Subproject A5.6

Modeling of Micro-Disk Resonator Arrays

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Introduction and Summary

Waveguides and resonators comprise the basic building blocks for the realization of an integrated optics. Loosely speaking, waveguides transport light between elements and resonators are used to “store” the light by means of constructive interference. This means that in a resonator light bounces back and forth between mirrors or, for our purposes equivalently, light runs around in loops. Efficient “trapping” can only occur for selected frequencies – the resonance frequencies that very sensitively depend on the resonator’s geometrical and material properties. Upon judiciously coupling such resonators with other resonators and/or with one or several waveguides one can thus realize a number of more complex functional elements. For instance, one can functionalize the resonator’s surface in order to allow for the deposition of specific molecules or proteins. This added material will alter the resonator’s properties, for instance, its resonance frequency. As frequencies – more precisely frequency shifts – can be detected with extremely high sensitivity this suggests that efficient and highly parallel sensing schemes may be constructed based on coupled waveguide-resonator systems.

This utility of coupled waveguide-resonator systems presents a number of rather significant challenges regarding modeling. The structures to be investigated are generally characterized by vastly different length scales. To be specific, we focus on systems that are investigated experimentally in the group of Heinz Kalt within subproject A.5.4 *Optical Biosensors on the Basis of Micro-Disk Resonators*. In order to obtain high Q-values, the resonator structures are typically large compared to the operation wavelength while the (evanescent) coupling between resonator and waveguide involves a narrow gap with typical sizes of 1/10 of the operation wavelength. This suggests a dual approach for quantitative analyses. Exact numerical methods can be utilized to determine the spectral response of, say, a single resonator coupled to one or two waveguides. In addition, exact numerical simulations can extract effective parameters that are used as input parameters for effective descriptions based on coupled-mode theory. Such semi-analytical coupled-mode approaches can be (and have to be) tailored to specific applications and their ranges of validity have to be gauged by comparing with corresponding exact numerical results. Once this has been accomplished, coupled-mode theory provides detailed insight into the underlying physics and thus allows for a educated optimization of the corresponding system.

In order to accomplish the modeling task outline above, we have utilized the Discontinuous Galerkin Time-Domain (DGTD) method which we have been developed in subproject A1.2 *Light-Matter Interaction in Nano-Photonic Systems*. DGTD combines spatial adaptivity through unstructured meshes with high-order spatial discretization and high-order time-stepping capabilities. In order to facilitate the above exact numerical simulation tasks, we have significantly improved the time-stepping characteristics well beyond what has originally been proposed [1-4] and have recently been able to adapt our code for high-performance-computation purposes using graphic processors. In addition, in collaboration with Dr. Kiran Hiremath (now Zuse-Institute Berlin) we have developed a coupled-mode theoretical (CMT) approach [5] that has allowed us to understand an unexpected effect of waveguide-coupled slotted-ring resonators. This effect allows to significantly modify the Q-value of certain resonances by rather minimal changes to the resonators’ specifications and, therefore, is rather well suited for sensing schemes and perhaps even for certain optomechanical applications..

1. Coupled Waveguide-Resonator Systems – Exact Numerical Approach via DGTD

In order to illustrate the challenges associated with exact numerical modeling of coupled waveguide-resonator systems, we consider a two-dimensional example of a silicon micro-disk resonator (diameter 5 μm) that is coupled via a (relatively) gap of 232 nm to two silicon waveguides (width 300 nm) as depicted in Fig. 1. This four-port device is operated at wavelengths centered around 1.55 μm for light with an electric field polarized along the z-axis.

