# WNA-Porto-2019 WORKSHOP ON NUMERICAL ANALYSIS dedicated to Claude Brezinski and Michela Redivo-Zaglia

Analysis Area of Center of Mathematics of University of Porto (CMUP) Department of Mathematics of Faculty of Sciences of University of Porto

Porto, July 15th, 2019



# Welcome to WNA-Porto-2019, Workshop on Numerical Analysis

The **WNA-Porto-2019** is a one day meeting organized by the Analysis Area of Center of Mathematics of University of Porto (CMUP) and will take place at Department of Mathematics of Faculty of Sciences of University of Porto. This year, it is dedicated to **Claude Brezinski** and **Michela Redivo-Zaglia** due to theirs important contributions to this field of research.

This event aims to gather PhD, Post-Doc students, members of CMUP and other researchers, in order to promote scientific actualization and exchanging of ideas around common themes in this area.

We would like to thank Claude Brezinski and Michela Redivo-Zaglia for accepting our invitation and all speakers who made this event possible.

This workshop is divided into two parts: in the morning, the lectures by Claude Brezinski and Michela Redivo-Zaglia will be presented and accessible via streaming at https://www.youtube.com/channel/UCHnYYI2uRnH8CVOF55Irw3g/live. The videos of the lectures of Claude Brezinski and Michela Redivo Zaglia are available at https://www.youtube.com/watch?v=DM2gXVtJO0g&feature=youtu.be and https://www.youtube.com/watch?v=XsWb2tAu6cM&feature=youtu.be respectively.

In the afternoon eight contributed talks will took place.

We hope this day will be fruitful and pleasant for all participants.

The organizers,

Zélia da Rocha and Paulo B. Vasconcelos

# Claude Brezinski

**Emeritus Professor** 

## Laboratoire Paul Painlevé University of Lille France

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**Claude Brezinski** is Emeritus Professor at the University of Lille, France. After his studies in mathematics and physics at the University of Paris, he spent some years as a research engineer at several places. After obtaining, in 1971, his Doctorat d'État in mathematics at the University of Grenoble under the supervision of Prof. Noël Gastinel, he got an associate (and then full) professorship at the University of Lille where he was the head of the Laboratoire d'Analyse Numérique et d'Optimisation for almost 30 years. He is a member of the Royal Academy of Sciences of Zaragoza, Spain. He retired in 2005. His research interests concern convergence acceleration by extrapolation methods, Padé approximation, continued fractions, orthogonal polynomials, numerical linear algebra, and history of sciences. He wrote 20 books and over 230 research papers. He supervised 60 thesis. He was an invited speaker at many international conferences and universities for short and long visits. He was fortunate enough to meet Michela Redivo-Zaglia 30 years ago, and they are collaborating since then. He was a member of the editorial boards of several international journals and, in 1991, he founded Numerical Algorithms which is now in the top rank of numerical analysis journals. He is still its editor-in-chief.



## Michela Redivo-Zaglia

Associated Professor European Ph.D.

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Michela Redivo-Zaglia got her degree in Mathematics in Padua in 1975 and her PhD degree (European label) in Lille, in France, in 1992. She is Associate Professor of Numerical Analysis since 1998 (habilitation to Full Professor in 2013). She was Vice-Director of the Department of Mathematics of Padua University (2008-2011) and from 2005 she belongs to the board of the Padua's Doctoral School in Mathematics (Coordinator and Delegate of the Computational Mathematics branch 2013-2017). She was the Head of the Computer Center of the Department of Electronics and Computer Sciences of the University of Padova from 1984 to 1998. Her research focuses primarily on Numerical Linear Algebra, Extrapolation and Convergence Acceleration Methods, and applications. She obtained important results in these fields of research that received many quotations. As author or coauthor, she published about 75 papers in recognized international journals, seven software packages, and seven books. One of these books is still now one of the main references on extrapolation methods. She has been invited as Visiting Professor in several European Universities and also in USA, South-Africa, Canada, Russia, China, and Hong Kong, giving there seminars and courses. Her scientific results have been presented at about 75 international conferences, 15 of them as invited or plenary speaker. She has been member of the committees and editor of the proceedings of many international conferences. She is currently member of the editorial board of three international journals. She has been member of PhD examination committees in foreign countries, and was, and is, responsible or participant in more than forty funded projects. She devoted a large part of her efforts in the training of young researchers and students. Moreover, she was one of the member of the starting group of pioneers of the project Teaching4Learning at the Padua University.

