Computational techniques & considerations in optics

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Applied NanoPhotonics Workshop
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Outline

- Motivation
- Basic numerical analysis
- Scalar time-frequency picture of light
- Spatiotemporal evolution of light
- Concluding remarks

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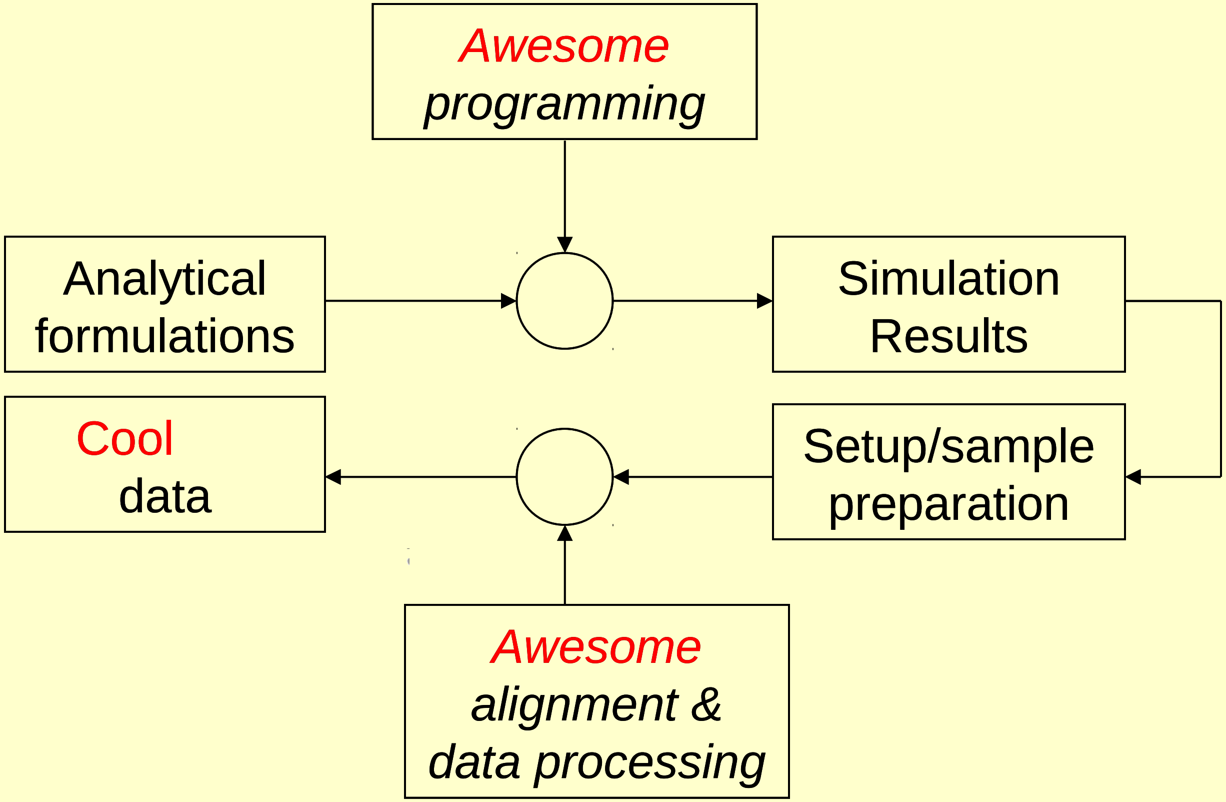
Motivation

- Systematic data assessment for all



Awesome programming

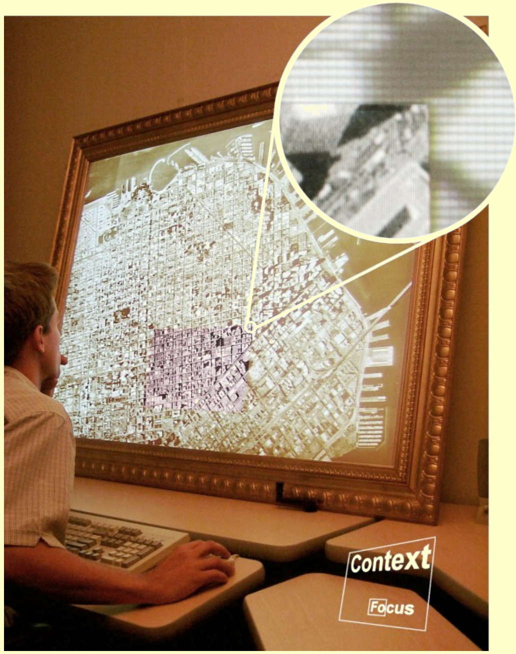
Analytical formulations

Simulation Results

Setup/sample preparation

Cool data

Awesome alignment & data processing



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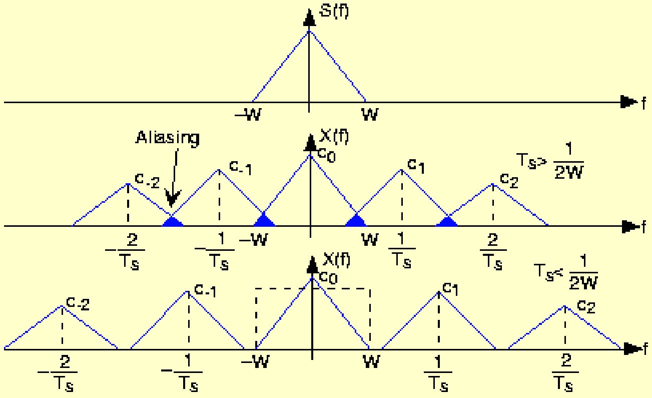
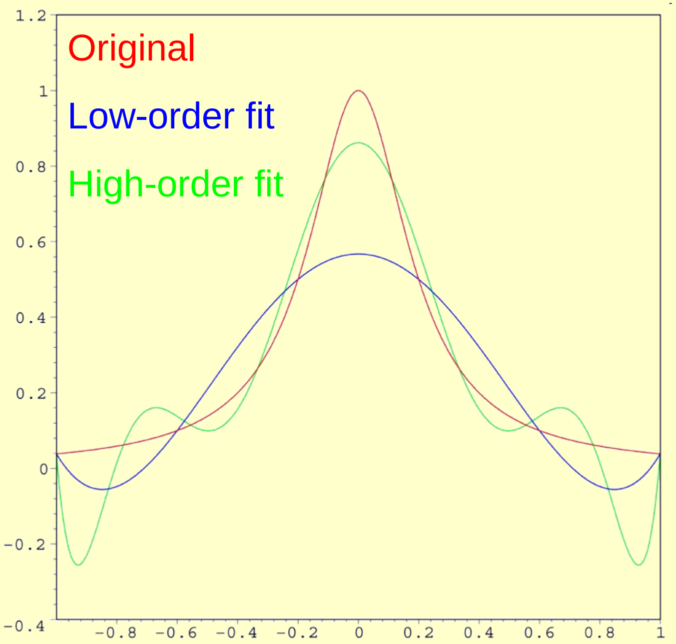
Elementary numerical concepts

