Time-domain simulations of nonlinear interaction in microring resonators using finite-difference and coupled mode techniques

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Abstract: Nonlinear interactions within compact, on-chip microring resonant cavities is a topic of increasing interest in current silicon photonics research. Frequency combs, one of the emerging nonlinear applications in microring optics, offers great potential from both scientific and practical perspectives. However, the mechanisms of comb formation appear to differ from traditional frequency combs formed by pulsed femtosecond lasers, and thus require detailed elucidation through theory and simulation. Here we propose a technique to mimic the accuracy of finite-difference time domain (FDTD) full wave nonlinear optical simulations with only a small fraction of the computational resources. Our new hybrid approach combines a single linear FDTD simulation of the key interaction parameters, then directly inserts them into a coupled-mode theory simulation. Comparison of the hybrid approach and full FDTD shows a good match both in frequency domain and in time domain. Thus, it retains the advantage of FDTD in terms of direct connection with experimental designs, while finishing much faster and sidestepping stability issues associated with direct simulation of nonlinear phenomena. The hybrid technique produces several key results explored in this paper, including: demonstrating that comb formation can occur with both anomalous and normal dispersion; suggesting a new mechanism for incoherent (Type II) frequency comb formation; and illustrating a method for creating soliton-like pulses in on-chip microresonators.

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OCIS codes: (130.4310) Nonlinear; (190.3270) Kerr effect; (190.4380) Nonlinear optics, fourwave mixing; (140.4780) Optical resonators.

References and links

- 1. P. Del'Haye, A. Schliesser, O. Arcizet, T. Wilken, R. Holzwarth, and T. J. Kippenberg, "Optical frequency comb generation from a monolithic microresonator," Nature **450**, 1214–1217 (2007).
- 2. J. Ye and S. T. Cundiff, *Femtosecond Optical Frequency Comb: Principle, Operation, and Applications* (Kluwer, 2005).

P. Del'Haye, S. B. Papp, and S. A. Diddams, "Hybrid electro-optically modulated microcombs," Phys. Rev. Lett. 109, 263901 (2012).

I. S. Grudinin, N. Yu, and L. Maleki, "Generation of optical frequency combs with a CaF₂ resonator," Opt. Lett. 34, 878–880 (2009).

