Developing a method for predicting the whispering gallery mode spectrum of microresonators

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Introduction

Background: Optical microresonators represent an important tool for biological sensing [1], especially in non-invasive treatment of a patient. Microscopic spheres of a high refractive-index material are able to exhibit optical phenomena known as Whispering Gallery Modes [2].

What are Whispering Gallery Modes (WGMs)?
Electromagnetic waves travelling within a symmetrical medium can produce resonances along the surface, similar to the way sound bounces around the edges of the Whispering Gallery of St Paul's Cathedral.

The azimuthal mode number, *n*, is related to the number of nodes on the surface. (Fig. 1).

There is also a radial mode number, *m*, related to the depth of the mode.

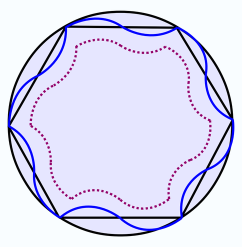
Figure 1 | Illustration of WGMs in a resonator.

Why are WGMs important?
• Because they can be easily adapted for biological and *in vivo* sensing, due to their high sensitivity to the external environment of the resonator.

• They are capable of extremely high quality(Q)-factors [3], which represent their power output relative to the background radiation, and the precision of their wavelength range. This makes the WGMs potentially very distinguishable from one another in the power spectrum. Changes to the WGMs can also be tracked easily, since only certain mode wavelengths are available for a given resonator size.

Why is this work novel?
While previous studies have predicted WGMs using mainly analytic models [4], here, for the first time, the excitation of the WGMs microresonators is investigated for point-source electric dipoles in the vicinity of the resonator. This provides an analogue for embedded nanoparticles, potentially exhibiting different mode excitation properties to that of incident plane-waves.

Research Aims:
• To develop a customisable, predictive tool for simulating the behaviour of a microresonator, and to predict the WGMs from the output spectrum.

• To investigate a variety of methods for exciting WGMs, and optimise the power coupling for a specific wavelength range, or specific modes.

• To be able to preselect specific optical properties for a resonator prior to fabrication, dramatically reducing material costs.

• To assess the viability of a resonator for use in biosensing, by scanning over a range of parameters, and comparing with experimental results.

Methods

Finite-Difference Time-Domain Method (FDTD):
The FDTD technique [5] discretises a volume of space into a 3D spatial lattice, and solves for the electromagnetic fields at each point. This is repeated for a finite number of time increments as the system evolves.

• FDTD constitutes a comprehensive solution of an optical system, with all radiation modes present. The only approximations involve discretisation and finite-volume effects, and ideal material properties.

• This method is suitable for accessing transient or unexpected electro-magnetic properties, as each time step is evaluated individually.

• However, the method is computationally expensive, each simulation of a few hundred wave periods requiring up to 100 hrs of supercomputer time (~30 CPUs) for a converged result.

The power spectrum is a useful quantity for representing the positions and Q-factors of the excited modes [6]. A flux-collection region is introduced a certain distance from the microresonator, and the output power is obtained by integrating over the Poynting vector, $S = E \times H$:

$$I(\lambda) = \int S(\lambda) \cdot n \, dA$$

Example: A microsphere, 6μm in diameter, is excited by an electric dipole source placed tangentially to the surface. (Fig. 2).

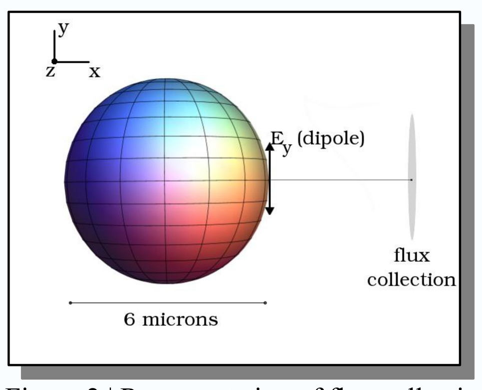

Figure 2 | Representation of flux collection from a microsphere, excited by a tangential electric dipole source.

Analytic model:
To check the mode positions predicted by FDTD, an analytic model is used, in which Maxwell's Equations are solved in a dielectric medium with boundary [7].

• The analytic model is only capable of estimating the wavelengths of the transverse electric (TE) and magnetic (TM) modes for an ideal geometry, assuming no mode superposition, and assumes excitation always occurs from an incoming plane wave.

• However, the analytic model represents an important test for the FDTD simulation. Accurate matching of the mode structure of the spectrum allows one to identify the dominant contributions to the prominent features of the spectrum. This identification facilitates future experimental studies in the reduction or enhancement of these features.

