the data on the cubic. To prevent non natural cusps and loops, we introduce a regularization parameter λ that multiplies the ingratl of the square of the second derivative of the cubic. The choice of λ is decided minimising the Generalised Cross Validation. We gather these information of the local cubics (one for each cluster of data) to build the global matrix of the optimisation problem, which takes into account the contribution of the least squares distance and the integral of the second derivative. This problem is then solved via a QR factorisation.

As an application example we propose the reconstruction of a Formula 1 circuit track, which is acquired as a list of sampled planar points. The data are first smoothed with the proposed algorithm and then the refined points and tangents are interpolated with clothoid curves, which are desirable curves in the automotive field.

Keywords: Bezier; Least Squares; Clustering

Barycentric rational Hermite interpolation with no poles and high rates of approximation

Emiliano Cirillo, Kai Hormann

In this talk we study an iterative approach to the Hermite interpolation problem, which first constructs an interpolant of the function values at $n+1$ nodes and then successively adds m correction terms to fit the data up to the m-th derivative. In the case of polynomial interpolation, this simply reproduces the classical Hermite interpolant, but the approach is general enough to be used in other settings. In particular, we focus on the family of barycentric rational Floater--Hormann interpolants, which are based on blending local polynomial interpolants of degree d with rational blending functions. For this family, the proposed method results in rational Hermite interpolants of degree $(m+1)(n+1)-1$, which converge at the rate of $O(h^{(m+1)(d+1)})$ as the mesh size h converges to zero.

Keywords: interpolation;approximation;Hermite interpolation

A Fourier Approach to Spline Hermite Interpolation

Costanza Conti, Lucia Romani, Michael Unser

The aim of this talk is to discuss the construction of minimally supported basis functions for Hermite interpolation. We consider both, the univariate (as in [1]) and the bivariate case and show how to get advantage from the deep relationship between Hermite and Bézier representation of piecewise polynomials. We will discuss how the use of Greens' function allows us to unreveil all theoretical properties of the Hermite basis functions.

In the bivariate case our model relies on three directional grids and Box-splines (see [2] but also [3]). The proposed model meets practical requirements such as invariance to affine transformations and minimal approximation properties. One of its great advantages is its non tensor-product structure which avoids the use of mixed derivatives and makes it suitable to Hermite-like representation of images in terms of samples with local tangents.

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Keywords: Hermite splines, box-splines, three directions grids, Fouier, Bezier representation.

On Polynomial Reproduction of Hermite Subdivision

Costanza Conti, Svenja Huening

Refinement rules of discrete data, so-called subdivision schemes, are iterative procedures producing smooth limit curves which approximate the given data [1]. In this talk we consider Hermite subdivision schemes where the sequence of input data consists of vectors, representing the value and the derivatives of a function [2]. We analyse the polynomial reproduction property of binary Hermite subdivision schemes of any order. In particular, we give algebraic conditions on the mask of the scheme describing polynomial reproduction [3]. We illustrate our results by several examples.

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Keywords*:* Hermite subdivision schemes, polynomial reproduction, algebraic conditions.

Fast and Accurate Interpolation of Scattered Hermite Type Data

Francesco Dell'Accio

We propose fast and accurate algorithms for the solution of the Hermite interpolation problem for scattered data. The major ingredients of the method are the Little's basis functions and the Hermite interpolant on the simplex by Sturm and an improvement which uses derivatives up to the order 2.
Although combinations of the Little's basis function with polynomial interpolants on triangles have been already considered, the possibility to reach approximation of order O(h^4) makes the method of interest for a wide class of researchers in industrial and applied mathematics.

Keywords: Hermite interpolation; scattered data; Shepard method

SPH Method: Numerical Investigations and Applications

Elisa Francomano, Marta Paliaga

In this paper we discuss on the enhancements in accuracy and computational demanding in approximating a function and its derivatives via Smoothed Particle Hydrodynamics. The standard method is widely used nowadays in various physics and engineering applications [1],[2],[3]. However it suffers of low approximation accuracy at boundaries or when scattered data distributions are considered. In this paper we discuss on some numerical behaviors of the method. Some variants of the process are analyzed and results on the accuracy and the computational demanding, dealing with different sets of data and bivariate functions, are proposed. (INDAM-GNCS Project 2018 " Metodi, algoritmi e applicazioni dell'approssimazione multivariata")

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Keywords: Meshless methods; accuracy; applications

Construction of a New Family of Non-stationary Hermite Subdivision Schemes Reproducing Exponential Polynomials

Byeongseon Jeong, Jungho Yoo

In this study, we present a new family of non-stationary Hermite subdivision schemes reproducing exponential polynomials with tension parameters. Acting on the vector data representing function values and corresponding first-order derivatives, the proposed Hermite subdivision scheme in this family reproduces a certain set of exponential polynomials. The exponential polynomial reproducing property provides flexibility in designing curves and surfaces, and is closely related to the approximation order of the associated scheme.

We analyze the convergence and smoothness of our non-stationary Hermite subdivision schemes by exploiting the factorization tools of non-stationary subdivision operators.

Some numerical results are given to illustrate the performance of the proposed schemes.

