Application of a non-uniform FFT to spectral resampling in Fourier transform specrometry

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A Spectral Resampling Problem

Let $s : \mathbb{R} \to \mathbb{R}$ be a continuous band-pass spectrum such that $s(v) = 0$ when $v \notin (v_{\text{min}}, v_{\text{max}})$.

Consider the uniform frequency grid with one point at $v = 0$ and

$$\delta v = \frac{2(v_{\text{max}} - v_{\text{min}})}{N}$$

where $N \in \mathbb{N}$.

Also, assume

$$\frac{v_{\text{min}}}{\delta v} \in \mathbb{N}.$$

A Spectral Resampling Problem (cont.)

Let $\mathrm{s} \in \mathbb{R}^N$ be

$$\mathrm{s} = \begin{bmatrix} s(v_{\mathsf{min}}) \\ s(v_{\mathsf{min}} + \delta v) \\ s(v_{\mathsf{min}} + 2\delta v) \\ \vdots \\ s(v_{\mathsf{min}} + q\delta v) \\ s(-\{v_{\mathsf{min}} + p\delta v\}) \\ \vdots \\ s(-\{v_{\mathsf{min}} + 2\delta v\}) \\ s(-\{v_{\mathsf{min}} + \delta v\}) \end{bmatrix}$$

where

$$p = \text{floor}\left(\frac{N-1}{2}\right) \quad \text{and} \quad q = \text{floor}\left(\frac{N}{2}\right).$$

A Spectral Resampling Problem (cont.)

Let $\tilde{f}_j \in \mathbb{R}$ be

$$\tilde{f}_j = \sum_{k=0}^{q} e^{\frac{2\pi i}{N} j(k(1-\rho)-\beta)} s(v_{\text{min}} + k\delta v) + \sum_{k=1}^{p} e^{-\frac{2\pi i}{N} j(k(1-\rho)-\beta)} s(-\{v_{\text{min}} + k\delta v\}),$$

and $\tilde{\mathbf{f}} \in \mathbb{R}^N$ be

$$\tilde{\mathbf{f}} = \begin{bmatrix} \tilde{f}_0 \\ \tilde{f}_1 \\ \tilde{f}_2 \\ \vdots \\ \tilde{f}_q \\ \tilde{f}_{-p} \\ \vdots \\ \tilde{f}_{-2} \\ \tilde{f}_{-1} \end{bmatrix}.$$

A Spectral Resampling Problem (cont.)

Let $\mathbf{E}(\rho, \beta) \in \mathbb{C}^{N \times N}$ be the operator such that

$$\mathbf{E}\mathbf{s} = \tilde{\mathbf{f}},$$

as a function of ρ and β, $\mathbf{E} : \mathbb{R}^2 \rightarrow \mathbb{C}^{N \times N}$.

Given $\tilde{\mathbf{f}}$, the problem is to estimate $\mathbf{s}$ by some $O(N \log N)$ operation.

Let $\mathbf{F} \in \mathbb{C}^{N \times N}$ be the DFT operator. We will

1. show that $\mathbf{E}^H$ could be a good approximation to $N\mathbf{E}^{-1}$,

2. approximate $\mathbf{E}^H$ by $\mathbf{F}^H = N\mathbf{F}^{-1}$ and

3. use FFT to solve the above problem.

An Approximation to $\mathbf{E}^{-1}$

Consider one element of $\mathbf{E}(\rho, \beta)$

$$e^{\frac{2\pi i}{N} j(k(1-\rho)-\beta)}.$$

Clearly

- $\mathbf{E}(0,0) = \mathbf{F}$ and $\mathbf{E}^H(0,0) = \mathbf{F}^H$, and

- $\mathbf{E}$ and $\mathbf{E}^H$ are continuous on $\mathbb{R}^2$,

hence

- $\mathbf{E}^H\mathbf{E}$ is continuous at $(\rho = 0, \beta = 0)$, and

- $\left(\mathbf{E}^H\mathbf{E}\right)(\rho, \beta) \approx \mathbf{F}^H\mathbf{F} = N\mathbf{I}$ if $\sqrt{\rho^2 + \beta^2}$ is small enough.

An Approximation to $\mathbf{E}^H$

Let $\mathbf{D}, \tilde{\mathbf{I}} \in \mathbb{R}^{N \times N}$ and $\mathbf{C}, \mathbf{S} : \mathbb{R} \to \mathbb{R}^{N \times N}$ be diagonal matrices such that

- $\text{diag}(\mathbf{D})^T = [0, 1, 2, \cdots, q, -p, \cdots, -2, -1]$

- $\text{diag}(\tilde{\mathbf{I}})^T = [\underbrace{-1, -1, -1, \cdots, -1}_{q+1}, \underbrace{1, \cdots, 1, 1}_{p}]$

- $\text{diag}\left(\mathbf{C}(\beta)\right) = \cos\left(\frac{2\pi}{N}\beta \, \text{diag}(\mathbf{D})\right)$

- $\text{diag}\left(\mathbf{S}(\beta)\right) = \sin\left(\frac{2\pi}{N}\beta \, \text{diag}(\mathbf{D})\right)$

An Approximation to $\mathbf{E}^H$ (cont.)

The sample element of $\mathbf{E}$ can be rewritten as

$$e^{\frac{2\pi i}{N} j(k(1-\rho)-\beta)} = \cos\left(\frac{2\pi}{N}\beta j\right) e^{\frac{2\pi i}{N} jk(1-\rho)} - i \sin\left(\frac{2\pi}{N}\beta j\right) e^{\frac{2\pi i}{N} jk(1-\rho)}.$$

After rewriting all elements of $\mathbf{E}$ as above and some factorization we get

$$\mathbf{E} = \mathbf{C}\mathbf{E}_0 + i\mathbf{S}\mathbf{E}_0\tilde{\mathbf{I}}$$

where

$$\mathbf{E}_0 = \mathbf{E}(\rho, 0).$$

An Approximation to $\mathbf{E}^H$ (cont.)

