Numerical integration, integral equations and transforms

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List of contributions

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10:30 – 12:30				G. Milovanovic T. Okayama M. Weimar S. Falletta	S. Notaris M. G. Russo M. Bulai
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Modeling metastatic tumor growth, numerical resolution and prediction

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Abstract: Iwata and coauthors in [1], based on [2] and [3], assumed that the new born generated metastasis can be only of the same size (1 cell). Latter in [4] has been shown that a metastasis generated by the primary tumor can be formed both by single cells and cluster of several cells. More importantly in [5] using a multicolor lineage tracing they have demonstrated that polyclonal seeding by cell clusters is a frequent mechanism in a common mouse model of breast cancer, accounting for $> 90\%$ of metastases.

Based on the biological evidence of the metastatic "born" mechanism we consider here the more general model where we assume that the metastatic emission at time t_0 can have a size different than 1 cell, i.e.$V_m(t = 0) = V_{m0}$.

Before solving the more general model we introduce five different tumor growth laws in Iwata partial differential equation model used to describe the metastatic growth. The models included in the study comprised the exponential, power law, Gompertz, generalized logistic and von Bertalanffy, all of them already introduced in [6].

The numerical method introduced in [7] was used to solve the Iwata model, based on a Volterra-integral equation method, with the tumor growths introduced above, considering two case studies such as lung and breast tumors. Last we conclude our work by using the same numerical method to solve the more general model and see how the value of V_{m0} affect the metastatic mass and the number of metastasis.

This is a joint work with Maria Carmela De Bonis, Concetta Laurita and Valeria Sagaria.

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A boundary integral equation method for linear elastodynamics problems on unbounded domains

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Abstract: We consider transient 3D elastic wave propagation problems in unbounded isotropic homogeneous media, which can be reduced to corresponding 2D ones. This is the case, for example, of problems defined on the exterior of a bounded rigid domain, which are invariant in one of the cartesian directions. The linear elastodynamics problem that characterizes small variations of a displacement field $\mathbf{u}(\mathbf{x},t) = (\mathrm{u}_1(\mathbf{x},t), \mathrm{u}_2(\mathbf{x},t))$, $\mathbf{x} = (x_1, x_2)$ in a homogeneous isotropic elastic medium Ω^e, caused by a body force $\mathbf{f}$, initial conditions $\mathbf{u}_0, \mathbf{v}_0$ locally supported and a Dirichlet datum $\mathbf{g}$, is defined by the following system:

$$\begin{cases} \rho \dfrac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x},t) - (\lambda+\mu)\nabla(\mathrm{div}\,\mathbf{u})(\mathbf{x},t) - \mu\,\nabla^2\mathbf{u}(\mathbf{x},t) & = \mathbf{f}(\mathbf{x},t) \quad (\mathbf{x},t) \in \Omega^e \times (0,T) \\ \mathbf{u}(\mathbf{x},t) & = \mathbf{g}(\mathbf{x},t) \quad (\mathbf{x},t) \in \Gamma \times (0,T) \\ \mathbf{u}(\mathbf{x},0) & = \mathbf{u}_0(\mathbf{x}) \quad \mathbf{x} \in \Omega^e \\ \mathbf{u}_t(\mathbf{x},0) & = \mathbf{v}_0(\mathbf{x}) \quad \mathbf{x} \in \Omega^e, \end{cases}$$

where $\rho > 0$ is the constant material density, $\lambda > 0$ and $\mu > 0$ are the Lamé constants. By applying a classical Helmholtz decomposition, $\mathbf{u} = \nabla\varphi_P + \mathbf{curl}\,\varphi_S$ and $\mathbf{f} = \nabla \mathrm{f}_P + \mathbf{curl}\,\mathrm{f}_S$, we split the elastic vector equation into a couple of scalar wave equations, describing, respectively, the propagation of P-waves (Primary or longitudinal) and S-waves (Secondary or transverse):

$$\begin{cases} \dfrac{\partial^2 \varphi_P}{\partial t^2}(\mathbf{x},t) - v_P^2 \nabla^2 \varphi_P(\mathbf{x},t) & = \dfrac{1}{\rho}\mathrm{f}_P(\mathbf{x},t) \\ \\ \dfrac{\partial^2 \varphi_S}{\partial t^2}(\mathbf{x},t) - v_S^2 \nabla^2 \varphi_S(\mathbf{x},t) & = \dfrac{1}{\rho}\mathrm{f}_S(\mathbf{x},t). \end{cases}$$