Keywords: Hermite subdivision scheme; exponential polynomial reproduction; smoothness

Reconstruction of Images with Discontinuities via Variably Scaled Discontinuous Kernels: Applications to MPI

Francesco Marchetti, Stefano De Marchi, Emma Perracchione

We consider the problem of reconstructing a 2D image, i.e. the computational issue consisting in approximating an underlying function given a set of data points and a set of data values. More precisely, we consider the interpolation problem; we look for a function such that it exactly matches the data values at the nodes. Since in applications we usually know the real data values at just few points (possibly scattered), in this work we focus on *Radial Basis Function* (RBF) interpolation. Indeed, it is meshfree and easy to implement in any dimension, differently from polynomial-based methods. Therefore, we consider the function space determined by a strictly positive definite and symmetric kernel which depends on a *shape parameter*. When dealing with images whose underlying functions have discontinuities or steep gradients, a fundamental task is to reduce the well-known Gibbs phenomenon, which affects the quality of the reconstruction causing oscillations and distortions in the whole image. A possible approach is to consider *Variably Scaled Kernels* (VSKs) [2], where the shape parameter is substituted by a *scale function*. VSKs turn out to be particularly effective when considering steep gradients, but the choice of the scale function is crucial. In our setting, in order to obtain a *mask matrix* of the image as scale function, we use an edge detector on a preliminary RBF reconstruction. We present some results involving different functions and sets of nodes. Finally, we apply this procedure in the context of Magnetic Particle Imaging (MPI) [1], using Lissajous nodes as data sites and showing that the proposed method outperforms the classical polynomial reconstruction in [3].

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Keywords: RBF approximation; Variably Scaled Kernels; Lissajous sampling

B-spline Bases on the Interval for the Numerical Solution of Fractional Differential Problems

Enza Pellegrino, Laura Pezza, Francesca Pitolli

Due to the nonlocal behavior of derivatives of fractional order, physical processes with memory and hereditary properties can be best described by fractional differential equations [1,2]. In general, it is not easy to derive the solution of fractional differential equations in a closed form. Therefore, efficient and accurate numerical methods are required for their solution. Our aim is to use the collocation method introduced in [3,4] to solve fractional differential problems on bounded intervals by means of B-spline bases. To this end, we give the analytical expression of the fractional derivatives in the Caputo sense for boundary B-spline functions. Thus, we can use B-spline bases on the interval to solve fractional differential problems. The numerical results confirm the accuracy of the proposed method.

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Keywords: fractional B-spline, collocation method

A Kinetic Neural Network Approach for Absolute Quantification and Change Detection in Positron Emission Tomography

Davide Poggiali

When dealing with absolute quantification of the tracer kinetics in Positron Emission Tomography (PET), one of the most reliable family of methods are the physiologically-consistent compartmental ODE models [3]. In this work we introduce the kinetic neural Network (kNN), a novel technique for absolute quantification inspired by compartmental models and Neural Networks commonly used in Deep Learning.

The ODE model's explicit solution is computed symbolically with the Python package sympy [2], by using the Padè approximation of the exponential matrix [1]. The model is evaluated voxel-by-voxel with PET data and fitted using the Gradient Descent technique. We applied this method on a set of PET images of the same subjects before and after an intervention. At last, we compared the derived parameter images by using Hostelling's t-squared statistic to evaluate the regions of the brain affected by the treatment.

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Keywords: PET, ODE, kinetics, Neural Network

MS2

MODELLING AND SIMULATION
OF
COMPLEX BIOLOGICAL SYSTEMS

Organizer

Gabriella Bretti

Describing Cell Behavior and Motion with PDE Chemotaxis Models

Gabriella Bretti

In recent years many studies have been carried out to understand and reproduce the movement of individuals on networks and on particular domains. With the aim of describing the dynamics of individuals moving on networks, we present mathematical PDE models of chemotaxis for two different biological applications and their numerical treatment.

The first model of chemotaxis we consider aims at describing the behavior of slime mold moving on networks during its feeding process: in accordance with laboratory experiments on Physarum polycephalum, individuals are able to select the shortest path among the competitive paths.

The second model, describes the behavior of tumor-associated macrophages, namely classically activated (M1) and alternatively activated (M2) cells, responsible for cancer inflammation. The aim is to understand the mechanism behind the switch from M1 to M2 and viceversa.

Keywords: networks; cell migration; chemotaxis; natural algorithm; shortest path; cancer invasion

Non-local Hybrid Model for Collective Cell Migration

Annachiara Colombi

A wide range of physio-pathological biological phenomena, from morphogenesis to cancer invasion, are characterized by collective cell dynamics. More specifically, the macroscopic evolution of cell aggregates, visible by looking at the totality of cells as a whole, results from the phenomenology of the single component cells, i.e., by individual behaviors and mutual interactions. Discrete particle models are widely used in this field, since they are focused on the cell-level of abstraction and are able to preserve the identity of single individuals reproducing their behavior.In this context, a fundamental role in determining the usefulness and the realism of a particle mathematical approach for cell spatial pattern is played by the choice of a intercellular pairwise interaction kernel and by the estimate of its parameters. The concept of H-stability, deriving from statistical mechanics, can have important implications in this respect. It in fact allows to a priori predict the stable configuration of a cell system for any given interaction kernel and relative coefficient setting. This is a starting point to model biological phenomena where the collective migration of the system results from the coexistence of multiple cell populations characterized by selected migratory determinants, as well as interactions with the surrounding environment.

