Kick-off *Workshop on Efficient Simulation and Computation for Sea, Health and Industry*

http://www.mat.uc.pt/~alma/ESC4SHI2019/

24-25 January 2019 — Department of Mathematics, University of Coimbra, Portugal

Agenda

Thursday, 24 January 2019

10:00 - 10:30 Welcome and coffee
10:30 - 11:00 Project presentation (broad lines)
11:00 - 13:15 Talk session 1
13:15 - 14:30 Lunch break
14:30 - 16:00 Talk session 2
16:00 - 16:30 Coffee & tea break
16:30 - 17:30 Project presentation (by each institution)

Friday, 25 January 2019

09:00 - 11:15 Talk session 3
11:15 - 11:30 Coffee & tea break
11:30 - 12:45 Organisation of project activities, team tasks, workshop and congress
12:45 - 13:00 Closure

Organising committee

Adérito Araújo, University of Coimbra
Sílvia Barbeiro, University of Coimbra
Stéphane Clain, University of Minho
Jorge Figueiredo, University of Minho
Rui Pereira, University of Minho

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João Miguel Nóbrega, University of Minho
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Alberto Proença, University of Minho
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List of communications

The abstracts of the communications are presented in the following pages.

VERY HIGH-ORDER ACCURATE FINITE VOLUME METHODS FOR COMPUTATIONAL RHEOLOGY AND ADVANCED APPLICATIONS

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ABSTRACT

The computational modeling of fluid flow problems in engineering applications often involve material systems whose complex molecular and microscopic structure gives rise to non-trivial and, sometimes, counter intuitive rheological behavior. In this respect, and contrarily to the classical models in computational fluid dynamics, the coupled governing partial differential equations must account for complex material properties, expressed by means of constitutive equations. Additional modeling and numerical challenges are then raised, which classical computational fluid dynamics methods are unable to properly solve. Aiming to overcome these limitations, the emerging field of computational rheology focus on bridging the gap between computer simulation and fluid flow problems involving complex rheological behavior. Nevertheless, the development of mathematical models, numerical methods, and computational codes in this subject has been uneven with the ever-increasing complexity of a wide range of fluid flow problems, from both the perspective of the fundamental science and the engineering practice.

Rheological constitutive equations have, generally, a partial differential nature, which results into larger non-linear systems to solve and, therefore, leads to an increased computational effort. Moreover, the computation of these constitutive equations are prone to instabilities and present poor robustness from their hyperbolic dominated nature, which deteriorate solution accuracy and convergence and, therefore, also significantly increase the demand of computational resources. Consequently, there is a growing concern that standard and outdated numerical methods, widely implemented in commercial and open-source codes used in industry, are improved or replaced by new and innovative alternatives, aiming to obtain more accurate solutions, more stable computation procedures, and significant computational gains. In that regard, the proposed research targets the investigation, development, and verification of a new class of methods for the computational rheology context.

The proposed new class of methods are developed within the high-order accurate finite volume framework, where error convergence higher than the classical first- and second-orders are achieved under mesh refinement, therefore resulting into substantial accuracy gains. Moreover, recent and comprehensive research on this topic has demonstrated that significant gains in computational efficiency, both in terms of time and memory usage, are also achieved when higher-order accurate methods are used to obtain the same solution accuracy level given by lower-order ones. A comprehensive analysis and verification, both of the numerical developments and the computational implementation, are planned to ensure that the proposed methods and tools are understood, assessed, and efficient. Also, validation with viscoelastic fluid flow problems in the context of micro-injection moulding, with the collaboration of the industrial partners, are targeted to prove the effectiveness and usefulness of the proposed tools. Additionally, although traditional polymer processing applications, such as extrusion and injection moulding, usually require less complex constitutive equations, validation with problems in this context is crucial before applying the proposed methods in more advanced and computationally demanding applications.

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ESTRUTURAS COSTEIRAS E TSUNAMI: APROXIMAÇÃO NUMÉRICA

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ABSTRACT

Desde o início da história das civilizações, as áreas costeiras estão tipicamente associadas a localizações estratégicas e grandes infraestruturas, nomeadamente portos e polos industriais e de turismo. É uma tendência mantida na atualidade, com nove em cada dez das maiores cidades do mundo localizadas em áreas costeiras. No entanto, as regiões costeiras são expostas a fenómenos naturais, como os tsunamis. Seis das cidades costeiras são expostas ao perigo do tsunami.

