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Model order reduction based solver for discontinuous Galerkin element approximation of time-domain Maxwell's equations in dispersive media

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 - Artificial validation case
 - Scattering of a plane wave by a Au-nanowire
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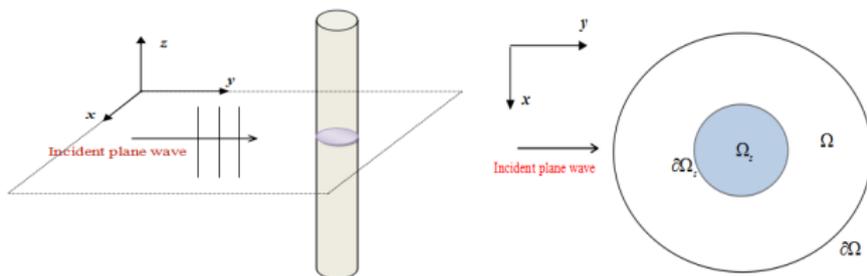
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Time-domain Maxwell-Drude equations

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{H}}{\partial t} + \operatorname{curl} \mathbf{E} = 0 \quad \text{in } \Omega \times (0, t_f], \\ \varepsilon_\infty \frac{\partial \mathbf{E}}{\partial t} - \operatorname{curl} \mathbf{H} + \mathbf{J} = 0 \quad \text{in } \Omega \times (0, t_f], \\ \frac{\partial \mathbf{J}}{\partial t} + \gamma_d \mathbf{J} - \omega_d^2 \mathbf{E} = 0 \quad \text{in } \Omega_s \times (0, t_f], \\ \mathbf{E}(\mathbf{x}; 0) = \mathbf{E}_0(\mathbf{x}), \mathbf{H}(\mathbf{x}; 0) = \mathbf{H}_0(\mathbf{x}) \quad \text{in } \Omega, \\ \mathbf{J}(\mathbf{x}; 0) = \mathbf{J}_0(\mathbf{x}) \quad \text{in } \Omega_s. \end{array} \right. \quad (1)$$

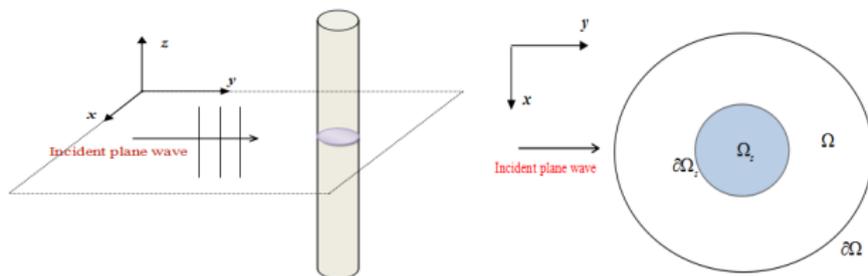
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- $\Omega \in \mathbb{R}^d$, $d = 2, 3$, t_f is the final physical time.
- \mathbf{E} , \mathbf{H} , and \mathbf{J} respectively denote the electric field, the magnetic field and the dipolar current vector.

Boundary condition

Hard-wall condition [Schmitt N, Scheid C, Lanteri S, et al, JCP, 2016.]:

$$\mathbf{n} \cdot \mathbf{J} = 0 \quad \text{on } \partial\Omega_s. \quad (2)$$

Perfect electric conductor condition (PEC):

$$\mathbf{n} \times \mathbf{E} = 0 \quad \text{on } \Gamma_m. \quad (3)$$

First order Silver-Müller absorbing boundary condition (ABC):

$$\mathbf{n} \times \mathbf{E} + z\mathbf{n} \times (\mathbf{n} \times \mathbf{H}) = \mathbf{n} \times \mathbf{E}^{inc} + z\mathbf{n} \times (\mathbf{n} \times \mathbf{H}^{inc}) \quad \text{on } \Gamma_a. \quad (4)$$

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- $\Gamma_m \cap \Gamma_a = \emptyset$, $\Gamma_m \cup \Gamma_a = \partial\Omega$, \emptyset is an empty set.
- \mathbf{n} denotes the unit normal vector pointing outward to $\partial\Omega$.
- \mathbf{E}^{inc} and \mathbf{H}^{inc} are the incident fields.
- $z = \sqrt{\mu/\varepsilon}$.

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Motivation

At present, most of numerical solvers for (1) with (2)-(4) can be summarized as: FDTD, FETD, FVTD, DGTD, etc. The DGTD methods has many advantages compared with the previous numerical methods:

- the use of unstructured possibly non-conforming meshes.
- easily obtained high order accuracy.
- *hp* -adaptivity.
- natural parallelism.
- ...

Motivation

DOFs of the DGTD method: $N_{dof} = \sum_{i=1}^{n_t} d_i$.

- n_t is the number of elements.
- d_i is the number of DOFs on element i .
 - 1D: $d_i = p + 1$.
 - 2D: $d_i = \frac{1}{2}(p + 1)(p + 2)$.
 - 3D: $d_i = \frac{1}{6}(p + 1)(p + 2)(p + 3)$.

Motivation

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Thus, it becomes an important problem how to get a low dimensional system that has the same response characteristics as the original system, while

- sufficiently accurate numerical solutions.
- far less storage requirements and much lower evaluation time.