Keywords: collective dynamics; cell aggregates; discrete approach

On Chip Reconstitution of Complex Biological Systems: a Bridge between Biology and Mathematical Models

Adele De Ninno

The development of theoretical frames able to describe complex biological systems has been a leitmotif in the work of many physicists and mathematicians and it is deeply linked with the possibility to obtain measurements of the parameters and variables describing the systems under observation. Recent advances in nano-biotechnology, 3D printing, biomaterials and microfluidic technologies have inspired new frontier solutions to reproduce, ex vivo, the complexity of biological systems in living multicellular micro-cultures. The idea to reconstitute subset of organs functionalities, on small, microscopy compliant, low cost, plastic devices is today a reality with concrete industrial applications and is known as the organs-on-chip approach. Combining microfluidics with the ability of cellular imaging enable to collect quantitative data from complex biological systems at a single-cell level, performing multi-parameter measurements of changes of hundreds of different cells and their microenvironment and offering access to various biological processes that are often concealed in the crowded in vivo environment. In this context the immune system is a striking example of an integrated information network engaged in coordinated host protective activities, able to fetch data from the body, analyse them and activate the needed countermeasures. When monitoring immune systems, the interplay between different cell types and the impact of functional responses reflect the roles of players and goals, respectively.

In the past years the combined efforts of our groups led us to set up to realize reproducible and controllable cancer-immune on chip models because of their exquisite capability to visualize multiple cell type interactions in real-time and to extract meaningful kinetics and behavioral data in unbiased and under therapeutic treatments including anticancer chemotherapy or immunotherapies. Smart implementation of image processing algorithms enable to quantify the simultaneous long-time interactions of huge number of cells and accurately solve the practical problems encountered in multi-cell type context. The experimental setup allowed us to describe the effects of drugs or genetic modifications in heterogeneous tumor-Immune microenvironments highlighting or confirming important mechanisms in boosting the immune response against cancer. In our vision the final goal will be to obtain an integrated experimental environment allowing for science experiments, pre-clinical trials and industrial testing, based on the synergistic use of organs/functional biological units based on advanced fabrication, biomaterial development and co-culture protocols (organs on chip, 3d bioprinting organoid approaches, tissue engineering), advanced measuring tools (microscopy, electrical, biochemical) in-silico models (agent based, systems biology, etc) and complexity science approaches.

A One-dimensional Vertical Ecosystem Model for Lake Dynamics

Fasma Diele, Mariasilvia Giamberini, Carmela Marangi, Angela Martiradonna, Antonello Provenzale

We present a modified version of an existing lake ecosystem model [1] describing a trophic chain generated by nutrients, phytoplankton, zooplankton and planktivorous fishes. The new model takes into account the vertical dynamics of the biomasses of the main species following the approach in [2]. We taylor the model to specific ecosystems by including seasonality in the dynamics of the various compartments. Moreover different species exhibit a different behaviour with respect to diffusion and to the rate of sinking and emerging. We simulate the evolution of the ecosystems hosted in alpine lakes located in study sites of a H2020 project. This work has been carried out within the H2020 project `ECOPOTENTIAL: Improving Future Ecosystem Benefits Through Earth Observations'. The project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 641762.

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Keywords: lake ecosystem model; one-dimensional vertical dynamics; trophic chain

Collective Dynamics: Mathematical Modelling and Numerical Simulations

Marta Menci

We present some results concerning mathematical models aiming at reproducing behaviors emerging in *collective motions*. In the literature, that terminology refers to the dynamics of groups of interacting agents, regardless of their nature. After a briew review of models, we focus on applications relating to biological phenomena, in which collective motions of cells occur. The approach is *hybrid*, meaning that cells are treated as discrete entities, whereas chemical signals, influencing the dynamic, are described as a continuum.

From an analytical point of view, we present a result for existence and uniqueness of the solution for systems of differential equations, arising from that kind of approach.

Finally, we focus on a hybrid mathematical model for the cardiospheres (CSps) formation, in relation to human cardiac stem cells. In particular, our work aims at modelling the earlier stage of in vitro formation, in which interacting cardiac progenitor cells begin to cluster, assuming the shape of a sphere.

By a numerical point of view, we have developed a suitable two-dimensional approximation scheme, based on finite differences, to simulate the model. The obtained results are in good agreement with laboratory experiments .

Keywords: collective motions; cardiospheres; finite difference scheme

MS3

SIGNAL AND DATA PROCESSING:

THEORY AND APPLICATIONS

Organizers

Vittoria Bruni, Mariantonia Cotronei, Milvia Rossini

A Normalized Information Based Method for Efficient Signal Representation

Vittoria Bruni, Lorenzo Della Cioppa, Domenico Vitulano

In this paper we present a novel and automatic method for the selection of the expansion coefficients of a signal in a given basis, useful in non-linear approximation problems. To this aim we evaluate signal complexity by means of a normalized information measure[2]. The latter is an entropic version of the normalized information distance (NID), which is a universal metric based on Kolmogorov complexity[1][3][4].

Specifically, the proposed method is able to set two distinct thresholds. The first one selects those coefficients able to represent signal content complexity. The latter discards redundant coefficients, i.e. those coefficients whose contribution is negligible in signal approximation with respect to standard quality measures, such as L2-based measures (MSE, SNR), L1 norm.

The proposed entropic version of NID relies on the representation of signal entropy in terms of a monotonic rearrangement of the same signal[2]. As a result, the two aforementioned thresholds correspond to two critical points of the proposed complexity measure, which can be computed using a fast and simple procedure.

Numerical results show that the proposed method is efficient in terms of computing time, in contrast to other information metrics such as normalized compression distance (NCD)[3]. In addition, it is able to tune the involved thresholds in an adaptive and automatic manner, without user's intervention or additional parameters to be tuned[2].

