Validation Report

Name of Report	Demonstration of the increase in Frequency resolution obtained with the Q calculator in OmniSim/Crystalwave
Performance Date	07 November 2007
Performed By	Klearchos Chaloulos
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Product Version & Compile Date	Version 4.2
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External Files	Q-calculator validation.prj, RingResonator_OmniSim.prj

Demonstration of the increase in Frequency resolution obtained with the Q calculator in OmniSim/Crystalwave

Outline

We are going to demonstrate how the use of the Q calculator feature allows us to achieve the correct resonance spectrum by using fewer time steps. We are going to study a 2D photonic crystal resonator with two closely spaced resonances. The result of the Q-calculator will be compared to the usual Fourier Transform spectrum, obtained with a much bigger duration.
Similar tasks will then be performed in the case of a large 3D ring resonator. For this large simulation, the gain in time attained by the use of the Pade transform is enormous. With the Q-calculator a simulation running for 10 hours gives good resolution. The Fourier transform needs more than 80 hours to get something similar.

2D photonic crystal Resonator

Structure

The structure can be seen on Fig 1. It is a 2D photonic crystal. The excitation is within the complete band gap of the photonic crystal. The losses occur because of the finite extend of the photonic crystal. The light that makes it to the simulation boundaries is absorbed by the PMLs there. Had the photonic crystal been infinite, there would be no losses at all.

We are going to examine two resonances that appear close to each other, and study the required length of the simulation (number of time steps) required in order to clearly distinguish them.

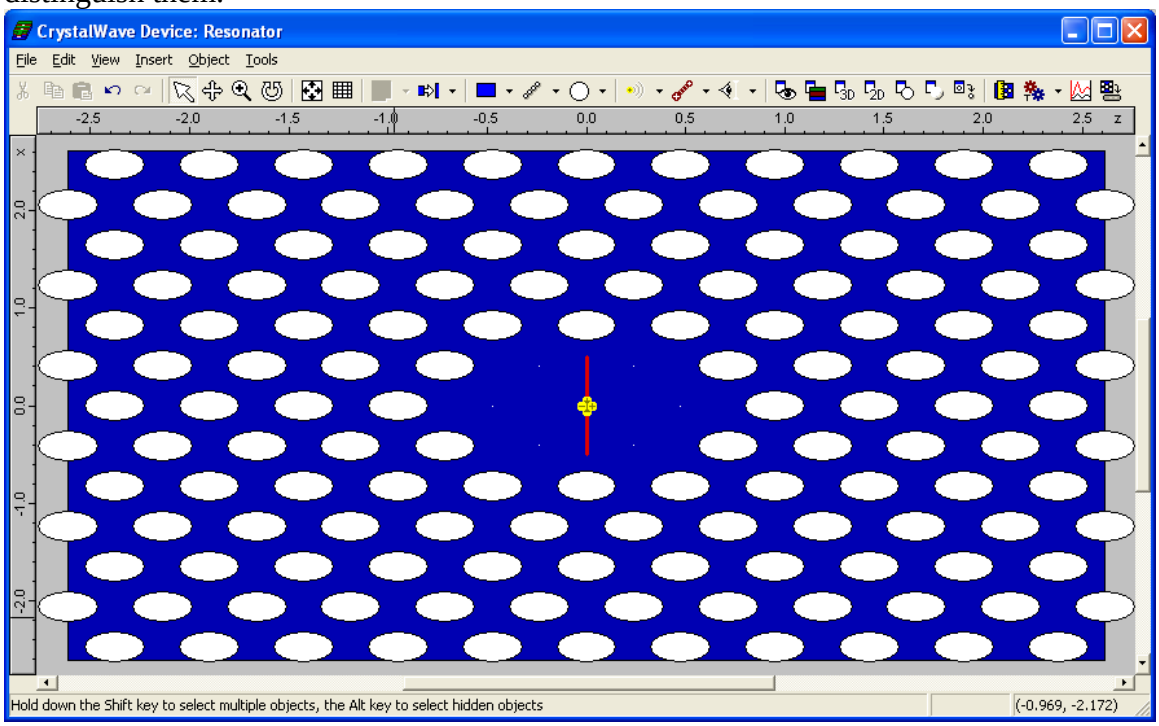

Figure 1: Resonant cavity in a 2D photonic crystal. It consists of air holes in a material of index 2.5. Some holes are removed to form the cavity. The period of the crystal is 0.475um and it is a triangular lattice.

Simulation

We simulate the above device with FDTD, using a grid of 0.475/15 um (15 points per period). For a duration of 120000 time steps (8215fs) we obtain the Fourier spectrum seen in Fig. 2.