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MOR

- Proper orthogonal decomposition (POD) methods [Holmes P, Lumley J L, Berkooz G, 1998].
- Krylov subspaces methods.
 - Padé-via-Lanczos (PVL) [R Freund, P Feldmann, 1993].
 - the Arnoldi method.
 - the multi-point rational Krylov subspaces [K Gallivan, E Grimme, 1996].
 - ...
- Balanced truncation methods [Moore B, 1981]
- ...

Notations

- K_i : an element of the mesh.
- N_Ω : the set of indices of the mesh elements.
- F_h^I : the union of all interior interfaces.
- F_h^B : the union of all boundary interfaces.
- F_{ij} : the common face of the K_i and K_j , K_j is a adjacent element.
- $\nu_i := \{j | K_i \cap K_j \neq \emptyset\}$: the set of indices of the elements which are neighbors of K_i .

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For a face $F_{ij} \in F_h^I$, we define average values $\{\cdot\}$:

$$\{\mathbf{v}\}_{F_{ij}} = \frac{1}{2}(\mathbf{v}_j + \mathbf{v}_i)$$

where \mathbf{v}_j and \mathbf{v}_i respectively stand for the traces of \mathbf{v} on F_{ij} from the interior of K_j and K_i . The finite dimensional subspace can be defined by:

$$\mathbf{V}_h^p := \{\mathbf{v} \in (L^2(\Omega))^3 \mid \mathbf{v}|_{K_i} \in (\mathbb{P}_p(K_i))^3, \forall i \in N_\Omega\}.$$

The restrictions of \mathbf{V}_h^p in Ω_s is denoted by $\tilde{\mathbf{V}}_h^p$.

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Weak variation

The DG method seeks an approximate solution $(\mathbf{E}_h, \mathbf{H}_h, \mathbf{J}_h)$ in the space $\mathbf{V}_h^p \times \mathbf{V}_h^p \times \tilde{\mathbf{V}}_h^p$ that should satisfy for all K_i in Ω_h :

$$\begin{cases} \left(\frac{\partial \mathbf{H}_h}{\partial t}, \mathbf{v} \right)_{K_i} + (\text{curl} \mathbf{E}_h, \mathbf{v})_{K_i} = 0, \quad \forall \mathbf{v} \in \mathbf{V}_h^p, \\ \left(\varepsilon_\infty \frac{\partial \mathbf{E}_h}{\partial t}, \mathbf{v} \right)_{K_i} - (\text{curl} \mathbf{H}_h, \mathbf{v})_{K_i} + (\mathbf{J}_h, \mathbf{v})_{K_i} = 0, \quad \forall \mathbf{v} \in \mathbf{V}_h^p, \\ \left(\frac{\partial \mathbf{J}_h}{\partial t}, \mathbf{v} \right)_{K_i} + (\gamma_d \mathbf{J}_h, \mathbf{v})_{K_i} - (\omega_d^2 \mathbf{E}_h, \mathbf{v})_{K_i} = 0, \quad \forall \mathbf{v} \in \tilde{\mathbf{V}}_h^p. \end{cases} \quad (5)$$

Using appropriate Green's formulas and replacing the boundary terms by numerical traces \mathbf{E}_h^* and \mathbf{H}_h^* in (5), which are also known as numerical fluxes, we have:

$$\begin{cases} \left(\frac{\partial \mathbf{H}_h}{\partial t}, \mathbf{v} \right)_{K_i} + (\mathbf{E}_h, \text{curl} \mathbf{v})_{K_i} - \langle \mathbf{E}_h^* \times \mathbf{n}, \mathbf{v} \rangle_{\partial K_i} = 0 \quad \forall \mathbf{v} \in \mathbf{V}_h^p, \\ \left(\varepsilon_\infty \frac{\partial \mathbf{E}_h}{\partial t}, \mathbf{v} \right)_{K_i} - (\mathbf{H}_h, \text{curl} \mathbf{v})_{K_i} + (\mathbf{J}_h, \mathbf{v})_{K_i} + \langle \mathbf{H}_h^* \times \mathbf{n}, \mathbf{v} \rangle_{\partial K_i} = 0 \quad \forall \mathbf{v} \in \mathbf{V}_h^p, \\ \left(\frac{\partial \mathbf{J}_h}{\partial t}, \mathbf{v} \right)_{K_i} + (\gamma_d \mathbf{J}_h, \mathbf{v})_{K_i} - (\omega_d^2 \mathbf{E}_h, \mathbf{v})_{K_i} = 0 \quad \forall \mathbf{v} \in \tilde{\mathbf{V}}_h^p. \end{cases}$$

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Space-discrete formulation

Proper choice of numerical traces \mathbf{E}_h^* and \mathbf{H}_h^* is essential for the correctness and the convergence of the scheme. For the sake of simplicity, we choose to use a fully centered numerical flux, i.e.

$$\mathbf{E}_h^* = \{\mathbf{E}_h\}_{F_{ij}}, \quad \mathbf{H}_h^* = \{\mathbf{H}_h\}_{F_{ij}}, \quad \forall i \in N_\Omega, \quad \forall j \in \nu_i.$$

