Information for simulations in Wave Propagation

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1 Consistent units

Although is a good practice to convert the equations to their dimensionless versions, we still need to plug numbers into our numerical algorithms. For that aim we need to use consistent units, as presented in the following table.

Quantity	SI	SI (mm)	US (ft)	US (inch)
Length	m	mm	ft	in
Force	N	N	lbf	lbf
Mass	kg	tonne (10^3 kg)	slug	lbf s^2/in
Time	s	s	s	s
Stress	Pa (N/m^2)	MPa (N/mm^2)	lbf/ft^2	psi (lbf/in^2)
Energy	J	mJ (10^{-3})	ft lbf	in lbf
Density	kg/m^3	tonne/mm^3	slug/ft^3	lbf s^2/in^4

2 Relations between elastic constants

K: Bulk modulus, λ: Lamé's first parameter, E: Young's modulus, G: Shear modulus, ν: Poisson's ratio, M: P-wave modulus.

	$K =$	$E =$	$\lambda =$	$G =$	$\nu =$	$M =$
(K, E)	K	E	$\frac{3K(3KE)}{9K-E}$	$\frac{3KE}{9K-E}$	$\frac{3K-E}{6K}$	$\frac{3K(3K+E)}{9K-E}$
(K, λ)	K	$\frac{9K(K-\lambda)}{3K-\lambda}$	λ	$\frac{3(K-\lambda)}{2}$	$\frac{\lambda}{3K-\lambda}$	$3K - 2\lambda$
(K, G)	K	$\frac{9KG}{2K+G}$	$K - \frac{2G}{3}$	G	$\frac{3K-2G}{2(3K+G)}$	$K + \frac{4G}{3}$
(K, ν)	K	$3K(1 - 2\nu)$	$\frac{3K\nu}{1+\nu}$	$\frac{3K(1-2\nu)}{2(1+\nu)}$	ν	$\frac{3K(1-\nu)}{1+\nu}$
(E, G)	$\frac{EG}{3(3G-E)}$	E	$\frac{G(E-2G)}{EG-E}$	G	$\frac{E}{2G} - 1$	$\frac{G(4G-E)}{3G-E}$
(E, ν)	$\frac{E}{3(1-2\nu)}$	E	$\frac{E\nu}{(1+\nu)(1-2\nu)}$	$\frac{E}{2(1+\nu)}$	ν	$\frac{E(1-\nu)}{(1+\nu)(1-2\nu)}$
(ν, G)	$\lambda + \frac{2G}{3}$	$\frac{G(3\lambda+2G)}{\lambda+G}$	λ	G	$\frac{\lambda}{2(\lambda+G)}$	$\lambda + 2G$
(ν, λ)	$\frac{\lambda(1+\nu)}{3(1-2\nu)}$	$\frac{\lambda(1+\nu)(1-2\nu)}{\nu}$	λ	$\frac{\lambda(1-2\nu)}{2\nu}$	ν	$\frac{\lambda(1-\nu)}{\nu}$
(G, λ)	$\frac{2G(1+\nu)}{3(1-2\nu)}$	$2G(1 + \nu)$	$\frac{2G\nu}{1-2\nu}$	G	ν	$\frac{2G(1-\nu)}{1-2\nu}$
(G, M)	$M - \frac{4G}{3}$	$\frac{G(3-M-4G)}{M-2G}$	$M - 2G$	G	$\frac{M-2G}{2(M-G)}$	M

3   Relations for elastic wave speeds

The P-wave is a dilatational wave with speed α given by

$$\alpha^2 = \frac{\lambda + 2G}{\rho}, \qquad \alpha^2 = \frac{G(1 - \nu)}{\rho},$$
$$\alpha^2 = \frac{M}{\rho}, \qquad \alpha^2 = \frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)\rho},$$
$$\alpha^2 = \frac{2\beta^2(1 - \nu)}{1 - 2\nu}.$$

