VALPARAISO'S MATHEMATICS AND ITS APPLICATIONS DAYS

Quinto Encuentro de la Matemática y sus Aplicaciones

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso

Valparaíso, 07, 08 y 09 de Enero de 2015

PROGRAMA

1. INTRODUCCIÓN

El **Quinto 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 **CC 1-35** en la Casa Central 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 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 5**.

Comité Organizador

Valparaíso, Enero de 2015

2. MIERCOLES, 07 DE ENERO

11.10-11.15 BIENVENIDA

11.15-12.00 MACIEJ PASZYNSKI: *Multi-thread multi-frontal direct solver with GALOIS scheduler for adaptive grids.*

12.00-12.45 DAVID PARDO: *Dimensionally Adaptive Methods for the Simulation and Inversion of Resistivity Geophysical Measurements.*

[Moderador: M. Barrientos]

12.45-15.00 ALMUERZO

15.00-15.30 DIEGO PAREDES: *Multiscale Hybrid-Mixed Method for Porous Media Problems.*

15.30-16.00 LUIS FRIZ: *Exponential stability of the magneto-micropolar fluids.*

16.00-16.30 PATRICIO CUMSILLE: *Spatial modeling of tumor drug resistance: the case of liver gist metastases.*

[Moderador: S. Ossandón]

16.30-17.00 COFFEE BREAK

17.00-17.30 CARLOS SPA: *An efficient implementation of a finite-difference room acoustics model in CUDA.*

17.30-18.00 ALEJANDRO ALLENDES: *Adaptive stabilized methods for the NavierStokes equations in three dimensions.*

[Moderador: E. Hernández]

3. JUEVES, 08 DE ENERO

11.15-12.00 JAIME ORTEGA: *Some Ideas on Inverse Geometric Problems in Water Waves*

12.00-12.45 HECTOR RAMIREZ: *On optimal strategies for feeding in minimal time a Sequential Batch Reactors with several species.*

[Moderador: E. Hernández]

12.45-15.00 ALMUERZO

15.00-15.30 FABIO CARRERA: *Development of a dynamical biomodel of anaerobic sludge thickening*

15.30-16.00 ALEJANDRO ROJAS: *Comparison between the MINC and MRMT configurations: The n-dimensional case.*

16.00-16.30 ANDRES DONOSO: *Optimization in biogas processes production. The importance of global sensitivity analysis, optimization procedure and uncertainty analysis.*

[Moderador: M. Barrientos]

16.30-17.00 COFFEE BREAK

17.00-17.30 DANTE KALISE: *Numerical methods for Hamilton-Jacobi-Bellman equations and applications in optimal control.*

17.30-18.00 MAURICIO BARRIENTOS: *A Moving Mesh Method Applied to a Biological Problem.*

[Moderador: S. Ossandón]

20:30 CENA DE CAMARADERIA

4. VIERNES, 09 DE ENERO

FORO INVESTIGACIÓN: Reunión para discusión e intercambio de ideas

15.30-17.00 LUGAR: *INSTITUTO DE MATEMÁTICAS, PUCV. SALA IM 2-1*

[Moderador: I. Muga]

V-MAD 5

Quinto Encuentro en Aplicaciones de la Matemática

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

Adaptive stabilized methods for the Navier–Stokes equations in three dimensions

Alejandro Allendes * Abner H. Poza † Richard Rankin ‡

Abstract

This work proposes and analyses an adaptive finite element scheme for the fully non-linear incompressible Navier-Stokes equations in a three dimensional space. The a posteriori error analysis is based on a Ritz projection of the residuals of the equation in conjunction with the construction of equilibrated boundary fluxes leading to the resolution of a local Neumann-type problem, for which minimized explicit solutions are constructed. The analysis is performed for a Residual Local Projection (RELP) finite element method, but can be easily modified to obtain error estimators for other stabilized methods, such as SUPG or SDFEM schemes. Finally, several numerical tests are performed to validate the analysis and test the performance of the error estimator.