A sample element of $\mathbf{E}_0 : \mathbb{R} \to \mathbb{R}^{N\times N}$ is

$$e^{\frac{2\pi i}{N} jk(1-\rho)},$$

which is an analytic function of ρ. The $m+1\ \underline{st}$ term of its Taylor series expansion at $\rho = 0$ is

$$\frac{1}{m!}\alpha^m j^m\ e^{\frac{2\pi i}{N} jk}\ k^m \rho^m \quad \text{where} \quad \alpha = -\frac{2\pi i}{N},$$

hence the $m+1\ \underline{st}$ term of the Taylor series expansion of $\mathbf{E}_0$ at $\rho = 0$ is

$$\frac{1}{m!}\alpha^m \mathbf{D}^m \mathbf{F} \mathbf{D}^m \rho^m.$$

The Taylor series expansion of $\mathbf{E}_0$ is

$$\mathbf{F} + \alpha \mathbf{D}\mathbf{F}\mathbf{D}\rho + \frac{1}{2!}\alpha^2 \mathbf{D}^2 \mathbf{F} \mathbf{D}^2 \rho^2 + \cdots$$

An Approximation to $\mathbf{E}^H$ (cont.)

By the same method used to approximate $\mathbf{E}$,

$$\mathbf{E}^H = \mathbf{E}_0^H \mathbf{C} - i\tilde{\mathbf{I}}\mathbf{E}_0^H \mathbf{S}$$

and the Taylor series expansion of $\mathbf{E}_0^H$ is

$$\mathbf{F}^H + \bar{\alpha}\mathbf{D}\mathbf{F}\mathbf{D}\rho + \frac{1}{2!}\bar{\alpha}^2\mathbf{D}^2\mathbf{F}^H\mathbf{D}^2\rho^2 + \cdots + \frac{1}{m!}\bar{\alpha}^m\mathbf{D}^m\mathbf{F}^H\mathbf{D}^m\rho^m + \cdots,$$

where $\bar{\alpha} = \frac{2\pi i}{N}$.

Performance

A second method for estimating $\mathbf{s} \in \mathbb{R}^N$ requires a zero-padded FFT and Shannon linear interpolation. Based on experience, $\tilde{\mathbf{f}}$ should be zero padded to at least 64 times its original size;

- $O(64N \log(N) + 64 \log(64) N)$ flops for FFT

- N linear interpolations.

Our method produces "similar" result if $\mathbf{E}_0(\rho)$ is replaced by its quadratic approximation;

- $O(6N \log(N))$ flops for FFT

- $23N$ other flops

- N cos and N sin evaluations.

Examples

Let

- c = compression factor due to off-axis
- d = Doppler shift due to velocity
- s = *slope* ($2^{\underline{nd}}$ order freq. correction)
- o = *offset* ($2^{\underline{nd}}$ order freq. correction).

Then to correct $\tilde{\mathbf{f}}$ for c let

$$\rho = c \quad \text{and} \quad \beta = \rho \frac{v_{\mathsf{min}}}{\delta v},$$

for d, s and o let

$$\rho = 1 - \frac{d}{s} \quad \text{and} \quad \beta = \rho \frac{v_{\mathsf{min}}}{\delta v} + \frac{o}{\delta v}$$

and for c, d, s and o together let

$$\rho = 1 - \frac{d}{s}(1 - c) \quad \text{and} \quad \beta = \rho \frac{v_{\mathsf{min}}}{\delta v} + \frac{o}{\delta v}.$$

Example #1

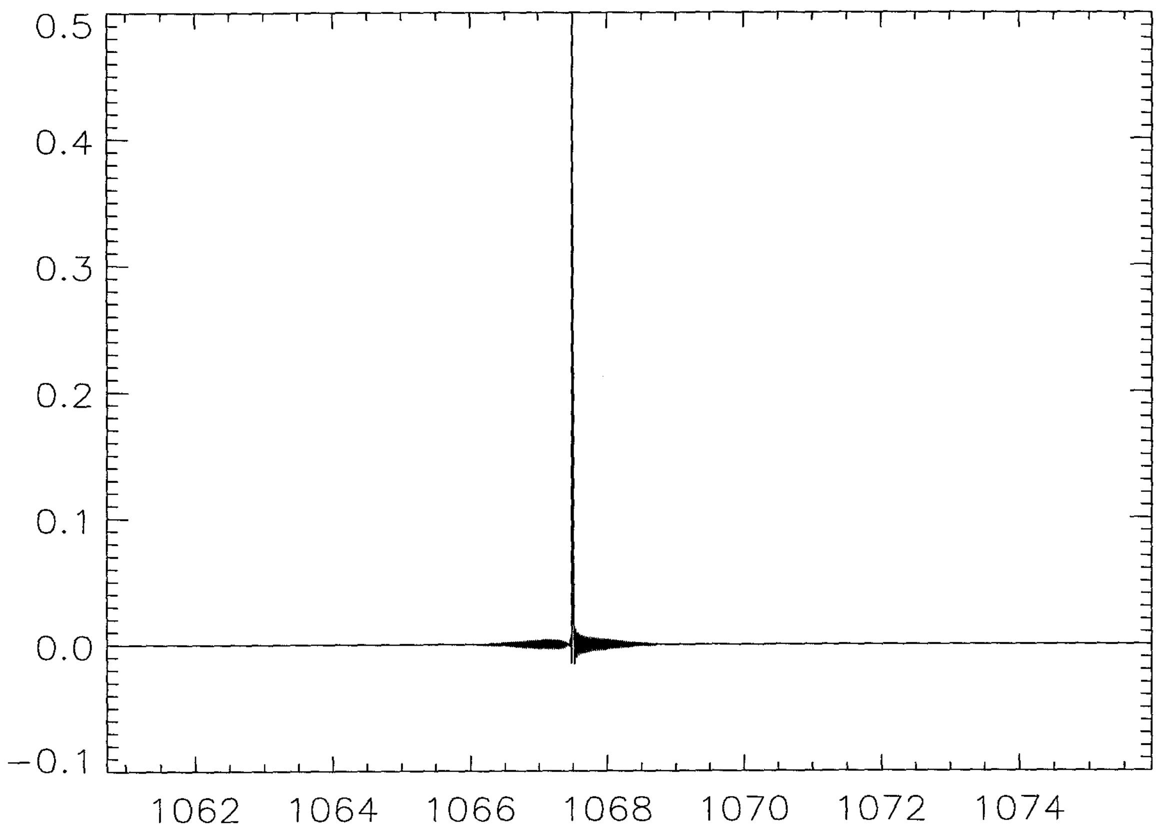
For a monochromatic, 1067.50 (cm^{-1}), spectrum s where