- W. C. Jiang, X. Lu, J. Zhang, O. Painter, and Q. Lin, "Ultra-bright photon-pair generation on a silicon chip," in *Frontiers in Optics 2012/Laser Science XXVIII*, OSA Technical Digest (online) (Optical Society of America, 2012), paper FW6C.10.
- B. E. Little, S. T. Chu, P. P. Absil, J. V. Hryniewicz, F. G. Johnson, F. Seiferth, D. Gill, V. Van, O. King, and M. Trakalo, "Very high order microring resonator filters for WDM applications," IEEE Photon. Technol. Lett. 16, 2263–2265 (2004).
- T. Barwicz, M. A. Popović, P. T. Rakich, M. R. Watts, H. A. Haus, E. P. Ippen, and H. I. Smith, "Microringresonator-based add-drop filters in SiN: fabrication and analysis," Opt. Express 12, 1437–1442 (2004).
- J. S. Levy, A. Gondarenko, M. A. Foster, A. C. Turner-Foster, A. L. Gaeta, and M. Lipson, "CMOS-compatible multiple-wavelength oscillator for on-chip optical interconnects," Nat. Photon. 4, 37–40 (2010).
- L. Razzari, D. Duchesne, M. Ferrera, R. Morandotti, S. Chu, B. E. Little, and D. J. Moss, "CMOS-compatible integrated optical hyper-parametric oscillator," Nat. Photon. 4, 41–45 (2010).
- F. Ferdous, H. Miao, D. E. Leaird, K. Srinivasan, J. Wang, L. Chen, L. T. Varghese, and A. M. Weiner, "Spectral line-by-line pulse shaping of on-chip microresonator frequency combs," Nat. Photon. 5, 770–776 (2011).
- S. B. Papp and S. A. Diddams, "Spectral and temporal characterization of a fused-quartz-microresonator optical frequency comb," Phys. Rev. A 84, 053833 (2011).
- T. J. Kippenberg, R. Holzwarth, and S. A. Diddams, "Microresonator-based optical frequency combs," Science 332, 555–559 (2011).
- A. B. Matsko, A. A. Savchenkov, W. Liang, V. S. Ilchenko, D. Seidel, and L. Maleki, "Mode-locked Kerr frequency combs," Opt. Lett. 36, 2845–2847 (2011).
- M. Popovic, *Theory and design of High-Index-Contrast microphotonic circuits* (MIT libraries thesis collection, Cambridge, MA, 2008).
- A. Rodriguez, M. Soljacic, J. Joannopoulos, and S. Johnson, "Chi(2) and Chi(3) harmonic generation at a critical power in inhomogeneous doubly resonant cavities," Opt. Express 15, 7303–7318 (2007).
- T. Herr, K. Hartinger, J. Riemensberger, C. Y. Wang, E. Gavartin, R. Holzwarth, M. L. Gorodetsky, and T. J. Kippenberg, "Universal formation dynamics and noise of Kerr-frequency combs in microresonators," Nat. Photon. 6, 480–487 (2012).
- 17. Y. K. Chembo and N. Yu, "Modal expansion approach to optical-frequency-comb generation with monolithic whispering-gallery-mode resonators," Phys Rev. A 82, 033801 (2010).
- E. Granados, D. W. Coutts, and D. J. Spence, "Mode-locked deep ultraviolet Ce:LiCAF laser," Opt. Lett. 34, 1660–1662 (2009).
- L. A. Lugiato and R. Lefever, "Spatial dissipative structures in passive optical systems," Phys. Rev. Lett. 58, 2209–2211 (1987).
- S. Coen, H. G. Randle, T. Sylvestre, and M. Erkintalo, "Modeling of octave-spanning Kerr frequency combs using a generalized mean-field Lugiato-Lefever model," Opt. Lett. 38, 37–39 (2013).
- M. R. Lamont, Y. Okawachi, and A. L. Gaeta, "Route to stabilized ultrabroadband microresonator-based frequency combs," Opt. Lett. 38, 3478–3481 (2013).
- M. Haelterman, S. Trillo, and S. Wabnitz, "Dissipative modulation instability in a nonlinear dispersive ring cavity," Opt. Commun. 91, 401–407 (1992).
- 23. A. Yariv and P. Yeh, Photonics: Optical Electronics in Modern Communications (Oxford University, 2007).
- A. B. Matsko, W. Liang, A. A. Savchenkov, and L. Maleki, "Chaotic dynamics of frequency combs generated with continuously pumped nonlinear microresonators," Opt. Lett. 38, 525–527 (2013).
- T. Hansson, D. Modotto, and S. Wabnitz, "On the numerical simulation of Kerr frequency combs using coupled mode equations," Opt. Commun. 312, 134–136 (2014).
- M. Peccianti, A. Pasquazi, Y. Park, B.E. Little, S.T. Chu, D.J. Moss, and R. Morandotti, "Demonstration of a stable ultrafast laser based on a nonlinear microcavity," Nature Comm. 3, 765 (2012).
- Y. Dumeige, C. Arnaud, and P. Feron, "Combining FDTD with coupled mode theories for bistability in microring resonators," Opt. Commun. 250, 376–383 (2005).
- A. F. Oskooi, D. Roundy, M. Ibanescu, P. Bermel, J. D. Joannopoulos, and S. G. Johnson, "MEEP: A flexible free software package for electromagnetic simulations by the FDTD method," Comp. Phys. Commun. 181, 687-702 (2010).
- V. A. Mandelshtam, "FDM: the filter diagonalization method for data processing in NMR experiments," Prog. Nucl. Mag. Res. Sp. 38, 159–196 (2001).
- B. E. Little, S. T. Chu, H. A. Haus, J. Foresi, and J. P. Laine, "Microring resonator channel dropping filters," J. Lightwave Technol. 15, 998–1005 (1997).
- W. Yang, A. Josh, and X. Min, "Effects of side-coupling on the phase response of cascaded microring all-pass filters," Opt. Commun. 232, 209–216 (2004).
- 32. Rosen Center for Advanced Computing: Carter User Information. http://www.rcac.purdue.edu/userinfo/resources/carter/, last accessed on May 31, 2013.
- 33. G. P. Agrawal, Fiber-Optic Communications Systems, 3rd ed. (John Wiley, 2002).
- F. Leo, S. Coen, P. Kockaert, S. P. Gorza, P. Emplit, and M. Haelterman, "Temporal cavity solitons in onedimensional Kerr media as bits in an all-optical buffer," Nat. Photon. 4, 471–476 (2010).

1. Introduction

Optical frequency comb formation is a very powerful technology, in which optical narrowband signals are created at predetermined frequency intervals with precisely controlled amplitudes and phases [1]. With a bandwidth of at least an octave (frequencies from ω to 2ω), coherent combs can be generated to span a very broad frequency spectrum. Optical frequency combs have a number of important current and potential applications, including precision metrology for improved GPS [2, 3], pulse shaping [4], terahertz spectroscopy and sensing, RF modulation [4], quantum photonics [5] and high-harmonic generation for extended UV (XUV) sources for lithography. Typically, optical combs are generated by using a pulsed femtosecond laser. However, such a solution tends to be relatively bulky and expensive. With recent advances in fabrication techniques, on-chip microresonators have recently been developed [6, 7]. If these microresonators are then excited by common continuous-wave (cw) pump lasers, optical frequency combs can now be generated within a compact form factor [1-5, 8-13]. Additionally, the microresonator combs have enabled novel features, including in particular very large (hundreds of GHz or above) free spectral range, increased flexibility in dispersion matching, and especially very high field intensities compared to macroscopic resonators [14]. For four-wave mixing processes, a 1,000-fold increase in intensity associated with photonic mode confinement can increase signal and idler generation by a factor of 1,000,000 or more [15].

