

High order curvilinear DGTD method for local and nonlocal plasmonics

Advanced computational methods for nano-optical applications (1A4)

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Spatial dispersion effects in metals

- Various models exist for modeling metal dispersion for the study of plasmon waves
- The most famous is the Drude model describing permittivity function of noble metals
- Such models share a common assumption: the **local response assumption (LRA)**
- LRA states that, at any point of the metal, the polarization of the electrons only depends on the electromagnetic fields at this precise point
- For scales approaching the nanometer, plasmons exhibit features that cannot be correctly predicted in the LRA framework
- **Modified models are required, called non-local models (NLM), owing to their accounting for what happens in the vicinity of the electron to determine its response**
- **Quantum HydroDynamic (QHD)** is one popular (semiclassical) theory

Numerical modeling of QHD

- Frequency-domain and time-domain settings
- Mostly considered in 2D with finite element (FE) and finite difference (TD) methods
- **Resource demanding (CPU and memory) in 3D**

Numerical modeling of QHD: some related works

- Time-domain setting (FDTD)
J.M. McMahon, S.K. Gray and G.C. Schatz
Phys. Rev. B 82, 035423, 2010
M. Fang, Z. Huang, W.E.I. Sha, X.Y.Z. Xiong and X. Wu - PIER, Vol. 157, 2016
And many other references ...
- Time-domain setting (DGTD)
A. Hille, M. Moeferd, C. Wolff, C. Matyssek, R. Rodriguez-Oliveros, C. Prohm
J. Niegemann, S. Grafström, L.M. Eng and K. Busch
J. Phys. Chem. C, Vol. 120, No. 2, 2016
Y. Grynko, T. Zentgraf, T. Meier and J. Förstner
Appl. Phys. B, Vol. 122, 2016
- Frequency-domain setting (FEM)
K.R. Hiremath, L. schiedrich and F. Schmidt
J. Comp. Phys., Vol. 231, No. 17, 2012
N.A. Mortensen, S. Raza, M. Wubs, T. Sndergaard and S.I. Bozhevolnyi
Nature Comm., Vol. 5, 2014
- Frequency-domain setting (HDG - Hybridized DG)
L. Li, S. Lanteri, N.A. Mortensen and M. Wubs
Comput. Phys. Comm., Vol. 219, 2017

Context and objective of the study

Context: development of high order finite element type solvers for time-domain plasmonics

Objective: impact of high order treatment of curvilinear geometries on accuracy and performance of a DGTD method for studying nonlocal dispersion effects

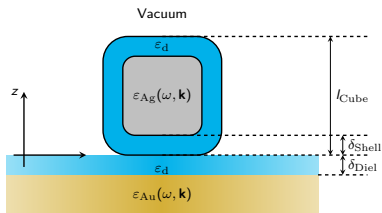
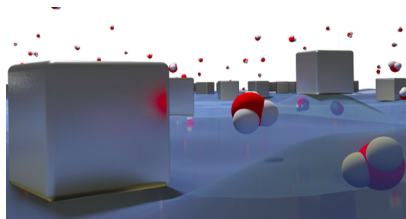
Modeling setting: linearized nonlocal hydrodynamic Drude model

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



Left figure: molecule sensing with nanocubes.

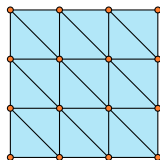
Right figure: nanocube setup to study the influence of nonlocal dispersion on gap plasmons (ongoing work in collaboration with A. Moreau, Institut Pascal, France).

