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Extracting Large Quality Factors in Photonic Crystal Double Heterostructure Cavities Using the Padé Method

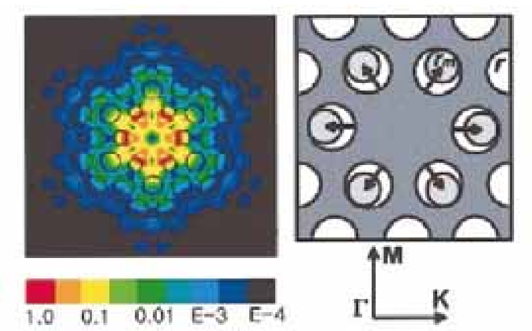
Adam Mock and John O'Brien

University of Southern California
Microphotonic Device Group

September 2, 2008
NUSOD - TuB3

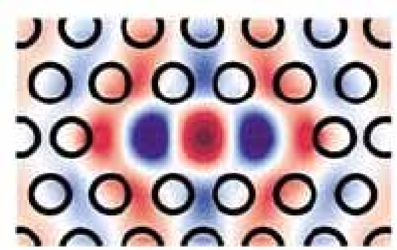
High quality factor photonic crystal cavities

D1 cavity, Q ~ 10^6



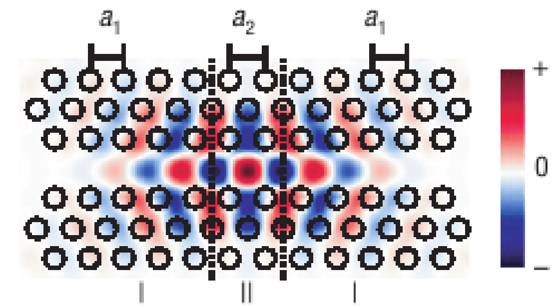
H. Y. Ryu, M. Notomi, Y. H. Lee Appl. Phys. Lett. **83** 4294 2003

L3 cavity, Q ~ 10^5



Y. Akahane, T. Asano, B.-S. Song, S. Noda Nature **425** 944 2005

PCDH cavity, Q ~ 10^6-10^9



B.-S. Song, S. Noda, T. Asano, Y. Akahane Nature Materials **4** 207 2005

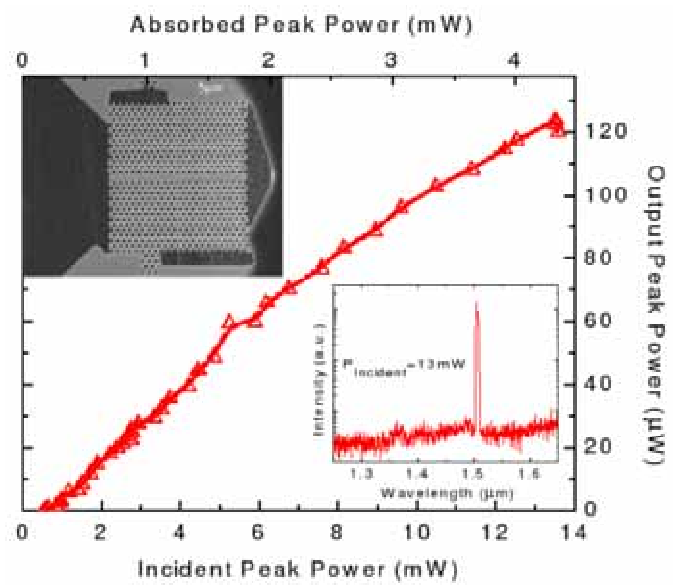
Biological and chemical sensors

Slow light (optical memory and buffers)

Lasers and filters for chip-scale photonic integration

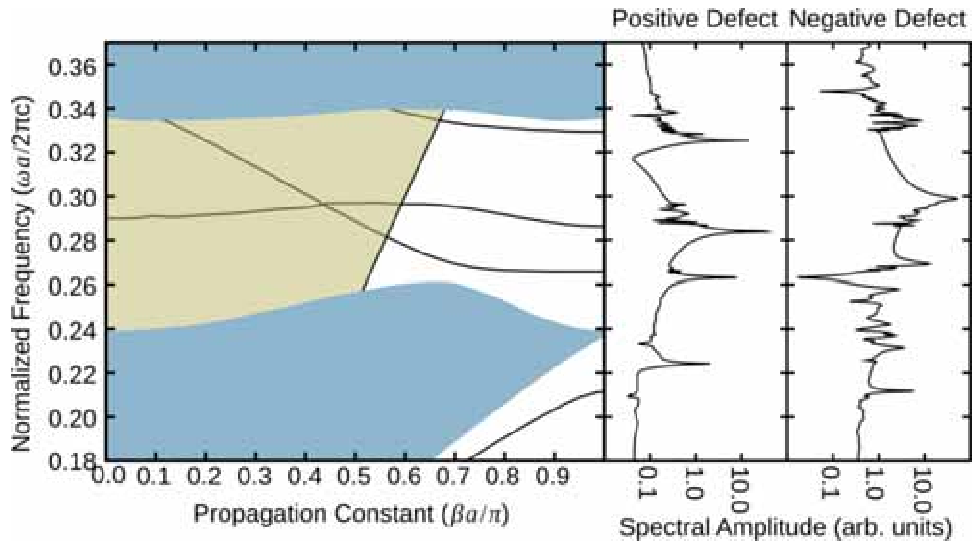
Photonic crystal double heterostructure lasers and cavities

>100μW edge-emitting output power



L. Lu, A. Mock, J. O'Brien, *et al*.
CLEO paper CMV3 (2007).

bound state formation near dispersion extrema



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Presentation outline

Finite-Difference Time-Domain numerical simulation technique

Optical loss in photonic crystal resonant cavities

Discrete Fourier transform + Padé interpolation method for quality factor estimation

Application to photonic crystal double heterostructure cavities

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Finite-difference time-domain analysis of photonic crystal resonant cavities

Discretized spatial derivatives

$$\frac{\partial D_x^{i,\,j+1/2,\,k+1/2}}{\partial t} = \frac{1}{\Delta y}\left(H_z^{i,\,j+1,\,k+1/2} - H_z^{i,\,j,\,k+1/2}\right) - \frac{1}{\Delta z}\left(H_y^{i,\,j+1/2,\,k+1} - H_y^{i,\,j+1/2,\,k}\right)$$

$$\frac{\partial B_x^{i-1/2,\,j+1/2,\,k+1}}{\partial t} = \frac{1}{\Delta z}\left(E_y^{i-1/2,\,j+1,\,k+3/2} - E_y^{i-1/2,\,j+1,\,k+1/2}\right) - \frac{1}{\Delta y}\left(E_z^{i-1/2,\,j+3/2,\,k+1} - E_z^{i-1/2,\,j+1/2,\,k+1}\right)$$

Discretized time derivatives

$$\frac{\partial D_x^{i,\,j+1/2,\,k+1/2}}{\partial t} = \left[\varepsilon\,\frac{E_x^{n+1/2} - E_x^{n-1/2}}{\Delta t}\right]^{i,\,j+1/2,\,k+1/2}$$

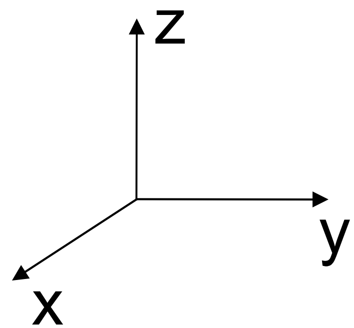
$$\frac{\partial B_x^{i-1/2,\,j+1,\,k+1/2}}{\partial t} = \left[\mu\,\frac{H_x^{n+1} - H_x^{n}}{\Delta t}\right]^{i-1/2,\,j+1,\,k+1/2}$$

