k-Wave short course – Part 4
Modelling sources

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Initial value problems (IVPs)

- The simplest way to include a source is to define an initial condition
- k-Wave supports setting an initial pressure distribution, `source.p0`

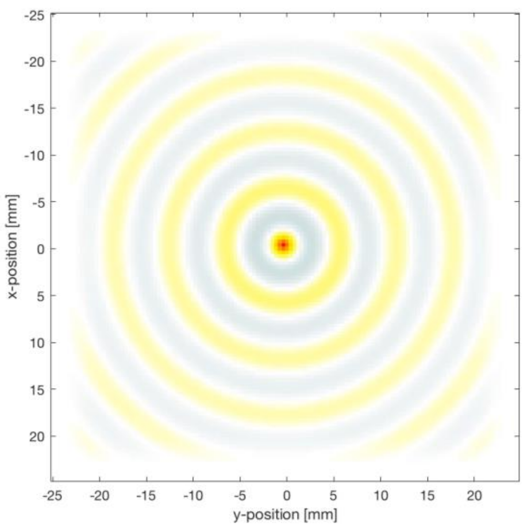
- k-Wave sets the initial particle velocity to zero by making it anti-symmetric about time zero: $u^{\frac{1}{2}} = -u^{-\frac{1}{2}}$
- This models photoacoustics, betraying k-Wave's origin

- BEWARE when doing convergence testing: Changing grid resolution changes frequency content with IVPs

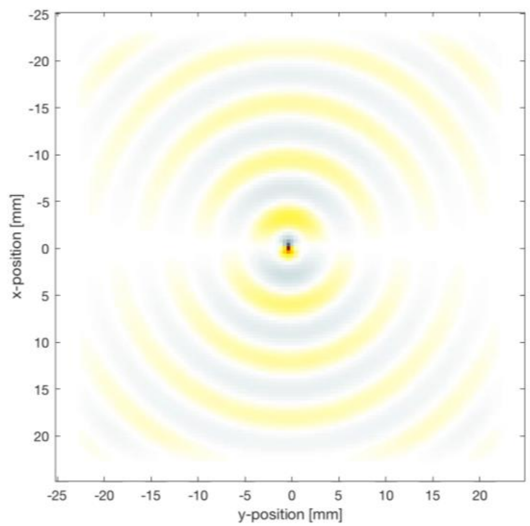
Time-varying sources

- Sources varying arbitrarily in time can be defined:
  - `source.p`, pressure (or mass) source
  - `source.ux`, velocity (or force) source
- Velocity sources are directional
- Sources can only be added at grid points

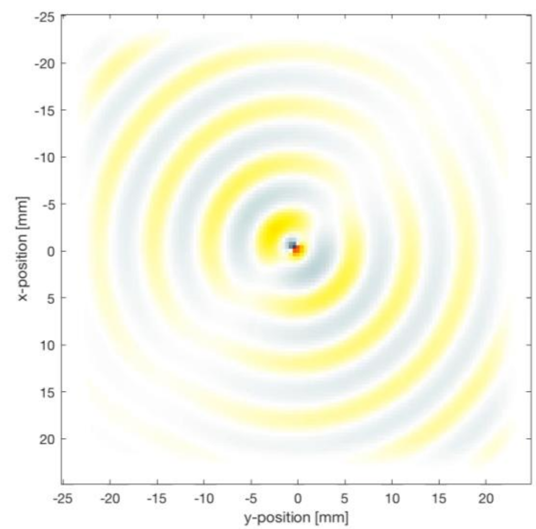
pressure source



velocity source



velocity source



Time-varying sources

- There are essentially two types of time-varying sources:

`source.p_mode = 'additive'`

The source is <u>added</u> to the acoustic field at the points defined in `source.p_mask`. (Default)

`source.p_mode = 'dirichlet'`

The source <u>replaces</u> the value of the acoustic field at the points defined in `source.p_mask`.

- Similar notation for `source.u_mask`, `source.u_mode`

Additive sources

- Discrete equations (without the PML), no source terms

$$u^{n+\frac{1}{2}} = u^{n-\frac{1}{2}} - \frac{\Delta t}{\rho_0}\mathcal{F}^{-1}\left\{ik_x\kappa e^{ik_x\Delta x/2}\mathcal{F}\left\{p^n\right\}\right\}$$

$$\rho^{n+1} = \rho^n - \Delta t\rho_0\mathcal{F}^{-1}\left\{ik_x\kappa e^{-ik_x\Delta x/2}\mathcal{F}\left\{u^{n+\frac{1}{2}}\right\}\right\}$$

$$p^{n+1} = c_0^2\rho^{n+1}$$

- with a <u>velocity</u> (or force) source

$$u^{n+\frac{1}{2}} = u^{n-\frac{1}{2}} - \frac{\Delta t}{\rho_0}\mathcal{F}^{-1}\left\{ik_x\kappa e^{ik_x\Delta x/2}\mathcal{F}\left\{p^n\right\}\right\} + \mathcal{F}^{-1}\left\{\sigma\mathcal{F}\left\{S_F^n\right\}\right\}$$

- with a <u>pressure</u> (or mass) source

$$\rho^{n+1} = \rho^n - \Delta t\rho_0\mathcal{F}^{-1}\left\{ik_x\kappa e^{-ik_x\Delta x/2}\mathcal{F}\left\{u^{n+\frac{1}{2}}\right\}\right\} + \mathcal{F}^{-1}\left\{\sigma\mathcal{F}\left\{S_M^{n+\frac{1}{2}}\right\}\right\}$$

Tabei et al. JASA, 111, 53–63 (2002). Treeby & Cox, J. Biomed. Opt., 15, 021314 (2010).

k-space correction factors

$$u^{n+\frac{1}{2}} = u^{n-\frac{1}{2}} - \frac{\Delta t}{\rho_0}\mathcal{F}^{-1}\left\{ik_x\kappa e^{ik_x\Delta x/2}\mathcal{F}\left\{p^n\right\}\right\} + \mathcal{F}^{-1}\left\{\sigma\mathcal{F}\left\{S_F^n\right\}\right\}$$

- The factor κ exactly corrects the phase error introduced by the finite-difference time derivative approximation

$$\kappa = \sin(c_0 k \Delta t/2)$$

- The factor σ is applied to time-varying sources so their temporal sampling can be as low as 4 points-per-period

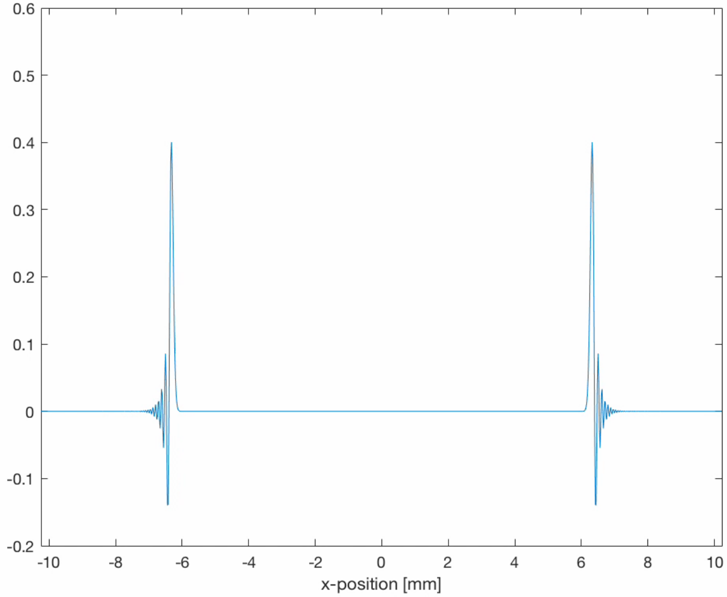
$$\sigma = \cos(c_0 k \Delta t/2)$$

- For a single frequency source $\sigma = \cos(\omega_0 \Delta t/2)$

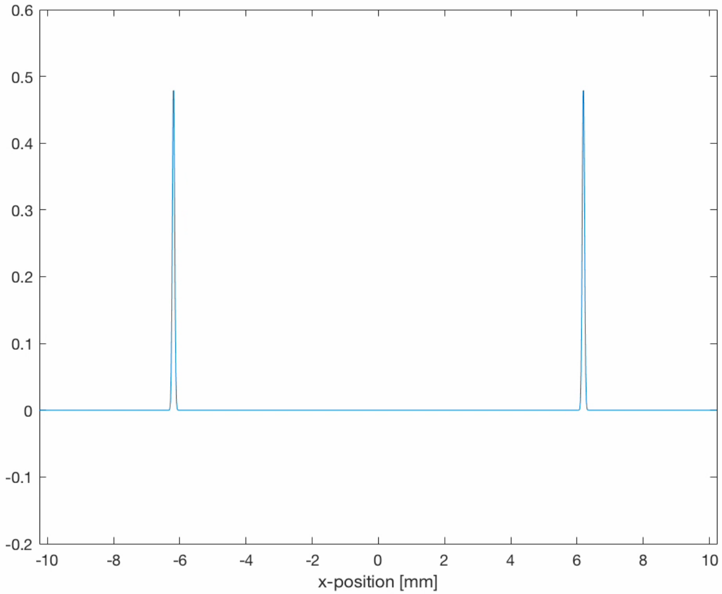
Tabei et al. JASA, 111, 53–63 (2002). Cox & Treeby, Proc. IEEE International Ultrasonics Symposium (2018)

