Eine Kleine OPT Musik: Ensemble Control in NMR

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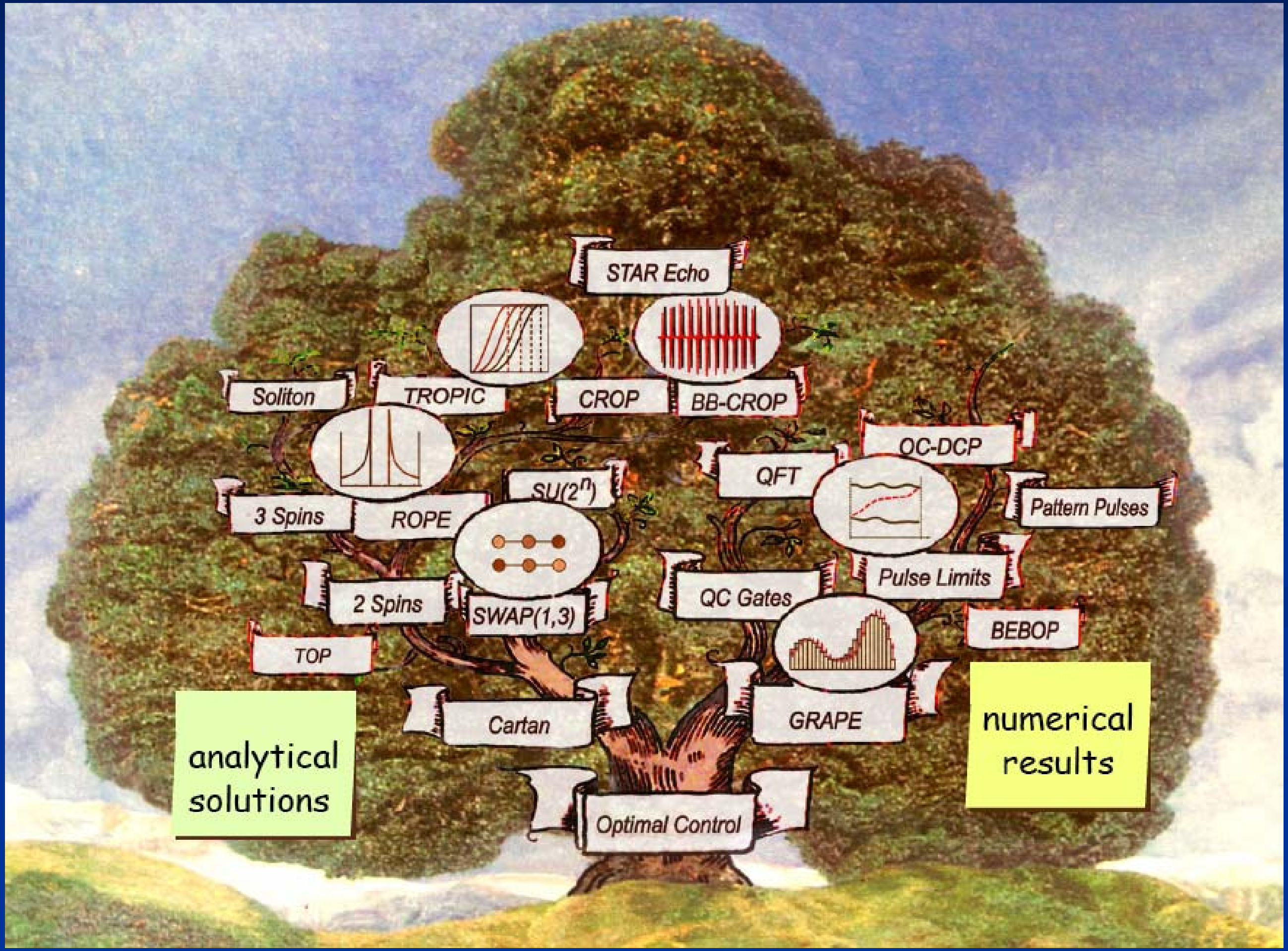
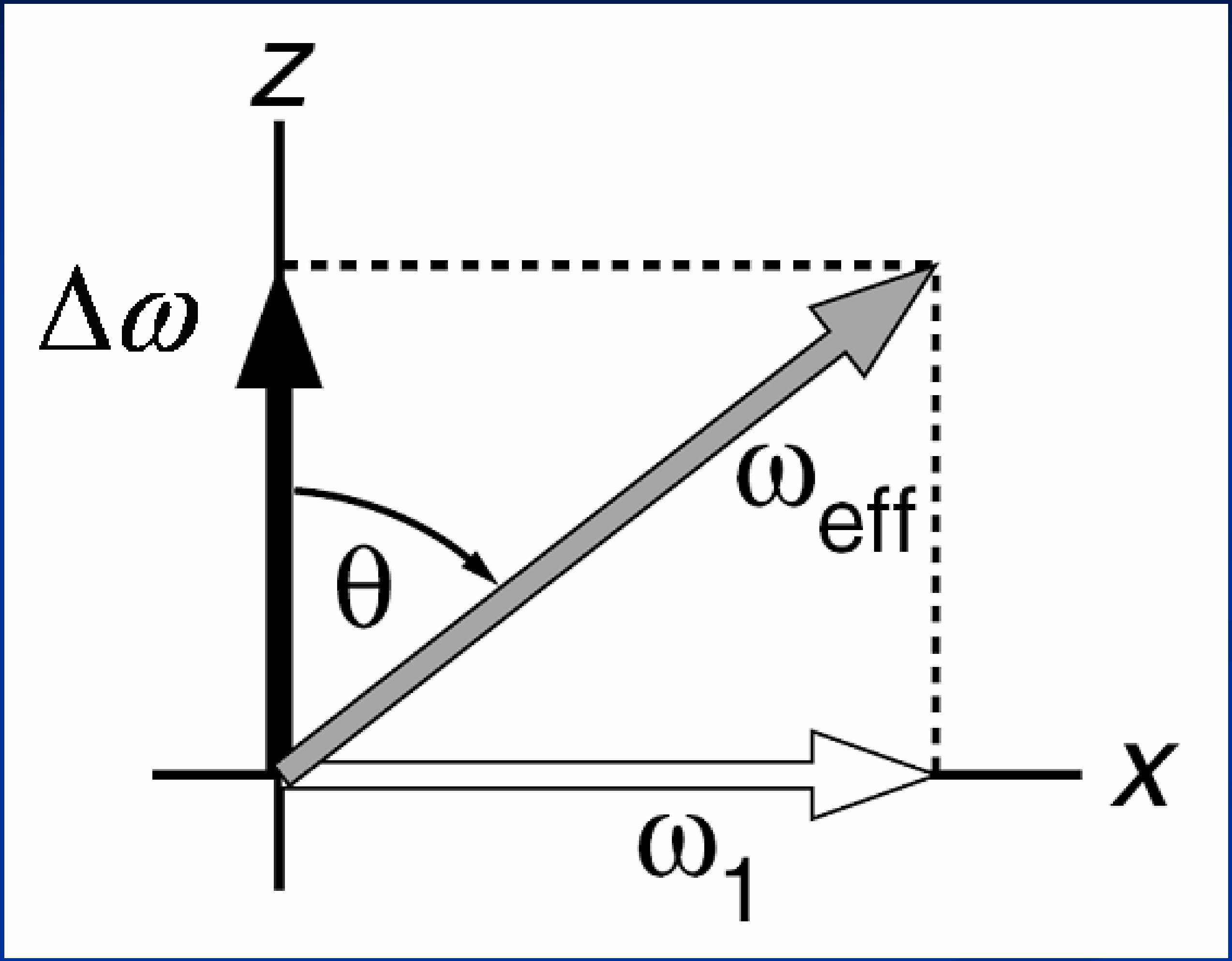
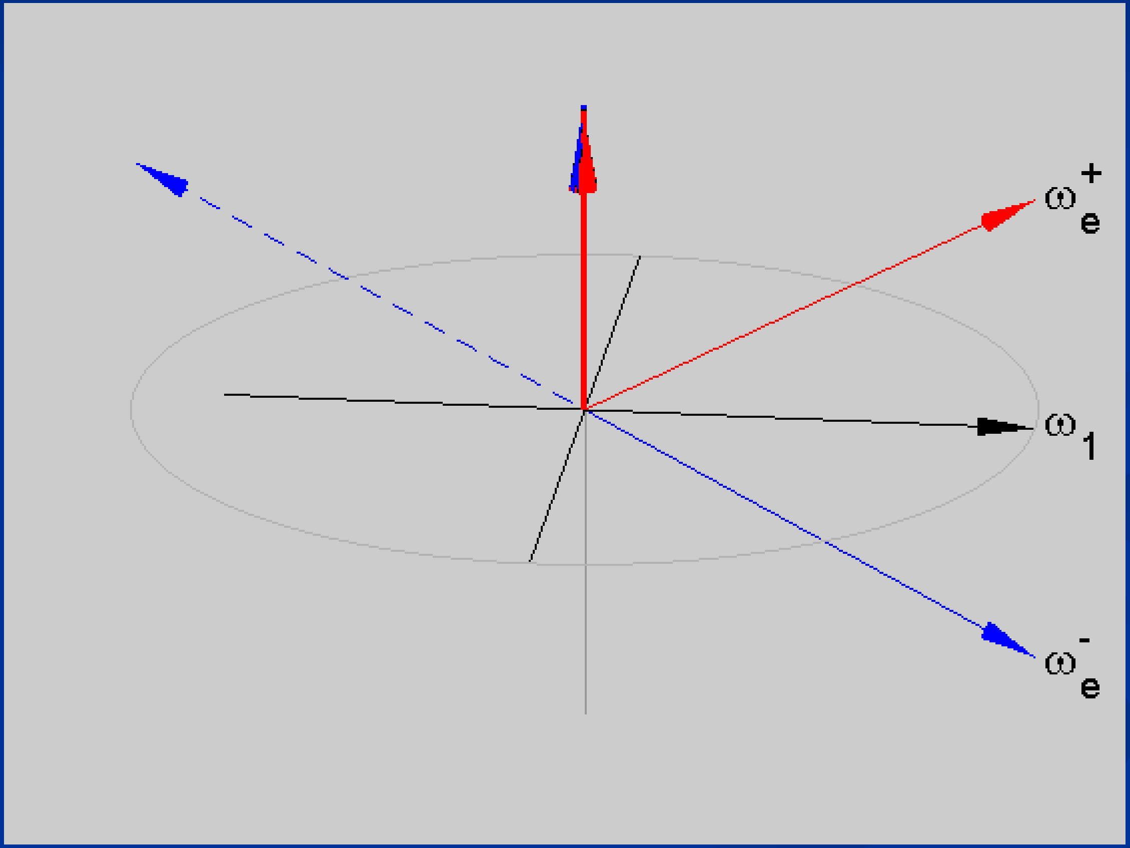
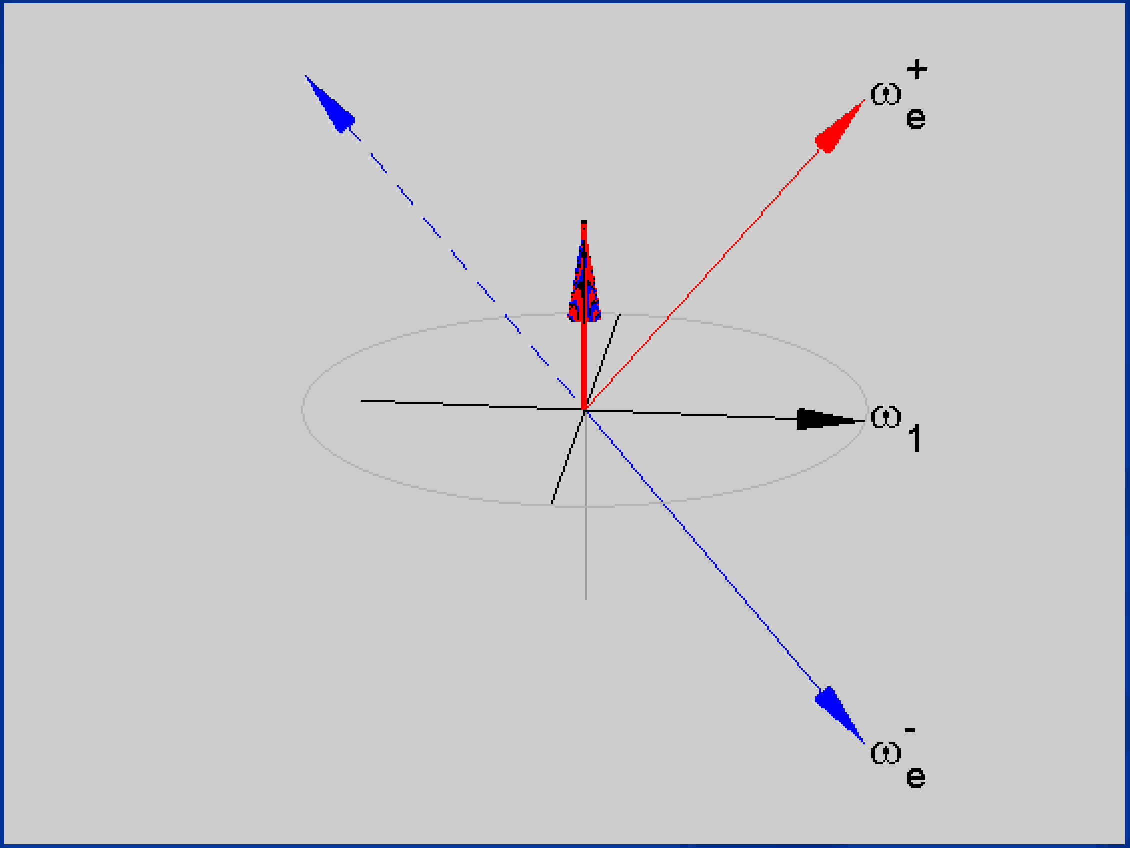