The S-wave is a distorsional wave with speed β given by

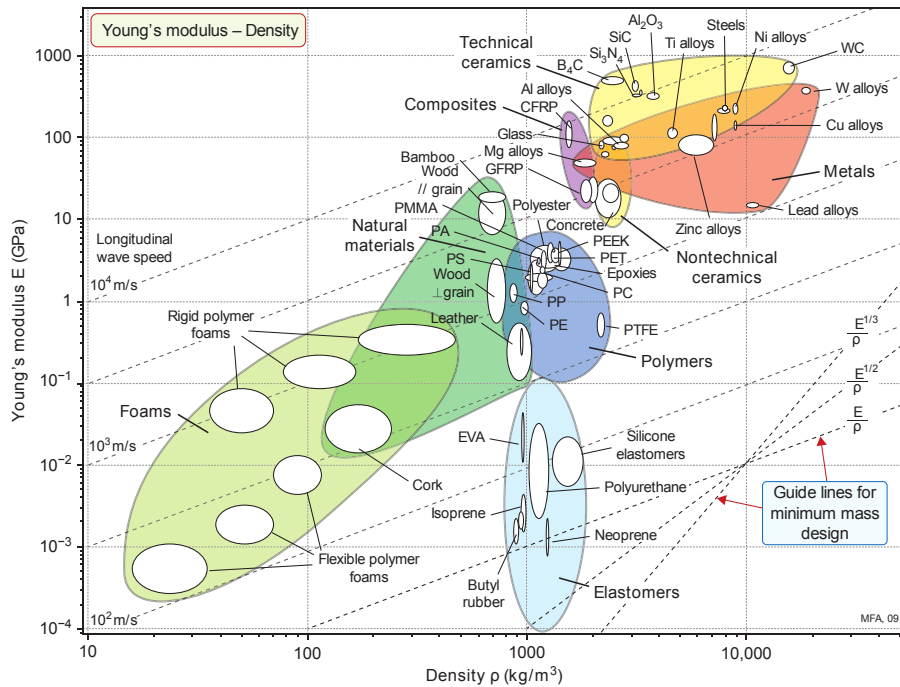$$\beta^2 = \frac{G}{\rho}$$
$$\beta^2 = \frac{E}{2(1 + \nu)\rho},$$
$$\beta^2 = \frac{\alpha^2(1 - 2\nu)}{2(1 - \nu)}.$$

Some particular values for the ratio

$$\frac{\alpha^2}{\beta^2} = \frac{2(1 - \nu)}{1 - 2\nu}$$

are

$$\frac{\alpha^2}{\beta^2} = \frac{4}{3} \quad \text{for } \nu = -1 \; ,$$

$$\frac{\alpha^2}{\beta^2} = 2 \quad \text{for } \nu = 0 \; ,$$

$$\frac{\alpha^2}{\beta^2} = 4 \quad \text{for } \nu = \frac{1}{3} \; ,$$

$$\frac{\alpha^2}{\beta^2} \to \infty \quad \text{when } \nu \to \frac{1}{2} \; .$$

Figure 1. Ashby chart for Young Modulus vs density. The lines show the sound speed, that is the speed for a wave in a rod made of this material and is between the longitudinal and shear wave speeds –for Poisson ratios in (-0.5,0.5). Taken from *Ashby, Michael F. "Materials selection in mechanical design." MRS BULLETIN 30 (2005): 995.*

4 Courant-Friedrichs-Lewy condition

The Courant-Friedrichs-Lewy condition (CFL condition) is a necessary condition for convergence while solving certain partial differential equations (usually hyperbolic PDEs) numerically by the method of finite differences. It arises when explicit time-marching schemes are used for the numerical solution. The condition is named after Richard Courant, Kurt Friedrichs, and Hans Lewy who described it in their 1928 paper [2].

The criterion could be stated as

$$C = v_x \frac{\Delta t}{\Delta x} \leq C_{max} \qquad \text{in 1D ;}$$

$$C = v_x \frac{\Delta t}{\Delta x} + v_y \frac{\Delta t}{\Delta y} \leq C_{max} \qquad \text{in 2D ;}$$

$$C = v_x \frac{\Delta t}{\Delta x} + v_y \frac{\Delta t}{\Delta y} + v_z \frac{\Delta t}{\Delta z} \leq C_{max} \qquad \text{in 3D ;}$$

Where v_{x_i} is the phase speed (for wave phenomena) in the x_i direction, Δx_i is the minimum spatial discretization in x_i direction, Δt is the time step and C_{max} is the maximum allowable value for C, which depends on the time discretization scheme but should be less than 1.