Dispersion correction example

pseudo-spectral time domain

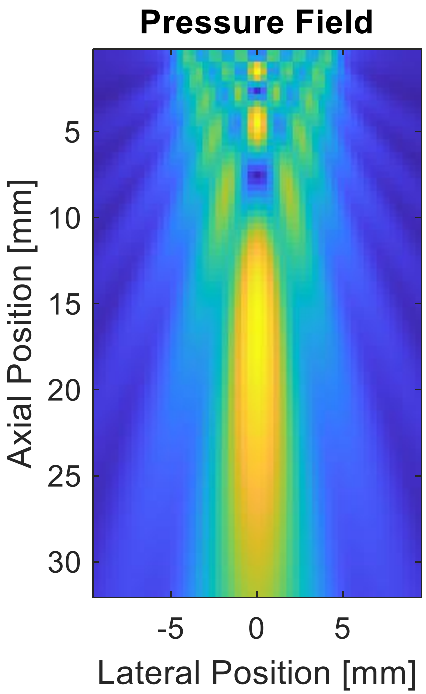


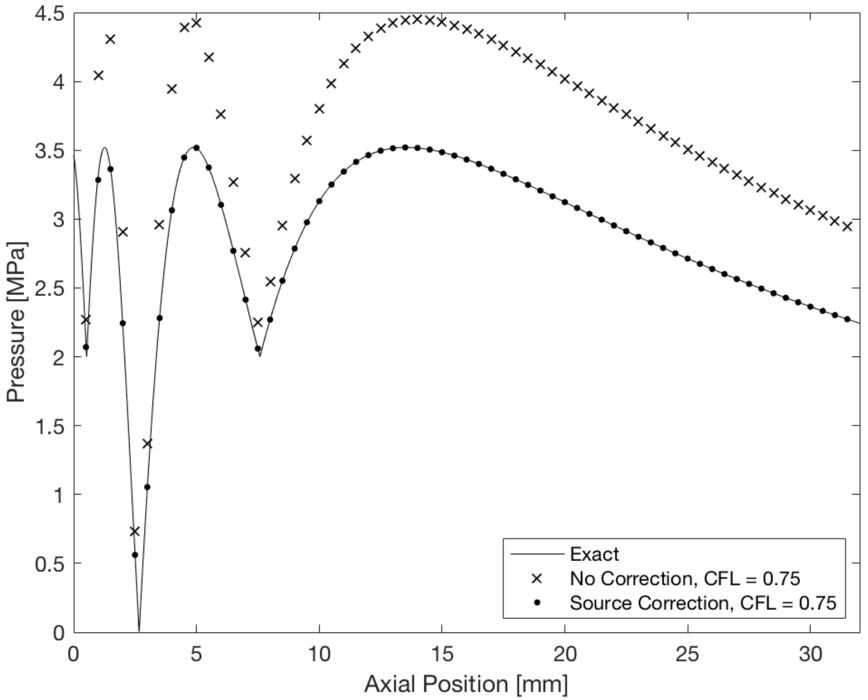
k-space corrected



Time-varying source correction example

- Circular piston transducer, 5mm radius
- 0.5 and 1 MHz simultaneously, 3D simulation
- 3 points-per-wavelength, 4 points-per-period
- Exact solution: Eq. 5-7.3 in Pierce “*Acoustics…*”, 1989.





Effect of staggered grids

- Note the timeshift between source and output
  - In `'additive'` mode, the output samples are `dt/2` ahead of the source samples
  - For the pressure output to correspond to times `0`, `dt`, `2dt`,... the `source.p` must be given at times `-dt/2`, `dt/2`, `3dt/2`,...
- Example: The time series generated by these commands are identical (bar a scaling factor, see below)

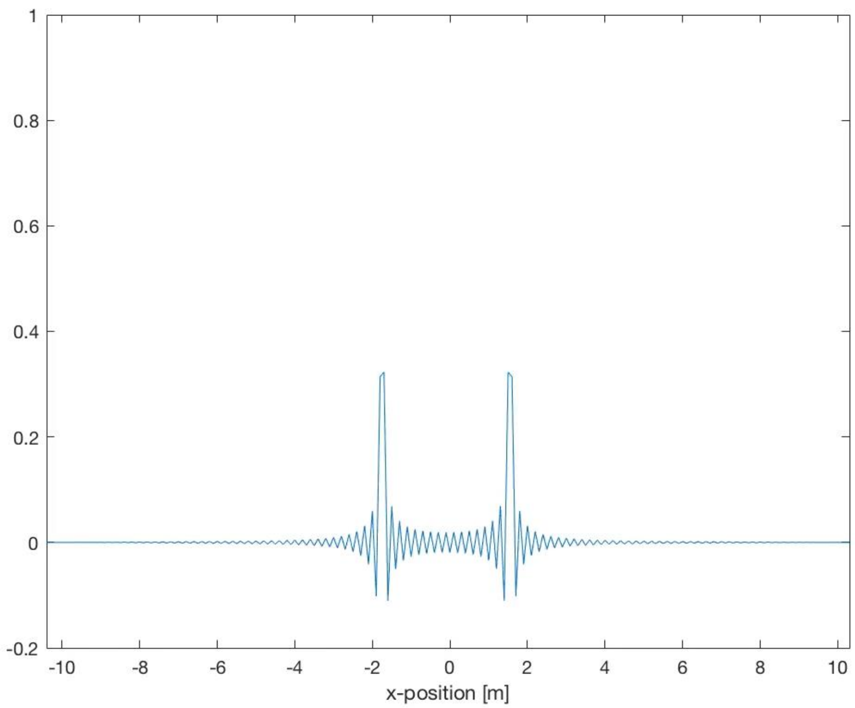
```
source.p0 = <binary_pattern>
```

```
source.p_mask = <binary_pattern>
source.p = [0.5 0.5]
```

To understand k-Wave, understand its Bandlimited Interpolant

Unintuitive behaviour 1: oscillations

- Initial condition: zero at all but one grid point
- Unexpected oscillations in the pulse as it propagates



The bandlimited interpolant (BLI)

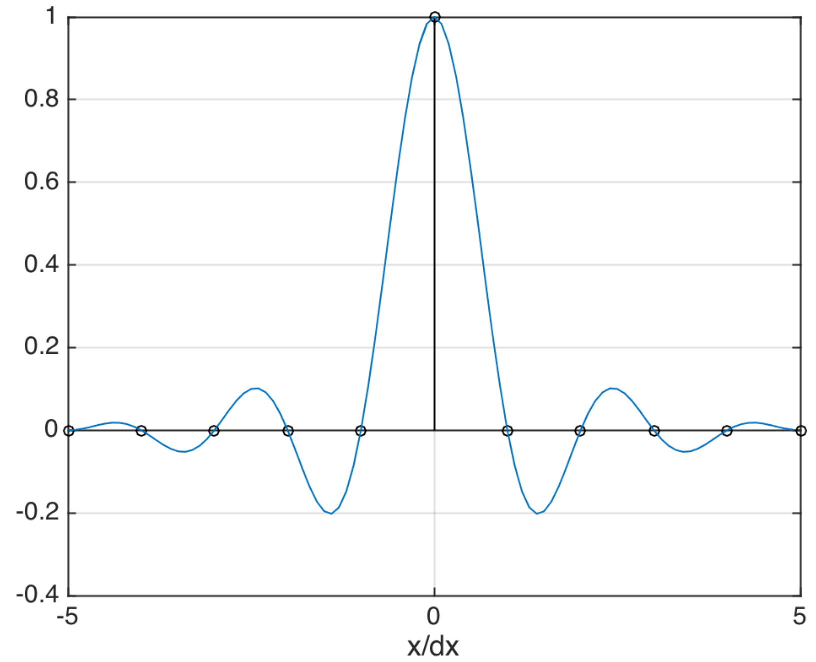
- Sources are defined on the grid: the values between grid points are implied
- For k-Wave, the implied intermediate values are known

$$p_0(x_n) = \begin{cases} 1 & \text{when } x_n = 0 \\ 0 & \text{otherwise} \end{cases}$$

$$P(k_m) = \sum_{n=-N/2}^{N/2-1} p_0(x_n) e^{2\pi i m n/N} = 1 \quad \forall m$$

$$p_0(x) = \frac{1}{N} \sum_{m=-N/2}^{N/2-1} P(k_m) e^{-2\pi i m x/\Delta x N}$$

$$= \frac{1}{N} \cot\left(\frac{x\pi}{\Delta x N}\right) \sin\left(\frac{x\pi}{\Delta x}\right)$$