STAR Echo
TROPIC
CROP
BB-CROP
Soliton
OC-DCP
QFT
SU(2^n)
3 Spins
ROPE
Pattern Pulses
Pulse Limits
2 Spins
SWAP(1,3)
QC Gates
BEBOP
TOP
Cartan
GRAPE
analytical solutions
numerical results
Optimal Control


z
Δω
θ
ω_eff
x
ω_1

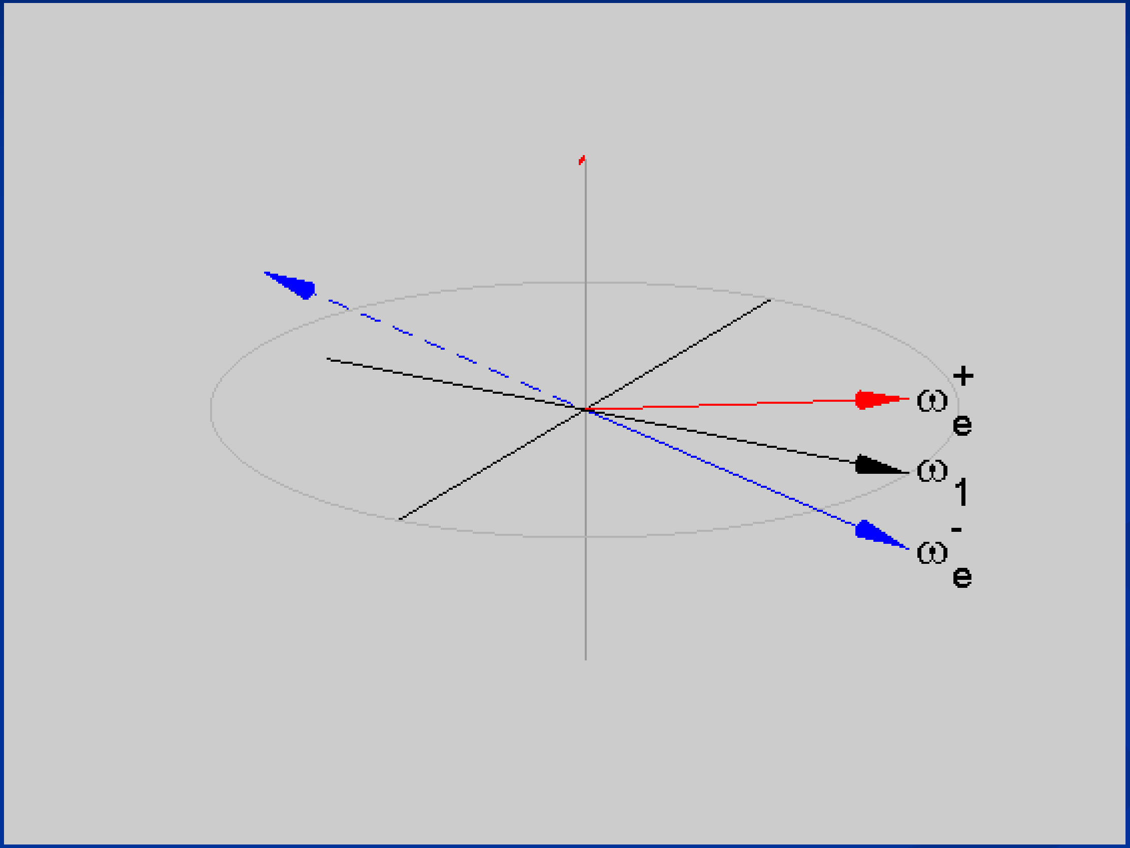


ω
+
e
ω
1
ω
-
e



ω_e^+
ω_1
ω_e^-

Composite π Pulse



MRI Applications

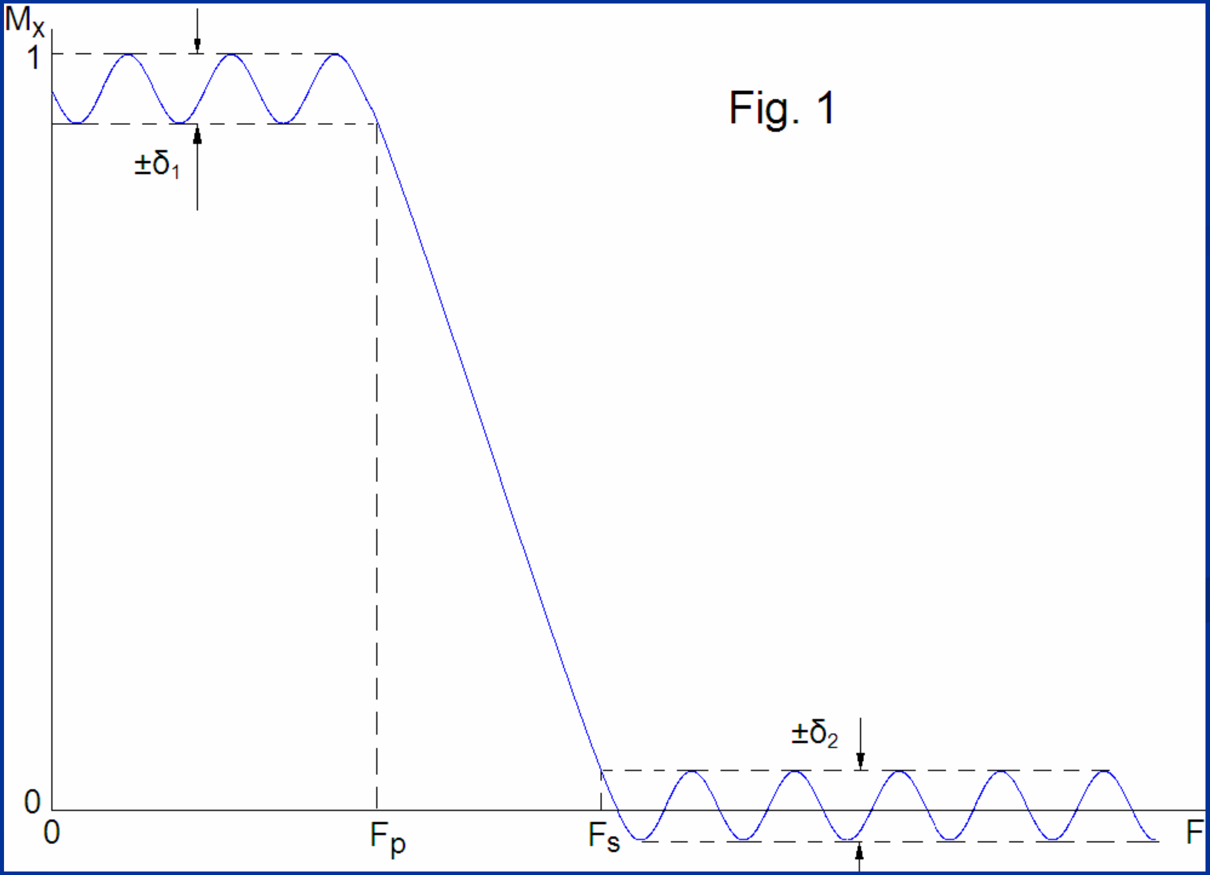
S. Conolly, D. Nishimura, and A. Macovski, Optimal control solutions to the magnetic resonance selective excitation problem, ***IEEE Trans. Med. Imag*****. MI-5**, 106-115 (1986).

J. Mao, T. H. Mareci, K. N. Scott, and E. R. Andrew, Selective inversion radiofrequency pulses by optimal control, *J. Magn. Reson.* **70**, 310-318 (1986).

D. Rosenfeld and Y. Zur, Design of adiabatic selective pulses using optimal control theory, Magn. Reson. Medicine **36**, 401-409 (1996).

OC → Shinnar-LeRoux (SLR)

- Fast & Powerful
- Well-defined empirical relations
- Constrained



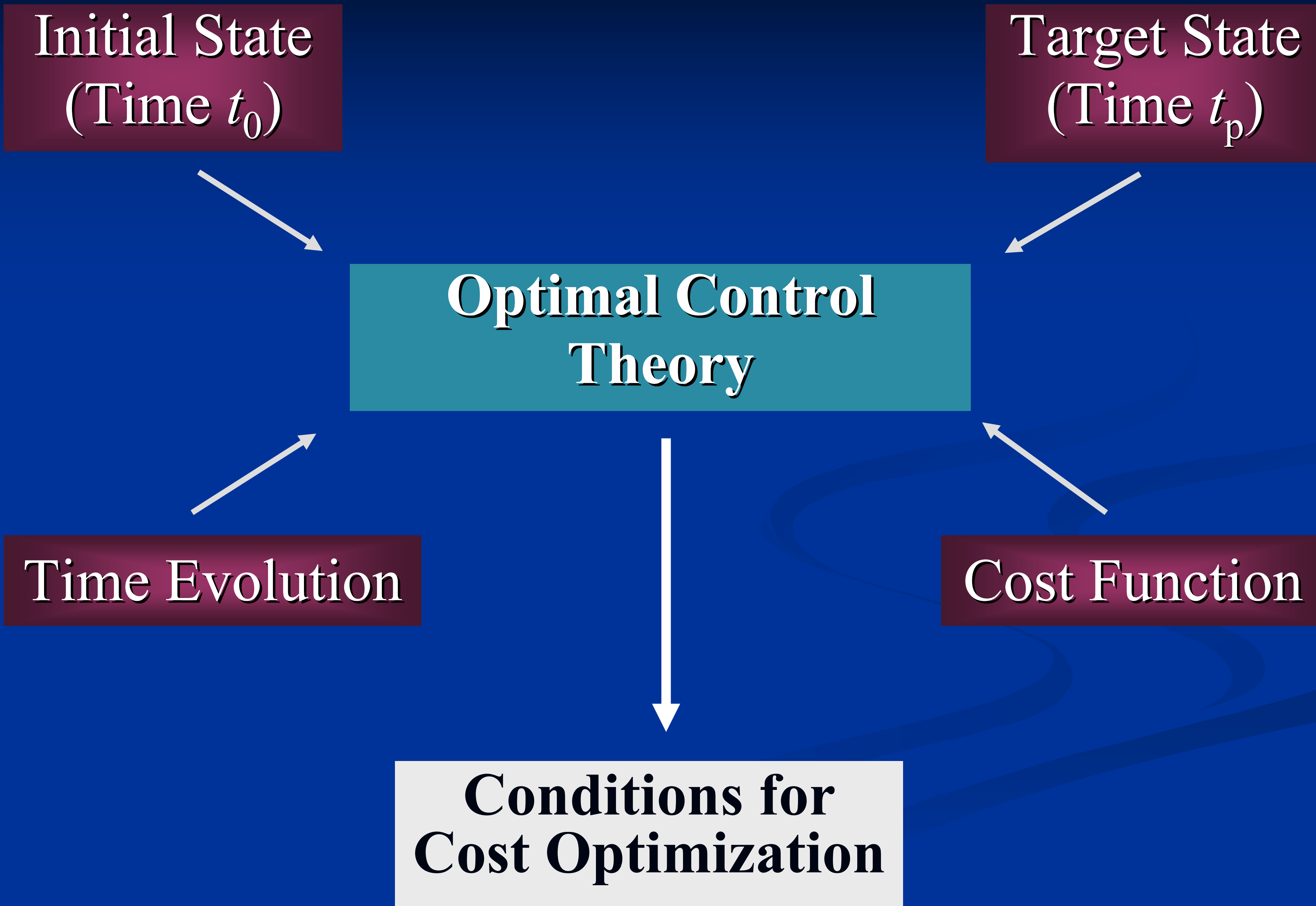
High Resolution NMR ↔ Imaging

Different requirements/opportunities

- Broadband non-selective pulses
  - Infinite transition width
- Often large, well-defined gaps in spectra
- Need refocused pulses
  - Chemical shift vs Gradient-induced dispersion
- 1H −13C − 15N coupling networks
  - Coherence transfer

- RF inhomogeneity/miscalibration
- Relaxation losses

Ingredients



M

F

Optimal Control Theory

Bloch Equation

$$dM/dt = \omega_e \times M$$
$$= \Omega M$$

$$\Phi(t_p) = \langle \mathbf{M} \mid \mathbf{F} \rangle$$
$$\rightarrow \mathbf{M} \cdot \mathbf{F}$$

Conditions for RF Controls to Optimize Cost

$$h = \langle \lambda \mid \mathrm{d}M/\mathrm{dt} = \omega_e \times M \rangle - L$$