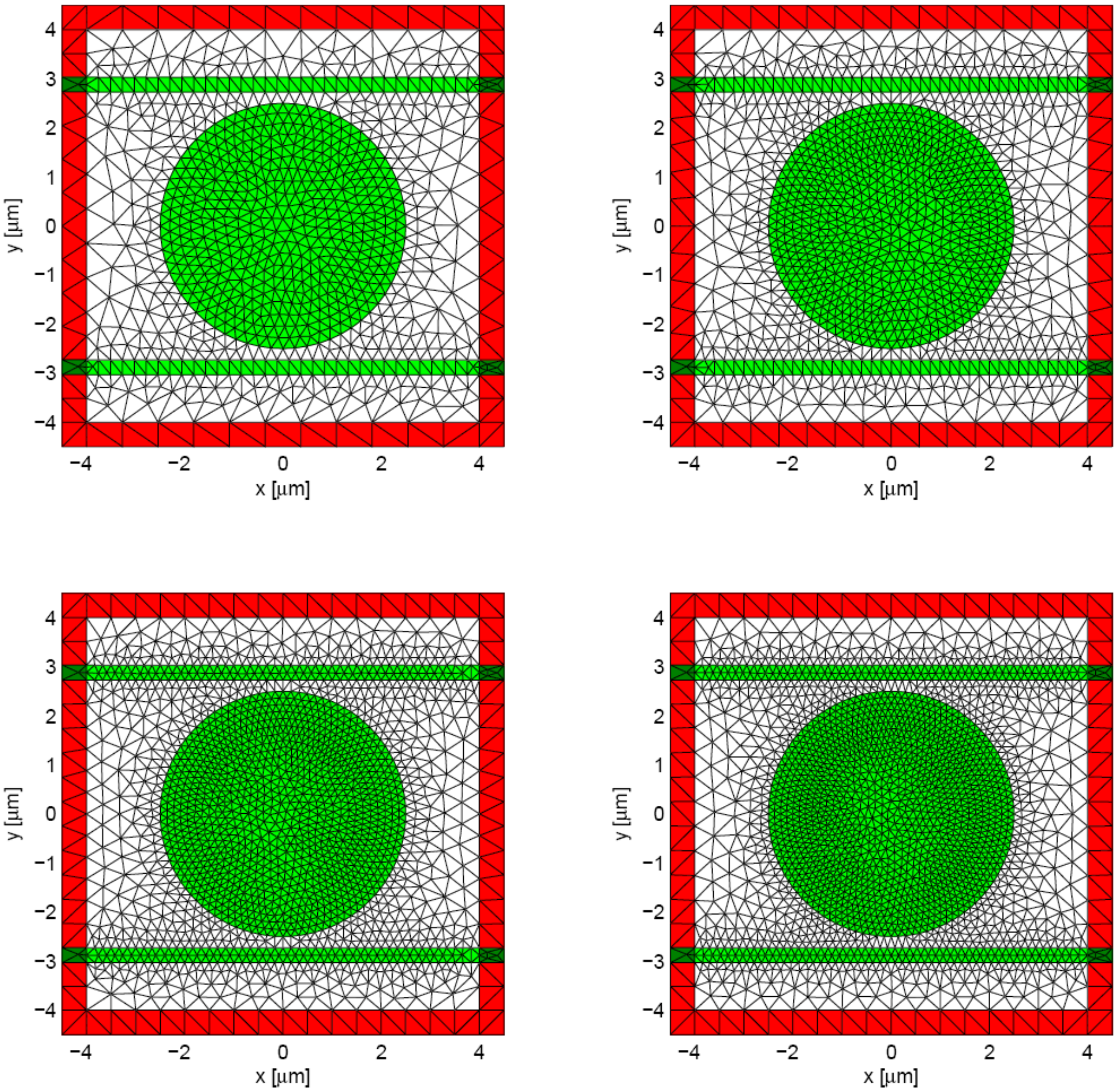

Fig.1: Typical finite-element meshes (M1: top left, M2: top right, M3: lower left, M4: lower right) used for the calculations of resonance frequencies and spectra for a typical realization of a coupled resonator-waveguide system. In all computations we employ 4^{th}-order polynomials to represent the field on each triangular element. Green and white shaded areas correspond to silicon and air, respectively, while red shaded areas denote perfectly matched layer absorbing boundaries.

Determining the spectral properties of such a device is already challenging for a time-domain method – clearly, one would rather want to use a frequency-domain method in order to find the resonances and their Q-values. However, one should bear in mind that, eventually, we want to analyze fully three-dimensional structures such as the goblet-shaped structures developed by the group of Heinz Kalt [6]. These goblets have typical diameters of several 10μm so that a frequency-domain approach quickly runs into serious issues related to computational resources, notably memory consumption when solving the corresponding system of equations.