Results

Identifying the Whispering Gallery Modes of a polystyrene microsphere:

FDTD simulation details: A spherical microresonator of polystyrene (n = 1.59) with a diameter of 6μm and placed in an air medium, is excited by a source, placed on the surface of the sphere (Fig. 2.). The source is a Gaussian electric dipole, with a range of wavelengths: 530-670nm, and a central wavelength of 600nm. It is oriented tangentially to the sphere's surface.
The power is then collected from a circular flux plane of diameter 2.58μm, placed a distance of 240nm from the sphere's surface, with a collection time of 300 periods, or 6×10^{-13}s. The normalised power spectrum is shown in Fig. 3, and is compared to the results from the analytic model.

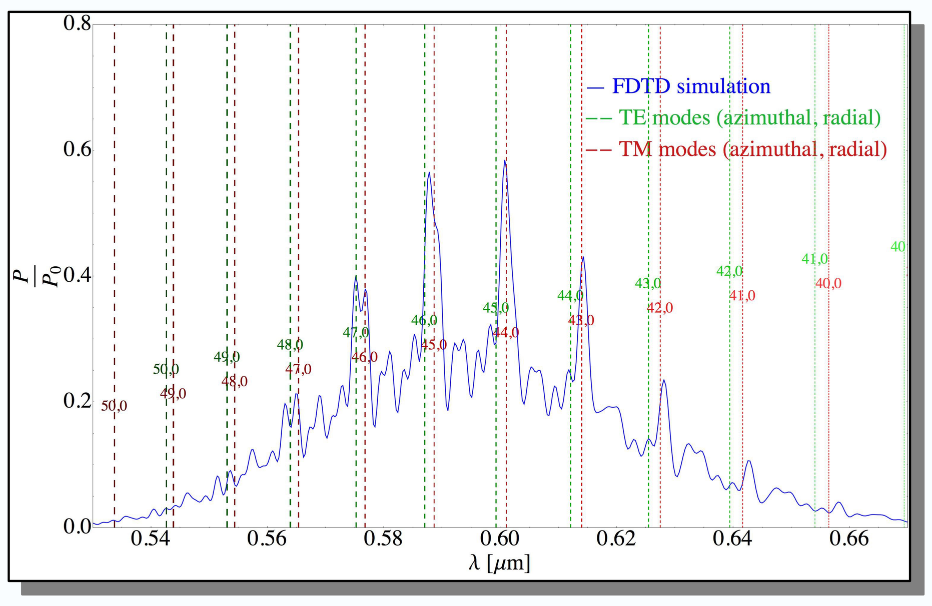

Figure 3 | FDTD simulation of the power spectrum for a polystyrene microsphere, 6μm in diameter. WGMs are excited from a tangential electric dipole source. Vertical dashed lines indicate predictions of fundamental radial TE (green) and TM (red) modes derived from the analytic model.

Features:
• Figure 3 demonstrates fairly good agreement between the FDTD calculation and the analytic model. The evenly-spaced dominant peaks correspond to the fundamental radial *(m=0)* TM modes, with azimuthal mode numbers of *n ~ 40-50.* This is to be expected from a tangentially oriented source, which predominantly excites the lower order radial modes.

• Nearby secondary peaks correspond to the equivalent TE modes. Spherical symmetry means that contributions from both TE and TM modes are present in the spectrum. Modes excited in close proximity to one another are slightly shifted away from the positions expected from the analytic model.

Different methods of exciting the modes:
A comparison of WGM mode excitation from a tangential and radial dipole source is shown in Fig. 4. Though the same modes are present, the power coupling is distributed differently, resulting in different peak heights. A radial source is more likely to excite higher order radial WGMs.

Figure 5 shows that peak height increases with flux collection time, until it reaches a steady state. However, some information about the double-peak structure is lost, as the power for intermediate modes builds up. Note that, for maximum collection times, $P/P_0 > 1$, indicating a Purcell enhancement.

Angular flux distribution:
FDTD can also provide information about the angular distribution of flux, as shown in Figs. 6 and 7. By comparing power output for different flux-plane distances from the microsphere, or flux-plane diameters, the spatial distribution of the Poynting vector, *S*(*r*), is sampled differently. One can investigate this further to map out a 3D image of the total distribution.