In the case of elastodynamics and for a spatial discretization with the finite element method, the criterion could be re-stated as

$$C \leq \alpha \frac{\Delta t}{h} \leq C_{max} \qquad \text{in 1D ;}$$

$$C \leq 2\alpha \frac{\Delta t}{h} \leq C_{max} \qquad \text{in 2D ;}$$

$$C \leq 3\alpha \frac{\Delta t}{h} \leq C_{max} \qquad \text{in 3D ;}$$

where α is the phase speed for the P-wave and h is the minimum distance between consecutive nodes. This give us the maximum allowable timestep as

$$\Delta t \leq C_{max} \frac{h}{\alpha} \qquad \text{in 1D ;} \tag{1}$$

$$\Delta t \leq \frac{C_{max}}{2} \frac{h}{\alpha} \qquad \text{in 2D ;} \tag{2}$$

$$\Delta t \leq \frac{C_{max}}{3} \frac{h}{\alpha} \qquad \text{in 3D .} \tag{3}$$

A graphical representation of the criterion is given in Figure 2. Intuitively, we can think about the CFL condition as a limit in the speed for transferring information from one node to its neighbors; this *speed* should be less than the speed for propagation of phenomena in the wave.
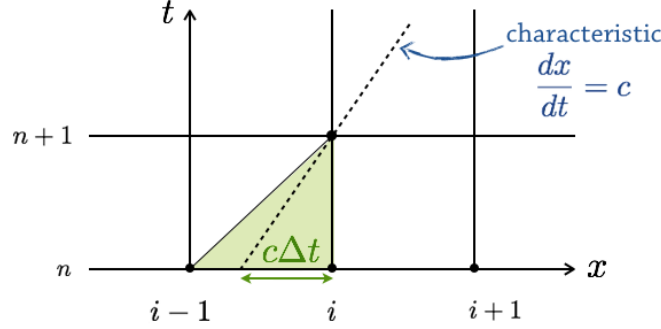
Figure 2. Graphic representation of the CFL condition in 1D. *L.A. Barba et al. Practical Numerical Methods with Python, 2014.*

5 Nyquist criterion

The Nyquist–Shannon sampling theorem (also Nyquist-Shannon-Whittaker theorem), after Harry Nyquist and Claude Shannon, in the literature more commonly referred to as the Nyquist sampling theorem or simply as the sampling theorem, is a fundamental result in the field of information theory, in particular telecommunications and signal processing. Sampling is the process of converting a signal (for example, a function of continuous time or space) into a numeric sequence (a function of discrete time or space). Shannon's version of the theorem states [3, 7, 6, 8]:

> If a function $x(t)$ contains no frequencies higher than B hertz, it is completely determined by giving its ordinates at a series of points spaced $1/(2B)$ seconds apart.

This theorem implies for us in the numerical simulation of wave propagation that

$$h \le \frac{\lambda}{2} \ ,$$

where h is the maximum distance between consecutive nodes and λ is the shortest wavelength that want to be sampled. So, the selection of h is commonly

$$h = \frac{\lambda}{k} \ \ ,$$

where $k > 2$ is a factor that depends on the numerical method. For finite element methods k is commonly 10, and for spectral element methods k is reduced to 5 [4].

6 Information for different pulse signals

In wave propagation problems we must work with time signals that are finite in time, let's say wave pulses (or wave packets in the Quantum Mechanics jargon). Some times we are interested in wave pulses because they are useful as wavefronts representation. Furthermore, wave packets are important since we cannot store information in a wave with a single frequency[1]. There is a trade off between the localization in time (duration of the pulse) and frequency (concentration of the energy around a specific value). This fact is well discussed in Quantum Mechanics texts since it re ects the discussion about waveparticle duality and uncertainty principle [9]. When we have finite time signals its corresponding Fourier transform will be in the whole frequency domain. In general terms, while more concentrated in the time domain, more spread in the frequency domain. From a numerical point of view we need to truncate the maximum frequency allowed for our simulations.

