Anales de la Academia Nacional de
Ciencias Exactas, Físicas y Naturales
Argentina
Tomo 73, 2022

NOVEL MATHEMATICAL AND COMPUTATIONAL METHODS FOR SCIENCE AND ENGINEERING

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Keywords
Computational science
Numerical analysis
Numerical methods
Partial differential equations
Fast methods
High-order methods

Abstract These notes present a conceptual narrative concerning a new class of highly accurate and efficient methods for the numerical solution of partial differential equations. This contribution, which is not offered as a text for specialists, has as its main objective to convey, to a presumptive audience with diverse scientific and technological interests, the character of these new methodologies, as well as their potential for effective computational simulation in vast areas of science and engineering.

Palabras clave
Ciencia computacional
Análisis numérico
Métodos numéricos
Ecuaciones en derivadas parciales
Métodos rápidos
Métodos de alto orden

Resumen Nuevos métodos matemáticos y computacionales para las ciencias y la ingeniería. Estas notas presentan una descripción conceptual de una nueva clase de métodos altamente precisos y eficientes para la solución numérica de ecuaciones en derivadas parciales. Este aporte, que no se presenta como un texto para especialistas, tiene como principal objetivo trasmitir, a una presunta audiencia con diversos intereses científicos y tecnológicos, el carácter de estas nuevas metodologías, así como su potencial para la simulación computacional efectiva en vastas áreas de ciencia e ingeniería.

1. Introduction

In spite of enormous progress in many areas of mathematics, numerical analysis, computational science and computer hardware, the efficient and reliable computational simulation of physical phenomena has continued to pose significant challenges in many scientific and technological contexts. In recent years, novel "fast", "high-order" and "spectral" techniques have emerged which can effectively tackle highly complex natural and engineered structures. The purpose of these notes is to present a conceptual narrative concerning these new computational methods. In this spirit, and to facilitate a descriptive presentation, bibliographical citations are avoided in this text—with the

expectation that the nomenclature used should easily enable an interested reader to access full references without difficulty.

As a specific motivating example, which will facilitate the introduction of a number of key concepts, we first consider the important problem of propagation and scattering of electromagnetic waves. This is a problem of significant impact on a wide range of areas of science and engineering, including optics, remote sensing, photonics, electronics, communications, etc. Numerical methods based on finite-element (FEM) and finite-difference (FD) approximations for such problems are accurate and capable of fine spatial resolution. These methods do require use of fine volumetric discretizations, however, not only in specific regions near boundaries, to adequately model complex engineered structures, but also *throughout the computational domain* to counter their inherent numerical dispersion and diffusion errors (described below). For problems with general temporal dependence, further, these fine spatial discretizations require use of small time-steps to ensure stability in the time evolution. As a result, electromagnetic simulations of large (and possibly complex) structures by means of volumetric discretizations require vast amounts of computing time and memory and have remained impractical. Fortunately, novel techniques have recently emerged that have significantly expanded the applicability of numerical methods to configurations previously not considered tractable within any reasonable accuracy.

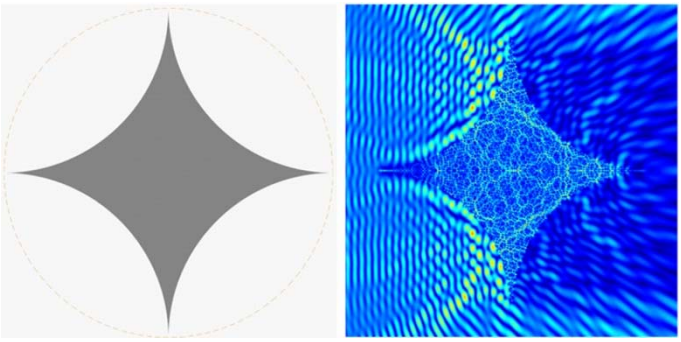

Fig. 1. The left image presents a notional structure made of a material that is penetrable to electromagnetic radiation such as e.g., visible light. The structure is 80 wavelengths at its widest; at wavelengths of the order of 1 μm, the structure is approximately 80 μm in size. Structures of such sizes, and even smaller, are designed, engineered, and manufactured, with features of the order of a single wavelength in some cases, to deliver a particular effect within a photonic structure on a photonic chip. The simulation, produced by this author in collaboration with A. Pandey, was obtained by means of a Chebyshev discretization of the relevant Helmholtz equation in conjunction with a Green-function formulation.

