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微纳尺度计算电磁学——领域思考与未来发展

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摘　要　从目标或器件尺寸与电磁波长的关系出发,总结了计算电磁学领域的常用理论和数值方法,以及最新的发展趋势.在分析该领域目前存在问题的基础上,指出了微纳尺度计算电磁学方向的重要性、独特性和对应的挑战.最后,给出个人对该方向发展的建议,并粗略综述了国内学者的工作,展望了领域的未来.

关键词　计算电磁;微纳尺度
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Nanoscale computational electromagnetics—personal thinking and future development

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Abstract　Starting from electrical sizes of objects and devices, commonly adopted theories and numerical methods together with recent advances in research area of computational electromagnetics (CEM) are summarized. Then, based on analysis of the existing problems in this area, the importance, peculiarities, and corresponding challenges of nanoscale CEM are expounded. Finally, personal suggestions for research directions of the nanoscale CEM are presented. Moreover, the research works done by Chinese researchers are reviewed, and outlook of the CEM area is discussed.

Keywords　computational electromagnetics; nanoscale

引　言

麦克斯韦方程是电磁学和光学学科的主导方程,决定了电磁波和光场的物理行为以及物理过程(包括辐射、传播、散射、吸收、转化),在科学技术和工程应用领域影响巨大.如果电磁目标或器件尺寸远远小于电磁波波长,依托低频分析和电路原理,数值模型采用静态法或准静态法[1-2]来处理.如果目标或器件尺寸远远大于电磁波波长,则依托高频分析和射线理论,数值模型采用射线追踪[3]、物理光学[4-5]、几何光学[4-5]、物理绕射[6]、几何绕射[5, 7]、抛物线方程法[8]等处理.如果尺寸和波长可比,依托中频分析和波动物理,数值模型除了采用三大主流方法积分方程[9-10]、有限差分[11-12]、有限元法[13-14]外,也涌现出了相应的快速计算方法[15-16](多层快速多极子[17-20]、快速傅里叶变换[21-25]、多层格林函数插值[26]、稀疏矩阵规则网格[27]、自适应交叉近似[28]、低秩分解[29]、$\mathcal{H}^2$-matrix[30-31]、多重网格法[32]等),低频与宽带方法(Loop-Tree 和 Loop-Star 基函数[33-34]、Buffa-Christiansen 基函数[35]、Calderón 预条件[36]、增广电场积分方程[37]、矢量-标量位方程[38]、低频和宽带多极子[39-43]等),及其它的一些数

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值技术（高阶[44-50]、伪谱[51]、多分辨率分析[52-53]、无条件稳定[54-58]、混合方法[59-60]、并行技术[17,61-62]等）. 近年来，计算电磁学的研究热点集中在间断伽辽金法[63-64]、区域分解法[65-66]、直接法[67-70]、多项式混沌法[71-72]、与频率无关的高频技术[73-75]、特征模分析[76-79]等. 计算电磁学发展至今已有近 60 年，研究者对电磁理论的理解逐步加深，对麦克斯韦方程时空离散的策略也日益精进，对网格[80-85]、边界[86-96]处理与基函数选择[97-99]，对微积分算子特征与空间几何，对矩阵性态与压缩、迭代、预处理等方面都做了极其深入的数学分析和数值实验，学术成果和工业应用丰富.

一方面，基于不同计算电磁学方法和数值技术，HFSS、CST、FEKO、FDTD Solutions、RSoft、COMSOL、Eastwave 等商业软件的功能和服务逐步完备，造成了电磁场与微波学科的科学家、工程师、学者把工作重心放在物理分析和工程设计上. 在高等院校和科研院所，电磁专业的大部分研究生已对算法细节知之甚少，计算电磁学的人才成匮乏态势. 计算电磁学领域的科研影响力有所下降，大部分的科学研究都更专注于物理概念的提出、工程设计的方案、数值结果的分析、产品性能的优劣，而很少人对算法过程、计算机资源过多关心. 许多计算电磁学领域内的年轻学者也时常抱怨领域发展滞缓、研究方向模糊、招生困难等头疼难题. 计算电磁学的未来之路何去何从，需要大家深入思考、集体智慧，更需要解决问题的新方向、新思路、新办法.

1　微纳计算电磁的新特点与挑战

另一方面，由于实验科学的突破革新，精密制备微米和纳米级电磁器件已无技术障碍；纳米科技飞速发展，工业产品层出不穷. 相比经典计算电磁学，微纳计算电磁学有如下新特点：1）工程设计更关心精细结构的近场仿真，而不是电大目标的远场仿真；2）凋落波、表面波及传播波之间的耦合和转换强，且所有材料为色散损耗媒质，没有理想导体的概念；3）感兴趣的物理参数不再是散射问题中的雷达散射截面、辐射问题中的方向性系数与增益，而是消光截面、吸收截面、电磁局域态密度、结构的等效极化率、器件的外量子效率等；4）除了激励问题，非均匀电磁系统的特征值问题、数值格林函数问题变得尤为重要；5）周期、随机、准周期、多层及混合结构多，材料的非线性效应明显；6）电磁与粒子（电子、空穴、离子、激子）混合系统的多物理场耦合呈现强非线性，不同方程的时间、空间网格划分有深度多尺度问题；7）在极弱场强条件下，电磁场波动性变弱，粒子性显著，经典麦克斯韦方程需要量子化处理，但色散损耗媒质中的量子化方案缺乏系统的理论与严格的模型；8）不少微纳尺度电磁多物理问题没有解析解、半解析解，甚至没有明确的数学物理方程，对仿真结果的评估、对仿真模型的改进难度大. 微纳结构的电磁模型，除了经典的线性麦克斯韦方程（材料构成可以是色散损耗煤质），还包括考虑非局域、非线性以及量子效应的多物理场、多尺度模型，如麦克斯韦-流体动力学模型，引入新的界面电磁参数的微观麦克斯韦方程及量子化的麦克斯韦旋度方程，相应公式分别如下：