- 1 Numerical framework: the DG method
- 2 Quantum HydroDynamic (QHD) modeling of spatial dispersion
- 3 Curvilinear DGTD method for the Maxwell-QHD equations
- 4 Numerical results
- 5 Software
- 6 Closure

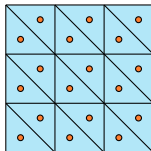
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Context

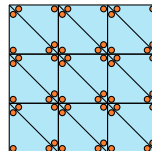
- Somewhere between a finite element and a finite volume method, gathering many good features of both
- Extensively developed by the CFD community
- Application to wave propagation problems naturally followed
- J.S. Hesthaven and T. Warburton (Springer, 2008)
Nodal discontinuous Galerkin methods: algorithms, analysis, and applications



(a) Finite elements:
continuous,
non-constant-per-cell
solution



(b) Finite volumes:
discontinuous,
constant-per-cell
solution



(c) Discontinuous
Galerkin:
discontinuous,
non-constant-per-cell
solution

Classical DG formulation

- Naturally adapted to heterogeneous media and discontinuous solutions
- Can easily deal with unstructured, possibly non-conforming meshes (h -adaptivity)
- High order with compact stencils and non-conforming approximations (p -adaptivity)
- Usually rely on polynomial interpolation but can also accommodate alternative basis expansions
- **But leads to larger problems compared to continuous finite element methods**

DGTD: Discontinuous Galerkin Time-Domain method

- Increasingly studied since 2000
J.S. Hesthaven and T. Warburton, *J. Comput. Phys.*, Vol. 181, 2002
L. Fezoui, S. Lanteri, S. Lohrengel and S. Piperno, *ESAIM: M2AN*, Vol. 39, No. 6, 2005
- For nanophotonics
K. Busch, M. König and J. Niegemann, *Las. Photon. Rev.*, Vol. 5, No. 6, 2011
- Commercial implementations: HFSS-TD (2010), Lumerical Device (2018)

DG for electromagnetic wave propagation in heterogeneous media

- Heterogeneity is ideally treated at the element level
 - Discontinuities occur at material (i.e element) interfaces
 - Mesh generation process is simplified
- Wavelength varies with ε and μ
 - For a given mesh density, approximation order can be adapted at the element level in order to fit to the local wavelength

Discretization of irregularly shaped domains

- Unstructured simplicial meshes
- The basic support of the DG method is the **element** (triangle in 2D and tetrahedron in 3D)
- Local refinement is facilitated by allowing non-conformity
- Non-conformity opens the route to the coupling of different discretization methods (e.g structured/unstructured)
- For time-domain problems, mass matrix is block diagonal (worst case) or diagonal
J. Xin and W. Cai, J. Sci. Comput., Vol. 50, 2012

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Constitutive equations for metals

- Electric polarization: $\mathbf{P} = \mathbf{P}_b + \mathbf{P}_f$
 - \mathbf{P}_b is the background polarization of the bound electrons
 - \mathbf{P}_f models the currents in the free electron gas

- Generalized dispersion model for bound electrons

S. Lanteri, C. Scheid and J. Viquerat - *SIAM J. Sci. Comput.*, Vol. 39, No. 3, 2017

$$\varepsilon_b(\omega) = \varepsilon_\infty - \frac{\sigma}{i\omega} - \sum_{l \in L_1} \frac{a_l}{i\omega - b_l} - \sum_{l \in L_2} \frac{c_l - i\omega d_l}{\omega^2 - e_l + i\omega f_l}$$

- QHD electron response: free gas modeled by a nonlinear fluid equation

$$m_{\text{elec}} (\partial_t + \mathbf{v} \cdot \nabla) \mathbf{v} = -\mathbf{q}_{\text{elec}} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) - m_{\text{elec}} \gamma \mathbf{v} - \nabla \left(\frac{\delta G[n]}{\delta n} \right)$$

$$\partial_t n + \nabla \cdot (n\mathbf{v}) = 0 \quad (\text{continuity equation})$$

where $\frac{\delta G[n]}{\delta n}$ is the **quantum pressure**

- Selection of quantum mechanical effects through the energy functional $G[n]$
C. Ciraci and F. Della Sala - *Phys. Rev. B*, Vol. 93, No. 20, 2016

$$G[n] \approx G_\eta[n] = T^{\text{TF}}[n] + \frac{1}{\eta} T^{\text{W}}[n] + W_{\text{XC}}$$

Terms: kinetic (T), exchange correlation and potential energy (XC)