# Venue: FC1 Maths Building

# Place: Room FC1.031

# Shedule: Monday, July 15th

10h	Registration	
10h 15m	Opening Session	
10h 30m	Claude Brezinski	Lille, France
11h 30m	Michela Redivo-Zaglia	Padova, Italy
12h 30m	Lunch	
14h 30m	Semyon Yakubovich	Porto, Portugal
15h	Ana Matos	Lille, France
15h 30m	Sílvio Gama	Porto, Portugal
15h 50m	Rúben Sousa	Porto, Portugal
16h 10m	Zélia da Rocha	Porto, Portugal
16h 30m	Coffee break	
17h	Marco Martins Afonso	Porto, Portugal
17h 20	José Matos	Porto, Portugal
17h 40m	Paulo Vasconcelos	Porto, Portugal
18h	Closing	

# PROGRAMME

- 10h Registration
- 10h 15m Opening Session
- 10h30m 11h30m

Claude Brezinski - University of Lille, France

Shanks' transformations, Anderson acceleration, and applications to systems of equations

The video of this lecture is available at https://www.youtube.com/watch?v=DM2gXVtJO0g&feature=youtu.be

### • 11h30m - 12h30m

Michela Redivo-Zaglia - University of Padova, Italy

Extrapolation: a useful tool for linear and nonlinear algebra problems

The video of this lecture is available at https://www.youtube.com/watch?v=XsWb2tAu6cM&feature=youtu.be

## 12h 30m - 14h 30m Lunch at Circulo Universitário

• 14h 30m - 15h

Semyon Yakubovich, University of Porto

Orthogonal polynomials with ultra-exponential weight functions: an explicit solution to the Ditkin-Prudnikov problem

• 15h - 15h 30m

Ana Matos, University of Lille, France

Working with rational functions in a numeric environment - some contributions

## • 15h 30m - 15h 50m

Sílvio Gama, University of Porto

Computation of kinematic and magnetic eddy diffusivities by Padé Approximation employing Mathematica

• 15h 50m - 16h 10m

Rúben Sousa, University of Porto

On generalized convolutions for Sturm-Liouville and elliptic operators

## • 16h 10m- 16h 30m

Zélia da Rocha, University of Porto On some properties of zeros of perturbed Chebyshev polynomials

## 16h 30m - 17h Coffee Break

• 17h - 17h 20m

Marco Martins Afonso, University of Porto An application of multivariate Hermite polynomials in fluid mechanics

- 17h 20m 17h 40m José Matos, ISEP Tau Toolbox: Tau method for integro-differential problems
- 17h 40m 18h Paulo B. Vasconcelos, University of Porto Tau Toolbox: Current achievements and plans

18h Closing

# ABSTRACTS

• Shanks' transformations, Anderson acceleration, and applications to systems of equations

### Claude Brezinski

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Laboratoire Paul Painlevé, University of Lille, France

## Abstract:

We present a general framework for Shanks' transformations of sequences of elements in a vector space. It is shown that the Minimal Polynomial Extrapolation (MPE), the Modified Minimal Polynomial Extrapolation (MMPE), the Reduced Rank Extrapolation (RRE), the Vector Epsilon Algorithm (VEA), and the Topological Epsilon Algorithm (TEA), which are standard general techniques for accelerating arbitrary sequences, all fall into this framework. Their properties are studied.

Then, we discuss the application of these methods to the solution of systems of linear and nonlinear equations. Their connections with quasi-Newton and Broyden methods are studied.