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Keywords: Information measure; non-linear approximation; entropy representatio

An Iterative Spectrogram Reassignment of Frequency Modulated Multicomponent Signals

Vittoria Bruni, Michela Tartaglione, Domenico Vitulano

Improving time-frequency resolution is a fundamental goal in nonstationary signal analysis. In case of multicomponent signals, where the individual modes interfere, linear time-frequency representations and quadratic distributions suffer from the presence of misleading interference terms. In order to overcome this drawback and improve time-frequency readability, nonlinear methodologies, such as reassignment and synchrosqueezing, have been proposed. These methods properly move points in the time-frequency plane in order to better localize signal components. Unfortunately, if the basic assumption of separability is not satisfied (i.e., individual modes are not sufficiently apart), reassigned and synchrosqueezed versions do not disclose a good modes discrimination.

In this work, it is first proved that the modulus of the Short Time Fourier Transform (STFT), referred to as spectrogram, of a linear combination of frequency modulated (FM) signals obeys a time-frequency evolution law, whose isolevel curves depend on signal instantaneous frequency (IF). Based on this result, an iterative Newton-like method for the spectrogram is proposed in order to move information content, concerning each component, toward the corresponding ridge curve, i.e. the isolevel curve where the spectrogram of a single and isolated mode would reach its maximum. This procedure allows us to obtain a time-frequency representation which better localizes the individual modes of the signal.

The proposed reallocation method is twofold advantageous: first, it allows us to overcome the limits of classical reassignment method, i.e. number of transforms (STFT) to compute and sensitiveness to kernel size; second, a simple check on the convergence order of the Newton-like method makes it able to adapt to regions where signal individual modes strongly interfere. Computational gain and robustness to interference effects make the proposed method suitable for accurate IF estimation, which is required in various applications involving radar, acoustic emissions, surveillance, music analysis.

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Keywords: Time-frequency reassignment;multicomponent signals;instantaneous frequency

Pattern recognition in X-ray CT and PET images

C. Campi, M. C. Beltrametti, A. M. Massone

In this talk we present some recent developments on X-ray computed tomography (CT) and Positron Emission Tomography (PET) images segmentation, in order to extract metabolic information in the case of oncological and neurodegenerative diseases. PET images, although being the gold standard for the assessment of pathological metabolic activity in human tissues, are characterized by a low resolution. The recognition of tissue borders is a difficult task, and we took advantage of anatomical information coming from high resolution X-ray CT images, acquired simultaneously with PET images, to enhance the region of interest identification.

Here we show how active contours [1] were successfully employed for the recognition of compact bone [2], while a generalization to algebraic curves [3] of Hough transform [4] was proposed for the identification of spinal canal. The developed methods have been applied to Adult Advanced Chronic Lymphocytic Leukemia (ACLL) [5] and Amyotrophic lateral sclerosis (ALS) [6].

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Keywords: pattern recognition; image processing; biomedical applications

Computational Bayesian Methods for ECG Denosing

Salvatore Cuomo, Rosanna Compagna, Raffaele Farina

In the signal processing field, data-driven approaches that smartly use some a "priori" information on data are recently studied to efficiently exploit the performances of processing algorithms and models.

The ECG filtering problem is a widely explored research topic and these novel recalled methodologies can be effectively adopted to achieve significant improvements in the ECG signal processing. In this work, we propose a modification of recursive filtering (RF) by considering a probabilistic Bayesian framework that is developed to selectively remove noise and artifacts from the acquired signals. Moreover, an interesting feature of our algorithm is that it is able to preserve any crucial medical information on the acquired data.

In this work, we highlight its computational efficiency that makes it ready as a useful tool for its implementation on mobile device applications. Finally, numerical experiments have been carried-out on real data to assess the advantages of the proposed model.

Keywords: Inverse Problems, Signal Denoising, ECG signals.

Learning Conditional Independence Graphs via Sparsity

Daniela De Canditiis, Armando Guardasole

It is well known in literature that for multivariate Gaussian distribution the precision matrix (the inverse of covariance) encodes the undirected graph representing conditional dependence.The notion of conditional dependence is more suited than the concept of dependence in order to catch the "direct link" between variables; this is the reason why recent interest in these types of graphs is greatly increased in many applications fields, like biological, medical, social and financial.

In this work, we deal with the problem of learning the conditional dependent graph given a set of *n* independent and identically distributed samples from a *p*-variate Gaussian distribution.When the sample size *n* is large, much larger than *p*, then the sample covariance estimator and its inverse are good estimators of their population counterparts. However, in the high dimensional case, i.e. when *n-p* is small or even when $n < p$, the sample covariance estimator is unstable and often not invertible. In such high dimensional cases, assuming a sparsity constrain on the number of non-zero coefficients of the precision matrix (i.e. on the number of edges in the graph), two different types of procedure can be applied. Global procedures, where the precision matrix (the graph structure) is learned through a penalized Maximum Likelihood Estimator and node-wise procedures, where the neighbourhoods of each node/variable is learned independently from the others. In this work, we want to show how combining these two approaches we can improve the estimation performance. In particular, we propose to apply a node-wise learning procedure which acts simultaneously on each node/variable incorporating the sparsity constraints via a group penalty. Our contribution is to study empirically how these different type of techniques work using different type of penalties, namely LASSO (Least Absolute Shrinkage and Selection Operator), SCAD (Smoothed Clipped Absolute Deviation) and MCp (Maximum Concave penalty). All these techniques are implemented using a Block-wise Coordinate Descendent algorithm, which make feasible all the procedures also in the high dimensional setting.