In this manuscript, we will explore the detailed behavior of microresonator optical frequency combs, since recent experiments to characterize their performance have revealed several surprising phenomena. In particular, as input power increases, the mode spacing decreases, and the total bandwidth of all modes generated increases dramatically, as does the noise. However, experimental microresonator combs typically experience too much incoherence for full spectral control at this time. Several theories have been proposed to explain the generation of coherent and incoherent combs, including multilevel comb growth [16], modulation instability [13], and deterministic chaos [17, 18]. To date, not enough theoretical or experimental work has been performed to distinguish between the different mechanisms, and accurately predict qualitative and quantitative behavior.

There have been several theoretical microresonator frequency comb studies performed using approaches such as Lugiato-Lefever (L-L) equation [19, 20] and the closely related general nonlinear Schrodinger equation [13]. These methods can provide excellent agreement with the experiment [21] under certain approximations. In particular the L-L equation takes the meanfield limit of the Maxwell-Bloch equations while also dropping higher-order spatial derivatives along the axis of propagation. Thus, systems with rapidly changing field intensity and spatial field variation may not be treated completely accurately using this model [22]. This may lead to less accurate results for systems under fast excitation (relative to the round trip time of the cavity) and small-scale devices such as small radius microresonators. Additionally, the use of these methods will not be appropriate for multimode-family analysis where sub-FSR mode spacing is required. Alternatively, coupled mode theory (CMT) [23-26] circumvents the described obstacles and has been extensively used to model nonlinear processes in microcavities. However, a one-to-one match between realistic comb formation processes in microring systems obtained with fully vectorial methods and corresponding coupled mode theory parameters has not been directly demonstrated in the previous work. In order to study the comb formation in the regime approaching experimental systems we implement a hybrid simulation method. In this approach, the key degrees of freedom are modeled through coupled mode theory with parameters such as mode profiles, mode frequencies and quality factors calculated in finite-difference time-domain (FDTD) simulations. A similar approach has been used previously to analyze bistability in the single mode cavity coupled to a waveguide [27]. In our study, we have shown that the hybrid CMT/FDTD method can be extended to model interactions of multiple modes occupying the same volume, subject to conservation rules and nonlinear coupling. This approach assumes perfect k-matching and dispersion was implemented via mode frequency definitions. Over the course of our studies, good agreement between CMT/FDTD and direct nonlinear FDTD simulations have been demonstrated.

For all cases where FDTD direct simulations are too time-consuming, and analytical estimates of nonlinear CMT parameters are unavailable or may not present an accurate picture of real performance (e.g., for small-radius microring resonators), our CMT/FDTD technique offers a potential advantage. There are many situations where this could be true because the field profile of even a microring resonator with any external symmetry breaking may no longer be given by Bessel functions. This method can be particularly useful to solve the cases when the eigenmodes of the cavity are significantly perturbed via coupling to other microrings or waveguides. Additionally, this method is extremely general, and encompasses not only microring systems with broken symmetry, but also has great potential for emerging nonlinear systems including but not limited to photonic crystals, plasmonics and metamaterials.

In the remainder of the paper we present a theory that shows the connection between the structure, generated FDTD field profiles, and CMT coupling parameters. We compare results obtained using hybrid CMT/ FDTD and FTDTD methods in the different dispersion regimes. After establishing a close match between solutions we explain advantages of the hybrid approach. We then explore the example of bright soliton-like mode formation in a microring, and show again that the hybrid method offers accurate, experimentally relevant results. Finally, we propose a mechanism explaining Type II frequency comb formation through the emergence of soliton-like pulses.

2. Theory

We can derive the equations of motion for Kerr nonlinear coupled mode theory as follows. We begin with the well-known electromagnetic field Hamiltonian:

$$H = \int dr \left[\varepsilon E(r)^2 + \frac{1}{\mu} B(r)^2 \right] \tag{1}$$

In the presence of a Kerr medium, we can generally write the refractive index as follows:

$$\boldsymbol{\varepsilon}(r) = \boldsymbol{\varepsilon}_o(r) + \boldsymbol{\varepsilon}_2 |\boldsymbol{E}(r)|^2 \tag{2}$$

Substituting this expression in yields:

$$H = \int dr \left[\varepsilon_o(r) + \varepsilon_2 |E(r)|^2 \right] \left[E(r)^2 + \frac{1}{\mu \varepsilon} B(r)^2 \right]$$
(3)

We can represent the electric field associated with mode k in terms of quadrature operators:

$$E_k(r) = C_k \cdot g_k(r)(a_k + a_k^{\dagger}) \tag{4}$$

where a_k is the annihilation operator, a_k^{\dagger} is the creation operator and $g_k(r)$ is the normalized amplitude function. C_k is a normalization constant, to be determined.