Replacing surface integrals using centered fluxes in (6) and, re-integrating by parts yields:

$$\begin{cases} \left(\frac{\partial \mathbf{H}_h}{\partial t}, \mathbf{v} \right)_{K_i} = -\frac{1}{2} \left((\operatorname{curl} \mathbf{v}, \mathbf{E}_h)_{K_i} + (\operatorname{curl} \mathbf{E}_h, \mathbf{v})_{K_i} \right) + \frac{1}{2} \sum_{l \in \nu_i} \langle \mathbf{E}_l \times \mathbf{n}, \mathbf{v} \rangle_{F_{il}}, \\ \left(\varepsilon_\infty \frac{\partial \mathbf{E}_h}{\partial t}, \mathbf{v} \right)_{K_i} = \frac{1}{2} \left((\operatorname{curl} \mathbf{v}, \mathbf{H}_h)_{K_i} + (\operatorname{curl} \mathbf{H}_h, \mathbf{v})_{K_i} \right) - \frac{1}{2} \sum_{l \in \nu_i} \langle \mathbf{H}_l \times \mathbf{n}, \mathbf{v} \rangle_{F_{il}}, \\ \left(\frac{\partial \mathbf{J}_h}{\partial t}, \mathbf{v} \right)_{K_i} = -(\gamma_d \mathbf{J}_h, \mathbf{v})_{K_i} + (\omega_d^2 \mathbf{E}_h, \mathbf{v})_{K_i}. \end{cases} \quad (7)$$

Space-discrete formulation

We now define a set of scalar basis functions φ_{ik} ($1 \leq k \leq d_i$) on the element K_i , and then vectorize the basis functions (as well as the test functions), so in a 3D setting we have $\forall i \in N_\Omega$, $0 \leq k \leq d_i$, the vectorial basis functions

$$\Phi_{ik}^1 = (\varphi_{ik}, 0, 0)^T, \quad \Phi_{ik}^2 = (0, \varphi_{ik}, 0)^T \text{ and } \Phi_{ik}^3 = (0, 0, \varphi_{ik})^T.$$

The test function \mathbf{v} can be chosen as the $3d_i$ vectors Φ_{ik}^m ($1 \leq k \leq d_i$, $1 \leq m \leq 3$). Then the problem (7) can be denoted by an equivalent matrix form:

$$\begin{cases} \mathbf{M}_i \frac{d\mathbf{H}_i}{dt} = -\mathbf{K}_i \mathbf{E}_i + \sum_{l \in \nu_i} \mathbf{S}_{il} \mathbf{E}_l, \\ \varepsilon_\infty \mathbf{M}_i \frac{d\mathbf{E}_i}{dt} = \mathbf{K}_i \mathbf{H}_i - \mathbf{M}_i \mathbf{J}_i - \sum_{l \in \nu_i} \mathbf{S}_{il} \mathbf{H}_l, \\ \frac{d\mathbf{J}_i}{dt} = -\gamma_d \mathbf{J}_i + \omega_d^2 \mathbf{E}_i. \end{cases} \quad (8)$$

Space-discrete formulation

Here, the 3×3 block diagonal mass matrix \mathbb{M}_i , the 3×3 block diagonal stiffness matrix \mathbb{K}_i , and the 3×3 block diagonal surface matrix \mathbb{S}_{il} are defined by their respective diagonal blocks:

$$\begin{cases} (\tilde{\mathbb{M}}_i^m)_{jk} = (\Phi_{ij}^m, \Phi_{ik}^m)_{\mathcal{K}_i}, & \text{of size } d_i \times d_i, \quad 1 \leq m \leq 3, \\ (\tilde{\mathbb{K}}_i^m)_{jk} = \frac{1}{2}((\Phi_{ij}^m, \text{curl} \Phi_{ik}^m)_{\mathcal{K}_i} + (\text{curl} \Phi_{ij}^m, \Phi_{ik}^m)_{\mathcal{K}_i}), & \text{of size } d_i \times d_i, \quad 1 \leq m \leq 3 \\ (\tilde{\mathbb{S}}_{il}^m)_{jk} = \langle \Phi_{ij}^m, \Phi_{ik}^m \times \mathbf{n}_{il} \rangle_{F_{il}}, & \text{of size } d_i \times d_i, \quad l \in \nu_i, \quad 1 \leq m \leq 3, \end{cases}$$

here, d_l denotes the number of DOFs on face $l \in \nu_i$.

Space-discrete formulation

Remark 1. For a metallic boundary face $F_{ij} \in \Gamma_m \cap F_h^B$, the metallic boundary condition is $\mathbf{E}_{h|F_{ij}} = 0$. We therefore define

$$\mathbf{E}_{j|F_{ij}} = -\mathbf{E}_{i|F_{ij}}, \quad \mathbf{H}_{j|F_{ij}} = \mathbf{H}_{i|F_{ij}}. \quad (9)$$

For an absorbing boundary face $F_{ij} \in \Gamma_a \cap F_h^B$, we can define

$$\begin{cases} \mathbf{E}_{j|F_{ij}} = z_i N_{ij} \mathbf{H}_{i|F_{ij}} + \mathbf{E}_{i|F_{ij}}^{inc} - z_i N_{ij} \mathbf{H}_{i|F_{ij}}^{inc}, \\ \mathbf{H}_{j|F_{ij}} = -z_i^{-1} N_{ij} \mathbf{E}_{i|F_{ij}} + \mathbf{H}_{i|F_{ij}}^{inc} + z_i^{-1} N_{ij} \mathbf{E}_{i|F_{ij}}^{inc}, \end{cases} \quad (10)$$

where $N_{ij} = \begin{pmatrix} 0 & n_{ijz} & -n_{ijy} \\ -n_{ijz} & 0 & n_{ijx} \\ n_{ijy} & -n_{ijx} & 0 \end{pmatrix}$, and $\mathbf{E}_{i|F_{ij}}^{inc}$, $\mathbf{H}_{i|F_{ij}}^{inc}$ are given incident fields.