We will produce simulation results under different sample size and sparsity scenarios explaining advantages and disadvantages of all these modern inference techniques. Finally, we will show an application to a real data set.

Keywords: undirected graph, conditional dependence, graphical lasso

On a Class of Fractional Refinable Functions

E. Pellegrino, L. Pezza, F. Pitolli

Recently, several experimental studies found out that some physical phenomena are well described by differential equations containing fractional derivatives with respect to the time and/or to the space. We refer, for example, to anomalous diffusion in viscoelastic materials or in biological tissues and to population dynamics [1].

To numerically solve fractional differential problems by collocation methods, we need a class of approximating functions that is closed with respect to the fractional derivative operator. A class of this type is the class of fractional refinable functions introduced in [2]. These refinable functions generate a MRA on $L_2(R)$ and have good approximation properties. Moreover, their fractional derivative has an analytical expression that involves fractional refinable functions belonging to the same class [3]. The aim of this talk is to study the properties of the functions in that class and analyze their performances when used to solve fractional differential problems.

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Keywords: Fractional differential problems, collocation method, fractional refinable functions

Background Subtraction - Adaptive SVD revealing Moving Objects

Günther Reitberger

One important task when processing sensor data is to distinguish relevant data from irrelevant one. Image and video data is no exception. With static cameras, e.g. in video surveillance, the background, e.g houses or trees, largely stays constant over a series of frames, whereas the foreground, consisting of objects of interest, e.g. cars or humans, causes differences in image sequences. Background subtraction aims to create a model of the background based on previous image sequences and subtracts it from newly incoming images resulting in the moving objects contained in the foreground. This work describes how a newly developed method for an iterative and adaptive calculation of a singular value decomposition can be used to maintain a model of the background via singular vectors spanning a subspace of the image space. The method provides a way to determine, in a computationally efficient manner, the amount of new information of an image regarding the singular vectors spanning the background space and provides the ability to perform block-wise updates. Both properties contribute to a fast and robust algorithm. The effects of these two properties and the success of the overall method to perform a state of the art background subtraction are shown in qualitative and numerical evaluations.

Keywords: Image Processing, Background Subtraction, SVD

Multiple Multiresolution for Images

Dörte Rüweler, Tomas Sauer

To extract features from an image, in particular directed edges, one can use multiple filterbanks with anisotropic dilation matrices.

Applying it once gives a level one decomposition of the image. An iterative application of the same filterbank results in a multiresolution decomposition of the image similar to a discrete wavelet decomposition which is helpful to extract features of different resolutions. Finally, multiple filterbanks in each level of the decomposition give a multiple multiresolution decomposition of the image.

This decomposition can be considered as a tree and different paths give directional information corresponding to different sequences of applied filterbanks. Experiments show that such decompositions already provide good detection of directed edges with a relatively small depth.

We will present an implementatio of this approach and show some examples of decompositions for different filterbanks as well as applications like denoising or compression.

Keywords: Filterbanks, multiple MRA, multiresolution analysis

The Phase Retrieval Problem in Ptychographical Imaging

Nada Sissouno

Measurements achieved with ptychographical imaging are a special case of diffraction measurements. They are generated by illuminating small parts of a sample with a focused X-ray. By shifting the sample finally a set of far-field diffraction patterns of the whole sample are obtained. From a mathematical point of view those measurements are the squared modulus of the windowed Fourier transform. Thus, we are facing a phase retrieval problem which will be introduced and analyzed from an applied and mathematical perspective in this talk. This is joint work with Rayan Saab (UCSD), Christian Schroer (DESY, Hamburg), and Frank Filbir (HMGU, Munich).

Big Data Challenges in Imaging from Computer Tomography

Tomas Sauer

Besides its well-known application in medicine as a fundamental tool for diagnostics, Computer Tomography in its industrial form has become a major tool in nondestructive testing or even just as one component in a multimodal sensor system.

The technical advantages of recent years allow to scan complex and large objects in very high resolution which leads to an immense amount of data: 1TB per scan is no exception any more. In order to handle such methods and to extract information or at least relevant data from the big data requires new approaches in image processing. The talk will present some of the challenges and some of the methods developed in the Passau Fraunhofer group for "Knowledge based Image Processing".

Keywords: Computer tomography; knowledge based image processing; big data

Mathematical Algorithms for Digital Image Processing and Applications

Gianluca Vinti

Some approximation results by means of sampling type operators will be presented and the results obtained will be applied, after implementation, to digital image processing. Finally, some applications to concrete problems in the medical and engineering fields, will be considered.

Keywords: sampling operators, digital image processing, approximation

Characterization of Hölder-Zygmund Spaces via Non-shift-invariant Tight Frames

Alberto Viscardi

Hölder-Zygmund spaces are classical spaces when it comes to the regularity analysis of signals and it is known they can be characterized by the decay of wavelet coefficients. We generalize, under suitable assumptions, the known characterization of Hölder-Zygmund spaces to the case of non-shift-invariant tight frames. We exploit such characterization to approximate the regularity of semi-regular subdivision schemes using for the analysis the Dubuc-Deslauriers family of semi-regular tight frames.