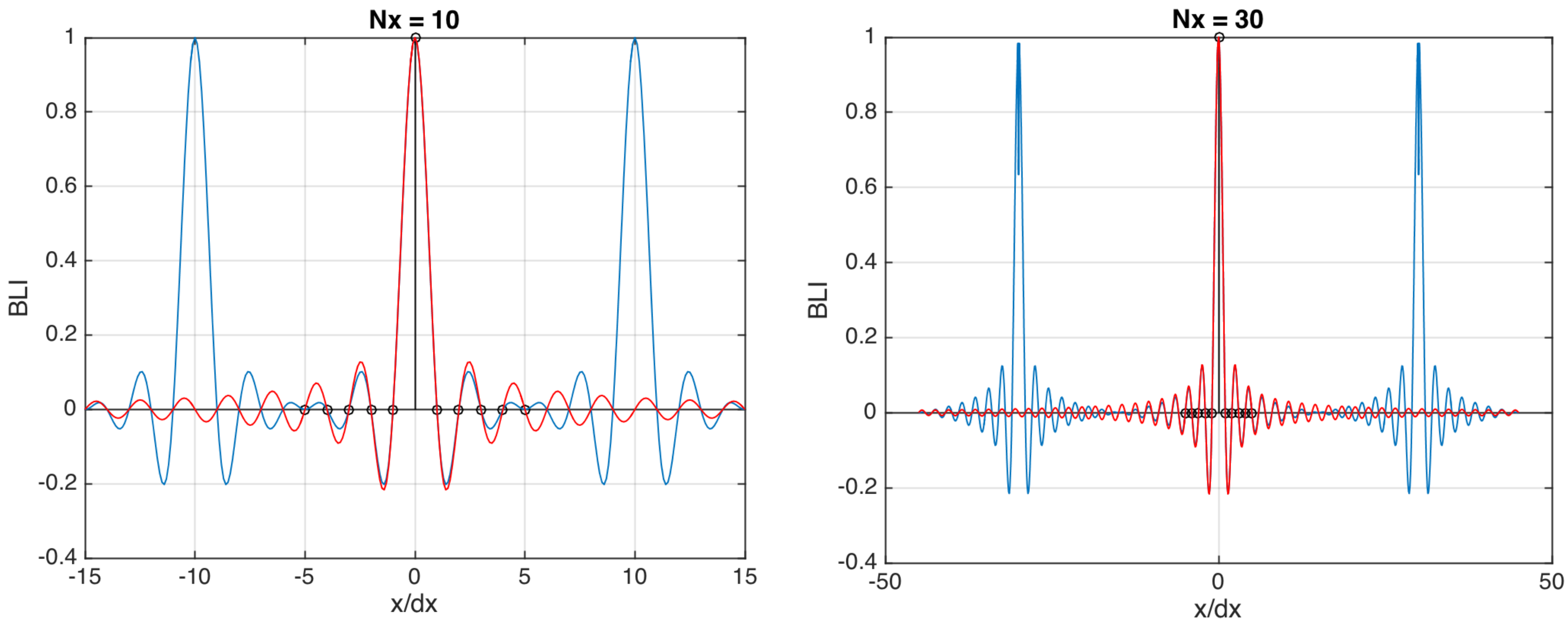
BLI = sum of sinc functions

The BLI can be written as a sum of sinc functions (one per periodic domain):

$$BLI_{1D}(x;0) = \frac{1}{N_x}\cot\left(\frac{x\pi}{\Delta x N_x}\right)\sin\left(\frac{x\pi}{\Delta x}\right) = \sum_{m=-\infty}^{\infty}\mathrm{sinc}\left(\frac{(x \pm m N_x \Delta x)\pi}{\Delta x}\right)$$

The first term is a good approximation:
(It improves as the domain size grows.)

$$BLI_{1D}(x;x_n) \approx \mathrm{sinc}\left(\frac{(x - x_n)\pi}{\Delta x}\right)$$

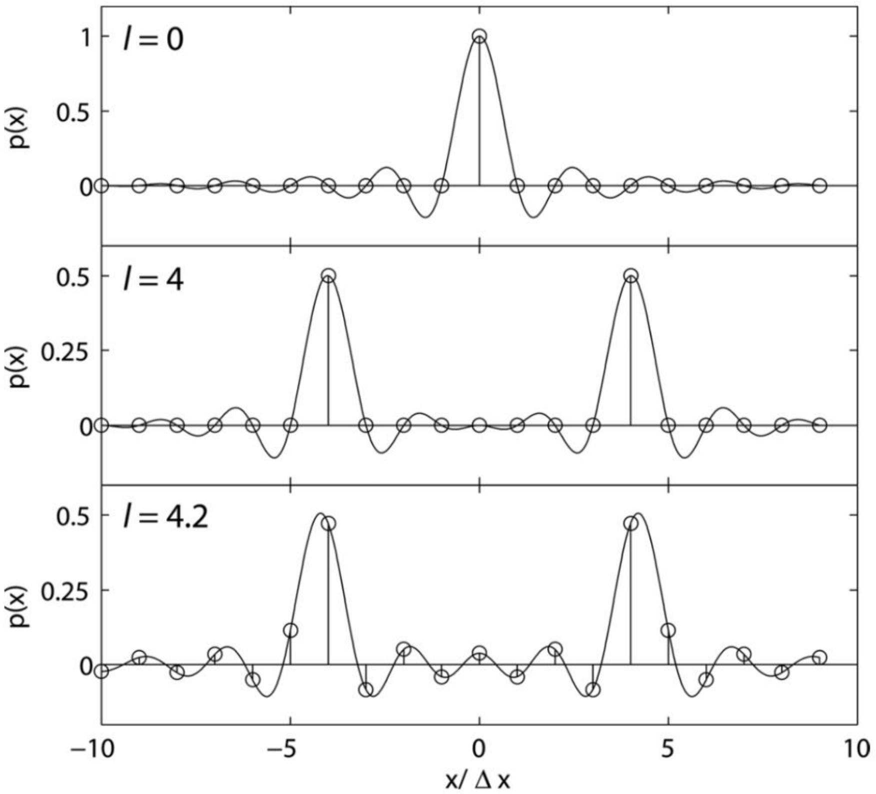


Unexpected oscillations explained

- Pulse propagating in 1D
- Shown at times $t = l\Delta x/c$

time is an integer multiple of $\Delta x/c$

time is non-integer multiple of $\Delta x/c$

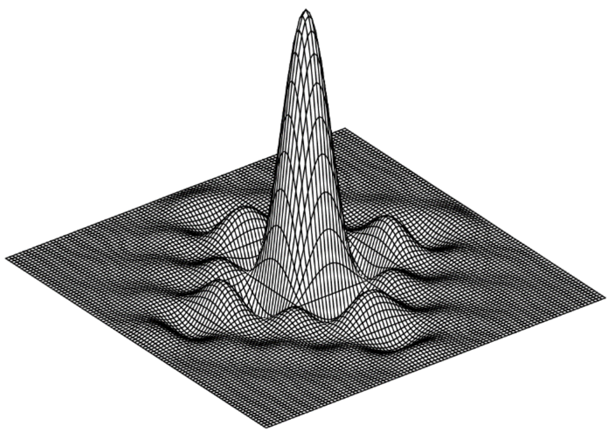


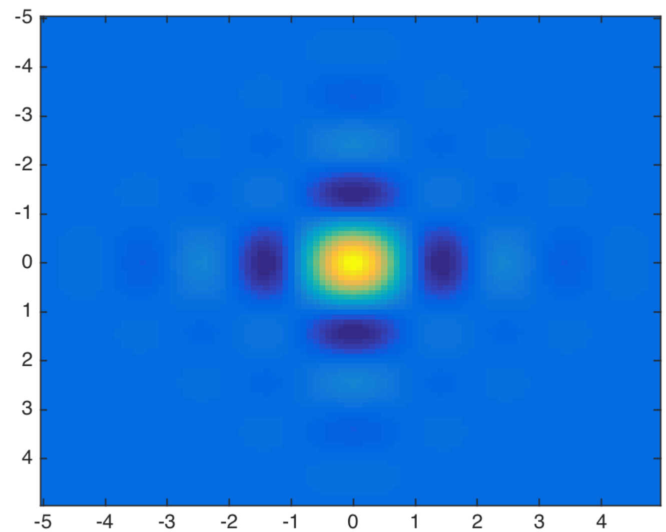
- When the pulse has moved by a non-integer multiple of the spacing, oscillations will show up

The bandlimited interpolant in 2D & 3D

$$BLI_{2D}(x - x_n, y - y_n) \approx \operatorname{sinc}\left(\frac{(x - x_n)\pi}{\Delta x}\right) \operatorname{sinc}\left(\frac{(y - y_n)\pi}{\Delta y}\right)$$

$$BLI_{3D}(x - x_n, y - y_n, z - z_n) \approx \operatorname{sinc}\left(\frac{(x - x_n)\pi}{\Delta x}\right) \operatorname{sinc}\left(\frac{(y - y_n)\pi}{\Delta y}\right) \operatorname{sinc}\left(\frac{(z - z_n)\pi}{\Delta z}\right)$$





The anisotropy or ‘squareness’ of the BLI is related to the fact that k-Wave samples a square (cubic) region of k-space, not a circular (spherical) region.