References

[1] Alejandro Allendes, Francisco Durán and Richard Rankin, *Right inverse of the divergence operator and its application to the a posteriori error analysis of finite element approximations, submitted*, 2014.

[2] Rodolfo Araya, Abner H. Poza and Frédéeric Valentin, *An adaptive residual local projection finite element method for the Navier–Stokes equations. To appear in Advances in Computational Mathematics*, 2014.

[3] J. Tinsley Oden, Weihan Wu, and Mark Ainsworth, *An a posteriori error estimate for finite element approximations of the Navier-Stokes equations.* Comput. Methods Appl. Mech. Engrg., 111(1-2):185202, 1994.

[4] R. Verfürth., *A posteriori error estimates for nonlinear problems. Finite element discretizations of elliptic equations.* Math. Comp., 62(206):445475, 1994.

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V-MAD 5

Quinto Encuentro en Aplicaciones de la Matemática

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

A Moving Mesh Mothod Applied to a Biological Problem

Mauricio Barrientos * Karina Vilches †

Abstract

In this work we study a parabolic problem arised from Keller-Segel model for chemotaxis. A new formulation of the system of partial differential equations is obtained by the introduction of a new variable, which is approximated via mixed finite element methods. At this point, the applicability of adaptive moving meshes theory is carried out with the purpose of obtain a cheap and better description of the behavior of the particles close to the blow up.

References

[1] M.J. Baines, M.E. Hubbard and P.K. Jimack, *Velocity-Based Moving Mesh Methods for Nonlinear Partial Differential Equations*, Commun. Comput. Phys., vol. 10 (3) (2011) 509–576.

[2] E.F. Keller and L.A. Segel, *Traveling bands of chemotactic bacteria*, J. Thoer. Biol., vol. 30 (1971) 235–248.

[3] R. Marlow, M.E. Hubbard and P.K. Jimack, *Moving mesh methods for solving parabolic partial differential equations.* Comput. & Fluids, vol. 46 (2011), 353–361.

[4] A. Morrocco, *Numerical Simulation of Chemotactic Bacteria Aggregation via Mixed Finite Elements*, ESAIM: M2AN., vol. 37 (4) (2003) 617–630.

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Quinto Encuentro en Aplicaciones de la Matemática

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

Development of a dynamical biomodel of anaerobic sludge thickening*

F. Carrera-Chapela[a,b,c] A. Torrico[d] A. Donoso-Bravo[a,b]
A. Osses[d] Jose A. Gonzalez[c] Héctor Ramírez C.[b,d] G. Ruiz-Filippi[a,b]

Abstract

During treatment of sewage urban, sludge are generated and should be stabilized, usually via anaerobic digestion prior to subsequent deposition on land or landfill. After anaerobic digestion, sludge are thickened and in this point gases released into the atmosphere (as hydrogen sulfide) are generators bad odor. In order to evaluate the impact of the residual biological activity in the sludge content in the thickener, a dynamic model (BDEL) which includes conversion of organic matter into biogas and hydrogen sulfide was developed, including the hydrodynamic described by Takacs model.

The results obtained using the BDEL model shown the emission flow rates of methane and hydrogen sulphide in amounts sufficient to have a negative impact on the environment as emission of greenhouse gas effect and odorant compound. The results indicate that the biological activity in the thickener is of great importance in the emission of these compounds into the atmosphere.

References

[1] Kalyuzhnyi, S.V. and Fedorovich, V.V., *Mathematical modelling of competition between sulphate reduction and methanogenesis in anaerobic reactors*, Bioresource Technology, vol. 65, 3, pp. 227–242, (1998).

[2] Lebrero, R., Bouchy, L., Stuetz, R. and Muñoz, R. *Odor Assessment and Management in Wastewater Treatment Plants: A Review*, Critical Reviews in Environmental Science and Technology, vol. 41, 10, pp. 915–950, (2011).