Of course, there is no free lunch. The price one has to pay for using a time-domain approach is given by excessive CPU time consumption. However, here we have a certain degree of leverage as on DGTD, the time-stepper can be chosen almost arbitrary. For instance, for a 4^{th}-order spatial discretization, we typically use a 4^{th}-order low-storage Runge-Kutta scheme as initially proposed by Hesthaven and Warburton [7]. With this approach our DGTD-computations of the above device for require about 100 times less memory and are about 10 times faster than corresponding FDTD-computations using the MEEP-package [8]. For the illustrative example described in Fig. 1, we display the field distribution of several modes of different radial order in Fig. 2. The corresponding spectra can be found in Fig. 3.

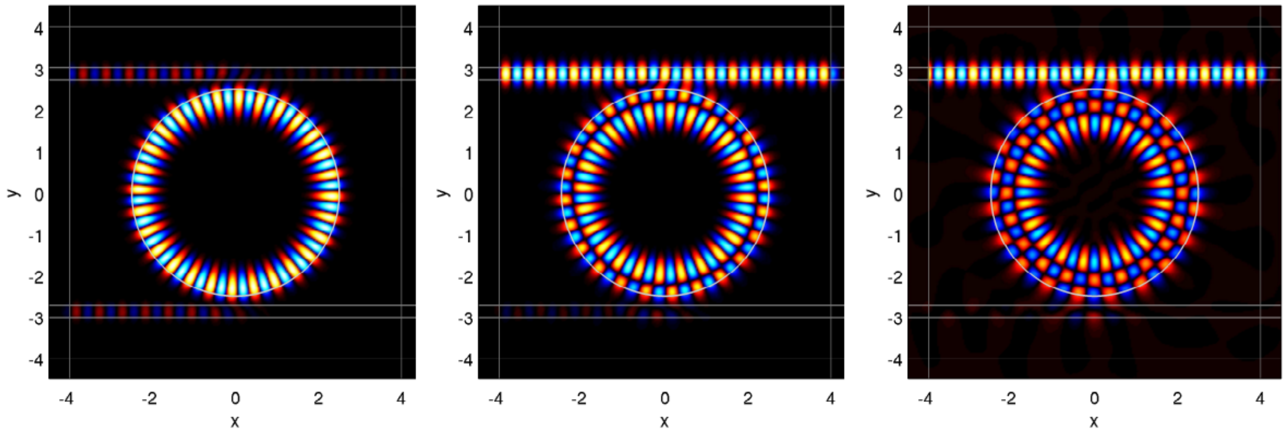

Fig.2: Field plots of the E_z-component of the system depicted in Fig. 6 after excitation with waveguide modes of different frequencies: The left panel shows a first-order radial mode with wavelength 1.529μm, the center panel a second-order radial mode with wavelength 1.5112μm, and the right panel a third-order radial mode with wavelength 1.5357μm.