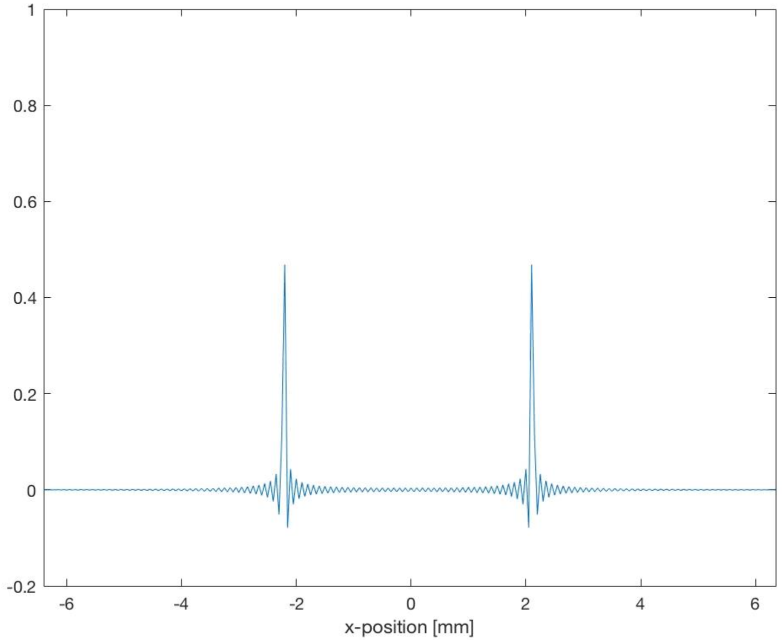
Spatial smoothing for IVPs

- When solving an IVP defined by `source.p0`, k-Wave defaults to the option: `'Smooth', true`.
- This uses a radially symmetric window to remove the high spatial frequencies (using the function `smooth`).

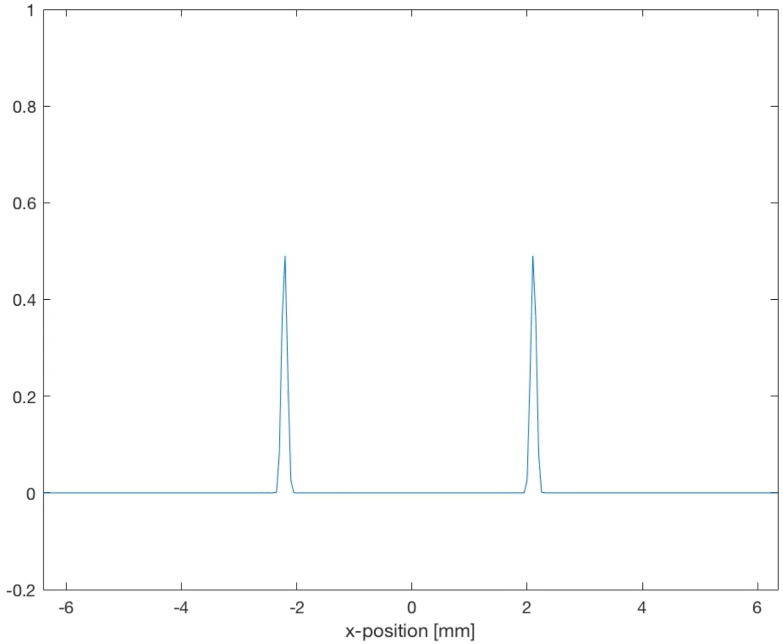
- There are two reasons for this:
  - In 2D & 3D k-Wave supports waves to higher frequencies if they are propagating diagonally across the grid than if they are propagating along the axis directions. Smoothing removes this behaviour.
  - Cosmetic: smoothing removing oscillations due to the BLI