MS4

MATHEMATICAL MODELLING IN MATERIALS WITH MEMORY AND NONLINEAR PHENOMENA

Organizers

Sandra Carillo, Federico Zullo

A Phase Transition Model for Auxetic Materials

Elena Bonetti

We introduce a nonlinear PDE system to describe auxetic materials behaviour by use of phase transition theory. Auxetic materials are smart materials showing shape memory effects combined with negative Poisson's coefficient. We introduce two phase parameters representing the different microscopic configurations of the lattice producing different responses of the material to external loads. The model is derived by a generalization of the principle of virtual powers including microscopic forces balance. We prove existence of (weak) solutions for a suitable variational formulation of the problem.

This research is a joint paper with Mauro Fabrizio and Michel Fremond.

Viscoelastic and Magneto-viscoelastic Materials: an Overview on Recent Results

Sandra Carillo

Integro-differential problems can be introduced to describe the mechanical behaviour of a viscoelastic material. The key feature of materials with memory is represented by the dependence of their mechanical behaviour on the previous history and non only on the actual behaviour. The kernel in the integro-differential equation represents the relaxation modulus. According to the classical model, studied in the celebrated article [1], a regular kernel is assumed. However, a relaxation modulus which satisfies the classical regularity assumptions is not suitable to describe the physical behaviour of all materials. In [2] a variety of non-classical memory kernels in linear viscoelasticity is presented; the evolution problem of further examples of viscoelastic materials can be studied on introduction of different kinds of generalised forms of the relaxation modulus. Accordingly, Integro-differential equations whose kernel is unbounded at the origin, are considered in [3,4] where, respectively, a one or three dimensional body is considered. A kernel which is continuous but not differentiable is considered in [5]. Finally, the case of a magnetically sensible viscoelastic material is investigated in [6,7,8], where the model is represented by an integro-differential nonlin- ear system. It takes into account the coupling of the linear viscoelasticity equation with the nonlinear differential equation which models the magnetic effect. Regular as well as singular problems are mentioned.

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Keywords: Materials with memory; viscoelasticity; magneto-viscoelasticity; integro-differential problem; regular kernel; singular kernel.

Thermoelectric Efficiency of Graded SicGe1-c Alloy

Vito Antonio Cimmelli, Patrizia Rogolino

We consider SicGe1-c graded systems of length L = 3 mm and L = 100 nm, under the action of an electric field **E**, and crossed by an electrical current **i**, the two sides of which are kept at two different temperatures Th and Tc. The dependence on composition and temperature of the thermal conductivity is analyzed. We evaluate the thermal conductivity in correspondence of the constant temperatures T = 300K; T = 400K and T = 500K, and investigate the thermoelectric efficiency of the system as function of the stoichiometric variable c and of the effective temperature gradient (Th-Tc)/L. For each temperature, we calculate the values of c in the interval [0; 1] which realize the optimal efficiency of the thermoelectric energy conversion. The corresponding values of the thermal conductivity are determined as well.

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Keywords: Graded systems; efficiency of thermoelectric energy conversion; figure-of-merit; minimum rate of energy dissipated

A Viscoelastic Equation with Nonlinear Density and Memory Effects

Monica Conti

We study a nonlinear viscoelastic equation suitable to modeling extensional vibrations of thin rods characterized by two main features: (1) nonlinear material density depending on the velocity (2) memory effects. We discuss the well-posedness of the model and the long-term behavior of the associated semigroup in the past-history framework. In particular, we show that the sole weak dissipation given by the memory term is enough to ensure existence and optimal regularity of the global attractor.

Keywords: viscoelasticity; global attractors

Steady States and Nonlinear Buckling of Cable-suspended Beam Systems

Claudio Giorgi, Elena Vuk, Ivana Bochicchio

This paper deals with the equilibria of an elastically-coupled cable-suspended beam system, where the beam is assumed to be extensible and subject to a compressive axial load. When no vertical load is applied, necessary and sufficient conditions in order to have nontrivial solutions are established, and their explicit closed-form expressions are found. In particular, the stationary solutions are shown to exhibit at most two non-vanishing Fourier modes and the critical values of the axial-load parameter which produce their pitchfork bifurcation (buckling) are established. Depending on two dimensionless parameters, the complete set of resonant modes is devised.
As expected, breakdown of the pitchfork bifurcations under perturbation is observed when a distributed transversal load is applied to the beam. In this case, both unimodal and bimodal stationary solutions are studied in detail. Finally, the more complex behavior occurring when trimodal solutions are involved is briefly sketched.

Keywords: Cable-suspended beam; nonlinear oscillations; stationary solutions; pitchfork bifurcation; biparametric resonance

Modeling Particle-Laden and Poroacoustic Flow Phenomena via the Generalized Continua Approach

Pedro M Jordan

With a focus on acoustic phenomena, we investigate several dual-phase (i.e., fluid-solid) flows using the generalized continua (GC) modeling approach, where by "GC" we mean modern generalizations of the constitutive relations of classical continuum mechanics that seek to capture the impact of sub-scale structure/dynamics on the (macroscopic) field variables. Working under the finite-amplitude framework, we derive and analyze generalizations of the weakly-nonlinear versions of the Euler and Navier--Stokes equations for the case of particle-laden and poroacoustic flows. Using both analytical and numerical methods, we examine the impact of the solid phase on the propagation and evolution of (1D) traveling and acceleration waves. Along the way, the advantages and disadvantages of this modeling approach will be discussed and applications to other fields noted.
(Work supported by ONR funding.)

Keywords: Nonlinear acoustics; generalized continua; dual-phase flows

Boundary Value Problems in Irregular Domains

Maria Rosaria Lancia, Simone Creo, Paola Vernole

In this talk we present some recents results on vector boundary value problems in irregular domains, possibly with fractal boundary.