In the following *subsections* we exposed some truncation tips for different wave pulses. This is important because numerically we cannot consider the complete spectrum of a pulse, since normally they cover the whole frequency domain. We will refer to the function in time as $f(t)$, and to its Fourier transform as $\hat{f}(\omega)$. Since the "energy" carried for the wave per frequency is proportional to the square of the absolute value of the Fourier transform $\hat{f}^2(\omega)$, we can compare the energy in the frequency interval $[0, \omega_{\max}]$ to the

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[1]That's why phase speed of waves can be higher than speed of light. For non-dissipative media, the energy (and so the information) travel with the group velocity [1].

energy content in $[0, \infty)$[2]. Thus, as a figure of merit we define

$$R(\omega_{\max}) = \frac{\int\limits_0^{\omega_{\max}} \hat{f}^2(\omega) \ \mathrm{d}\omega}{\int\limits_0^{\infty} \hat{f}^2(\omega) \ \mathrm{d}\omega} \times 100\% \ , \tag{4}$$

and tell us the proportion of energy taken into account if we neglect circular frequencies higher than $\omega_{\max}$.

6.1 Ricker wavelet

It is common to use a Ricker wavelet as the input signal in simulations since it has the energy concentrated around a circular frequency ω_c. Let's write the signal as

$$f(t) = \left(\frac{12t^2}{b^2} - 1 \right) e^{-\frac{6t^2}{b^2}} \ ,$$

where b is the elapsed time between the peaks in the time domain [5]. The Fourier transform for this signal is

$$\hat{f}(\omega) = -\frac{\sqrt{\pi} b^3 \omega^2 e^{-\frac{b^2 \omega^2}{24}}}{2 \ 6^{3/2}} \ ,$$

with a characteristic[3] circular frequency

$$\omega_c = \frac{2\sqrt{6}}{b}.$$

To satisfy the sampling theorem we need to design our simulations thinking about the shortest wavelength, so we need to think about the maximum frequency. To know where to trunk the signal (in the frequency domain) we could compute how much energy is in $[0, \omega_{max}]$ and compare this value with the energy stored in the interval $[0, \infty)$. Some particular values are :
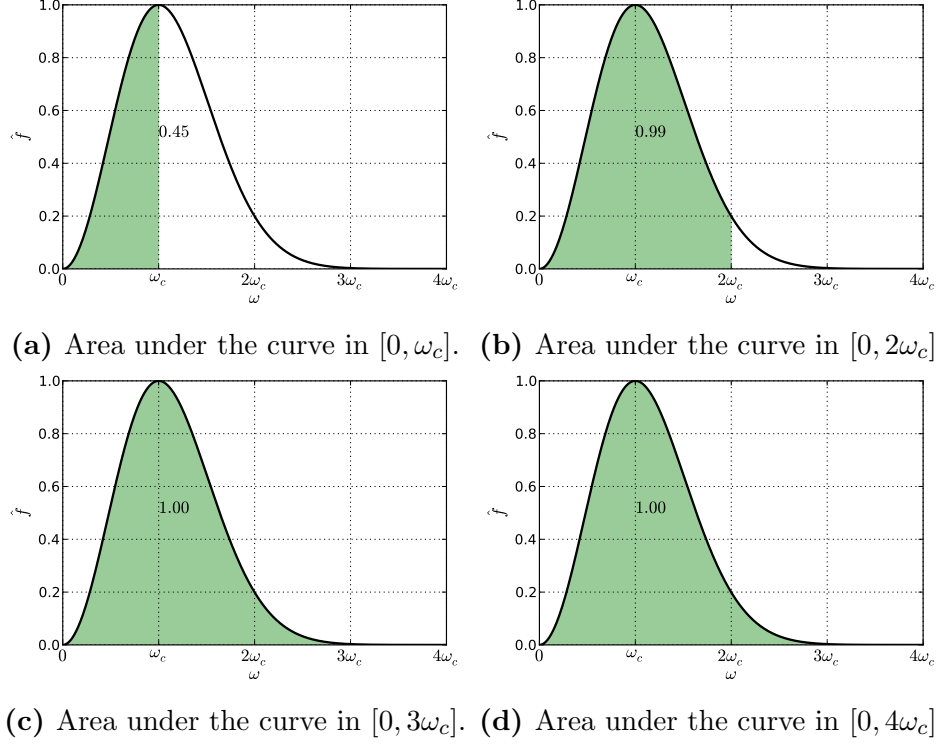
$$R(1.0\omega_c) = 45.06\% \ ;$$
$$R(1.5\omega_c) = 89.09\% \ ;$$
$$R(2.0\omega_c) = 99.32\% \ ;$$
$$R(3.0\omega_c) = 99.99\% \ ;$$
$$R(4.0\omega_c) = 100.00\% \ .$$

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[2]We just need to compute one halfspace because the other half has the same values.
[3]The characteristic frequency is the value at which the peak appears.