Para a recomendação de medidas eficazes de mitigação do risco de tsunami, é necessário o conhecimento do fenómeno físico. Dado o escasso número de eventos e a disponibilidade apenas recente de instrumentação para registar os dados, é comum o recurso a experimentação laboratorial e a aproximações numéricas para adquirir e complementar informação.

Os modelos laboratoriais são menos económicos e mais morosos. Com a evolução computacional, a aproximação numérica tornou-se uma alternativa muito vantajosa, ainda que os modelos do tsunami e da sua interação com as estruturas sejam complexos e computacionalmente exigentes.

O projeto ESC4SHI prevê a aplicação de métodos e ferramentas numéricas para contribuir para o estudo das fases de propagação e inundação do tsunami, incluindo a sua interação com as estruturas costeiras.

O comportamento dos fluidos é descrito pelas equações diferenciais de Navier-Stokes, NS. A depender do problema a abordar, podem adotar-se simplificações.

Para simular a propagação e a inundação do tsunami, é desenvolvida/validada uma ferramenta numérica baseada no Método dos Volumes Finitos que resolve as equações não-lineares do tipo *Shallow-Water*, SW, obtidas pela integração das NS em altura e considerando o fluido incompressível e invíscido, com capacidade de tratar descontinuidades, batimetrias complexas, interação seco-molhado, força de inércia de convexão e força de fricção do fundo oceânico para reproduzir comportamento da onda quando se aproxima da costa, manter a propriedade C, responsável por manter a situação de repouso da fluido quando não é atuado exteriormente, geração de *nesting* para garantir maior precisão e menores gastos computacionais e cálculo da inundação.

Para simular a interação do tsunami com a estrutura, existe a particularidade de os fluidos terem uma discretização Euleriana e os sólidos uma discretização Lagrangiana. É desenvolvida/validada uma formulação Lagrangiana para discretizar o fluido e uma metodologia numérica *Smoothed-Particle-Hydrodynamic*, SPH, para resolver o sistema de equações.

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COMPUTATIONAL RHEOLOGY ET AL. @ IPC/UMINHO

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ABSTRACT

The current capabilities of numerical codes, which are able to model very complex processes, and the availability of powerful computational resources, clearly promote the use of numerical modelling tools to assist any design related tasks.

For more than a decade, the Computational Rheology Group, from the Institute for Polymers and Composites at the University of Minho (IPC/UMinho), has been developing and exploiting modelling codes to aid the design of different tools, with a special focus on polymer processing applications.

This talk aims to provide an overview of the computational rheology related work done at IPC/UMinho, by a large group of researchers, in many cases in close cooperation with industry.

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ASSESSING MICROSTRUCTURAL CHANGES ON OCULAR DISEASES THROUGH SIMULATION OF LIGHT PROPAGATION IN OCULAR TISSUES

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ABSTRACT

The early stages of ocular diseases are characterized by microstructural changes on tissue components, namely cells and collagen fibers, affecting their properties and their spatial organization. These changes impact light propagation on ocular media, through alterations on refractive properties and tissue transparency, and may cause vision impairment or even blindness.

A computation tool comprising accurate models of ocular tissues microstructure, numerical simulation of light propagation in ocular media and mathematical modeling of imaging techniques, like Optical Coherence Tomography (OCT), has the potential to elucidate the early changes associated to different pathologies, extending the knowledge on eye physiopathology.

In this presentation, we will introduce the basic structure of the human eye and its main components. The fundamentals and features of OCT imaging will be reviewed and a new technique, capable of imaging the organization of collagen fibers in the corneal stroma - Second Harmonic Generation – will be discussed. We will present our previous work on modeling light propagation in the retina and the results obtained on the assessment of cell level alterations responsible for OCT data on Diabetic Macular Edema. The presentation will end by addressing future research on modeling and simulation of ocular tissues, focusing on stroma collagen organization, a key factor for eye transparency.

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DISCONTINUOUS GALERKIN METHODS FOR TIME-DEPENDENT MAXWELL'S EQUATIONS

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ABSTRACT

Motivated by a real application, which encompasses modeling electromagnetic wave's propagation through the eye's structures, we propose an explicit iterative leap-frog discontinuous Galerkin method for time-domain Maxwell's equations in anisotropic materials. We focus on deriving stability and convergent estimates of the fully discrete scheme. We consider anisotropic permittivity tensors, which arise naturally in our application of interest. An important aspect in computational electromagnetic problems, which will be discussed, is the implementation of the boundary conditions.