To motivate our description, we consider the simple notional example depicted in Fig. 1. The image on the left presents a material structure made of a "penetrable" material—in this case, a material, such as e.g., silicon or glass, that is at least partially transparent to electromagnetic illumination at certain frequencies. As light impinges on the object, part of it reflects directly, as from glass or water, and, as in such cases, part of the light penetrates the

material. For the type of material considered in the figure, the propagation wavelength in the material is smaller than that in the ambient free space: as can be appreciated in the figure, the interior waves oscillate spatially on a finer scale than those in the exterior.

The illuminating radiation, incident from the left in the present example, thus impinges upon the obstacle, and gives rise to a highly complex pattern of reflected and transmitted waves, wherein transmitted waves travel within the material and then themselves impinge upon other material boundaries, giving rise to multiple scattering, each time including reflection and transmission, etc., in accordance with Maxwell's equations.

In classical FD and FEM numerical methods, the continuum differential equations governing a particular physical problem, such as the Maxwell equations in our present illumination example, are discretized via approximation of derivatives by means of FD or FEM approximations. Thus, in the case illustrated in the figure, a fine volumetric discretization would need to be utilized—at the very least, of the order of a few points per wavelength, since, clearly, it would be impossible to resolve the details in the electromagnetic field with discretizations that contain one or fewer points per wavelength. And, if the details of fields are not resolved at the level of the wavelength, then the accuracy of the solution overall is compromised, potentially resulting in completely incorrect predictions.

The use of a fixed number of points per wavelength is therefore manifestly necessary, but unfortunately it is generally not sufficient to maintain a prescribed accuracy in general solutions of the Maxwell equations. To demonstrate this, we consider an experiment in which a fixed number of points per wavelength are used for the solution of problems for smaller and smaller wavelengths, with a fixed overall geometry–such as, say, the one depicted in Fig. 1. At a fixed number of points per wavelength, the error in approximation of continuous derivatives by discrete derivatives remains constant, but the number of times such approximations are used grows as the wavelength decreases and the number of wavelengths spanned by the domain grows. This leads to so-called "dispersion" errors that grow without bound as the number of wavelengths spanned by the domain grows. Equivalently, to maintain a certain accuracy, the number of points used *per wavelength* must be increased.

The precise selection of numbers of points per wavelength that are necessary to maintain accuracy depend on the *order of accuracy* inherent in the finite-difference or finite-element used for the approximation of spatial derivatives. Algorithms of higher orders of accuracy give rise to slower growth in the number of discretization points necessary to maintain accuracy as the size of the problem grows. But such slower growth is accompanied by other challenges, such as potential losses in stability and requirement of reduced

time steps in time-dependent problems, as well as difficulties concerning enforcement of boundary conditions, and, especially for large three-dimensional problems, computational cost. Still, high order finite-difference and finite-element methods can be successfully implemented, and they remain powerful, widely used numerical techniques for the types of problems under consideration.

2. Novel Numerical Methods

Various alternatives to FEM and FD discretization approaches, which avoid some of the drawbacks mentioned above, are discussed in what follows. These methods rely on use of representations of solutions in terms of explicit functions over large regions in the physical simulation domain. In the context of electromagnetic scattering problems, for example, we mention methods which represent the electromagnetic fields in terms of the electrical currents that exist at the interfaces between materials: as discussed in Section 4, field values can be produced from the surface currents, as linear combinations of a number of explicit functions, each one of which provides a contribution to the physical field over the complete simulation domain. (Or, equivalently, but using a different terminology: field values can be evaluated everywhere in space by means of surface integrals with integrands given by products of electrical currents and Green functions.) For problems in fluid-dynamics, in turn, spectral representations based on Fourier series or Chebyshev expansions might be used where, once again, linear combinations of explicit functions are used to represent solutions either through the complete simulation domain, or at least over large regions thereof. Although they effectively resolve the difficulties associated with the dispersion errors mentioned in the previous section, these methods themselves present certain practical challenges, as described briefly in what follows, and with more detail in Sections 3 and 4.