We present existence and uniqueness results for the weak solution.

The numerical approximation in some test cases will be discussed.

Keywords: fractals, irregular domains, vector boundary value problem

On the Zeros of Entire Functions.

Federico Zullo

The zeros of entire functions of complex variable appear in a great number of problems in physics and engineering. In this talk we discuss the distribution and localization of the zeros of entire functions, giving a method to construct a recursion satisfied by them and present some properties related to this recursion.

An application to the zeros of Airy functions and to the poles of Painlevé 1 equation is given.

Keywords: entire function; value distribution

MS5

MESH GENERATION AND ADAPTION FOR SIMULATION-BASED ENGINEERING

Organizer

François Guibault

GPU parallelization of mesh adaptation techniques by node movement in a Riemanian metric

William Bussière, Francois Guibault

In numerical fluid mechanics, mesh adaptation provides an efficient mechanism to enhance the precision of an approximate solution while limiting the consumption of computerr esources [1]. By an iterative process of consecutive resolution-adaptation phases, the shape and size of the elements are adapted to the curvature of the approximate solution to reduce interpolation error. With the ever increasing size of the problems studied in numerical fluid mechanics, multiple parallelization techniques have been developed to reduce the time needed by solvers to compute solutions. However, if mesh adaptation algorithms do not benefit from similar parallelization efforts, their computing time may soon dominate the overall resolution-adaptation iterative process. This study aims to determine whether GPUs are able to accelerate the adaptation process while producing meshes of a quality that matches the one produced by current methods on the CPU.

By Cea's lemma, it is known that the approximation error is bounded by the interpolation error. Computed as an a posteriori error estimator [3], the metric function species to the adapter the ideal length of an edge in a given location to obtain a specic interpolation error. Topological and geometrical operations modify an initial mesh in order to maximize element conformity to a specied metric. The present study focuses on node relocation algorithms that already demonstrated their suitability for efficient parallelization on GPU [2]. The manipulation of non-simplicial elements and the precise sampling of a 3Dmetric function yield, however, signicant challenges which must be tackled in the context of mesh adaptation procedures on GPU for numerical uid mechanics applications. Specialized mesh adaptation software was developed to cope with the specicities of parallelism on GPU. While on the CPU, the metric function is sampled on a backgroundmesh by local search, the present approach proposes to sample the metric function in a texture on the GPU side. A series of node relocation algorithms are implemented and compared on both types of processor, including the Laplacian smoothing, gradient descent and Nelder-Mead. A new version of Laplacian smoothing for mesh adaptation in a Riemannian metric is proposed. Furthermore, in addition to the node axis, this study proposes two new parallelization axes for node relocation algorithms: the elements and positions axes. Important implementation issues involved in porting the node relocation algorithms on the GPU are discussed, including processors synchronization and the translation of data structures. Two technologies for the development of GPU kernels are compared: GLSL and CUDA.

The results clearly show that the sampling of the metric function by local search is not practical on the GPU because of excessive instruction count and thread divergence. On the contrary, metric sampling through a texture demonstrates encouraging acceleration rates.

Even though texture sampling presents some precision flaws for the most difficult metric functions, the present study demonstrates that by increasing the resolution of the textures by a reasonable amount, it is possible to meet background mesh precision. Concerning node relocation algorithms, local optimization algorithms stand out when compared to Laplacian smoothing for their efficacy, both on tetrahedral and hexahedral meshes. In particular, the Nelder-Mead algorithm stands out for its high speed both on the CPU and on the GPU. The newly explored parallelization axes on the GPU allow doubling implementation acceleration rates. For instance, the multi-axis version of the gradient descent algorithm achieves between 48 and 110 acceleration speedup on sample 3D testcases, while the multi-element version of the Nelder-Mead algorithm is approximately 50 times faster than its sequential version. In short, the selected optimal adaptation pipeline samples the metric function in a texture and uses a multi-element version of the Nelder-Mead algorithm written in CUDA to move mesh nodes on the GPU. Despite GLSL's high portability compared to CUDA, its implementation of the optimal pipeline shows lower acceleration rates and often lacks in robustness.

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Keywords: Mesh Adaptation, Mesh Smoothing, Parallelization, GPU, Riemanian Metric

Simulations in Large Tridimensional Discrete Fracture Networks (DFN): I. Geometric Modeling and Mesh Generation

Patrick Laug, Geraldine Pichot

Fractures in the Earth's subsurface have a strong impact in many physical and chemical phenomena, as their properties (in particular their permeabilities) are very different from those of the surrounding rocks. They play a major role in diverse fields of applications such as groundwater extraction, oil and gas exploitation, geothermal energy production, CO2 sequestration, etc. In this presentation, we focus on the well-known Discrete Fracture Network (DFN) models and on efficient techniques to mesh them. The generated meshes are subsequently used to carry out numerical simulations*.

In the DFN models, fractures are represented by ellipses that are randomly generated in the tridimensional space, following experimental statistics. To make this model suitable for classical surface and volume meshers, it is necessary to add some information, which is accomplished in several steps: computation of the intersections between fractures, selection of fractures using a graph structure, and construction of a conforming set of edges that can be used as input for a mesh generator. All these steps present special difficulties if there are large numbers of fractures with distances, lengths and angles spanning over several orders of magnitude. Computational times are also critical, and only linear time algorithms can be accepted. In this talk, a methodology for modeling and meshing DFNs will be presented, and recent meshes up to hundreds of thousands of fractures will be shown.