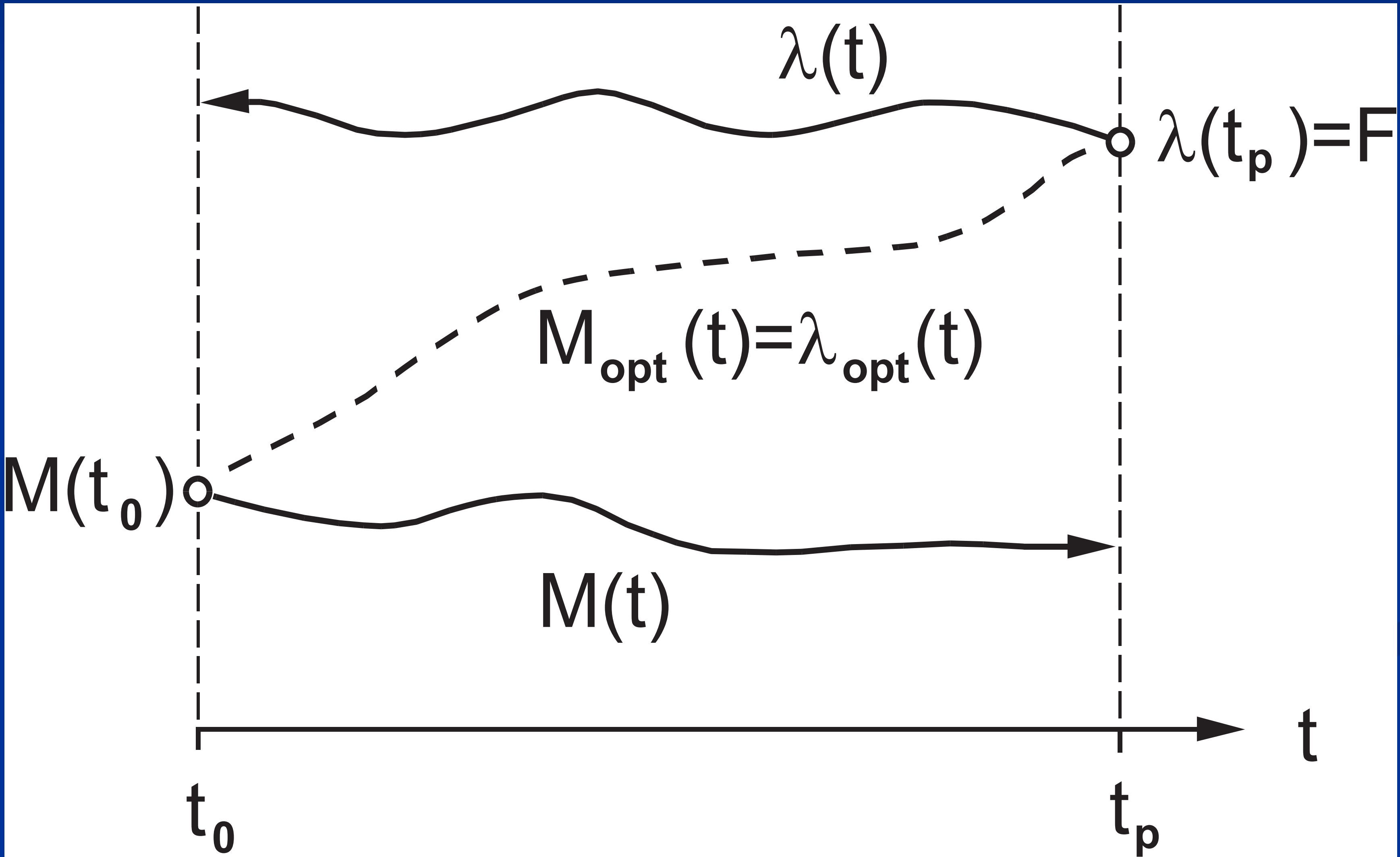
$$\rightarrow \lambda \cdot (\omega_e \times M)$$
$$= M \cdot (\lambda \times \omega_e)$$
$$= \omega_e \cdot (M \times \lambda)$$

$$dh/d\lambda = \dot{M}$$
$$dh/dM = -\dot{\lambda}$$
$$dh/d\omega_e = G \rightarrow 0$$

$$h = \langle \lambda \mid f \rangle - L$$
$$\rightarrow \langle \lambda \mid \Omega M \rangle$$
$$\langle \lambda \mid H \Psi \rangle \leftrightarrow \langle \lambda \mid [H , \rho] \rangle$$

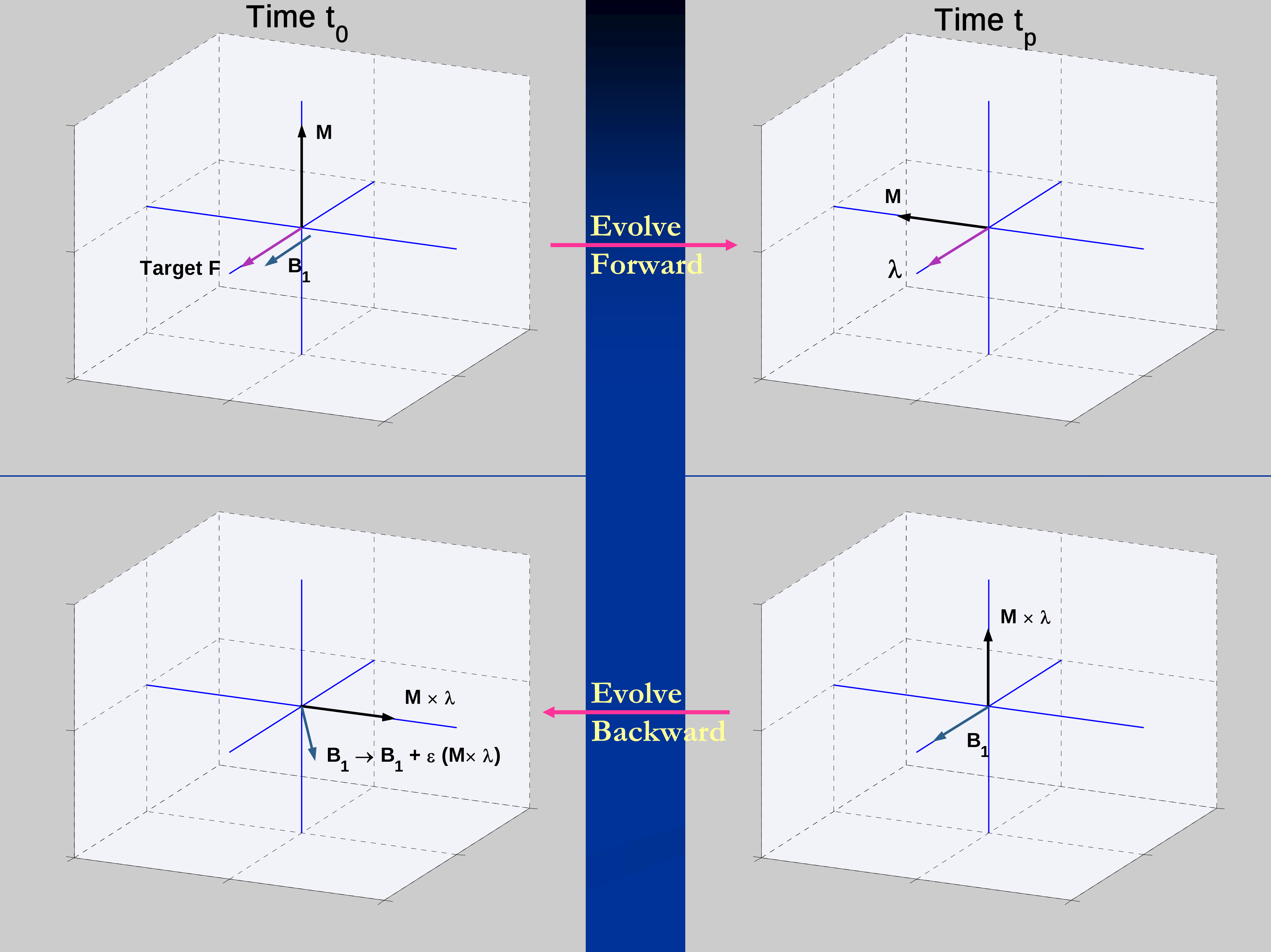
$$\langle A \mid B \rangle \leftrightarrow A^{\dagger} \cdot B \leftrightarrow \mathrm{Tr}(A^{\dagger} B)$$
$$\mathrm{Tr}(ABC) = \mathrm{Tr}(CAB) = \mathrm{Tr}(BCA)$$

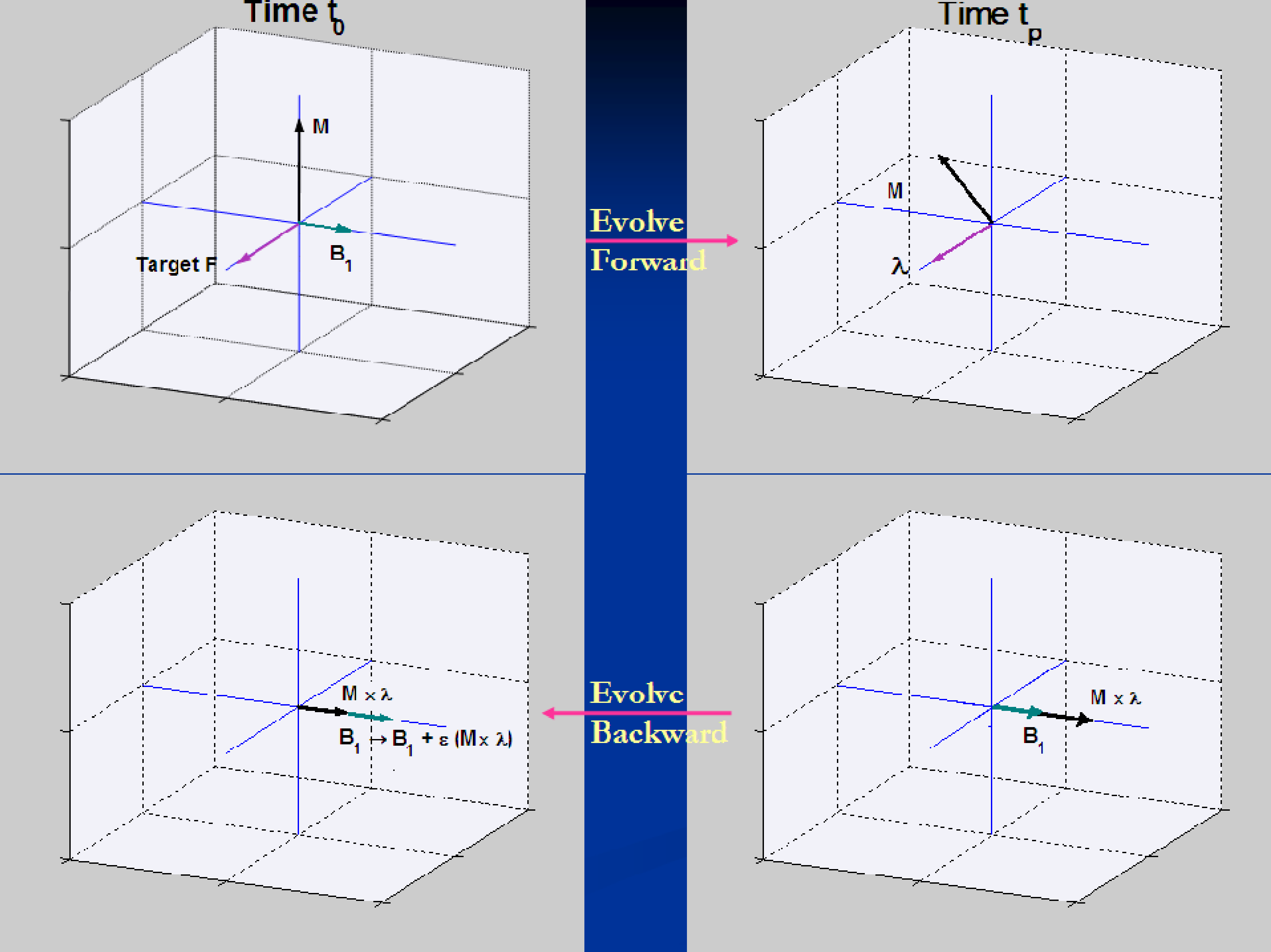
- Lagrange multiplier **λ** : $\lambda(t_p) = \partial\Phi / \partial\mathbf{M} = \mathbf{F}$
  - **Also obeys Bloch Equation**
- $\mathbf{M} \times \boldsymbol{\lambda} = 0$



“Design” a Hard 90^o Pulse

- Initial state **M** along z-axis
- Target **F** along x-axis
- Cost = < F | M > → **M·F**
  - λ = **F**
- Choose $\mathbf{B}_1 * t_P \rightarrow 90^o$
  - “Guess” $\mathbf{B}_1$ along x-axis


Time t_0
M
Target F
B_1
Evolve
Forward
Time t_p
M
λ
M × λ
$B_1 \to B_1 + \varepsilon\ (M \times \lambda)$
Evolve
Backward
M × λ
B_1



Time t_0
M
Target F
B_1
Evolve Forward
Time t_p
M
λ
Evolve Backward
$M \times \lambda$
$B_1 \mapsto B_1 + \varepsilon (M \times \lambda)$
$M \times \lambda$
B_1

Design a "Calibration-Free" Broadband Excitation Pulse

- t_{90} ~ 10–25 μs for typical ^{13}C probes
  - ~ 10–20 kHz peak RF
- Uniformly excite 200 ppm ^{13}C chemical shift range
  - ~ 40 kHz bandwidth at 800 MHz

- Initial state **M** along z-axis   Target **F** along x-axis
- Average **M** × **λ** resulting from range of RF and resonance offsets
- Cost $\Phi = \mathbf{M} \cdot \mathbf{F}$

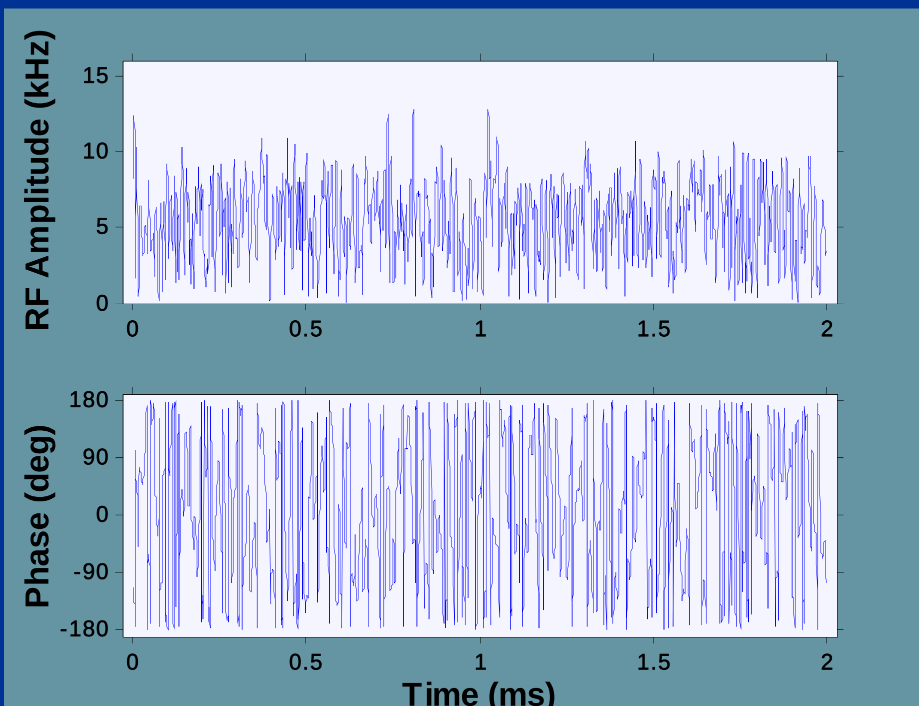
  $$\leftrightarrow ||\mathbf{M} - \mathbf{F}||^n \quad \text{(weighted)}$$
- Clip nominal peak RF at 15 kHz