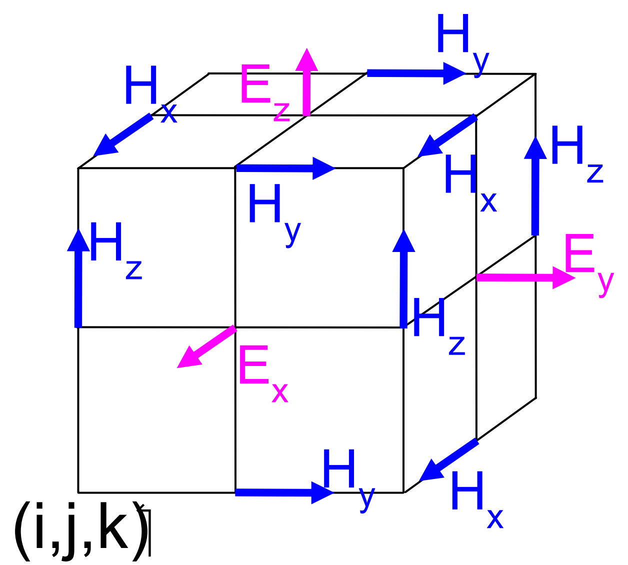
FDTD simulation parameters

$$\Delta t \le \frac{\Delta x}{c\sqrt{3}} \qquad \Delta t = 0.87\,\frac{\Delta x}{c\sqrt{3}}$$

$$\Delta x = \frac{a}{20}$$

Effectively 40 samples per lattice constant

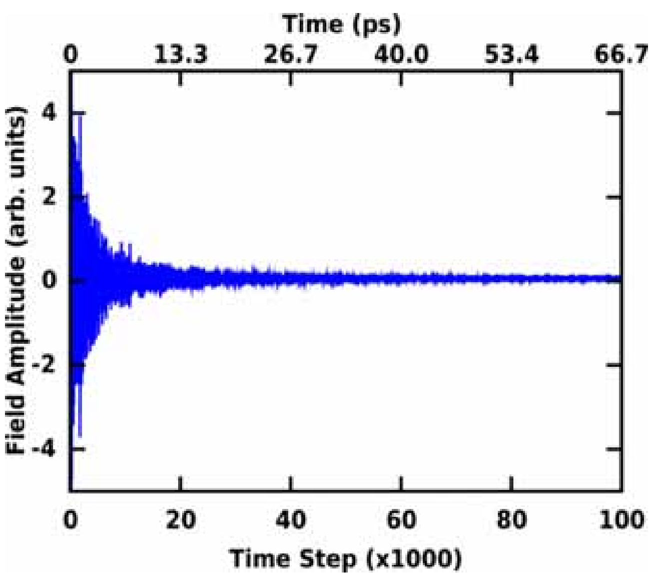




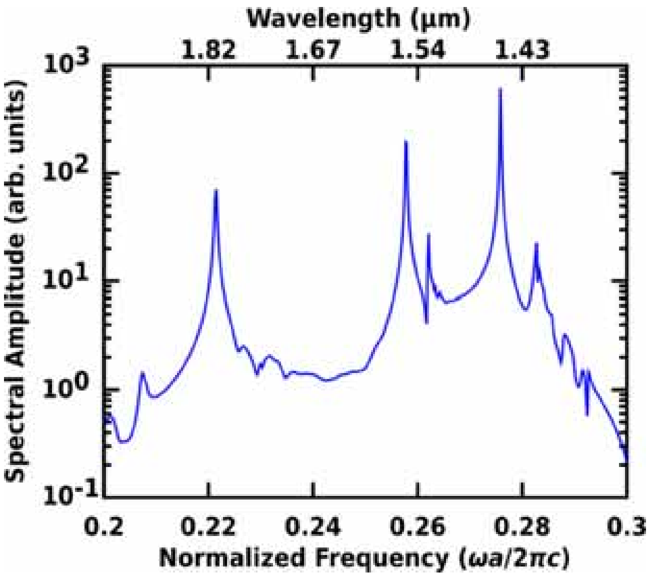
Numerical analysis method

- Broadband initial condition to excite all cavity resonances
- Propagate the fields in time for 10^5 FDTD time steps
- 15 layers of PML on all boundaries to absorb leaky radiation from the cavity
- Spectral analysis using discrete Fourier transform on resulting time sequence

Time Sequence



DFT of Time Sequence



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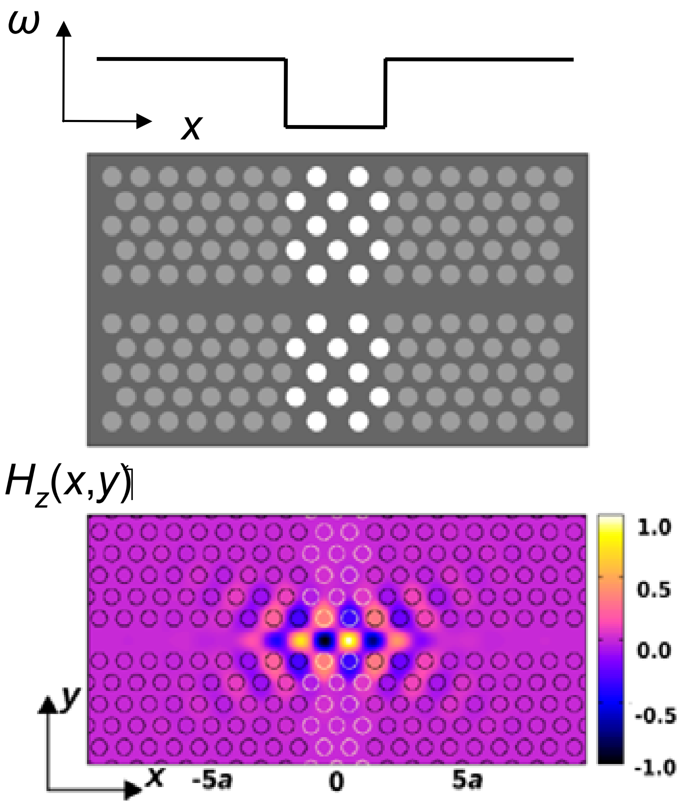
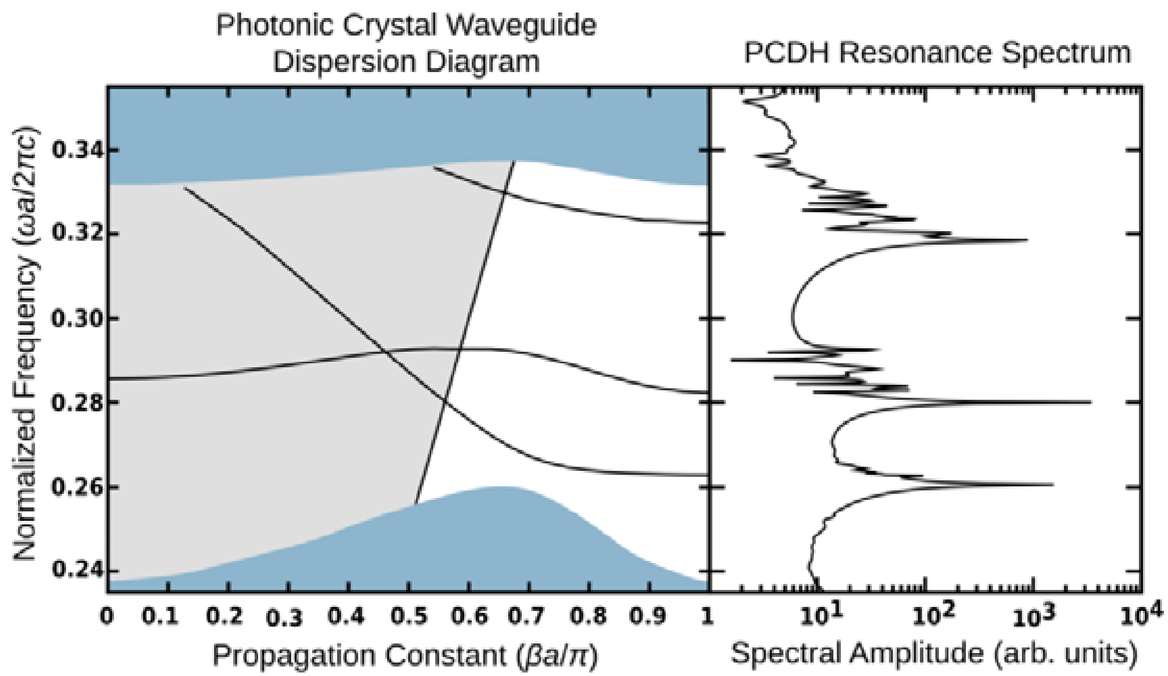
Photonic crystal double heterostructure resonant cavities

