VALPARAISO'S MATHEMATICS AND ITS APPLICATIONS DAYS

Séptimo Encuentro de la Matemática y sus Aplicaciones

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso

Valparaíso, 12 y 13 de Enero de 2017

PROGRAMA

1. INTRODUCCIÓN

El **Séptimo Encuentro de la Matemática y sus Aplicaciones** ha sido organizado en conferencias secuenciales de **45 y 30 minutos** de duración (40 y 25 minutos de exposición, respectivamente, y 5 minutos para preguntas y comentarios). Todas las charlas se llevarán a cabo en la sala **IMA 2-3** en el segundo piso del Instituto de Matemáticas de la Pontificia Universidad Católica de Valparaíso.

En la siguiente página se detalla la programación correspondiente, incluyendo autor y título de la charla.

La organización agradece al Instituto de Matemáticas y al GEAGAM Network por su gran apoyo para llevar a cabo este evento. Igualmente, extiende su reconocimiento y gratitud a todos los expositores, quienes gracias a su buena voluntad de participar, han hecho posible la realización de este **VMAD 7**.

Comité Organizador

Valparaíso, Enero de 2017

2. JUEVES, 12 DE ENERO

10.10-10.15 BIENVENIDA

10.15-11.00 DAVID PARDO: *Refined Isogeometric Analysis (rIGA).*

11.00-11.30 SERGIO ROJAS: *An efficient 1.5D Galerkin method for geophysics.*

[Moderador: M. Barrientos]

11.30-12.00 COFFEE BREAK

12.00-12.30 PAULINA SEPÚLVEDA: *A spacetime DPG method for the Schrodinger equation.*

12.30-13.00 TOMÁS BARRIOS: *Analyses of DG approximations for Stokes problem based on velocity-pseudostress formulation.*

[Moderador: I. Muga]

13.00-15.00 ALMUERZO

15.00-15.30 FERNANDO CÓRDOVA: *Impulsive differential equations with dynamical pulse times. Applications towardas the biological systems.*

15.30-16.00 KARINA VILCHES: *Modelling the environmental influence in chemotaxis movements.*

16.00-16.30 PATRICIO CUMSILLE: *Classical Mathematical Modeling for Description and Prediction of Experimental Tumor Growth: the case of melanoma.*

[Moderador: D. Paredes]

16.30-17.00 COFFEE BREAK

17.00-17.30 CRISTÓBAL BERTOGLIO: *Estimation of pressure drop in blood flows from MRI.*

17.30-18.00 PABLO MOISSET de ESPANES: *A mathematical insight into intracellular iron regulation: the buffering behavior of ferritin is explained by large capacity and small exchanges.*

[Moderador: M. Barrientos]

3. VIERNES, 13 DE ENERO

10.15-11.00 RYAN McCLARREN: *High Fidelity, Moment-Based Methods for Particle Transport: The confluence of PDEs, Optimization, and HPC.*

11.00-11.30 CARLOS JERES-HANCKES: *Uncertainty Quantification for Electromagnetic Scattering by 1D PEC Gratings.*

[Moderador: D. Paredes]

11.30-12.00 COFFEE BREAK

12.00-12.30 PAUL ESCAPIL: *Wave Diffraction by Random Surfaces: Uncertainty Quantification via Sparse Tensor Boundary Elements.*

12.30-13.00 IGNACIA FIERRO: *Electromagnetic scattering at a telescope mirror.*

[Moderador: M. Barrientos]

13.00-15.00 ALMUERZO

15.00-15.30 ELWIN VAN'T WOUT: *High-performance computing of multiple wave scattering with boundary element methods*

15.30-16.00 CONSUELO FUENZALIDA: *Sparse Tensor Approximations and Smolyak Quadratures for Estimating Second-Order Statistical Moment for Neutron Flux.*

16.00-16.30 CAROLINA URZÚA-TORRES: *Optimal Operator Preconditioning for Boundary Elements on 3D screens.*

[Moderador: I. Muga]

16.30-17.00 COFFEE BREAK

17.00-17.30 GINO MONTECINOS: *A strategy for the treatment of Dirichlet boundary conditions in the context of ADER scheme for one-dimensional conservation laws.*

17.30-18.00 CRISTÓBAL CASTRO: *Numerical methods for hyperbolic equation. Applications to shallow water and linear elasticity.*

[Moderador: M. Barrientos]

20:30 CENA DE CAMARADERIA

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Analyses of DG approximations for Stokes problem based on velocity-pseudostress formulation

Tomás P. Barrios * Rommel Bustinza † Felipe Sánchez ‡

Abstract

In the present paper we propose two families of local discontinuous Galerkin methods for the numerical approximation of Stokes equations in their (nonsymmetric) velocity-pseudostress formulation. Because of a characterisation of the discrete kernel of the relevant bilinear form is not straightforward in the present setting, the well-posedness of the first kind of problems could follow from the Babuska-Brezzi theory only in the case of high-order approximations. For low-order methods (which may be more attractive in view of the associated computational complexity of tensor field-based discretisations), one Raviart-Thomas projection in combination with the Fredholm alternative allows to conclude the bijectivity of the solution operator. Error estimates are then derived, always under the assumption that the divergence of the approximation space of stresses is contained in the discrete velocity space, and that the gradient of the velocity space is contained in the pseudo-stress approximation space. Next, we relax these last restrictions by proposing two stabilised schemes: one incorporating a div-div term, and a second one bearing a Galerkin least-squares residual. The analysis of the stabilised methods is also presented, and the behaviour of the three schemes are illustrated via a few numerical examples.