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[3] Metcalf and Eddy, *Wastewater engineering: Collection and pumping of wastewater* McGraw-Hill, New York, N.Y.,1981.

[4] Stellacci, P., Liberti, L., Notarnicola, M. and Haas, C.N., *Hygienic sustainability of site location of wastewater treatment plants* Desalination, vol. 253, 1-3, pp. 51–56, (2010).

[5] Takacs, I., Nolasco, G. and Patryioand, D.,*Clarification-Thickening Process*, Water Research, vol. 10, 25, pp.1263–1271, (1991).

[6] Bernard, O., Hadj, Z., Dochain, D., Genovesi, A. and Steyer, J.P., *Dynamical model development and parameter identification for an anaerobic wastewater treatment process* Biotechnology and bioengineering, vol. 75, 4, pp. 424–438, (2001).

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Quinto Encuentro en Aplicaciones de la Matemática
Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

Spatial modeling of tumor drug resistance: the case of liver gist metastases

Thierry Colin * Francois Cornelis † Patricio Cumsille ‡ Guillaume Lefebvre § Clair Poignard ¶ Olivier Saut ‖

Abstract

This work is devoted to modeling gastrointestinal stromal tumor (GIST) metastases in the liver, their growth and resistance to therapies. More precisely, resistance to two standard treatments based on tyrosine kinase inhibitors (imatinib and sunitinib) is observed clinically. Using observations from medical images, we build a spatial model consisting in a set of nonlinear partial differential equations. After calibration of its parameters with clinical data, this model reproduces qualitatively and quantitatively the spatial tumor evolution of one specific patient. Important features of the growth such as the appearance of spatial heterogeneities and therapeutic failures may be explained by our model. We then investigate numerically the possibility of optimizing the treatment in order to increase the progression free survival time and the minimum tumor size reachable by varying the dose of the first treatment. We find that according to our model, the progression free survival time becomes flat with respect to this dose. We also demonstrate numerically that the spatial structure of the tumor may provide much more insights on the cancer cell activities than the standard RECIST criteria, which only consists in the measurement of the tumor diameter.

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References

[1] T. Colin, F. Cornelis, P. Cumsille, G. Lefebvre, C. Poignard, and O. Saut, *Spatial modeling of tumor drug resistance: the case of liver gist metastases*, Submitted to Mathematical Medicine and Biology (2014).

[2] F. Cornelis, O. Saut, P. Cumsille, D. Lombardi, A. Iollo, J. Palussiere, and T. Colin, *In vivo mathematical modeling of tumor growth from imaging data: Soon to come in the future?*, Diagnostic and Interventional Imaging, 94 (2013), pp. 593–600.

[3] F. Billy, B. Ribba, O. Saut, H. Morre-Trouilhet, T. Colin, D. Bresch, J.-P. Boissel, E. Grenier, and J.-P. Flandrois, *A pharmacologically based multiscale mathematical model of angiogenesis and its use in investigating the efficacy of a new cancer treatment strategy*, Journal of Theoretical Biology, 260 (2009), pp. 545–562.

[4] H. M. Byrne, *Dissecting cancer through mathematics: from the cell to the animal model*, Nature Reviews Cancer, 10 (2010), pp. 221–230.

[5] T. Colin, A. Iollo, D. Lombardi, and O. Saut, *System identification in tumor growth modeling using semi-empirical eigenfunctions*, Mathematical Models and Methods in Applied Sciences, 22 (2012), p. 1250003.

[6] F. Lignet, S. Benzekry, S. Wilson, F. Billy, O. Saut, M. Tod, B. You, A. A. Berkane, S. Kassour, M. Wei, E. Grenier, and B. Ribba, *Theoretical investigation of the efficacy of antiangiogenic drugs combined to chemotherapy in xenografted mice*, Journal of Theoretical Biology, 320 (2013), pp. 86–99.

[7] B. Ribba, T. Colin, and S. Schnell, *A multiscale mathematical model of cancer, and its use in analyzing irradiation therapies*, Theoretical Biology and Medical Modelling, 3 (2006), p. 7.