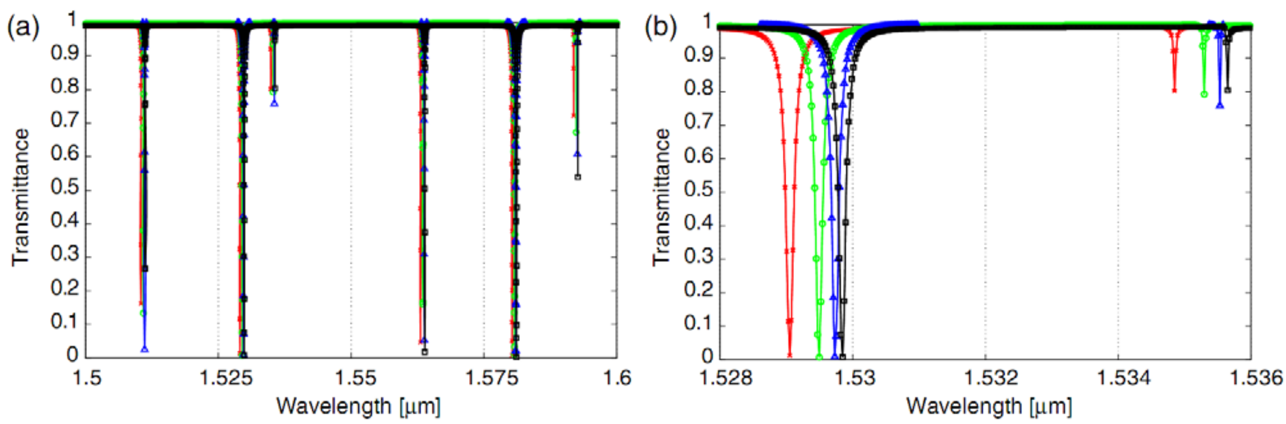

Fig.2: Spectra for meshes M1 (crosses),M2 (circles),M3 (triangles) and M4 (squares). All calculations were done in fourth order. (a) shows a broader spectrum around the wavelength of interest, while (b) contains a close-up of the spectrum around 1.53 μm.

Obviously, the rather extreme accuracy required to obtain converged results has forced us to work on the time-stepping characteristics of the DGTD approach. Therefore, we have focused on constructing dedicated low-storage Runge-Kutta schemes that yield stability regions that are better adapted to the spectra of typical nano-photonic system operators [3,4] relative to the originally proposed scheme [7]. To make a long story short, we have managed to improve the execution speed of our code by about 40% to 50%, merely by changing 12 numbers within several thousand lines of code. In addition, we have introduced curvilinear elements [9] to better resolve rounded geometries.

Only with these improvements have we been able to accurately simulate a slightly more complex setup, i.e., a waveguide-coupled slotted-ring resonator as described in the next section.

2. Coupled Waveguide-Resonator Systems – Coupled-Mode Theory

The principal aim of coupled-mode theoretical (CMT) approaches to complex photonic systems is to concentrate on the essential physics of the problem by considering the dominant modes of certain simpler subsystems and their coupling. This raises the question of which modes to consider (and which to leave out) and how good the corresponding approximations are. Very often, both questions can only be answered by comparing with exact numerical results for certain test systems.

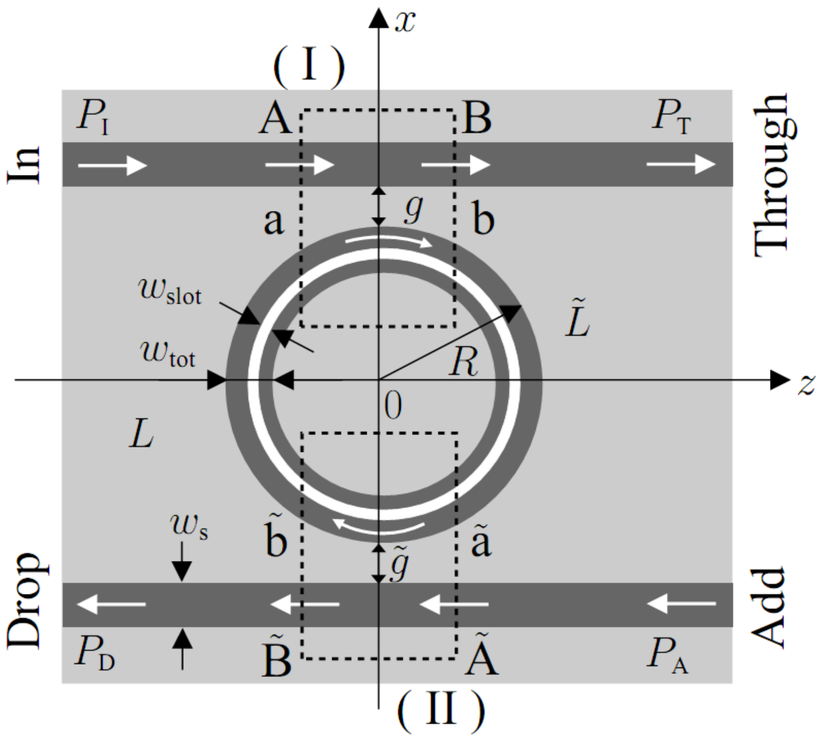

Fig. 4. Schematics for a slotted-resonator based 4-port device where the slot's position inside the ring is varied. This slotted resonator is coupled to two identical straight waveguides that realize input and output ports. The device performance may be characterized via the power levels associated with the input ports, P_I and P_A (In- and Add-port), and the output ports, P_T and P_D (Through- and Drop-port), respectively. Within a coupled-mode theoretical approach this device is further decomposed into several functional elements. Two couplers, (I) and (II), delineated with dashed-line boxes, are connected via two identical segments of bent slotted waveguides of different length and each of these couplers is further connected to two identical input and output port waveguides (see Ref. [5] for more details).