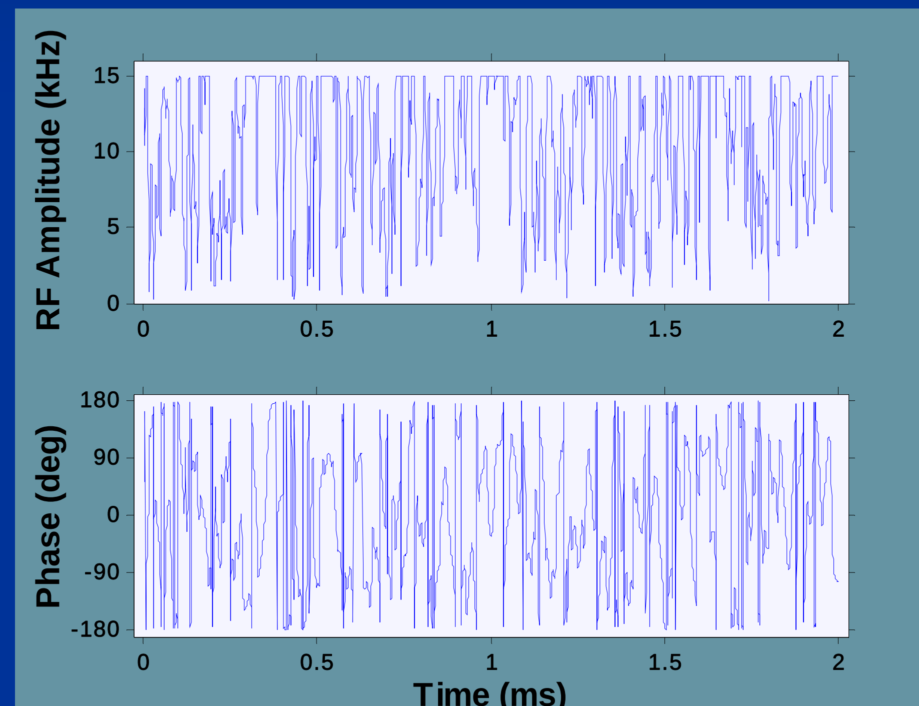
Input Noise

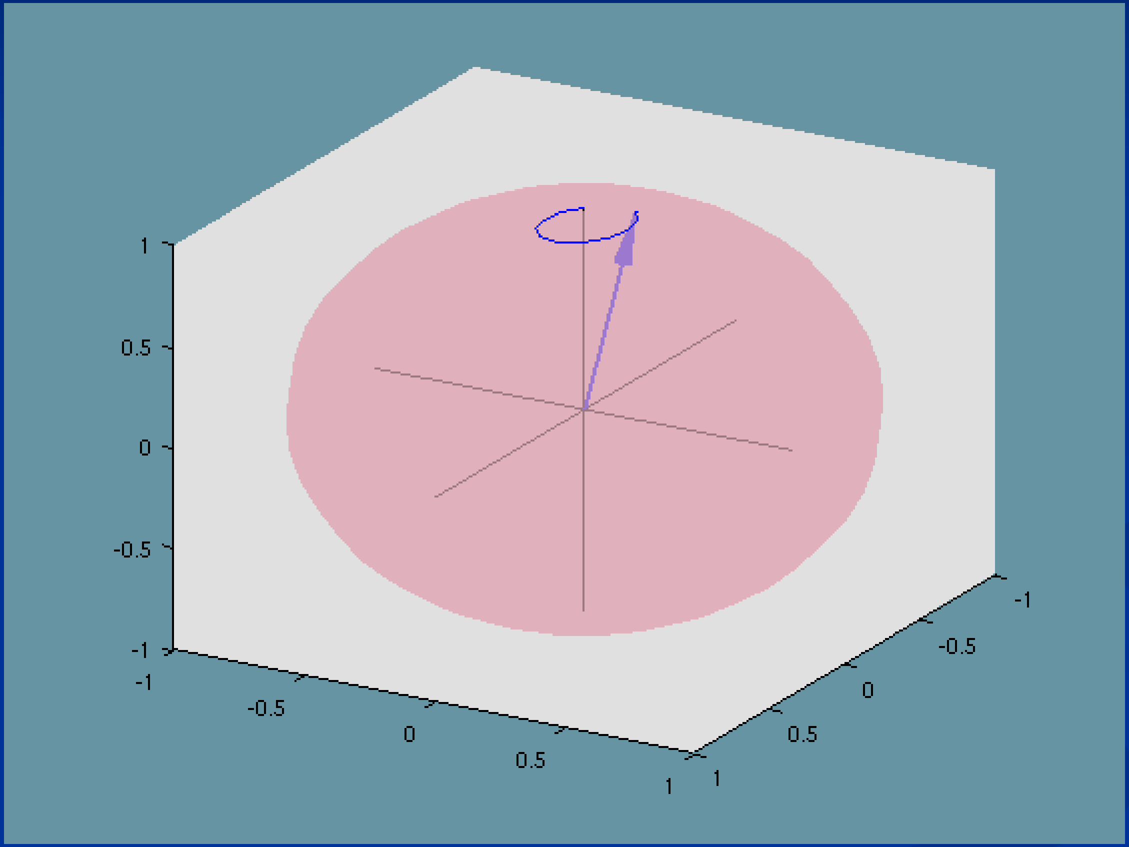
Optimal

Control

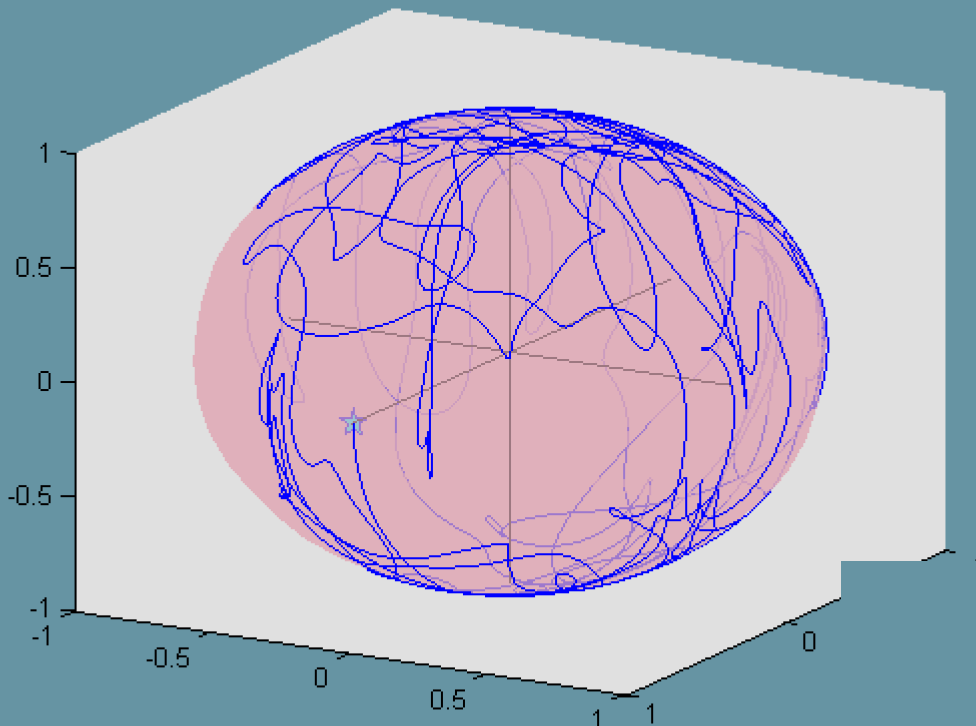
Output ?