The two equations are coupled by the problem Dirichlet boundary conditions $\nabla\varphi_P + \mathbf{curl}\,\varphi_S = \mathbf{g}$ on Γ. This splitting has been used in [1] to solve an interior problem by a finite element method. Instead, in [2] the two aforesaid scalar equations are reformulated in terms of their associated space-time BIE representations. This approach, inherently allows to include P- and S-wave sources. The two scalar equations are discretized by combining a time convolution quadrature with a classical space collocation method. Several numerical results, including comparisons with the well known vector space-time boundary integral formulation approach are presented and discussed.

This talk comprises joint work with Giovanni Monegato and Letizia Scuderi, Dipartimento di Scienze Matematiche, Politecnico di Torino.

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Orthogonal Systems in the Complex Plane and Quadrature Processes

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Abstract: A few classes of polynomials and rational functions, orthogonal in the complex plane with respect to the Hermitian and non-Hermitian inner products are considered, as well as some applications in numerical analysis.

The first results on this subject were obtained for orthogonal polynomials on the semicircle $\Gamma = \{z = \mathrm{e}^{\mathrm{i}\theta} \,|\, 0 \le \theta \le \pi\}$ with respect to the non-Hermitian inner product defined by

$$(f, g) = \int_{\Gamma} f(z)g(z)w(z)(\mathrm{i}z)^{-1}\mathrm{d}z,$$

where $z \mapsto w(z)$ is a *complex* weight function holomorphic in the half disk $D_+ = \{z \in \mathbb{C} \,|\, |z| < 1, \, \mathrm{Im}\, z > 0\}$ (see [1], [2], [3]).

Beside the construction and analysis of these new orthogonal systems, the corresponding quadrature formulas of the highest degree of exactness are also constructed. The obtained results allow a very efficient application in the integration of quasi-singular integrals (see [4]).

Keywords: Complex orthogonal systems, Quadrature formula, Quasi-singular integrals, Recurrence relations, Zeros.

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Anti-Gaussian quadrature formulae of Chebyshev type

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Abstract: Laurie (cf. [3]), in 1996, in an attempt to estimate practically the error of the Gauss quadrature formula, developed the anti-Gaussian quadrature formula, which is an $(n+1)$-point interpolatory formula designed to have an error precisely opposite to the error of the Gauss formula for all polynomials of degree up to $2n+1$. The anti-Gaussian formula enjoys nice properties: Its nodes interlace with the Gauss nodes and, with the possible exception of the first and the last one, they are contained in the support interval; its weights are all positive; and the formula has precise degree of exactness $2n-1$ and it can easily be constructed.

A Chebyshev type quadrature formula is an n-point interpolatory formula having equal weights, real nodes and degree of exactness (at least) n (cf. [2]). Equally-weighted quadrature formulae are useful in practice, because they minimize both the number of computations involved and the effect of random errors in the function values (cf. [1, Chapter 9]). Furthermore, the study of Chebyshev type formulae is an intriguing mathematical problem.

In this talk, we examine whether there are positive measures admitting anti-Gaussian formulae of Chebyshev type.

