Numerical solution

Nature Photonics spoke to Allen Taflove, father of the finite-difference time-domain technique, about the birth of Maxwell's equations and their impact on the world after 150 years.

Who were the most important contributors to Maxwell's equations?
Clearly, the work of Faraday and Ampere was essential for Maxwell to achieve his unification. Had their experiments not taken place, Maxwell would have had no physical basis. Their results founded the very thought that there was a missing term, the displacement current.

However, there should be no question that the laws of classical electrodynamics are really Maxwell's discovery. Not only did he add the displacement current term, he really put everything together, albeit with 20 equations and 20 unknowns. To this day his achievement remains the physical basis of much of the electro-technology that separates our society from that of the nineteenth century.

Did they realize the impact at that time?
Scientists of Maxwell's era could have no idea of the impact of his synthesis. They didn't even understand the fundamental concept of electromagnetic wave propagation, requiring a 'luminiferous aether' for this function. Commonplace modern technology dependent on Maxwell's equations, such as smartphones, would absolutely mystify the scientists of Maxwell's time.

Up to the 1950s, what types of problems were tackled?
There was fundamental work related to plane electromagnetic wave propagation and reflection/refraction at material interfaces, as well as foundational work on radiation from electric and magnetic dipoles.

Notably, the Sommerfeld half-plane problem was arguably the first solved problem in diffraction theory. Subsequently, this led to advances in integral equation techniques and the Wiener–Hopf method — powerful techniques in applied mathematics that persist to this day.

Sommerfeld and Brillouin precursors were theoretically predicted in the first decade or two of the twentieth century. Other important results include Mie (eigenfunction) solutions of time-harmonic plane-wave interactions with spheres and infinite cylinders of circular cross-section, eigenfunction solutions of time-harmonic propagation in metal waveguides, Schelkunoff's field equivalence theorems and Bethe's theory of diffraction by small holes.

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Tell us about Kane Yee and his pioneering work on the numerical solution of Maxwell's equations.
Yee's paper published in May 1966 represented a complete paradigm shift in how to solve Maxwell's equations (*IEEE Trans. Antennas Propag.* **14**, 302–307; 1966). Essentially all previous solution techniques were based on Fourier-domain concepts in the broadest sense. By this, I mean an a priori assumption of one or more of the following: a time-harmonic (sinusoidal steady-state) variation of all field quantities; a particular set of spatial modes; a particular geometry-appropriate Green's function; a particular integral equation projected to a particular abstract function space; and perhaps a particular short-wavelength asymptotic field behaviour.

In essence, Yee's technique advanced the electromagnetic field directly in space and time, just as occurs in nature, with no fundamental assumptions other than a particular space-time discretization. If any spatial modes were present, they would evolve from the background as an emergent property of the system. The same could be said for the Green's function.

Not many people know that Kane Yee was simply learning how to program in Fortran, as he told me 20 years later. He chose Maxwell's time-dependent curl equations as the basis of his self-study because he wanted an initial-value problem that had both time and space derivatives.

Yee's technique required dimensionally less computer storage and running time for modelling electromagnetic wave interactions with material structures of volumetric complexity greater than anything previously reported in the literature. Furthermore, it allowed the solution of impulsive, broadband electromagnetic wave interactions using just a single modelling run, and permitted a natural, direct incorporation of material nonlinearities.

However, Yee's paper had several deficiencies including an incorrect numerical stability condition and a computationally inefficient means to generate the incident electromagnetic wave as an initial condition. Furthermore, Yee's use of perfectly reflecting walls as the outer boundaries of his computation space prevented the modelling of important open-region problems involving radiation and scattering. Finally, he reported no confidence-building validations.

How did you get involved with numerically solving the equations?
In 1972, during a seminar course at Northwestern University, my graduate adviser, Professor Morris Brodwin (who sadly passed away in November 2014), asked me to look at the problem of assessing microwave exposure levels causing human ocular cataracts, which had been reported during the Second World War by radar technicians. I initially thought that Brodwin's problem was intractable as it seemed to require the solution of around 100,000 E- and H-field vector components. In 1972, the best computers could solve for only a few hundred field components using the available time-harmonic integral-equation techniques, which required generating and inverting large matrices.

Having almost given up on Brodwin's problem, I spotted Yee's 1966 paper by accident while randomly leafing through back issues of journals. I had seen no citations to Yee. The thought occurred that, using Yee's technique, I could cram the volumetric human eye model into Northwestern's Control Data CDC-6400 computer. Yee's incorrect numerical stability bound caused me considerable grief for a while until I derived the correct limit, and proceeded to code simple two-dimensional grids.

To his credit, Brodwin agreed to let me pursue this topic for my PhD thesis, even though it was not in the mainstream of his research. By 1975, my algorithm development, coding and validations had progressed to the point where a fully three-dimensional model of the microwave-irradiated human eye could be implemented. That year I published my results in two papers in *IEEE Transactions on Microwave Theory and Techniques* and earned my PhD. But, like Yee's paper, my work remained uncited.