- Sources of error
  - Numerical and physical
- Noise suppression
  - Reformulating differentiation
- Sampling (pixelation)
  - Sampling rate, overlapping replica (aliasing), A/D issues



Data processing

- Linear filtering
  - Moving average
    - Phase shift
- Nonlinear filtering
  - Median
    - Spikes, salt-pepper noise
  - Fitting
    - Scaling and centering
    - Polynomials, splines, orthogonal bases
- Optimization
  - Local optima
  - Evolutionary algorithms



Impact of increasing polynomial order on error

Expansion: $f(x)=\Sigma a_n x^n$ (decreasing error)

Fitting: $f(x)=\Sigma a_n x^n$ (**<u>enhancing error</u>**)

Known/Unknown

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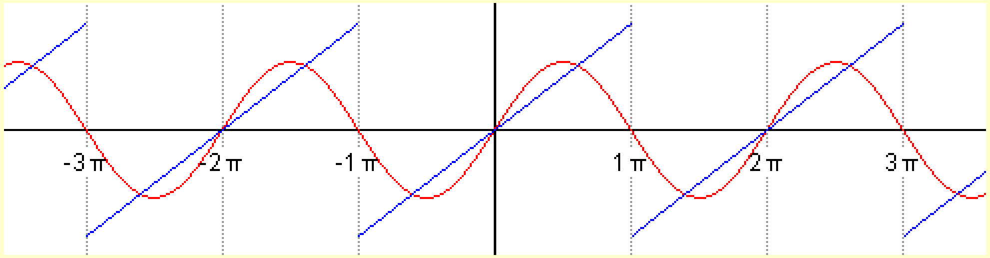
Fourier transform(s): *A tale of two sinusoidals*

- Sign convention (Engineering vs. Physics)
- Continuous vs. Discrete Fourier transform (DFT)
- Fast computation of DFT (FFT)
  - FFT is neither an operator, nor an algorithm
  - Notation and a class of algorithms
  - The “1/N” pre-factor

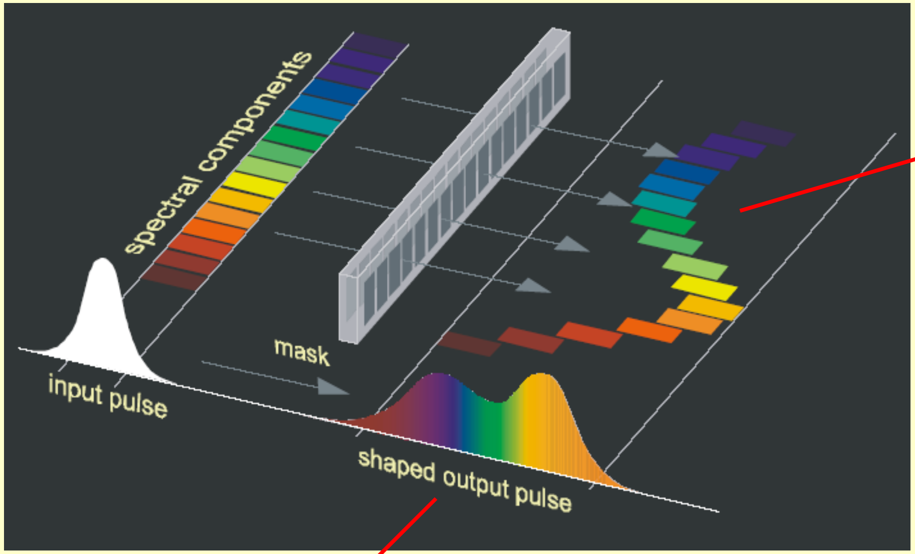
$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi)\, e^{2\pi i x \xi}\, d\xi, \qquad \hat{f}(\xi) := \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i x \xi}\, dx,$$

$$x_n = \frac{1}{N} \sum_{k=0}^{N-1} X_k e^{\frac{2\pi i}{N} kn} \qquad n = 0, \dots, N-1 \qquad X_k = \sum_{n=0}^{N-1} x_n e^{-\frac{2\pi i}{N} kn} \qquad k = 0, \dots, N-1$$



Phase

- Wrapped phase vs. unwrapped phase
- Phase vs. delay
- Real vs. complex signals



Group delay *profile*, $t_g(\omega)$

$\downarrow$

$\int d\omega$

$\downarrow$

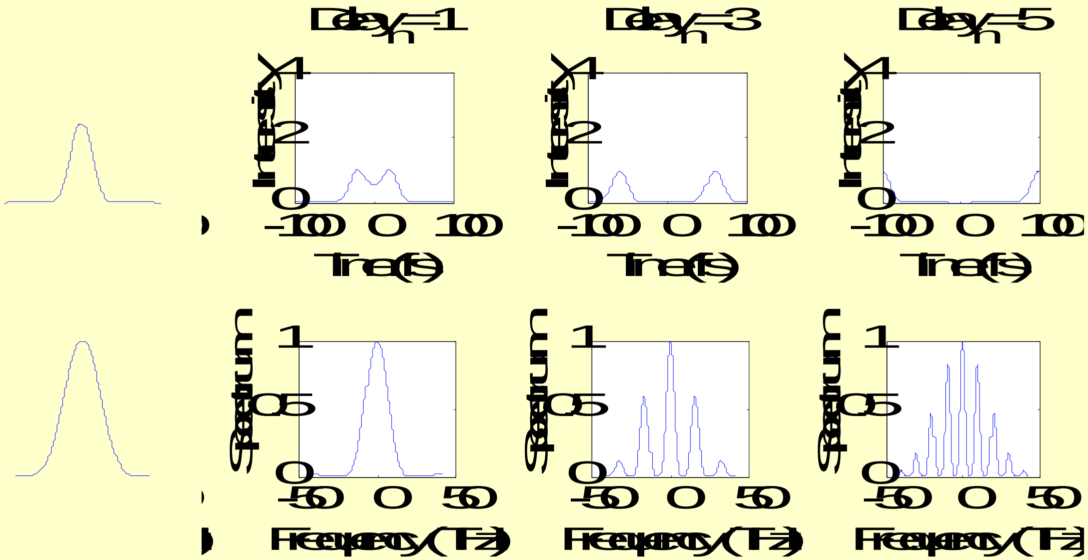
Unwrapped phase, $\varphi(\omega)$

Temporal profile, $E(t)$

$E(t)$ ← Fourier transform → $E(\omega)=|E(\omega)|e^{i\varphi(\omega)}$

Resolution and range

- Temporal range ↔ spectral resolution
    - Physical resolution (diffraction)
    - Numerical resolution (of all elements)
    - Temporal artifacts
- Trade-off between resolution and range
    - Trade-off between resolutions in the two domains