We illustrate the theoretical results with numerical examples. We also present the results of simulations which aim to represent simple examples of light scattering in the outer nuclear layer of the retina.

This work was developed in the framework of a more general project that aims develop a computational model to simulate the electromagnetic wave's propagation through the eye's structures to create a virtual optical a virtual optical coherence tomography scan.

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VERY HIGH ORDER SCHEMES MASSIVE MULTI-THREADED ALTERNATING DIRECTION IMPLICIT TYPE METHOD (ADI) FOR THE STEADY STATE 2D CONVECTION-DIFFUSION EQUATION ON CURVED DOMAINS.

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ABSTRACT

We present an ADI type method with structured grids to solve the steady state 2D Convection Diffusion equation on curved boundary domains. The two main objectives are: the design of a highly parallelized method for multi-thread implementation; the adaptation of the ROD method to provide very high order with complex geometries. The Ghost cells layer (1 or 2 rings), are evaluated using the ROD technology where we prescribe the necessary information from the points in the curved boundary to the barycenter to provide the expected order of convergence using polynomial reconstruction. The massive multi-threading code, takes advantage of the ADI formulation that solve independently 1D problem corresponding to each line or each column. AIM: Efficient data structures and creating an optimal algorithms to avoid the memory bounded problem that provide excellent speed-up even for a very large number of cores.

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THE MOOD TECHNIQUE IN THE FRAMEWORK OF A HIGH-ORDER FINITE VOLUME SCHEME TO SOLVE THE SHALLOW-WATER PROBLEM

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ABSTRACT

The shallow-water system models a wide class of river or ocean flows for both engineering and environmental purposes. Moreover, extreme phenomena such as tsunami or flooding can have dramatic consequences to the environment and populations and could be considered in this framework. Therefore, producing very efficient numerical schemes to obtain accurate approximations for the solution of the shallow-water system and deliver reliable previsions is a constant challenging objective. We present a finite volume scheme for the 1D/2D shallow-water problem that involves a local polynomial reconstruction combined with an appropriate Multi-dimensional Optimal Order Detection (MOOD) technique [1, 2, 3]. This technique allows to obtain very accurate approximations for smooth solutions and preserves the stability in the vicinity of discontinuities. We describe the interplay between polynomial reconstruction and the MOOD technique and present examples that illustrate the application of this numerical scheme. The tests show that this numerical scheme is well-balanced allowing to reach up to 6th-order accuracy in the numerical solutions.

REFERENCES

[1] S. Clain, S. Diot, R. Loubère, A high-order finite volume method for hyperbolic systems: Multi-dimensional Optimal Order Detection (MOOD), J. Comput. Phys. 230 Issue 10 (2011) 4028–4050.

[2] S. Diot, S. Clain, R. Loubère, Improved detection criteria for the Multi-dimensional Optimal Order Detection (MOOD) on unstructured meshes with very high-order polynomials, Comput. & Fluids 64 (2012) 43–63.

[3] S. Diot, R. Loubère, S. Clain, The MOOD method in the three-dimensional case: very-high-order finite volume method for hyperbolic systems, Int. J. Numer. Meth. Fluids 73 (2013) 362–392.

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ESTUDO DA ESTABILIDADE LINEAR EM TEMPO DE ORDEM ELEVADA

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ABSTRACT

O objetivo do trabalho é realizar um estudo detalhado da estabilidade da acoplagem entre um esquema de tipo Runge-Kutta multistage e um operador linear discreto (por exemplo a convecção-difusão unidimensional). A idea é deixar alguns graus de liberdade para melhor controlar a estabilidade para aumentar o passo de tempo, nomeadamente RK com sub-estágios adicionais e um esquema de tipo diferenças finitas com $2k+1$ pontos para o operador espacial, onde os coeficientes são ajustados em função do Péclet.
Nesta apresentação consideramos um esquema numérico em espaço com 5 pontos, obtendo-se assim um sistema semi-discreto de EDOs. Este sistema está associado a um operador com um conjunto de valores próprios dependentes de 6 parâmetros e do número de Péclet. Numa primeira abordagem, pretendemos estudar a relação entre os parâmetros e o número de Péclet de modo a garantir a consistência, ordem e estabilidade do operador.

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