$$\frac{\partial \boldsymbol{v}_n}{\partial t}+\boldsymbol{v}_n\cdot\nabla\boldsymbol{v}_n+\frac{\boldsymbol{v}_n}{\tau_m}=-\frac{q}{m^*}(\boldsymbol{E}+\boldsymbol{v}_n\times\boldsymbol{B})-\frac{1}{m^*}\nabla V; \tag{1}$$

$$\begin{cases}D_\perp^+-D_\perp^-=d_\parallel\nabla_\parallel\cdot(\boldsymbol{D}_\parallel^+-\boldsymbol{D}_\parallel^-)\\ B_\perp^+-B_\perp^-=0\\ \boldsymbol{E}_\parallel^+-\boldsymbol{E}_\parallel^-=-d_\perp\nabla_\parallel(E_\perp^+-E_\perp^-)\\ \boldsymbol{H}_\parallel^+-\boldsymbol{H}_\parallel^-=\mathrm{i}\omega d_\parallel(\boldsymbol{D}_\parallel^+-\boldsymbol{D}_\parallel^-)\times\boldsymbol{n}\end{cases}; \tag{2}$$

$$\begin{cases}\nabla\times\hat{\boldsymbol{E}}(\boldsymbol{r},t)=-\dfrac{\partial\hat{\boldsymbol{B}}(\boldsymbol{r},t)}{\partial t}\\ \nabla\times\hat{\boldsymbol{H}}(\boldsymbol{r},t)=\hat{\boldsymbol{J}}(\boldsymbol{r},t)+\dfrac{\partial\hat{\boldsymbol{D}}(\boldsymbol{r},t)}{\partial t}\end{cases}. \tag{3}$$

式(1)中的 $\boldsymbol{v}_n$ 是电子速度，τ_m 是弛豫时间，V 是包含量子压力、交换、相关等效应的势能项. 该式通过电流连续性方程，与麦克斯韦方程耦合；电子密度的初始值可由等离子体频率或第一性原理仿真得出. 引入界面电流和电荷后，修正边界条件(2)中的 $d_\parallel$ 和 $d_\perp$ 表面微观电磁参数，需要根据实验结果拟合得出. 式(3)中的量子场量和激励源都是算子形式，具体求解必须采用特征模式展开或非均匀空间的格林函数法，并将算子作用在光子波函数上.

上述涉及前沿电磁理论及应用的课题，有大量技术细节商业软件没法解决，许多功能模块商业软件也未能提供. 涉及到新出现的多物理场分析仿真和工程设计问题，COMSOL 软件也无能为力. 常常需要人工输入多物理方程的变分形式和边界条件，且技术细节处理的一般性、通用性可能导致具体问题的结果不正确（例如，多物理系统的电荷守恒，能量守恒，动量、角动量守恒，电流连续性等可能被破坏）.

在微纳电磁学研究方向亟待解决的前沿科学和工程问题中，计算电磁学人的参与却不多，究其原因

有四.首先,计算电磁学领域的研究生和学者的知识结构仍以传统工程电磁学和数值分析为基础,对交叉学科涉及的物理概念、理论及应用并不熟悉,包括固体物理、半导体器件、量子力学、微纳电磁学、非线性光学、量子电动力学等,而对现代数学(微分几何、群论、拓扑学等)的发展也了解不足.其次,从事新领域的计算仿真要和其他领域的研究者交流合作,缺乏合作渠道和彼此的有效沟通也是一个普遍存在的问题.再次,计算电磁学以算快、算准、算省、算大为目标,许多研究者对问题本身欠缺理论基础和物理视野,这就造成了数值结果无法有逻辑的组织、阐释,物理机制和设计准则无从挖掘,数值结果无法用课题领域相关的语言和思维描述.进一步导致无法将研究成果发表在高影响力的期刊上,或即使发表,论文的可读性也不好.此外,大部分相关领域的读者对算法本身兴趣不大,也造成了计算电磁学有关论文阅读量的大幅降低,领域影响力显著削减.最后,学科交叉、不同领域的交叠已是大势所趋,但相关的复合课程、教材却仍未更新,相关的跨领域学术交流还未成型.而且在有限的研究生培养时间和年轻学者的科研时间中,他们无法有效学习其他领域的知识.同时,采用创新的数值模型挖掘创新的物理概念和优化工程设计,将占据大量时间,投入产出比低,一般的博士生也无法在3～4年的学业中完成.