Linearized QHD model

- Pure Thomas-Fermi theory
- First order linearized term of the quantum pressure: $\beta^2 \frac{1}{n_0} \nabla n$
- Three-dimensional Fermi gas: $\beta = \sqrt{\frac{3}{5}} v_F$ where v_F is the Fermi velocity
- No von Weizsäcker contribution as well as exchange correlation
- Linearizing around an equilibrium state, i.e. $u(\mathbf{x}, t) \approx u_0 + u_1(\mathbf{x}, t)$ for $u \in \{n, \mathbf{v}, \mathbf{E}, \mathbf{B}\}$, keeping the linear terms only and omitting the index $(\cdot)_1$

$$m_{\text{elec}} \partial_t \mathbf{v} = -q_{\text{elec}} \mathbf{E} - m_{\text{elec}} \gamma \mathbf{v} + m_{\text{elec}} \beta^2 \frac{1}{n_0} \nabla n \quad (1)$$

$$\partial_t n = -n_0 \nabla \cdot \mathbf{v} \quad (2)$$

assuming $\partial_t n_0 = \mathbf{v}_0 = \mathbf{E}_0 = \mathbf{B}_0 = 0$.

- Using $\mathbf{J}_{\text{free}} = n_0 q_{\text{elec}} \mathbf{v}$, the current density of free electrons in the fluid, and (2) in $\partial_t(1)$

$$\partial_{tt} \mathbf{J}_{\text{free}} + \gamma \partial_t \mathbf{J}_{\text{free}} - \beta^2 \nabla (\nabla \cdot \mathbf{J}_{\text{free}}) - \omega_P^2 \epsilon_0 \partial_t \mathbf{E} = 0 \quad \text{with } \omega_P = \sqrt{\frac{n_0 b q_{\text{elec}}^2}{\epsilon_0 m_{\text{elec}}}}$$

- First order form

$$\partial_t \mathbf{J}_{\text{free}} + \gamma \mathbf{J}_{\text{free}} - \beta^2 \nabla Q - \omega_P^2 \epsilon_0 \mathbf{E} = 0$$

$$\partial_t Q - \nabla \cdot \mathbf{J}_{\text{free}} = 0$$

Time-domain Maxwell-QHD equations

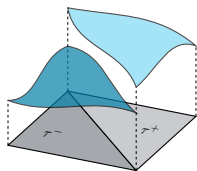
$$\begin{aligned}
 \nabla \times \mathbf{E} + \mu_0 \partial_t \mathbf{H} &= 0 \\
 \nabla \times \mathbf{H} - \varepsilon_0 \varepsilon_\infty \partial_t \mathbf{E} - \mathbf{J}_{\text{free}} - \mathbf{J}_{\text{bound}} &= 0 \\
 \partial_t \mathbf{J}_{\text{free}} + \gamma \mathbf{J}_{\text{free}} - \beta^2 \nabla Q - \omega_p^2 \varepsilon_0 \mathbf{E} &= 0 \\
 \partial_t Q - \nabla \cdot \mathbf{J}_{\text{free}} &= 0 \\
 -\mathbf{J}_{\text{bound}} + \mathcal{J}_0 + \sum_{l \in L_1} \mathcal{J}_l + \sum_{l \in L_2} \mathcal{J}_l &= 0 \\
 -\mathcal{J}_0 + \left(\sigma + \sum_{l \in L_2} d_l \right) \mathbf{E} &= 0 \\
 -\mathcal{J}_l + a_l \mathbf{E} - b_l \mathcal{P}_l &= 0 \quad \forall l \in L_1 \\
 -\partial_t \mathcal{P}_l + \mathcal{J}_l &= 0 \quad \forall l \in L_1 \\
 -\partial_t \mathcal{J}_l + (c_l - d_l f_l) \mathbf{E} - f_l \mathcal{J}_l - e_l \mathcal{P}_l &= 0 \quad \forall l \in L_2 \\
 -\partial_t \mathcal{P}_l + d_l \mathbf{E} + \mathcal{J}_l &= 0 \quad \forall l \in L_2
 \end{aligned}$$

with $\{\varepsilon_\infty, \sigma, a_l, b_l, c_l, d_l, e_l, f_l\} \in \mathbf{R}$ and $L_{1,2}$ being the number of first and second order poles, respectively, in the GDM for local dispersion.

