High performance cOmputing and SCientific dAta management dRiven by highly demanding applications

Achievements and perspectives on numerical schemes for wave propagation problems

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Fifth Workshop of the CNPq-Inria HOSCAR project
High Performance Computing and Scientific Data Management
Driven by Highly Demanding Applications
Inria Sophia Antipolis - Méditerranée, France

Outline

HOSCAR project: generalities

- The HOSCAR project is a CNPq - Inria collaborative project between Brazilian and French researchers, in the field of computational sciences
- The project is also sponsored by the French Embassy in Brazil
- Starting date: July 2012
- Duration: 4 years
- Web: http://www-sop.inria.fr/hoscar

HOSCAR project: objectives

- The general objective of the project is to setup a multidisciplinary Brazil-France collaborative effort for taking full benefits of future high-performance massively parallel architectures
- The targets are the very large-scale datasets and numerical simulations relevant to a selected set of applications in natural sciences
  1. Resource prospection
  2. Reservoir simulation
  3. Cardio-vascular system modeling
  4. Astronomy data management

HOSCAR project: organization and partnership

- The project involves computer scientists and numerical mathematicians divided in 3 fundamental research groups:
  1. Numerical schemes for PDE models (Group 1),
  2. Scientific data management (Group 2),
  3. High-performance software systems (Group 3).
- Several Brazilian institutions are participating to the project among which:
  - LNCC (Laboratrio Nacional de Computao Cientfica),
  - COPPE/UFRJ (Instituto Alberto Luiz Coimbra de Ps-Graduao e Pesquisa de Engenharia/Alberto Luiz Coimbra Institute for Graduate Studies and Research in Engineering, Universidade Federal do Rio de Janeiro),
  - INF/UFRGS (Instituto de Informtica, Universidade Federal do Rio Grande do Sul),
  - LIA/UFC (Laboratrios de Pesquisa em Cincia da Computao Departamento de Computao, Universidade Federal do Cear).
- The French partners are research teams from several INRIA research centers

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Organization: group 1

- Numerical schemes for PDE models
  - Research activities are concerned with the numerical treatment of PDE systems modeling wave propagation and fluid flow problems
  - Related issues are concerned with the discretization in space and time taking into account the characteristics of the physical phenomena underlying the target applications such as, heterogeneity of the media, geometrical complexity (e.g. faults, geological layers, wells, etc.), variation in space and time scales among others
  - Emphasize is put on finite element type discretization methods and associated techniques for the scalable construction of adapted discrete models of the problems at hand

HOSCAR project: organization and partnership

Organization: group 2

- Scientific data management
  - Develop scientific data management techniques that will provide a transparent view (virtualized data view) over distributed scientific data and images
  - Build on the techniques proposed by Google Bigtable and the MapReduce paradigm, and extend QEF, a distributed and parallel query engine framework that the participating groups have been developing, to integrate Hadoop
  - Design strategies to distribute the catalogue according to multiple dimensions, including very precise double data type measurements and spatial coordinates
  - Investigate parallel analysis techniques in HPC that can support efficient analysis of huge datasets

Organization: group 3

- High performance software systems
  - The experience of major supercomputing centers points out that the development of scientific applications that are able to take profit of the ever-increasing capability of HPC systems is as challenging as building such systems
  - It is far from uncommon that applications need to be reprogrammed to scale and the scientists' skill in efficiently employing HPC resources is therefore paramount to achieve the desired performance
  - Objective is to propose different strategies for abstracting away from such scientists the algorithms and techniques that enable such performance at the system level, thus allowing such scientists to concentrate in the coding of typical idioms for their domain of knowledge

HOSCAR project: organization and partnership

- Allocated budget is used for:
  - Organizing the annual workshop of the project (1 week),
  - Supporting inter-groups short-term visits of researchers and students,
  - Organizing summer schools.
- 1st workshop, July 25-27 2012, Inria Sophia Antipolis-Mditerrané, France
- 2nd workshop: September 10-13 2012, LNCC, Ptropolis, Brazil
- 3rd workshop: September 2-6 2013, INRIA Bordeaux - Sud-Ouest, France
- 4th workshop: September 15-18, Gramado, Brazil

Outline

Joint activities on wave propagation PDE models

Context at Inria

- DGDT (Discontinuous Galerkin Time-Domain) methods
- High order DGTD methods formulated on unstructured meshes
- System of Maxwell equations for electromagnetic wave propagation
- System of elastodynamic equations for seismic wave propagation
- Study of Theoretical and numerical issues
- Software developments in 2d and 3d
- High performance computing aspects (e.g. hybrid MIMD/SIMD strategy)