Space-discrete formulation

For all element, we can get a descriptor system of first order in time for (8) as following:

$$\begin{cases} \mathbf{M} \frac{d\mathbf{H}_h}{dt} = -\mathbf{K}\mathbf{E}_h + \mathbf{S}^i\mathbf{E}_h + \mathbf{S}^e\mathbf{E}_h + \mathbf{B}^h u_h(t), \\ \varepsilon_\infty \mathbf{M} \frac{d\mathbf{E}}{dt} = \mathbf{K}\mathbf{H}_h - \mathbf{S}^i\mathbf{H}_h - \mathbf{S}^h\mathbf{H}_h - \mathbf{M}\mathbf{J}_h + \mathbf{B}^e u_e(t), \\ \frac{d\mathbf{J}_h}{dt} = -\gamma_d \mathbf{J}_h + \omega_d^2 \mathbf{E}_h. \end{cases} \quad (11)$$

The descriptor system of first order in time can then be written as:

$$\begin{cases} M\dot{x}(t) = Kx(t) + bu(t), \\ y(t) = p^T x(t), \end{cases} \quad (12)$$

with initial condition $x(0) = x_0 = [\mathbf{E}_0(x), \mathbf{H}_0(x), \mathbf{J}_0(x)]^T$, where $M, K \in R^{N \times N}$, $p, b \in R^N$, and $N = 9N_{dof}$.

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POD-DGTD formulations

Let

$$W = [x(t_{n_1}), x(t_{n_2}), \dots, x(t_{n_\ell})] \in R^{N \times \ell}$$

be a collection of **snapshots** of the solution of (12). We compute the singular value decomposition and truncate depending on how fast the singular values decay:

$$W = U \Sigma V^T \approx U_n \Sigma_n V_n^T, \quad n \leq r \leq \ell \ll N.$$

Here, $r = \text{rank}(W)$, U and V are $N \times N$ and $\ell \times \ell$ unitary matrices. Let $U = (\psi_1, \psi_2, \dots, \psi_N)$ and $V = (\phi_1, \phi_2, \dots, \phi_\ell)$, then the POD reduced basis is the set $U_n = \{\psi_i\}_{i=1}^n (n \leq r)$.

POD-DGTD formulations

Then considering the approximation of the state vector $x(t)$ by another state vector, constrained to stay in the subspace spanned by the columns of U_n , namely,

$$x(t) \approx U_n z(t), \quad z(t) \in R^n,$$

yields an linear system with respect to the state variable $z(t)$:

$$\begin{cases} MU_n \dot{z}(t) = KU_n z(t) + bu(t), \\ \tilde{y}(t) = p^T U_n z(t). \end{cases}$$

After left-multiplying the first equation by U_n^T , we have

$$\begin{cases} U_n^T MU_n \dot{z}(t) = U_n^T KU_n z(t) + U_n^T bu(t), \\ \tilde{y}(t) = p^T U_n z(t). \end{cases}$$

Then an n th reduced-order model of the linear system (12) in the time domain is naturally defined, and the quadruples (M_n, K_n, b_n, p_n^T) can be simply expressed as $(U_n^T MU_n, U_n^T KU_n, U_n^T b, p^T U_n)$.

POD-DGTD formulations

Remark 2. For the discrete scheme (8), the number of DOFs ($9N_{dof}$) is very large, but the number DOFs n of the POD-DGTD formulations (22) is very small as we will show from the numerical results.

Remark 3. The choice of the dimension d of the POD basis is not obvious. We denote by $\varepsilon(\psi_1, \psi_2, \dots, \psi_d) = \sum_{j=d+1}^r \lambda_j$ the POD energy or error in the POD basis. If we want the POD energy to be less than some prescribed tolerance ρ , i.e., that

$$\varepsilon(\psi_1, \psi_2, \dots, \psi_n) \leq \rho,$$

we can choose d to be the minimum of positive integer such that

$$\pi(n) = \frac{\sum_{j=1}^n \lambda_j}{\sum_{j=1}^r \lambda_j} \geq 1 - \rho. \quad (13)$$

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Krylov-subspace based operator exponential approach

Introducing the system matrix A as

$$A = -M^{-1}K,$$

stable field approximations can be computed as [Zimmerling J, Wei L, Urbach P, et al, JCP, 2016]

$$x(t) = u(t) * 2\eta(t) \operatorname{Re}[\eta(A) \exp(-At) M^{-1}b] \quad \text{for } t > 0,$$

where $\eta(t)$ is the Heaviside unit step function. The central approximation of the Krylov subspace techniques described then reads as

$$\exp(-At) M^{-1}b = V_n \exp(-H_n t) \mathbf{e}_1,$$

\mathbf{e}_1 being a first unit basis vector, n being the dimensional of the reduced order system, and V_n, H_n can be obtained by Arnoldi-process or rational Lanczos-process.