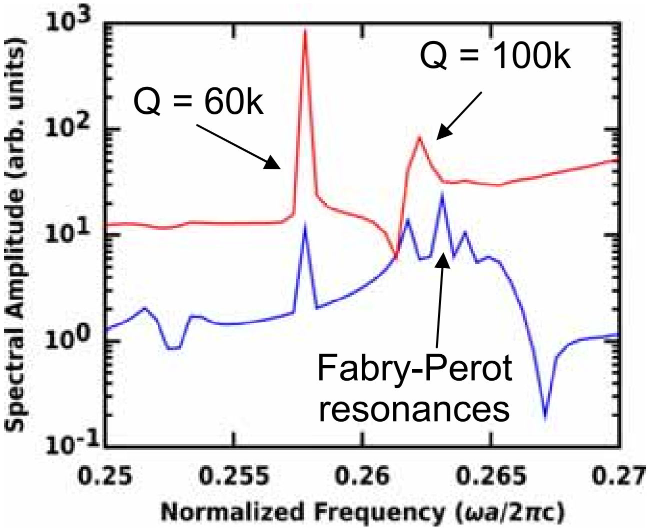


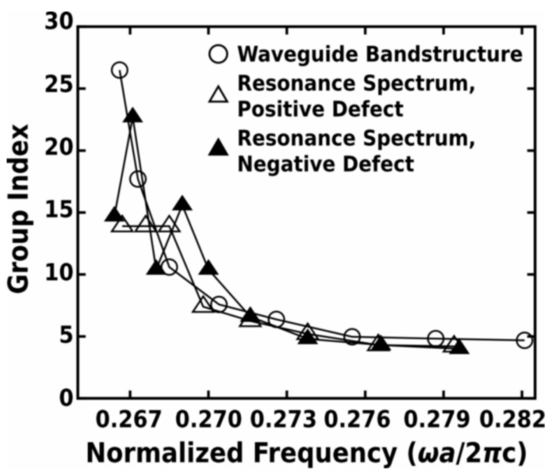


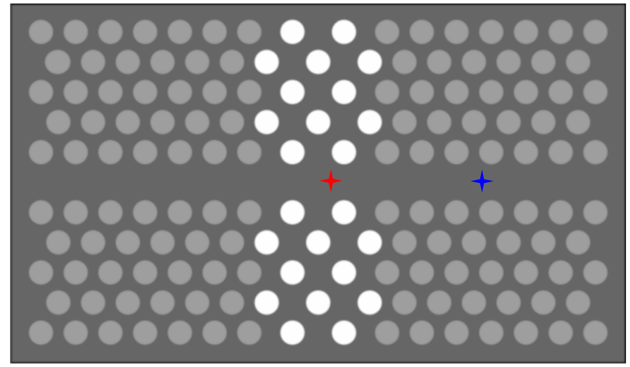
20 PCWG periods each side
8 PC rows top and bottom

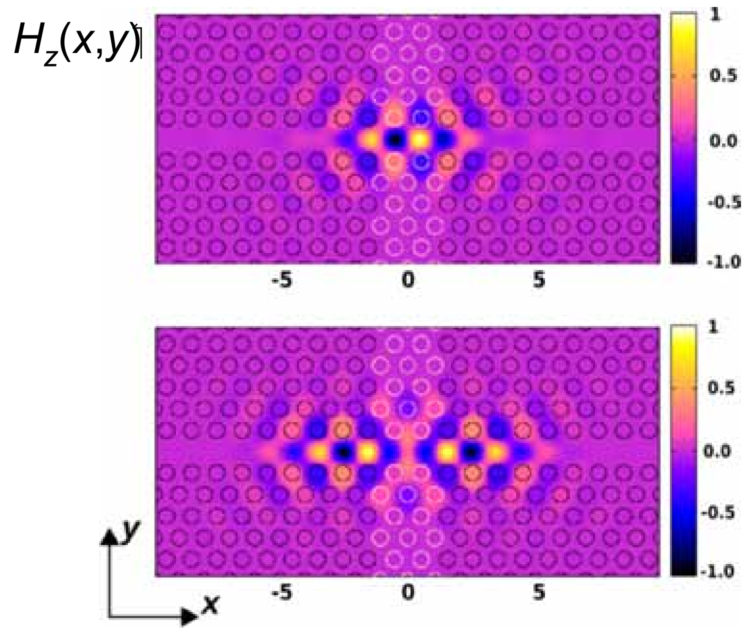
<u>Computational resources</u>
950 x 340 x 200 spatial points
100 processors
20 hours for 200k time steps

Photonic crystal double heterostructure: Free spectral range









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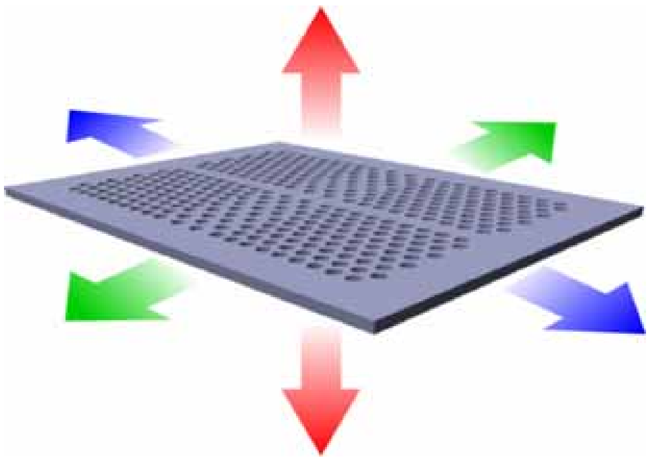
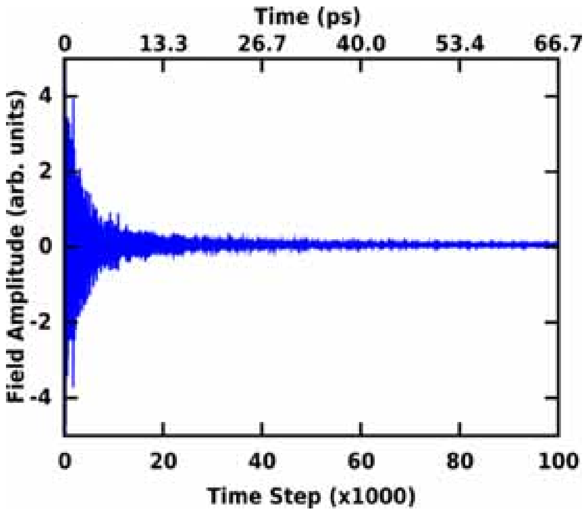
Leakage mechanisms in PCDH cavities