This can be depicted in Figure 3

(a) Area under the curve in $[0, \omega_c]$. **(b)** Area under the curve in $[0, 2\omega_c]$.

(c) Area under the curve in $[0, 3\omega_c]$. **(d)** Area under the curve in $[0, 4\omega_c]$.

Figure 3. Energy distribution in the spectrum of the Ricker wavelet.

6.2 Gaussian wavelet

One option to obtain a wavelet with the energy concentrated in a single frequency value is to use a signal which spectrum is a Gaussian function (Normal distribution) of the form[4]

$$\hat{f}(\omega) = \frac{1}{\omega_\sigma \sqrt{2\pi}} \left[e^{-\frac{(\omega - \omega_0)^2}{2\omega_\sigma^2}} + e^{-\frac{(\omega + \omega_0)^2}{2\omega_\sigma^2}} \right] \quad , \tag{5}$$

where ω is the angular frequency, ω_0 is the value of angular frequency for the highest density (mean value), ω_σ is the value around ω_0 to have roughly 80%

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[4]Both, the positive and negative frequencies are *valid*. That's why we should include the second term in brackets.

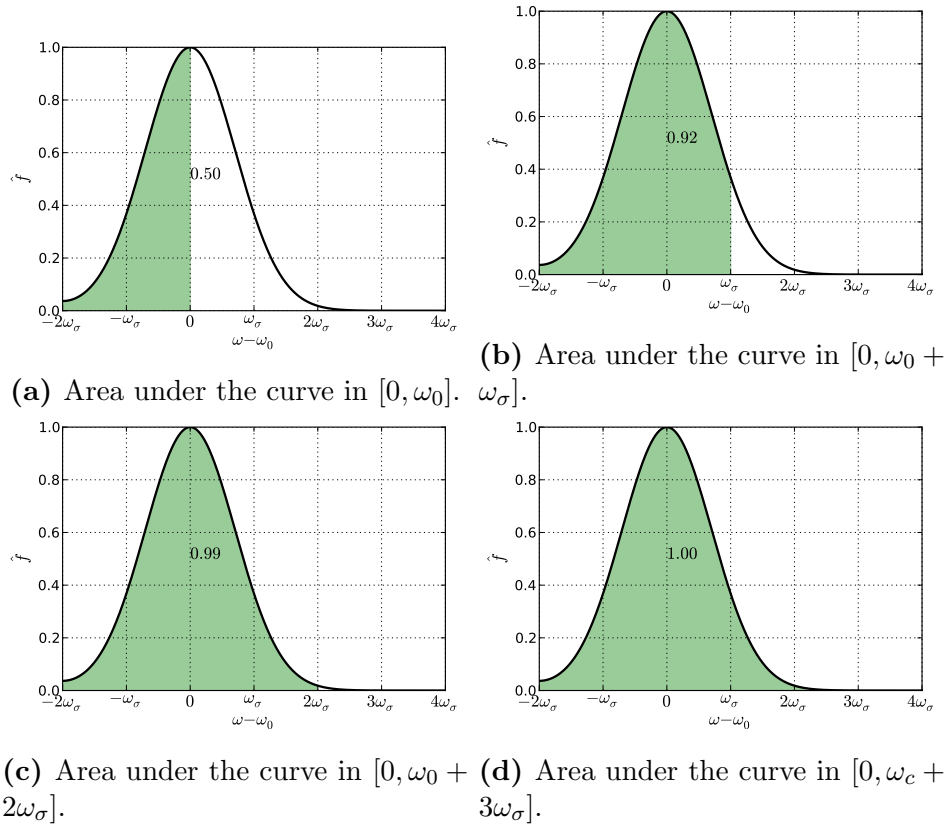of the energy (standard deviation). In the time domain, the signal looks like

$$f(t) = 2e^{-\frac{(\omega_\sigma t)^2}{2}} \cos(\omega_0 t) \ , \tag{6}$$

that is, basically, a harmonic function modulated by a Gaussian.