The references for Krylov-subspace based operator exponential approach:

- Zimmerling J, Wei L, Urbach P, et al. A Lanczos model-order reduction technique to efficiently simulate electromagnetic wave propagation in dispersive media. *Journal of Computational Physics*, 2016, 315: 348-362.
- Botchev M A. Krylov subspace exponential time domain solution of Maxwell's equations in photonic crystal modeling. *Journal of computational and applied mathematics*, 2016, 293: 20-34.
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- ...

Padé approximation and moment-matching

Taking a Laplace transform for the descriptor system (12), assuming zero initial conditional, and then we obtain the following frequency domain formulation of (12):

$$\begin{cases} sMX(s) = KX(s) + bU(s), \\ Y(s) = p^T X(s) \end{cases} \quad (14)$$

where $X(s)$, $Y(s)$, and $U(s)$ respectively denotes the Laplace transform of $x(x)$, $y(x)$, and $u(x)$. Eliminating $X(s)$ in (14) leads to a transfer function of the original system (12) as

$$H(s) = \frac{Y(s)}{U(s)} = p^T (sM - K)^{-1} b, \quad (15)$$

where $s \in \mathbb{C}$, and $H(s) \in R_{N-1,N}$ is a scalar rational function.

Padé approximation and moment-matching

The Taylor series expansion of $H(s)$ about $s_i \in \mathbb{C}$ ($i = 1, 2, \dots, l$) is given by

$$H(s) = \sum_{j=0}^{\infty} m_j(s_i)(s - s_i)^j, \quad (16)$$

where $m_j(s_i) = p^T [-(s_i M - K)^{-1} M]^j (s_i M - K)^{-1} b$ are called moments about s_i , l is the number of expansion points. We seek a reduced order system such that the Taylor expansion of the corresponding transfer function at s_i has the form

$$H_n(s) = \sum_{j=0}^{\infty} \hat{m}_j(s_i)(s - s_i)^j, \quad (17)$$

where $\hat{m}_j(s_i)$ are called moments about s_i for a reduced order system.

Padé approximation and moment-matching

The function $H_n(s) \in R_{n-1,n}$ is said to be an n th multi-point Padé approximation of $H(s)$ about the expansion point s_i ($i = 1, 2, \dots, l$) if it matches with the moments of $H(s)$ as far as possible, i.e.

$$m_j(s_i) = \hat{m}_j(s_i), \quad j = 0, 1, 2, \dots, j_i - 1, \quad i = 1, 2, \dots, l,$$

where $j_i > 0$ denotes the number of the moments corresponding at s_i , and $n = \sum_{i=1}^l j_i$. Then,

$$H(s) = H_n(s) + \sum_{j=j_i}^{\infty} (m_j(s_i) - \hat{m}_j(s_i))((s - s_i)^j), \quad (18)$$

where the last summation term denotes the error between the frequency response of the original system and that of the reduced-order system. If $l = 1$, (17) is a standard n th Padé approximant for $H(s)$.

Padé approximation and moment-matching

If the transfer function $H_n(s)$ of the reduced-order system is expressed as a scalar rational function

$$H_n(s) = \frac{P_{n-1}(s)}{Q_n(s)}, \quad (19)$$

where the numerator $P_{n-1}(s)$ and the denominator $Q_n(s)$ are defined respectively

$$\begin{cases} P_{n-1}(s) = \sum_{j=0}^{n-1} a_j (s - s)^j, \\ Q_n(s) = 1 + \sum_{j=1}^n b_j (s - s)^j, \end{cases}$$

and the coefficients $\{a_j\}$ and $\{b_j\}$ are unknown, we can obtain a total of $2n$ linear equations by (18) and (19) by collecting the coefficients of the polynomials. Unfortunately, the coefficient matrix of the linear equations, which is called the Hanker matrix, usually is ill-conditioned.

Padé via Lanczos ($l = 1, s_0$)

For the matrix $B = -(K - s_0 M)^{-1} M$, the vector $r = (K - s_0 M)b$, and a left starting vector p , the n th Krylov subspace $\mathcal{K}_n(B, r)$ is spanned by a sequence of n column vectors:

$$\mathcal{K}_n(B, r) = \text{span}\{r, Br, B^2 r, \dots, B^{n-1} r\}.$$

This is sometimes called the right Krylov subspace. When the matrix B is nonsymmetric, there is a left Krylov subspace generated by B^T and a starting vector p defined by

$$\mathcal{K}_n(B^T, p) = \text{span}\{p, B^T p, (B^T)^2 p, \dots, (B^T)^{n-1} p\}.$$

Note that the first $2n$ moments m_i of $H(s)$ are connected with Krylov subspaces through computing the inner products between the left and right Krylov sequences:

$$m_{2i} = ((B^T)^i p)^T \cdot (B^i b)^T, \quad m_{2i+1} = ((B^T)^i p)^T \cdot (B^{i+1} b)^T,$$

for $i = 1, 2, \dots, n-1$.