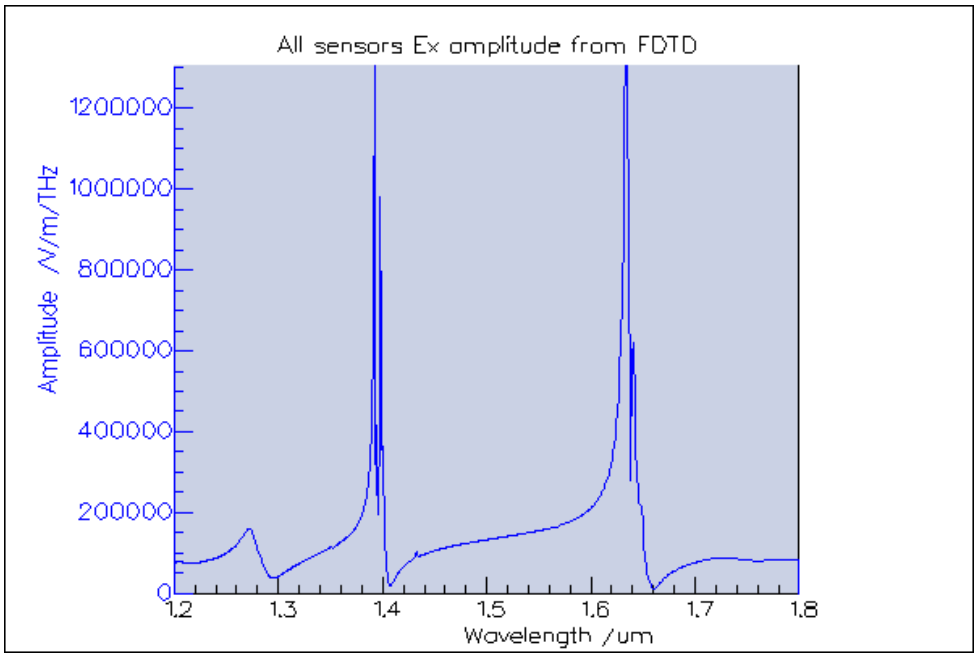

Figure 2: Ex amplitude at the centre of the sensor of Fig. 1, vs wavelength. Duration=120000 time steps.

We will study the closely spaced resonances near 1.4um. In Fig. 3 we present several plots of the spectrum obtained with the Fourier transform and the Pade transform (Q calculator). In both cases we compare spectra obtained for different durations. For the Q calculator, we manually specified the beginning of the time window to be at the first time step. We did the same for the Fourier transform, in order to obtain directly comparable results. For the same reason, we squared the output of the Fourier transform, as this is field amplitude (Ex^2), while the Pade transform returns intensity (again Ex was chosen as the component to be used).