Methods based on use of Green functions for Maxwell's equations, for example, rely heavily on evaluation of certain "surface reflections"—thus accounting for the way into which every elementary element of surface reflects light upon every other element of surface. For a total of, say N relevant surface elements, a total of N^2 interactions need to be accounted for—which leads to a computational cost that is generally unacceptably high, except for sufficiently small and simple simulation contexts. Additionally, these methods depend upon accurate representation of interface boundaries as well as evaluation of challenging operators involving Green functions—which require numerical calculation of large numbers of integrals over the interface surfaces, each one of which contains an unbounded integrand.

Some of these difficulties also arise in the context of spectral methods: here a total of N functions must be evaluated and combined at a number of

the order of N points, at a cost that, once again, could generally unacceptably high: of the order of N^2 operations. Spectral methods present a number of additional challenges—since, e.g., Fourier series and Chebyshev expansions are natively designed to be applicable in separable domains such as Cartesian boxes or spherical shells or deformation thereof via suitable mappings, and since the first ones require a stringent assumption of periodicity, while the second ones give rise to extremely fine discretizations near boundaries, and thus, for problems with general time dependence, require use of extremely small time-steps for numerical stability.

Novel trends in the field of numerical analysis and computational science have sought to negotiate these challenges with the goal of reaping the benefits of explicit-function numerical representations in terms of Green functions, Fourier, and Chebyshev expansions, etc., but with applicability to realistic, spatio-temporally challenging, scientific, and engineering configurations. In the following two sections we discuss recent progress in this regard, drawing in part from recent work by the author and collaborators on Green-function and spectral methods, and with reference to other related methods and techniques.

3. Spectral Methods in General Domains and the FC method

In the context of spectral methods, the Fast Fourier Transform (FFT) provides a central guiding light, albeit not the complete answer to all the ailments arising from the use of spectral methods. By exploiting a certain algebra-manipulation trickery applicable to certain set of spectral methods, including Fourier- and Chebyshev-based methods, the FFT lends a capability of evaluating the combined effect of all N functions at all N discretization points at a cost of the order of merely $N \log N$ operations—significantly smaller than the cost, of the order of N^2 operations, required for evaluation of each one of the N functions at each one of the N points. The acceleration provided by the FFT algorithm makes it feasible to apply the highly accurate and dispersionless spectral methods to important large scale scientific and engineering configurations.

Simulations based on classical Fourier spectral methods are restricted to periodic problems on a rectangular domains, since, for non-periodic functions, Fourier series incur the Gibbs phenomenon—a crippling approximation error that manifests itself in the form of wild oscillations in tight intervals around the discontinuity points. Chebyshev-based methods are more geometrically friendly. They do not require the stringent periodicity conditions inherent in Fourier spectral methods and, as a result, they can be applied over multiple subdomains, each mapped to a square, leading to possible applicability to relatively complex geometrical structures. The Chebyshev methods are extraordinarily accurate, and they can deliver

excellent engineering accuracies on the basis of very sparse meshes. They derive these qualities from certain graded spatial meshes which cluster discretization points near the boundaries of the (cubic or square) simulation domains. Chebyshev methods can therefore be used as excellent approximation elements for problems independent of time, at a cost comparable to that required by FEM or FDM approaches. The situation is more challenging for time domain problems—which, in view of the fine spatial spacing between certain discretization points, leads to a requirement of an extremely fine time discretization mesh, for stability, on account of the CFL stability constraint (Courant-Friedrichs-Lewy) or, as an alternative, use of (expensive) implicit time-stepping algorithms.

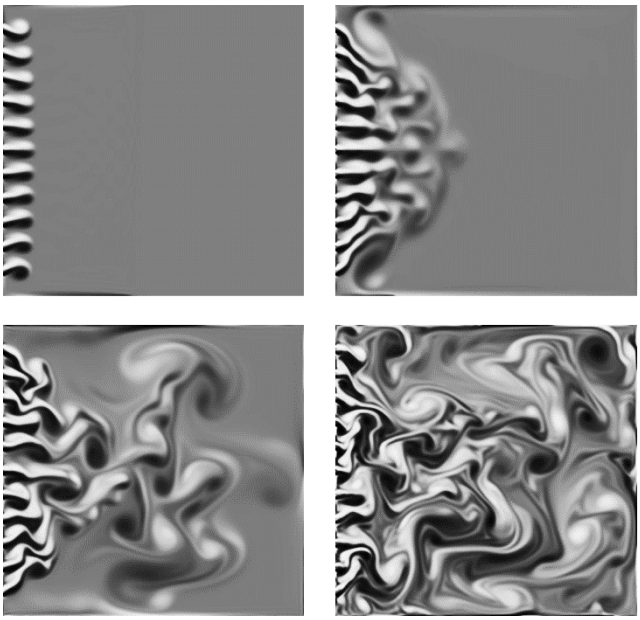

Fig. 2. Solution of the compressible Navier-Stokes's equations corresponding to a flow of gas into a that results from an influx of eleven gas jets (impinging at slightly vertically asymmetric angles). Simulation produced by the Fourier-Continuation methods presented in work by the author with N. Albin. A total of $100 = 10 \times 10$ FC expansions where used. The spatial dependence of the density is displayed at four different points in time.