Modeling context

- Interaction of electromagnetic (EM) waves with biological tissues
- Microwave regime (300 MHz to 300 GHz)

Applications

- Assessment of biological effects of human exposure to EM waves emitted from wireless systems
- Design of medical diagnostic and therapeutic systems

Modeling challenges

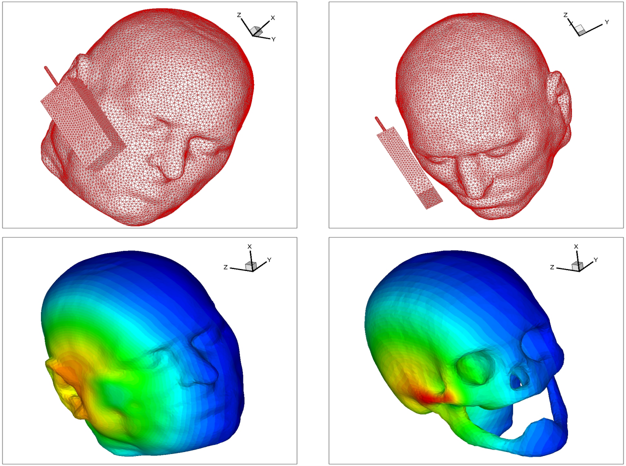
- Heterogeneous media with high water content
- Shapes of tissues and tissue interfaces
- Coupling with complex source devices (mobile phone, antenna array, etc.)

Mathematical model

- System of time-domain Maxwell equations
- Dispersion model: Debye or Cole-Cole

Joint activities on wave propagation PDE models

Context at Inria: computational biolectromagnetics



Exposure of head tissues to an electromagnetic wave emitted by a localized source. Top figures: surface triangulations of the skin and the skull. Bottom figures: contour lines of the amplitude of the electric field.

Joint activities on wave propagation PDE models

Context at Inria: computational geoseismics

Modeling context

- Interaction of seismic waves with geological media

Applications

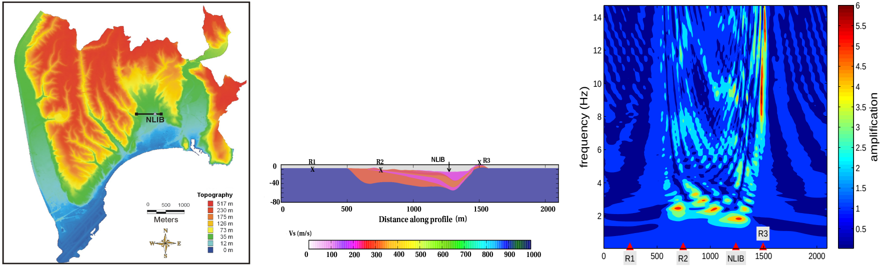
- Seismic hazard assessment
- Natural resource prospection

Modeling challenges

- Heterogeneous media, free surfaces
- Faults, solid-liquid zones
- Localized non-linear effects

Mathematical model

- System of time-domain elastodynamic equations
- Viscoelasticity model: Generalized Maxwell Body, Generalized Zener Body

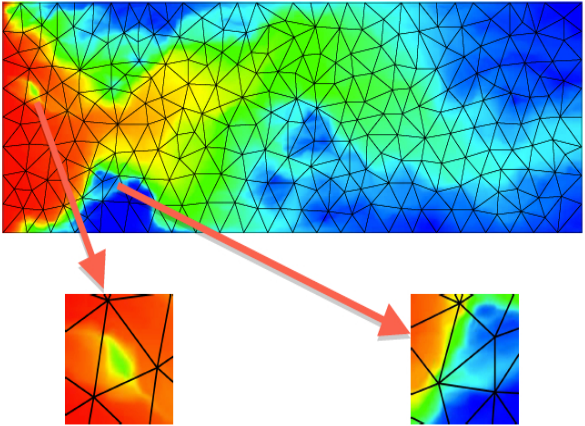


Propagation of a plane wave in a heterogeneous model of Nice area (model provided by CETE Méditerranée). Left figure: topography of Nice and location of the cross-section used for numerical simulations (black line). Middle figure: S-wave velocity distribution along the cross-section in the Nice basin. Right figure: transfer functions (amplification) for a vertically incident plane wave ; receivers every 250 m at the surface. This numerical simulation was performed using a numerical method for the solution of the elastodynamics equations coupled to a Generalized Maxwell Body (GMB) model of viscoelasticity (PhD thesis of Fabien Peyrusse).