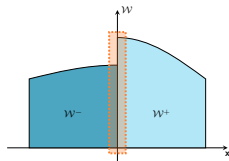
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Main principles of a DG method

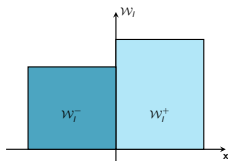
- 1 Definition of the computational domain
 - Unstructured mesh with **tetrahedral** elements
 - Structured or unstructured mesh with **hexahedral** elements
 - Local refinement (possibly non-conforming)
- 2 Discretization in space
 - **Element-wise** weak formulation
 - **Numerical traces** (fluxes) at inter-element boundaries to recover consistency
⇒ Solution of a Riemann problem
 - Numerical integration of elementary terms on a reference element
- 3 Time integration of the semi-discrete equations
 - Explicit scheme (in most of the cases)
 - Implicit scheme or locally implicit scheme
 - Local time stepping



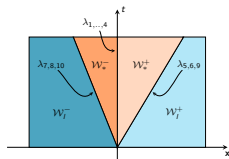
(d) Field discontinuity at the interface of two mesh cells



(e) Generalized Riemann problem at a cell interface



(f) Leading Riemann problem at the cell interface



(g) Solution of the leading term Riemann problem

Riemann problem. Figure (d) illustrates a field discontinuity at the interface of two mesh cells. Generally, this is subject to a generalized Riemann problem as shown in (e). Considering only the leading term within the vicinity of the interface (orange region), simplifies the generalized Riemann problem to a standard Riemann problem with a piecewise constant solution (f). Its solution in the $(x - t)$ space is shown in (g).

Main principles of a DG method

- Z : impedance - Y : admittance - α : upwinding parameter

$$\{\mathbf{A}\}_{-+} := \mathbf{A}^- + \mathbf{A}^+, \quad \llbracket \mathbf{A} \rrbracket_{-+} := \mathbf{A}^- - \mathbf{A}^+,$$

- Numerical flux for the Maxwell part

$$\mathbf{n} \times \mathbf{H}_*^- = \frac{1}{Z^- + Z^+} (\mathbf{n} \times \{\mathbf{ZH}\}_{-+} - \alpha \mathbf{n} \times (\mathbf{n} \times \llbracket \mathbf{E} \rrbracket_{-+})),$$

$$\mathbf{n} \times \mathbf{E}_*^- = \frac{1}{Y^- + Y^+} (\mathbf{n} \times \{\mathbf{YE}\}_{-+} + \alpha \mathbf{n} \times (\mathbf{n} \times \llbracket \mathbf{H} \rrbracket_{-+}))$$

- Numerical flux for the hydrodynamic Drude model part

$$(\beta^-)^2 Q_*^- = \frac{\beta^- \beta^+}{\beta^- + \beta^+} (\{\beta Q\}_{-+} - \alpha (\mathbf{n} \cdot \llbracket \mathbf{J} \rrbracket_{-+})),$$

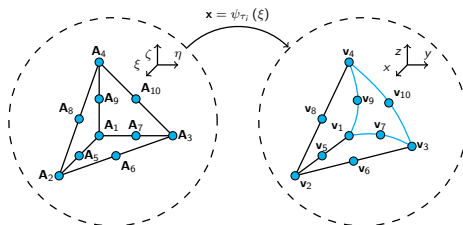
$$(\beta^-)^2 \mathbf{n} \cdot \mathbf{J}_*^- = \frac{(\beta^-)^3 (\beta^+)^3}{(\beta^-)^3 + (\beta^+)^3} \left(\mathbf{n} \cdot \left\{ \frac{\mathbf{J}}{\beta} \right\}_{-+} - \alpha \llbracket Q \rrbracket_{-+} \right)$$

with on the boundary of the nonlocal dispersive domain

$$Q_*^- |_{\partial\Omega_{\text{NL}}} = Q^- \quad \text{and} \quad \mathbf{n} \cdot \mathbf{J}_*^- |_{\partial\Omega_{\text{NL}}} = 0$$