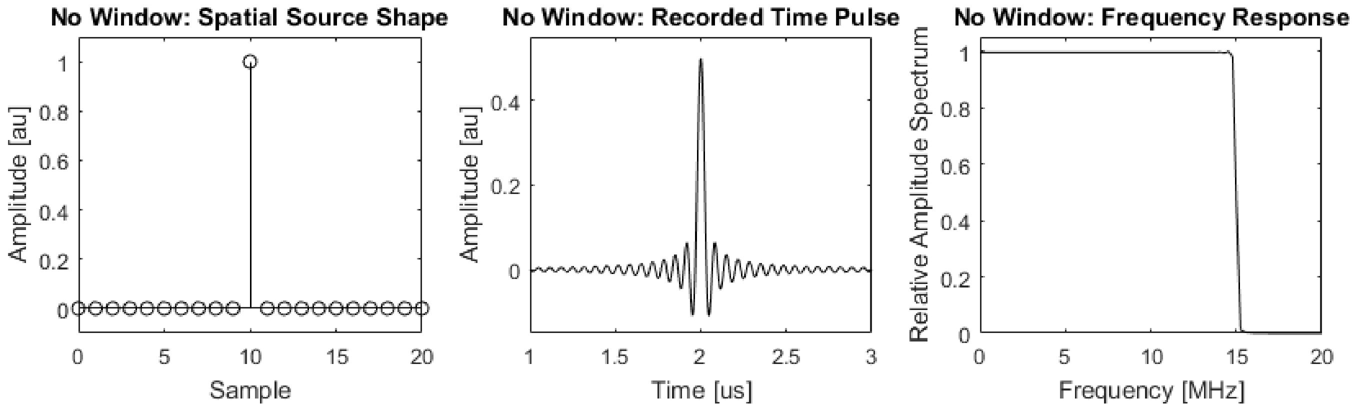
Spatial smoothing for IVPs

Unsmoothed



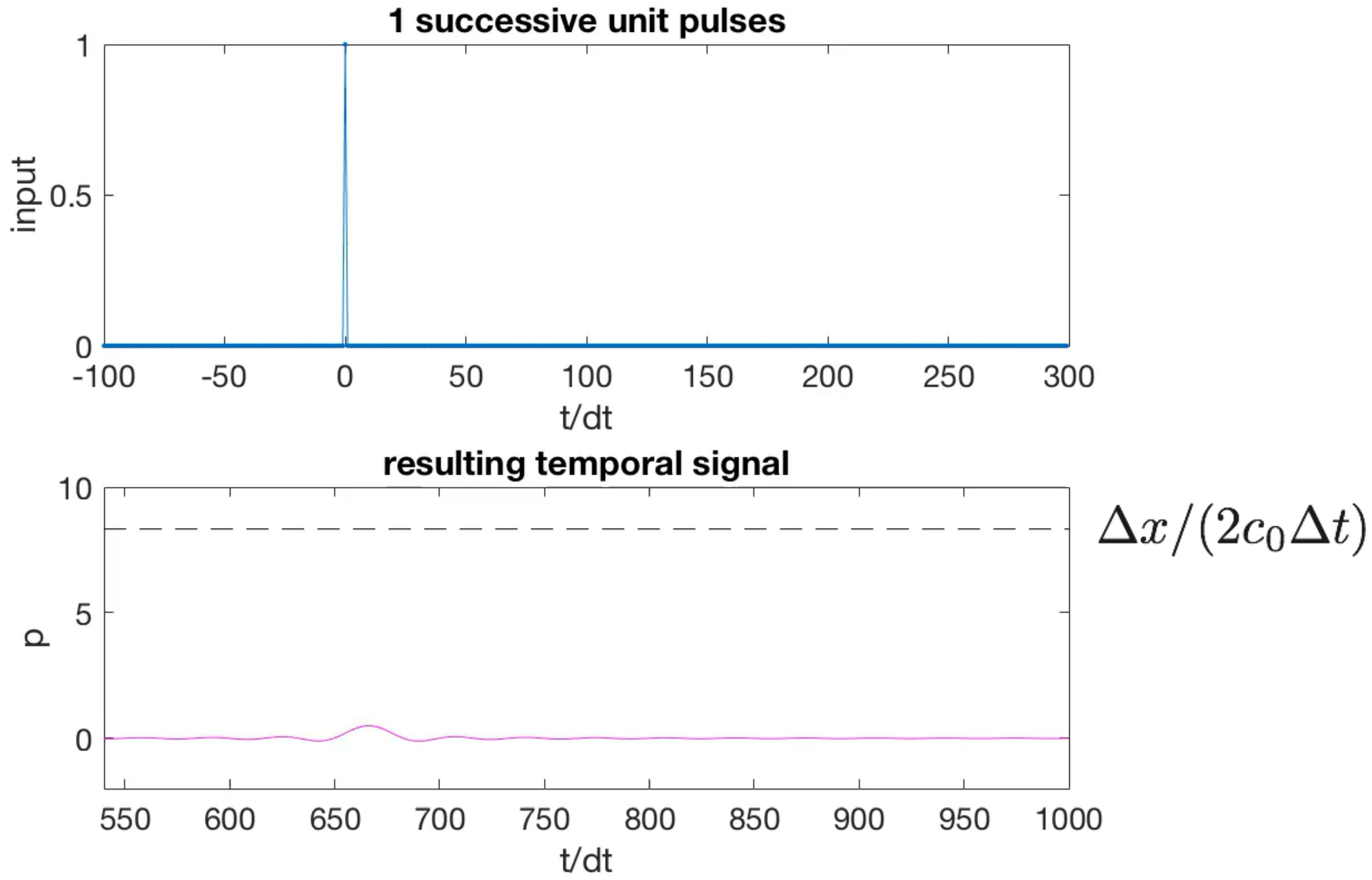
Smoothed




No Window: Spatial Source Shape
Amplitude [au]
1
0.8
0.6
0.4
0.2
0
0
5
10
15
20
Sample
No Window: Recorded Time Pulse
Amplitude [au]
0.4
0.2
0
1
1.5
2
2.5
3
Time [us]
No Window: Frequency Response
Relative Amplitude Spectrum
1
0.8
0.6
0.4
0.2
0
0
5
10
15
20
Frequency [MHz]

Unintuitive behaviour 2: scaling

- The duration of a source signal affects the amplitude
- Converges to $\Delta x/(2c_0\Delta t)$ for long signals $N \gg \Delta x/c_0\Delta t$



Scaling factor explained

- The field from a string of N ones will be a sum of N BLIs each shifted by $\pm c\Delta t$
- For a source at the origin, the pressure field can be written as:

$$p(x, t = N\Delta t) = \frac{1}{2}\sum_{n=0}^{N}\left(BLI(x + cn\Delta t) + BLI(x - cn\Delta t)\right)$$

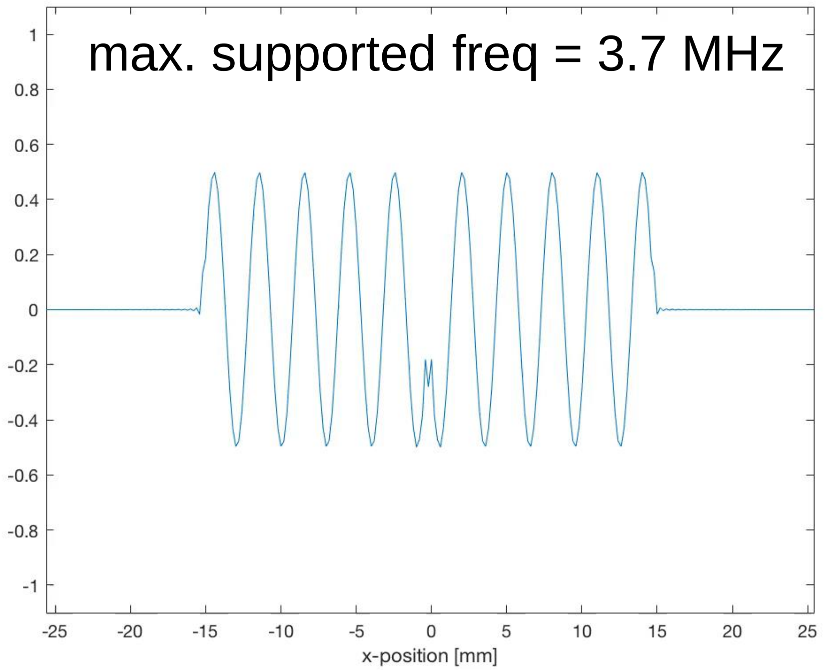
$$= \frac{1}{2}\sum_{n=0}^{N}\left(\mathrm{sinc}\left(\frac{\pi}{\Delta x}(x + cn\Delta t)\right) + \mathrm{sinc}\left(\frac{\pi}{\Delta x}(x - cn\Delta t)\right)\right)$$

- For sufficiently large N, the maximum pressure amplitude will converge to

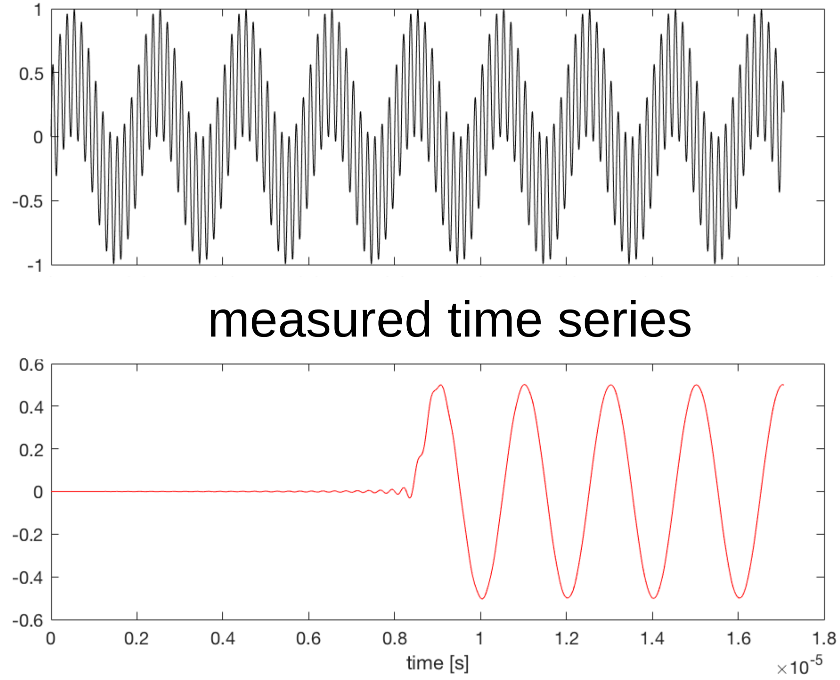
$$\frac{1}{2}\sum_{n=-\infty}^{\infty}\mathrm{sinc}\left(\frac{\pi cn\Delta t}{\Delta x}\right) = \frac{\Delta x}{2c\Delta t}$$

Unintuitive behaviour 3: frequency cutoff

- Source components above the *maximum supported frequency* $f_{\max} = c_0/2\Delta x$ will not propagate.
- These high frequencies are *not* aliased to lower frequencies, the energy is simply lost.