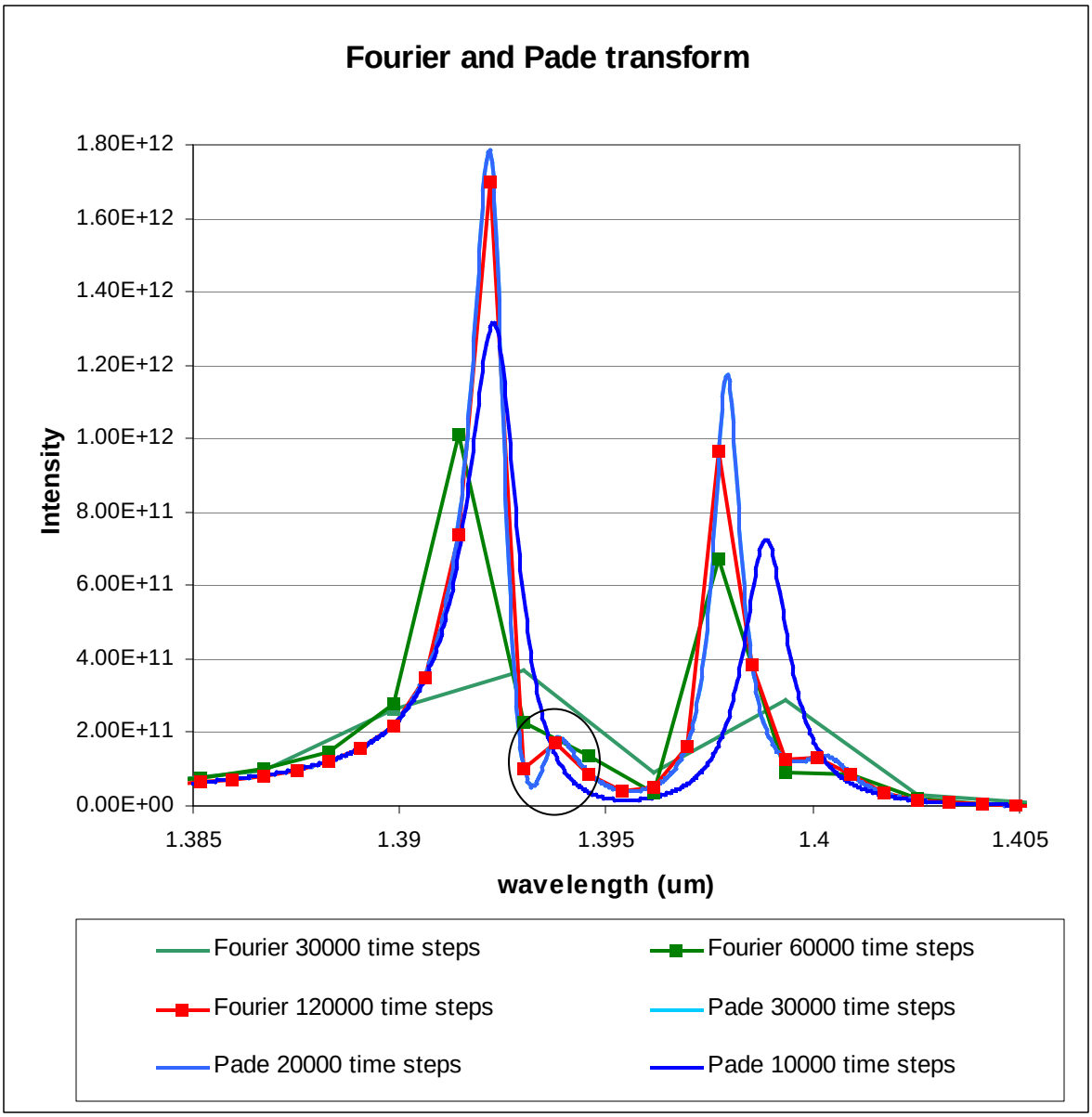

Figure 3: Comparison of the Fourier transform and the Pade transform for different durations. The Fourier lines are the lines with data points plotted. The Pade lines do not have data points plotted because of the much higher resolution. We can see that the Pade transform has converged from a duration of 20000. Actually the 20000 and 30000 lines fall on top of each other. The Fourier transform needs 120000 time steps in order to converge. Note also the third weak resonance in the circle. Fourier Transform needs 120000 time steps to resolve it, while Pade Transform sees it with 20000 time steps.

From Fig 3 we see that the spectrum obtained from the Q-calculator has a much higher resolution for the same duration of the simulation. Note also that a third weak resonance becomes visible at120000 time steps with the Fourier Transform, while the Pade Transform of the Q calculator resolves it at 20000 time steps.
Another advantage of the Q-calculator is that the user can specify the resolution by setting the steps parameter (Fig 4). Also, we can get the Q-factor of our resonances directly.