Out-of-plane: wavevector components not totally internally reflected
In-plane: finite number of photonic crystal cladding periods
finite number of photonic crystal waveguide periods





20 PCWG periods each side
8 PC rows top and bottom

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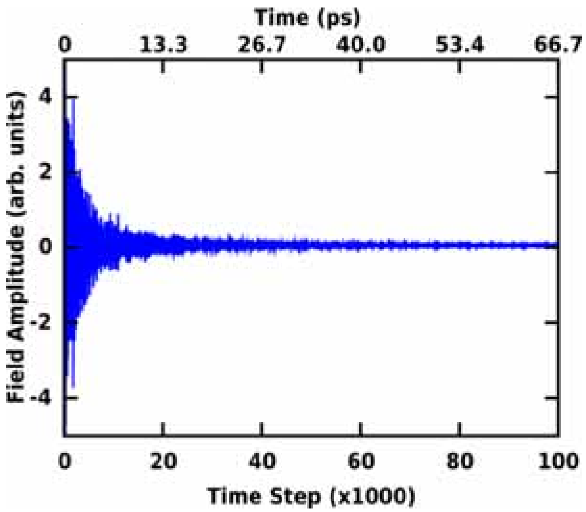
P(out-of-plane) / P(in-plane) = 1.8

P(waveguide) / P(pc cladding) = 0.2

Methods of calculating the quality factor

- Physical definition of *Q*

$$Q = \omega_0 \frac{\langle U \rangle}{\left\langle \frac{dU}{dt} \right\rangle}$$



- Damped cosine time function (Filter Diagonalization)

$$f[n] = f_0 e^{-\omega_0 n\Delta t / 2Q} \cos(\omega_0 n \Delta t)$$

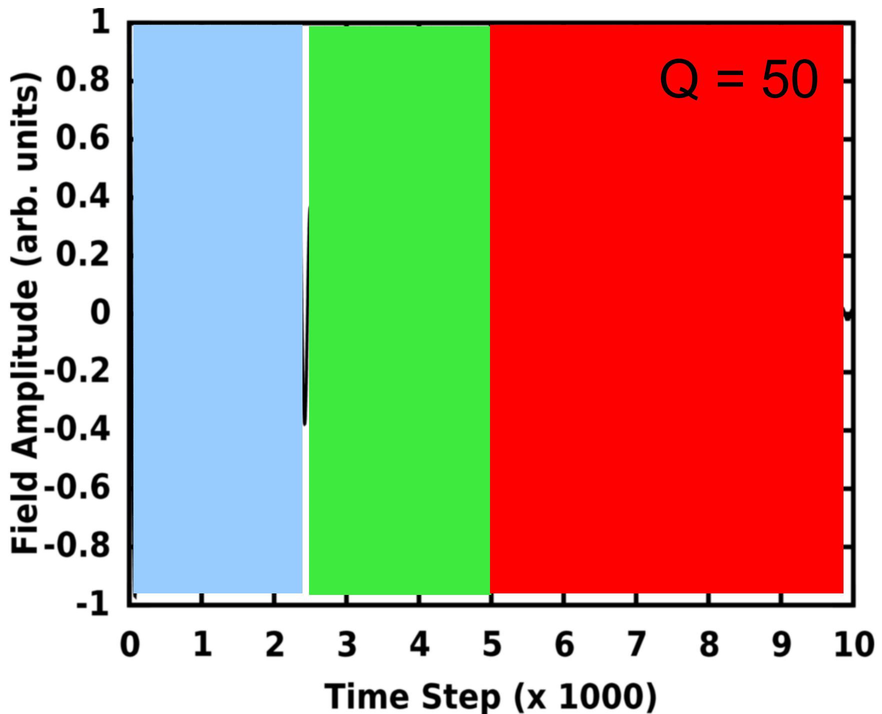
- Fourier transform is a Lorentzian function (Padé interpolation)

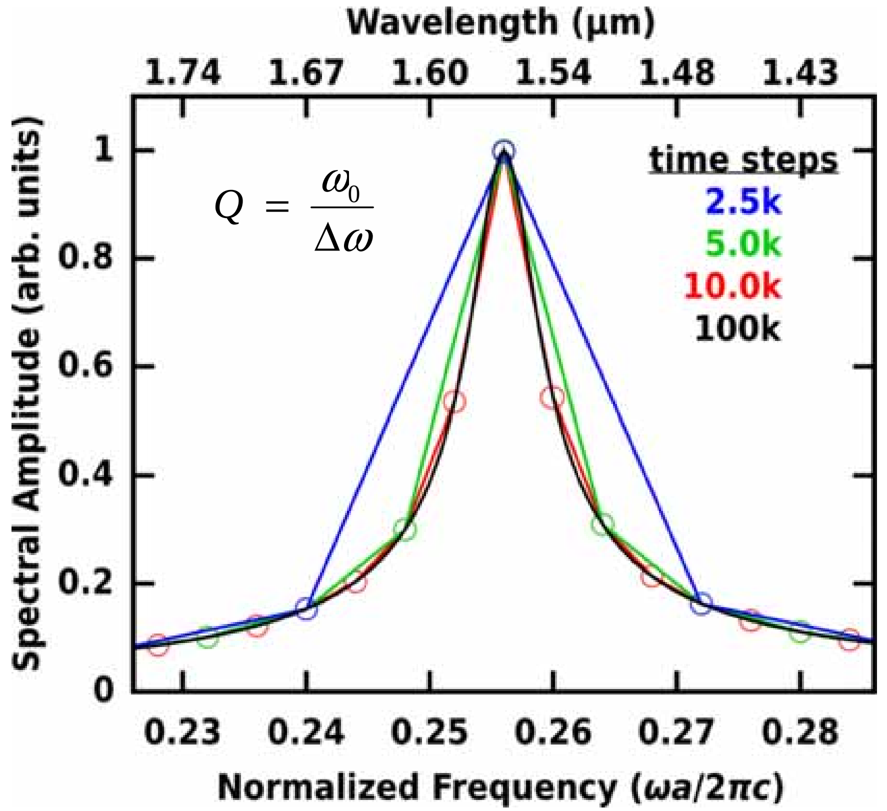
$$F(\omega) = \frac{f_0 / 2}{\frac{\omega_0}{2Q} - i(\omega - \omega_0)} \Rightarrow Q = \frac{\omega_0}{\Delta\omega}$$