Joint activities on wave propagation PDE models

Context at LNCC

- MHM (Multiscale Hybrid Methods)
- Darcy equation, elasticity equation, reaction-advection-diffusion equation
- Include local upscaling and crossing interfaces
- Capture boundary layers on coarse meshes
- Easy access to an estimator for mesh adaptivity
- Study of Theoretical and numerical issues
- Software developments in 2d and 3d
- High performance computing aspects (e.g. SPiNMe adaptation)



Transport in heterogeneous media: advection dominated flow in the subsurface.

Joint activities on wave propagation PDE models

Achievements in the context of the HOSCAR project

- 17 months stay of Frédéric Valentin in the Nachos team form october 2013 to january 2015
- 3 months visti of Diego Paredes in the Nachos team from may to july 2014
- Study of MHM formulations for wave propagation models
  - System of time-domain Maxwell equations
    Cf. talk of Raphaël Léger and Claire Scheid
  - System of time-domain elastodynamic equations
    Cf. talk of Marie-Hélène Lallemand-Tenkes

Outline

HPC4E : High Performance Computing for Energy

EUB-2-2015 : High Performance Computing (HPC)

Project objectives

The HPC4E project aims to apply the new exascale HPC techniques to energy industry simulations, customizing them if necessary , and going beyond the state-of-the-art in the required HPC exascale simulations for different energy sources that are the present and the future of energy:

- wind energy production and design,
- efficient combustion systems for biomass-derived fuels (biogas),
- and exploration geophysics for hydrocarbon reservoirs.

Partnership

- Barcelona Supercomputing Center (BSC)
- Inria
- Lancaster University (ULANC)
- Centro de Investigaciones Energdéticas Medioambientales y Tecnolégicas (CIEMAT)
- Iberdrola Renovables Energa
- Repsol
- Total

- Fundaäo Coordenaäo de Projetos, Pesquisas e Estudos Tecnoclógicos (COPPE)
- LNCC
- Instituto Tecnolgíco de Aeronáutica
- Petroleo Brasileiro (Petrobras)
- Universidade Federal do Rio Grande do Sul (INF-UFRGS)
- Universidade Federal de Pernambuco (CER-UFPE)

Wave propagation related activities

- Hiepacs, Magique3D and Nachos project-teams
- LNCC
- Total

- MHM for the system of time-domain elastodynamic equations
- HDGM for the system of frequency-domain elastodynamic equations
- Exploitation of high performance sparse linear solvers
- Scalable inplementations in 3d
- Applications in petroleum resource prospection

Outline

The HOMAR associate team

Supporting entities

- Inria, European and International Partnerships Department
- FAPERJ

Partners

- Inria Sophia Antipolis-Méditerranée, Nachos project-team
  - Stéphane Lanteri
  - Marie Hélène Lallemand
  - Raphaël Léger
  - Claire Scheid
- LNCC, Petrópolis, Brazil
  - Antônio Tadeu Azevedo Gomes
  - Alexandre Madureira
  - Antonio André Novotny
  - Frédéric Valentin
- Instituto de Matemticas, Universidad Católica de Valparaiso, Chile
  - Diego Paredes

General objectives

- Study of time dependent wave propagation problems with strong multiscale features (in space and time)
- Design, analysis and implementation of a family of innovative high performance numerical methods for the simulation of multiscale wave propagation problems

Specific objectives

1. To design and analyze new MHM methods for the system of time-domain Maxwell equations coupled to models of physical dispersion, in view of their application to light interaction with nanometer scale structures
2. To design and analyse new MHM methods for the system of time-domain elastodynamic equations for modeling elastic wave propagation in anisotropic media
3. To devise appropriate discrete versions of the proposed MHM methods using DG (Discontinuous Galerkin) formulations for the discretization of the local solvers, and to study the mathematical properties (stability, convergence) of the combined MHM-DGTD strategies
4. To implement the proposed MHM-DGTD solution strategy on modern parallel computing architectures combining coarse grain (MIMD - Multiple Instruction Multiple Data) and fine grian (SIMD - Single Instruction Multiple Data) processing units
5. To demonstrate the capabilities of the developed MHM-DGTD parallel solution strategies for the simulation of selected problems in the fields of nanophotonics and elastodynamics