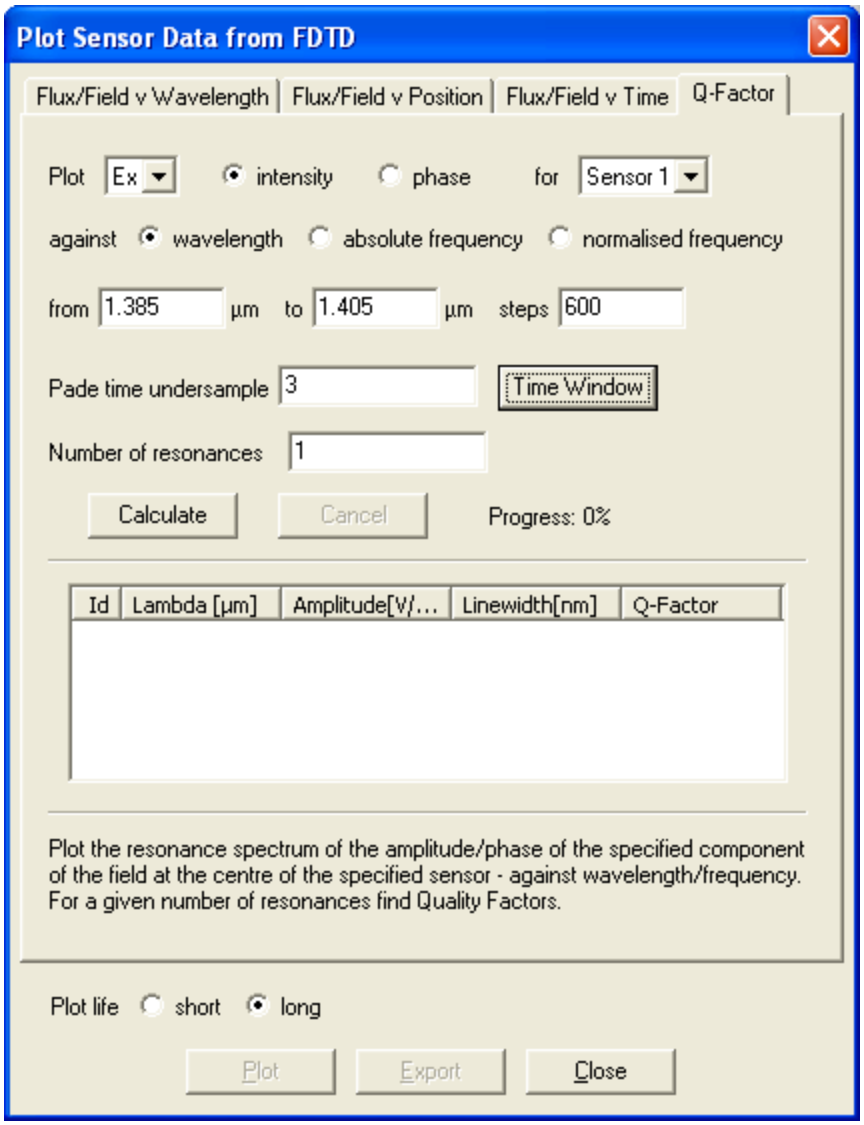

Figure 4: Q calculator window.

Q factor convergence

We will study the convergence of the Q factor calculated for the stronger resonance of Fig. 3, vs the number of time steps. We see that the Q returned from the Q-calculator converges for much fewer time steps (at 20000), while the Q calculated from the Fourier transform needs 120000 time steps to stabilize.

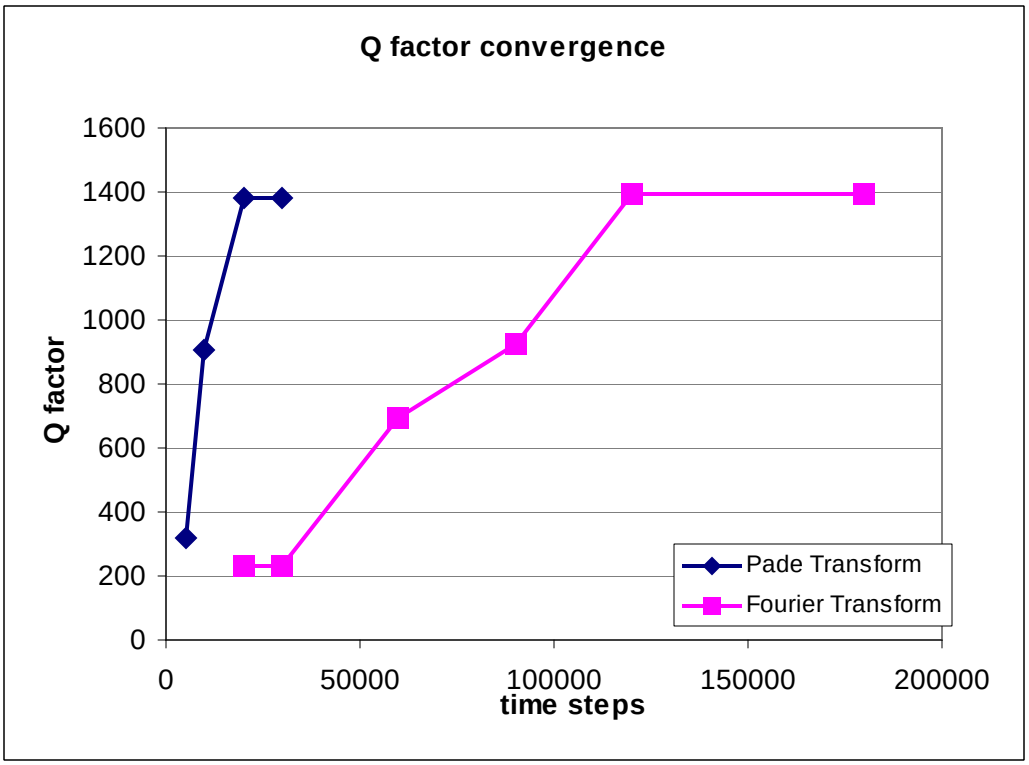

Figure 5: Convergence of the Q-factor, calculated for the stronger resonance of Fig. 3, from the Pade transform and the Fourier transform. It is evident that the Pade transform converges much quicker than the Fourier transform. It needs less than ¼ of the time steps required for the Fourier transform.