- $v_{\text{min}} = 1060.7366$ (cm^{-1})
- $v_{\text{max}} = 1075.8752$ (cm^{-1})
- $\delta v = 0.014798222$ (cm^{-1})
- $N = 2048$
- $c = 1.818000 \times 10^{-5}$
- $d = 0.99999500$
- $s = 0.99992401$
- $o = 0.01000000$

we have

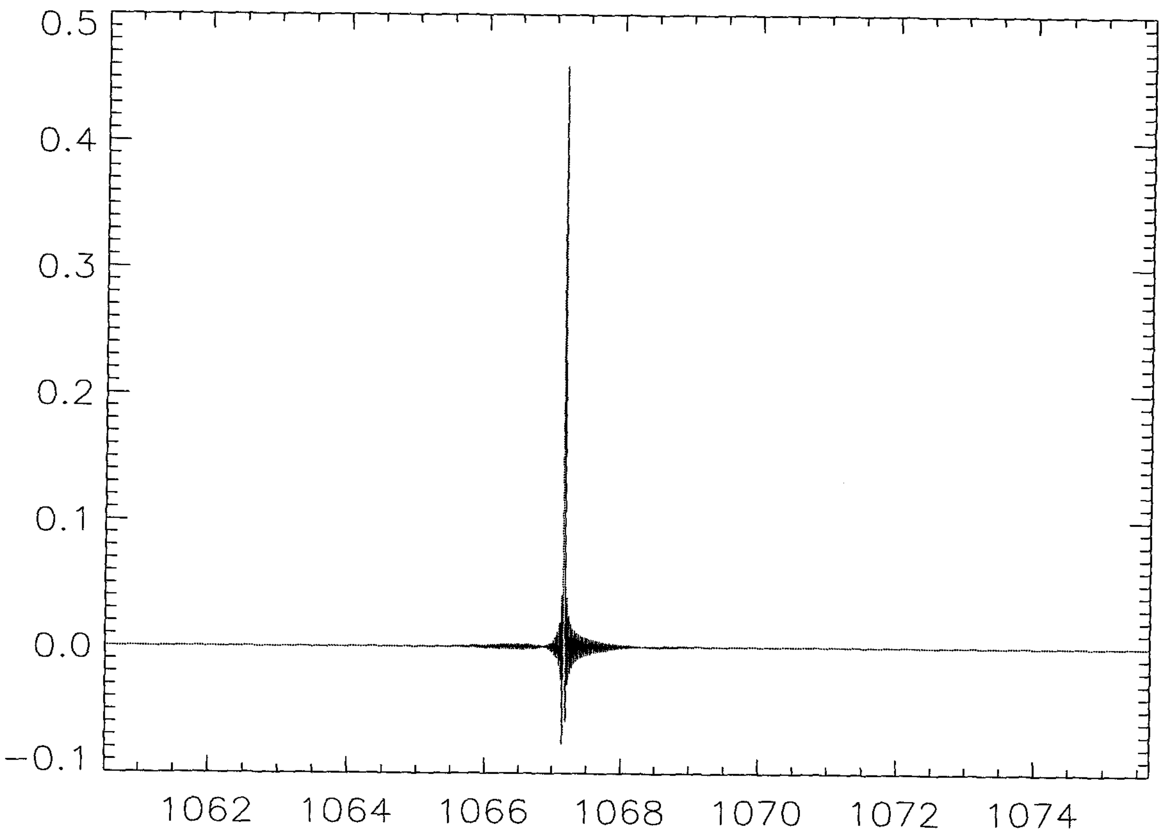
$$\frac{v_{\text{min}}}{\delta v} = 71680.0$$

Example #1 (cont.)