We can simplify Eq. (3) by considering only the electric field contribution to the energy in the absence of nonlinearities:

$$H_{el} = C_k^2 \int \varepsilon_0(r) g_k(r)^2 (a_k + a_k^{\dagger})^2 dr$$
(5)

$$H_{el} = C_k^2 \int \varepsilon_0(r) g_k(r)^2 dr (a_k^2 + a_k a_k^{\dagger} + a_k^{\dagger} a_k + a_k^{\dagger 2})$$
(6)

Canceling quadratic terms and adding linear terms from the magnetic energy part of the Hamiltonian, the total energy becomes:

$$H = 2C_k^2 \int \varepsilon_0(r)g_k(r)^2 dr(a_k a_k^{\dagger} + a_k^{\dagger} a_k)$$
⁽⁷⁾

In order for mode k to evolve with its characteristic frequency ω_k through the Heisenberg equation of motion, the following equality must also hold:

$$H = \frac{1}{2}\hbar\omega_k (a_k a_k^{\dagger} + a_k^{\dagger} a_k) \tag{8}$$

Therefore:

$$C_k = \frac{1}{2} \sqrt{\frac{\hbar \omega_k}{\int \varepsilon_0(r) g_k(r)^2 dr}}$$
(9)

Then the total field in the cavity can be written as:

$$E(r) = \sum_{k} \frac{1}{2} \sqrt{\frac{\hbar \omega_k}{\int \varepsilon_0(r) g_k(r)^2 dr}} g_k(r) (a_k + a_k^{\dagger})$$
(10)

Including nonlinear terms in Eq. (3) leads to the following result:

$$H = \sum_{k} \hbar \omega_{k} (a_{k}^{\dagger} a_{k} + \frac{1}{2}) + \frac{\hbar^{2} \varepsilon_{2}}{2} \sum_{i,j,k,l} \sqrt{\omega_{i} \omega_{j} \omega_{k} \omega_{l}} M_{ijkl} a_{i}^{\dagger} a_{j}^{\dagger} a_{k} a_{l} e^{i(\omega_{k} + \omega_{l} - \omega_{i} - \omega_{j})t}$$
(11)

where

$$M_{ijkl} = \frac{\int g_i(r)g_j(r)g_k(r)g_l(r)dr}{\left[\int \varepsilon_0(r)g_i(r)^2 dr\right]^{1/2} \left[\int \varepsilon_0(r)g_j(r)^2 dr\right]^{1/2} \left[\int \varepsilon_0(r)g_k(r)^2 dr\right]^{1/2} \left[\int \varepsilon_0(r)g_l(r)^2 dr\right]^{1/2}}$$
(12)

Applying Heisenberg equations of motion with commutator relations:

$$\frac{da_i}{dt} = \frac{1}{i\hbar} [a_i, H] \tag{13}$$

$$\left[a_{i},a_{j}^{\dagger}\right] = \delta_{ij} \tag{14}$$

$$[a_i, a_j] = 0 \tag{15}$$

yields to :

$$\frac{da_i}{dt} = -i\omega_i a_i - i\frac{\hbar^2 \varepsilon_2}{2} \sqrt{\omega_i \omega_j \omega_k \omega_l} M_{ijkl} e^{i(\omega_k + \omega_l - \omega_i - \omega_j)t} a_j^{\dagger} a_k a_l,$$
(16)

Self-phase modulation coupling is given by:

$$M_{iiii} = \frac{\int g_i(r)^4 dr}{\left(\int \varepsilon_0(r)g_i(r)^2 dr\right)^2}$$
(17)

while cross-phase modulation coupling is given by:

$$M_{ijij} = \frac{\int g_i^2(r)g_j^2(r)dr}{\int \varepsilon_0(r)g_i(r)^2 dr \int \varepsilon_0(r')g_j(r')^2 dr'}$$
(18)

3. Numerical methods

In this manuscript, we will perform a comprehensive set of simulations to predict and characterize the performance of photonic microresonator-based optical combs. The uniqueness of our approach will come from combining two distinct simulations in a unified framework: finitedifference time domain and coupled mode theory. We will essentially perform two types of time domain simulations: first is a direct simulation of the whole problem, including Kerr nonlinearities; the second will be a simulation of only the *linear* properties of the system, to be used as inputs for the coupled-mode theory.

A key enabling strategy will be reducing quasi-2D experimental structures consisting of approximately 14 million degrees of freedom down to about 11 weakly-coupled degrees of freedom - a reduction in complexity by a factor of a million. This greatly simplified approach captures the key dynamics of the system in terms of weakly coupled independent resonant waveguide and cavity modes, including both linear and nonlinear interactions. This can also be thought of in terms of lumped circuit-element models used in electrical engineering design. While the system behavior in the linear regime can be obtained semi-analytically, detailed analysis of nonlinear interactions requires numerical solutions of the appropriate (coupled) ordinary differential equations. The predictions of this approach will be confirmed computationally through comparison with separate, direct full-wave simulation of the same design.



Fig. 1. (a) Radial distribution of the normalized amplitude function |g(r)| for the fundamental normal dispersion mode (b) Radial distribution for the order 1 anomalous dispersion mode. The boundaries of the microring core region are shown as dotted lines.