References

[1] T.P. Barrios and R. Bustinza: *An augmented discontinuous Galerkin method for elliptic problems*. Comptes Rendus de l'Academie des Sciences, Series I, vol. 344, pp. 53-58, (2007).

[2] T.P. Barrios and R. Bustinza: *A priori and a posteriori error analyses of an augmented discontinuous Galerkin formulation*. IMA Journal of Numerical Analysis, vol 30, 4, pp. 987-1008, (2010).

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[3] T.P. Barrios and R. Bustinza: *An augmented discontinuous Galerkin method for stationary Stokes problem*. Preprint 2010-25, Departamento de Ingeniera Matemtica, Universidad de Concepcin, Chile, 2010.

[4] T.P. Barrios, R. Bustinza, G. C. García, and E. Hernández: *On stabilized mixed methods for generalized Stokes problem based on the velocity-pseudostress formulation: A priori error estimates*. Computer Methods in Applied Mechanics and Engineering, vol. 237-240, pp. 78-87, (2012).

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Estimation of pressure drop in blood flows from MRI

Cristóbal Bertoglio* David Nolte Axel Osses

Abstract

Blood flow velocity, hemodynamic pressure gradients, arterial stiffness, etc are very important clinical indexes of the cardiovascular condition. To date, clinical gold standard are invasive procedures or imaging techniques requiring exogenous contrast agents or x-rays. Recent advancements in inverse problems and numerical hemodynamics have shown their potential to use coupled fluid-solid models and medical images in order estimate non-invasively hemodynamic quantities from medical images [1, 2, 3].

In this talk we will focus on strategies to estimate pressure gradients from velocity data. We will detail two approaches: (a) efficient methods for the pressure gradient computation assuming the velocity is measured everywhere in space (at a certain spatial resolution), as it can be obtained by 3D Phase-Contrast MRI [4], and (b) an optimization-based approach with the incompressible Navier-Stokes equations as constraints, that may allow a reduced amount of data (e.g. 2D Phase-Contrast MRI).

References

[1] C. Bertoglio, P. Moireau, and JF. Gerbeau, *Sequential parameter estimation in fluid-structure problems. Application to hemodynamics.* Int.J.Num.Meth.Biomed.Eng., 28:434–455, (2016).

[2] C. Bertoglio, D. Chapelle, M. Fernández, JF. Gerbeau, and P. Moireau, *State observers of a vascular fluid-structure interaction model through measurements in the solid.*. Comp.Meth.Appl.Mech.Engrg., 256:149–168, (2013).

[3] C. Bertoglio, D. Barber, N. Gaddum, I. Valverde, M. Rutten, P. Beerbaum, P. Moireau, R. Hose, and JF. Gerbeau., *Identification of artery wall stiffness: in vitro validation and in vivo results of a data assimilation procedure applied to a 3D fluid-structure interaction model.* J.Biomech., 47(5):1027–1034, (2014).

[4] C. Bertoglio, R. Nuñez, F. Galarce, D. Nordsletten, A. Osses, *Relative pressure estimation from 4D velocity measurements in blood flows: state-of-the-art and new approaches.* Preprint hal-01323289, v2 (2016).

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Numerical methods for hyperbolic equations. Applications to shallow water and linear elasticity

Cristóbal Castro *

Abstract

One of the main characteristic of hyperbolic equations is the development of discontinuous solution even for smooth initial data. In order to address this condition a robust and accurate Riemann solver is necessary. In most cases, the exact solution is not available or not desirable due to computational complexity. If we consider Euler equations as example, there are number of approximate Riemann solver in the literature [3]. In this presentation we show recent developments of numerical method for solving hyperbolic equations. In particular we present an approximate, general equation of state, Riemann solver for Euler equations [4]. Another interesting aspect of hyperbolic equations is the wave propagation capability. In geophysical problems the propagation of small amplitude for long distance and time pose a mayor challenge. We show applications of tsunami [2] and seismic wave propagation [1].

References

[1] Cristóbal E. Castro, Martin Käser, and Gilbert B. Brietzke. Seismic waves in heterogeneous material: subcell resolution of the discontinuous galerkin method. *Geophys. J. Int.*, 182(1):250–264, 2010.

[2] Cristóbal E. Castro, Eleuterio F. Toro, and Martin Käser. ADER scheme on unstructured meshes for shallow water: simulation of tsunami waves. *Geophys. J. Int.*, 189(3):1505–1520, 2012.