If we consider that $\omega_0/\omega_\sigma > 0$ we can have the expressions

$$R(\omega_0) = 50\%;$$
$$R(\omega_0 + \omega_\sigma) = 84.27\%;$$
$$R(\omega_0 + 2\omega_\sigma) = 97.73\%;$$
$$R(\omega_0 + 3\omega_\sigma) = 99.87\%;$$
$$R(\omega_0 + 4\omega_\sigma) = 100.00\%$$

that is depicted in Figure 4

(a) Area under the curve in $[0, \omega_0]$.

(b) Area under the curve in $[0, \omega_0 + \omega_\sigma]$.

(c) Area under the curve in $[0, \omega_0 + 2\omega_\sigma]$.

(d) Area under the curve in $[0, \omega_c + 3\omega_\sigma]$.

Figure 4. Energy distribution in the spectrum of the Gaussian wavelet.

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6.3   Square pulse

A square pulse with duration Δt is given by

$$f(t/\Delta t) = \begin{cases} 0 & \text{if } |t| >= \Delta t/2 \\ 1 & \text{if } |t| < \Delta t/2 \end{cases} \tag{7}$$
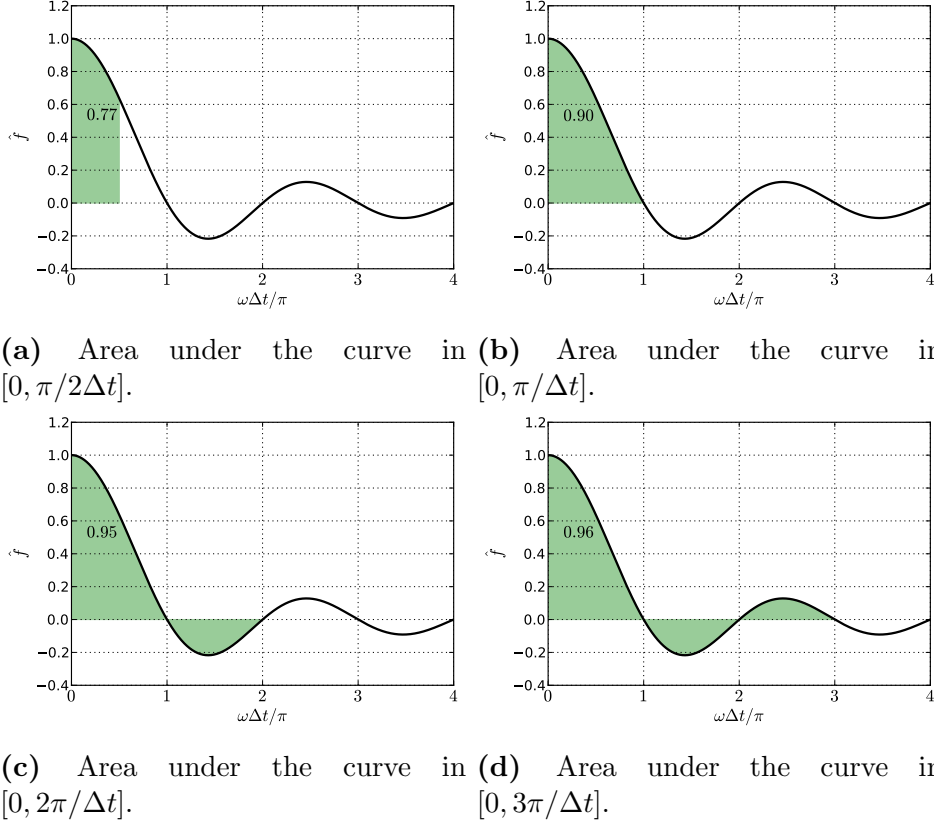
And the Fourier transform is given by

$$\hat{(f)}(\omega\Delta t) = \frac{\sin\left(\frac{\omega\Delta t}{2}\right)}{\left(\frac{\omega\Delta t}{2}\right)} \quad, \tag{8}$$

for this case, the ratios R are:

$$R(\pi/2\Delta t) = 77.37\%;$$
$$R(\pi/\Delta t) = 90.28\%;$$
$$R(2\pi/\Delta t) = 94.99\%;$$
$$R(3\pi/\Delta t) = 96.64\%.$$

This can be depicted in Figure 5

(a) Area under the curve in $[0, \pi/2\Delta t]$.