2 计算电磁发展的新思路

怎样解决上述问题,拓展计算电磁学的新方向、提升领域的影响力,值得每一个计算电磁学人思考.而电磁前沿方向的软件平台,可能成为西方对我国技术禁运的下一个目标,成为将来的“卡脖子”问题.从电磁场和粒子相互作用的角度,其涉及到未来的光伏和照明技术,涉及到未来的量子信息、量子计算机技术,涉及到未来的电磁、光-生物检测技术,也涉及到无线传输-大数据技术等等.与此同时,西方各国则针对电磁学未来面对的技术挑战,调整了教学系统和相关课程,重组了院系,新工科(即物理加工程的培养模式)在欧洲高校已初具规模.经过深入思考,我仅从个人角度,针对我国学科特点、人才结构、专业现状,给出如下几点建议.1)改进电磁场与微波学科的教学体系及课程设置,翻新教材,鼓励研究生跨院系、跨专业选课.除研修电磁学科的传统专业课外,学习1～2门电磁交叉学科的基本知识.2)开展针对年轻学者和研究生的暑期课程或讨论班,举行聚焦前沿课题的小型研讨会,增强交叉专业知识、把握前沿动态、加强跨领域的学科交流、寻找合作机会、扩大领域影响.3)利用网络资源,开展视频讲座活动、开展源代码及程序的开源分享、开展领域成果宣传,降低编写、使用前沿计算程序的门槛,进一步扩大领域影响力,寻找项目合作.4)从纯数值计算,算快、算准、算省、算大为目标,转变到以解决前沿电磁学问题及实际工程应用为目标,以数值模型和算法为基础,以数值结果组织、处理、优化、解释、利用为核心,以开发面向问题的专用工程软件平台为成果的研究思路上来.5)开展高影响力期刊投稿、组织材料、撰写论文、修改申诉的培训,利用一切可利用的资源,提升研究成果的质量、可见度、影响力.

3 国内微纳计算电磁的研究工作

在微纳电磁学数值建模和电磁-粒子混合系统的多物理场分析等交叉前沿方向,据我不完全的了解,国内计算电磁学学者已经做了大量工作:毛军发、尹文言等学者对微纳电子系统“电-热-力”耦合效应的多物理场分析[100-103]、对二维材料的电磁响应建模[104-105],李尔平、陈红胜、陈文超等学者对微纳电子设备的多物理仿真与设计[106-107],学者段宝岩对电子装备的机电热场耦合建模[108],夏明耀、郭立新、陈彬等学者对电磁目标-等离子体相互作用的建模[109-113],王建国等学者对电磁波与相对论带电粒子相互作用及介质强场击穿的模拟[114-116],黄卡玛等学者对微波化学方向的研究[117-118],聂在平、何十全等学者对金属纳米结构的仿真[119],盛新庆、潘小敏等学者对光学力的模拟分析[120-121],陈如山、丁大志等学者对电磁结构和半导体器件的多物理耦合建模[122]、对粒子高次谐波生成的仿真[123],崔铁军、杨帆、李懋坤等学者对超材料、超表面的电磁建模[124-127],吴先良、黄志祥、熊晓燕等学者对增益材料[128]、非线性材料的建模及设计[129-132],胡俊、陈涌频等学者对非均匀电磁环境下的分子自发辐射的模拟[133-134],孙胜等学者对与量子系统无缝连接的矢量-标量位方程的建模[135-136],沙威等学者对太阳能[137-139]、量子电磁学[140-142]的数值分析,曹礼群、陈强等学者对量子半经典框架的数值分析[143-144],童美松等学者对弹性波的仿真[145],刘英、张欢欢等学者对辐射降温[146-148]的建模等等.还有其他相关工作,由于本人刚回国,可能有所疏漏,未能列出,敬请谅解.

4 展 望

上述利用计算电磁技术,对科学和工程前沿领

域的探索，表明我国计算电磁学人面对困难和挑战、奋勇而上的信心，也表明我们对最新电磁交叉领域的知识学习和再创造的能力. 只要国内计算电磁学人团结在一起，加强合作，勇于改革，甘于吃苦，乐于挑战，无私奉献，我国计算电磁学的未来发展将充满新的契机，迎来新的突破，并为推动人类科学和工程的进步发挥重大的作用.

参考文献

[1] DAVIDSON. D B. Computational electromagnetics for rf and microwave engineering[M]. New York: Cambridge University Press, 2011.

[2] PETERSON A F, RAY S L, MITTRA R. Computational methods for electromagnetics[M]. New York: Wiley-IEEE Press, 1997.

[3] LING H, CHOU R C, LEE S W. Shooting and bouncing rays: calculating the RCS of an arbitrarily shaped cavity[J]. IEEE transactions on antennas and propagation, 1989, 37 (2): 194-205.

[4] KNOTT E F, SCHAEFFER J F, TULLEY M T. Radar cross section[M]. 2nd ed. Raleigh: SciTech Publishing Inc., 2004.

[5] 汪茂光. 几何绕射理论[M]. 西安：西安电子科技大学出版社，1994.

[6] UFIMTSEV P Y. Fundamentals of the physical theory of diffraction[M]. New Jersey: Wiley-IEEE Press, 2014.

[7] BOROVIKOV V A, KINBER B Y. Geometrical theory of diffraction[M]. London: IET, 1994.

[8] LEVY M. Parabolic equation methods for electromagnetic wave propagation[M]. London: IEE, 2000.

[9] GIBSON W C. The method of moments in electromagnetics[M]. 2nd. Boca Raton: CRC Press, 2015.

[10] HARRINGTON R F. Field computation by moment methods[M]. New York: Wiley-IEEE Press, 1993.

[11] SULLIVAN D M. Electromagnetic simulation using the FDTD method [M]. New York: Wiley-IEEE Press, 2000.

[12] TAFLOVE A, HAGNESS S C. Computational electrodynamics: the finite-difference time-domain method [M]. 3rd ed. Boston: Artech House, 2005.

[13] JIN J M. The finite element method in electromagnetics[M]. 3rd ed. New York: Wiley-IEEE Press, 2014.

[14] VOLAKIS J L, CHATTERJEE A, KEMPEL L C. Finite element method for electromagnetics: antennas, microwave circuits, and scattering applications [M]. New York: Wiley-IEEE Press, 1998.

[15] CHEW W C, JIN J M, LU C C, et al. Fast solution methods in electromagnetics[J]. IEEE transactions on antennas and propagation, 1997, 45(3): 533-543.