[3] E. F. Toro. *Riemann Solvers and Numerical Methods for Fluid Dynamics, Third Edition.* Springer-Verlag Berlin Heidelberg, 2009.

[4] Eleuterio F. Toro, Cristóbal E. Castro, and Bok Jik Lee. A novel numerical flux for the 3D Euler equations with general equation of state. *J. Comput. Phys.*, 303:80–94, 2015.

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Impulsive differential equations with dynamical pulse times. Applications towardas the biological systems.

Fernando Córdova-Lepe *

Abstract

A type of impulsive differential equations (IDE) with dynamical pulse times is presented. These equations were introduced by Córdova-Lepe et al in the year 2012, [1]. In addition, some applications in mathematical modeling of biological systems are given. More precisely, some models in epidemiology (pulse vaccination), bioeconomics (pulse fishery) and bioprocess (pulse control) are discussed, see [2, 3, 4].

References

[1] F. Córdova–Lepe, M. Pinto and E. González–Olivares. A new class of differential equations with impulses at instants dependingof preceeding pulses. Applications to management of renewable resources. Nonlinear Analysis (RWA), 13:2313–2322. 2012.

[2] F. Córdova–Lepe, R. Del Valle and G. Robledo. A pulse vaccination strategy at variable times depending on incidence. Journal of Biological Systems, 19:1–16, 2011.

[3] F. Córdova–Lepe, R. Del Valle and G. Robledo. A pulse fishery model with closures as function of the catch: Conditions for sustainability. Mathematical Bioscience, 239:169–177, 2012.

[4] F. Córdova–Lepe, R. Del Valle and G. Robledo. Stability analysis of a selfcycling fermentation model with stat- edependent impulse times. Mathematical Methods in the Applied Sciences. 37:1460–1475, 2014.

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Classical Mathematical Modeling for Description and Prediction of Experimental Tumor Growth: the case of melanoma

Patricio Cumsille * Andrés Rodríguez †

Abstract

In this work we study classical mathematical models of tumor growth (see [2, 5]) in order to describe and predict melanoma development (melanoma is the most serious type of skin cancer). To do so, firstly an experimental methodology will be carry out: human melanoma cells will be grown in a culture medium RPMI-1640 with a pH of 7.2, supplemented with serum at 5% in order to stimulate division. Once confluent, cells will be suspended in a sterile medium. Next, 200,000 of these melanoma cells will be injected in the skin of two group of mice, from which daily growth will be observed starting from the 7th day post injection, by using a Caliper, measuring the length and the width of melanoma tumor for each group, control and experimental, data which will be used in order to make parameters estimation of mentioned models, thereby describing and forecasting tumor growth. Control group is composed by wild-type mice, whereas experimental group consists of mice to which Adenosine receptor of type A2 has been knocked out, with the aim to investigate the influence of Adenosine in tumor growth, since this proteine has a role as an angiogenesis modulator by enhancing vascular endothelial growth factor (VEGF)[1] activity (see [1]).

The numerical methodology required in order to make parameters estimation of the classical mathematical models, based upon ordinary differential equations (ODE), consists in employing Trust-Region-Reflective Algorithm (see [3]), a non linear optimization method specially designed to solve parameters estimation problems by non linear least squares criterion. This algorithm is implemented in Matlab© through lsqnonlin function (see [7]). In order to use it, we will give as input data of this function: the experimental data (the length and the width measured at certain times, in days), the ODE solution, if an explicit formula is available (in the case where this is not available, we use the ode45 solver of Matlab© in order to numerically solve the ODE for each

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[1]VEGF is the most important pro-angiogenic molecule triggered under hypoxic conditions.

model), an initial guess of the optimal value of the parameter vector (which in general is unknown, but exploring the relative square error, in evaluating it as a function of parameters space, we achieve an initial guess to start the optimization procedure), the Jacobian matrix of the residuals (when an explicit solution of the ODE model is available), and lower and upper bounds for the parameters (obtained also by the exploratory method mentioned before). Next, we will apply statistical methods based upon non linear least squares regression tools (see [4, 6]) in order to assess goodness of fit for parameters estimated, as well as, performance of prediction to each model studied.

The expected results of this work are: 1) establish the descriptive power of each model, using several goodness-of-fit metrics and a study of parametric identifiability, 2) assess the models ability to forecast tumor growth, this for both groups of individuals, under experimental conditions described before, and 3) conclude that both groups come from different populations, that is to say, the fact of knocking out the type A2 Adenosine receptor influences tumor growth, which will be achieved through validation of mathematical models with experimental data.

References

[1] F. Azuaje, F. Léonard, M. Rolland-Turner, Y. Devaux, and D. R. Wagner, *Proof-of-principle investigation of an algorithmic model of adenosine-mediated angiogenesis*, Theoretical Biology and Medical Modelling, 8 (2011), p. 7.