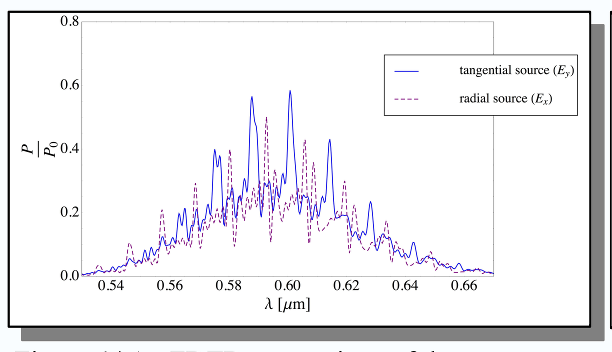
Figure 4 | An FDTD comparison of the power spectra for 6μm diameter microspheres, excited by tangential or radial electric dipole sources.

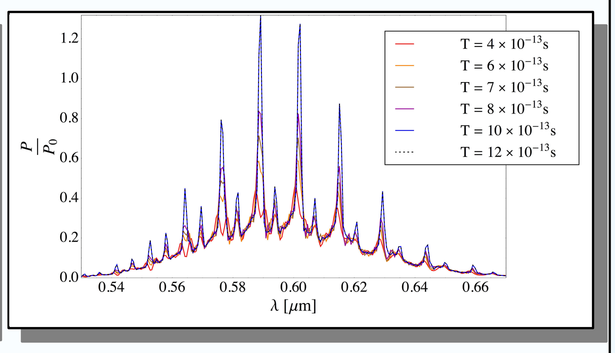
Figure 5 | A comparison of the power spectra for increasing flux collection time.

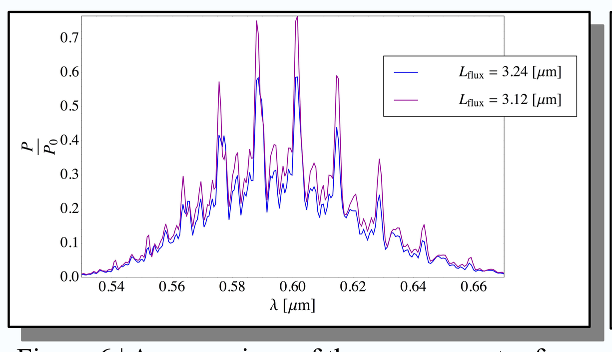
Figure 6 | A comparison of the power spectra for flux collection planes different distances, L_{flux}, from the centre of the sphere.

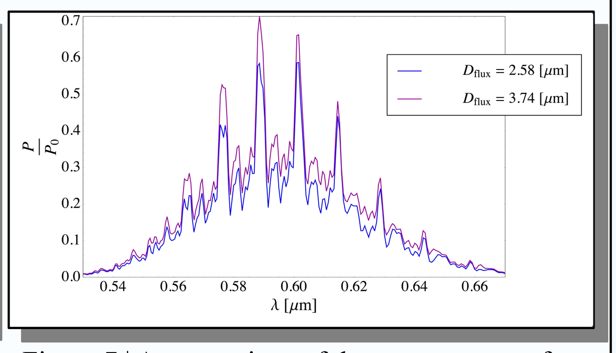
Figure 7 | A comparison of the power spectra for different flux collection diameters, D_{flux}.

Example: The flux density, *S*(*r*), is shown in an example plot in Fig. 8 at a time slice of 6×10^{-13}s.
The flux collection region is shown in the *x-y* plane, with lighter colour corresponding to a larger value of *S*.

An analysis of the flux distribution can provide a way to distinguish modes at different time slices, and transient resonant phenomena.

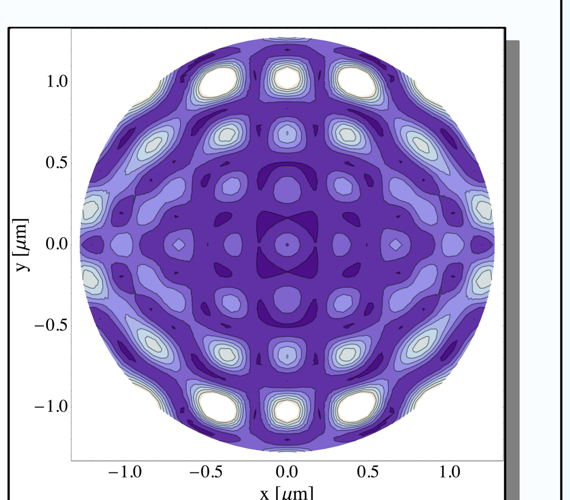
Figure 8 | The spatial distribution of the flux density, *S*, in the circular collection region, $t = 6 \times 10^{-13}$s.