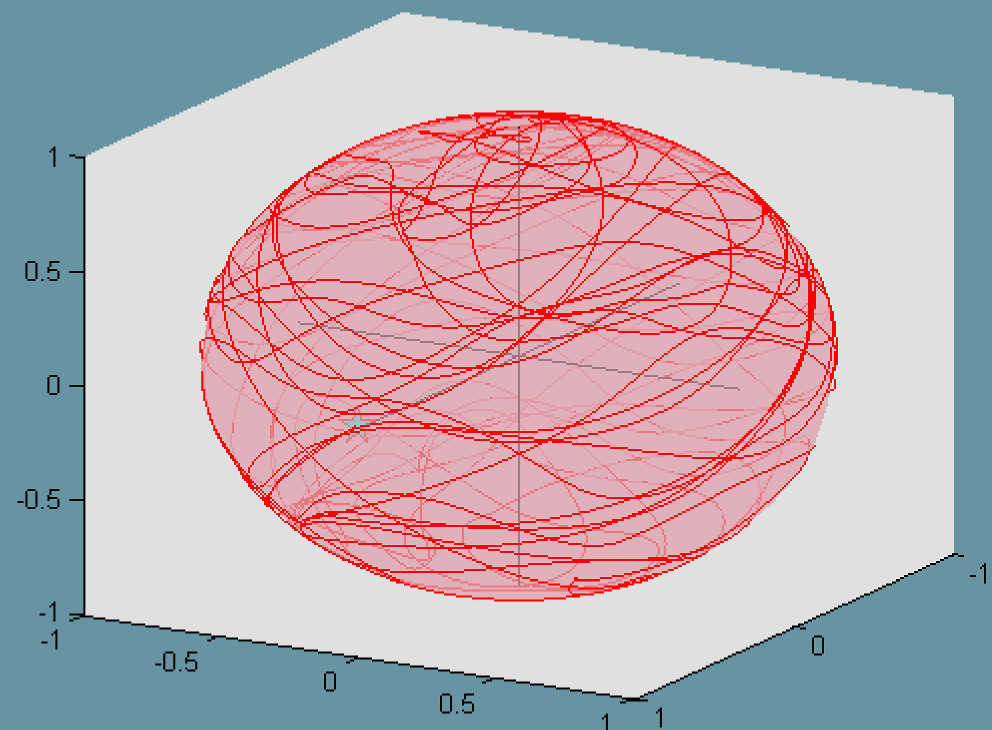


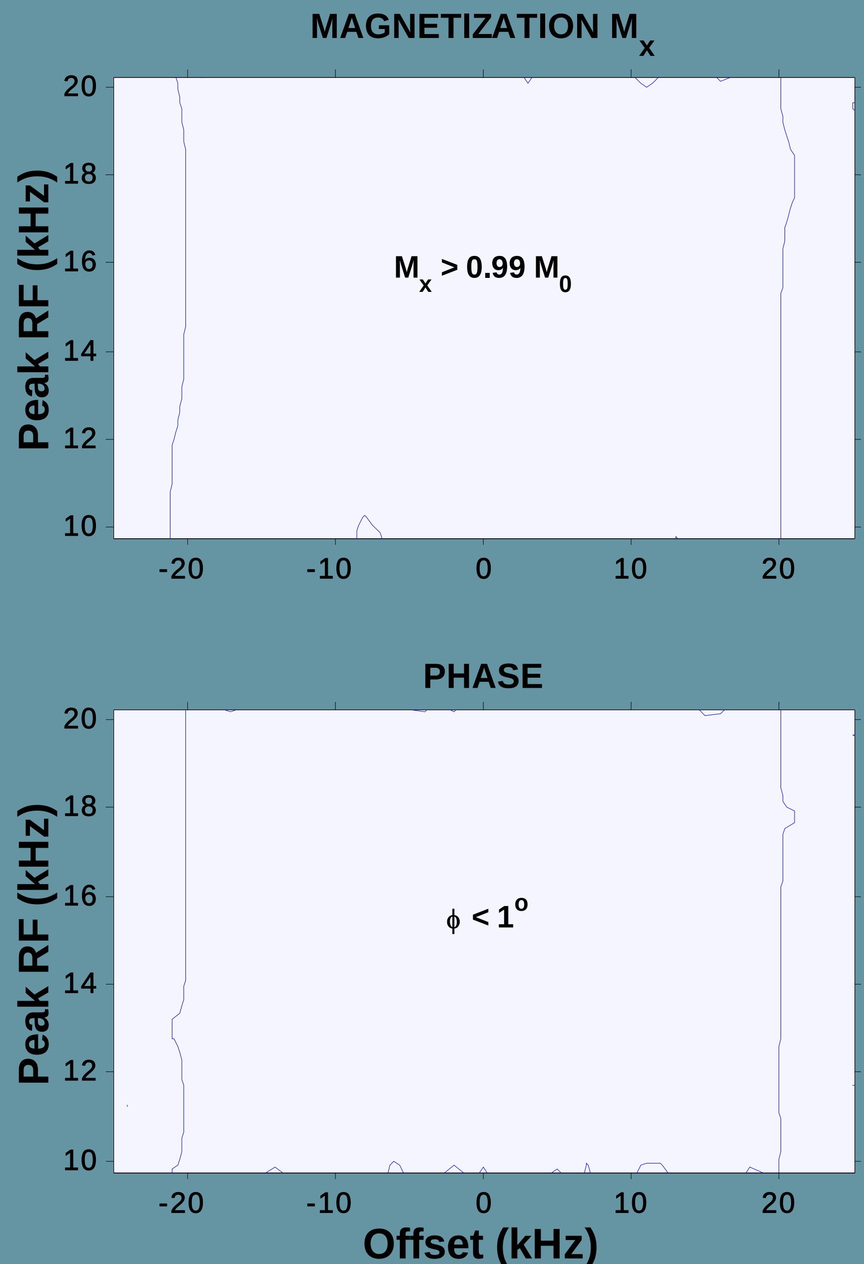




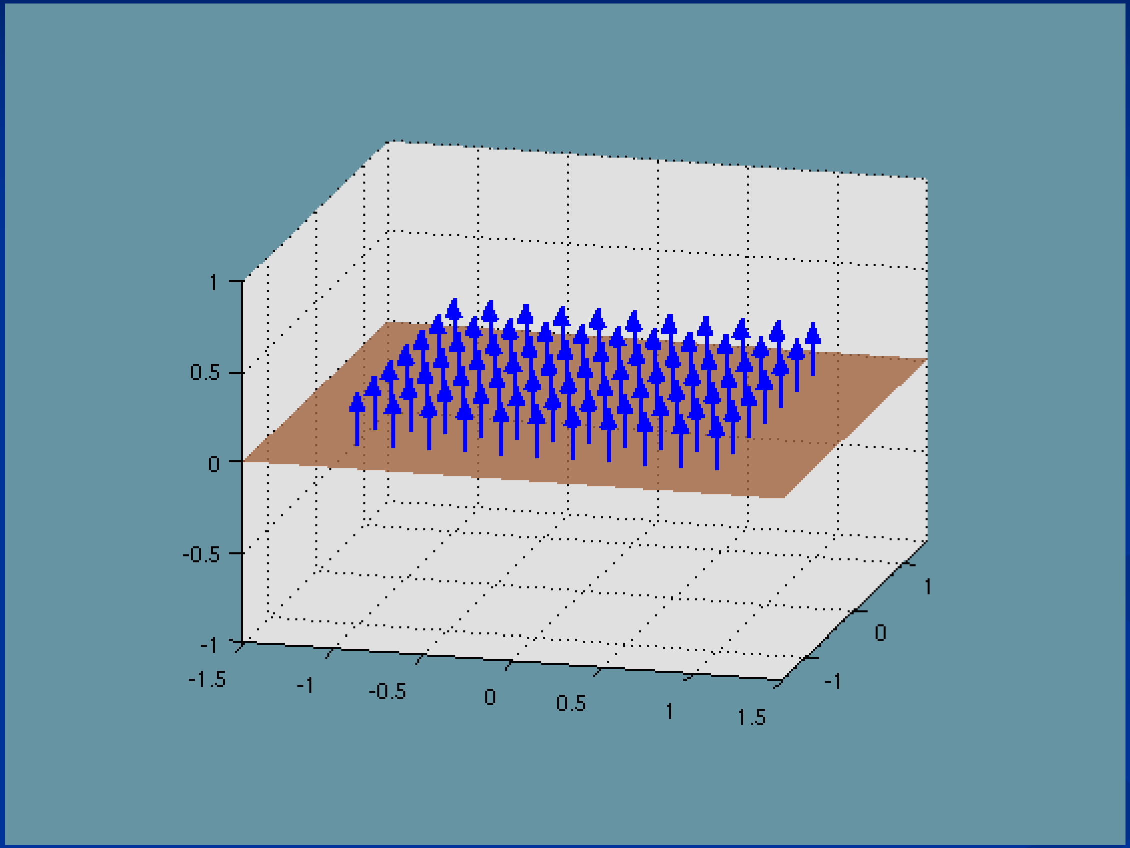
1
0.5
0
-0.5
-1
-1
-0.5
0
0.5
1
-1
-0.5
0
0.5
1


1
0.5
0
-0.5
-1
-1
-0.5
0
0.5
1
1
0

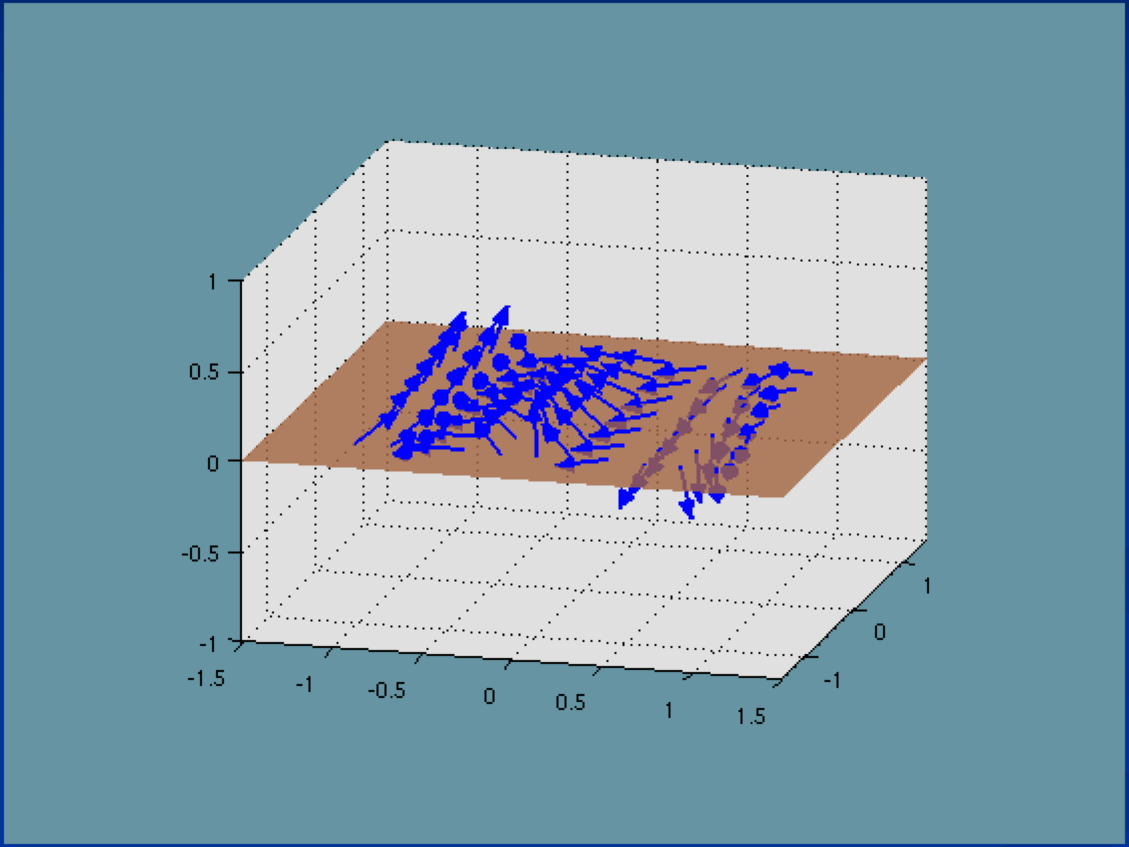

1
0.5
0
-0.5
-1
-1
-0.5
0
0.5
1
1
0
-1



MAGNETIZATION M_x
Peak RF (kHz)
20
18
16
14
12
10
$M_x > 0.99\ M_0$
-20
-10
0
10
20
PHASE
$\phi < 1^o$
Offset (kHz)

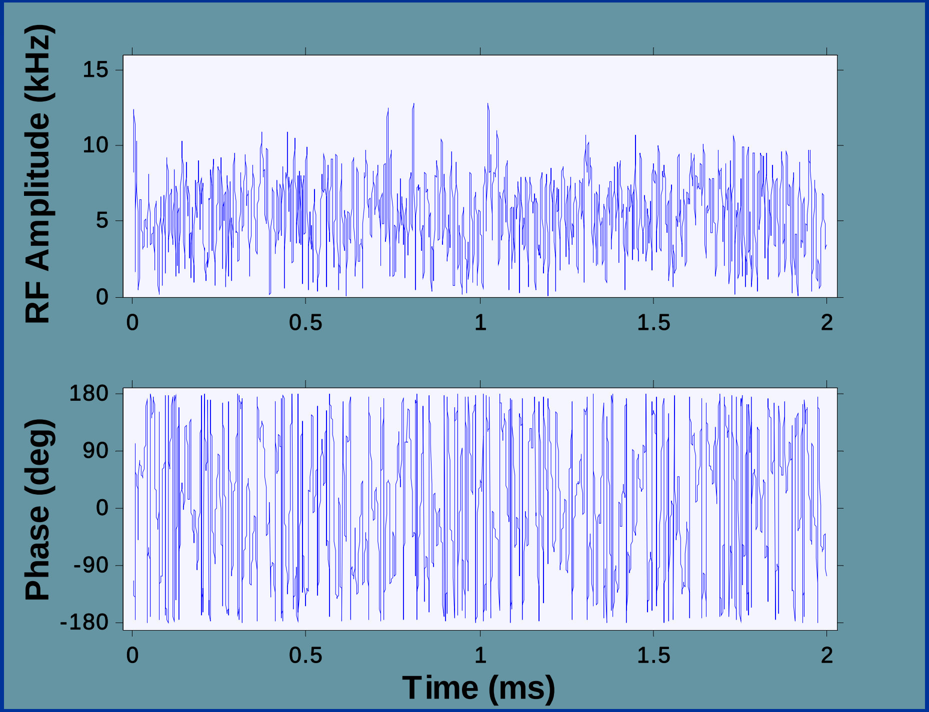


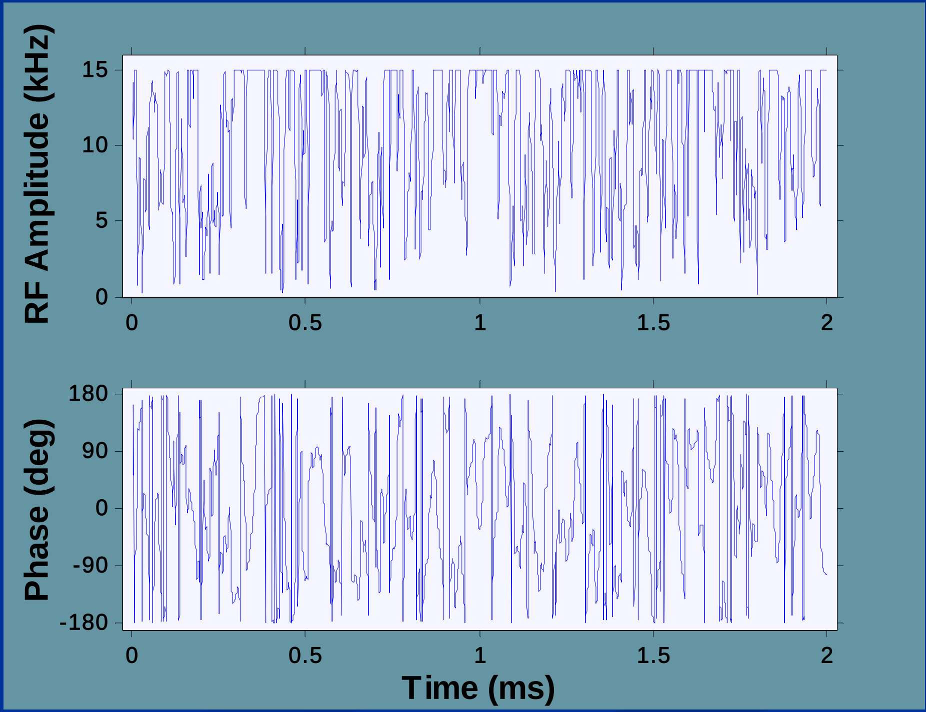
1
0.5
0
-0.5
-1
-1.5
-1
-0.5
0
0.5
1
1.5
1
0
-1