The Fourier Continuation method (FC) is a spectral alternative to the Fourier and Chebyshev approaches which addresses difficulties encountered in these and other spectral methods. As other approaches, the FC method approximates a given function $y = f(x)$ defined on an interval I of the real line by a Fourier series expansion of a required order, but it does so by (a) relying only on an equi-spaced grid, and (b) in manner that is specifically designed to avoid the approximation error associated with the aforementioned Gibbs phenomenon. (Note that the Gibbs phenomenon occurs, even if f is smooth throughout the interval I, unless f is "smoothly-periodic in I" in the sense that the periodic extension of f is a continuous and smooth function of x, up to and including the endpoints of I.) In order to eliminate the Gibbs phenomenon, the basic FC algorithm, called FC(Gram)

method (in view of its reliance on Gram polynomials for certain near-boundary operations), constructs an accurate Fourier approximation of f, but where the Fourier expansion is periodic in an interval J which strictly contains I: J ⊃ I.

To do this, the FC algorithm first uses available function values at a few (e.g., five) discretization points near each endpoint of the interval I to produce discrete function values on the interval J but outside I so that, in all, a discrete sampling of a smoothly periodic function f^c defined on the interval J is obtained which coincides with f in the interval I. The discrete continuation function values are obtained by means of certain linear algebra procedure based on evaluation of QR factorization of matrices in high-precision computer accuracy. (The high precision QR factorization used, which eliminates the ill conditioning inherent in the continuation procedure, is a "universal" precomputation—whose results can be stored in a small file in computer disc and uploaded at the beginning of every application of the FC algorithm.) Once the "periodic" vector of function values has been obtained the coefficients of the FC expansion can be efficiently produced by means of the FFT algorithm applied in the interval J. In particular, the Fourier expansion of the function f^c and its derivatives closely approximate the original function f and its derivatives throughout the original interval I, up to and including its endpoints. The extension of this technique to higher dimensions is straightforward, by producing one-dimensional FC-based derivatives one dimension at a time, including arbitrary mixed derivatives of any given order.

The FC method has been applied to a variety of problems in two- and three-dimensional space, including problems in hydro- and gas-dynamics, seismology, acoustics, heat conduction, linear transport theory (e.g. neutron transport, radiative transfer), elasticity, turbulence, etc. In most cases, the applications make use of multiple overlapping (generally curvilinear subdomains) in conjunction with applications of the FC method in curvilinear coordinate systems to match a given structure. One of the most significant advantages of the FC method is its reliance on equi-spaced meshes, which lend a number of benefits, including, as suggested above, manageable CFL constraints on time-steps for time-dependent problems, and simplicity in the domain decomposition and meshing, in addition to spectral-like character leading to low dispersion and diffusion.

A range of applications of FC methods in various areas of science, including computation of seismograms, flow past obstacles, radiative transfer, magneto-hydrodynamics, turbulence, complex shock dynamics, etc., have recently been demonstrated. Here we present a simple application, illustrated in Fig. 2, which concerns the solution of the compressible Navier-Stokes's equations corresponding to a flow of gas into a chamber resulting from an influx of eleven gas jets. The four subfigures in Fig. 2 depict the

values of the mass density at four different points of time. The jets were arranged in a close-to-symmetric but non-symmetric fashion along the y axis around $y = 0$. The results depicted were produced by means the FC-based algorithms introduced by the author in collaboration with N. Albin, by means of an array of $100 = 10 \times 10$ equisized squares spanning the computational domain. The solution on each one of these squares was produced via Fourier continuation, so that one-hundred different FC expansions are combined in the density values depicted in the figure. In particular it is easy to appreciate that, in view of their accuracy, the decomposition into one-hundred different subdomains does not give rise to visible numerical artifacts at the boundaries between different square subdomains. The aforementioned contributions demonstrate, in each particular instance, the accuracy and efficiency resulting from the algorithms. As demonstrated in these references, in many cases the approach leads to significant efficiency and accuracy gains over the performance provided by other existing algorithms.