*See Pichot et al. MASCOT 2018 abstract, Simulations in Large Tridimensional Discrete Fracture Networks (DFN): II. Flow Simulations.

Simulations in Large Tridimensional Discrete Fracture Networks (DFN): II. Flow Simulations

Geraldine Pichot, Patrick Laug, Jocelyne Erhel, Romain Le Goc,
Caroline Darcel, Philippe Davy, Jean-Raynald de Dreuzy

We start this presentation by assuming that a model and a mesh of the DFNs have been computed*. We focus here on the numerical methods to solve efficiently single-phase flow problems.

We will present the software NEF-Flow dedicated to solving single phase flow in large scale DFNs. NEF stands for Numerical Experiments involving Fractures. The software NEF-Flow is written in Matlab and implements the mixed-hybrid finite element method in an optimized way, using vectorization to decrease the computational time. It handles either matching or non-matching meshes at the intersection between fractures, sink/source terms and contrasts in transmissivities.

A large set of benchmark test cases will be presented. Typically, we extended those proposed in [1, 2] to DFNs generated with the UFM framework [3,4]. These DFNs are large scale DFNs where the fracture size distribution matches the observations and where fractures are organized so that large fractures inhibit the smaller ones, creating T-termination configurations. They may contain hundreds of thousands of fractures. Hydraulic properties will be computed efficiently on these networks. (*See Laug et al. MASCOT 2018 abstract, Simulations in large tridimensional Discrete Fracture Networks (DFN): I. Geometric modeling and mesh generation)

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Implementation of a Learning Environment for Grid Generation

Ricardo Camarero

As the geometric complexity of engineering applications increases, the role of the grid generation has become a critical step in the overall procedure of numerical simulations. The progress achieved in meshing techniques stems from the requirements of industrial applications and has followed the capabilities of geometric modelling, workstation technologies and computational geometry.

The early developments were carried out for a given problem, usually written by the end user. This was followed by a shift towards a dynamic commercial sector which made the major advances available to engineers and analysts, through innovative software environnements by computer science professionals. Initially a specialized problem-dependent issue, this has led to the development of generic software applicable to many fields of engineering, and has become a new discipline with a wide range of methodologies.

The training requirements of this community of students, researchers and practitionners have been met by a hands-on, practice-based and product-oriented approach.

This paper presents a model of engineering education whose role is not only to train technical experts but also to train engineers who master the scientific fundamentals of grid generation while acquiring the skills required to develop complex value-added engineering analysis tools in a modern IT environment,

How are these skills taught ?

Such a comprehensive goal cannot be achieved by the use of commercial or research codes which are too problem-specific and lack the necessary variety in methods, algorithms and data structures necessary for a generic education. Instead, what is proposed is a software rich learning environment based on an open architecture. This comprises geometric and topological representations and operations covering the requirements of most current meshing methodologies.

The pedagological approach is based on a problem-based model which mimics the progression of the apprentice to the expert engineer. The fundamental knowledge and skills acquisition is a parallel, self-reinforcing process whereby the student develops several algorithms spanning a wide range of current meshing classes, on significant, yet simple, geometries. These learning outcomes are achieved maintaining a close relation with the basic meshing algorithms where specialized computer chores are encapsulated into services functions through fully integrated modules.

Mesh Generation for Building Aerodynamics: Challenges, Best Practices and Lessons Learned

Alessandro Gambale

This presentation focuses on the specific requirements, strategies and key choices for mesh generation in Computational Fluid Dynamics (CFD) simulation of air flows around buildings. CFD has established as a valuable tool in building engineering for predicting the value of relevant flow properties such as velocity, pressure, turbulence intensity, temperature. Architectural Aerodynamics deals with large and complex geometries consisting of buildings, roads, green areas, a number of other smaller objects such as cars, trees, pedestrians and others. Each of those objects has on its surface a number of details with dimensions even several orders of magnitude smaller than the object they belong to. This large range of dimensions is a major challenge to the creation of a high-quality computational mesh.The computational cost and the quality of results of simulations are largely influenced by how the computational domain is created, by the choice of which objects and what details are included and which are discarded and by the meshing strategy and algorithm. Special care must be paid to the regions close to the solid surfaces, so that an appropriate cell dimension is achieved, in accordance with the turbulence model that will be applied.Guidelines from relevant literature and lessons learned from professional and academic practice will be presented to serve as an introduction to this fascinating and challenging field of numerical simulation.

Keywords: Computational Fluid Dynamics, CFD, building aerodynamics, mesh generation, turbulence, architectural aerodynamics, urban design, building engineering

POSTERS

ClusterKDE Algorithm for Clustering Data Based on Kernel Density Estimation

Solange Regina dos Santos

In this work we present an algorithm for clustering based on univariate kernel density estimation, named ClusterKDE. It consists of an iterative procedure that in each step a new cluster is obtained by minimizing a smooth kernel function. Although in our applications we have used the univariate Gaussian kernel, any smooth kernel function can be used. The proposed algorithm has the advantage of not requiring a priori the number of cluster. Furthermore, the ClusterKDE algorithm is very simple, easy to implement, well-defined and stops in a finite number of steps, namely, it always converges independently of the initial point. We also illustrate our findings by numerical experiments which are obtained when our algorithm is implementedin the software Matlab and applied to practical applications. The results indicate that the ClusterKDE algorithm is competitive and fast when compared with the well-known Clusterdata and K-means algorithms, used by Matlab to clustering data.

Keywords: Kernel density estimation; Gaussian kernel; Clustering data

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