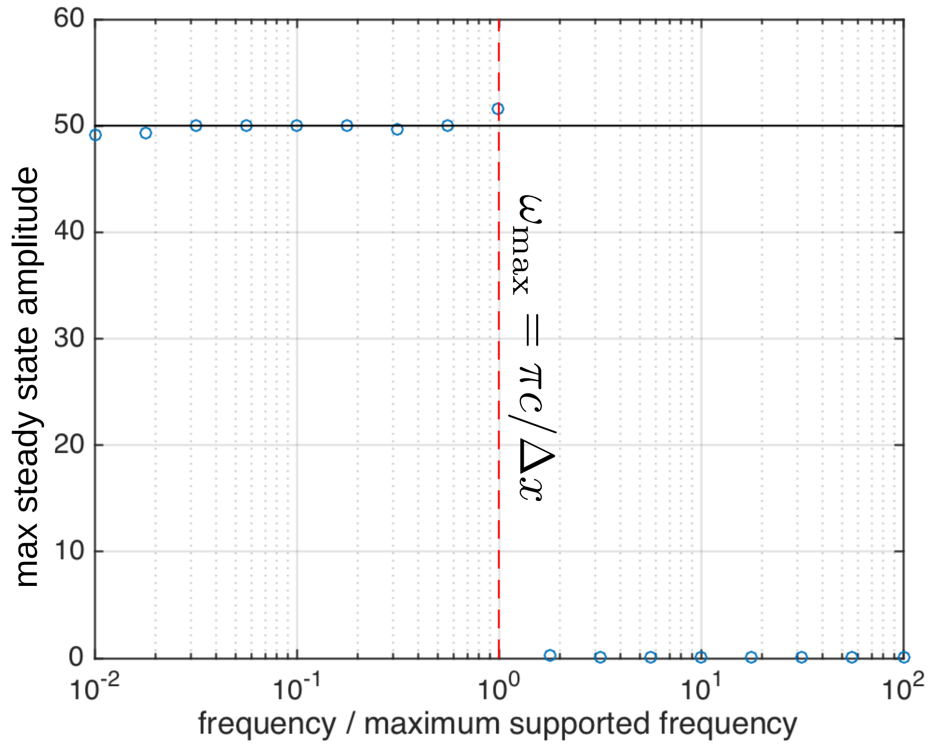


source 6 MHz + 0.5 MHz



Frequency cutoff explained

The scaling factor and cut-off frequency for the cw case can be calculated



$$p(x, t = N\Delta t) =$$

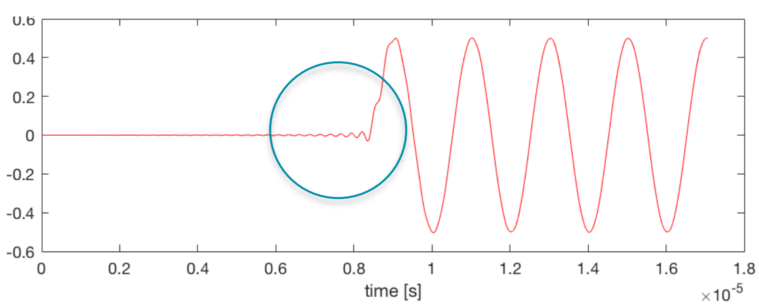
$$\frac{1}{2} \sum_{n=0}^{N} \cos(\omega n \Delta t) \mathrm{sinc}\left(\frac{\pi}{\Delta x}(x \pm cn\Delta t)\right)$$

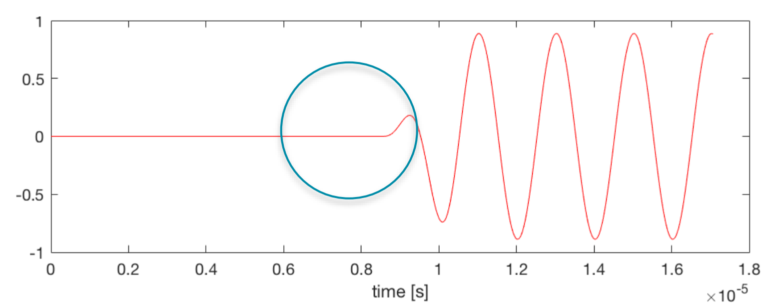
source shifted BLIs

$$\frac{1}{2} \sum_{n=-\infty}^{\infty} \cos(\omega n \Delta t) \mathrm{sinc}\left(\frac{cn\Delta t \pi}{\Delta x}\right) = \begin{cases} \frac{\Delta x}{2c\Delta t} & \text{when } \omega < \omega_{max} \\ \frac{\Delta x}{4c\Delta t} & \text{when } \omega = \omega_{max} \\ 0 & \text{when } \omega > \omega_{max} \end{cases}$$

Temporal filtering of sources

- Nevertheless, it can be helpful to filter the signal `source.p` using the function `filterTimeSeries`
- Two reasons:
  - Ramp up to avoid transient start-up oscillations
  - Filter out above cut-off frequency to avoid non-propagating frequencies in `source.p`
  - Causal filtering by default

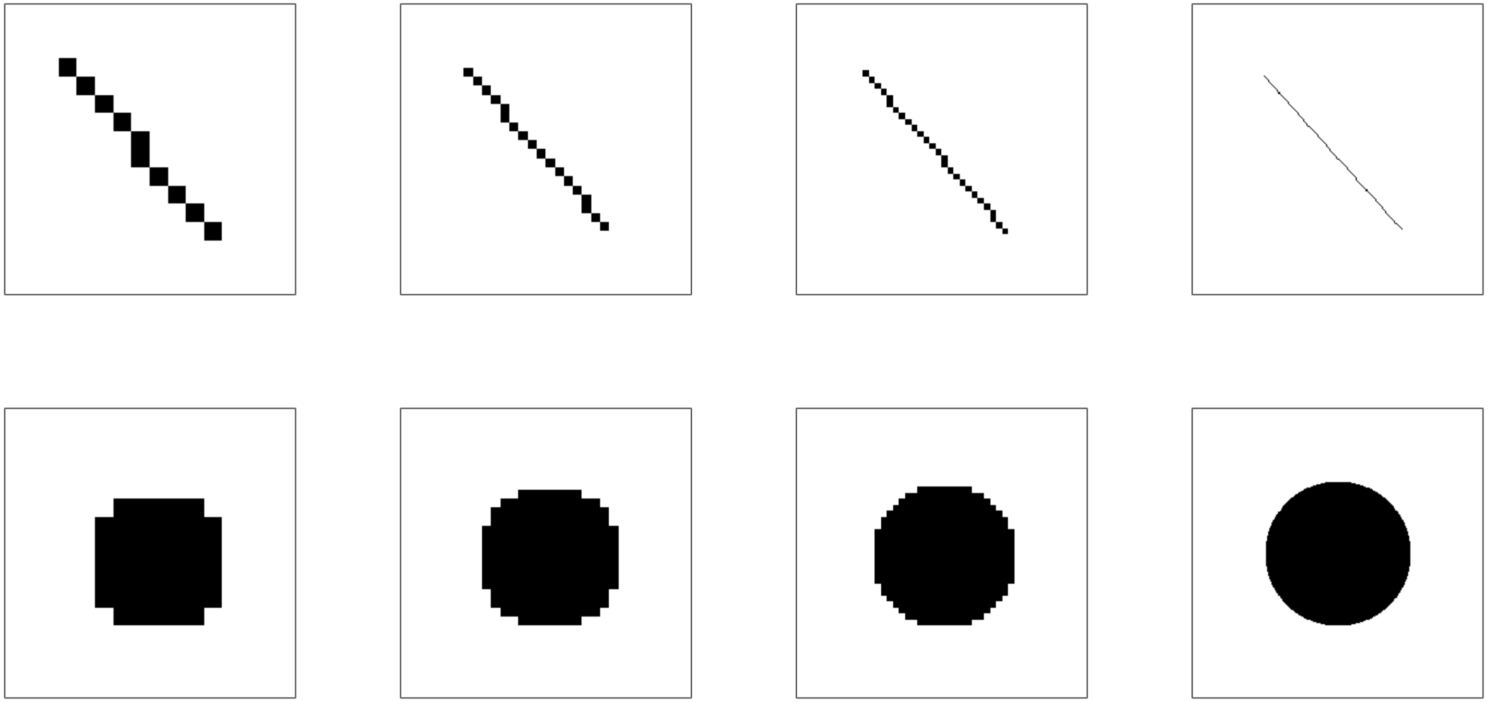




Exploiting the fact we know k-Wave's Bandlimited Interpolant

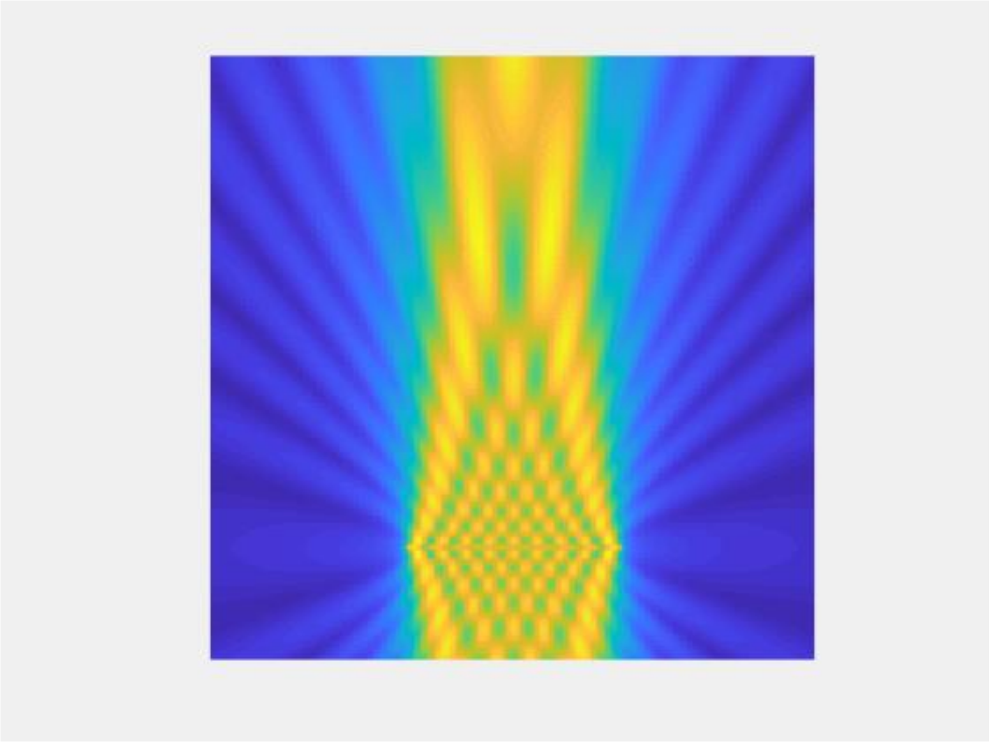
Source staircasing

- Representing continuous sources on a grid leads to 'staircasing', which can lead to unexpected results