1
0.5
0
-0.5
-1
-1.5
-1
-0.5
0
0.5
1
1.5
1
0
-1

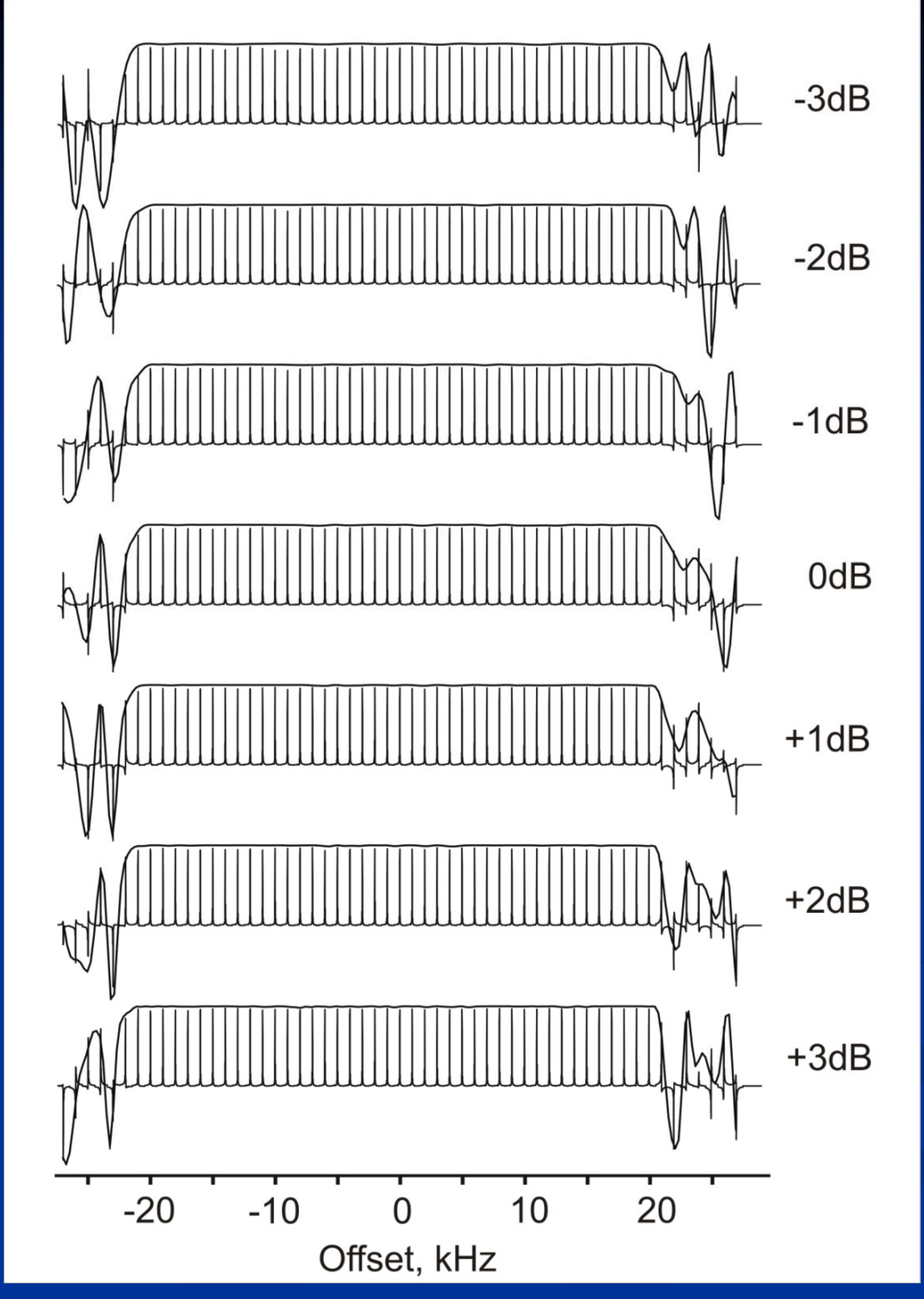
Input Noise → Optimal Control → Output





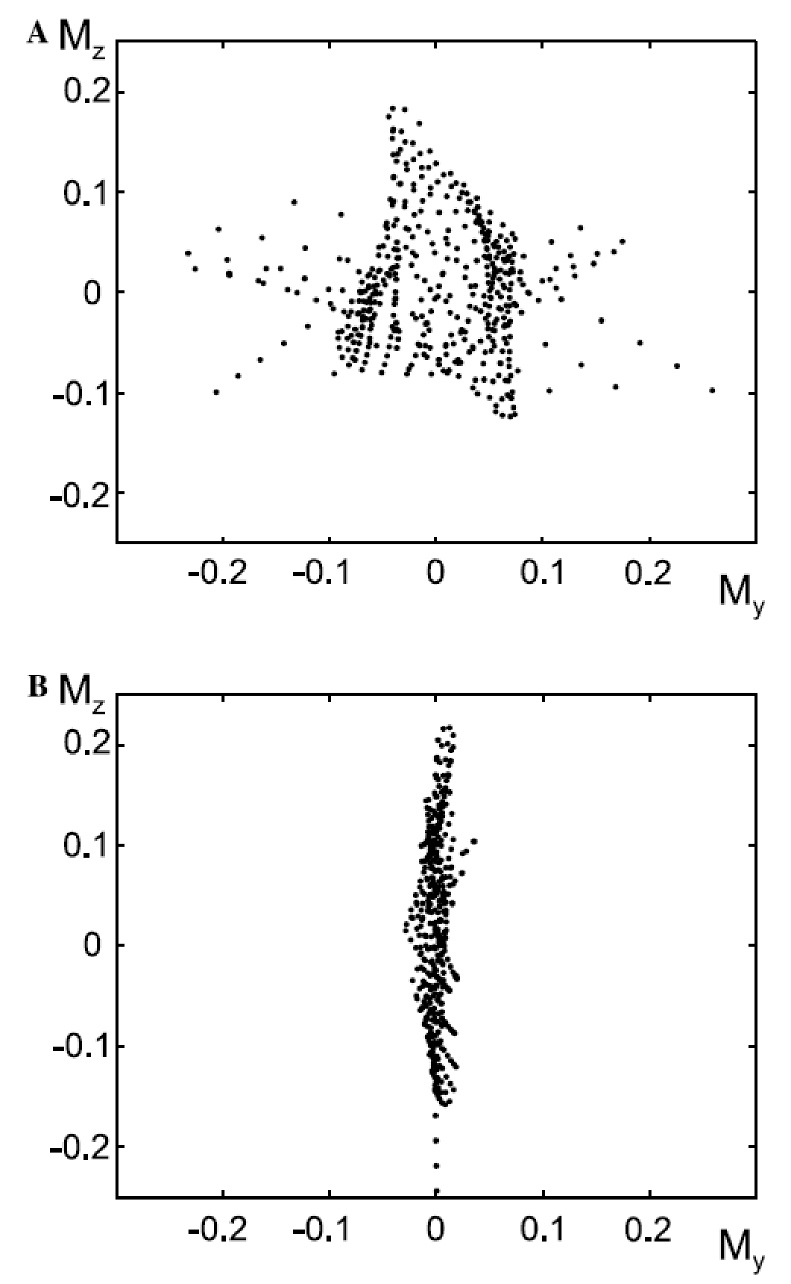
Glendower: I can call spirits
from the vasty
deep.

Hotspur: Why, so can I,
or so can any man;
But will they come
when you do call
for them?



-3dB
-2dB
-1dB
0dB
+1dB
+2dB
+3dB
-20
-10
0
10
20
Offset, kHz

Tailoring the Cost Function to Performance



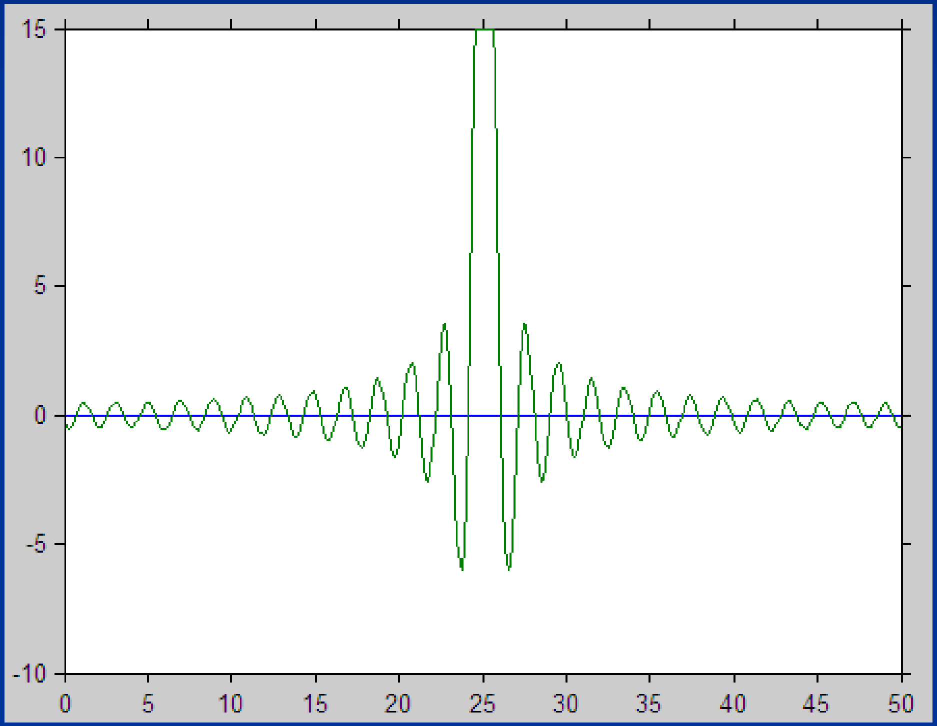
Cost $\Phi = \mathbf{M} \cdot \mathbf{F}$

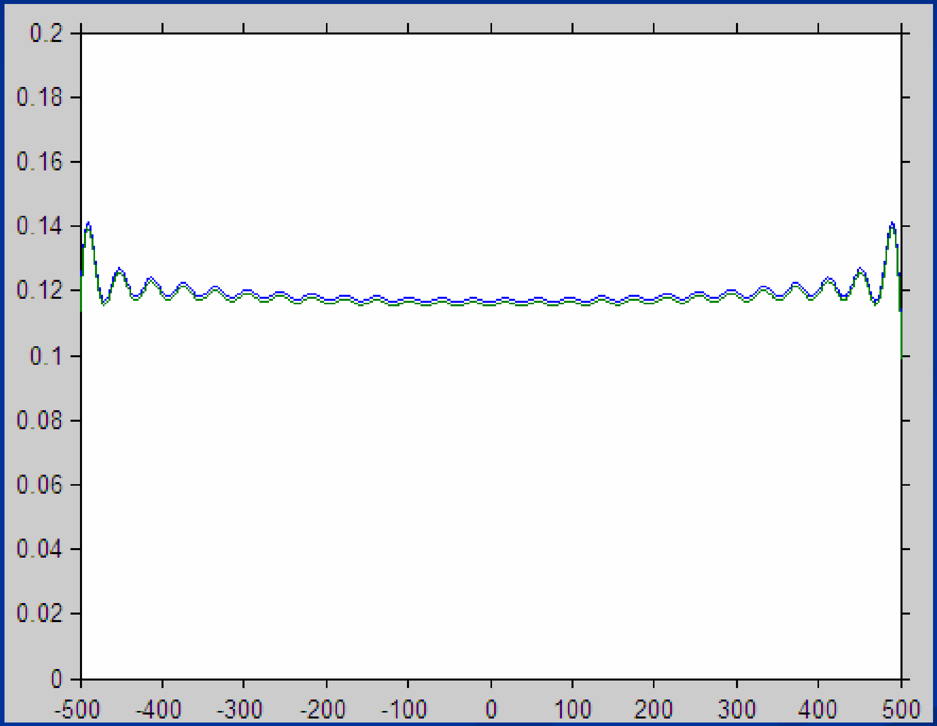
$$\Phi = \sum_{i=1}^{3} a_i (M_i - F_i)^2$$

$\mathbf{a} = (1, 1, 0)$

Extreme Spectral Bandwidth

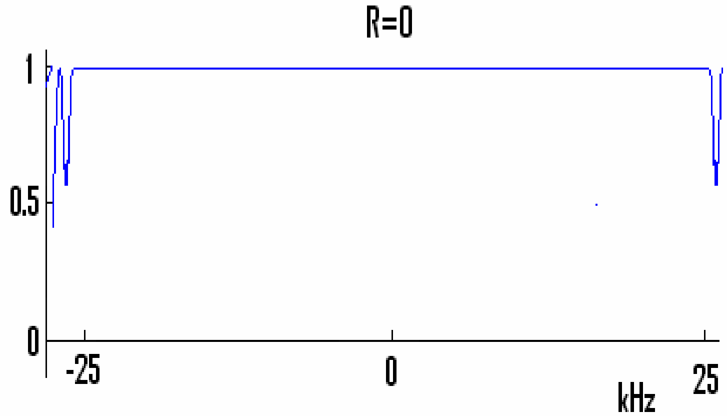
EPR Applications?