[8] B. Ribba, O. Saut, T. Colin, D. Bresch, E. Grenier, and J. Boissel, *A multiscale mathematical model of avascular tumor growth to investigate the therapeutic benefit of anti-invasive agents*, Journal of Theoretical Biology, 243 (2006), pp. 532–541.

[9] B. Ribba, O. Saut, T. Colin, D. Bresch, E. Grenier, and J. P. Boissel, *A multiscale mathematical model of avascular tumor growth to investigate the therapeutic benefit of anti-invasive agents*, Journal Theoretical Biology, 243 (2006), pp. 532–541.

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Quinto Encuentro en Aplicaciones de la Matemática

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

Optimization in biogas processes production. The importance of global sensitivity analysis, optimization procedure and uncertainty analysis

Andres Donoso-Bravo[a,*] Fabio Carrera-Chapela[a,b,*]
Gonzalo Ruiz-Filippi[*]

Abstract

Biogas produced during the anaerobic degradation of the organic matter from waste and wastewater has become an important source of renewable energy. Mathematical modeling can help to predict and control the system behavior in order to assure process stability and biogas production maximization. The identifiability of anaerobic digestion models presents serious difficulties mostly due to the lack of reliable measurements, usually only ethe biogas flow. In this study, an assessment of the optimization of an anaerobic digestion model in a batch test is presented based on the application of global sensitivity analysis, multi-start optimization procedure and parameters uncertainty estimation. In regards to the experimental information two different conditions that can be actually manipulated, were assessed: the initial conditions in terms of substrate and biomass in the batch test and the sampling frequency of the biogas flow.

The results indicate that if methane is considered as the sole experimental output, the variations of the initial conditions regarding the substrate and inoculum in a batch test does not improve the models parameters sensitivity in a significant way. Adding some off-line measurement of another variable, such as a substrate concentration, will enhance the parameters sensitivity. In terms of the optimization procedure, the frequency of the sampling (on-line or off-line) exert a significant influence specially in regards to dodging to get trapped in local minima. The use of a multi-start strategy is strongly recommended since it gives a more clear and wide vision of the optimization results by sweeping a large range of possible initial guesses. Both the Fisher information Matrix and the Hessian may yield different results depending on the complexity of the model, the parameters to be identified and the minimization criteria chosen for the optimization. Further research on optimization of anaerobic digestion models is encouraged.

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References

[1] Bernard, O., Hadj-sadok, Z., Dochain, D., Genovesi, A., Steyer, J., Project, C. and Cedex, S., *Dynamical Model Development and Parameter Identification for an Anaerobic Wastewater Treatment Process*, Biotechnol. Bioeng. vol.75, pp. 424–438, (2001).

[2] Donoso-Bravo, A., Mailier, J., Martin, C., Rodríguez, J., Aceves-Lara, C.A. and Vande Wouwer, A., *Model selection, identification and validation in anaerobic digestion: a review*, Water Res., vol. 45, pp. 5347–5364, (2011).

[3] Kelessidis, A. and Stasinakis, A.S., *Comparative study of the methods used for treatment and final disposal of sewage sludge in European countries*, Waste Manag., vol. 32, pp. 1186–1195, (2012).

[4] Marsili-Libelli, S. and Checchi, N., *Identification of dynamic models for horizontal subsurface constructed wetlands.*, Ecol. Modell., vol. 187, pp. 201–218, (2005).

[5] Vanlier, J., Tiemann, C.A., Hilbers, P.A.J. and Riel N.A.W. Van, *Parameter uncertainty in biochemical models described by ordinary differential equations*, Math. Biosci., vol. 246, pp. 305–314, (2013).

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Quinto Encuentro en Aplicaciones de la Matemática

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

Exponential stability for magneto-micropolar fluids

Pablo Braz e Silva * Luis Friz † Marko Rojas Medar ‡

Abstract

The objective of the present work is to study the exponential stability for strong solutions of the evolution equations governing the motion of incompressible micropolar (asymmetric) fluids in a bounded domain. In other words, the solutions of the magneto-micropolar fluids system tend to the stationary solutions when the time t goes to infinity both L^2-norm than L^p-norm.