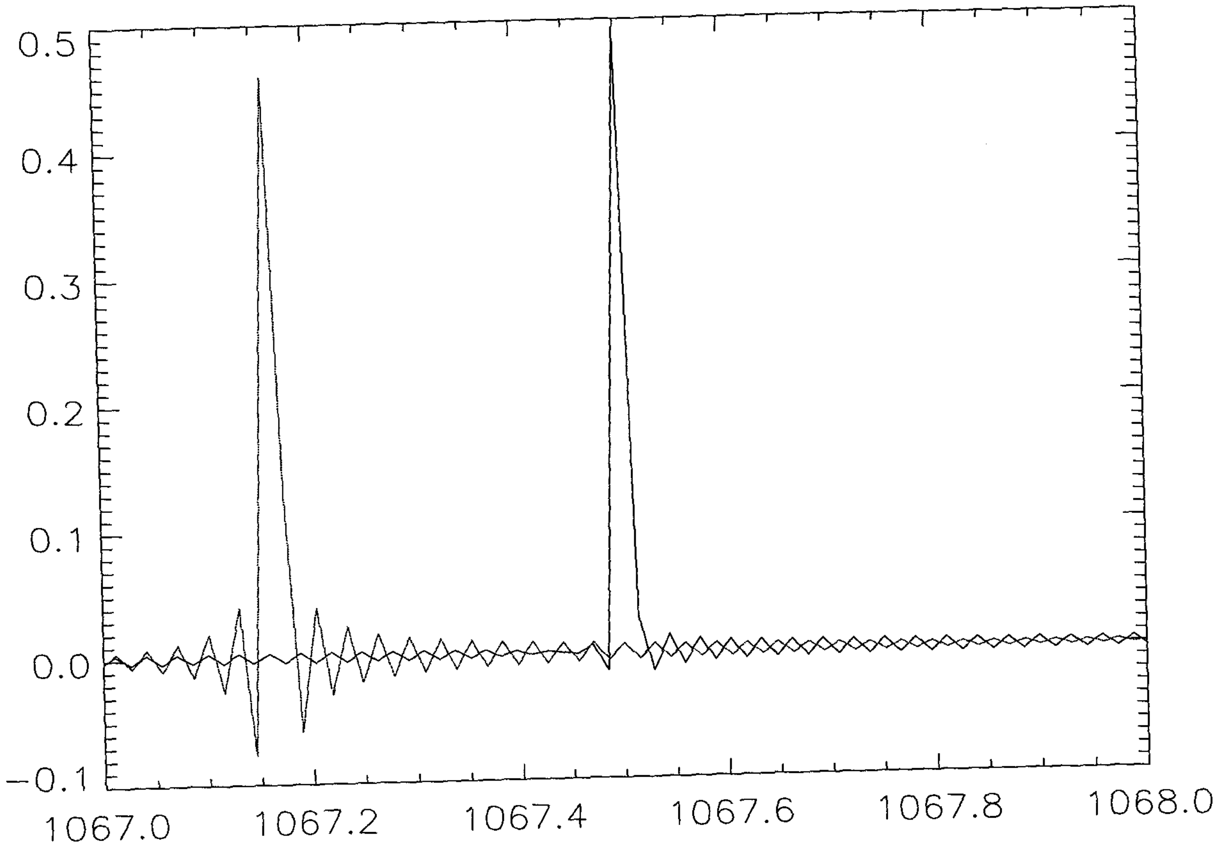
$$\mathbf{s} = \mathbf{E}^{-1}\tilde{\mathbf{f}}$$

Example #1 (cont.)



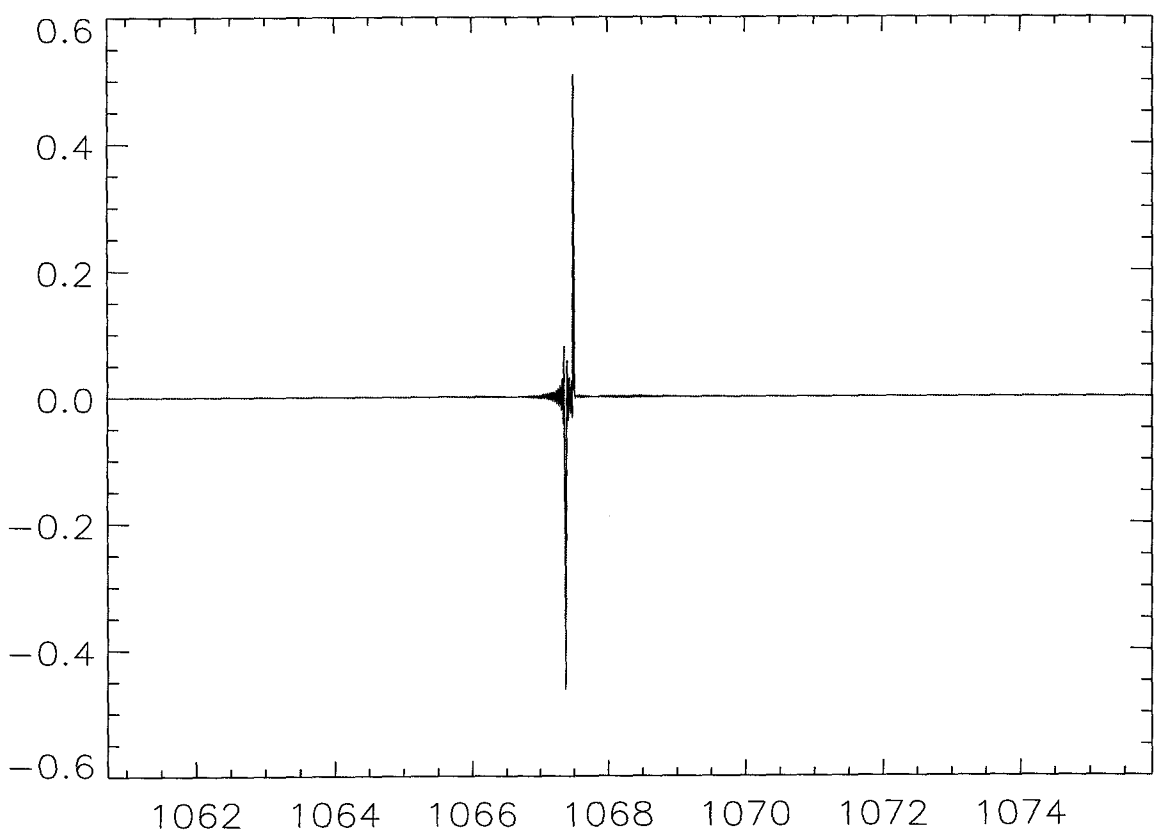
$$\tilde{\mathbf{s}} = \frac{1}{N}\mathbf{F}^H\tilde{\mathbf{f}} = \mathbf{F}^{-1}\tilde{\mathbf{f}}$$

Example #1 (cont.)