Fourier analysis & nonlinearity

- Phasor
    - Time-domain analysis (single-frequency)
    - Frequency-domain *appearance*
- Linear system theory
    - Multiplication in the **frequency domain**
        - $E_{out}(\omega)=E_{in}(\omega)H(\omega)$
        - Equivalence to phasor analysis

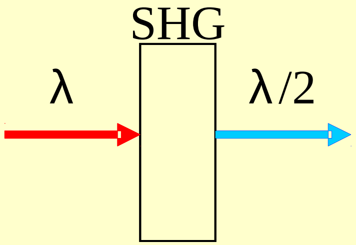
$$\underbrace{e_{in}(t) \xrightarrow{F} E_{in}(\omega)}_{\text{Superposition}} \longrightarrow \underbrace{\boxed{H(\omega)}}_{\text{Superposition}} \longrightarrow \underbrace{E_{out}(\omega) \xrightarrow{F^{-1}} e_{out}(t)}_{\text{Superposition}}$$

- Nonlinear system with sinusoidal excitation
    - **Phasor notation does not imply frequency-domain analysis**

$$\underbrace{e_{in}(t) \xrightarrow{F} E_{in}(\omega)}_{\text{Superposition}} \longrightarrow \underbrace{\boxed{\text{No } H_{\omega}}}_{\textbf{No superposition}} \longrightarrow \underbrace{E_{out}(\omega) \xrightarrow{F^{-1}} e_{out}(t)}_{\text{Superposition}}$$

Frequency domain: “f” or “λ”?

- “t” forms a Fourier transform pair with “f”
  - 100 fs ←→ 4.5THz (9.5nm@800nm, 38nm@1600nm)
- Measurement/shaping in the pixel (wavelength) domain
- Conversion
  - Weight factor: $I_f(f)=I_\lambda(c/f) * [c/f^2]$
  - Equally-spaced points in “f” needed for DFT (re-sampling needed)
- Comparing “bandwidths” in a nonlinear process
  - $\Delta f_{SHG}/\Delta f=1.4>1$, $\Delta\lambda_{SHG}/\Delta\lambda=0.35<1$



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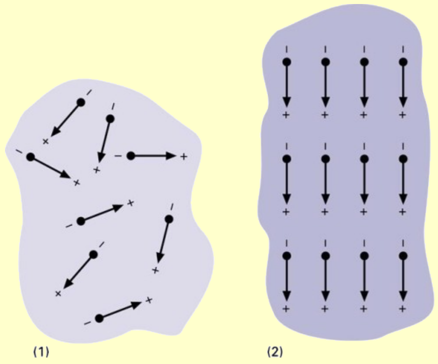
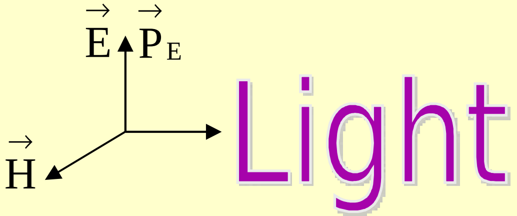
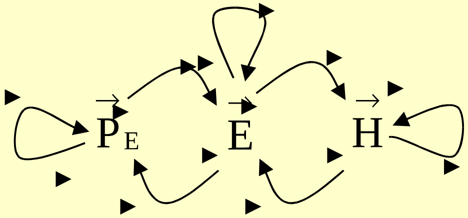
Maxwell’s equations

- Light-matter interaction
  - Induced polarization
- Coupling between spatial and temporal variations







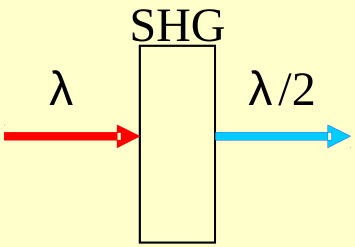
$$\vec{\nabla}\times\vec{H} = \vec{J} + \frac{\partial}{\partial t}(\varepsilon_0\,\vec{E} + \vec{P}_E)$$

$$\vec{\nabla}\times\vec{E} = \vec{0} - \frac{\partial}{\partial t}(\mu_0\,\vec{H})$$

Scalar vs. wave picture: SHG test case

Scalar model

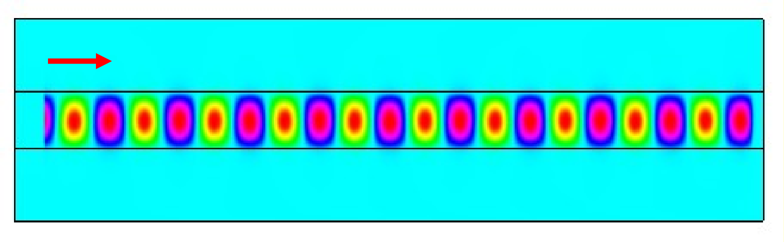
Assumptions: Homogeneous medium, plane wave excitation, low efficiency …