[2] S. Benzekry, C. Lamont, A. Beheshti, A. Tracz, J. Ebos, L. Hlatky, and P. Hahnfeldt, *Classical mathematical models for description and prediction of experimental tumor growth*, PLoS Comput. Biol., 10 (2014), p. e1003800.

[3] M. A. Branch, T. F. Coleman, and Y. Li, *A subspace, interior, and conjugate gradient method for large-scale bound-constrained minimization problems*, SIAM Journal on Scientific Computing, 21 (1999), pp. 1–23.

[4] K. P. Burnham and D. R. Anderson, *Model selection and multimodel inference : a practical information-theoretic approach*, Springer, New York, 2002.

[5] P. Cumsille, A. Coronel, C. Conca, C. Quiñinao, and C. Escudero, *Proposal of a hybrid approach for tumor progression and tumor-induced angiogenesis*, Theoretical Biology and Medical Modelling, 12 (2015), p. 13.

[6] C. J. W. George A. F. Seber, *Nonlinear Regression*, Wiley Series in Probability and Statistics, Wiley, 2003.

[7] The Mathworks Inc., *Nonlinear least squares (curve fitting)*. `https://www.mathworks.com/help/optim/nonlinear-least-squares-curve-fitting.html`, 2016. [Online; accessed 2016].

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Wave Diffraction by Random Surfaces: Uncertainty Quantification via Sparse Tensor Boundary Elements

Paul Escapil-Inchauspé * Carlos Jerez-Hanckes †

Abstract

We consider the numerical solution of time-harmonic scattering of acoustic and electromagnetic waves from obstacles with uncertain geometries. Using first-order shape derivatives, we derive deterministic boundary integral equations for the mean field and the two-point correlation function of the random solution for a soft-obstacle Dirichlet problem. Sparse tensor Galerkin discretizations of these equations are implemented with the so-called *combination technique*. Similar discretization errors for the covariance is achieved with $\mathcal{O}(N \log N)$ degrees of freedom instead of $\mathcal{O}(N^2)$. Performance comparison of our approach to classic Monte-Carlo Galerkin formulation is given for different shapes. Finally, we verify the robustness of the sparse tensor approximation and compare it to low-rank approximations techniques.

References

[1] H. Harbrecht, R. Schneider, and C. Schwab, *Sparse second moment analysis for elliptic problems in stochastic domains*, Numerische Mathematik, 109 (2008), pp. 385–414.

[2] H. Harbrecht, M. Peters and M. Siebenmorgen, *Combination technique based k-th moment analysis of elliptic problems with random diffusion*, Journal of Computational Physics, **252** (2013), pp. 128–141.

[3] C. Jerez-Hanckes and C. Schwab, Electromagnetic wave scattering by random surfaces: Uncertainty quantification via sparse tensor boundary elements, *IMA Journal of Numerical Analysis* (2016).

[4] R. Potthast, *Frechet differentiability of boundary integral operators in inverse acoustic scattering*, Inverse Problems, 10 (1994), p. 431.

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[5] S. Sauter and C. Schwab, *Boundary Element Methods*, Springer Series in Computational Mathematics, Springer Berlin Heidelberg, 2010.

[6] T. von Petersdorff and C. Schwab, *Sparse finite element methods for operator equations with stochastic data*, Applications of Mathematics, 51 (2006), pp. 145–180.

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Electromagnetic scattering at a telescope mirror

María Ignacia Fierro Piccardo *

Abstract

This presentation is part of a ModEM project, which has as a main objective finding out out how defects on a telescope mirror could cause noise its observations. The hipothesis is that gaps on a telescope surface produce changes on the polarizarion of the field scattered by the mirror. This problem is usually attacked by high frequency methods, as Physical Optics (PO) or Physical Theory of Diffraction (PTD), but in order to validate the results obtained by those methods, we propose to use the Boundary Elements Method on a common problem with the PO/PTD methods. For this reason, in this presenntation we show some of the preliminar results that will allow us to decide about the effect of the defects on the telescope mirror and, in a future, to validate or refutate the results obtained by PO/PTD.

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Sparse Tensor Approximations and Smolyak Quadratures for Estimating Second-Order Statistical Moment for Neutron Flux

María Consuelo Fuenzalida * Carlos Jerez * Ryan McClarren †

Abstract

In this work, we develop a novel method to compute the second order statistical moment of neutron flux inside a reactor by solving the neutron transport equation for its moments. Randomness comes from the lack of precise of knowledge of external sources as well as of cross-section parameters. Thus, the flux is itself a random variable and we are interested in computing its moments directly instead of using Monte-Carlo simulations. This approach, however, entails the appearance of the so-called curse of dimensionality. By assuming as given both the second moment of sources and probability distributions of cross-section parameters, we present an efficient method based on a sparse tensor finite-element method approximation as well as the use of Smolyak quadratures.

References

[1] Ayres, D. and Eaton, M.D., *Uncertainty quantification in nuclear criticality modelling using a high dimensional model representation.* Annals of Nuclear Engineering, vol. 80, 5, pp. 379-402, (2015).