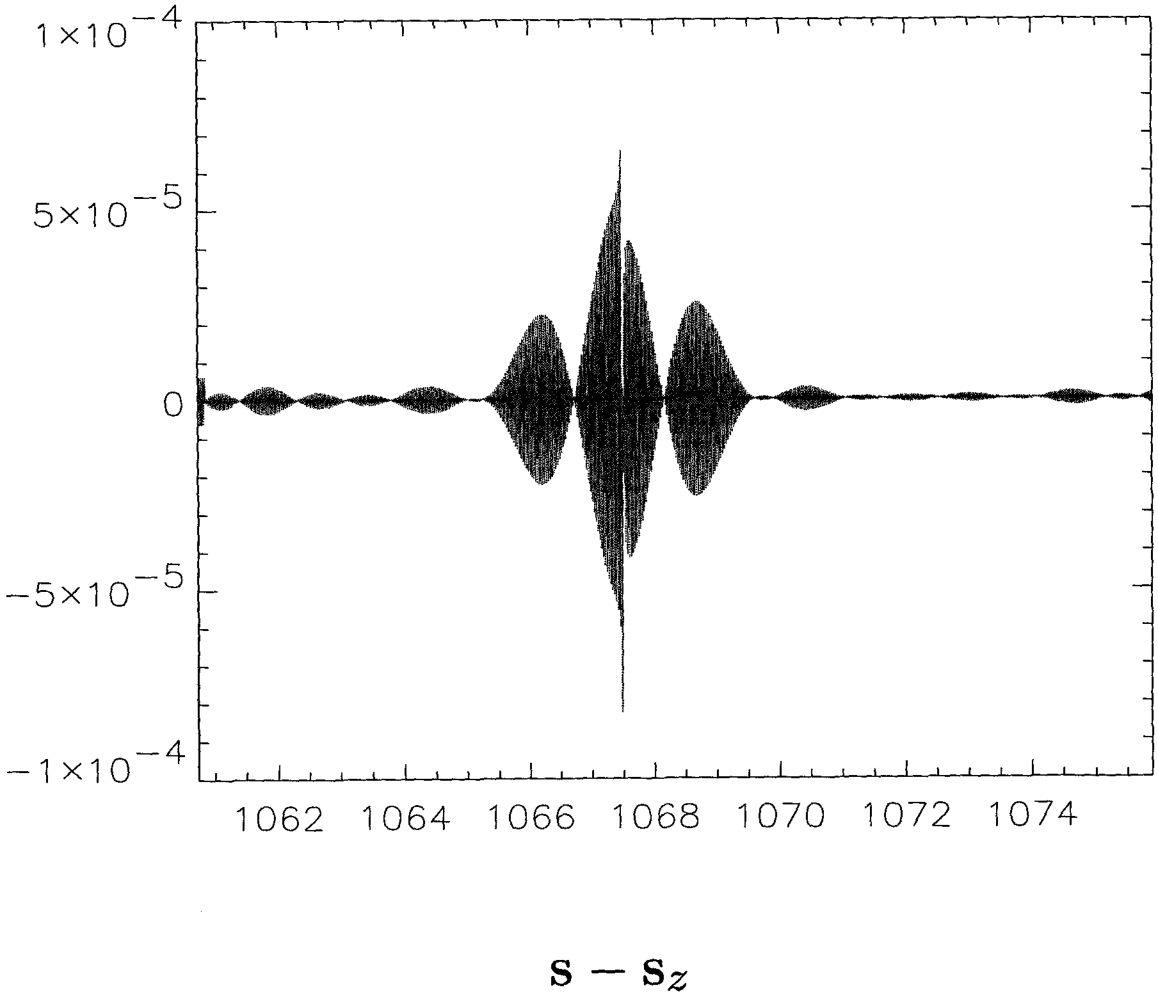
$\tilde{s}$ over plotted on s (zoomed in)

Example #1 (cont.)