4. Green-Function Methods

We now turn to problems whose solutions can be expressed in terms of certain "Green functions", also called "Fundamental Solutions", for a given differential equation at hand. A Green function $G(x,y)$ for a differential equation in the variable x is a special solution of the equation for each y, which results as sources concentrated at the single point $x = y$ are prescribed. The importance of Green functions is that, for *linear* differential equations, a solution of the equation can be obtained for an arbitrary source function $f(x)$ as a linear combination of $G(x,y)$ (or, more precisely, as an integral of the product $G(x,y)\varphi(y)$ with a "integral density" function $\varphi(y)$) over a range of values of the variable y.

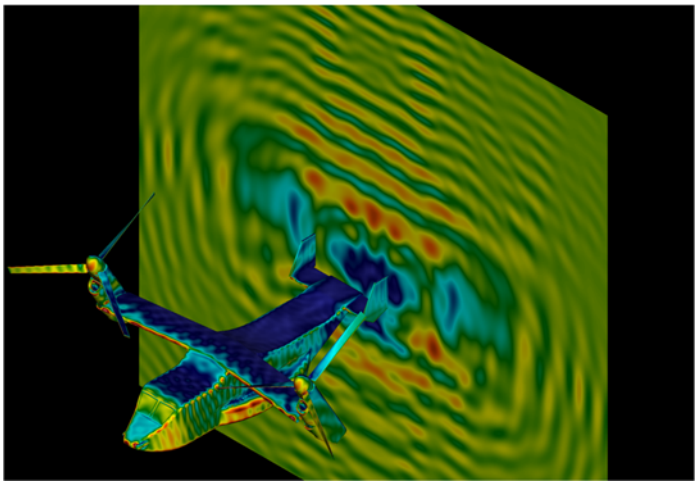

Fig. 3. Solution of problem of scattering produced by means of a commercial implementation of Green function methods introduced by the author and collaborators J. Guzman, V. Kononov and L. Voss.

As indicated above, Green functions can only be utilized for linear problems such as, e.g., the wave propagation problem considered in Section 1; on account of nonlinearity, Green functions are not applicable to problems such as those considered in Section 3. But even for linear equations there are significant restrictions in the use of Green functions as part of efficient computational methods, mainly on account of the high cost required for Green function evaluation—except in the small number of cases for which the Green functions can be *computed in closed form*.

(Under various conditions often met in practice, Green functions for linear equations can be expressed in terms of Fourier transforms. This is indeed so for differential equations with constant coefficients, as established by the celebrated Malgrange–Ehrenpreis theorem. Further, Green functions for equations with certain types of variable coefficients—which only take a finite number of constant values, each one on a simple region such as a half-space or an otherwise separable domain—can in some cases be obtained by means of Fourier transformation and "Sommerfeld Integrals". Unfortunately, explicit numerical calculations of necessary Green function values by such methods often require a prohibitive computational cost when applied to numerical solution of differential equations.)

In spite of these challenges, Green function-based approaches have had very significant impact in many areas of science and technology. This is due mainly to the fortuitous fact that closed-form Green-function expressions do indeed exist for some of the most important problems in present-day application areas. Thus, Green function methods find direct applicability in electromagnetism, elasticity, heat transfer and acoustics, and they play central supporting roles in the numerical solution of certain nonlinear problems—most famously in hydrodynamics, where Green function methods for the solution of the Poisson equation are often used in an algorithmic step that enforces the incompressibility condition in the *nonlinear* Navier-Stokes equations. Naturally, these Green function methods can be used as components of numerical solvers for multi-physics problems, such as, e.g., the problem of magneto-hydrodynamics—that governs the mutual interactions between gas-dynamics and electromagnetism time evolution of stars as well as the design of nuclear fusion reactors.