50 μs RF pulse
RFmax = 15 kHz

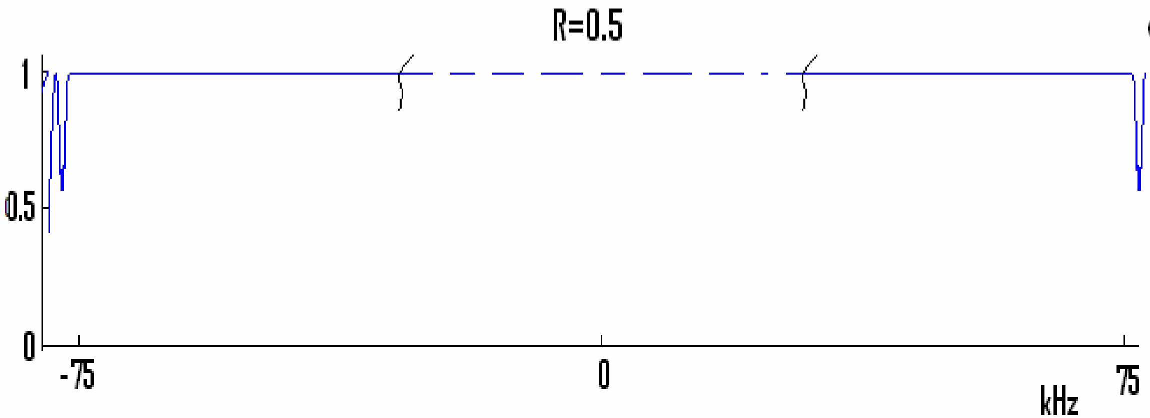
Mx as function of offset ±500 kHz

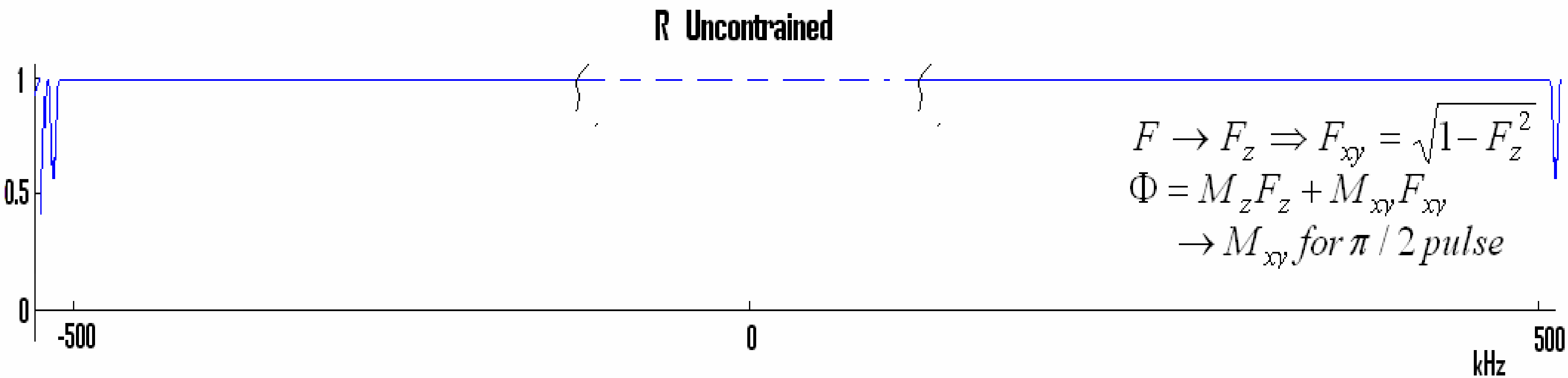


$$F = \cos\varphi \cdot \hat{x} + \sin\varphi \cdot \hat{y}$$

$$R(\Delta\omega \cdot Tp)$$

$$\Phi = \langle F \mid M \rangle = \vec{M} \cdot \vec{F}$$





$$F \rightarrow F_z \Rightarrow F_{xy} = \sqrt{1 - F_z^{\,2}}$$

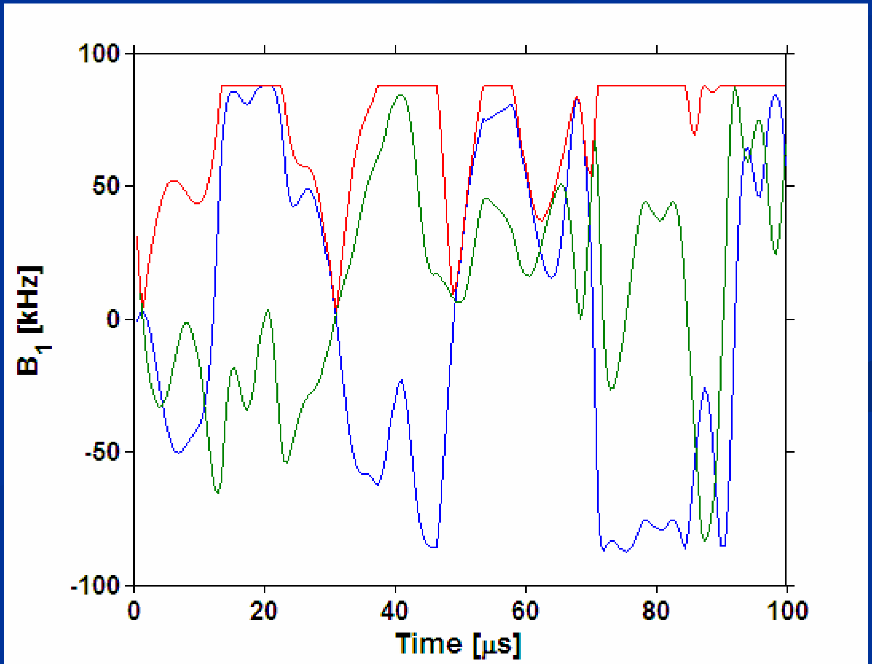
$$\Phi = M_z F_z + M_{xy} F_{xy}$$

$$\rightarrow M_{xy}\, for\, \pi / 2\, pulse$$

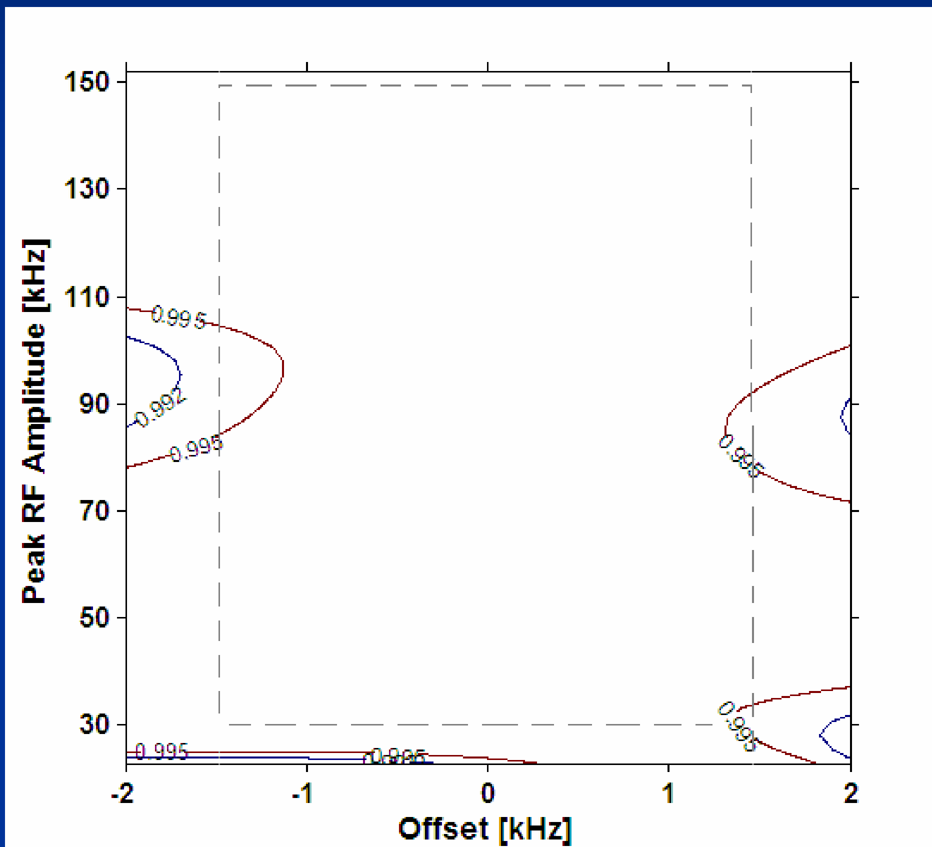
Extreme Tolerance to RF Inhomogeneity

Toroid Cavity Detectors

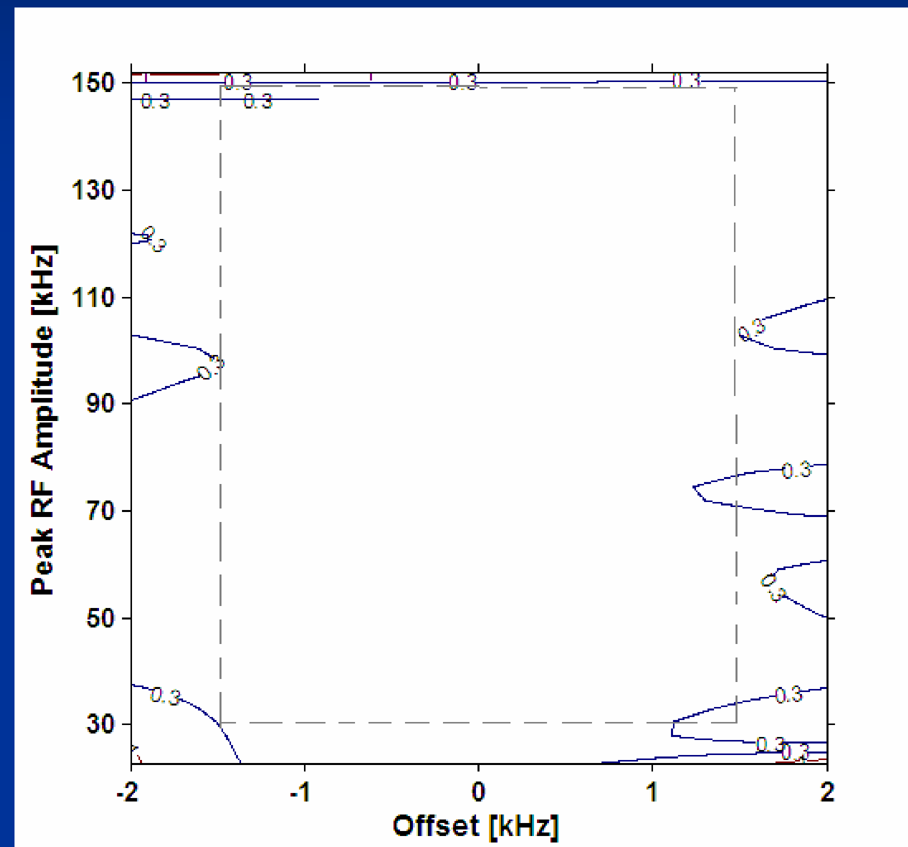
- High P (→ 300 barr), T (→ 250 °C)
  - Monitor *in situ* catalytic reactions
- Large RF gradient (factor of 5-10)
- Chemical shift imaging



Extreme Tolerance to RF Inhomogeneity



M_x as function of offset and ingomogeneity.



Phase deviation from x-axis (in degrees) as function of offset and ingomogeneity.

Relaxation-Compensated Broadband Excitation Pulses

$$\dot{\boldsymbol{M}}(t) = \boldsymbol{\omega}_e(t) \times \boldsymbol{M}(t) + D[\boldsymbol{M}_0 - \boldsymbol{M}(t)]$$

$$D = \begin{pmatrix} 1/T_2 & 0 & 0 \\ 0 & 1/T_2 & 0 \\ 0 & 0 & 1/T_1 \end{pmatrix}$$

$$h(t) = \boldsymbol{\lambda}(t) \cdot \dot{\boldsymbol{M}}(t) = \boldsymbol{\lambda} \cdot [\boldsymbol{\omega}_e \times \boldsymbol{M} + D(\boldsymbol{M}_0 - \boldsymbol{M})]$$

$$\dot{\boldsymbol{M}} = \partial h / \partial \boldsymbol{\lambda}$$

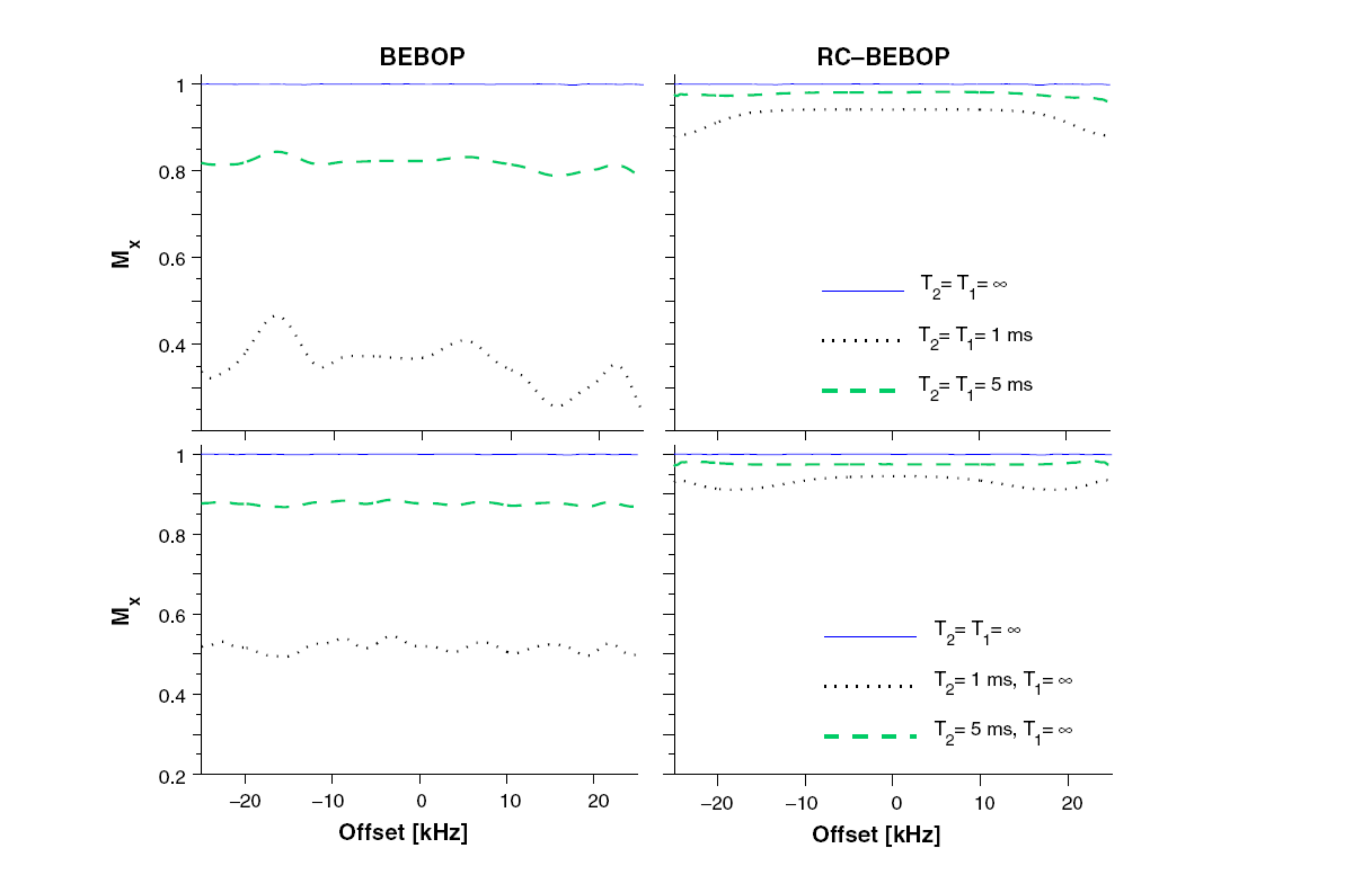
$$\begin{aligned} \dot{\boldsymbol{\lambda}}(t) &= -\,\partial h / \partial \boldsymbol{M} \\ &= \boldsymbol{\omega}_e(t) \times \boldsymbol{\lambda}(t) + D\boldsymbol{\lambda}(t) \end{aligned}$$