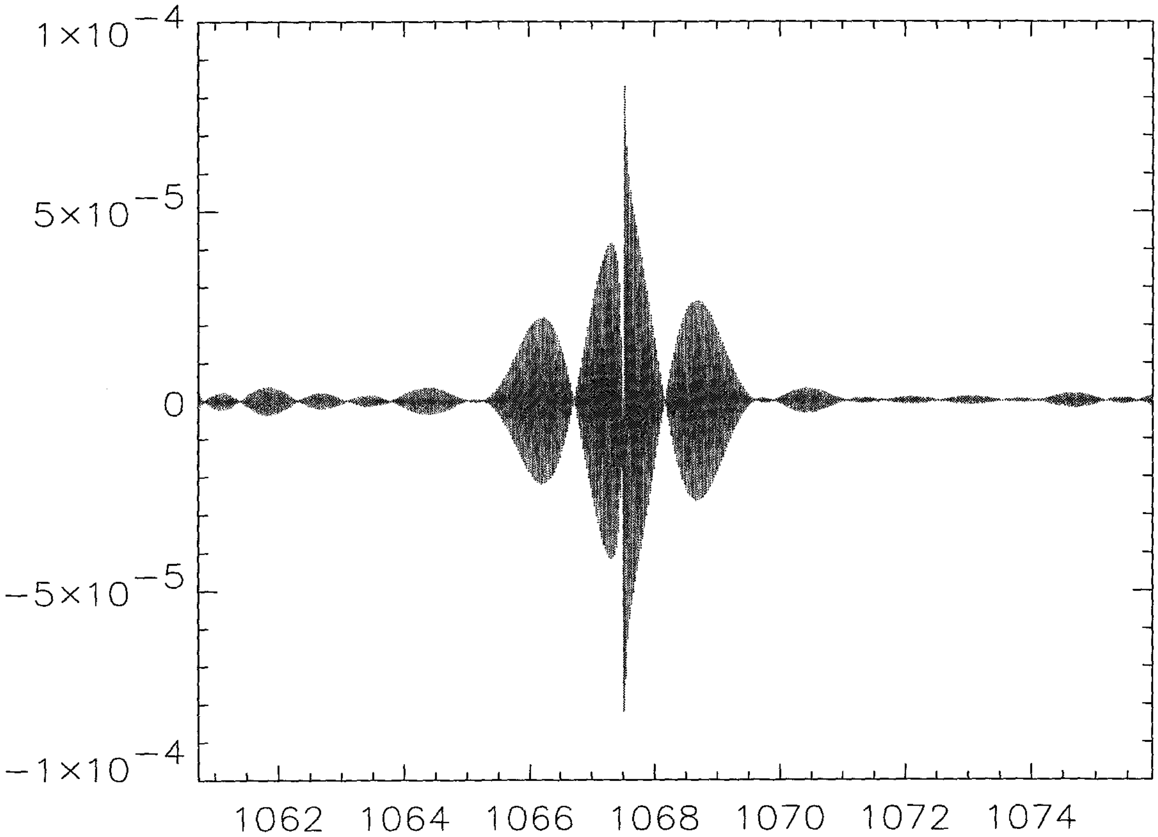
$$\mathbf{s} - \tilde{\mathbf{s}} = \mathbf{E}^{-1}\tilde{\mathbf{f}} - \mathbf{F}^{-1}\tilde{\mathbf{f}}$$

Example #1 (cont.)



where $\mathbf{s}_z$ is an estimate of $\mathbf{s}$ obtained through zero-padded FFT and Shannon linear interpolation

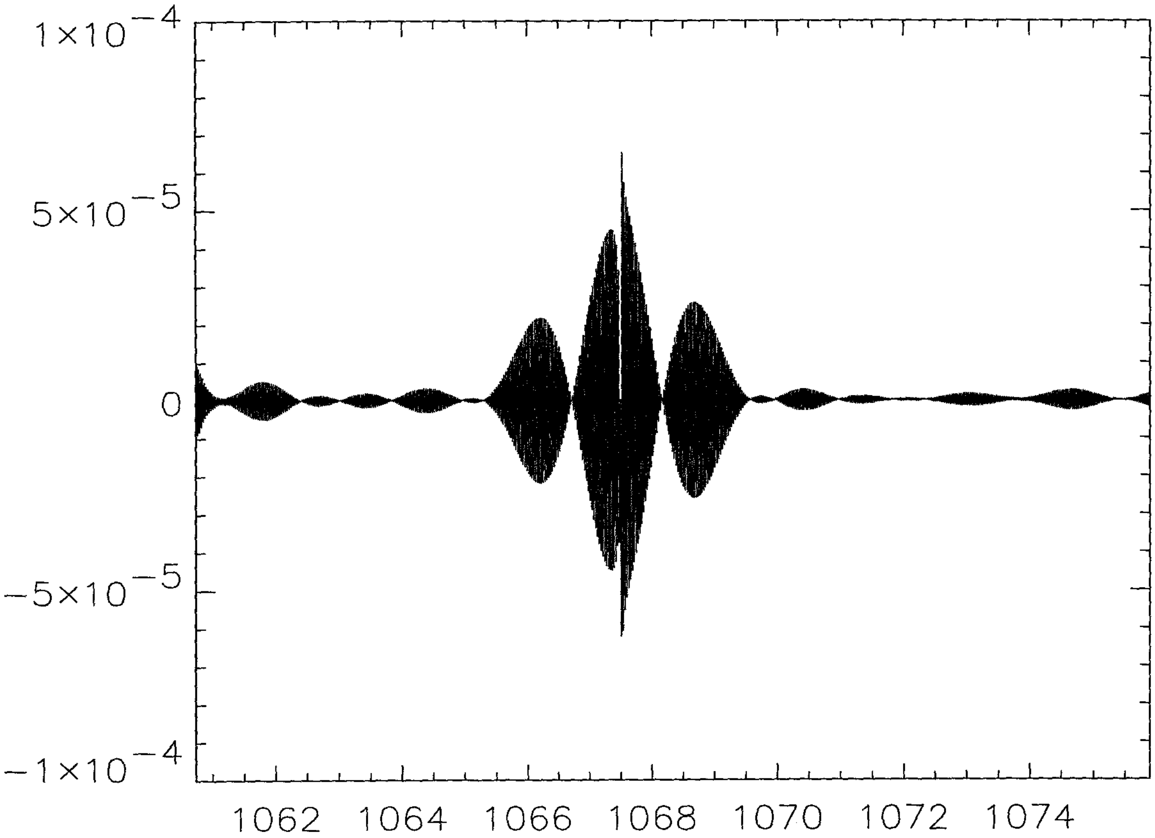
Example #1 (cont.)



$$\mathbf{s} - \frac{1}{N}\mathbf{E}(\rho, \beta)^H \tilde{\mathbf{f}}$$

where $\rho = 1 - \frac{d}{s}(1 - c)$, $\beta = \rho \frac{v_{\text{min}}}{\delta v} + \frac{o}{\delta v}$ and $\mathbf{E}_0(\rho)^H$ is replaced by its quadratic approximation at $\rho = 0$