As an illustration, we consider the construction of a CMT for systems such as the waveguide-coupled slotted-resonator depicted in Fig. 4. Here, the input and output waveguides have been chosen such that they support only one propagating mode (actually two counter-propagating modes) for the frequency range for which operation of the device shall be considered. Similarly, the modes for a circular slotted waveguide can be found by a standard approach using cylindrical coordinates. In both cases, the results are mode profiles and propagation constants – in the case of the circular slotted waveguide they are complex, signaling that light is not strictly guided.

A naïve CMT approach would consist in retaining only that mode of the circular slotted waveguide that exhibits the lowest losses. However, a comparison with exact numerical results quickly reveals that this is inadequate. Here, a word of caution is required. In order to obtain converged results for this system, we have had to push DGTD very hard. As a matter of fact, for the meshes depicted in Fig. 5 we have obtained convergence only when using 6^{th}-order spatial discretization and curvilinear elements in the slot region. This analysis also reveals that one needs to take into account all the modes of the slotted ring resonator whose effective group index at the operation frequency exceeds the value of the background dielectric constant. In the present case, this amounts to considering the fundamental and 1^{st}-order radial modes simultaneously, although they do exhibit substantially different imaginary parts in their propagation constants.

The actual construction of the CMT is another matter for which we would like to refer to Ref. [5]. Suffice it to say that – as usual in most CMT approaches – we rely on an “adiabatic approximation” which disregards the backscattering processes into the counter-progating modes. This adiabaticity is less and less justified the closer we bring the waveguides to the slotted resonator. This is clearly seen in Fig. 6, where we display a comparison of the input-output characteristics for different waveguide-resonator separations.

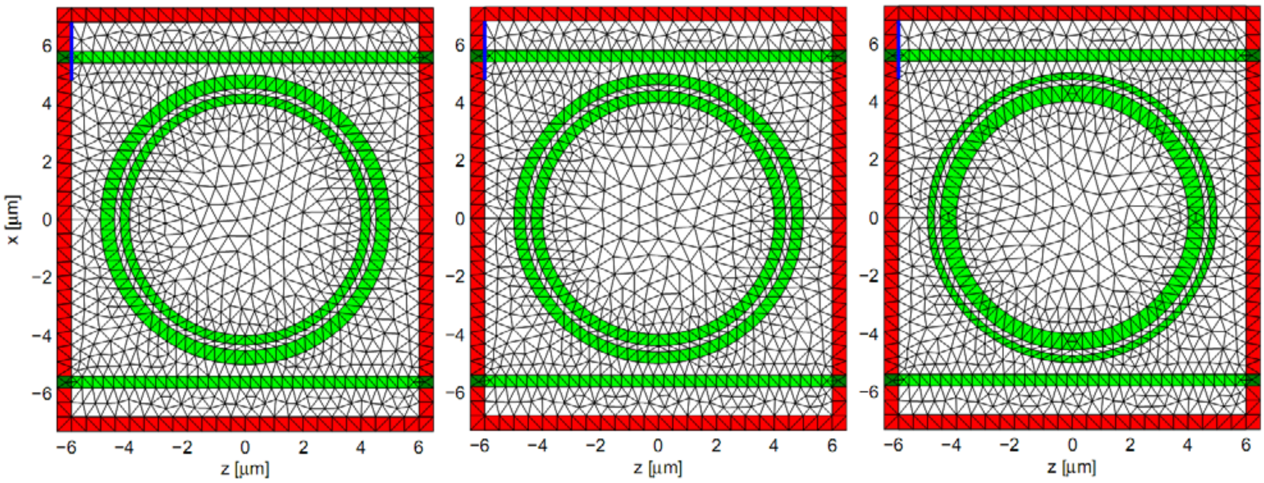

Fig. 5. Meshes that have been used for the DGTD computations of the slotted resonator device sketched in Fig. 5. From left to right, the slot position corresponds to η = 0.4, η = 0.5, and η = 0.7 respectively. The computational domain is enclosed by perfectly matched layers as indicated by the finite-width outermost box. In order to determine the spectral response of the device a broad-band pulse for is injected in the upper left waveguide. The flux through the output ports is recorded and subsequently Fourier-transformed.