[16] CHEW W C, MICHIELSSEN E, SONG J M, et al. Fast and efficient algorithms in computational electromagnetics[M]. Norwood: Artech House Inc., 2001.

[17] ERGUL O, GUREL L. The multilevel fast multipole algorithm (MLFMA) for solving large-scale computational electromagnetics problems [M]. New York: IEEE-WILEY Press, 2014.

[18] SONG J M, LU C C, CHEW W C. Multilevel fast multipole algorithm for electromagnetic scattering by large complex objects[J]. IEEE transactions on antennas and propagation, 1997, 45(10): 1488-1493.

[19] GREENGARD L, ROKHLIN V. A fast algorithm for particle simulations[J]. Journal of computational physics, 1987, 73(2): 325-348.

[20] 胡俊. 复杂目标矢量电磁散射的高效方法：快速多极子方法及其应用[D]. 成都：电子科技大学，2000.

[21] CATEDRA M F, GAGO E, NUNO L. A numerical scheme to obtain the RCS of three-dimensional bodies of resonant size using the conjugate gradient method and the fast Fourier transform[J]. IEEE transactions on antennas and propagation, 1989, 37(5): 528-537.

[22] SARKAR T, ARVAS E, RAO S. Application of FFT and the conjugate gradient method for the solution of electromagnetic radiation from electrically large and small conducting bodies[J]. IEEE transactions on antennas and propagation, 1986, 34(5): 635-640.

[23] PHILLIPS J R, WHITE J K. A precorrected-FFT method for electrostatic analysis of complicated 3-D structures[J]. IEEE transactions on computer-aided design of integrated circuits and systems, 1997, 16 (10): 1059-1072.

[24] SEO S M, LEE J F. A fast IE-FFT algorithm for solving PEC scattering problems[J]. IEEE transactions on magnetics, 2005, 41(5): 1476-1479.

[25] BLESZYNSKI E, BLESZYNSKI M, JAROSZEWICZ T. AIM: adaptive integral method for solving large-scale electromagnetic scattering and radiation problems[J]. Radio science, 1995, 31(5): 1225-1251.

[26] WANG H G, CHAN C H. The implementation of multilevel Green's function interpolation method for full-wave electromagnetic problems[J]. IEEE transactions on antennas and propagation, 2007, 55 (5): 1348-1358.

[27] PAK K, TSANG L, JOHNSON J. Numerical simu-

lations and backscattering enhancement of electromagnetic waves from two-dimensional dielectric random rough surfaces with the sparse-matrix canonical grid method[J]. Journal of the Optical Society of America A, 1997, 14: 1515-1529.

[28] ZHAO K, VOUVAKIS M N, LEE J F. The adaptive cross approximation algorithm for accelerated method of moments computations of EMC problems[J]. IEEE transactions on electromagnetic compatibility, 2005, 47(4): 763-773.

[29] LIBERTY E, WOOLFE F, MARTINSSON P G, et al. Randomized algorithms for the low-rank approximation of matrices[J]. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104 (51): 20167-20172.

[30] HACKBUSCH W, BÖRM S. $\mathcal{H}^2$-matrix approximation of integral operators by interpolation[J]. Applied numerical mathematics, 2002, 43(1): 129-143.

[31] CHAI W, JIAO D. An $\mathcal{H}^2$-matrix-based integral-equation solver of reduced complexity and controlled accuracy for solving electrodynamic problems [J]. IEEE transactions on antennas and propagation, 2009, 57(10): 3147-3159.

[32] ZHU Y, CANGELLARIS A C. Multigrid finite element methods for electromagnetic field modeling[M]. New York: IEEE-Wiley Press, 2006.

[33] EIBERT T F. Iterative-solver convergence for loop-star and loop-tree decompositions in method-of-moments solutions of the electric-field integral equation [J]. IEEE antennas and propagation magazine, 2004, 46 (3): 80-85.

[34] VECCHI G. Loop-star decomposition of basis functions in the discretization of the EFIE [J]. IEEE transactions on antennas and propagation, 1999, 47 (2): 339-346.

[35] BUFFA A. CHRISTIANSEN S H. A dual finite element complex on the barycentric refinement [J]. Mathematics of computation, 2007, 76: 1743-1769.

[36] ANDRIULLI F P, COOLS K, BAGCI H, et al. A multiplicative Calderon preconditioner for the electric field integral equation[J]. IEEE transactions on antennas and propagation, 2008, 56(8): 2398-2412.

[37] QIAN Z G, CHEW W C. An augmented electric field integral equation for high-speed interconnect analysis [J]. Microwave and optical technology letters, 2008, 50(10): 2658-2662.

[38] CHEW W C. Vector potential electromagnetics with generalized gauge for inhomogeneous media: formulation[J]. Progress in electromagnetics research, 2014, 149: 69-84.

[39] JIANG L J, CHEW W C. A mixed-form fast multipole algorithm[J]. IEEE transactions on antennas and propagation, 2005, 53(12): 4145-4156.

[40] CHENG H, CRUTCHFIELDW Y Z, GIMBUTAS L F, et al. A wideband fast multipole method for the Helmholtz equation in three dimensions[J]. Journal of computational physics, 2006, 216(1): 300-325.

[41] BOGAERT I, PEETERS J, OLYSLAGER F. A nondirective plane wave MLFMA stable at low frequencies[J]. IEEE transactions on antennas and propagation, 2008, 56(12): 3752-3767.

[42] ZHAO J S, CHEW W C. Integral equation solution of Maxwell's equations from zero frequency to microwave frequencies[J]. IEEE transactions on antennas and propagation, 2000, 48(10): 1635-1645.