Dealing with *geometry approximation error*

- NURBS-enhanced finite element method (NEFEM)
M. Dawson, R. Sevilla and K. Morgan, *Appl. Math. Model.*, Vol. 55, 2018
High order DGTD method for computing resonant frequencies and modes
- Isogeometric analysis
Directly employs the geometric basis functions as approximation space
A. Buffa, G. Sangalli and R. Vázquez
Comp. Meth. Appl. Mech. Engng., Vol. 199, No. 17-20, 2010
- Our setting: isoparametric FEM



Second order mapping from the reference element $\hat{\tau}_i$ to the physical element τ_i

Validation: standing wave in a spherical PEC cavity

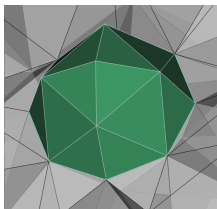
	α	M1		M2		M3		M4	
		Rect.	Curv.	Rect.	Curv.	Rect.	Curv.	Rect.	Curv.
\mathbb{P}_1	0	-	-	2.01	-	1.85	-	1.51	-
	1	-	-	2.14	-	2.03	-	2.01	-
\mathbb{P}_2	0	-	-	2.19	2.85	2.14	2.29	2.03	2.30
	1	-	-	2.20	3.25	2.03	3.08	2.01	3.06
\mathbb{P}_3	0	-	-	2.19	4.17	2.14	3.82	2.03	3.55
	1	-	-	2.20	4.36	2.03	4.03	2.03	4.03
\mathbb{P}_4	0	-	-	2.18	4.37	2.14	4.25	2.03	4.04
	1	-	-	2.18	4.36	2.03	4.26	2.03	4.05

Convergence rates of the spherical cavity case for different approximation orders and fluxes, with linear and curvilinear meshes of increasing refinement (α is the upwinding parameter).

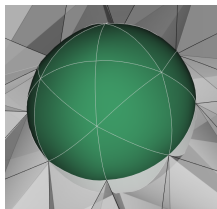
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Numerical results

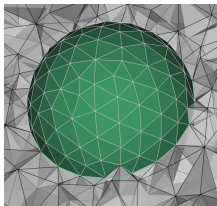
Scattering by a gold nanosphere



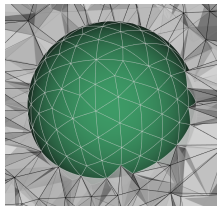
(h) Mesh M1 without high order cells.



(i) Mesh M1 with quadratic cells.



(j) Mesh M2 without high order cells.

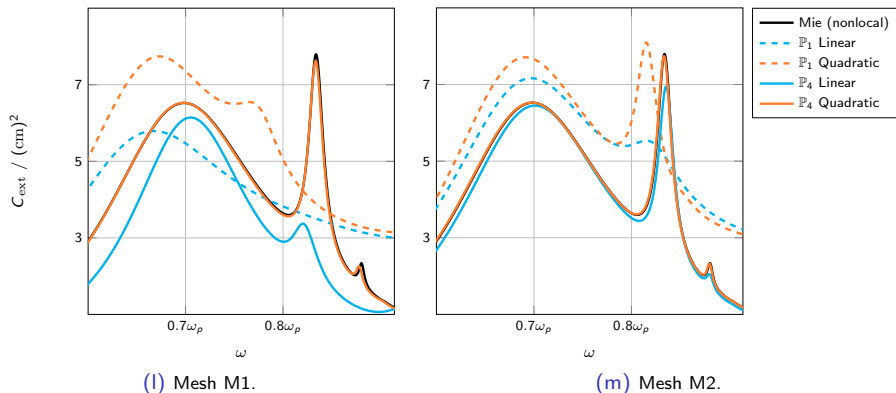


(k) Mesh M2 with quadratic cells.

Four different discretization for a scattered sphere in vacuum. Figures (a) and (b) have the same number of elements and differ by the geometric representation order from linear to quadratic. Figure (c) is a refined version of (a) and (d) is the high order version.