It is useful to visualize the character of Green function methods in the context of propagation and scattering of light; analogous descriptions apply in other application contexts. In the light scattering context, the Green function $G(x, y)$ is expressed in closed form in terms of certain derivatives of the expression $\frac{1}{4\pi}\mathrm{e}^{k|\mathrm{x}-\mathrm{y}|}/|\mathrm{x}-\mathrm{y}|$, where $k = 2\pi/\lambda$ denotes the spatial frequency or "wavenumber" corresponding to the wavelength λ. The Green function admits a compelling physical interpretation: the quantity $G(x, y)$ corresponds to the light that would be observed at point x arising from a source of unit

"intensity" located at the single point y. Clearly, such a source, as a small (infinitesimal) bulb in the otherwise featureless three-dimensional space, generates a spherical illumination wave that expands at the speed of light and which, as time tends to infinity, covers all space. This final time state, as $t \to \infty$, of the point-source illuminated space, is precisely the Green function $G(x, y)$.

Then, according to Fresnel spectacular interpretation, which, in particular, allowed him to postulate the wave-like structure of light, every point on an illuminated surface reflects a point source $\varphi(y)G(x, y)$ as described in the previous paragraph. According to Fresnel, the combination (sum) of all of these point sources is precisely what we experience as the light that is scattered (reflected) by the surface. Putting aside certain subtleties concerning the vector character of light which were ignored in the early theory, Fresnel interpretation is in accord with the predictions of the subsequent Maxwell's theory of electromagnetism.

The numerical methods based on Green functions harness Fresnel's ideas, as well as their extensions to other types of problems for which similar Green functions can be obtained in closed form, or for which Green functions can otherwise be computed numerically with adequate computational efficiency. In the Green function method outlined above, a numerical approximation of the unknown function $\varphi(y)$ is sought. Once this function is determined, the field at any point in space can be obtained by summation, or, more precisely, integration, with respect to y over the given scattering surface.

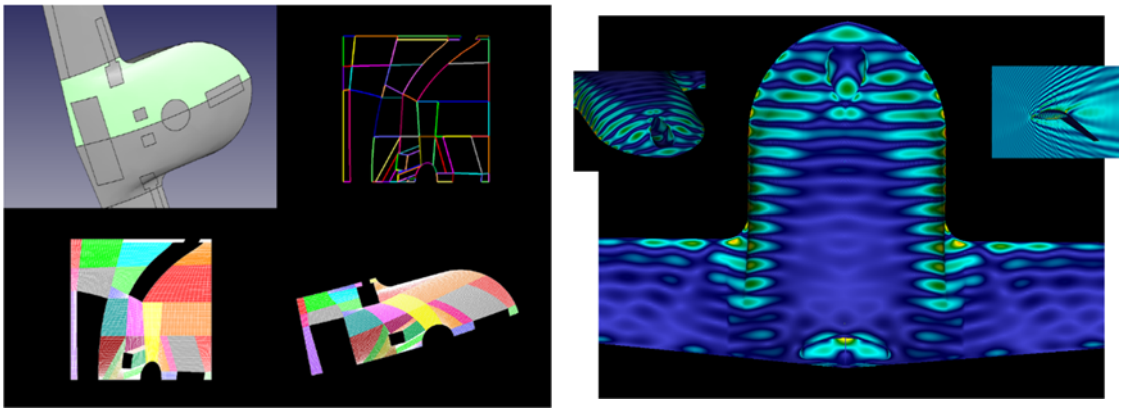

Fig. 4. Left: curved quadrilateralization CAD-file processing resulting from a commercial implementation of methods introduced by J. Guzman and the author and mentioned in Section 4. Right: Surface density (an electromagnetic version of the density φ mentioned in the text, which actually corresponds to the electrical current), and the resulting spatial electric field, obtained by integration.

The unknown function φ can be discretized in a number of ways, including finite-element approximations on the scattering surfaces, which gives rise to one of the preferred approaches in many areas of engineering,

namely, the Boundary Element Method (BEM), called Method of Moments in the electrical engineering literature. Other approaches for the discretization of the function φ are based on point sampling. In either case, for any assignment of values of the discretized density φ, whether or not these discrete values collectively satisfy the physical surface scattering conditions, a value of the integral can be obtained. Using the surface scattering conditions this representation results in a matrix equation for the discretized density φ, whose solution yields this quantity and thus, by integration, as suggested above, the field at any point in space.