References

[1] Eringen, A.C., *Theory of micropolar fluids.* J. Math. Mech. 16, 1-8, (1966).

[2] G. Lukaszewicz, G., *Micropolar fluids: Theory and Applications* Birkhäuser, Boston, (1999).

[3] Ortega-Torres E.E. and Rojas-Medar, M.A., *Magneto-micropolar fluid motion: global existence of strong solutions.* Abstract and Applied Analysis 4, 109-125 (1999).

[4] Qu, C. and Wang, P., *L^p exponential stability for the equilibrium solutions of the Navier-Stokes equations*, J. Math. Anal. Appl. 190, 419-427 (1995).

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Quinto Encuentro en Aplicaciones de la Matemática
Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

Numerical methods for Hamilton-Jacobi-Bellman equations and applications in optimal control

Dante Kalise *

Abstract

In this talk we will review some classical and recent results concerning the link between Hamilton-Jacobi equations and optimal control, its numerical approximation, and different applications. A standard tool for the solution of optimal control problems is the application of the Dynamic Programming Principle proposed by Bellman in the 50s. In this context, the value function of the optimal control problem is characterized as the solution of a first-order, fully nonlinear Hamilton-Jacobi-Bellman (HJB) equation. A major advantage of the approach is that a feedback mapping connecting the current state of the system and the optimal control can be obtained by means of the Pontryagin principle. However, since the HJB equation has to be solved in a state space of the same dimension as the system dynamics, the approach is only feasible for low dimensional dynamics. In the first part of the talk, we will present the main results related to HJB equations, viscosity solutions and links to optimal control. The second part will be devoted to the construction of efficient and accurate numerical schemes for the approximation of HJB equations.

References

[1] Alla, A., Falcone, M., and Kalise, D., *An efficient policy iteration algorithm for the solution of dynamic programming equations.* to appear in SIAM Journal on Scientific Computing, 21 pp. (2014).

[2] Bokanowski, O., Falcone, M., Ferretti, R., Grüne, L., Kalise, D., and Zidani., H., *Value iteration convergence of ϵ-monotone schemes for stationary Hamilton-Jacobi equations.* to appear in Discrete and Continuous Dynamical Systems - Series A, 34 pp. (2014).

[3] Falcone, M., and Kalise, D., *A high-order semi-Lagrangian/finite volume scheme for Hamilton-Jacobi-saacs equations.* System Modeling and Optimization 443, pp. 105–117 (2014).

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Quinto Encuentro en Aplicaciones de la Matemática

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

Dimensionally Adaptive Methods for the Simulation and Inversion of Resistivity Geophysical Measurements

David Pardo * Shaaban Bakr † Carlos Torres-Verdín ‡

Abstract

A number of three dimensional (3D) simulators of geophysical logging measurements have been developed during the last two decades for oil-industry applications. These simulators have been successfully used to study and quantify different physical effects occurring in 3D geometries. Despite such recent advances, there are still many 3D effects for which reliable simulations are not available. Furthermore, in most of the existing results, only partial validations have been reported, typically obtained by comparing solutions of simplified model problems against the corresponding solutions calculated with a lower dimensional (2D or 1D) numerical method. The lack of 3D simulation results (as opposed to 2D results) is due to major difficulties encountered when solving geometrically challenging problems. Namely, for mesh-based methods (Finite Elements, Finite Differences, Boundary Elements, etc.), the size of the system of linear equations becomes excessively large to be solved in real time.

When solving inverse geophysical problems (as opposed to forward simulation problems), the cost of computations dramatically increase, making the use of 3D simulators impractical. Often, even 2D simulators cannot be afforded due to their elevated computational cost.