[43] WALLEN H, SARVAS J. Translation procedures for broadband MLFMA[J]. Progress in electromagnetics research, 2005, 55: 47-78.

[44] GEORGAKOPOULOS S V, BIRTCHER C R, BALANIS C A, et al. Higher-order finite-difference schemes for electromagnetic radiation, scattering, and penetration, part I: theory[J]. IEEE antennas and propagation magazine, 2002, 44(1): 134-142.

[45] GEORGAKOPOULOSS V, BIRTCHER C R, BALANIS C A, et al. Higher-order finite-difference schemes for electromagnetic radiation, scattering, and penetration, part 2: applications[J]. IEEE antennas and propagation magazine, 2002, 44 (1): 92-101.

[46] JORGENSEN E, VOLAKIS J L, MEINCKE P, et al. Higher order hierarchical Legendre basis functions for electromagnetic modeling[J]. IEEE transactions on antennas and propagation, 2004, 52(11): 2985-2995.

[47] SILVESTER P. A general high-order finite-element analysis program waveguide[J]. IEEE transactions on microwave theory and techniques, 1969, 17(4): 204-210.

[48] ZHAO S, WEI G W. High-order FDTD methods via derivative matching for Maxwell's equations with material interfaces[J]. Journal of computational physics, 2004, 200(1): 60-103.

[49] WEBB J P. Hierarchal vector basis functions of arbitrary order for triangular and tetrahedral finite elements[J]. IEEE transactions on antennas and propagation, 1999, 47(8): 1244-1253.

[50] YOUNG J L, GAITONDE D, SHANG J S. Toward

the construction of a fourth-order difference scheme for transient EM wave simulation: staggered grid approach[J]. IEEE transactions on antennas and propagation, 1997, 45(11): 1573-1580.
[51] LIU Q H. PSTD algorithm: a time-domain method requiring only two cells per wavelength[J]. Microwave and optical technology letters, 1997, 15(3): 158-165.
[52] KRUMPHOLZ M, KATEHI L P B. MRTD: new time-domain schemes based on multiresolution analysis[J]. IEEE transactions on microwave theory and techniques, 1996, 44(4): 555-571.
[53] CHEN Y, CAO Q, MITTRA R. Multiresolution time domain scheme for electromagnetic engineering [J]. New York: Wiley, 2005.
[54] SUN G, TRUEMAN C W. Unconditionally stable Crank-Nicolson scheme for solving two-dimensional Maxwell's equations[J]. Electronics letters, 2003, 39(7): 595-597.
[55] ZHEN F, CHEN Z, ZHANG J. Toward the development of a three-dimensional unconditionally stable finite-difference time-domain method[J]. IEEE transactions on microwave theory and techniques, 2000, 48 (9): 1550-1558.
[56] SHIBAYAMA J, MURAKI M, YAMAUCHI J, et al. Efficient implicit FDTD algorithm based on locally one-dimensional scheme [J]. Electronics letters, 2005, 41(19): 1046-1047.
[57] HE Q, GAN H, JIAO D. Explicit time-domain finite-element method stabilized for an arbitrarily large time step[J]. IEEE transactions on antennas and propagation, 2012, 60(11): 5240-5250.
[58] TAN E L. Unconditionally stable LOD-FDTD method for 3-D Maxwell's equations[J]. IEEE microwave and wireless components letters, 2007, 17(2): 85-87.
[59] SHENG X Q, JIN J M, SONG J, et al. On the formulation of hybrid finite-element and boundary-integral methods for 3-D scattering[J]. IEEE transactions on antennas and propagation, 1998, 46(3): 303-311.
[60] TZOULIS A, EIBERT T F. A hybrid FEBI-MLFMM-UTD method for numerical solutions of electromagnetic problems including arbitrarily shaped and electrically large objects[J]. IEEE transactions on antennas and propagation, 2005, 53(10): 3358-3366.
[61] PAN X M, PI W C, YANG M L, et al. Solving problems with over one billion unknowns by the MLFMA[J]. IEEE transactions on antennas and propagation, 2012, 60(5): 2571-2574.
[62] TABOADA J M, ARAUJO M G, BERTOLO J M, et al. MLFMA-FFT parallel algorithm for the solution of large-scale problems in electromagnetics[J]. Progress in electromagnetics research, 2010, 105: 15-30.
[63] COCKBURN B, SHU C W. TVB Runge-Kutta local projection discontinuous Galerkin finite element method for conservation laws. II. general framework[J]. Mathematics of computation, 1989, 52 (186): 411-435.
[64] HESTHAVEN J S, WARBURTON T. Nodal high-order methods on unstructured grids: I. time-domain solution of Maxwell's equations[J]. Journal of computational physics, 2002,181: 186-221.
[65] LEE S C, VOUVAKIS M N, LEE J F. A non-overlapping domain decomposition method with non-matching grids for modeling large finite antenna arrays [J]. Journal of computational physics, 2005, 203(1): 1-21.
[66] LI M K, CHEW W C. Wave-field interaction with complex structures using equivalence principle algorithm[J]. IEEE transactions on antennas and propagation, 2007, 55(1): 130-138.
[67] DUFF I S, ERISMAN A M, REID J K. Direct methods for sparse matrices[M]. Oxford: Oxford University Press, 2017.
[68] GILLMAN A, YOUNG P M, MARTINSSON P G. A direct solver with O(N) complexity for integral equations on one-dimensional domains[J]. Frontiers of mathematics in China, 2012, 7(2): 217-247.
[69] MARTINSSON P G, ROKHLIN V. A fast direct solver for boundary integral equations in two dimensions[J]. Journal of computational physics, 2005, 205(1): 1-23.
[70] DAVIS T A, DUFF I S. An unsymmetric-pattern multifrontal method for sparse LU factorization[J]. SIAM journal on matrix analysis and applications, 1997, 18 (1): 140-158.
[71] XIU D, HESTHAVEN J S. High-order collocation methods for differential equations with random inputs [J]. SIAM journal on scientific computing, 2005, 27 (3): 1118-1139.
[72] BAGCI H, YUCEL A C, HESTHAVEN J S, et al. A fast stroud-based collocation method for statistically characterizing EMI/EMC phenomena on complex platforms[J]. IEEE transactions on electromagnetic compatibility, 2009, 51(2): 301-311.
[73] BETTESS P, LAGHROUCHE O, PERREY-DEBAIN