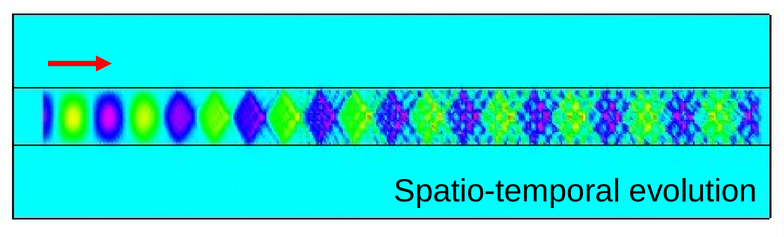
Wave model

Arbitrary medium, source, efficiency …

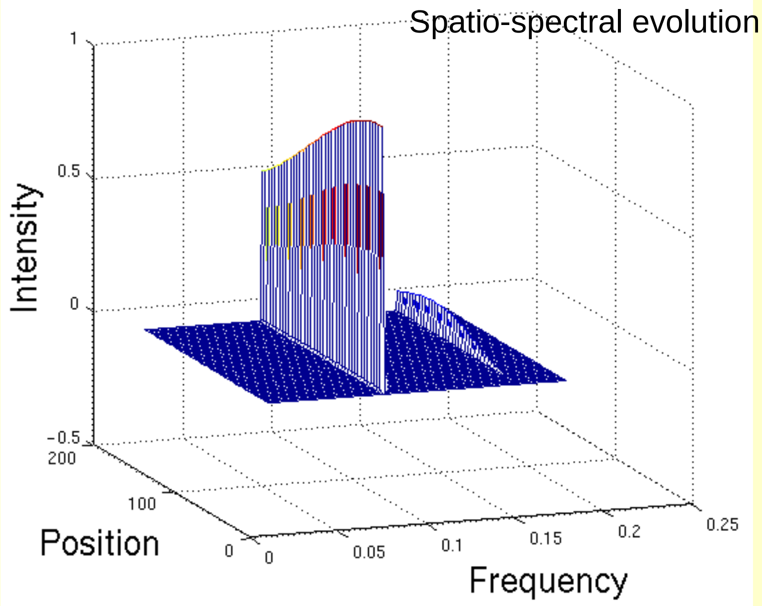
Field snapshot in a (linear) slab waveguide



Field snapshot in a nonlinear ($\chi^{(2)}$) slab waveguide



Spatio-temporal evolution

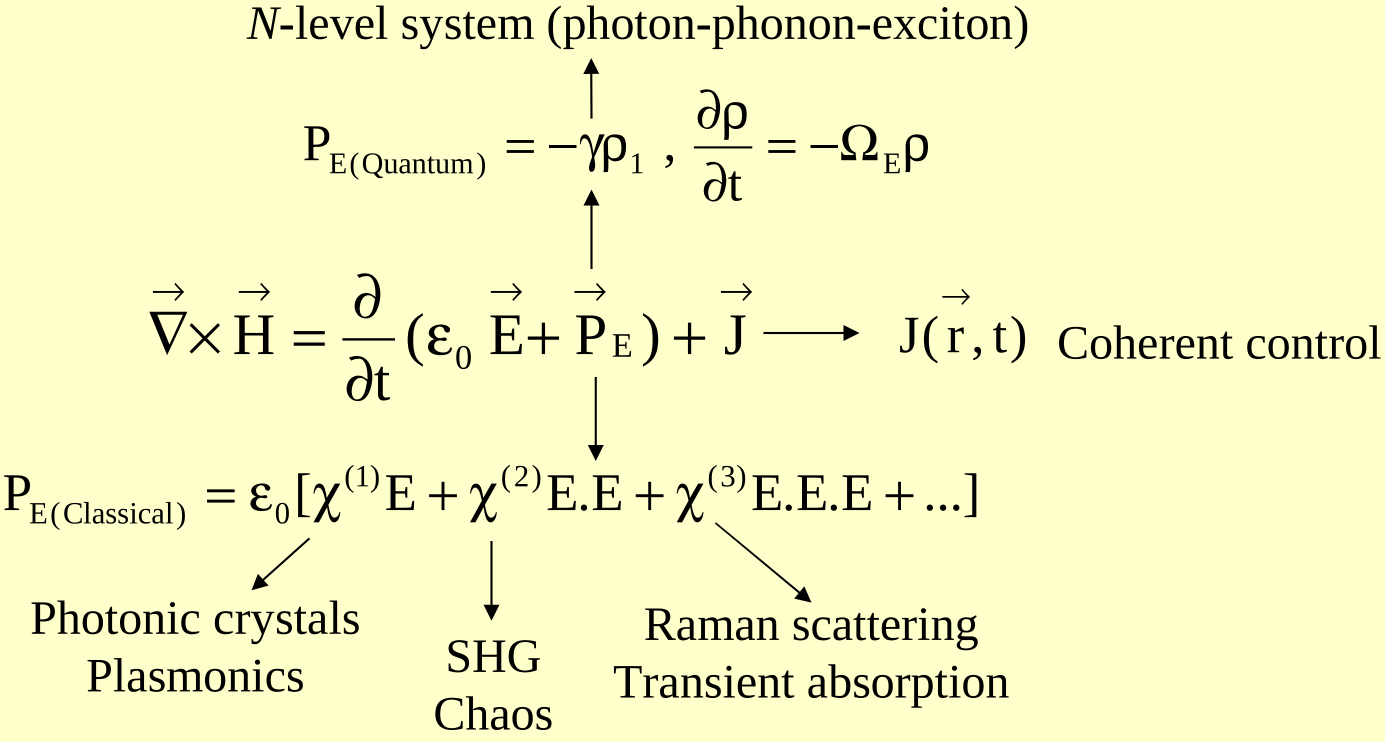


Spatio-spectral evolution

Journal of Lightwave Technology ***24****, 624 (2006)*

Classical and semi-classical electromagnetics

- Induced polarization characterizing light-matter interaction



N-level system (photon-phonon-exciton)

$$P_{E(\text{Quantum})} = -\gamma\rho_1 \ , \ \frac{\partial\rho}{\partial t} = -\Omega_E\rho$$

$$\vec{\nabla}\times\vec{H} = \frac{\partial}{\partial t}(\varepsilon_0\vec{E}+\vec{P}_E) + \vec{J} \longrightarrow J(\vec{r},t)$$

Coherent control

$$P_{E(\text{Classical})} = \varepsilon_0[\chi^{(1)}E + \chi^{(2)}E.E + \chi^{(3)}E.E.E + \ldots]$$

Photonic crystals
Plasmonics

SHG
Chaos

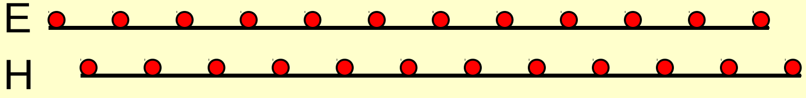
Raman scattering
Transient absorption

Quantitative solutions of wave equation

- Time-domain vs. frequency-domain
  - Reduced number of independent variables (f)
  - Fundamental insight (f)
  - Simplicity (t)
  - Speed (f)
  - Field patterns (t/f)
  - Spatial and temporal “transients” (t)
  - Material dispersion/absorption (f)
  - Nonlinear analysis beyond common approximations (t)
  - Inherent errors (f)
    - Grid vs. structure
  - Sensitivity (t/f)
    - Slow-light
    - Sharp resonance
- Boundary conditions
  - Perfect electric conductor (PEC): $E_{\text{tangential}}=0$
  - Perfectly matched layer (PML): $E_{\text{“reflected”}}=0$