[2] Harbrecht, H., Schneider, R. and Schwab, C., *Sparse second moment analysis for elliptic problems in stochastic domains.* Numerische Matematik, vol. 109, pp. 385-414, (2008).

[3] Larsen E, G.N., Morel, J. and Miller, W., *Asymptotic Solution of Numerical Transport Problems in Optically Thick, Diffusive Regimes.* Journal of Computational Physics, vol. 69, pp. 283-324, (1987).

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Uncertainty Quantification for Electromagnetic Scattering by 1D PEC Gratings

R. Aylwin* C. Jerez-Hanckes * G. Silva *,† P. Fay †

Abstract

We present a deterministic numerical method able to calculate efficiently first and second statistical moments of the scattered field by a periodic perfect electric conductor surface with stochastic perturbations on its surface. The electric field integral equation (EFIE) was solved using boundary elements method (BEM), and constant hierarchical bases, called Haar wavelets. To validate the BEM implementation the method was compared to COMSOL Multiphysics. On the other hand, to validate the stochastic calculations, the algorithm was compared to the Monte-Carlo simulation, obtaining good agreement in both cases. The proposed deterministic approach converges faster than Monte-Carlo simulation with $O(N \log N)$ computational effort.

References

[1] Solano, M. E., Faryad, M. , Monk, P. B., Mallouk, T. E., and Lakhtakia, A. *Periodically multilayered planar optical concentrator for photovoltaic solar cells*,' Applied Physics Letters, vol. 103, no. 19, p. 191115, 2013.

[2] Harbrecht, H., Schneider, R. and Schwab, C., *Sparse second moment analysis for elliptic problems in stochastic domains*. Numerische Matematik, vol. 109, pp. 385-414, (2008).

[3] Harbrecht, H., Schneider, R. and Schwab, C., *Multilevel frames for sparse tensor product spaces*, 2007.

[4] Bruno, O. P. and Haslam, M. C., *Efficient high-order evaluation of scattering by periodic surfaces: deep gratings, high frequencies, and glancing incidences*,' Journal of the Optical Society of America A, vol. 26, pp. 658 – 668, Feb. 2009.

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High Fidelity, Moment-Based Methods for Particle Transport: The confluence of PDEs, Optimization, and HPC

Ryan G. McClarren *

Abstract

The calculation of the transport of particles is important in many applications including rarefied gas dynamics, plasma physics, and the nuclear energy systems. In this talk I will motivate the choice of moment-based methods for solving particle transport problems, and discuss the difficulties such approaches have. To obtain physically-meaningful solutions the discretization of the original integro-differential equation can depend on the solution to an optimization problem. I will show how these optimization problems arise, what methods perform best in terms of cost and accuracy, and how these problems can be well-suited for high performance computing.

References

[1] McClarren, R.G., Holloway, J.P., and Brunner, T.A., *On solutions to the P_n equations for thermal radiative transfer.*. Journal of Computational Physics 227.5: 2864-2885 (2008).

[2] Hauck, C.D., and McClarren, R.G., *Positive P_N Closures.* SIAM Journal on Scientific Computing, 32(5), 2603-2626, (2010).

[3] Laiu, M.P., Hauck, C.D., McClarren, R.G., O'Leary, D.P. and Tits, A.L., *Positive filtered p n moment closures for linear kinetic equations.* SIAM Journal on Numerical Analysis, in press (2016).

[4] McClarren, R.G. and Hauck, C.D., *Simulating radiative transfer with filtered spherical harmonics.*. Physics Letters A, 374(22), pp.2290-2296 (2010).

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A mathematical insight into intracellular iron regulation: the buffering behavior of ferritin is explained by large capacity and small exchanges

P. Moisset de Espans * A. Olivera-Nappa † J. Soto ‡

Abstract

Ferritin is a highly conserved ubiquitous iron-storage protein present in archaea, bacteria and eukaryotic cells and is also thought to be the major iron concentration buffer inside cells. Ferritin is a hetero-24- mer formed by two different peptide chains that assemble in a hollow sphere multimeric structure. This molecular structure is strikingly different from all other intracellular metal ion concentration buffers and determines two unique ferritin functional features: ferritin fer- rooxidase activity sequesters soluble Fe2+ ions as insoluble Fe 3+ oxides inside the protein cavity, where they remain isolated from the external medium, and they can only be exchanged with the exterior through small channels that allow only a few iron atoms to pass simultaneously. The latter is exacerbated by the enzymatic activity itself, which imposes a kinetic limiting step on the amount of iron atoms that can be processed in a given period, in stark contrast with most common intracellular buffers that do not possess catalytic activity. Using a simple model based on mass action kinetics with minimal mechanistic hypothesis, we show that the isolation of iron atoms inside the protein and the exchange of few atoms at a time are sufficient to qualitatively determine ferritins dynamic behavior and to satisfy the stringent free iron intracellular concentration requirements. The main characteristics of this control profile are an almost constant free iron 1profile for a broad range of total iron concentrations, a single and globally stable equilibrium, a fast control velocity when faced to total iron concentration perturbations and an energy-efficient operation. This sophisticated and robust control response is radically different from those of other intra and extracellular buffer systems and has been achieved by using a surprisingly simple structurally and catalytically based strategy that do not require feedback control loops or sensing devices.