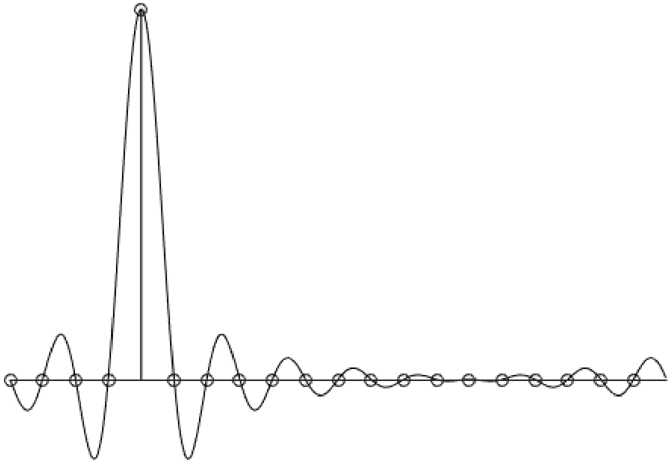
Source staircasing

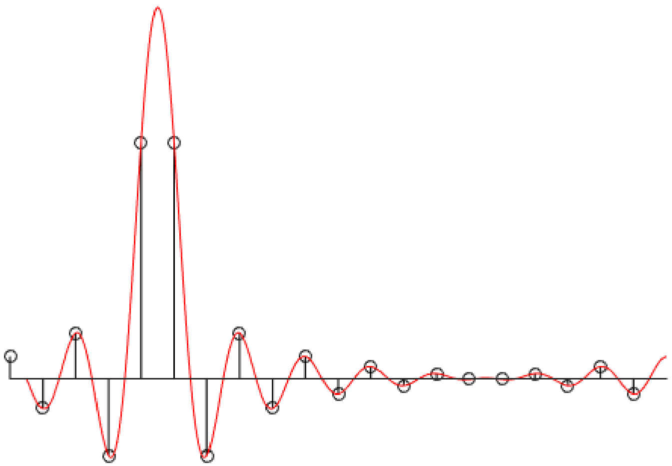
- The effect of staircasing on beam patterns



Off-grid source placement

- The more general problem: how can we place sources at points that are not grid points?





Modelling off-grid sources

- In a numerical model, the best achievable approximation of a desired continuous source distribution, $f(\mathbf{x})$, is its bandlimited version
- This is found by convolving with the BLI (the bandlimited delta function)

$$f_{\mathrm{BL}}(\mathbf{x}) = \int BLI(\mathbf{x} - \mathbf{x}')f(\mathbf{x}')d\mathbf{x}'$$

- Sampling this at the grid points gives the required source amplitudes for input to k-Wave

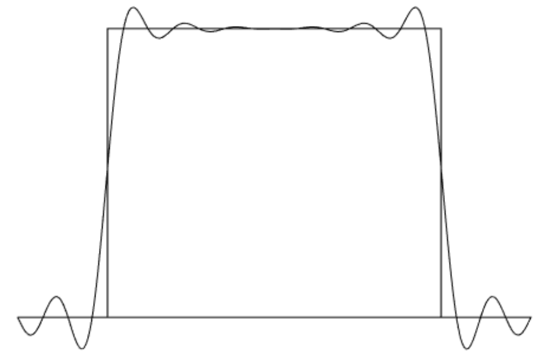
$$\hat{a}_n = f_{\mathrm{BL}}(\mathbf{x})\big|_{\mathbf{x}=\mathbf{x}_n}$$

Wise et al., JASA, 146, 278-288 (2019)