Finite Difference Time Domain (FDTD)

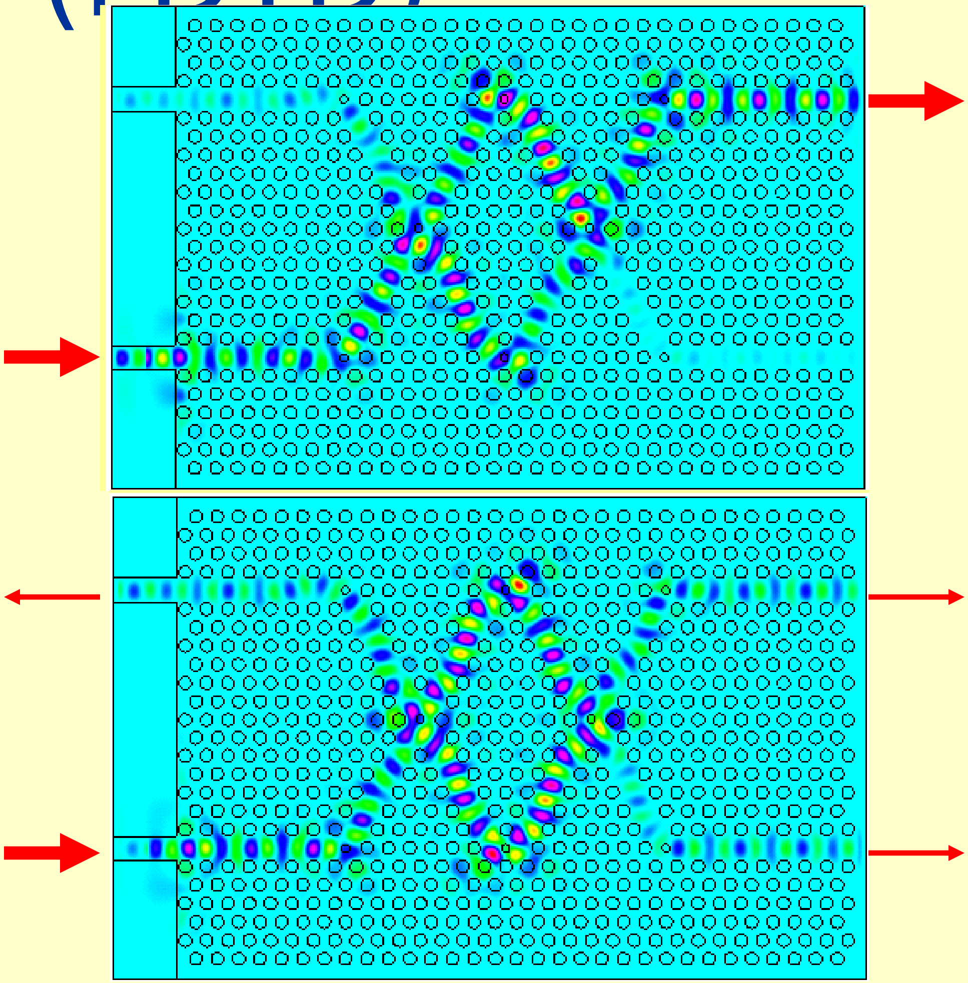
- Uniform sampling and Cartesian coordinate
- Approximation of field derivatives using half a step size
  - E and H fields calculated at points/instants half a step size apart
- Algorithm
  - Initialize E and H; Update E; Update H; Iterate
- Complexity
  - Just algebraic equations (no matrix or operator formalism)
- Where to get?
  - DIY (easy to code)!
  - Commercially available
  - MEEP (MIT *ab-initio*) for *open-source-philic* professionals
- Extension to static nonlinearities and semi-classical Emag
- 1-week workshop and coding in Excel
- *Caution:* No “awesome programming”!

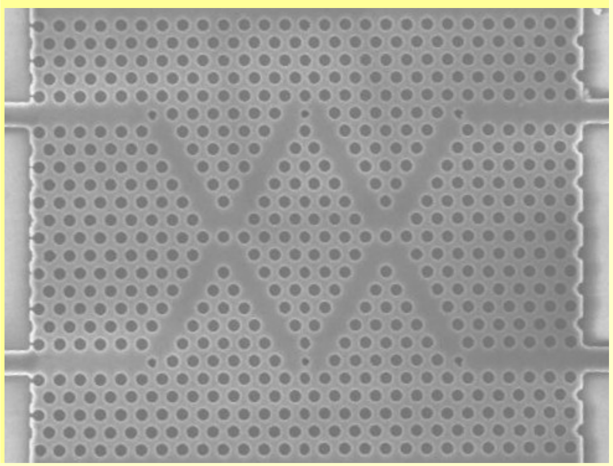


“x” and “t”

$$f'(x) \approx \frac{f(x+\Delta x/2) - f(x-\Delta x/2)}{\Delta x}$$

Classical 2D linear solver (FDTD)

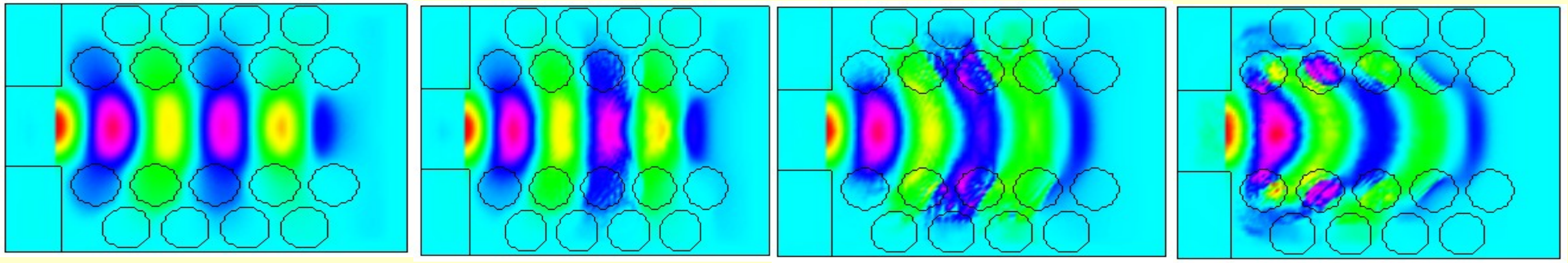




Controlled routing/beam-splitting (at different frequencies) in a multi-bend photonic crystal waveguide by tuning cavity (junction) holes