The FDTD simulations in this paper are performed using a freely available software package, known as MEEP [28]. To reduce the computational load while preserving accuracy, the system is treated in 2D (which makes the effective height of the ring large). For normal and anomalous dispersion cases we selectively coupled to the modes having fundamental and first harmonic radial profile (order 0 modes and order 1 modes respectively, Fig. 1). The distributed, soft-source excitation was positioned within the microring core. The source amplitude is set to $A_s = |A_s|e^{-(t-t_0)^2/2\tau^2}e^{-(\phi-\phi_0)^2/2\sigma^2}$ where τ is the standard deviation in time and σ is the standard deviation in azimuthal angle. The phase is given by $k_{\phi}\phi$ where k_{ϕ} corresponds to the azimuthal wavevector of the "cold" cavity. In the radial direction, for excitation of the fundamental mode follows a $\cos(r)$ profile with the maximum corresponding to the core center. Similarly, for excitation of order 1 mode, the radial variation has a $\sin(r)$ profile with zero corresponding to the core center. Polarization in all cases is in the *z* direction (into the plane in Fig. 2). The source center frequency was chosen to coincide with the natural resonant frequency of the microring obtained using filter diagonalization [29]. In both normal and anomalous dis-



Fig. 2. Distribution of the electric field of a mode with a fundamental radial profile. The component of the field going into the plane (E_z) is shown. Red designates positive values; blue negative; white zero.



Fig. 3. (a) Dispersion parameter data for normal dispersion region of fundamental radial (order 0) profile modes; (b) the anomalous dispersion region of order 1 modes.

persion case $|A_s|$ was set to produce the uniform "cold" cavity mode of amplitude 5 (V/a). In normal dispersion case source frequency was set to f = 0.5916 (c/a) and in anomalous case it was set to f = 0.3618 (c/a) where c is the velocity of light and $a = 1 \,\mu$ m is a unit length (MEEP units). These frequencies correspond to the source wavelengths $\lambda = 1.69 \,\mu$ m and $\lambda = 2.76 \,\mu$ m respectively. In this paper, two source excitation regimes were studied: narrowband source with $\tau = 1000$ (a/c) and $\sigma = 0.1$ rad that mimic CW single frequency excitation and broadband source with $\tau = 12.02$ (a/c) and $\sigma = 0.01$ rad to explore pulse propagation in the microring. There are several ways to introduce dispersion in the microring systems, such as adding material dispersion or perturbing the geometry [30, 31]. In order to avoid significant losses associated with large material dispersion, materials were taken to be dispersion-free, with dispersion being introduced via geometry. Furthermore, refractive indices were chosen to restrict the number of modes excited in the ring. Cladding refractive indices were set to $n_{clad}^{norm} = 2.33$ and $n_{clad}^{anom} = 2$ (based on tantalum pentoxide) for normal and anomalous dispersion, with the core refractive index fixed at $n_{core} = 2.53$ (based on titanium dioxide). Geometric dispersion (Fig. 3) was derived from the frequencies of the resonant modes of the specific family obtained using harminv, a filter diagonalization MEEP program. The core material Kerr susceptibility was set to $X^{(3)} = 0.004 \ (a^2/W)$. Dimensions of the microring used in simulation correspond to $r = 40 \,\mu$ m (microring outer radius) and $w = 2 \,\mu$ m (core width).

Resonance number	Frequency	Q	Amplitude	Relative error
	(c/a)		(MEEP units)	
1	0.585039	401172	0.0330443	5.789262e-11
2	0.586622	415560	0.0788294	2.503092e-11
3	0.588206	431139	0.146794	1.336046e-11
4	0.58979	447318	0.213382	9.271911e-12
5	0.591374	463984	0.242161	8.396964e-12
6	0.592958	481228	0.214549	9.278247e-12
7	0.594541	499082	0.148396	1.434943e-11
8	0.596125	517695	0.0801344	2.530687e-11
9	0.597708	536495	0.0337884	5.216343e-11

Table 1. Resonant mode parameters from FDTD and Haminv used in CMT

Coupled mode theory parameters were chosen to match those used in the FDTD simulation. Table 1 lists parameters extracted from a "cold" cavity FDTD simulation using harminv for normal dispersion case analysis. As before, a Gaussian current source was used, with $\tau = 16.7$ (a/c) and a point-like spatial distribution. The interpolated CMT frequencies were set to match the linear dispersion slope obtained from harminv frequencies with dispersion approximated up to B_2 parameter. The number of coupled modes playing significant role in the time dynamics was determined to be N = 15 in the normal case and N = 9 in the anomalous case, by inspection. Alternatively, we can find the number of modes *a priori* by making an initial guess for the CMT simulation, and then refining this number, such that the energy contained in the modes on the extremities of the steady-state spectrum would be below predefined threshold (< 1% of the pump energy in our case). The normalized amplitude function was found using steady state single mode field distribution as $g_i(r) = E_i(r)/E_{max}$, while the coupling coefficient M_{ijkl} was computed by assuming perfect spatial mode overlap between modes (following Eq. (12)). The resulting system of governing equations has the following form:

$$\frac{da_i}{dt} = -i\omega_i a_i - i\frac{\hbar^2 \varepsilon_2}{2} \sqrt{\omega_i \omega_j \omega_k \omega_l} M_{ijkl} e^{i(\omega_k + \omega_l - \omega_i - \omega_j)t} a_j^{\dagger} a_k a_l + s,$$
(19)

with the source term *s* given by:

$$s = E_{s} e^{-(t-t_{o})^{2}/2\tau^{2}} e^{i\omega_{s}t}$$
⁽²⁰⁾

where ω_s is the pump frequency, E_s is the pump amplitude and $\hbar = 1$ in all simulations. The resulting system of coupled differential equations was solved using the ode15s stiff ODE solver in MATLAB.