In the late 1970s the US Air Force Rome Air Development Center (RADC) was faced with a problem whereby radar beams emitted by 'friendly' aircraft caused one of its air-to-air missiles to go haywire. All attempts at modelling this problem had failed because the missile's internal geometry was far too complex. In 1977, employed as a staff engineer at IIT Research Institute in Chicago (IITRI), I proposed that RADC allow me to tackle the problem. Given the go-ahead, I adapted the Fortran code used for my PhD thesis to run efficiently on the new Control Data STAR-100 supercomputer, which had enough fast memory to contain the required 800,000 field-vector unknowns. I subsequently succeeded in determining the precise failure mechanism of the missile and the radar frequency at which the problem occurred. RADC was impressed. At this point, I was solving problems 1,000 times more complex (in terms of field-vector unknowns) than possible using Fourier-domain techniques.

Based on my work for RADC, I coined the descriptor 'finite-difference time-domain' and the acronym FDTD in a 1980 paper (*IEEE Trans. Electromagn. Compat.* **EMC-22,** 191–202; 1980). (Google Scholar currently shows 75,000 results for the search term 'finite-difference time-domain'). I knew that I had found a powerful tool. Unlike Yee, I didn't drop the subject for 20 years — I ran with it, determined to convince the community!

To this end, in the 1980s my IITRI colleague, Korada Umashankar, and I published the first rigorous validations of FDTD for the surface currents and far fields of 2D and 3D scattering objects, and electromagnetic coupling to wires and wire bundles located in free space or in multi-resonant cavities. After I joined Northwestern University in 1984, Evans Harrigan at Cray Research kindly arranged free access to Cray's corporate supercomputers, enabling the solution of ultralarge problems that no one could ignore.

■ It seems like it took decades for the technique to become widespread.

During most of the twentieth century, the engineering electromagnetics community was wedded to Fourier-domain concepts in the broadest sense, as mentioned earlier. FDTD was ignored, and at times even ridiculed. One such episode remains burned into my memory. In 1986, an internationally known professor actually laughed at me in an open meeting that had been called to consider the future of computational electromagnetics, because of my use of supercomputers. Pointing directly at me, he joked: "Look at Taflove over there. When he wakes up in the morning, he gets down on his knees, bows his head, and says, 'And now, let us Cray'." I was speechless and terrified — not yet being tenured at Northwestern University.

Nevertheless, I was granted tenure — and my research group continued to advance FDTD theory, algorithms and applications. These included the treatment of linear and nonlinear lumped circuit elements coupled to the electromagnetic field, curved surfaces in the context of Yee's Cartesian grid, and linear and nonlinear frequency-dispersive media. Our latter advance resulted in the first solutions directly from the time-dependent Maxwell's curl equations of the Sommerfeld and Brillouin precursors, as well as temporal and spatial optical solitons.

With advances in supercomputing, by the 1990s and early 2000s we were time-marching tens of millions to hundreds of millions of field-vector components to model entire aircraft for radar cross-section, to design complex phased-array antennas, to detect and image early-stage breast cancers using ultrawideband microwave radar, and to investigate ultra-low frequency geophysical phenomena within the global Earth-ionosphere waveguide.

A crucial event that helped popularize FDTD internationally was J-P. Berenger's 1994 publication of his split-field perfectly matched layer (PML) absorbing boundary condition (ABC) technique (*J. Comput. Phys.* **114,** 185–200; 1994). Now, the computational dynamic range of FDTD modelling for open-region problems was no longer limited by the ~1% reflection error of previous ABCs. With PML, such errors were reduced to mere parts per million.

Subsequently, Berenger's nonphysical split-field PML was reformulated to allow a potential physical realization via a stretched-coordinate mapping of Maxwell's curl equations. This work arguably motivated subsequent research in transformation electromagnetics/optics that has achieved acclaim with its promise of 'invisibility cloaks'. Concurrently, we have seen a tremendous expansion of FDTD modelling efforts involving metamaterials, nanophotonics and plasmonics.

Most recently, collaborating with my Northwestern University colleague, Professor Vadim Backman, we applied FDTD to create a 'microscope in a computer'. This tool solves Maxwell's curl equations with nanometre resolution within a biological specimen. Then, it rigorously transforms the computed near-fields through various apertures and lenses all the way to the image plane, where individual colour pixels are synthesized. Using this tool, we deduced the physical basis of Vadim's promising spectroscopic microscopy technique for early-stage cancer detection. Exciting!

■ What is the big electromagnetics problem for the future?

I'm excited by the prospect of self-consistently linking the time-domain Maxwell's equations to quantum electrodynamics (QED) in a computationally efficient manner. Nature does this every attosecond — can we emulate that?

Some small steps are already being made in this direction. For example, recent publications reported FDTD models of nonlocal dielectric functions, and an FDTD treatment of the coupling of classical electrodynamics for a nanoparticle with electronic structure theory for a nearby molecule, as described using real-time time-dependent density functional theory.

I foresee FDTD models of individual photons and vacuum fluctuations leading to the evolution of the Casimir effect directly in the time domain, models of the temporal dynamics of a variety of tunnelling phenomena and a deep investigation of quantum plasmonics.

Overall, I see the development of rigorous computational models of the time-dependent physics of nanometre-scale structures communicating their QED-based physical phenomena to the macroscopic world via Maxwell's equations.

INTERVIEW BY DAVID PILE