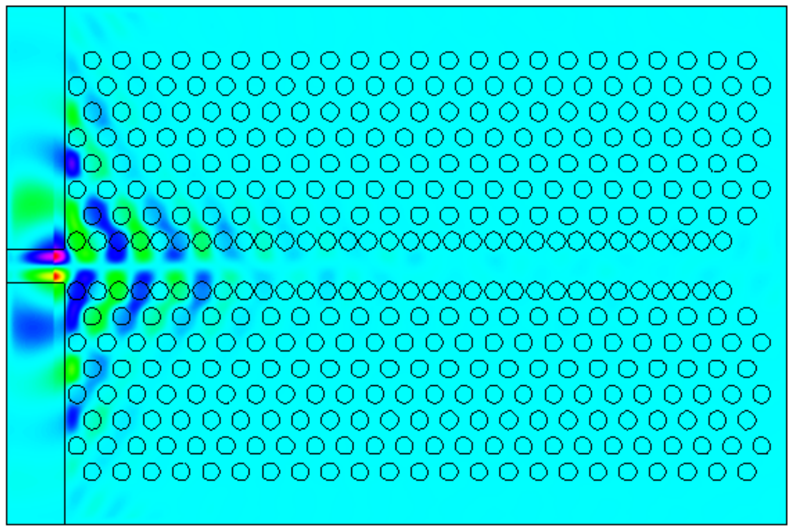
More field snapshots with FDTD

Photonic crystal waveguide; holes infiltrated with nonlinear $X^{(3)}$ material; TE polarization



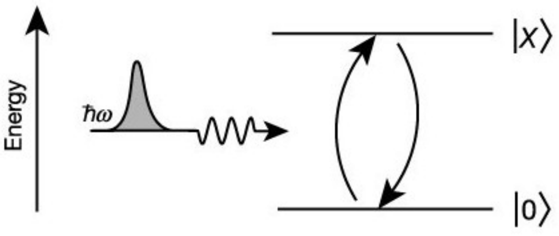
$X^{(3)}=0$ **$X^{(3)}_1$** **$X^{(3)}_2$** **$X^{(3)}_3$**

Exciting a complex odd mode in a photonic crystal waveguide (TM polarization)



Semi-classical 1D (nonlinear) model

- Liouville formulation (PRA **52**, 3082)
- Dipole matrix elements
  - ρ_1: Polarization
  - ρ_2: Quadrature polarization
  - ρ_3: Population difference (ρ_{30}=-1)
  - $\rho_1^2+\rho_2^2+\rho_3^2=1$ for a lossless system ($T_1=T_2=\infty$)



$$\frac{\partial}{\partial t}\rho = -\frac{i}{\hbar}[H,\rho]$$

Maxwell

$$\partial_t H_y = -\frac{1}{\mu_0}\partial_z E_x$$

$$\partial_t E_x = -\frac{1}{\epsilon_0}\partial_z H_y - \frac{1}{\epsilon_0}\partial_t P_x$$

$$= -\frac{1}{\epsilon_0}\partial_z H_y - \frac{N_{\text{atom}}\gamma}{\epsilon_0 T_2}\rho_1 + \frac{N_{\text{atom}}\gamma\omega_0}{\epsilon_0}\rho_2$$

Bloch

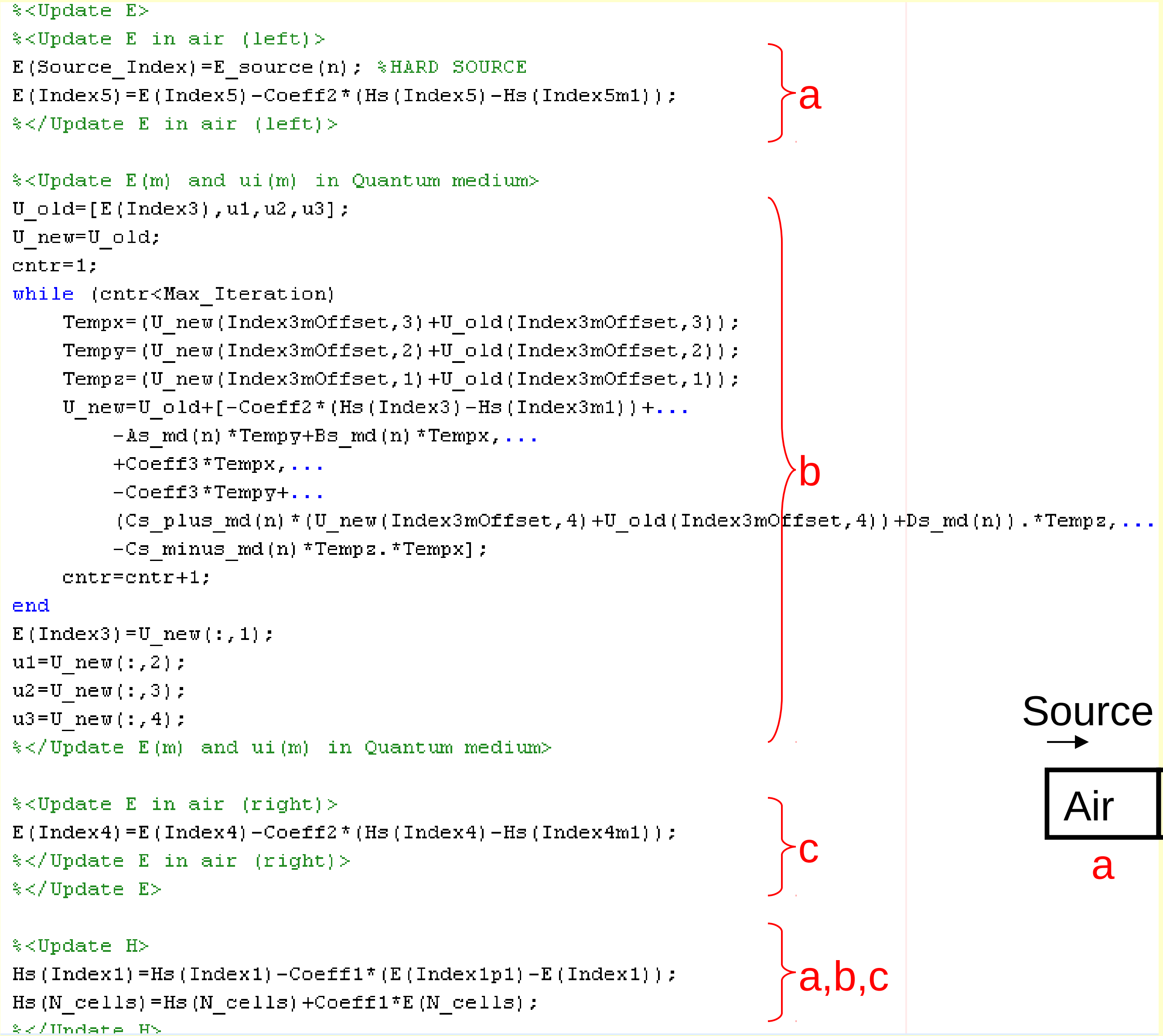
$$\partial_t\rho_1 = -\frac{1}{T_2}\rho_1 + \omega_0\rho_2,$$

$$\partial_t\rho_2 = -\omega_0\rho_1 - \frac{1}{T_2}\rho_2 + 2\frac{\gamma}{\hbar}E_x\rho_3,$$