In this presentation, we first explain how oil companies record different types of electromagnetic geophysical measurements. Then, we explain the main mathematical and computational difficulties associated to the simulation and inversion of such measurements. Subsequently, we analyze a number of mathematical features that a numerical method should possess in order to overcome the above challenges. Finally, we present a family of dimensionally adaptive methods that we are employing for solving such simulation and inversion problems.

One of the main objectives of this presentation is to raise the awareness and interest of the applied mathematics community on the topic, since its expertise is necessary in order to solve several mathematical problems that still remain open in the area.

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V-MAD 5

Quinto Encuentro en Aplicaciones de la Matemática

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

Multiscale Hybrid-Mixed Method for Porous Media Problems

Diego Paredes * Frédéric Valentin † Christopher Harder ‡

Abstract

Multiscale Hybrid-Mixed (MHM) finite element method have been recently developed for several operators, including hydro-dynamics and reaction-advection-diffussion models. The MHM method is a consequence of a hybridization procedure, and emerges as a method that naturally incorporates multiple scales while provides solutions with high-order precision. The computation of local problems is embedded in the upscaling procedure, which are completely independent and thus may be naturally obtained using parallel computation facilities. We conclude that the MHM method is naturally shaped to be used in parallel computing environments and appears to be a highly competitive option to handle realistic multiscale parabolic boundary value problems with precision on coarse meshes. Numerical experiments will also be shown in order to support the theoretical results.

References

[1] R. Araya, C. Harder, D. Paredes, and F. Valentin, *Multiscale hybrid-mixed method.* SIAM J. Numer. Anal., 51(6):35053531, (2013).

[2] C. Harder, D. Paredes, and F. Valentin, *On a multiscale hybrid-mixed method for advective-reactive dominated problems with heterogenous coefficients.* submitted to MMS.

[3] C. Harder, D. Paredes, and F. Valentin, *A family of multiscale hybrid-mixed finite element methods for the Darcy equation with rough coefficients.* Journal of Computational Physic, 245(0):107 130, (2013).

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V-MAD 5

Quinto Encuentro en Aplicaciones de la Matemática

Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

Multi-thread multi-frontal direct solver with GALOIS scheduler for adaptive grids.

Maciej Paszyński, Konrad Jopek *

Abstract

In this paper we present our new multi-frontal solver algorithm for 2D adaptive finite element method computations implemented in GALOIS system [1], and compare it to other state-of-the-art solver MUMPS [2, 3]. We try to answer the question what does it mean to have a faster solver, and how can we compare our new solver with other state-of-the-art solvers, in a fair way. We consider different measures for comparison of the two solvers, in particular (1) execution time, (2) number of Floating Point Operations (FLOPs), and (3) efficiency and speedup for parallel execution.

The execution time is the most common utilized measure:

- Using different machines may results in different execution times.
- Using different compilators may result in different execution times.
- Using different compilation flags (e.g. debug vs release) may result in different execution times.
- Using different libraries (e.g. BLAS, LAPACK etc. for sequential solvers, or ScaLAPACK, PLAPACK for parallel solvers) linked to the solver may result in redically different execution time.
- Using different algorithms for generation of the elimination tree that controls the execution of the multi-frontal solver algorithm (often called ordering algorithms) results in different execution times, e.g. the state-of-the-art MUMPS solver provides six different ordering algorithms, namely nested-dissection algorithm implemented in METIS library, Approximate Minimum Degree (AMD), Quasi-Approximate Minimum Degree (QAMD), Approximate Minimum Fill (AMF), SCOTCH, PORD [4].

Summing up, for the comparison of the execution time it is necessary to make sure that both solvers have been compiled in the same way (if possible) and linked with identical libraries (if possible).