E, et al. Prescribed error tolerances within fixed computational times for scattering problems of arbitrarily high frequency: the convex case[J]. Philosophical transactions: mathematical, physical and engineering sciences, 2004, 362(1816): 629-645.

[74] WU Y M, JIANG L J, CHEW W C. An efficient method for computing highly oscillatory physical optics integral [J]. Progress in electromagnetics research, 2012, 127: 211-257.

[75] WU Y M, JIANG L J, SHA W, et al. The numerical steepest descent path method for calculating physical optics integrals on smooth conducting quadratic surfaces[J]. IEEE transactions on antennas and propagation, 2013, 61(8): 4183-4193.

[76] CHEN Y, WANG C F. Characteristic modes: theory and applications in antenna engineering [J]. New Jersey: Wiley, 2015.

[77] CHEN Y, WANG C F. Electrically small UAV antenna design using characteristic modes [J]. IEEE transactions on antennas and propagation, 2014, 62 (2): 535-545.

[78] DAI Q I, WU J, GAN H, et al. Large-scale characteristic mode analysis with fast multipole algorithms [J]. IEEE transactions on antennas and propagation, 2016, 64(7): 2608-2616.

[79] SARKAR T K, MOKOLE E L, SALAZAR-PALMA M. An expose on internal resonance, external resonance, and characteristic modes[J]. IEEE transactions on antennas and propagation, 2016, 64 (11): 4695-4702.

[80] BRENGER J P. A Huygens subgridding for the FDTD method[J]. IEEE transactions on antennas and propagation, 2006, 54(12): 3797-3804.

[81] OKONIEWSKI M, OKONIEWSKA E, STUCHLY M A. Three-dimensional subgridding algorithm for FDTD[J]. IEEE transactions on antennas and propagation, 1997, 45(3): 422-429.

[82] DEY S, MITTRA R. A locally conformal finite-difference time-domain(FDTD) algorithm for modeling three-dimensional perfectly conducting objects[J]. IEEE microwave and guided wave letters, 1997, 7 (9): 273-275.

[83] XIAO T, LIU Q H. Enlarged cells for the conformal FDTD method to avoid the time step reduction[J]. IEEE microwave and wireless components letters, 2004, 14(12): 551-553.

[84] ZAGORODNOV I A, SCHUHMANN R, WEILAND T. A uniformly stable conformal FDTD-method in Cartesian grids[J]. International journal of numerical modelling-electronic networks devices and fields, 2003, 16(2): 127-141.

[85] YU W H, MITTRA R. A conformal FDTD algorithm for modeling perfectly conducting objects with curve-shaped surfaces and edges[J]. Microwave and optical technology letters, 2000, 27(2): 136-138.

[86] MUR G. Absorbing boundary-conditions for the finite-difference approximation of the time-domain electromagnetic-field equations[J]. IEEE transactions on electromagnetic compatibility, 1981, 23(4): 377-382.

[87] BERENGER J P. A perfectly matched layer for the absorption of electromagnetic waves[J]. Journal of computational physics, 1994, 114(2): 185-200.

[88] CHEW W C, WEEDON W H. A 3-D perfectly matched medium from modified Maxwells equations with stretched coordinates[J]. Microwave and optical technology letters, 1994, 7(13): 599-604.

[89] CAO Q S, CHEN Y C, MITTRA R. Multiple image technique (MIT) and anistropic perfectly matched layer (APML) in implementation of MRTD scheme for boundary truncations of microwave structures [J]. IEEE transactions on microwave theory and techniques, 2002, 50(6): 1578-1589.

[90] ELMAHGOUB K, YANG F, ELSHERBENI A Z. Scattering analysis of periodic structures using finite-difference time-domain method [M]. San Rafael: Morgan & Claypool Publishers, 2012.

[91] RODEN J A, GEDNEY S D. Convolution PML (CPML): an efficient FDTD implementation of the CFS-PML for arbitrary media[J]. Microwave and optical technology letters, 2000, 27: 334-339.

[92] CHOW Y L, YANG J J, FANG D G, et al. A closed-form spatial Green's function for the thick microstrip substrate[J]. IEEE transactions on microwave theory and techniques, 1991, 39(3): 588-592.

[93] BEGGS J H, LUEBBERS R J, YEE K S, et al. Finite-difference time-domain implementation of surface impedance boundary conditions[J]. IEEE transactions on antennas and propagation, 1992, 40(1): 49-56.

[94] MALONEY J G, SMITH G S. The efficient modeling of thin material sheets in the finite-difference time-domain (FDTD) method[J]. IEEE transactions on antennas and propagation, 1992, 40(3): 323-330.

[95] MEI K K, FANG J, Superabsorption-a method to improve absorbing boundary conditions (electromagnetic waves)[J]. IEEE transactions on antennas and propagation, 1992, 40(3): 1001-1010.