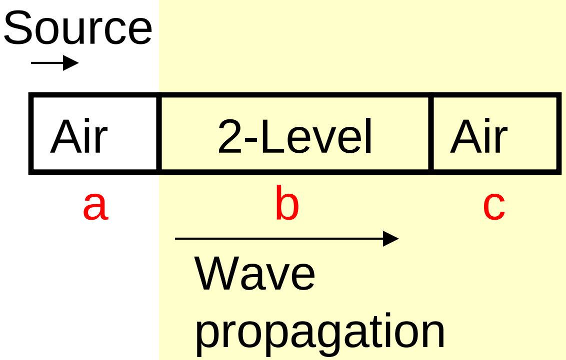
$$\partial_t\rho_3 = -2\frac{\gamma}{\hbar}E_x\rho_2 - \frac{1}{T_1}(\rho_3 - \rho_{30}).$$

$$P_x(t) = -N_{\text{atom}}\gamma\rho_1(t)$$

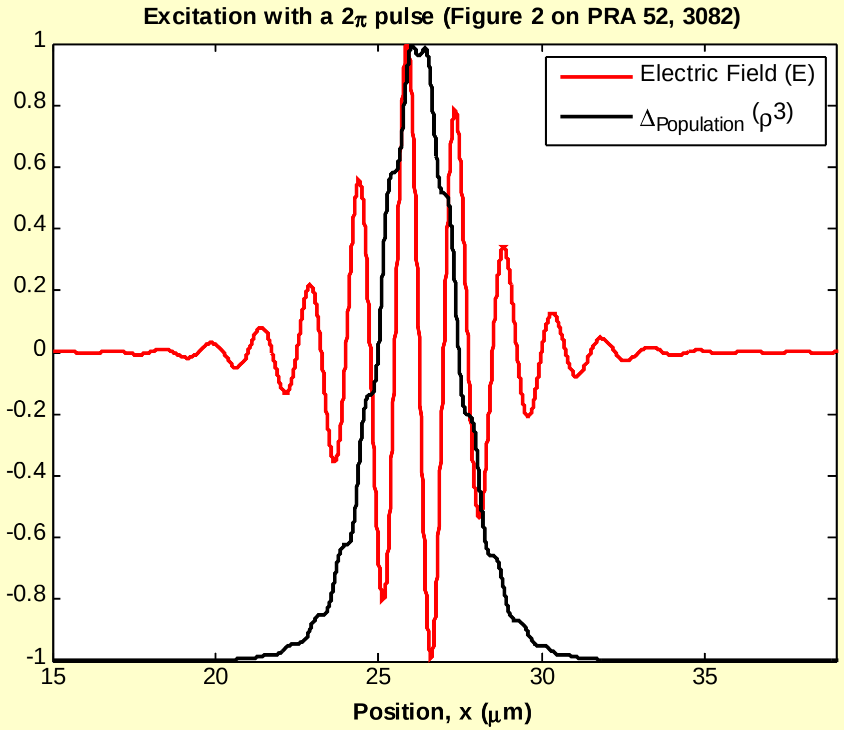
Core of an FDTD source code for a quantum system



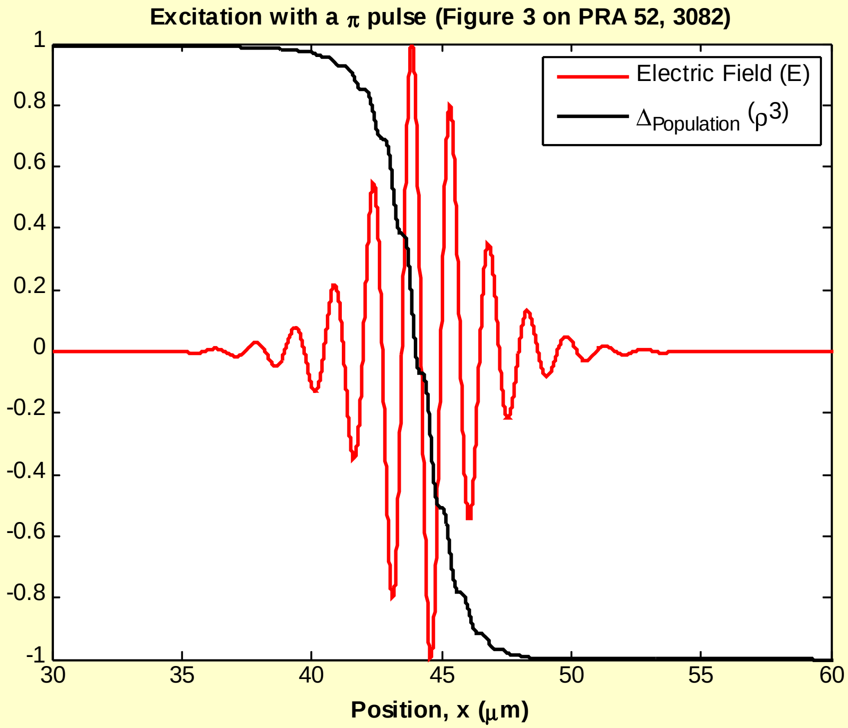
```
%<Update E>
%<Update E in air (left)>
E(Source_Index)=E_source(n); %HARD SOURCE
E(Index5)=E(Index5)-Coeff2*(Hs(Index5)-Hs(Index5m1));
%</Update E in air (left)>

%<Update E(m) and ui(m) in Quantum medium>
U_old=[E(Index3),u1,u2,u3];
U_new=U_old;
cntr=1;
while (cntr<Max_Iteration)
    Tempx=(U_new(Index3mOffset,3)+U_old(Index3mOffset,3));
    Tempy=(U_new(Index3mOffset,2)+U_old(Index3mOffset,2));
    Tempz=(U_new(Index3mOffset,1)+U_old(Index3mOffset,1));
    U_new=U_old+[-Coeff2*(Hs(Index3)-Hs(Index3m1))+...
        -As_md(n)*Tempy+Bs_md(n)*Tempx,...
        +Coeff3*Tempx,...
        -Coeff3*Tempy+...
        (Cs_plus_md(n)*(U_new(Index3mOffset,4)+U_old(Index3mOffset,4))+Ds_md(n)).*Tempz,...
        -Cs_minus_md(n)*Tempz.*Tempx];
    cntr=cntr+1;
end
E(Index3)=U_new(:,1);
u1=U_new(:,2);
u2=U_new(:,3);
u3=U_new(:,4);
%</Update E(m) and ui(m) in Quantum medium>

%<Update E in air (right)>
E(Index4)=E(Index4)-Coeff2*(Hs(Index4)-Hs(Index4m1));
%</Update E in air (right)>
%</Update E>

%<Update H>
Hs(Index1)=Hs(Index1)-Coeff1*(E(Index1p1)-E(Index1));
Hs(N_cells)=Hs(N_cells)+Coeff1*E(N_cells);
%</Update H>
```