Numerical results

Scattering by a gold nanosphere



Extinction cross-section spectra on meshes M1 and M2.

Comparison of the extinction cross-section spectra of a metallic nano-sphere in dependence of the polynomial interpolation order and the geometric mesh order, i.e. linear or quadratic mesh elements.

Numerical results

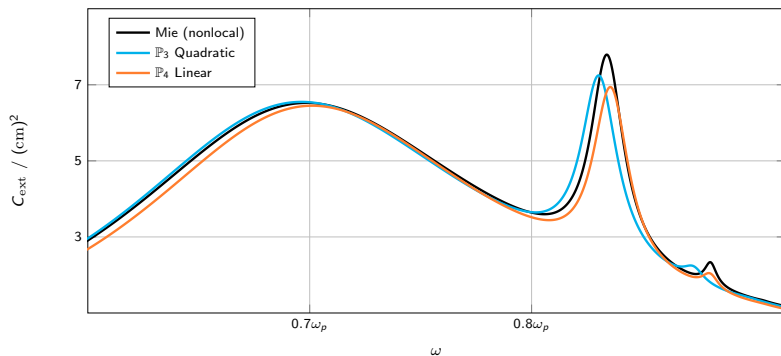
Scattering by a gold nanosphere

	\mathbb{P}_1	\mathbb{P}_2	\mathbb{P}_3	\mathbb{P}_4
M1 – Linear	33.33%	29.95%	28.83%	28.80%
M1 – Quadratic	43.67%	18.51%	6.60%	2.38%
M2 – Linear	33.50%	11.07%	7.18%	5.34%
M2 – Quadratic	39.40%	10.07%	3.58%	0.96%

Relative error is given with respect to the analytical nonlocal Mie solution

Numerical results

Scattering by a gold nanosphere



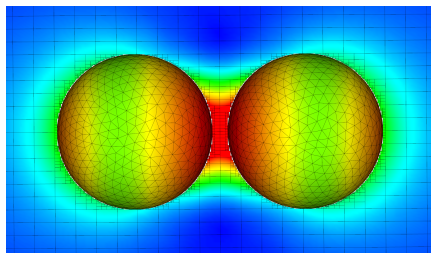
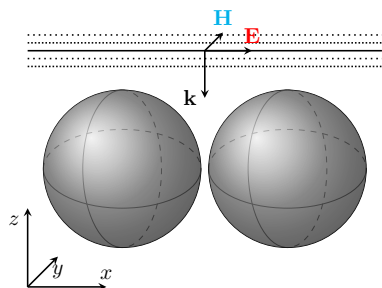
Extinction cross-section spectra on meshes M1 and M2.

Comparison of the extinction cross-section spectra of a metallic nanosphere in dependence of the polynomial interpolation order and the geometric mesh order, i.e. linear or quadratic mesh elements.

Numerical results

Nanosphere dimer

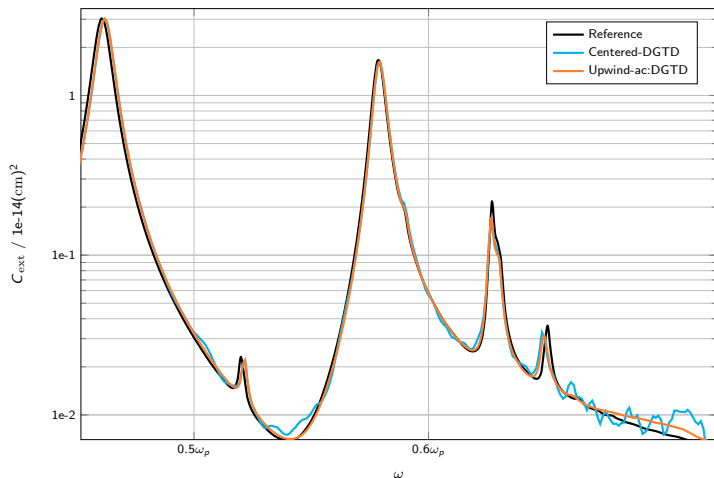
- Material: gold, $\omega_p = 1.39e + 16$ rad/s, $\gamma = 3.23e + 13$ rad/s and $\beta = 0.84$ m/s
- Sphere radius: 10 nm
- Gap size: 2 nm



Nanosphere dimer system. Left figure sketches the dimer setup with an e_x polarized incident plane wave. Right figure shows the 3D field distribution of the electric field on the dimer surface and on a cutting plane and along the dimer axis.