Padé via Lanczos

The left and right Krylov subspaces contain the desired information of moments, but the vectors $B^i r$ and $(B^T)^i p$ are unsuitable as basis vectors. The remedy is to construct more suitable basis vectors $\{v_1, v_2, \dots, v_n\}$ and $\{w_1, w_2, \dots, w_n\}$ such that they span the same desired Krylov subspaces. It is well-known that the Lanczos process is an elegant way to generate the desired basis vectors.

Lanczos process

Give a matrix B , a right starting vector r and a left starting vector p , the Lanczos process generates the basis vector $\{v_i\}$ and $\{w_i\}$, known as the Lanczos vector. Moreover, these Lanczos vector are constructed to be biorthogonal

$$(w_j)^T v_k = 0, \quad \text{for all } j \neq k.$$

The Lanczos vectors can be generated by two three-term recurrences. There recurrences can be stated compactly in matrix form as follows

$$\begin{cases} BV_n = V_n T_n + \rho_{n+1} v_{n+1} \mathbf{e}_n^T, \\ B^T W_n = \tilde{V}_n T_n + \eta_{n+1} w_{n+1} \mathbf{e}_n^T, \end{cases}$$

where T_n and \tilde{T}_n are the tridiagonal matrices.

Reduced Order Model

In general, the application of model order reduction to (12) yields a reduced order model by using the orthogonal projection $x(t) = V_n z(t)$

$$\begin{cases} M_n \dot{z}(t) = K_n z(t) + b_n u(t), \\ \tilde{y}(t) = p_n^T z(t), \end{cases} \quad (20)$$

where $M_n, K_n \in R^{n \times n}$, and $b_n, p_n \in R^n$ have a significantly smaller dimension $n \ll N$ than the original system (12), and

$$M_n = V_n^T M V_n, \quad K_n = V_n^T K V_n, \quad b_n = V_n^T b, \quad p_n = V_n^T p.$$

Why is the simple choice $l = 1, s_1 = s_0$?

- If $l > 1, s_i \in \mathbb{C} (i = 1, 2, \dots, l)$, e.g, the rational Arnoldi method, the selection of suitable expansion points (also called shifts) is crucial for the quality of the resulting reduced order model.
- If $l = 1, s_1 = \textit{infinite}$, e.g, PVL with expansion at infinity is fast while the accuracy of the method is very low.

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- 5 Summary

Information about test problems:

- The computational domain: the square $\Omega_{\square} = (x, y) \in [0, l] \times [0, l]$.
- The boundary condition: PEC.
- The Drude parameters: $\varepsilon_{\infty} = 3.7362$, $\omega_d = 1.3871e7$ GHz, $\gamma_d = 4.41544e4$ GHz.
- Codes: MATLAB 2013b (Memory: 8Gb).
- Method: DG methods with RK_4 , PVL-DGTD methods.

Table: Convergence results for the dispersive cavity problem.

	DGTD- \mathbb{P}_1			DGTD- \mathbb{P}_2			DGTD- \mathbb{P}_3			DGTD- \mathbb{P}_4		
h	L^2 -error	r	L^2 -error	r	L^2 -error	r	L^2 -error	r	L^2 -error	r		
3.678e-08	3.482e-08	-	9.364e-10	-	4.161e-11	-	6.735e-13	-				
1.839e-08	1.618e-08	1.106	1.965e-10	2.253	5.140e-12	3.017	4.091e-14	4.042				
9.194e-09	7.931e-09	1.028	4.678e-11	2.070	6.448e-13	2.995	2.585e-15	3.984				
4.597e-09	3.946e-09	1.007	1.161e-11	2.011	8.099e-14	2.993	1.644e-16	3.975				

It can be seen that the convergence order of numerical simulation is to satisfy the theoretical convergence order.

Table: Computational performance of the artificial problem.

Mesh	DGTD		PVL-DGTD		
	N	L^2 -error	n	s_0	L^2 -error
			\mathbb{P}_1		
M1	3744	3.482e-08	25	1300f	3.489e-08
M2	14976	1.618e-08	25	2100f	1.618e-08
M3	59904	7.931e-09	35	3500f	7.930e-09
			\mathbb{P}_2		
M1	7488	9.364e-10	35	1700f	9.366e-10
M2	29952	1.965e-10	35	3700f	1.964e-10
M3	119808	4.678e-11	90	12000f	4.684e-11
			\mathbb{P}_3		
M1	12480	4.161e-11	45	1500f	4.162e-11
M2	49920	5.140e-12	75	3100f	5.799e-12
M3	199680	6.448e-13	100	15000f	6.518e-13
			\mathbb{P}_4		
M1	18720	6.735e-13	52	2100f	6.907e-13
M2	74880	4.092e-14	90	10000f	4.292e-14
M3	299520	2.585e-15	150	20000f	3.473e-15

✓ the difference between the error calculated by the DGTD method and that calculated by the PVL-DGTD is small.

✓ while the dimension of the reduced order model is much smaller than that of the original system.

Table: Computational performance of the artificial problem.