Discrete Fourier transform resolution

$$\Delta f = \frac{1}{N\Delta t}$$

$$f[n] = f_0 e^{-\omega_0 n\Delta t/2Q}\cos(\omega_0 n\Delta t)$$





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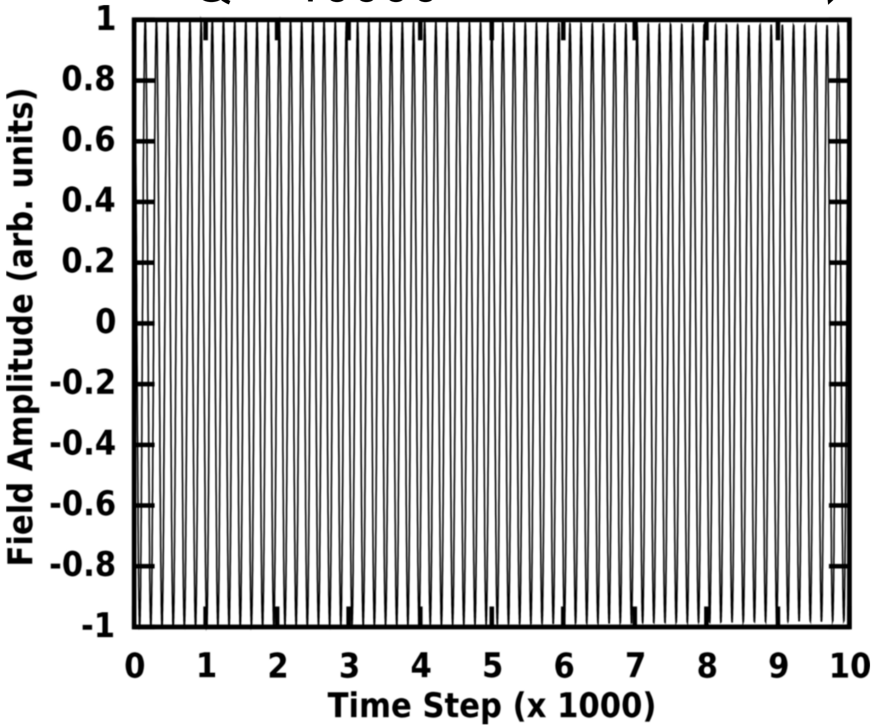
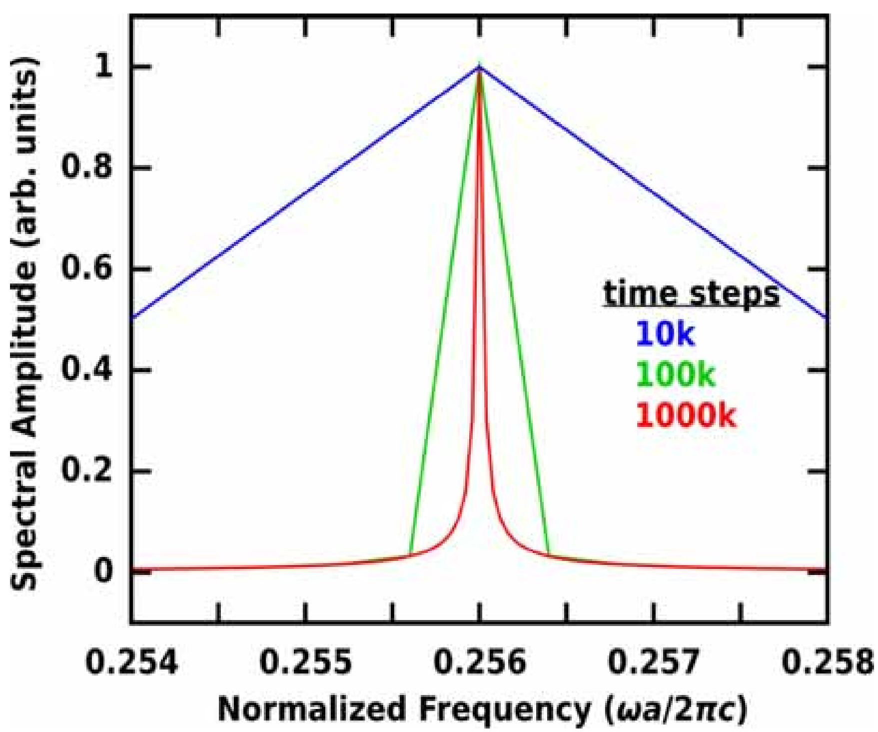
Discrete Fourier transform resolution

amplitude decreased to 0.98
after 10k time steps

Q = 10000





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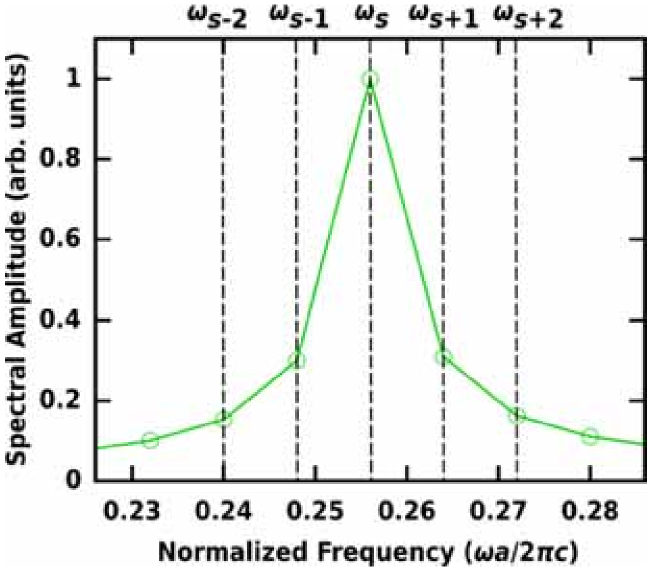
Padé interpolation method

$$\frac{\alpha_0 + \alpha_1\omega_s + \alpha_1\omega_s^2 + \cdots + \alpha_M\omega_s^M}{\beta_0 + \beta_1\omega_s + \beta_1\omega_s^2 + \cdots + \beta_N\omega_s^N} = \frac{Q_M(\omega_s)}{D_N(\omega_s)} = F(\omega_s)$$



where $\omega_s = s\Delta\omega$ is the *s*th DFT frequency sample

setting $\beta_0 = 1$ and multiplying both sides by the denominator yields

$$\alpha_0 + \alpha_1\omega_s + \alpha_1\omega_s^2 + \cdots + \alpha_M\omega_s^M = F(\omega_s)\left(1 + \beta_1\omega_s + \beta_1\omega_s^2 + \cdots + \beta_N\omega_s^N\right)$$

$$\alpha_0 + \alpha_1\omega_s + \alpha_1\omega_s^2 + \cdots + \alpha_M\omega_s^M - F(\omega_s)\left(\beta_1\omega_s + \beta_1\omega_s^2 + \cdots + \beta_N\omega_s^N\right) = F(\omega_s)$$

M+1 *α*-terms and N *β*-terms

linear equation with M+N+1 unknowns which requires M+N+1 DFT frequency samples for a unique solution

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S. Dey and R. Mittra, IEEE Microwave and Guided Wave Letters **8** 415 (1998)

Padé interpolation method for Lorentzian lineshapes

General Padé function

$$P(M,N)=\frac{Q_M(\omega_s)}{D_N(\omega_s)}=\frac{\alpha_0+\alpha_1\omega_s+\alpha_1\omega_s^2+\cdots+\alpha_M\omega_s^M}{\beta_0+\beta_1\omega_s+\beta_1\omega_s^2+\cdots+\beta_N\omega_s^N}$$

Damped cosine time function has Lorentzian function Fourier transform

$$f[n]=f_0e^{-\omega_0 n\Delta t/2Q}\cos(\omega_0 n\Delta t) \Longleftrightarrow F(\omega)=\frac{f_0/2}{\frac{\omega_0}{2Q}-i(\omega-\omega_0)}$$