Once we have the two solvers compiled and linked at the same way, we still do not know what does it mean that the execution time of one solver is smaller than the execution time of the other one, and we need to include some additional measure, like the number of floating point operations (FLOPs)

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- Using the FLOPs number it is necessary to remember that they measure only the amount of operations spent by the solver on factorization and forward / backward substitutions, it does not include memory transfers, reordering, reindexing etc.
- Using the FLOPs is platform indendent.
- However the compilation flags as well as the compilator kind may affect the number of FLOPs, since some compilators may perform optimization of codes.
- It may also depend on the implementation of the factorization routines, e.g. we may also use Cholesky LU factorization in one solver (if the problem is symmetric and positive definite) and pure LU factorization in the other solver.
- It may also depend on the libraries linked to the solver peforming basic algebraic operations, like BLAS and LAPACK.
- Using different eliminations tree result in different number of FLOPs.

In order to show that our solver has better elimination tree algorithm, we need to compare the same implementation of the solver executed with two different elimination trees. On the other hand to show that our solver has more optimized factorizaton routines, we need to execute the two solvers on the identical elimination trees.

Finally, the efficiency and speedup can be used as a measure only for the parallel execution of the solver algorithm.

- They measure only the relative performance on the parallel machine with respect to the sequential code.
- They strongly depend on the architecture of parallel machine.
- They strongly depend on the parallel efficiency / speedup of the linked libraries.
- They depend on the well-balance of the elimination tree.

We utilize all these measure to compare our solvers and we show that the GALOIS based solver outperform both sequential and parallel solvers.

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References

[1] Goik, D., Jopek, K., Paszyński, M., Lenharth, A., Nguyen, D., and Pingali, K., *Graph Grammar based Multi-thread Multi-frontal Direct Solver with Galois Scheduler*. Procedia Computer Science, vol. 29, pp. 960-969, (2014).

[2] Amestoy, P.R. and Duff, I.S., *Multifrontal parallel distributed symmetric and unsymmetric solvers*. Computer Methods in Applied Mechanics and Engineering, vol. 184, pp. 501-520, (2000).

[3] *MUlti-frontal Massively Parallel Sparse direct solver, http://http://mumps.enseeiht.fr/.*

[4] Paszyńsla. A., *Volume and neighbors algorithm for finding elimination trees for three dimensional h-adaptive grids*. Computers and Mathematics with Applications, in press. DOI: 10.1016/j.camwa.2014.09.012 (2014).

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Quinto Encuentro en Aplicaciones de la Matemática
Instituto de Matemáticas, Pontificia Universidad Católica de Valparaíso, 7–9 Enero, 2015

On optimal strategies for feeding in minimal time a SBR with several species.

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Abstract

In this paper we consider the optimal control problem consisting of feeding in minimal time a Sequential Batch Reactors (SBR) where several species compete for a single substrate, with the objective being to reach a given (low) level of the substrate. Following [8, Gajardo et al. Minimal Time Sequential Batch Reactors with Bounded and Impulse Controls for One or More Species. SIAM J. Control and Optimization, vol. 47, Issue 6, pp. 2827-2856, 2008], we allow controls to be bounded measurable functions of time plus possible impulses. A suitable modification of the dynamics leads to a slightly different optimal control problem, without impulsive controls, for which we apply different optimality conditions derived from the Pontryagin principle and the Hamilton-Jacobi-Bellman equation. We thus characterize the singular arcs of our problem as the extremal trajectories keeping the substrate at a constant level. We also establish conditions for which a immediate one impulse (IOI) strategy is optimal. Some numerical experiences are then included in order to show that those conditions are also necessary to ensure the optimality of the IOI strategy.

References

[1] GAJARDO, P., RAMÍREZ H. AND RODRÍGUEZ, J. C., *Tools for improving feeding strategies in a SBR with several species*. Bioprocess and Biosystems Engineering, vol. 37, pp. 63–71, (2014).

[2] GAJARDO, P., HARMAND, J., RAMÍREZ, H. AND RAPAPORT, A., *Minimal time bioremediation of natural water resources*. Automatica, vol. 47, 4, pp. 1764–1769, (2011).