Mesh	DGTD		PVL-DGTD			Speed-up
	$\bar{T}_{\text{construction}}(\text{s})$	$T_{\text{solution}}(\text{s})$	$\bar{T}_{\text{construction}}(\text{s})$	$T_{\text{PVL}}(\text{s})$	$T_{\text{solution}}(\text{s})$	
			\mathbb{P}_1			
M1	0.566	0.405	0.566	0.148	0.026	57.037%
M2	2.535	3.135	2.535	0.990	0.091	65.518%
M3	14.499	29.041	14.499	9.137	1.550	63.200%
			\mathbb{P}_2			
M1	0.601	3.109	0.601	0.613	0.059	78.385%
M2	2.873	28.020	2.873	3.725	0.437	85.146%
M3	22.994	285.670	22.994	58.094	8.376	76.732%
			\mathbb{P}_3			
M1	0.638	10.680	0.638	2.623	0.147	74.064%
M2	3.765	115.400	3.765	23.464	2.232	77.733%
M3	52.804	1135.300	52.504	224.765	28.818	77.664%
			\mathbb{P}_4			
M1	0.896	36.593	0.896	7.689	0.360	78.004%
M2	7.155	334.265	7.155	92.095	4.832	71.003%
M3	126.198	3148.400	126.198	783.482	74.960	72.734%

✓ It is seen that the PVL-DGTD method saves the required CPU time to yield a uniform accuracy level.

- The point with coordinates: $(4.560e-8, 6.625e-7)$;
- Methods: DGTD- \mathbb{P}_2 with M2, PVL-DGTD- \mathbb{P}_2 with M2.

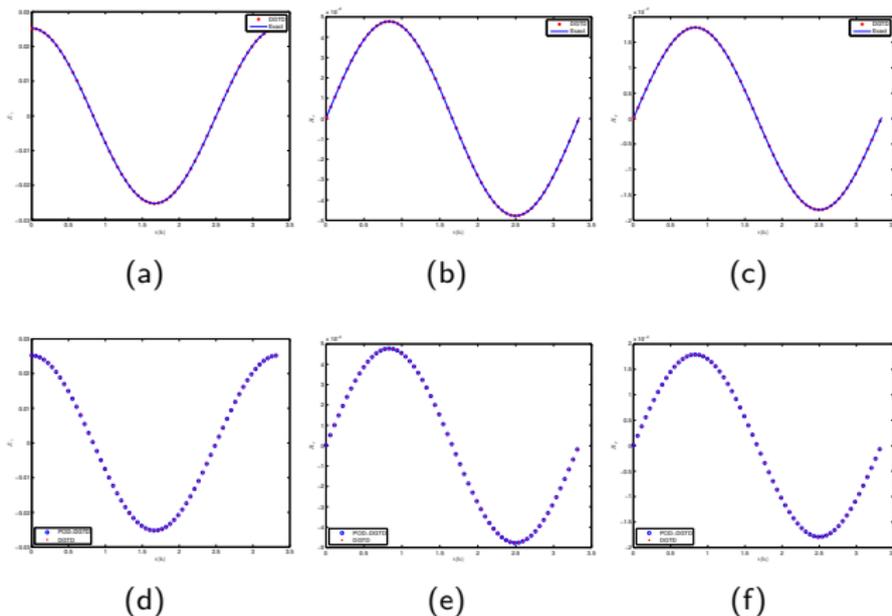


Figure: Comparisons between the usual DGTD methods and the PVL-DGTD methods. (a)~(c): the usual DGTD solutions for E_z , H_x , H_y . (d)~(f): the PVL-DGTD solutions for E_z , H_x , H_y .

■ Time: $t = 1e-6$;

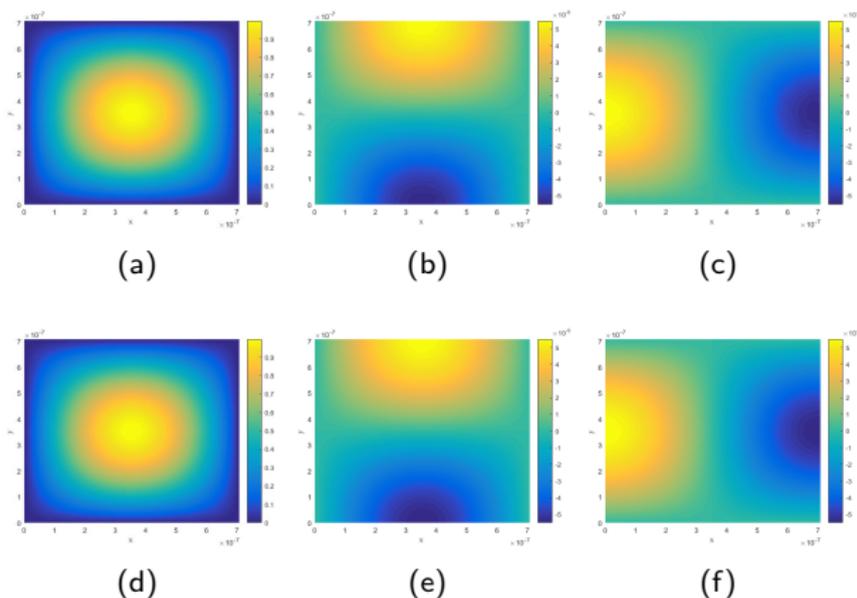


Figure: Comparisons between the usual DGTD methods and the PVL-DGTD methods. (a)~(c): the DGTD solutions for E_z , H_x , H_y . (d)~(f): the PVL-DGTD solutions for E_z , H_x , H_y .