Semi-classical 1D (FDTD): 2π-pulse vs. π-pulse



Excitation with a 2π pulse (Figure 2 on PRA 52, 3082)



Excitation with a π pulse (Figure 3 on PRA 52, 3082)

Frequency-domain simulations

- Numerical
  - COMSOL
    - Multi-physics
    - Finite-element
  - MIT *Photonic-Bands*
  - DIY!
- Semi-analytical
  - Single-scattering approximation (as in Green’s function and density of states calculations) is common.
- Note: Field patterns are <u>not</u> snapshots!

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Concluding remarks

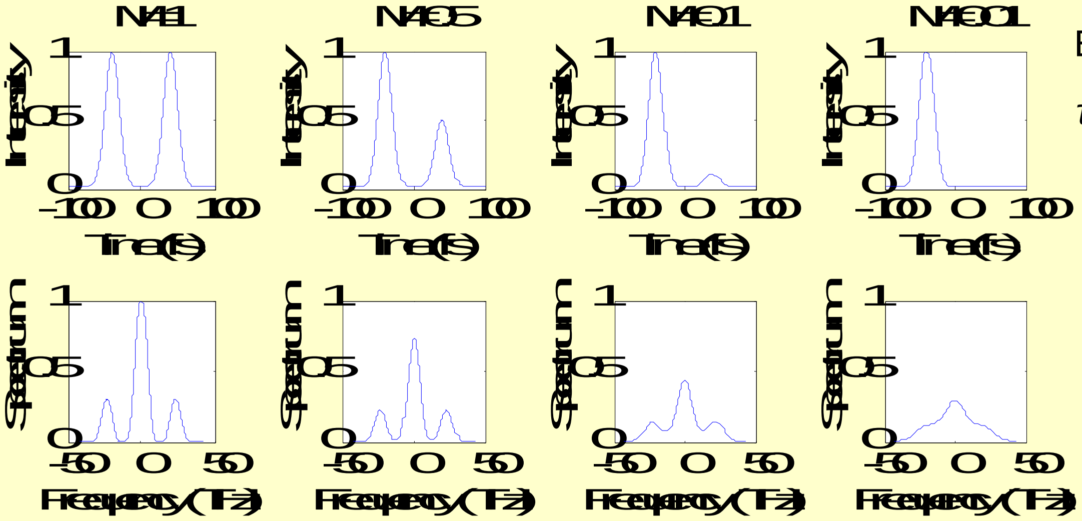
- Trade-off between the time man/machine think
- Avoiding critical errors
  - By use of newbies’ programming style
  - Writing down equations, function arguments …
- Computational skills different from math or programming skills

And a few miscellaneous points!

Spectral analyses: all techniques in a glance

Formalism	Time	Frequency	Notes
Fourier series	continuous, dt=0; Δt=∞	discrete, df=Const>0; Δf=∞	continuous f_0, harmonics
Fourier transform	**continuous, dt=0; Δt=∞**	**continuous, df=0; Δf=∞**	**“features”, sinusoidals, lock-in amp.**
Discrete time Fourier transform	discrete, dt>0; Δt=∞	continuous, df=0; Δf=1	periodic frequency
Discrete Fourier transform	**discrete, dt>0; Δt<∞**	**discrete, df>0; Δf=1<∞**	**FFT, frequency warping, aliasing**
Short-term Fourier transform	discrete, dt>0; Δt<∞	discrete, df>0; Δf<∞	Spectrogram
Laplace transform	continuous & real	continuous and complex	sinusoidal-exponential functions
Z transform	discrete & real	continuous, complex	Arbitrary discrete filters/models, “periodic”
Wavelet transform	discrete & continuous	discrete & continuous	decaying “sinusoidals”, optimized (dt,df)

Spectral resolution & amplitude artifact in time



$E(t) \leftarrow F \rightarrow E(\omega)$

$E(t)+mE(t-\tau) \leftarrow F \rightarrow E(\omega)(1+m\cos(\omega\tau))$

$\tau_n=2$; scanning m (modulation index, MI)

Small MI → poor fringe visibility

Low resolution → poor fringe visibility

Low resolution → spurious small MI

Spurious MI corrected by deconvlucy.m!

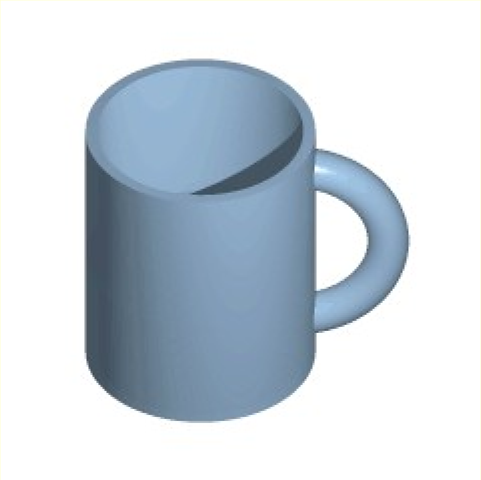
Grand prize

€50 for correct measurement of a double-pulse!

(FROG, SPIDER, MIIPS …), No deconvolution.

What topology is NOT?

- Topology is <u>not</u> a fancy word to use instead of “shape” or “geometry” for 3D objects.
- If we fold/stretch/reshape/… a piece of paper, the geometry changes, but the topology (“connectedness”) remains the same (unless we tear it).



Different geometries with the same topology