Experimental comparison:
Polystyrene microspheres coated with a fluorescent dye are excited by a 532nm laser. The dye emits at 570-650 nm. Coupling the spheres to a fibre [8] constrains the mode excitation to a particular direction.

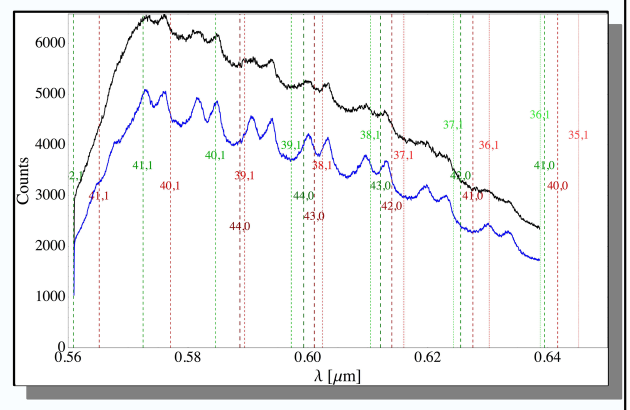
Figure 9 | Experimental result for the power spectra of 6μm diameter microspheres, both freely suspended (black line) and coupled to a fibre (blue line). Predictions from the analytic model are shown as vertical dashed lines, TE(*n*,*m*) and TM(*n*,*m*).

The output spectra for free and fibre-coupled spheres are shown in Fig. 9. The analytic model shows agreement with only a few modes, stimulating a need to provide predictions of WGMs that incorporate realistic physical characteristics in order to compare with experiment.

FDTD is able to provide such a realistic prediction through a comprehensive simulation of all modes, at each grid point. Upon making a robust comparison with experiment, different values of the simulation input parameters may be explored, in order to optimise the resonator for biosensing applications.

Conclusions

Novel features:
The FDTD method can be tailored for more realistic scenarios, when the assumptions in the analytic models make direct comparison with experiment difficult. Examples include: mixing effects of closely spaced modes, access to the angular flux distribution by modifying the flux collection region, simulation of the relative coupling efficiency to different modes, and calculation of the mode Q-factors.

An important novel feature of FDTD is the ability to investigate the choice of source used for mode excitation, as-yet unexplored in the literature. Dipole sources may be placed at a variety of positions and orientations on the surface of the sphere, which can serve as an analogue for nanoparticle coatings.

Towards a customisable tool for WGM prediction:
The computational tool FDTD represents a promising candidate in developing a WGM prediction tool for microresonators.

• It obtains a comprehensive output spectrum including all radiation modes and bound modes of light.

• Input parameters are easily modified to scan over attributes of interest, such as dielectric geometry, size, shape, refractive index contrast, flux region size, collection time, and method of excitation from a source.

• Though computationally expensive, a step-wise simulation in time allows for identification of transient resonant properties, such as the mode behaviour as a function of collection time, or the angular distribution of the flux density.

Further Research

The next step in this project is to establish a robust comparison with experimental results for a variety of sizes of microsphere. This may involve the introduction of evenly-distributed dipole sources of random orientation, to act as an analogue for fluorescent dye used in experiment.

The FDTD simulation is also able to address a variety of nonlinear optical effects, providing insight into the mode structure of a resonator.

Finally, tuning the characteristics of the resonator for optimal power coupling and identifying prominent spectral features will help to reduce fabrication costs, and aid the development of the next generation of biosensing tools.

References

[1] Vollmer, F., Braun, D., *et al.*, Appl. Phys. Lett. **80**, 21 (2002).
[2] Vahala, K., *Optical Microcavities*, World Scientific Publishing Co. Pte. Ltd, (2004).
[3] Armani, A. M., *et al.,* Science **317**, 783 (2007).
[4] Teraoka, I., Arnold, S., J. Opt. Soc. Am. B **23**, 7 (2006).
[5] Taflove, A., *Computational Electrodynamics: The Finite-Difference Time-Domain Method,* Artech House, Boston (1995).
[6] Henderson, M. R., Afshar V. S., Greentree, A. D., Monro, T. M., Optics Express **19**, 17, 16194 (2011).
[7] Johnson, B. R., J. Opt. Soc. Am. A **10**, 2 (1993).
[8] François, A., Rowland, K. J., Monro, T. M., Appl. Phys. Lett. **99**, 141111 (2011).

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