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Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 12 y 13 Enero, 2017

A strategy for the treatment of Dirichlet boundary conditions in the context of ADER scheme for one-dimensional conservation laws

G. I. Montecinos *

Abstract

ADER schemes are high-order numerical methods, which nowdays are very popular. The so called reconstruction procedure is one of their building block, see [1] for details. ADER method for general conservation laws, may lose accuracy if boundary conditions are not deal properly. In this work the treatment of Dirichlet boundary conditions, is concerned. The reconstruction procedure, near boundaries, demands for information outside the computational domain, which is carried out in terms of numerical solutions of auxiliary problems. These problems are hyperbolic and they are constructed from the conservation laws and the information at boundaries. The evolution of these problems, unlike to the usual manner, is done in space rather than in time due to that, these are named, *reverse problems*. The methodology can be seen as a numerical version of the inverse Lax-Wendroff procedure, [2]. Expected orders of accuracy for solving conservation laws by using the proposed strategy at boundaries, are obtained up to fifth-order in both space and time, [3] for details.

References

[1] E. F. Toro. *Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction*. Springer-Verlag, third edition, 2009. ISBN 978-3-540-25202-3.

[2] S. Tan and C.-W. Shu. Inverse Lax-Wendroff procedure for numerical boundary conditions of conservation laws. *Journal of Computational Physics*, 229(21):8144 – 8166, 2010.

[3] G. I. Montecinos. *A strategy to implement Dirichlet boundary conditions in the context of ADER finite volume schemes. One-dimensional conservation laws.* Computers & Fluids, 140: 357 - 370, 2016

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Refined Isogeometric Analysis (rIGA)

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Abstract

Isogeometric Analysis (IGA) is a discretization method commonly employed nowadays to solve numerical problems governed by partial differential equations (PDEs). This method employs Computed-Aided Design (CAD) functions as basis functions to build the discretization of the governing PDEs [1]. This choice avoids to define a secondary set of functions for the engineering analysis, which drastically reduces the time and implementation efforts of the pre-processing step. In addition, highly continuous CAD functions provide better approximation properties than traditional Finite Element method on a per-degree of freedom basis, suggesting IGA is an accurate and robust scheme to approximate the solution of PDEs [2, 3]. Unfortunately, a high degree in the continuity also degrades the performance of direct solvers, increasing the computational cost per degree of freedom, resulting in larger solution time and memory requirements [4].

In this work, we propose an approach to dramatically reduce the computational time employed to approximate the PDEs solution when using highly continuous IGA discretizations. This method adjusts locally the continuity of the basis functions according to how the solver of linear equations operates. Starting from a highly continuous C^{p-1} IGA, the method enriches the space by decreasing the continuity over certain hyperplanes. These hyperplanes correspond to: (a) the separators used during the elimination of the degrees of freedom (dof) when using direct solvers, and (b) the skeleton obtained after static condensation of certain macro-element unknowns for the case of iterative solvers. We denote this method as "refined Isogeometric Analysis" or rIGA [5].

Despite the fact that rIGA spaces are richer than those coming from highly continuous C^{p-1} IGA systems, the computational time required to solve the resulting system of linear equations for a given mesh and fixed polynomial order is reduced both in the

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cases of direct and iterative solvers with respect to their highly continuous C^{p-1} IGA counterpart.

For the case of direct solvers, this reduction factor is approximately p^2, being p the polynomial order. For instance, in a $2D$ quadrilateral mesh with four million elements and $p = 5$, the system resulting from rIGA is solved in almost *one* minute, while the system obtained from IGA requires approximately 22 minutes to be solved. In $3D$, when the mesh size is two million elements and $p = 3$, the rIGA system is solved in *one* hour, while the system obtained from IGA requires almost 15 hours to be solved.

For the case of iterative solvers, the savings of rIGA with respect to C^{p-1} IGA are more moderate and show an increment as the polynomial degree grows. For a mesh with four million elements and polynomial degree $p = 9$, rIGA delivers a reduction factor of approximately 3 with respect to C^{p-1} IGA.

References

[1] T. J. R. Hughes and J. A. Cottrell and Y. Bazilev., *Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement.* Comput. Methods Appl. Mech. Engrg., vol. 194, (39-41), pp. 4135-4195, (2005).

[2] V. P. Nguyen and C. Anitescu and S. P. A. Bordas and T. Rabczuk., *Isogeometric analysis: An overview and computer implementation aspects.* Mathematics and Computers in Simulation, vol. 117, pp. 89-116, (2015).