[96] HOPPE D J. Impedance boundary conditions in electromagnetics[J]. Boca Raton: CRC Press, 1995.

[97] PETERSON A F, WILTON D R, JORGENSON R E. Variational nature of Galerkin and non-Galerkin moment method solutions[J]. IEEE transactions on antennas and propagation, 1996, 44(4): 500-503.

[98] PRAKASH V V S, MITTRA R. Characteristic basis function method: a new technique for efficient solution of method of moments matrix equations[J]. Microwave and optical technology letters, 2003, 36: 95-100.

[99] GÜREL, SERTEL K, ŞENDUR Í K. On the choice of basis functions to model surface electric current densities in computational electromagnetics[J]. Radio science, 1999, 34(6): 1373-1387.

[100] CHEN W C, YIN W Y, JIA L, et al. Electrothermal characterization of single-walled carbon nanotube (SWCNT) interconnect arrays[J]. IEEE transactions on nanotechnology, 2009, 8(6): 718-728.

[101] KONG F Z, YIN W Y, MAO J F. Electro-thermo-mechanical characterizations of various wire bonding interconnects illuminated by an electromagnetic pulse [J]. IEEE transactions on advanced packaging, 2010, 33(3): 729-737.

[102] LI N, MAO J, ZHAO W S, et al. Electrothermal co-simulation of 3-D carbon-based heterogeneous interconnects [J]. IEEE transactions on components, packaging and manufacturing technology, 2016, 6: 518-526.

[103] XU J, YIN W Y, MAO J. Transient thermal analysis of GaN heterojunction transistors (HFETs) for high-power applications[J]. IEEE microwave and wireless components letters, 2007, 17(1): 55-57.

[104] CUI J P, ZHAO W S, YIN W Y, et al. Signal transmission analysis of multilayer graphene nano-ribbon (MLGNR) interconnects[J]. IEEE transactions on electromagnetic compatibility, 2011, 54(1): 126-132.

[105] WANG X H, YIN W Y, CHEN Z. Matrix exponential FDTD modeling of magnetized graphene sheet[J]. IEEE antennas and wireless propagation letters, 2013, 12: 1129-1132.

[106] CHEN W, CHENG R, WANG D W, et al. Electrothermal effects on hot-carrier reliability in SOI MOSFETs: AC versus circuit-speed random stress [J]. IEEE transactions on electron devices, 2016, 63(9): 3669-3676.

[107] CHEN W, LEBURTON J P, YIN W Y, et al. Multiphysics modeling and simulation of carrier dynamics and thermal transport in monolayer MoS2/WSe2 heterojunction[J]. IEEE transactions on electron devices, 2018, 65(10): 4542-4547.

[108] 段宝岩. 电子装备机电耦合理论、方法及应用[M]. 北京: 科学出版社, 2011.

[109] CHEN Q, CHEN B. Hybrid electrodynamics and kinetics simulation for electromagnetic wave propagation in weakly ionized hydrogen plasmas[J]. Physical review E, 201, 286(4): 046704.

[110] CHEN Q, CHEN B, CHEN P F, et al. A unified radiative magnetohydrodynamics code for lightning-like discharge simulations[J]. Physics of Plasmas, 2014, 21(3): 032901.

[111] ZHAO P C, GUO L X, LI H M. Effect of microwave frequency on plasma formation in air breakdown at atmospheric pressure [J]. Chinese physics B, 2015 (10): 336-339.

[112] QIAN J W, ZHANG H L, XIA M Y. Modelling of electromagnetic scattering by a hypersonic cone-like body in near space[J]. International journal of antennas and propagation, 2017: 3049532.

[113] XIE K, YANG M, BAI B, et al. Re-entry communication through a plasma sheath using standing wave detection and adaptive data rate control[J]. Journal of applied physics, 2016, 119(2): 023301.

[114] WANG Y, WANG J, CHEN Z, et al. Three-dimensional simple conformal symplectic particle-in-cell methods for simulations of high power microwave devices[J]. Computer physics communications, 2016, 205: 1-12.

[115] CAI L, WANG J, ZHU X, et al. Two-dimensional simulation research of secondary electron emission avalanche discharge on vacuum insulator surface[J]. Physics of plasmas, 2015, 22(1):013502.

[116] WANG J, ZHANG D, LIU C, et al. UNIPIC code for simulations of high power microwave devices[J]. Physics of plasmas, 2009, 16(3): 033108.

[117] WU L, ZHU H, HUANG K. Thermal analysis on the process of microwave-assisted biodiesel production, Bioresource technology, 2013, 133: 279-284.

[118] XIAO W, HUANG K, ZHANG W, et al. Modeling of argon plasma excited by microwave at atmospheric pressure in ridged waveguide[J]. IEEE transactions on plasma science, 2016, 44: 1075-1082.

[119] HE S, SHA W, JIANG L J, et al. Finite element based generalized impedance boundary condition for modeling plasmonic nanostructures[J]. IEEE transactions on nanotechnology, 2012,11(2): 336-345.

[120] PAN X M, XU K J, YANG M L, et al. Prediction of metallic nano-optical trapping forces by finite element-boundary integral method[J]. Optics express, 2015, 23(5): 6130-6144.

[121] XU K J, PAN X M, LI R X, et al. Fast and accurate algorithm for repeated optical trapping simulations on arbitrarily shaped particles based on boundary element method[J]. Journal of quantitative spectroscopy and radiative transfer, 2017, 195: 76-84.

[122] CHEN S, DING D, CHEN R. A hybrid volume: surface integral spectral-element time-domain method for nonlinear analysis of microwave circuit[J]. IEEE antennas and wireless propagation letters, 2017, 16: 3034-3037.