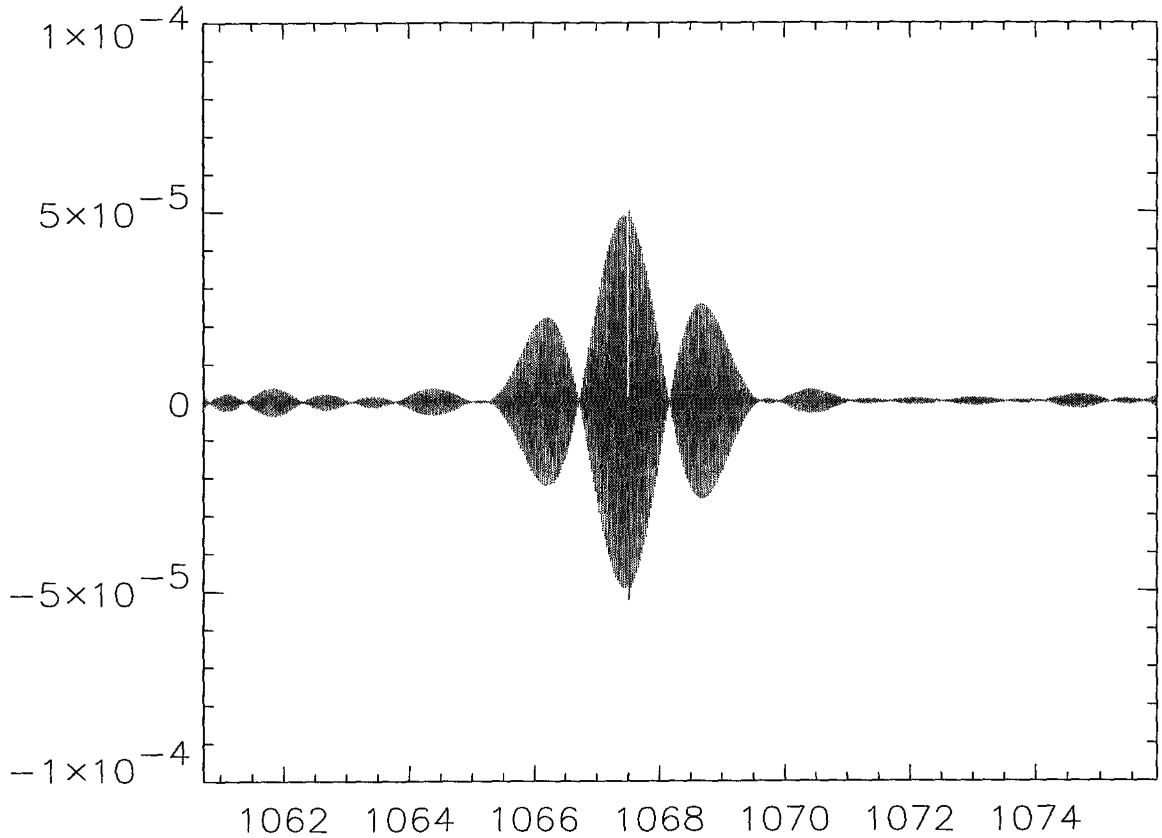
Example #1 (cont.)



$$\mathbf{s} - \frac{1}{N}\mathbf{E}(\rho_2, \beta_2)^H \left[\mathbf{F}\left\{\frac{1}{N}\mathbf{E}(\rho_1, \beta_1)^H \tilde{\mathbf{f}}\right\}\right]$$

where $\rho_1 = c$, $\beta_1 = \rho_1 \frac{v_{\text{min}}}{\delta v}$, $\rho_2 = 1 - \frac{d}{s}$ and $\beta_2 = \rho_2 \frac{v_{\text{min}}}{\delta v} + \frac{o}{\delta v}$, and $\mathbf{E}_0(\rho)^H$ is replaced by its quadratic approximation at $\rho = 0$

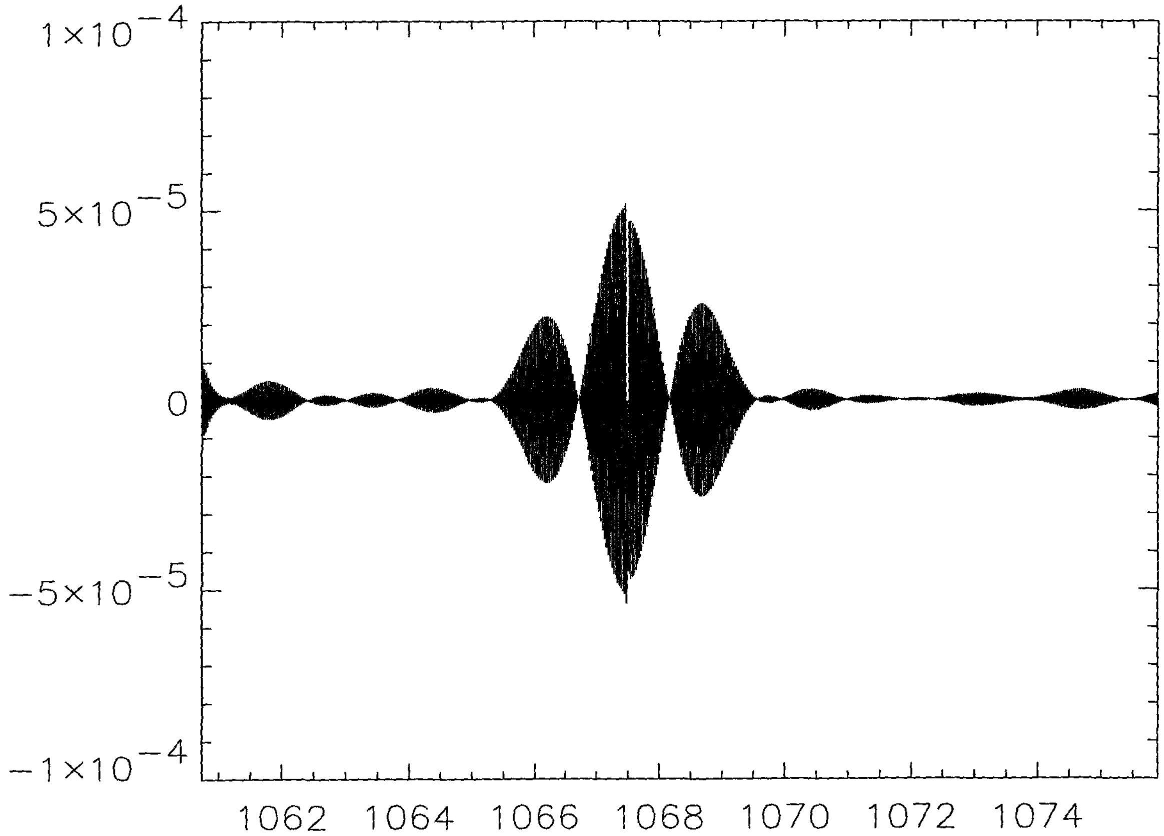
Example #1 (cont.)