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Yet another Sinc indefinite integration formula

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Abstract: By integrating both sides of Shannon's sampling formula, Haber [1] derived the so-called "Sinc indefinite integration" expressed as

$$\int_{-\infty}^{t} F(u)\,\mathrm{d}u \approx \sum_{j=-N}^{N} F(kh)J(j,h)(t), \quad t \in (-\infty,\infty), \tag{1}$$

where $J(j,h)(t) = \int_{-\infty}^{t} \mathrm{sinc}[(u-jh)/h]\,\mathrm{d}u$. This approximation is quite efficient if F is a rapidly decreasing function. Utilizing this fact, Haber also proposed to combine (1) with the "tanh transformation," $s = \psi(u) = \tanh(u/2)$, for indefinite integration over $x \in (-1,1)$ as

$$\int_{-1}^{x} f(s)\,\mathrm{d}s = \int_{-\infty}^{\psi^{-1}(x)} f(\psi(u))\psi'(u)\,\mathrm{d}u \approx \sum_{j=-N}^{N} f(\psi(jh))\psi'(jh)J(j,h)(\psi^{-1}(x)). \tag{2}$$

He also showed that its convergence rate is $\mathrm{O}(\exp(-c\sqrt{N}))$. After a decade, instead of the tanh transformation, Muhammad and Mori [2] proposed to employ the "double-exponential transformation," $s = \phi(u) = \tanh((\pi/2)\sinh u)$, which improves the convergence rate to $\mathrm{O}(\exp(-cN/\log N))$ [3].

However, the formula (2) has a drawback in computation of the basis function $J(j,h)(t)$, which contains the sine integral (a special function). To improve this situation, using the value table of $e_k = 1/2 + \int_0^k \mathrm{sinc}\,u\,\mathrm{d}u$, Stenger [4] derived another formula of the form

$$\int_{-1}^{x} f(t)\,\mathrm{d}t \approx \sum_{j=-N}^{N} c_j \omega_j(x), \tag{3}$$

where $c_j = h\sum_{i=-N}^{N} e_{i-j} f(\psi(ih))\psi'(ih)$, and $\omega_j(x)$ contains only elementary functions as

$$\begin{cases} \omega_{-N}(x) = \dfrac{2}{1-\psi(-Nh)}\left\{\dfrac{1-x}{2} - \displaystyle\sum_{k=-N+1}^{N}\left(\dfrac{1-\psi(kh)}{2}\right)\mathrm{sinc}[(\psi^{-1}(x)-kh)/h]\right\}, \\ \omega_j(x) = \mathrm{sinc}[(\psi^{-1}(x)-jh)/h] \quad (j=-N+1,\ldots,N-1), \\ \omega_N(x) = \dfrac{2}{\psi(Nh)+1}\left\{\dfrac{x+1}{2} - \displaystyle\sum_{k=-N}^{N-1}\left(\dfrac{\psi(kh)+1}{2}\right)\mathrm{sinc}[(\psi^{-1}(x)-kh)/h]\right\}. \end{cases}$$

The formula (3) can attain $\mathrm{O}(\exp(-c\sqrt{N}))$, which is the same as Haber's formula. In this talk, by replacing $\psi(u)$ with $\phi(u)$ in Stenger's formula, yet another formula is derived, which attains $\mathrm{O}(\exp(-cN/\log N))$. Numerical comparison is also presented.

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Gauss quadrature for linear functionals and Lanczos algorithm

Stefano Pozza
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Abstract: The Gauss quadrature can be naturally generalized to approximate quasi-definite linear functionals where the interconnections with (formal) orthogonal polynomials, (complex) Jacobi matrices, and Lanczos algorithm are analogous to those in the positive definite case. In particular, the existence of the n-weight (complex) Gauss quadrature corresponds to successfully performing the first n steps of the Lanczos algorithm. Moreover, such connections can also be extended to the case of the (look-ahead) Lanczos algorithm.

This is a joint work with M. Pranić, and Z. Strakoš.