We then consider Anderson Acceleration (AA) which is a method for solving systems of equations. In the linear case, it is known that AA and GMRES are 'essentially' equivalent in a certain sense while GMRES and RRE are mathematically equivalent. We discuss the connection between AA, the RRE, the MPE, and other methods in the nonlinear case. Finally, Anderson-type methods are presented.

#### References

[1] C. Brezinski, M. Redivo-Zaglia, Y. Saad, Shanks Sequence Transformations and Anderson Acceleration, SIAM Review, 60 (2018), pp. 646–669.

[2] C. Brezinski, M. Redivo Zaglia, Y. Saad, Applications of coupled topological Shanks transformations to systems of equations, in progress.

• Extrapolation: a useful tool for linear and nonlinear algebra problems

## Michela Redivo-Zaglia

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#### Abstract:

Several methods for solving linear and nonlinear algebra problems produce sequences of approximations of the solution. Let  $(\mathbf{S}_n)$  be a sequence of elements of a vector space E on a field  $\mathbb{K}$  ( $\mathbb{R}$  or  $\mathbb{C}$ ) which converges to a limit  $\mathbf{S}$ . If the convergence is slow, it can be transformed, by a sequence transformation, into a new sequence or a set of new sequences which, under some assumptions, converges faster to the same limit. When E is  $\mathbb{R}$  or  $\mathbb{C}$ , a well known such transformation is due to Shanks, and it can be implemented by the scalar  $\varepsilon$ -algorithm of Wynn. This transformation was generalized to sequences of elements of a general vector space E by the topological Shanks transformations that can be recursively implemented by the topological  $\varepsilon$ -algorithms of Brezinski (1975). They were recently greatly simplified, and they can now be applied not only to vectors, but also to matrices and tensors. The Matlab package EPSfun, which can be used for that purpose, is available in the public domain library netlib. Numerical results for many different problems are presented. • Orthogonal polynomials with ultra-exponential weight functions: an explicit solution to the Ditkin-Prudnikov problem

## Semyon Yakubovich

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## DM-FCUP, University of Porto, Portugal

### Abstract:

In this talk we give an interpretation of new sequences of orthogonal polynomials with ultra-exponential weight functions in terms of the so-called composition orthogonality. The 3-term recurrence relations, explicit representations, generating functions and Rodrigues-type formulae are derived. The method is based on differential properties of the involved special functions and their representations in terms of the Mellin-Barnes and Laplace integrals. Certain advantages of the composition orthogonality are shown to find a relationship with the corresponding multiple orthogonal polynomial ensembles. • Working with rational functions in a numeric environment - some contributions

#### Ana Matos

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#### Laboratoire Paul Painlevé, University of Lille, France

#### Abstract:

Rational functions like for instance Padé approximants play an important role in signal processing, sparse interpolation and exponential analysis. They have good theoretical properties in approximation and modeling. However, for a successful modeling with help of rational functions we want to make sure that there is no "similar" rational function being degenerate, i.e., having strictly smaller degree of both degrees of numerator and denominator. In particular, we prefer having rational functions without Froissart doublets (i.e., roots close to a pole) because their presence induce numerical instabilities: small variations in the argument of the function give rise to large variations in the function values.

In a numerical setting, we will bring out some quantities to control conditioning and stability of the computed rational functions. These quantities are based on the condition number of some matrices, numerical co-primeness of polynomials and spherical derivatives. They are reliable indicators of the good numerical properties of the functions and we can use them to choose the good class of functions or to construct new approximations. • Computation of kinematic and magnetic eddy diffusivities by Padé approximation employing Mathematica

## Sílvio Gama

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## DM-FCUP, University of Porto, Portugal

#### Abstract:

We consider the large-scale kinematic dynamo problem for three-dimensional flows of an incompressible electrically conducting fluid [1]. Application of Padé approximants [2,3,4] for computation of the tensor of magnetic eddy diffusivity for parityinvariant flows [5] have been explored using symbolic computing by Mathematica. We construct Padé approximants of the tensor expanded in power series in the inverse molecular diffusivity  $1/\eta$  around  $1/\eta = 0$  [6]. This yields the values of the minimum magnetic eddy diffusivity to satisfactory accuracy for  $\eta$  as small as 0.05. Algorithms for symbolic calculation of convolutions of trigonometric polynomials involved are presented.