Effect of the Time Window

Here we will explore the effect that the Time Window of the Pade Transform has on the calculation of Q. The Time window specifies which data is to be used for the input of the Pade Transform, e.g. data from time step 2000 to time step 5000.
In the previous calculation the Time window started right at the beginning of the calculation. This sometimes is not desired, as the excitation pulse will also be used in the calculation of the resonance spectrum. It has been seen that a better spectrum can be obtained when starting the Time Window from a later time step. The default setting in OmniSim is to start the Time Window when 75% of the energy has passed (Fig 6).

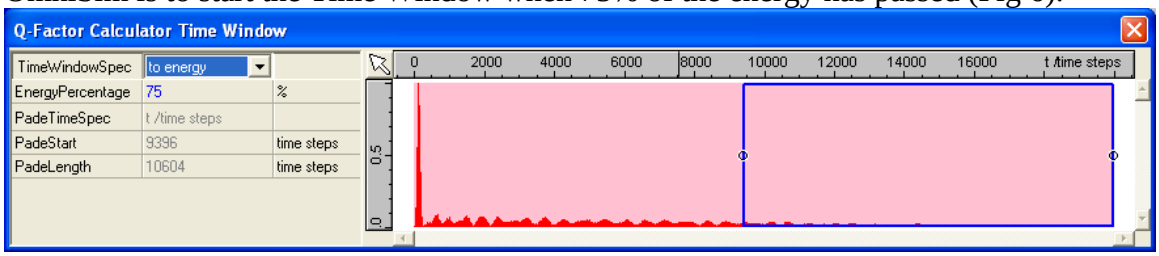

Figure 6: Q-Factor Calculator Time window, showing the input data used for the calculation. Here, data is used after 75% of the energy has passed.

We ran a simulation with a total duration of 60000 time steps, on the structure of Fig. 1. In Fig. 7, we plot the Q factor against the starting point of the Time Window. The starting point is defined from the amount of energy passed. So 0% means that no energy has passed, and we use all the data. 90% means that most of the energy has passed, and only data from time steps near the end of the simulation is used. During this test, we kept the duration of the time window to 20000 time steps for all starting points, so that the different durations would not affect the result. The only thing changing is the position of the time window. The Pade transform was applied from wavelength 1.385 to 1.395 um, with 300 points in between (wavelength resolution 0.0333nm).