$$\mathbf{s} - \frac{1}{N}\mathbf{E}(\rho, \beta)^H\tilde{\mathbf{f}}$$

where $\rho = 1 - \frac{d}{s}(1 - c)$, $\beta = \rho\frac{v_{\text{min}}}{\delta v} + \frac{o}{\delta v}$ and $\mathbf{E}_0(\rho)^H$ is replaced by its cubic approximation at $\rho = 0$

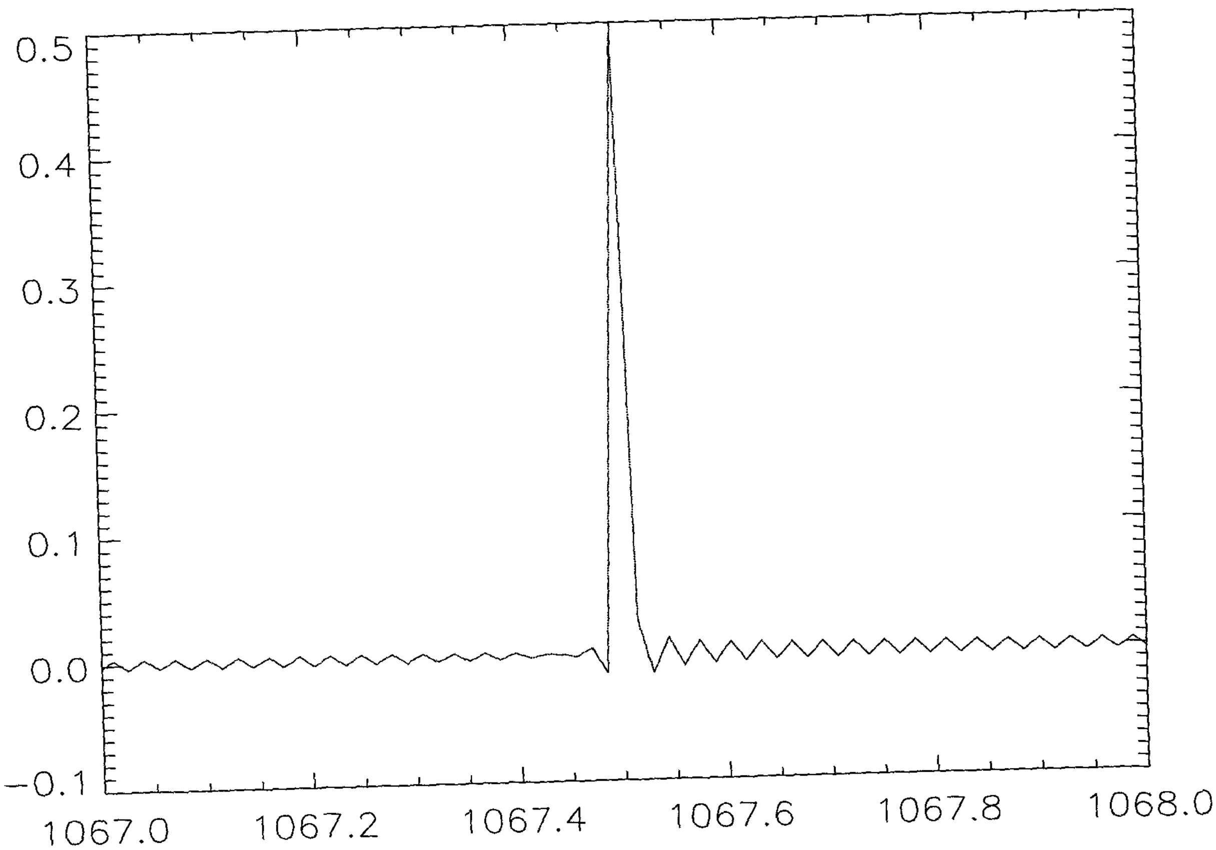
Example #1 (cont.)



$$\mathbf{s} - \frac{1}{N}\mathbf{E}(\rho_2, \beta_2)^H \left[\mathbf{F}\left\{\frac{1}{N}\mathbf{E}(\rho_1, \beta_1)^H \tilde{\mathbf{f}}\right\}\right]$$

where $\rho_1 = c$, $\beta_1 = \rho_1 \frac{v_{\text{min}}}{\delta v}$, $\rho_2 = 1 - \frac{d}{s}$ and $\beta_2 = \rho_2 \frac{v_{\text{min}}}{\delta v} + \frac{o}{\delta v}$, and $\mathbf{E}_0(\rho)^H$ is replaced by its cubic approximation at $\rho = 0$

Example #1 (cont.)



Corrected $\tilde{s}$ over plotted on s (zoomed in)