Physical context: wave/matter interaction on the nanoscale

- Electromagnetic wave ⇒ nanophotononics
- Elastodynamic wave ⇒ nanophononics

Nanophotonics

- Nanophotonics or nano-optics is the study of the behavior of light on the nanometer scale
- It is considered as a branch of optical engineering which deals with optics, or the interaction of light with particles or substances, at deeply subwavelength length scales
- Refers to phenomena of ultraviolet, visible and near IR light, with a wavelength of approximately 300 to 1200 nanometers
- The interaction of light with these nanoscale features leads to confinement of the electromagnetic field to the surface or tip of the nanostructure resulting in a region referred to as the optical near field

Main modeling features

- Metal nanoparticles and metal/dielectric interfaces
- Very strong localized EM field enhancements
- Local, non-local and possibly non-linear dispersion effects

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Applications

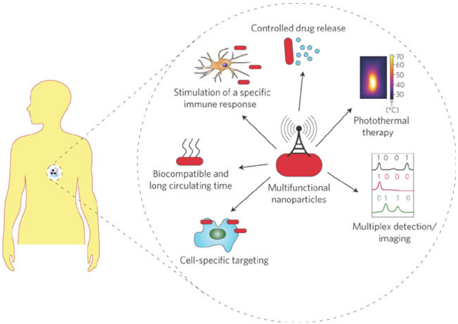
The enabling nature of nanophotonics means that the potential applications of nanophotonics are expected to be be broad.

Examples applications with potential commercial and/or societal impact are:

- Nano-engineered photonics materials
- Nanoscale quantum optics
- Nanoscale functional imaging
- Photovoltaics
- Communications and all-optical signal processing
- Chemical biosensors
- Plasmon-enhanced magnetic storage

Applications: nanoscale functional imaging

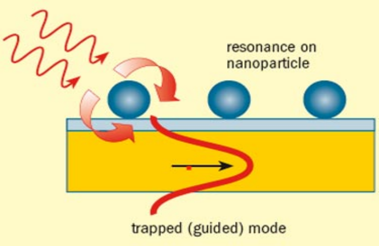
The optical antenna concept is very promising for achieving ultrahigh spatial resolution and sensitivity, but requires development for real-world applications



From: Tumour targeting: nanoantennas heat up
W. Zhao and J.M. Karp, Nature Materials 8, pp. 453-454, 2009

Applications: photovoltaics

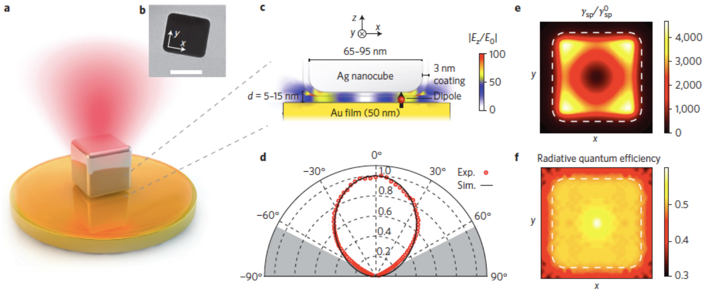
- In recent years, there has been rapid development in the field of nanoscale light trapping for solar cells
- This has been driven by the decrease in thickness of solar cells in order to reduce materials costs, as well as advances in fabrication technology and computer power for simulating nanoscale structures
- Most importantly, thin-film cell designs will need to incorporate nanophotonic light trapping in order to reach their ultimate efficiency limits



From: Nanoparticles inspire plasmonic solar cells
C. Richards, Optics & Laser Europe, March issue, 2009

Applications: nanoscale patch antenna (NPA)

- To move nanophotonic devices such as lasers and single-photon sources into the practical realm, a challenging list of requirements must be met, including directional emission, room-temperature and broadband operation, high radiative quantum efficiency and a large spontaneous emission rate (Purcell effect)
- On resonance, the maximum field enhancements in the gap can reach 200, resulting in up to 30,000-fold fluorescence intensity enhancement of molecules integrated into the gap



From: Probing the mechanisms of large Purcell enhancement in plasmonic nanoantennas G.M. Akselrod *et al.*, Nature Photonics, Vol. 8, pp. 835–840, 2014

Computational nanophotonics: some generalities

- Challenges with the simulation of ElectroMagnetic (EM) wave propagation
  - Geometrical characteristics of the propagation domain:
    - dimensions relatively to the wavelength,
    - irregularly shaped objects and singularities.
  - Physical characteristics of the propagation medium:
    - heterogeneity and anisotropy,
    - physical dispersion and dissipation.
  - Characteristics of the radiating sources and incident fields
- Starting point PDE model: the system of Maxwell equations