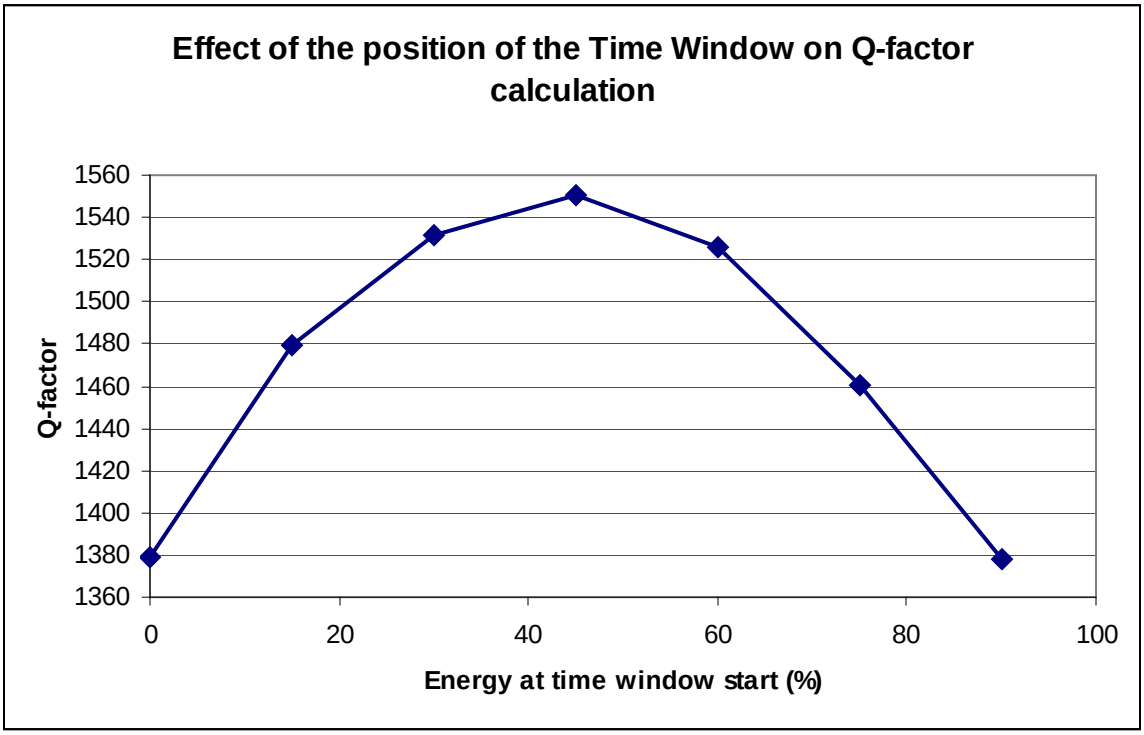

Figure 7: Q-factor for different positions of the Time window. The starting position of the time window is specified by the amount of energy that has passed (percentage). The duration of the time window was kept fixed at 20000 time steps. We see that the Q factor varies only be ~ 10%, which is a decent accuracy for this difficult calculation.

3D Ring Resonator

In this section we will use the Q calculator to find the Q factor of a 3D ring resonator. A direct simulation of a ring resonator in OmniSim is cumbersome, as the large structure requires a large amount of memory, and the high Q requires the simulation to be run for a very long time in order to obtain the needed frequency resolution. The Q-calculator can be of significant help in the last issue, as it allows us to obtain the required resolution with a much smaller duration.

Structure

The structure is a usual SOI structure. The waveguide is single mode. The radius of the ring is 7.5um.

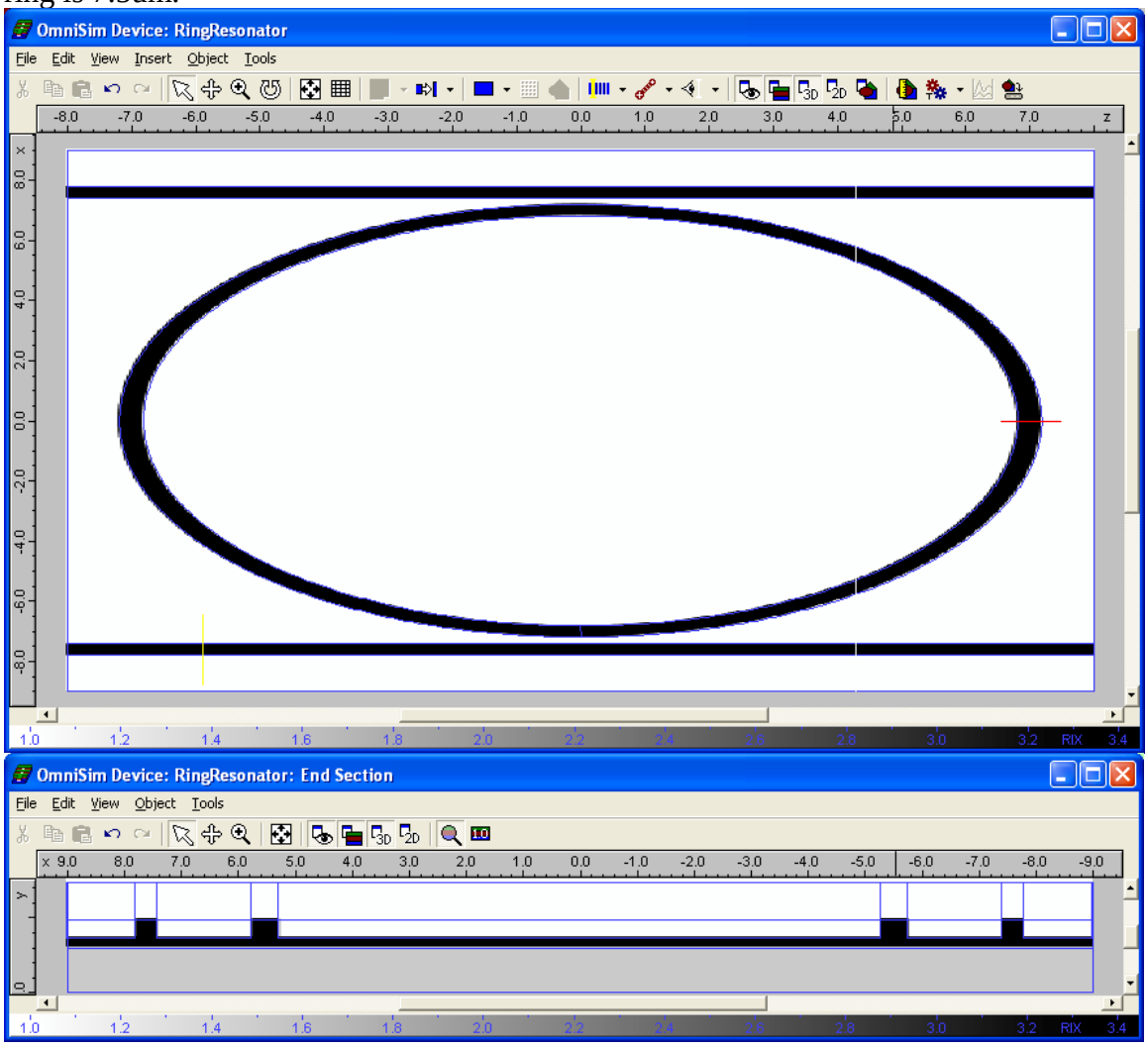

Figure 8: Top view (top) and cross-section view (bottom) of the 3D ring resonator. It is a usual SOI structure.