In order to directly compare FDTD results to CMT simulations, the electrical field E_z in FDTD was sampled at a single point, and compared to a sum of the cavity mode fields in the CMT simulation. The sampling location in FDTD was set at the point inside the microring core corresponding to the maximum of the radial mode profile (Fig. 1), 45° away from the source center. The resolution of the simulation was set to be 40 grid points / μ m (i.e., a grid spacing of 25 nm).



Fig. 4. Comparison of FDTD and CMT results for the normal dispersion case: (a) FDTD time domain; (b) CMT time domain; (c) FDTD frequency domain; and (d) CMT frequency domain.

4. Results and discussion

In this part of the manuscript, we show that our expectations of comb generation dynamics are confirmed with direct finite-difference time domain simulation, and show the corresponding coupled-mode theory simulations that corroborate our prior observations.

We can observe a close correlation between the FDTD and CMT simulations performed using narrowband excitation, from perspectives in the time domain in Figs. 4(a), 4(b), 5(a), and 5(b), as well as perspectives in the frequency domain in Figs. 4(c), 4(d), 5(c), and 5(d). In particular, the time domain envelopes of the CMT and FDTD simulations match very well with key features such as self-phase modulation induced initial peak and beat tones corresponding to round trip times in the cavity. The shapes of the periodic pulses are also closely matched in both cases. The low frequency beat tone present in the FDTD anomalous simulation shown in Fig. 5(a) is due to the coupling of the source having a mode 1 spatial profile to the mode 0 family. This coupling could not be completely eliminated in the anomalous case, as the two modes nearly coincide in frequency and propagation of mode 0 is allowed. In the normal case, we were able to prohibit mode 1 propagation by increasing the cladding index; hence, no lowfrequency beat tones were observed there.

As far as the frequency domain, the graphs can be seen to match well in terms of their bandwidth and frequency spacing. However, the FDTD simulation show a slight asymmetry in its frequency spectrum compared to CMT. We can again observe the effects of undesirable coupling in anomalous case seen as lowering of the FDTD spectral amplitude compared to CMT shown in Figs. 5(c) and 5(d), as some energy is channeled into the mode 0 family.



Fig. 5. Comparison of FDTD and CMT results for the anomalous dispersion case: (a) FDTD time domain; (b) CMT time domain; (c) FDTD frequency domain; and (d) CMT frequency domain.

We further investigate the root cause of the observed asymmetry in the spectrum shape. Taking advantage of the CMT ability to separate different nonlinear coupling mechanisms, we perform the time domain envelope comparison of FDTD with CMT selectively disabling different CMT coupling channels (Fig. 6). We compare simulations done using the full CMT approach, CMT with only self-phase modulation (SPM) terms included, and CMT with both SPM and cross-phase modulation (XPM) terms included. For the steady state region (t > 6000), the full CMT simulation provides the best match with FDTD, since it does not omit any terms. On the other hand, the SPM envelope is constant and SPM+XPM envelope modulation is significantly reduced, reflecting the fact that energy transfer to the sideband modes is inhibited. For the initial FDTD transient, a CMT simulation with only SPM provides a very good match, while CMT with both SPM and XPM quenches the initial peak. This implies that magnitude of XPM interactions in FDTD is reduced from those in CMT in the initial phase. To explain this observation, we can further note that the onset of CMT XPM interactions occurs as the envelope of the source starts to flatten - i.e., where the Gaussian input waveform reaches its peak. Indeed, when the Gaussian reaches its maximum value the amplitudes and consequently the frequencies of the sideband modes are stabilized and coupling with the pump mode will occur. It can be observed as quenching of the initial envelope As shown in Fig. 6(a): in the SPM+XPM case, labeled as CMT.SPM+XPM, and the full CMT case, labeled as CMT. However, in FDTD microring systems, the source pulse must travel around the microring. As a result, the stabilization does not take place everywhere simultaneously, but rather is reached gradually, leaving the initial transient unperturbed, as shown in Fig. 6(a) and labeled as FDTD. It seems feasible to design a more complex excitation procedure that will emulate the effects described above, if



Fig. 6. Time domain envelopes of different coupling and excitation regimes in FDTD and CMT: (a) Comparison of FDTD and CMT envelopes for different coupling mechanisms: (solid blue) FDTD results, (solid red) CMT results, (dashed black) CMT results with only self-phase modulation (SPM) terms, (dotted green) CMT results with only SPM and cross-phase modulation (XPM) terms, (solid cyan) amplitude scaled source transient; (b) Comparison of FDTD and CMT for different excitation regimes: (dotted green) uniform source, (solid red) source with $\sigma = 3.14$, (solid black) CMT results with only SPM terms and $\sigma = 0.1$.

one would like to achieve greater accuracy in the frequency domain.