Padé function corresponding to Lorentzian form

$$P(0,1)=\frac{\alpha_0}{1+\beta_1\omega}=\frac{-i\alpha_0/\beta_1}{-i/\beta_1-i\omega}=\frac{-i\alpha_0/\beta_1}{-i/\beta_1-i\omega_0-i(\omega-\omega_0)}$$

$$\boxed{-i/\beta_1-i\omega_0=\frac{\omega_0}{2Q}}$$

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Padé convergence – user defined time sequence

$$-i/\beta_1 - i\omega_0 = \frac{\omega_0}{2Q}$$

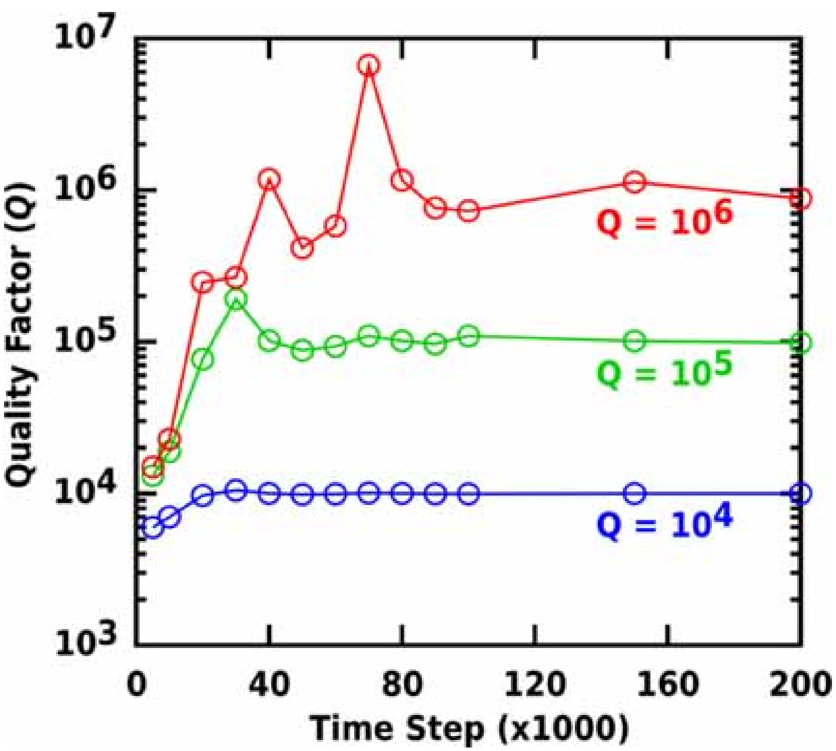
$$1/\beta_1 + \omega_0 = i\frac{\omega_0}{2Q}$$

complex number — real number — imaginary number

$$\mathrm{Re}[1/\beta_1] = -\omega_0$$

$$\mathrm{Im}[1/\beta_1] = \frac{\omega_0}{2Q}$$

$$\Rightarrow \quad Q = \frac{-\mathrm{Re}[1/\beta_1]}{2\,\mathrm{Im}[1/\beta_1]}$$



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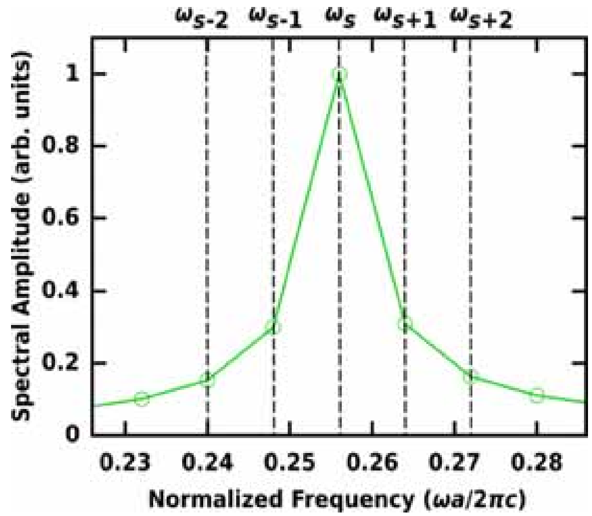
Padé convergence – user defined time sequence

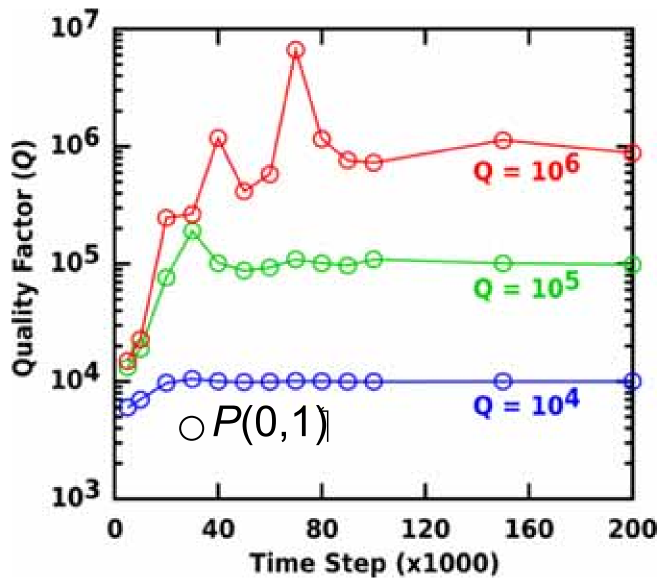
For $P(0,1)$, the Padé method requires M+N+1 = 0 + 1 + 1 = 2 DFT frequency samples for a unique solution

For $P(1,1)$, the Padé method requires M+N+1 = 1 + 1 + 1 = 3 DFT frequency samples for a unique solution

$$P(1{,}1) = \frac{\alpha_0 + \alpha_1\omega}{1+\beta_1\omega} = \frac{\alpha_1}{\beta_1} + \frac{\alpha_0 - \alpha_1/\beta_1}{1+\beta_1\omega}$$

$$\mathrm{Re}[1/\beta_1] = -\omega_0 \qquad \mathrm{Im}[1/\beta_1] = \frac{\omega_0}{2Q} \quad \Rightarrow \quad Q = \frac{-\mathrm{Re}[1/\beta_1]}{2\,\mathrm{Im}[1/\beta_1]}$$





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Padé convergence – user defined time sequence

For $P(0,1)$, the Padé method requires
M+N+1 = 0 + 1 + 1 = 2 DFT frequency samples
for a unique solution

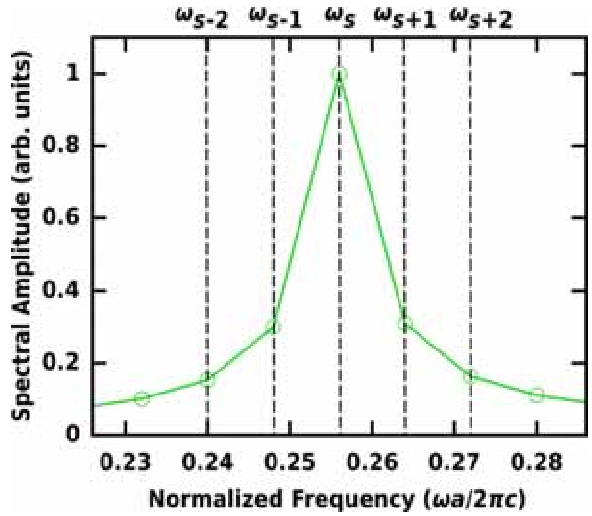
For $P(1,1)$, the Padé method requires
M+N+1 = 1 + 1 + 1 = 3 DFT frequency samples
for a unique solution