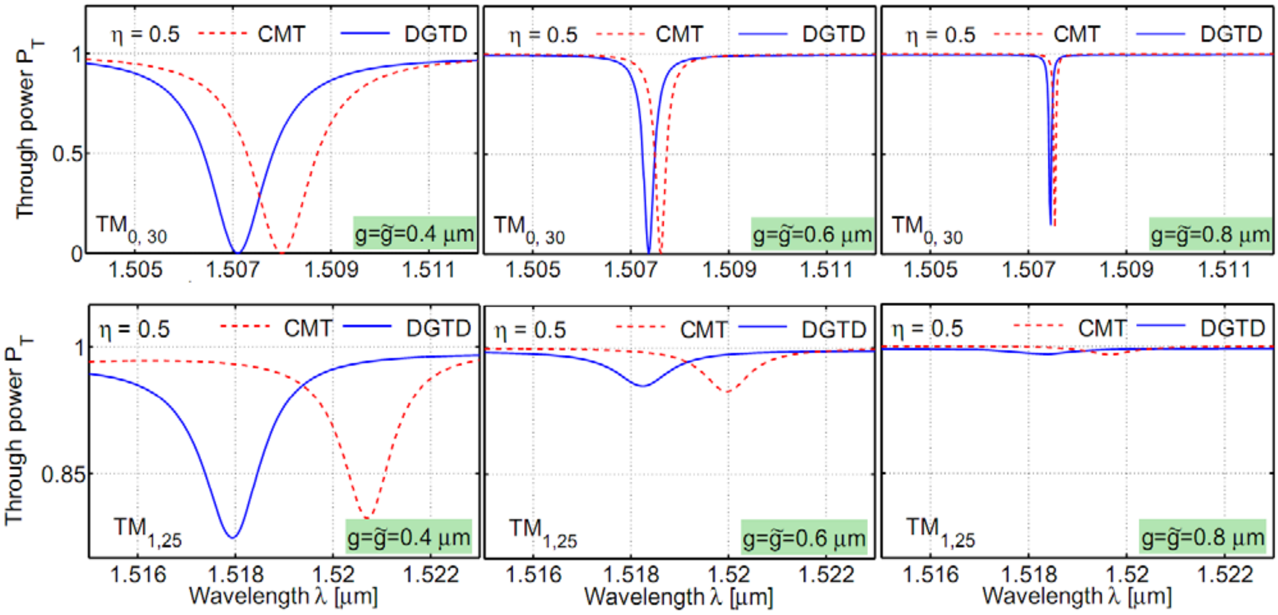

Fig. 6. Spectral response of the slotted resonator device depicted in Fig. 4 for a symmetric slot position (η = 0.5) for various minimal separations of the straight waveguides from the slotted resonator (see Ref. [5] for further details).

Nevertheless, CMT captures the essential physics of the problem. This is illustrated in Fig. 7, where we display the input-output characteristics for different locations of the slot within the ring, i.e., different values of the parameter η. Actually, it is this parameter that adjusts the relative coupling strength between the modes of the straight waveguides and the modes of the circular slotted waveguide sections. As a result, the resonator's resonances are profoundly modified, notably when the coupling to the more lossy 1st-order mode is practically eliminated for η = 0.7; in this case, the line widths of the fundamental resonances change by more than an order of magnitude. This somewhat unexpected effect may be exploited for the construction of highly sensitive sensing devices based on properly engineered waveguide-coupled slotted resonator systems. It is even conceivable that the asymmetric mode profile within the slot (that can be engineered via the slot's position) will find applications in optomechanical devices.