[3] GAJARDO, P., RAMÍREZ, H. AND RAPAPORT, A., *Minimal time sequential Batch Reactors with Bounded and Impulsive Controls for one or more species*. SIAM Journal on on Control and Optimization, vol. 47, 6, pp. 2827–2856, (2008).

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[4] Gajardo, P., Ramírez, H., Rapaport, A. and Riquelme, V., *Bioremediation of Natural Resources via Optimal Control Techniques.* BIOMAT 2011 International Symposium on Mathematical and Computational Biology, World Scientific, pp. 178–191, (2012).

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Quinto Encuentro en Aplicaciones de la Matemática

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Comparison between the MINC and MRMT configurations: The n-dimensional case*

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Abstract

In geosciences, models of fractured porous media are often described as a mobile zone driven by advection, and one or several immobile zones directly or indirectly connected to the mobile zone by diffusion terms. In order to modelling a flow process, it is possible to define different configurations between this zones. Example of these are the classical connections in series and parallel, both in noninteracting systems.

The models MINC (Multiple INteracting Continua) and MRMT (Multiple Rate Mass Transfer) are extensively used in transport phenomena. We believe that these models are also relevant to describe flows in soil or in porous media such as biofilms. In the same way, these models can be used to describe connections between bioreactors (general gradostat for instance).

The goal of this manuscript is determine conditions for the input-output equivalence of these configurations for n compartments using some important results of the linear system theory, control theory and numerical analysis. Some examples are given in order to validate our results.

References

[1] Chi-Tsong Shen, *Linear System Theory and Design*, Oxford University Press, 1999.

[2] Haggerty, R. and Gorelick, S. M., *Multiple-Rate Mass Transfer for Modeling Diffusion and Surface Reactions in Media with Pore-Scale Heterogeneity*, Water Resources Research, vol. 31, 10, pp. 2383–2400, (1995).

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[3] Harmand, J., Rapaport, A. and Trofino, A., *Optimal design of two interconnected bioreactors some new results*, American Institute of Chemical Engineering Journal, vol. 49, pp. 1433–1450, (1999).

[4] Harmand J., Rapaport, A. and Dramé, A., *Optimal design of two interconnected enzymatic reactors*, Journal of Process Control, vol. 14, pp. 785–794, (2004).

[5] Smith, H. and Waltman, P., *The Theory of Chemostat. Dynamics of Microbial Competition*, Cambridge Studies in Mathematical Biology, Cambridge University Press, 1995.

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An efficient implementation of a finite-difference room acoustics model in CUDA

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Abstract
In this work, we present a novel Graphic Processing Unit (GPU) implementation of a room acoustics model based on an explicit family of Finite-Difference Time-Domain (FDTD) algorithms. These algorithms are based on the formulation of two Partial Differential Equations (PDE): the discrete Wave equation for characterizing the sound propagation through the air and a locally-reacting impedance model for simulating the walls of the enclosure. We first develop a strategy for implementing a Frequency Independent (FI) impedance model which is free of warp divergences and then, we extend the model adding a Digital Impedance Filter (DIF) boundary subroutine able to compute the acoustic pressure of different nodes such as corners or edges without any performance penalty. Both implementations are validated and deeply analyzed by performing different 3-D numerical experiments. Finally, to compare our proposal to other GPU implementations, we define a performance metric which is capable to objectively measure the throughput of any implementation using a simple number. The robustness of this metric allows us to compare algorithms even if these have been run in different GPU cards or have been formulated with other explicit models.

References

[1] Kutruff, H., *Room Acoustics.* Spon Press, 4th edition; 2000.

[2] Kowalczyk, K. and van Walstijn, M., *Room acoustics simulation using 3-D compact explicit FDTD schemes.* IEEE Transactions on Audio, Speech, and Language Processing, 19(1), 34-46. 2011.

[3] López, J.J., Carnicero, D., Ferrando, N. and Escolano, J., *Parallelization of the finite-difference time-domain method for room acoustics modelling based on CUDA.* Mathematical and Computer Modelling. 57(7-8):1822-1831. 2013.

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