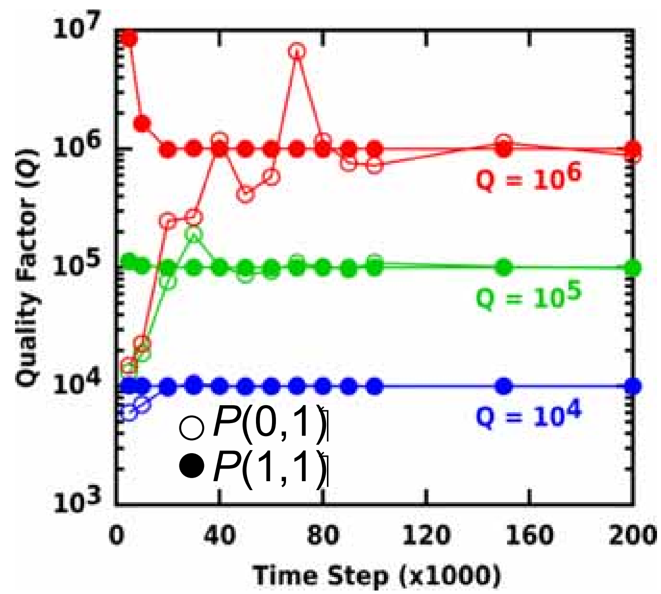
$$P(1,1) = \frac{\alpha_0 + \alpha_1 \omega}{1 + \beta_1 \omega} = \frac{\alpha_1}{\beta_1} + \frac{\alpha_0 - \alpha_1 / \beta_1}{1 + \beta_1 \omega}$$

$$\mathrm{Re}[1/\beta_1] = -\omega_0$$

$$\mathrm{Im}[1/\beta_1] = \frac{\omega_0}{2Q}$$

$$\Rightarrow \quad Q = \frac{-\mathrm{Re}[1/\beta_1]}{2\,\mathrm{Im}[1/\beta_1]}$$





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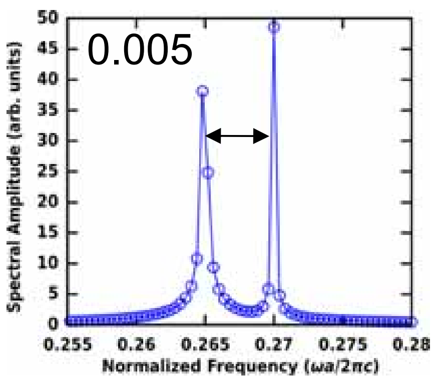
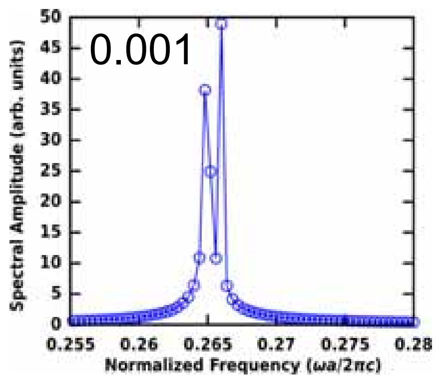
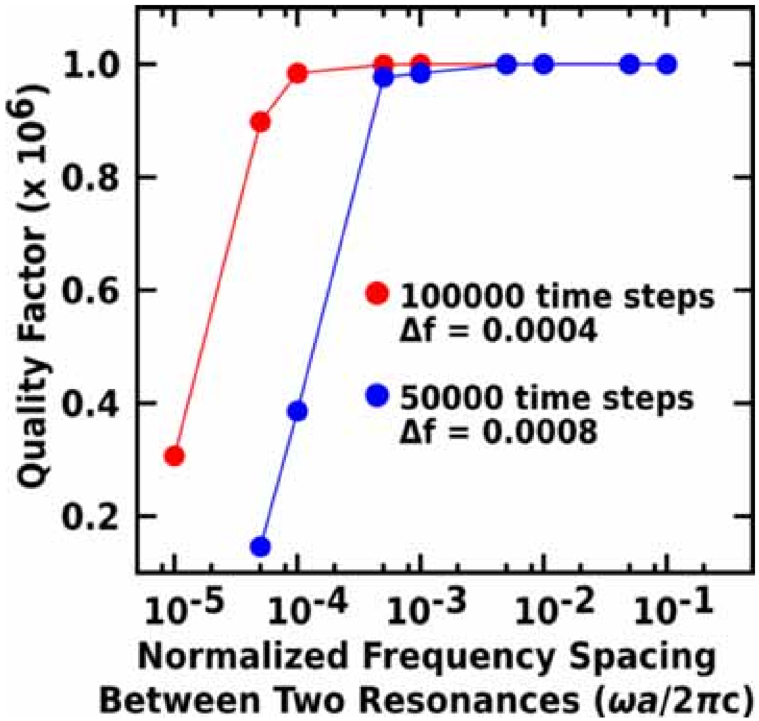
Padé convergence – user defined time sequence with two resonances

$$P(2,2)=\frac{\alpha_0+\alpha_1\omega+\alpha_2\omega^2}{1+\beta_1\omega+\beta_2\omega^2}=\frac{\alpha_2}{\beta_2}+\frac{\alpha_0+\alpha_1-\frac{\alpha_2}{\beta_2}-\frac{\alpha_2\beta_1}{\beta_2}\omega}{1+\beta_1\omega+\beta_2\omega^2}$$

$$P(2,2)=\frac{\alpha_2}{\beta_2}+\frac{C_1}{\frac{\omega_1}{2Q_1}-i(\omega-\omega_1)}+\frac{C_2}{\frac{\omega_2}{2Q_2}-i(\omega-\omega_2)}$$







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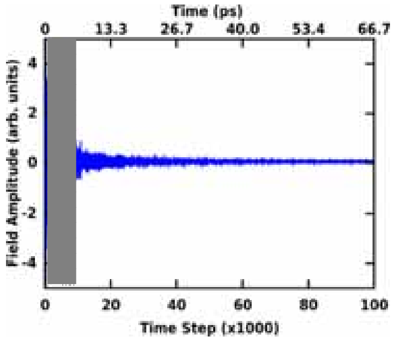
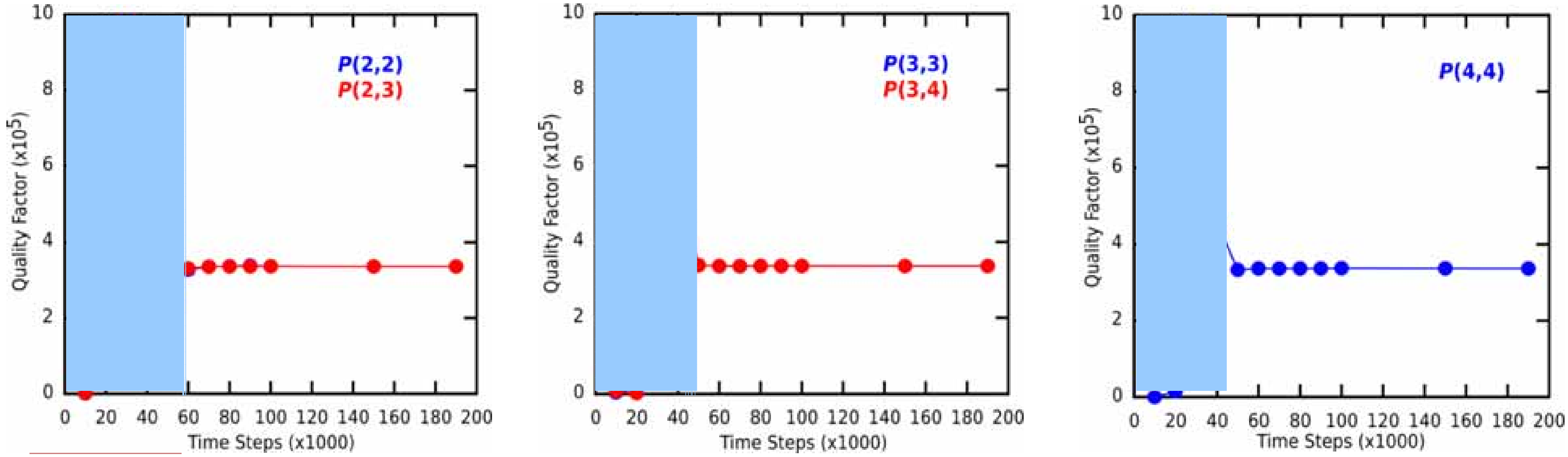
Padé convergence – FDTD analyzed PCDH cavity