As already noted, the Green-function methods considered in this section are based on discretization of the scattering boundaries. These methods thus require significantly smaller discretizations than would be needed to mesh a sufficiently large 3D domain around the scattering structure for use in conjunction with a volumetric finite-element or finite-difference discretization. Compounding challenges, such volumetric approaches require use of a sufficiently large buffer region to enable absorption of outgoing waves, by means of some sort of absorbing boundary condition algorithm such as the Perfectly Matched Layer method. As a counterpart, volumetric finite-element, and finite-difference discretizations result in very sparse matrices, which can be applied and inverted much more efficiently than do full matrices such as those resulting from Green function-based discretizations. The natural question concerning the potential relative benefits of volumetric- vis-à-vis surface-discretization approaches requires a nuanced answer and is considered in what follows.

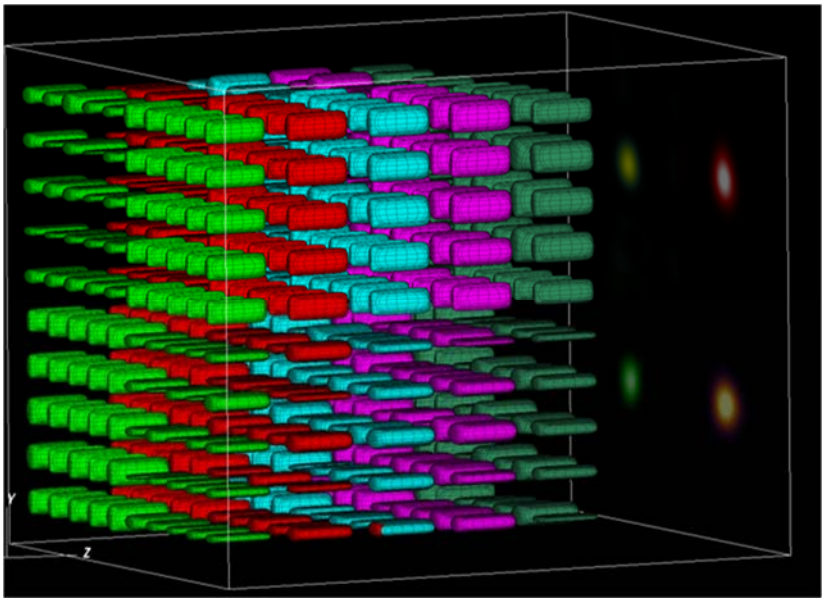

Fig. 5. 10 × 10 × 5 nanopost array designed to focus two different wavelengths and two different polarizations of light at four different points in space. TiO_2 nanoposts in SiO_2 matrix. Array size: 2,439 cubic μm. Design and simulation by A. Fernandez Lado, E. Garza, E. Jimenez, and the author, produced on the basis of accelerated Green function methods.

Useful preliminary indications in this regard can be obtained by considering the asymptotic growth of the computational cost as the size of the problem grows without bound. In detail, for problems of a size given by a certain number of wavelengths, a volumetric method in three-dimensional space requires use a number of the order of $N_V = n^3$ unknowns, where n denotes the number of discretization points used per spatial dimension of a notional discretized cube. For a problem of such a size, a Green function-based surface discretization method requires use of a number N_G of the order of n^2 unknowns (in asymptotic-order notation, $N_G = \mathcal{O}(n^2)$). A straightforward solution via Gaussian elimination for an $N \times N$ matrix requires a $\mathcal{O}(N^3)$ operations for general matrices, but the cost is lower for sparse finite-difference matrices, of the order of $\mathcal{O}(N^{8/3})$, so that, for direct solution the corresponding costs would be $\mathcal{O}(n^6)$ operations for the Green function method vs. $\mathcal{O}(n^8)$ operations for the volumetric approach. But there are multiple caveats to these simple-minded estimates, involving mainly fast alternatives to Gaussian elimination for the solution of the linear system under consideration.

On one hand, for sparse matrices such as those arising from finite-difference and finite-element methods, the frontal and multi-frontal matrix solvers introduced over the last several decades can obtain solutions in as few as $\mathcal{O}(N^2)$ operations, which significantly reduces the finite-difference cost to $\mathcal{O}(N_V^2) = \mathcal{O}(n^6)$ operations: comparable to the direct Gaussian elimination cost for the Green function-based solver. Unfortunately, the multifrontal methods do not produce any gains when applied to dense matrices, such as those arising from use of the Green-function approach.