As an alternative, a natural course of action would be to attempt to use an FDTD source with a spatially uniform envelope. Figure 6(b) shows the results for sources with uniform distribution (no angular variation) and source with angular standard deviation $\sigma = 3.14$ rad. Same as before the amplitudes we set to produce 5 (V/a) uniform "cold" cavity mode amplitude; the source bandwidth and nonlinear coefficient were held the same. Compared to the previous simulation in Figure 6(a) having $\sigma = 0.1$ rad, comb formation is strongly inhibited, suggesting that the uniform source does not produce enough intermode coupling to generate a comb from a single pump line, and that nonuniform "seeding" similar to modulation instability onset is required. In theory, spontaneous emergence of the modes with the uniform source can be achieved by properly setting the noise floor, but we anticipate that in that case obtained spectrum would be even more difficult to predict. This assumption will have to be verified in future work.

Overall, in all cases, the simulation times can be dramatically reduced by going from FDTD to CMT simulations. It took approximately 5 hours with 48 cores to run the FDTD simulation in MEEP on the Purdue University Rosen Center for Advanced Computing's Carter Community Cluster [32]. Note that the simulation was performed on 2D system with the infinite third dimension. For the full 3D system, the simulation time would be further multiplied. In the 2D case, MEEP scales well for this problem up to 48 cores and beyond - i.e., the number of corehours consumed is not strongly dependent on the number of cores used. However, the CMT simulation with our current MATLAB implementation only took 20 minutes as a serial process (single-core) on an Asus desktop machine. This represents a decrease in CPU core-hours by a factor of 720, or equivalently, 2.86 orders of magnitude. These results thus demonstrate a clear advantage in using the CMT method versus a fully vectorial approach. In future work, it would be desirable to achieve an even greater degree of improvement through fine-tuning of the ODE solution technique embedded in MATLAB. Subsequent topics for investigation may then include detailed exploration and optimization of microresonator comb design as a function of experimental parameter values, assuming modest nonlinear coefficients. A search technique such as this could enable a broad range of customized applications for these combs, which



Fig. 7. (a) Dispersion parameter data for order 0 modes (dotted blue) having normal dispersion and order 1 modes (solid red) with anomalous dispersion; (b) Field profile of the traveling pulses corresponding to order 0 modes and order 1 modes. All simulations were performed in the "cold" cavity.

may include but would not be limited to: signal and idler pair generation at arbitrary, targeted frequencies; enhanced third-harmonic generation; efficient terahertz generation; and arbitrary waveform generation.

5. Nonlinear phenomena in microring resonators

So far our discussion has been mainly focused on nonlinear interaction of the modes under narrowband excitation conditions. We can now consider nonlinear phenomena enabled by modes having broadband excitation and further expand on the theory of nontrivial selection rule dynamics during frequency comb formation.

One particularly intriguing nonlinear phenomenon is the bright temporal soliton, which can be excited in the waveguide system by appropriately balancing anomalous dispersion and nonlinearity by adjusting the amplitude and time duration of the traveling pulse [33, 34]. Considering a microring as a perturbed waveguide system and applying the same discussion we were able to predict existence of the soliton-like propagation for selected modes of the system. In order to confirm this, we used FDTD and CMT to analyze pulse propagation for the set of modes of radial order 1. Figure 7(a) displays in solid red the dispersion parameter plot for this family of modes. Figures 7(b) and 8 illustrate field profiles of the pulses and point field data corresponding to both families of modes simultaneously propagating in the "cold" cavity microring. Note from these plots that the pulses of different mode families have distinctly different group velocities allowing their temporal and spacial separation in the analysis. Figure 9(a) shows the results for FDTD mode 1 pulse evolution as it propagates in the microring generated using broadband source excitation. Both "cold" cavity case and the case of cavity with appropriate amount of Kerr nonlinearity were considered. Similarly, we performed CMT simulations using 59 coupled modes with the same set of parameters to emulate pulse propagation, as shown in Fig. 9(b). In order to further reduce CMT computational time, we implemented slow varying envelope approximation for these simulations. Results show a good match of pulse propagation dynamics in both linear and nonlinear case. In both FDTD and CMT cases, the spreading of the pulse due to dispersion is reduced when nonlinearity is added, confirming soliton-like behavior. For these simulations parameters were calculated according to [33] for fundamental soliton mode; nonlinear susceptibility was set to $X^{(3)} = 0.004 (a^2/W), \tau = 12.02(a/c)$, group velocity dispersion parameter $B_2 = -0.019 (a/c^2)$ and $|A_s| = 0.135 (V/a)$.