Computing the regularized minimal-norm solution of an overdetermined system of Fredholm integral equations of the first kind in a RKHS

Giuseppe Rodriguez
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Abstract: Overdetermined systems of first kind integral equations appear in many applications. When the right-hand side is discretized, the resulting finite-data problem is ill-posed and admits infinitely many solutions. We propose a numerical method to compute the minimal-norm solution of a system of the form

$$\begin{cases} \displaystyle\int_a^b k_\ell(x_{\ell,i},t)\, f(t)\, dt = g_\ell(x_{\ell,i}), \qquad \ell = 1,\dots,m, \quad i = 1,\dots,n_\ell, \\ f(a) = f_0,\ f(b) = f_1. \end{cases}$$

in the presence of boundary constraints. The algorithm is motivated by the Riesz representation theorem and operates in a reproducing kernel Hilbert space (RKHS). Since the resulting linear system is strongly ill-conditioned, we construct a regularization method, depending on a discrete parameter, based on the expansion of the minimal-norm solution in terms of the singular functions of the integral operator defining the problem. Numerical results demonstrate the excellent performance of the proposed method.

This is a joint work with Patricia Díaz de Alba, Luisa Fermo, and Federica Pes [1, 2].

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Averaged Gauss quadrature formulas: Properties and applications

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Abstract: Gauss quadrature rules associated with a nonnegative measure with support on (part of) the real axis find many applications in Scientific Computing. It is important to be able to estimate the quadrature error when replacing an integral by an ℓ-node Gauss quadrature rule in order to choose a suitable number of nodes. A classical approach to estimate this error is to evaluate the associated $(2\ell+1)$-node Gauss–Kronrod rule. However, Gauss–Kronrod rules are not guaranteed to exist. Laurie in '96 developed $(\ell+1)$-node anti-Gauss rules that together with the corresponding ℓ-node Gauss rule for sufficiently smooth integrands provide upper and lower bounds for the desired integral. Laurie also defined averaged rules that are the average of Gauss and anti-Gauss rules. Subsequently, Spalević described weighted averaged rules that match one more moment than Laurie's averaged rules. This talk proposes to use the difference between the ℓ-node Gauss rule and the associated averaged or weighted averaged Gauss rules to estimate the error in the Gauss rule. A novel application to the estimation of the error in matrix functions also is described. This talk presents joint work with N. Eshghi and M. Spalević.

Numerical methods for 2D linear Fredholm integral equations using Padua points

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Abstract: The talk deals with the numerical approximation of 2D Fredholm linear integral equations of the type

$$f(x,y) - \mu \int_S k(x,y,s,t) f(s,t) w(s,t) ds dt = g(x,y), \qquad (x,y) \in S,$$

where $S = [-1,1]^2$, g and k are known functions defined in S and S^2, respectively, μ is a fixed real parameter and f is the unknown in S. For this kind of equation several methods where proposed, based on piecewise polynomial approximation (see for instance [1], [3]) or on global approximation methods using tensorial operators (see [4]). The global approach leads to well conditioned, stable and convergent algorithms, in which the approximate solution behaves like the best polynomial approximation of the solution f in the appropriate spaces of functions. Nevertheless usually the global strategy means also a high computational cost, if compared with the methods based on the piecewise polynomial approximation. Here we propose numerical methods of Nyström and collocation type based on the sets of Padua points, using the cubature rule and the interpolation process introduced in [5] and [2]. These choices allows to preserve the good properties of the global approach as regards to the rate o convergence, but with a reduced computational effort.

This is a joint work with Anna Lucia Laguardia.

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Efficient numerical integration of permutation-invariant functions

Markus Weimar
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Abstract: Motivated by problems from computational quantum physics we study the efficient numerical integration of multivariate functions which are invariant under permutations (of subsets) of their arguments. We find an upper bound for the nth minimal worst case error of quasi-Monte Carlo schemes and show that, under certain conditions, it can be bounded independent of the number of dimensions. Special attention is paid to unshifted and randomly shifted rank-1 lattice rules in such a permutation-invariant problem setting. In particular, we present a component-by-component algorithm to find the generating vector for a shifted rank-1 lattice rule that obtains a rate of convergence arbitrarily close to $\mathcal{O}(n^{-\alpha})$, where $\alpha > 1/2$ denotes the smoothness of the underlying function space and n is the number of cubature nodes.

The talk is based on joint work [1, 2] with D. Nuyens and G. Suryanarayana from KU Leuven, Belgium.

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