[3] J. A. Evans and Y. Bazilevs and I. Babuška and T. J. R. Hughes., *n-Widths, supinfs, and optimality ratios for the k-version of the isogeometric finite element method.* Comput. Methods Appl. Mech. Engrg., vol. 198, (21-26), pp. 1726-1741, (2009).

[4] N. Collier and D. Pardo and L. Dalcin and M. Paszyński and V.M. Calo., *The cost of continuity: A study of the performance of isogeometric finite elements using direct solvers.* Comput. Methods Appl. Mech. Engrg., vol. 213-216, pp. 353-361, (2012).

[5] D. Garcia and D. Pardo and L. Dalcin and M. Paszyński and N. Collier and V. M. Calo., *The Value of Continuity: Refined Isogeometric Analysis and Fast Direct Solvers..* Comput. Methods Appl. Mech. Engrg., *in press*, (2016).

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An efficient 1.5D Galerkin method for geophysics.

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Abstract

To characterize hydrocarbon (oil and gas) bearing formations, usually maps of the Earth subsurface are estimated by interpreting resistivity measurements obtained from various electromagnetic impulses through the media. In logging-while-drillling (LWD) operations, it is required to estimate the resistivities ideally in real (logging) time (see [2, 5]).

In multiple reservoirs, it is customary to assume homogeneous materials along two spatial directions, making possible the dimensional reduction of the problem through a Hankel transform, obtaining a so called 1.5D formulation. Under this assumption, semi-analytical methods can be employed to solve a single forward problem in a fraction of a second (see [1, 3, 8], and more recently [4, 6, 7, 9]). However, these methods have several limitations, including: (a) they can only consider piecewise constant materials, and (b) it is difficult (and sometimes impossible) to obtain semi-analytical derivatives, forcing the use of expensive finite difference schemes. When considering Galerkin-type formulations for the 1.5D problem, more general models can be considered. Moreover, accurate approximations of the derivatives can be obtained through the resolution of an adjoint problem. Unfortunately, standard Galerkin methods are relatively slow when compared to the semi-analytical solution, as it occurs in practical applications.

In this talk, we present a novel Hankel-Galerkin multi-scale method that drastically reduces the total computational time. The method employs multi-scale basis functions. The resulting procedure is computationally expensive when comparing with a single forward resolution; however, it becomes competitive when solving multiple forward problems. In the presentation, we introduce the method for the acoustic an electromagnetic cases, and show numerical results validating its accuracy.

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References

[1] Chew, W.C., Chen, S.Y., *Response of a point source embedded in a layered medium.* Antennas and Wireless Propagation Letters, IEEE **2**(1), 254-258 (2003).

[2] Ijasan, O., Torres-Verdín, C., Preeg, W.E., *Inversion-based petrophysical interpretation of logging-while-drilling nuclear and resistivity measurements.* Geophysics **78**(6), D473-D489 (2013).

[3] Kong, J., *Electromagnetic fields due to dipole antennas over stratified anisotropic media.* Geophysics **37**(6), 985-996 (1972).

[4] Løseth, L., Ursin, B., *Electromagnetic fields in planarly layered anisotropic media.* Geophysical Journal International **170**(1), 44-80 (2007).

[5] Pardo, D., Torres-Verdín, C., *Fast 1D inversion of logging-while-drilling resistivity measurements for improved estimation of formation resistivity in high-angle and horizontal wells.* Geophysics **80**(2), E111-E124 (2015).

[6] Rojas, S., Muga, I., Pardo, D., *A quadrature-free method for simulation and inversion of 1.5D direct current (DC) borehole measurements.* Computational Geosciences, **20**(6), 1301-1318 (2016).

[7] Streich, R., Becken, M., *Sensitivity of controlled-source electromagnetic fields in planarly layered media.* Geophysical Journal International **187**(2), 705-728 (2011).

[8] Wait, J.R., *The magnetic dipole over the horizontally stratified Earth.* Canadian Journal of Physics 29(6), 577-592 (1951).

[9] Zhong, L., Li, J., Bhardwaj, A., Shen, L.C., Liu, R.C., *Computation of triaxial induction logging tools in layered anisotropic dipping formations.* Geoscience and Remote Sensing, IEEE Transactions on 46(4), 1148-1163 (2008).

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A spacetime DPG method for the Schrödinger equation

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Sriram Nagaraj [‡] Paulina Sepúlveda [§]

Abstract

The aim of this talk is to describe a spacetime Discontinuous Petrov Galerkin (DPG) method for the linear time-dependent Schrödinger equation. We show that it is possible to lose solutions if the second order Schrödinger equation is reformulated into a first order formulation. This makes spacetime methods based on a second order formulation particularly attractive for capturing irregular solutions. We show some numerical experiments motivated by pulse propagation in dispersive optical fibers.