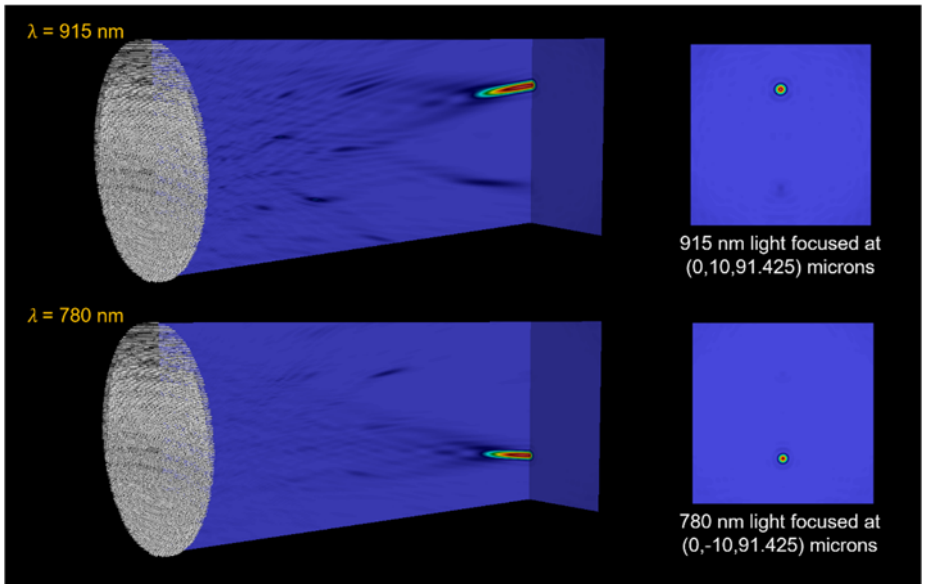

Fig. 6. Metamaterial "lens" consisting of 20,000 micron-sized nanomposts (a much larger variant of the nanopost array presented in Fig. 5). TiO2 nanoposts in SiO2 matrix. Array size: 2,439 cubic µm. Simulation by C. Bauinger, E. Jimenez, and the author.

Numerous additional significant advantages of all of these methods could be mentioned. In the context of time-domain finite-difference solvers we emphasize these solvers' ability to produce, by post-processing via Fourier transformation in the time variable, frequency-domain solutions for multiple frequencies as a result of a single time-domain solve, as well as their ability to effectively treat inhomogeneous media. The Green function-based solvers, on the other hand, when implemented with sufficient accuracy for integration of the infinite Green function and infinite currents at edges, and when adequately "accelerated", excel in their accuracy and applicability to large and geometrically complex problems—possibly involving three-dimensional scatterers hundreds or even thousands of wavelengths in electrical size and beyond.

Figs. 3 and 4 illustrate applications of a commercial implementation of Green function-based solvers proposed by the present author and his collaborators in recent years. In particular, the left panel in Fig. 4 demonstrates the software-based processing of the CAD file (Computer Aided Design) representing an engineering surface (an aircraft in this case) that yields a representation of the surface by a finite number of "logical quadrilaterals", that is, portions of the surface bounded by four smooth curves, which are given by an explicit parametrization from the unit square. This decomposition is then used by these algorithms to exploit Chebyshev expansions (which were briefly described in Section 3) as well as novel methods for accurate integration of functions that are infinite at certain points. Acceleration provides the final element that enables solution of challenging problems. The available acceleration methods, which include the Fast Multipole Method, the Adaptive Integral Method, and other related approaches, generally rely on Fast Fourier Transforms, and thus reduce the solution to computational costs of the order of $N_G\, log(N_G) = n^2\, log(n^2)$ operations—significantly less than those required by other approaches. A novel acceleration introduced recently by C. Bauinger and the author does not rely on use of FFTs, and it thus appears well poised for use in the context of parallel and GPU computing in large computational infrastructures. Various implementations of Green function algorithms and acceleration methods introduced by the author and collaborators are demonstrated in Figs. 3 through 6.

5. Conclusions

As suggested in Section 2, the spectral and Green-function methods considered in these notes derive a distinctive character from use of representation of solutions in terms of explicit functions over large regions in the physical simulation domain. As a result of such representations, these methods avoid the additive accumulation of errors incurred by the local discretizations of derivatives utilized in other approaches. When used in

conjunction with appropriate acceleration methods and algorithms for processing of geometric structures given by CAD representations, these approaches can be applied to (and deliver accurate solutions for) problems which were previously not considered tractable with any reasonable accuracy.