- 10k time step transient removed
- Converged Q = 336.7k
- < 1% fluctuation in the unshaded portion
- 10k transient + 50k for $P(3,3)$, $P(3,4)$, P(4,4)





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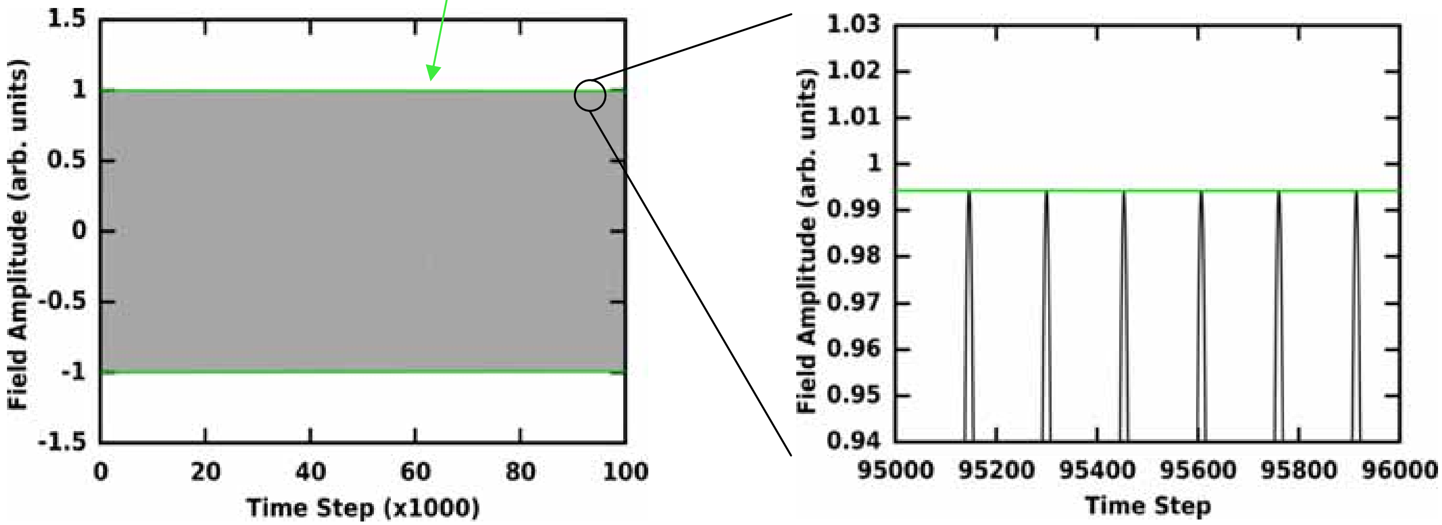
Verification of *Q* value using complementary methods

$$f[n] = e^{-\omega_0 n \Delta t / 2Q}$$



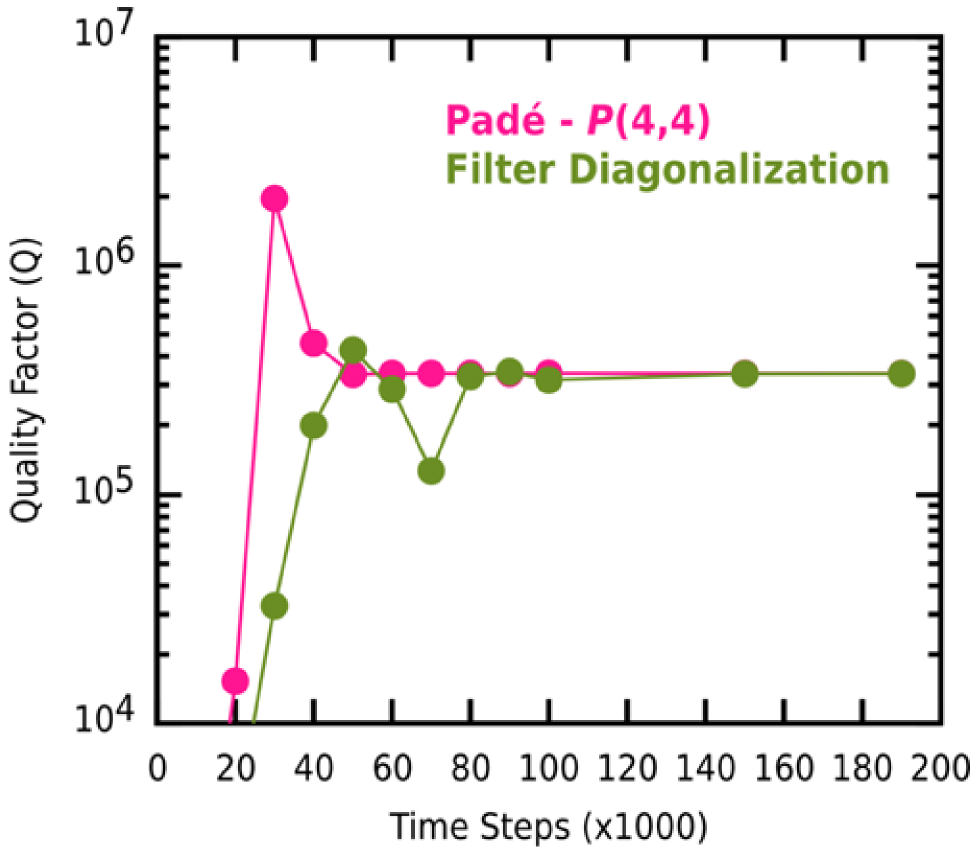
<u>Explicit calculation</u>

$$Q = \omega_0 \frac{\langle U \rangle}{\left\langle \frac{dU}{dt} \right\rangle}$$

Padé *Q* = 336.7k

Energy density *Q* = 329.3k

Comparison between Padé and filter diagonalization method



<u>Filter-Diagonalization</u>

M. R. Wall and D. Neuhauser, J. Chem. Phys **102** 8011 (1995).

V. A. Mandelshtam and H. S. Taylor, J. Chem. Phys. **107** 6756 (1997).

ab-initio.mit.edu/harminv/

Summary

FDTD analysis of PCDH cavities

Time sequence length – spectral resolution

Convergence properties of different Padé functions

Application to photonic crystal double heterostructure cavities

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