#### References

[1] Zheligovsky, V.A. Large-scale perturbations of magnetohydrodynamic regimes: linear and weakly nonlinear stability theory, Lecture Notes in Physics, vol. 829, Springer-Verlag, Heidelberg, 2011.

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[5] Gama, S., Vergassola, M., Frisch, U. "Negative eddy viscosity in isotropically forced two-dimensional flow: linear and nonlinear dynamics", *Journal of Fluid Mechanics* **260**, 95–126, 1994.

[6] Gama, S.M.A., Chertovskih, R., Zheligovsky, V. "Computation of kinematic and magnetic  $\alpha$ -effect and eddy diffusivity tensors by Padé approximation", *Fluids* 4(2), 110, 1–25, 2019.

• On generalized convolutions for Sturm-Liouville and elliptic operators

## Rúben Sousa

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### University of Porto

#### Abstract:

In this talk we address the following question: given an elliptic operator  $\mathcal{L}$  on a subset E of Euclidean space, can we construct a convolution-like operator which commutes with  $\mathcal{L}$ , in analogy with the corresponding property between the ordinary convolution and the Laplacian?

We will present a novel unified framework for the construction of convolutions associated with a general class of regular and singular Sturm-Liouville boundary value problems. This unified approach is based on the application of the Sturm-Liouville spectral theory to the study of the associated hyperbolic equation. We will then show that each Sturm-Liouville convolution gives rise to a Banach algebra structure in the space of finite Borel measures in which various probabilistic concepts and properties can be developed in analogy with the classical theory; in particular, this allows us to develop a generalized notion of Lvy process.

We will also discuss ongoing work on multidimensional elliptic operators. In this setting, it turns out that a positive answer to the above question depends on certain geometrical properties of the eigenfunctions of the elliptic operator. This will be illustrated through some numerical examples.

• On some properties of zeros of perturbed Chebyshev polynomials of second kind

## Zélia da Rocha

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## DM-FCUP, University of Porto, Portugal

## Abstract:

Orthogonal polynomials satisfy a recurrence relation of order two defined by two sequences of coefficients. If we modify one of these coefficients at a certain order, we obtain the so-called perturbed orthogonal sequence. In this work, we consider some perturbed of arbitrary order of Chebyshev polynomials of second kind. These families are of second degree and semi-classical [1,2]. From the connection relations of the perturbed sequence in terms of the original one [4], we obtain a location of extremal zeros of perturbed Chebyshev polynomials with respect to extremal zeros of Chebyshev polynomials [3,5]. From the connection relations of the perturbed sequence in terms of the connection relations of the perturbed sequence in terms of the associated Jacobi matrices, we derive the Geršgorin location for the set of zeros of these polynomials [5]. Using other relations deduced from Jacobi matrices, we deduce some results about points that do not depend on perturbation [3,5]. This work is illustrated by graphical representations and demonstrations done with *Mathematica*<sup>®</sup>.

**Key words:** Perturbed Chebyshev polynomials; connection relations; zeros; Jacobi matrix; Geršgorin disks.

## References

[1] Z. da Rocha, A general method for deriving some semi-classical properties of perturbed second degree forms: the case of the Chebyshev form of second kind, J. Comput. Appl. Math., 296 (2016) 677–689.

[2] Z. da Rocha, On the second order differential equation satisfied by perturbed Chebyshev polynomials, J. Math. Anal., 7(1) (2016) 53-69.

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[4] Z. da Rocha, On connection coefficients of some perturbed of arbitrary order of the Chebyshev polynomials of second kind, *J. Differ. Equ. Appl.*, 25:1 (2019) 97-118.