Results

A plot of the spectrum of one resonance of the ring can be seen on Fig. 9. We see again the Pade transform achieves equivalent resolution to the Fourier transform by using only a quarter of the time steps. For these large simulation the gain in time is tremendous; For 60000 time steps ~20 hours are required on a 3GHz Pentium 4 PC. This is a simulation you can run overnight. For 220000 time steps ~ 80 hours are needed. The simulation with 280000 time steps needed 20 hours on a cluster with 5 nodes. Also, as we can see from Fig. 10, the Q factor calculated from the Pade transform has converged from 30000 time steps, which means that ~10 hours are needed, compared to 80. We have to mention that ~ 20 minutes were needed for the calculation of the Pade spectrum (200 points between

1.4 and 1.555, resolution 0.07nm). This illustrates the tremendous gain in speed by using the Q calculator in high resonators and 3D simulations.

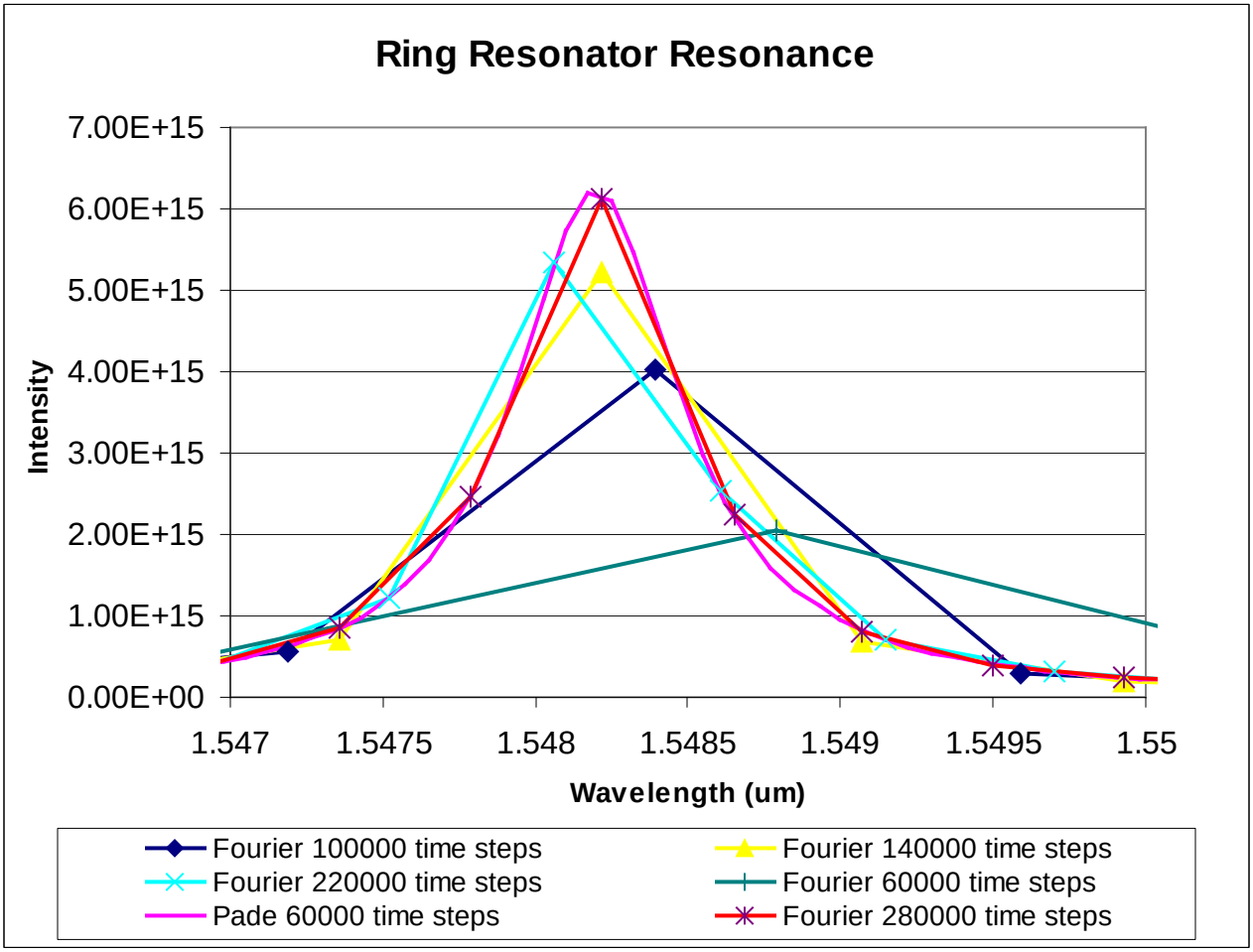

Figure 9: Spectrum of a resonance of the ring Resonator. We can see how few points the spectrum calculated with the Fourier transform has, compared to the Pade transform. Also, the Pade Transform for 60000 time steps looks better even from the Fourier transform at 280000 time steps. Note that for 60000 time steps we needed ~20 hours, s duration that can be run overnight. For 220000 time steps, ~80 hours the simulation needed 80 hours! The 280000 time steps simulation took 20 hours on a cluster with five nodes. Note also how few points the Fourier transform curves have. Even for the 280000 time steps case, there are 5 points describing the resonance.

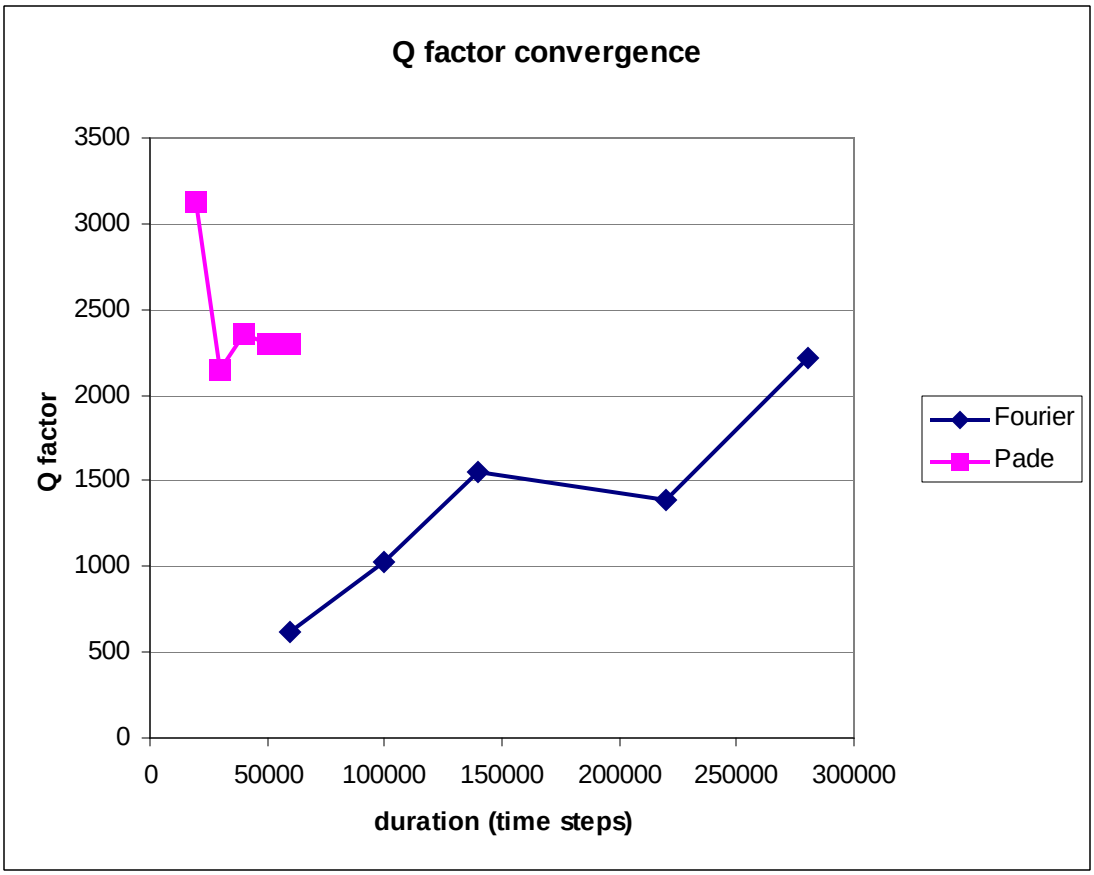

Figure 10: Q factor convergence, for different simulation durations. The Pade transform converges at about 30000 time steps. The Fourier Transform has not converged even at 220000.