James Clerk Maxwell (1831-1879)

The time-domain Maxwell-Drude equations

- In the frequency domain, the polarization $\mathbf{P}$ is linked to the electric field through the relation $\hat{\mathbf{P}} = -\dfrac{\varepsilon_0 \omega_d^2}{\omega^2 + i\gamma_d \omega}\hat{\mathbf{E}}$
- Time domain ODE for the polariaztion: $\dfrac{\partial^2 \mathbf{P}}{\partial t^2} + \gamma_d \dfrac{\partial \mathbf{P}}{\partial t} = \varepsilon_0 \omega_d^2 \mathbf{E}$
- Dipolar current vector: $\mathbf{J}_p = \dfrac{\partial \mathbf{P}}{\partial t}$

$$\left\{ \begin{array}{rcl} \dfrac{\partial \mathbf{H}}{\partial t} & = & -\nabla \times \mathbf{E} \\ \varepsilon_\infty \dfrac{\partial \mathbf{E}}{\partial t} & = & \nabla \times \mathbf{H} - \mathbf{J}_p \\ \dfrac{\partial \mathbf{J}_p}{\partial t} + \gamma_d \mathbf{J}_p & = & \omega_d^2 \mathbf{E} \end{array} \right.$$

Hydrodynamic Drude model

- Generalized definition of the electric permittivity

$$\varepsilon_r(k,\omega) = \varepsilon_\infty - \varepsilon_{\text{local}}(\omega) - \varepsilon_{\text{non local}}(k,\omega)$$

- Time-domain Maxell equations coupled to hydrodynamic Drude model

$$\left\{\begin{array}{rcl} \dfrac{\partial \mathbf{H}}{\partial t} & = & -\nabla \times \mathbf{E} \\ \varepsilon_\infty \dfrac{\partial \mathbf{E}}{\partial t} & = & \nabla \times \mathbf{H} - \mathbf{J}_l - \mathbf{J}_{nl} \\ \dfrac{\partial \mathbf{J}_l}{\partial t} + \gamma_l \mathbf{J}_l & = & \omega_l^2 \mathbf{E} \\ \dfrac{\partial \mathbf{J}_{nl}}{\partial t} + \gamma_{nl} \mathbf{J}_{nl} & = & \beta^2 \nabla Q_{nl} + \omega_{nl}^2 \mathbf{E} \\ \dfrac{\partial Q_{nl}}{\partial t} & = & \nabla . \mathbf{J}_{nl} \end{array}\right.$$

A. Moreau, C. Ciraci and D.R. Smith - Physical Review B 87, 045401 (2013)

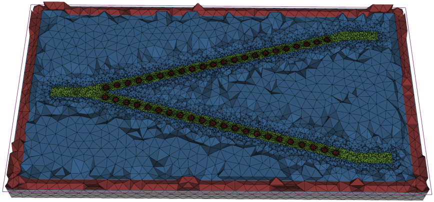
S. Raza, S.I. Bozhevolnyi, M. Wubs, N.A. Mortensen
J. Phys.: Condens. Matter 27, 183204 (topical review, 2015)

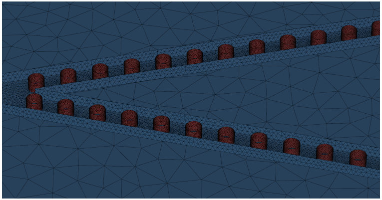
Links with HOMAR

- There are plenty of problems in nanophotonics that are heterogeneous and multiscale
- Optimization (structural and topological) has to be considered as one of the the next steps
- Exploit MHM methods in this context

Collaboration with applied physicists

- Prof. Hugo E Hernandez Figueroa
  School of Electrical and Computer Engineering
  University of Campinas
- Fotonicom
  National Institute of Photonics Science and Technology for Optical communication
  http://fotonicom.ifi.unicamp.br





Thank you for your attention !

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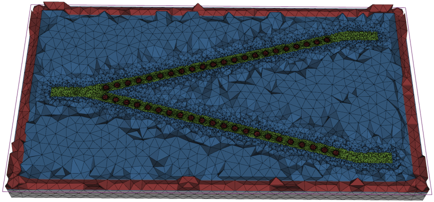

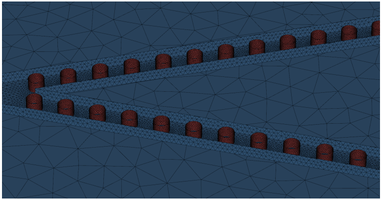

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