Numerical results

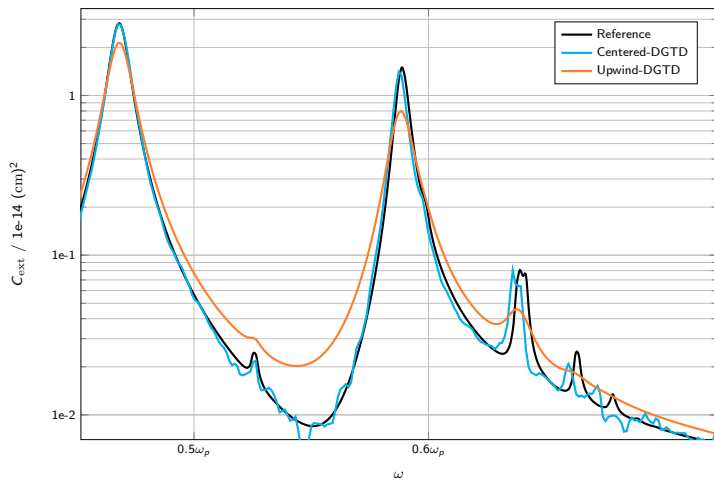
Nanosphere dimer



Nanosphere dimer - local. Comparison of the extinction CS spectra for a spherical dimer system on a linear mesh in dependence of the numerical flux choice. Black: reference DGTD solution with curvilinear elements. Blue: DGTD with centered fluxes and linear mesh cells. Orange: DGTD with upwind fluxes and linear mesh cells.

Numerical results

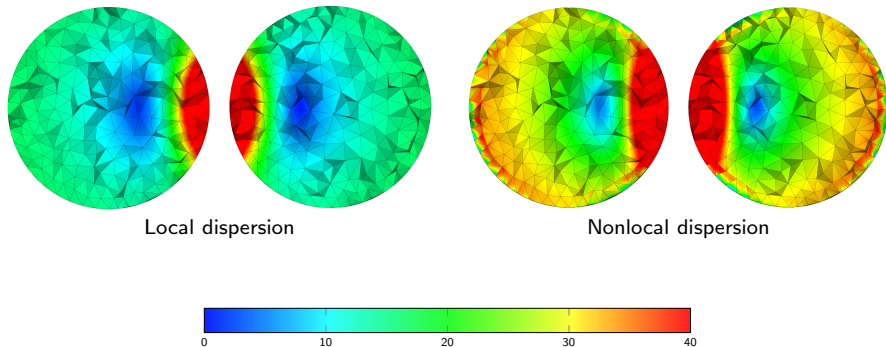
Nanosphere dimer



Nanosphere dimer - nonlocal. Comparison of the extinction CS spectra for a spherical dimer system on a linear mesh in dependence of the numerical flux choice. Black: reference DGTD solution with curvilinear elements. Blue: DGTD with centered fluxes and linear mesh cells. Orange: DGTD with upwind fluxes and linear mesh cells.

Numerical results

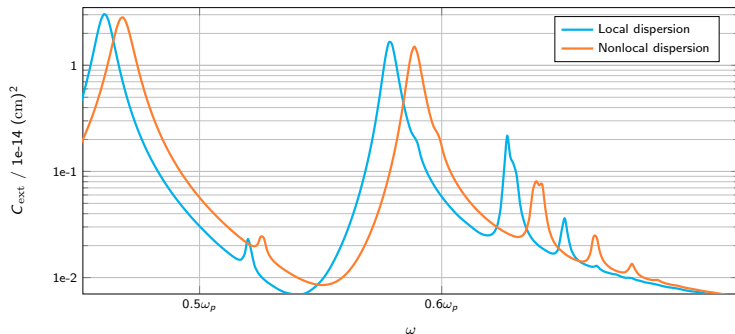
Nanosphere dimer



Nanosphere dimer field plot at the third resonance (volume). Left figure: 3D field distribution of the electric field if a local dispersion model is employed. Right figure: a nonlocal dispersion model is used. Nonlocality smears out vacuum-metal interface and builds up a *penetration* layer. The discontinuities of the DGTD method are clearly visible.