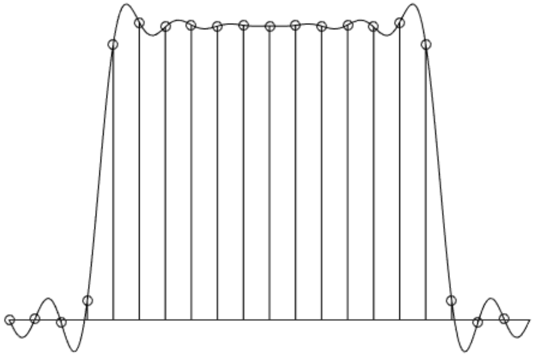
Modelling off-grid sources

desired continuous source

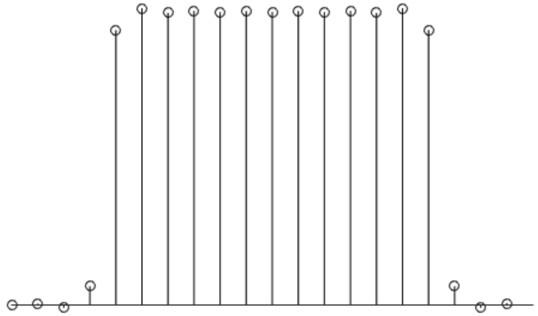
bandlimited version



sample the bandlimited version

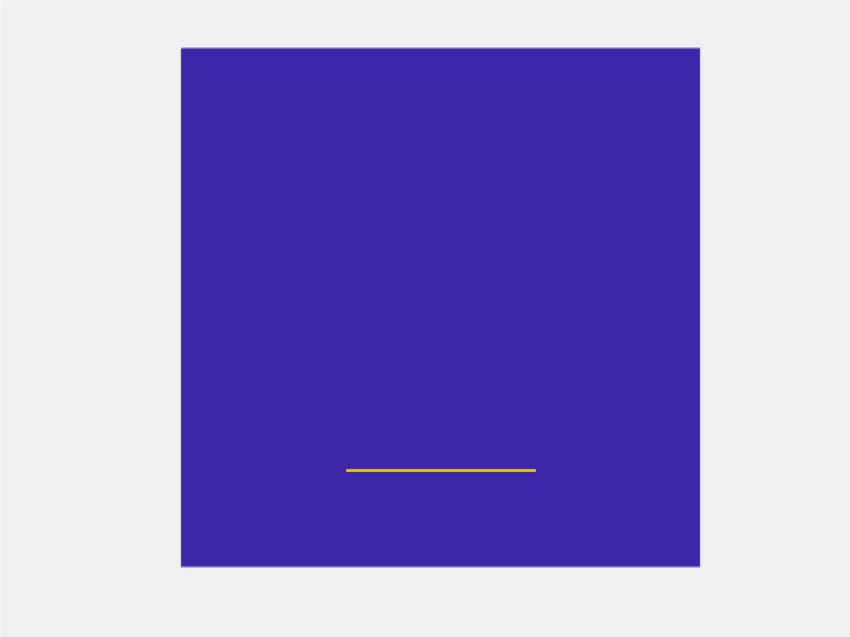


use these source amplitudes

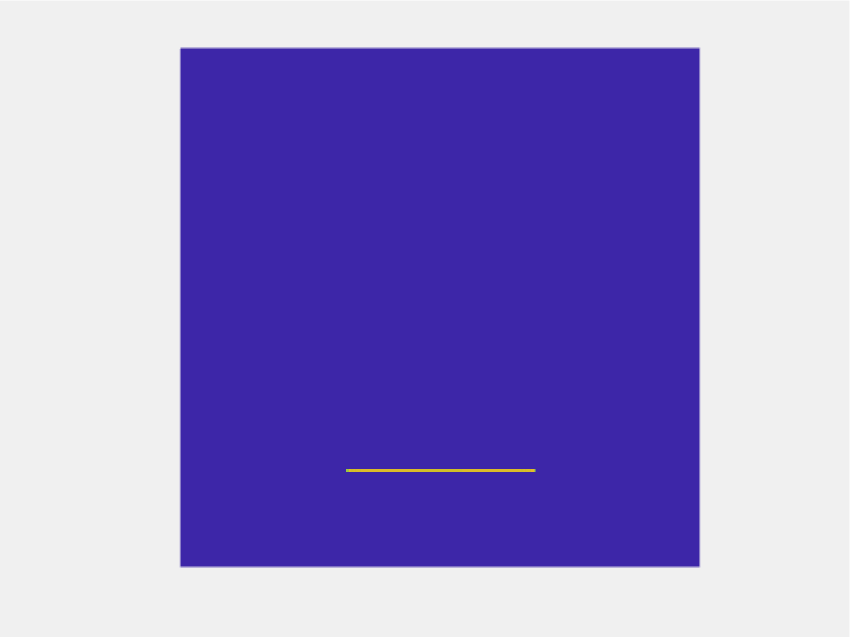


Modelling off-grid sources

- On-grid ‘line’ source

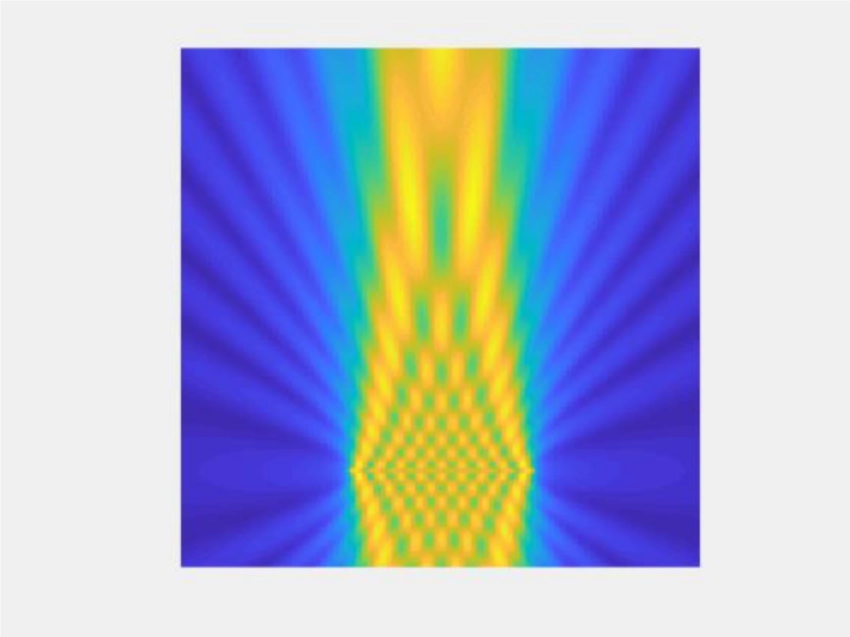


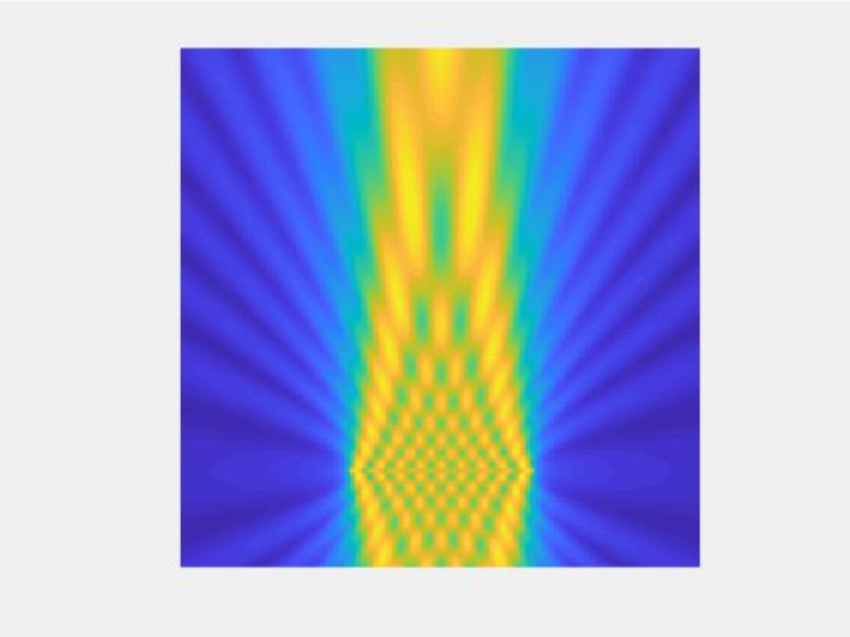
- Off-grid line source



Modelling off-grid sources

- On-grid ‘line’ source
- Off-grid line source



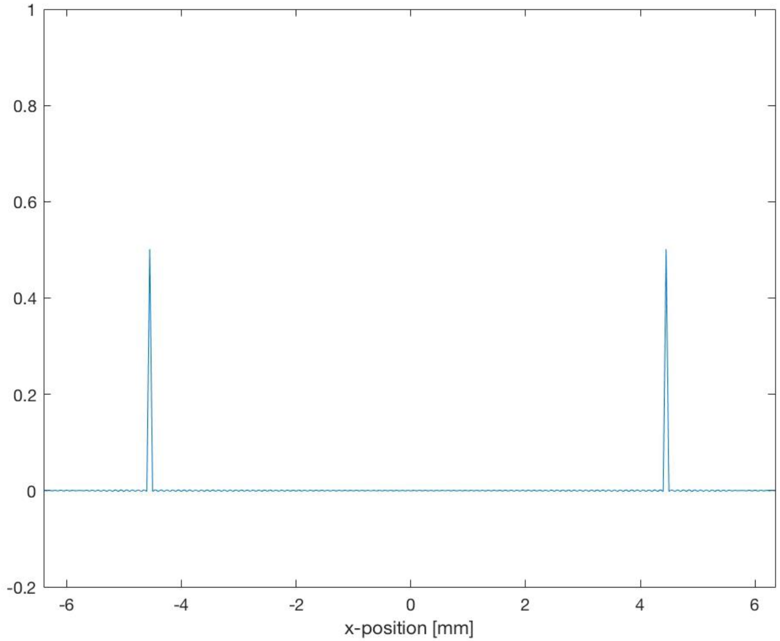


- Off-grid sources & detectors will be integrated into k-Wave as kWaveArray class
- alpha version is currently available: see this post on the k-Wave Forum: http://www.k-wave.org/forum/topic/alpha-version-of-kwavearray-off-grid-sources

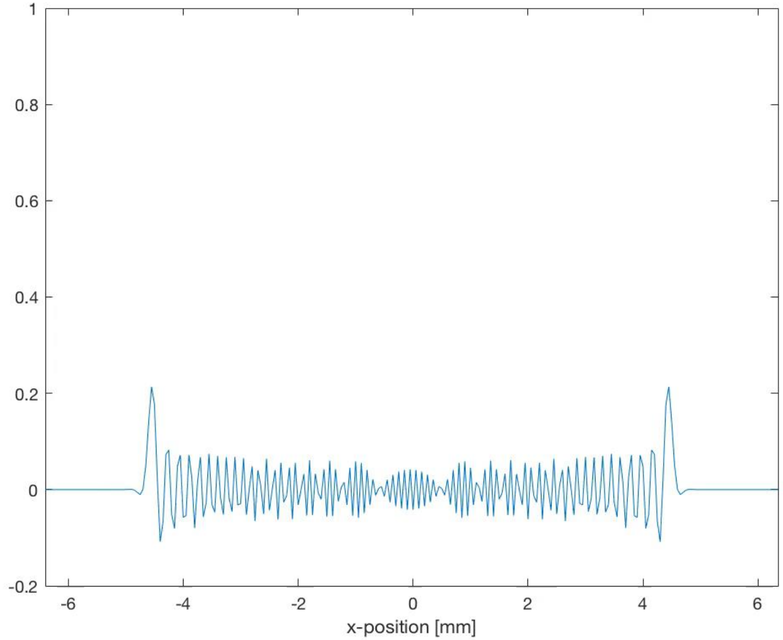
Wise et al., JASA, 146, 278-288 (2019)

BLIs are not unique to k-Wave!

Unsmoothed k-Wave



Unsmoothed finite difference
(fourth-order accurate)



- But k-Wave has the advantage that we know what the BLI is

Summary

- k-Wave can model initial value problems
- k-Wave can model the response to broadband, time-varying, pressure or velocity sources
- Many aspects of k-Wave's behaviour can be understood by considering its Bandlimited Interpolant (BLI)
- Source content at frequencies higher than supported by the grid are lost, not propagated.
- Off-grid sources can be used to ameliorate source staircasing