Fig. 8. (a) Time domain traveling pulses in the "cold" microring cavity with an order 1 source profile. (b) Corresponding frequency domain data, showing that the broadband excitation spectrum excites both order 0 and order 1 modes.



Fig. 9. Evolution of the propagating pulse in the cases of zero and $X^{(3)} = 0.004$ Kerr nonlinearity: (a) FDTD calculation (b) corresponding CMT simulation. A good match is observed. In both cases, pulse spreading is dramatically suppressed with appropriate level of nonlinearity, much like in a soliton.

Another phenomenon where pulse propagation in microring cavity plays an important role is the frequency comb dynamics, in particular formation of the Type II frequency combs. Type II is considered an undesirable path of frequency comb formation that appear along the lines of conventional Type I and it has been a subject of number of studies in the recent literature [10, 16]. In this research it has been confirmed that the Type II frequency comb is associated with formation of subcombs at multiple FSR (Δ) from the pump line. Frequencies of the lines in Type II combs can be described by the formula [16]:

$$\omega_n^i = \omega_p + \xi_i + n\sigma, \ n = 0, \pm 1, \pm 2...$$
 (21)

where *i* is a subcomb index σ is a cavity FSR, ω_p is a pump frequency and ξ_i is a frequency offset which arises due to *k*-conservation rules in the dispersive medium. We note that while the lines within a subcombs are separated by a single FSR, the spacing of different subcombs is governed by dispersion.

We would like to suggest a novel step-by-step mechanism of Type II comb formation and

offer methods for mitigating and eliminating Type II comb excitation. It is instructive to consider single modes and pulses in the "cold" microring cavity. On one hand, single modes that are uniform in space, similar to the one shown in Fig. 2, are constrained by azimuthal boundary conditions and therefore k-conservation rules. On the other hand, it can be seen from the field point data in Figs. 7(b) and 8(a) that traveling pulses remain localized in time and space, and hence are not subject to azimuthal boundary conditions. When the first four-wave mixing event occurs during Type II comb formation, energy from the uniform bound pump mode transfers to a signal and idler pair, following k-conservation rules. This event transforms single mode field distribution in the cavity into a modulated field with period $1/\Delta$. At the same time, a dispersion-induced frequency offset ξ_i will create a low frequency modulation and thus a pulselike periodic train. As this pulse-like waveform propagates, it will compress due to nonlinear interaction similar to soliton formation described above resulting in a localized pulse. For this pulse, azimuthal k-conservation rules are lifted, and the corresponding spectrum will be single FSR spaced. This produces frequency comb line spacings described by Eq. (21). The presented mechanism may explain why there are no consecutive multi-FSR combs in the spectrum (that is why a comb spectrum can have only single value of Δ), as the modes are constrained by the azimuthal k-matching only once, in the beginning of the comb formation. Therefore, based on the proposed comb formation dynamics, the most straightforward way to obtain a reproducible type I comb is a short-pulse pumping (e.g., with an ultra-fast laser) that will not be governed by azimuthal k-matching. Such pumping can occur with a period that is an integer multiple of the round trip of the resonator, which would allow for practical low frequency excitation approaches. Alternatively, one could design a ring structure that would no longer enforce the initial k-conservation condition (e.g., with significant sidewall scattering).

6. Conclusion

In this work, we studied the emerging class of on-chip microresonator-based nonlinear optical phenomena. We began our analysis with frequency comb formation, to which we applied powerful framework of coupled-mode theory derived rigorously from basic quantum mechanical principles in the presence of a finite number of weakly-coupled modes. In principle, it enabled us to quickly analyze millions of interactions by reducing them to the smallest reasonable number of degrees of freedom, which can be individually adjusted for each problem. At the same time, we demonstrated that we can implement this theory via direct simulation of experimental designs, to avoid ad hoc selection of parameter values in the coupled mode theory analysis. It was shown that the results of the hybrid CMT/FDTD and FDTD simulations match each other fairly closely. The exceptions to perfect matching are due to cross-coupling of FDTD excitation and imperfect initial condition matching. The approach can be used to examine the generation of optical combs in the presence of dispersion (both normal and anomalous), and our studies showed that comb generation from the single pump line is still permitted in both cases. Furthermore, the number of CPU core-hours required for the CMT simulation is reduced by a factor of 720 compared to the FDTD simulation, and may be amenable to further reduction. This significant speed-up should enable comprehensive automated design and optimization studies to achieve microresonator combs with tailored properties. Analyzing nonlinear pulse propagation phenomena in the same system, we demonstrated formation of the soliton-like pulses in higher order radial modes using both FDTD and CMT approaches, and presented a new mechanism for Type II frequency comb formation. This new computational framework can be leveraged for analyzing important optical applications of nonlinear phenomena in photonic crystals, plasmonics and metamaterials. Our approach can also be transferred to the analysis of weakly coupled system with nontrivial mode distribution and coupling, such as random lasers, nonlinear plasmonics, higher harmonic generation, ultrafast pulse shaping, and quantum photonics.

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