Numerical results

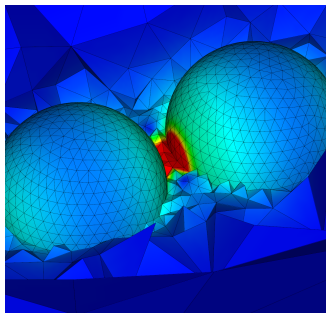
Nanosphere dimer



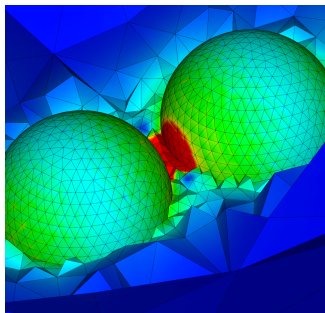
Nanosphere dimer: local vs. nonlocal dispersion. Comparison of local and nonlocal extinction CS.

Numerical results

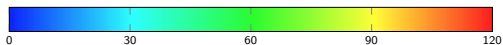
Nanosphere dimer



Local dispersion



Nonlocal dispersion



Nanosphere dimer: local vs. nonlocal dispersion. Left figure: 3D field distribution at third resonance of the electric field if a local dispersion model is employed. Right figure: a nonlocal dispersion model is used. Nonlocality widens the gap plasmon resonance due to stronger field enhancements.

Summary

- Centered DGTD solution almost is polluted by spurious modes
- Upwind DGTD introduces numerical dissipation and damps spurious modes
- The higher numerical dissipation of upwind DGTD can make the detection of weak resonances impossible
- Significant blue-shift for all resonances when switching to nonlocal dispersion
- Regarding the near-field distribution, nonlocality leads to a stronger penetration of the field
- Nonlocality leads to a field enhancement on the surface and widens the gap mode

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Development of a dedicated software suite for nanophotonics

DIOGENeS - DIscOntinuous GalErkin Nano Solvers
<https://diogenes.inria.fr>

- 3D time-domain and frequency-domain Maxwell equations
- High order DG and HDG (Hybridized DG) methods
- Drude, Drude-Lorentz and generalized dispersion models
- Linearized hydrodynamic Drude model
- Unstructured and hybrid cubic/tetrahedral meshes
- Affine and curvilinear elements
- Optimized low storage Runge-Kutta time schemes
- PDE-based and algebraic domain decomposition solvers (frequency-domain)
- Hybrid MIMD/SIMD parallelization based on MPI/OpenMP
- CFS-PML, TF/SF formulation, etc.



Positioning

- Not a commercial software but rather a tool to enable multi-disciplinary collaborations
- Main objectives
 - Enhance the capabilities of DG type methods for dealing with realistic scientific and technological applications
 - Contribute to solving concrete problems requiring advanced modeling and simulation, in addition to experimental design
 - Participate to collaborative projects with physicists facing difficulties with their own simulation tools
- Under development since December 2015
First official release planned for end of 2018



- 1 Numerical framework: the DG method
- 2 Quantum HydroDynamic (QHD) modeling of spatial dispersion
- 3 Curvilinear DGTD method for the Maxwell-QHD equations
- 4 Numerical results
- 5 Software
- 6 Closure**

Summary

- Improved numerical treatment of curvilinear geometries
- Higher order accuracy thanks to higher order mappings
- Better resolution of plasmonic features
- Computational efficiency thanks to coarser meshes

Future works

- Generalized nonlocal optical response (GNOR) model
- Spill-out models
- Nonlinear hydrodynamic Drude model



Thank you for your attention !