✓ We again find that PVL-DGTD solutions coincide with the DGTD solutions and the analytical solutions.

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- 5 Summary

Information about test problems:

- The computational domain: a gold disk of radius $r = 2nm$.
- The boundary condition: ABC, and propagating along the $-y$ axis.
- The incident plane wave (a sinusoidal modulated Gaussian pulse):

$$\{E_x^{inc}, H_z^{inc}\} \propto \sin(2\pi f_c(t - \tau)) \exp(-(\frac{t - \tau}{\alpha})^2).$$

- The Drude parameters: $\varepsilon_\infty = 1$, $\omega_d = 1.19e4$ THz, $\gamma_d = 141$ THz;
- Codes: MATLAB 2013b (Memory: 8Gb).

Table: Comparisons between the DGTD solutions and the POD-DGTD solutions on CPU times and errors for Au-nanowire.

		Usual DG(a)	Reduced-order DG(b)	Gain	$\max_{n \in [0, N_t]} e_d^n$
MS	\mathbb{P}_p	CPU time(s)	CPU time(s)	CPU_a/CPU_b	
	1	4.253	0.238	17.906	7.431e-12
M1	2	15.637	0.579	27.007	5.028e-12
	1	26.990	1.494	18.070	4.824e-12
M2	2	118.545	5.222	22.703	1.368e-12
	1	866.590	14.744	58.774	8.324e-13
M3	2	3496.236	43.743	79.926	5.531e-13

Field distributions. Time: $t = (6*(1e-16))$.

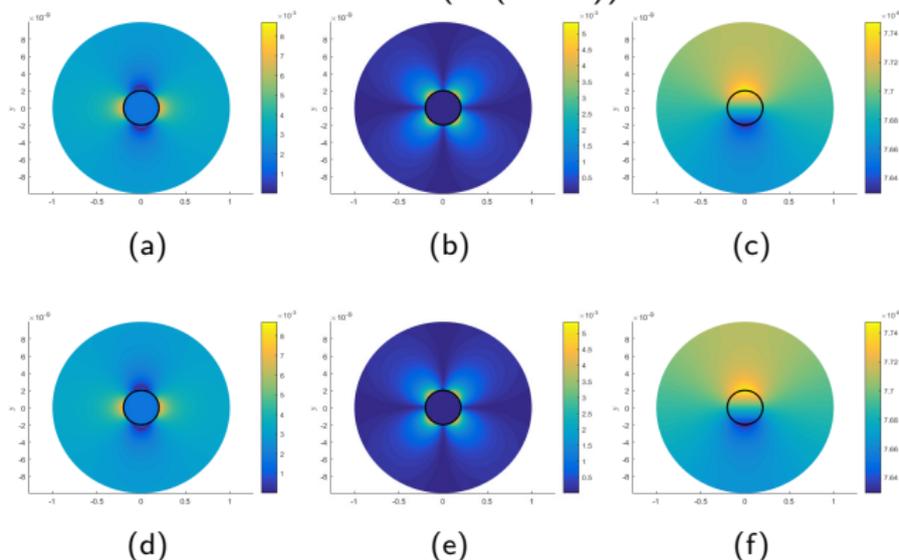


Figure: Field distributions for the simulation of the scattering a plane wave by a gold nanowire. We plot the contour lines of the fields in frequency domain, i.e. the fields are calculated by a DFT from the time-domain solutions by DGTD and POD-DGTD methods. (a)~(c): the DGTD solutions for E_x , E_y , H_z . (d)~(f): the POD-DGTD solutions for E_x , E_y , H_z .

- Field distributions: E_x .
- Time: $t = (6*(1e-16))$.

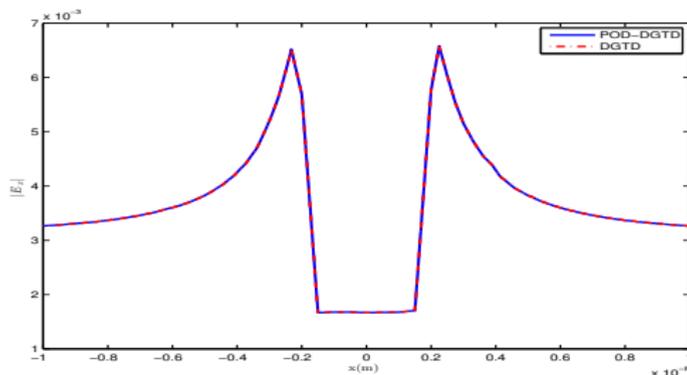


Figure: 1D distribution along the x for the modulus of E_x in the Fourier domain.

Conclusions and Future works

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Future works:

- More complex 3d realistic applications should be investigated;
- The error bounds between the usual DG solutions and the reduced-order DG solutions will be derived;
- The extension of this reduce-order method to more general physical model, e.g., Hydrodynamic Drude and generalized non-local modes.
- other MOR methods, such as, rational Krylov subspace technique.

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