[123] ZHANG L, ZENG H, CHEN R S. Full-quantum numerical scheme of finite difference time domain method for high-order harmonic generation[J]. IEEE journal on multiscale and multiphysics computational techniques, 2018, 3: 74-79.

[124] WANG K, ZHAO J, CHENG Q, et al. Broadband and broad-angle low-scattering metasurface based on hybrid optimization algorithm[R]. Scientific Reports 4, 2014: 5935.

[125] YOU J W, ZHANG J F, JIANG W X, et al. Accurate analysis of finite-volume lumped elements in metamaterial absorber design[J]. IEEE transactions on microwave theory and techniques, 2016, 64(7): 1966-1975.

[126] DANG X, LI M, YANG F, et al. Quasi-periodic array modeling using reduced basis method[J]. IEEE antennas and wireless propagation letters, 2016, 16: 825-828.

[127] DANG X, LI M, YANG F, et al. Quasi-periodic array modeling using reduced basis from elemental array [J]. IEEE journal on multiscale and multiphysics computational techniques, 2017, 2: 202-208.

[128] HUANG Z, KOSCHNY T, SOUKOULIS C M. Theory of pump-probe experiments of metallic metamaterials coupled to a gain medium[J]. Physical review letters, 2012, 108:187402.

[129] FANG M, HUANG Z, SHA W, et al. Full hydrodynamic model of nonlinear electromagnetic response in metallic metamaterials[J]. Progress in electromagnetics research, 2016, 157: 63-78.

[130] FANG M, SHEN N H, SHA W, et al. Nonlinearity in the dark: broadband terahertz generation with extremely high efficiency[J]. Physical review letters 2019, 122: 027401.

[131] XIONG X Y Z, AL-JARRO A, JIANG L J, et al. Mixing of spin and orbital angular momenta via second-harmonic generation in plasmonic and dielectric chiral nanostructures[J]. Physical review B, 2017, 95: 165432.

[132] XIONG X Y Z, JIANG L J, SHA W, et al. Strongly enhanced and directionally tunable second-harmonic radiation from a plasmonic particle-in-cavity nanoantenna[J]. Physical review A, 2016, 94: 053825.

[133] CHEN Y P, SHA W, JIANG L, et al. Graphene plasmonics for tuning photon decay rate near metallic split-ring resonator in a multilayered substrate[J]. Optics express, 2015, 23(3): 2798-2807.

[134] CHEN Y P, SHA W, CHOY W C H, et al. Study on spontaneous emission in complex multilayered plasmonic system via surface integral equation approach with layered medium Green's function[J]. Optics express, 2012, 20(18): 20210-20221.

[135] LI Y L, SUN S, DAI Q, et al. Vectorial solution to double curl equation with generalized coulomb gauge for magnetostatic problems[J]. IEEE transactions on magnetics, 2015, 51(8): 7002306.

[136] LIU Q S, SUN S, CHEW W C. A potential-based integral equation method for low-frequency electromagnetic problems[J]. IEEE transactions on antennas and propagation, 2018, 66(3): 1413-1426.

[137] REN X, WANG Z, SHA W, et al. Exploring the way to approach the efficiency limit of perovskite solar cells by drift-diffusion model[J]. ACS photonics, 2017, 4(4): 934-942.

[138] SHA W, CHOY W C H, WU Y, et al. Optical and electrical study of organic solar cells with a 2D grating anode[J]. Optics express, 2012, 20(3): 2572-2580.

[139] SHA W, ZHANG H, WANG Z S, et al. Quantifying efficiency loss of perovskite solar cells by a modified detailed balance model[J]. Advanced energy materials, 2018, 8 (8): 1701586.

[140] CHEN Y P, SHA W, JIANG L, et al. A unified Hamiltonian solution to Maxwell-Schrödinger equations for modeling electromagnetic field-particle interaction[J]. Computer physics communications, 2017, 215: 63-70.

[141] SHA W, LIU A Y, CHEW W C. Dissipative quantum electromagnetics[J]. IEEE journal on multiscale and multiphysics computational techniques, 2018, 3 198-213.

[142] CHEW W C, LIU A Y, SALAZAR-LAZARO C, et al. Quantum electromagnetics: a new look[J]. IEEE

journal on multiscale and multiphysics computational techniques, 2016, 1: 73-97.

[143] CHEN Q, QIN H, LIU J, et al. Canonical symplectic structure and structure-preserving geometric algorithms for Schrödinger-Maxwell systems[J]. Journal of computational physics, 2017, 349: 441-452.

[144] MA C, CAO L. A Crank-Nicolson finite element method and the optimal error estimates for the modified time-dependent Maxwell-Schrödinger equation[J]. SIAM journal on numerical analysis, 2018, 56: 369-396.

[145] CHEW W C, TONG M S, HU B. Integral equation methods for electromagnetic and elastic waves[J]. San Rafael: Morgan & Claypool Publishers, 2008.

[146] ZHANG H H, LIU Y, XIONG X Y Z, et al. Investigating thermal cooling mechanisms of human under exposure to electromagnetic radiation[J]. IEEE access, 2019. DOI:10.1109/ACCESS.2019.2891696

[147] ZHANG H H, SHA W, HUANG Z X, et al. Flexible and accurate simulation of radiation cooling with FETD method[R]. Scientific reports, 2018, 8: 2652.

[148] ZHANG H H, LIN Z C, SHA W, et al. Electromagnetic-thermal analysis of human head exposed to cell phones with the consideration of radiative cooling[J]. IEEE antennas and wireless propagation letters, 2018, 17(9):1584-1587.

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