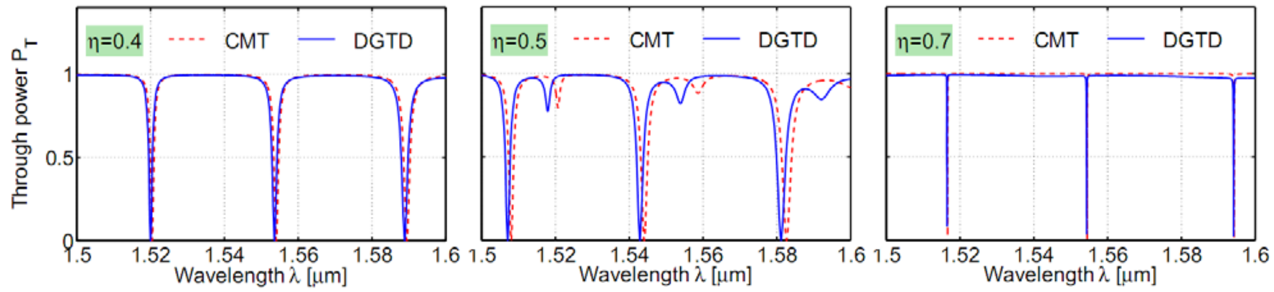

Fig. 7. Spectral response of the slotted resonator device depicted in Fig.4 for various slot positions within the ring (see Ref. [5] for details on the device parameters). The results of the CMT approach are compared with the results of numerically exact DGTD computations. Note the dramatic change in resonance line widths when going from η = 0.4 via η = 0.5 to η = 0.7.

3. Ongoing Developments

After having established a working CMT approach to waveguide-coupled resonator systems, we are now moving to construct a perturbation theoretical approach that will allow us to consider – within CMT – the effect of small perturbations on the resonances' position and linewidths. Clearly, this has to be compared with exact numerical results in order to understand its limitations. Once it has been established, this perturbation-theory-plus-CMT approach will allow us to develop optimized layouts for various purposes such as high-sensitivity sensing etc.

On the methodical side, we still consider DGTD too slow (although it definitely outperforms FDTD by a large margin). Therefore, we have embarked on transferring our code to high-performance-computing systems using graphic processor units (GPUs). The preliminary speedup characteristics are reported in Fig. 8. Given that current CPUs feature hexacore processors – for which we could parallelize our code via MPI – we estimate that we will eventually end up with a total GPU-speedup of a factor of about 10 relative to CPU.

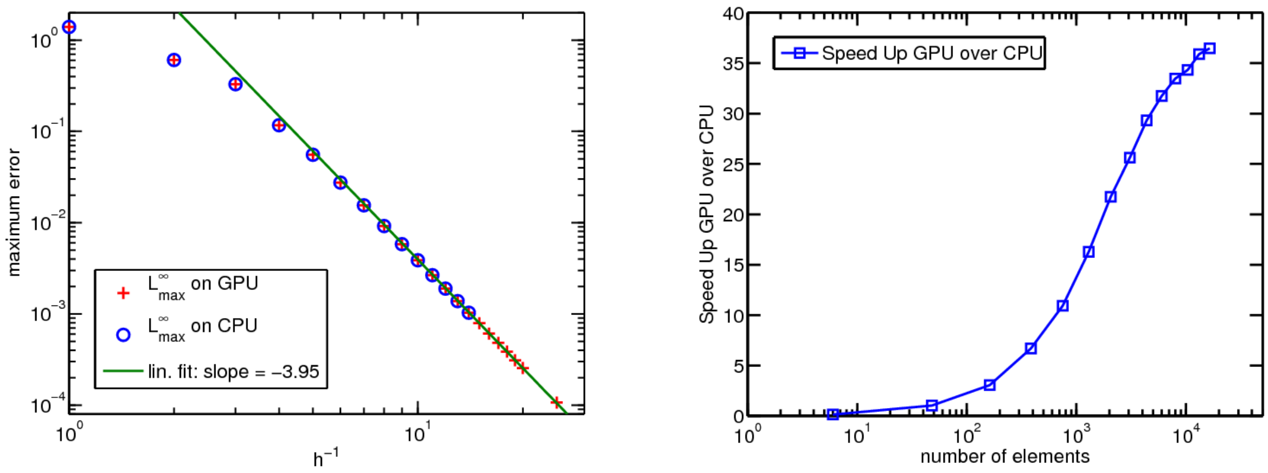

Fig. 8. Accuracy comparison (left panel) and speedup (right panel) of GPU-based computations relative to CPU computations with a single core for a test system. The computations are done with a DGTD-code with 4th-order accurate spatial discretization.

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