References

[1] Demkowicz, L., Gopalakrishnan, J., Nagaraj, S. and Sepúlveda, P., *A spacetime DPG method for the Schrodinger equation. ArXiV:1610.04678, (2016).*

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Optimal Operator Preconditioning for Boundary Elements on 3D screens

Ralf Hiptmair * Carlos Jerez-Hanckes † Carolina Urzúa-Torres ‡

Abstract

The discretization of first-kind boundary integral operators (BIOs) by low-order Galerkin BEM leads to ill-conditioned linear systems on fine meshes. Consequently, iterative solvers become prohibitely slow and preconditioning is necessary.

The standard "Calderón preconditioning" technique breaks down when considering open boundaries as when modeling screens. In this case, the double layer operator and its adjoint vanish. Moreover, the associated weakly singular and hypersingular operators no longer map fractional Sobolev spaces in a dual fashion.

We propose new Calderón-type preconditioners for the hypersingular and weakly singular operators arising from the Laplacian on screens. For their construction, we use operator preconditioning [1] and the bilinear forms induced by their recently found inverse BIOs over the disk [2, 4].

In addition, we are able to apply our preconditioning technique to non-uniform meshes [3]. This property poses a great advantage, as solutions of boundary integral equations on screens Γ feature a square-root type singularity at $\partial\Gamma$, which can be resolved by refining towards the boundary.

Numerical examples illustrate the optimality of our preconditioners when applied to different screens.

References

[1] Hiptmair, R. *Operator Preconditioning.* Computers and Mathematics with Applications. 52, pp. 699-706, (2006).

[2] R. Hiptmair, C. Jerez-Hanckes, C.Urzúa-Torres *Optimal Operator Preconditioning for the Hypersingular Operator Over 3D Screens.* Tech. Rep. 2016-09, Seminar for Applied Mathematics, ETH Zürich, (2016).

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[3] R. Hiptmair, C.Urzúa-Torres *Dual Mesh Operator Preconditioning On 3D Screens: Low-Order Boundary Element Discretization.* Tech. Rep. 2016-14, Seminar for Applied Mathematics, ETH Zürich, (2016).

[4] R. Hiptmair, C. Jerez-Hanckes, C.Urzúa-Torres *Optimal Operator Preconditioning for the Weakly Singular Operator Over 3D Screens.* (In preparation).

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Modelling the environmental influence in chemotaxis movements

Karina Vilches Ponce *

Abstract

In this presentation, we review the state of the art about the incorporation of the environmental influence in the chemotaxis classical modelling. The mathematical results obtained by different authors will be summarized and the remaining challenges in this subject will be given.

References

[1] Chae, M., Kang, K., & Lee, J. *Global existence and temporal decay in Keller-Segel models coupled to fluid equations.* Communications in Partial Differential Equations, 39(7), 1205-1235. (2014).

[2] Espejo, E., & Suzuki, T. *Reaction terms avoiding aggregation in slow fluids.* Nonlinear Analysis: Real World Applications, 21, 110-126.(2015).

[3] Lorz, A. *Coupled Keller-Segel-Stokes model: global existence for small initial data and blow-up delay.* Communications in Mathematical Sciences, 10(2), 2012. (2012).

[4] Tao, Y., & Winkler, M. *Locally bounded global solutions in a three-dimensional chemotaxis-Stokes system with nonlinear diffusion.* In Annales de l'Institut Henri Poincare (C) Non Linear Analysis (Vol. 30, No. 1, pp. 157-178). Elsevier Masson. (2013, February).

[5] Winkler, M. *Global large-data solutions in a chemotaxis-Navier Stokes system modeling cellular swimming in fluid drops.* Communications in Partial Differential Equations, 37(2), 319-351.(2012).

[6] Winkler, M. *Stabilization in a two-dimensional chemotaxis-NavierStokes system.* Archive for Rational Mechanics and Analysis, 211(2), 455-487. (2014).

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High-performance computing of multiple wave scattering with boundary element methods

Elwin van 't Wout *

Abstract

Computational simulation of wave scattering at multiple objects is of interest to different areas in engineering and physics. Two such applications are the prediction of acoustic scattering at rib cages for the planning of medical treatment procedures and the electromagnetic scattering at telescope mirrors for astronomical signal processing. Furthermore, both problems require the simulation of high-frequent wave fields at large-scale objects. Since the geometry is embedded in free space, the Boundary Element Method (BEM) is the prime choice of numerical algorithm. Because of the surface integral representation, the number of degrees of freedom scales favourably compared to volumetric methods. However, solving the dense set of linear equations poses severe limitations on the maximum frequency that can be used on present-day computing platforms. Here, a combination of parallelisation, preconditioning, and compression techniques will be used to achieve large-scale BEM simulations.

References

[1] E. van 't Wout, P. Gélat, T. Betcke, and S. Arridge, *A fast boundary element method for the scattering analysis of high-intensity focused ultrasound.* JASA, vol. 138, pp. 2726–2737, 2015.

[2] T. Betcke, E. van 't Wout, and P. Gélat, *Computationally Efficient Boundary Element Methods for High-Frequency Helmholtz Problems in Unbounded Domains.* Chapter to appear in "Modern solvers for Helmholtz problems", Geosystems Mathematics, Springer, 2017.

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