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• An application of multivariate Hermite polynomials in fluid mechanics

## Marco Martins Afonso

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### University of Porto

### Abstract:

In 1865 Charles Hermite introduced the multivariate version of his orthogonal polynomials, suitable for a multidimensional problem with a Gaussian weight in the Ornstein–Uhlenbeck formalism. Such tensorial polynomials have often been used in theoretical physics to describe the quantum harmonic oscillator, by means of Hermitianization process and second-quantization algorithm, introducing the vacuum state and the ladder (creation/annihilation) operators.

We will show an interesting application of this framework to classical fluid dynamics, in order to obtain the transport properties and the temporal evolution of the concentration of particles carried by a flow field. Namely, we study the sedimentation and diffusion of inertial particles, endowed with a small-but-finite radius and a mass density different from the surrounding environment, as well as their dispersion following a spatially-localized emission (a point source).

The theory provides generic formulae in the phase space, too hard to tackle even numerically. It is therefore necessary to focus on perturbative limits where the analytical investigation can proceed further, such as the cases of little particle inertia or of quasi-neutral buoyancy. After a power-series expansion — either regular or multiscale — in the corresponding small parameter, a projection on the basis of multivariate Hermite polynomials allows for a strong simplification of the problem to the physical space, with a huge reduction in the dimensionality and in the number of degrees of freedom. Tools such as Mathematica, Maple and Matlab can be extremely helpful in the symbolic calculus associated with this computational procedure.



Figure 1: Droplet collision and coalescence represent the last and essential stage of rain formation. This process is driven by the difference in settling between drops of different sizes, a phenomenon that can be attacked analytically by making use of the multivariate Hermite polynomials.



# Bibliografy

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[6] M. MARTINS AFONSO & S.M.A. GAMA, Point-source dispersion of quasineutrally-buoyant inertial particles, *Eur. Phys. J.* E **42**(1), 10:1–8 (2019).  Tau Toolbox: Tau method for integro-differential problems José A. Matos jma@isep.ipp.pt ISEP, Porto

#### Abstract:

The spectral Tau method was originally developed by Lanczos in the 30's to delivers polynomial approximations to the solution of differential problems. Initially developed for linear differential problems with polynomial coefficients, it has been used to solve broader mathematical formulations: non-polynomial coefficients, nonlinear differential and integro-differential equations. Several works applying the Tau method have been performed to approximate the solution of differential linear and non-linear equations. Nevertheless, in all these works the Tau method is tuned for the approximation of specific problems and not offered as a general purpose numerical tool. Another barrier to use the method as a general purpose technique has been the lack of automatic mechanisms to translate the integro-differential problem by an algebraic one. Furthermore and most importantly, problems often require high-order polynomial approximations, which brings numerical instability issues. The tau method inherits numerical instabilities from the large condition number associated with large matrices representing algebraically the actions of the integral, differential or integro-differential operator on the coefficients of the series solution. In this work numerical instabilities related with high-order polynomial approximations, in the tau method, are tackled allowing for the deployment of a general framework to solve integro-differential problems.

• Tau Toolbox: Current achievements and plans

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## FEP, University of Porto, Portugal

### Abstract:

Together with some hands-on examples for the TAU Toolbox library, envisaged future extensions will be exposed. Furthermore, recent current developments will be shared: differential eigenproblems and the use of multiprecision arithmetic. The former will provide Tau Toolbox with the ability to compute eigenpairs from differential problems. Preliminary results show the effectiveness of the spectral Tau method approach to solve linear, polynomial and nonlinear eigenvalue problems. The latter is important in cases where double precision arithmetic is not sufficient to provide results with the required accuracy. This is the case when facing ill-conditioned problems, which prevent stable algorithms from working within machine precision. Exploring higher precision of floating point arithmetic (e.g. quadruple precision) can overcome some of these issues. Experimental results on the computation of approximate solutions of differential problems via spectral methods will be exposed with resource to multiprecision arithmetic.

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