(b) Area under the curve in $[0, \pi/\Delta t]$.

(c) Area under the curve in $[0, 2\pi/\Delta t]$.

(d) Area under the curve in $[0, 3\pi/\Delta t]$.

Figure 5. Energy distribution in the spectrum for the square wavelet.
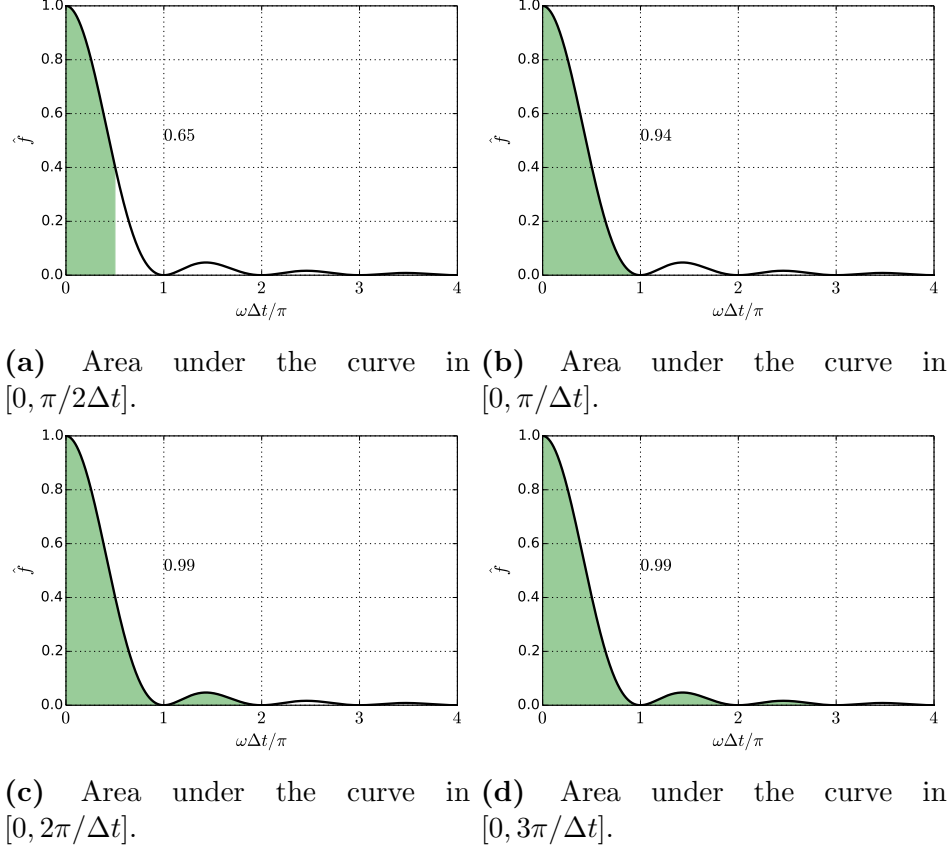
6.4 Triangle pulse

The triangle pulse is given by the convolution of two square pulses, and the Fourier transform is

$$\hat{f}(\omega) = \left[\frac{\sin(\omega/2)}{(\omega/2)}\right]^2 . \tag{9}$$

For this case the ratios are:

$$R(\pi/2\Delta t) = 65.77\%;$$
$$R(\pi/\Delta t) = 94.98\%;$$
$$R(2\pi/\Delta t) = 99.71\%;$$
$$R(3\pi/\Delta t) = 99.87\%.$$

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That are depicted in Figure 6

(a) Area under the curve in $[0, \pi/2\Delta t]$.

(b) Area under the curve in $[0, \pi/\Delta t]$.

(c) Area under the curve in $[0, 2\pi/\Delta t]$.

(d) Area under the curve in $[0, 3\pi/\Delta t]$.

Figure 6. Energy distribution in the spectrum for the triangle wavelet.

References

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[6] Wikipedia contributors, *Nyquist-Shannon sampling theorem*, Wikipedia, The Free Encyclopedia, `https://en.wikipedia.org/w/index.php?title=Nyquist%E2%80%93Shannon_sampling_theorem` (accessed May 26, 2016).

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