$$\lambda(t_p) = \partial \Phi / \partial \boldsymbol{M}$$

$$\Phi = \boldsymbol{M}(t_p) \cdot \boldsymbol{F}$$

$$\lambda(t_p) = \boldsymbol{F}$$

Calibration-free BEBOP pulse, $t_p = 1$ ms



Empirical Relations for OC Selective-Pulse Design

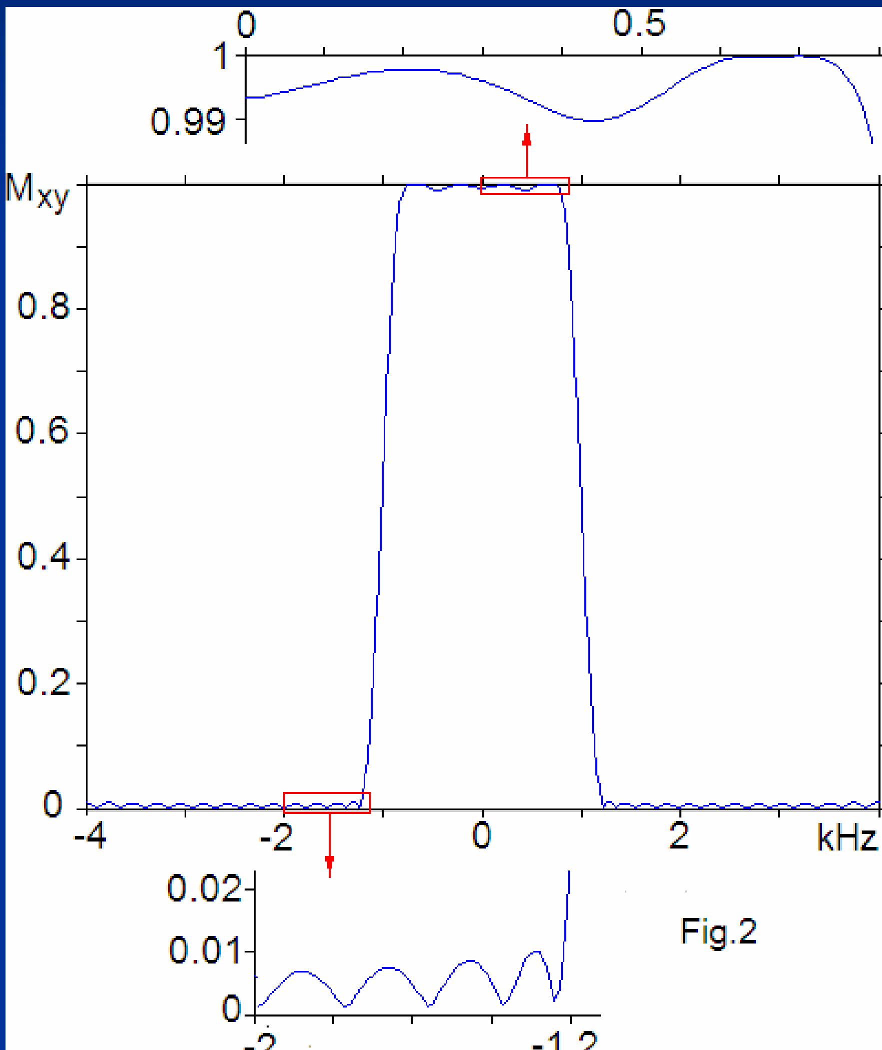


Fig.2

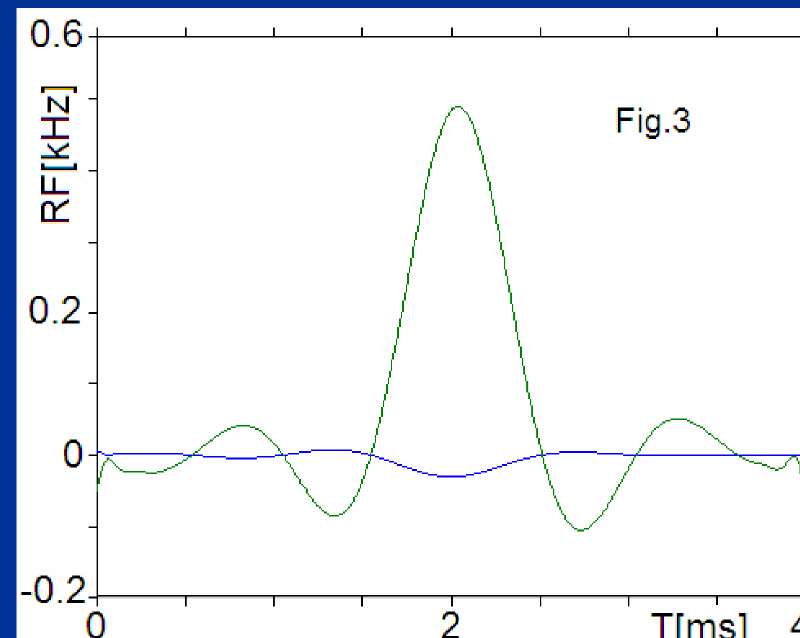
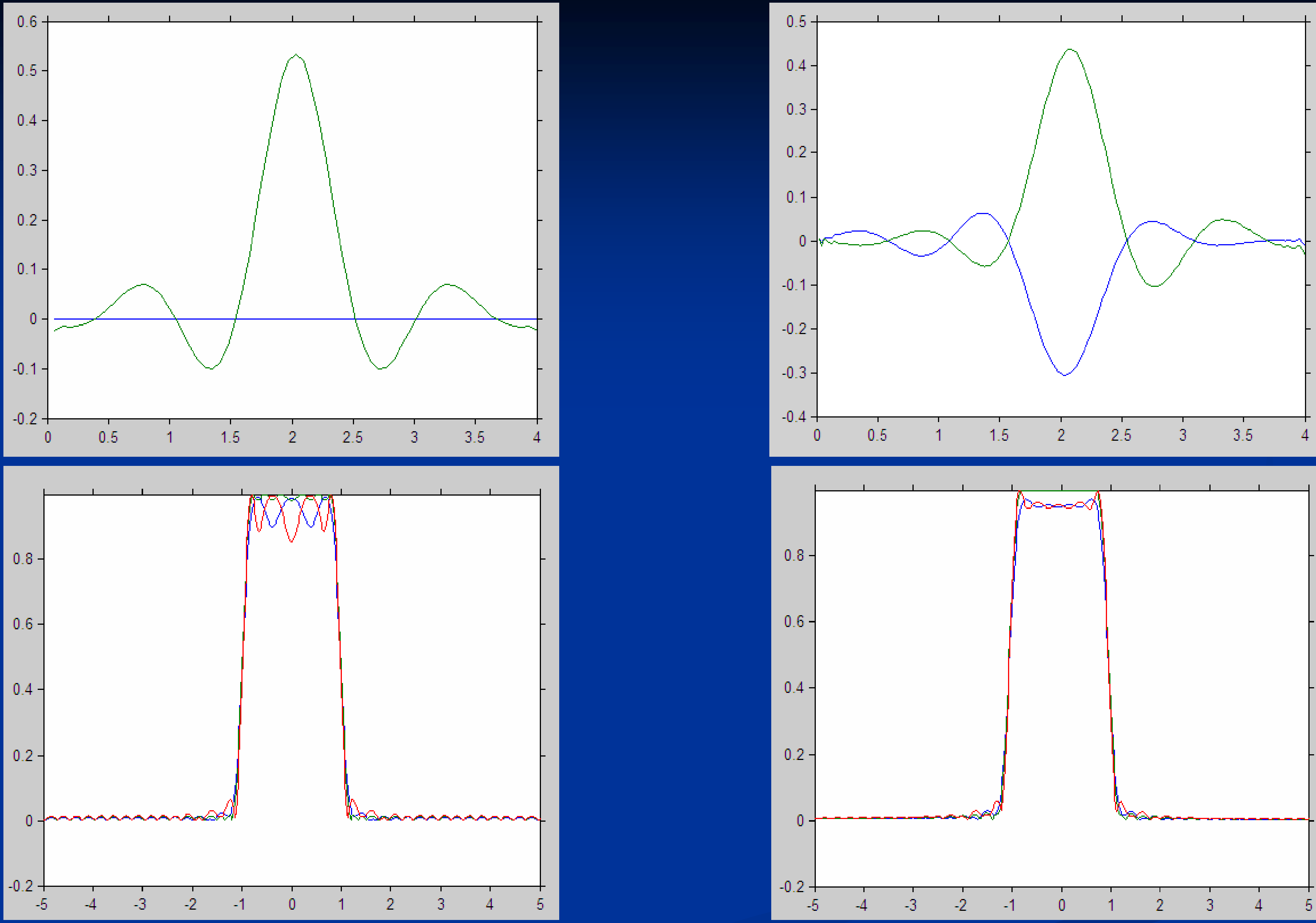


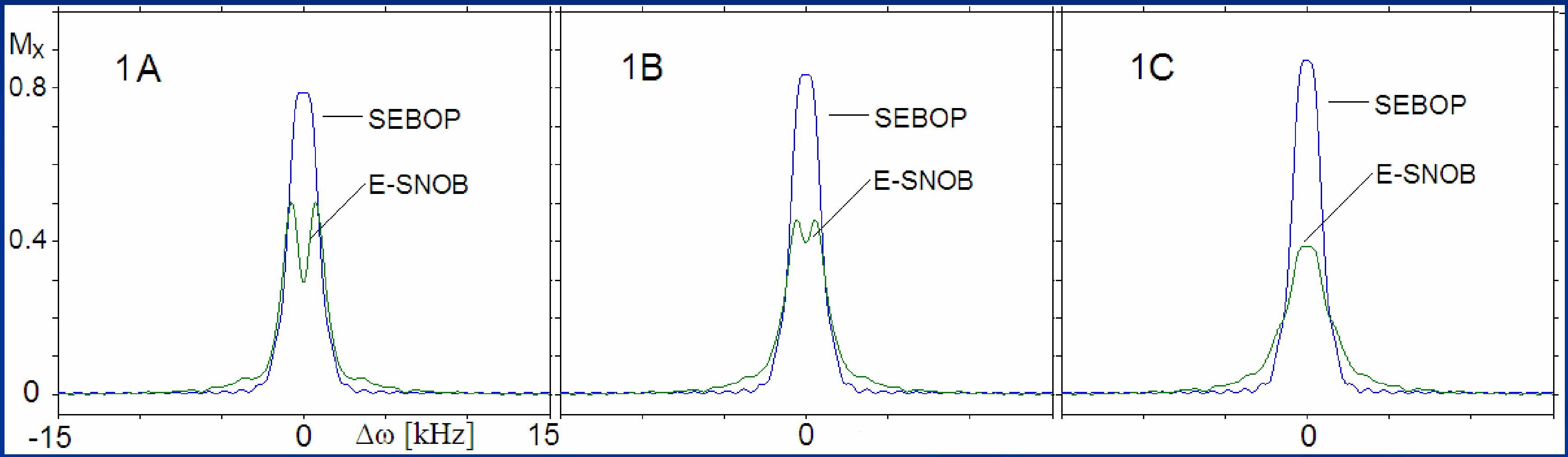
Fig.3



SLR (left) and OC (right) Pulse and Slice Profile

Ideal RF (green) Ideal + 20% (red) Ideal – 20% (blue)

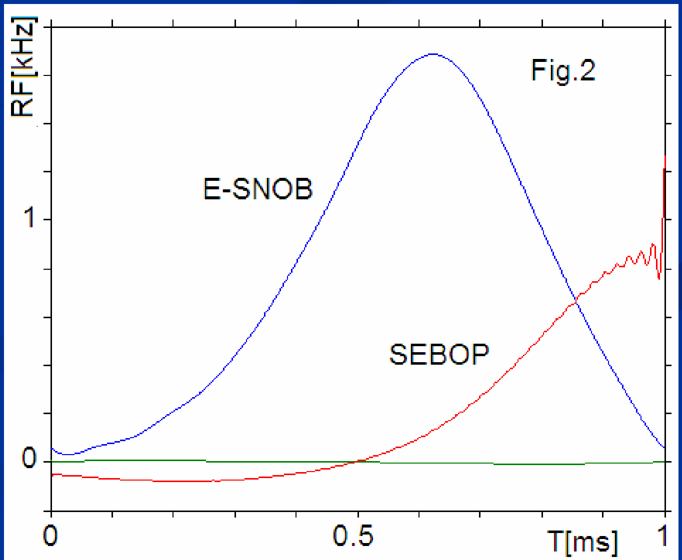
Relaxation-Compensated Selective Pulses

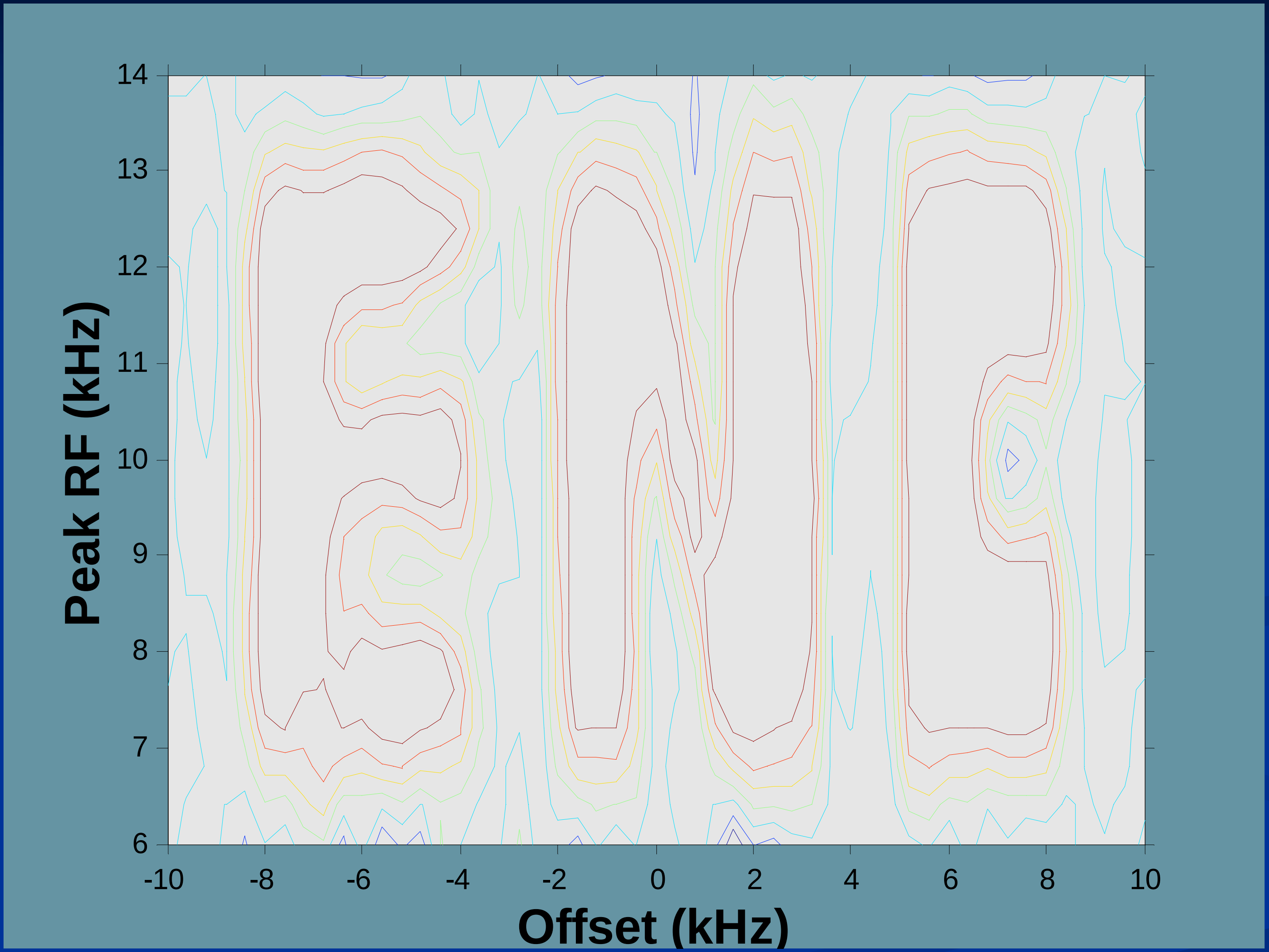


Simulated performance (*M*x versus frequency offset Δω) for the case $Tp = T_1 = T_2 = 1$ ms.

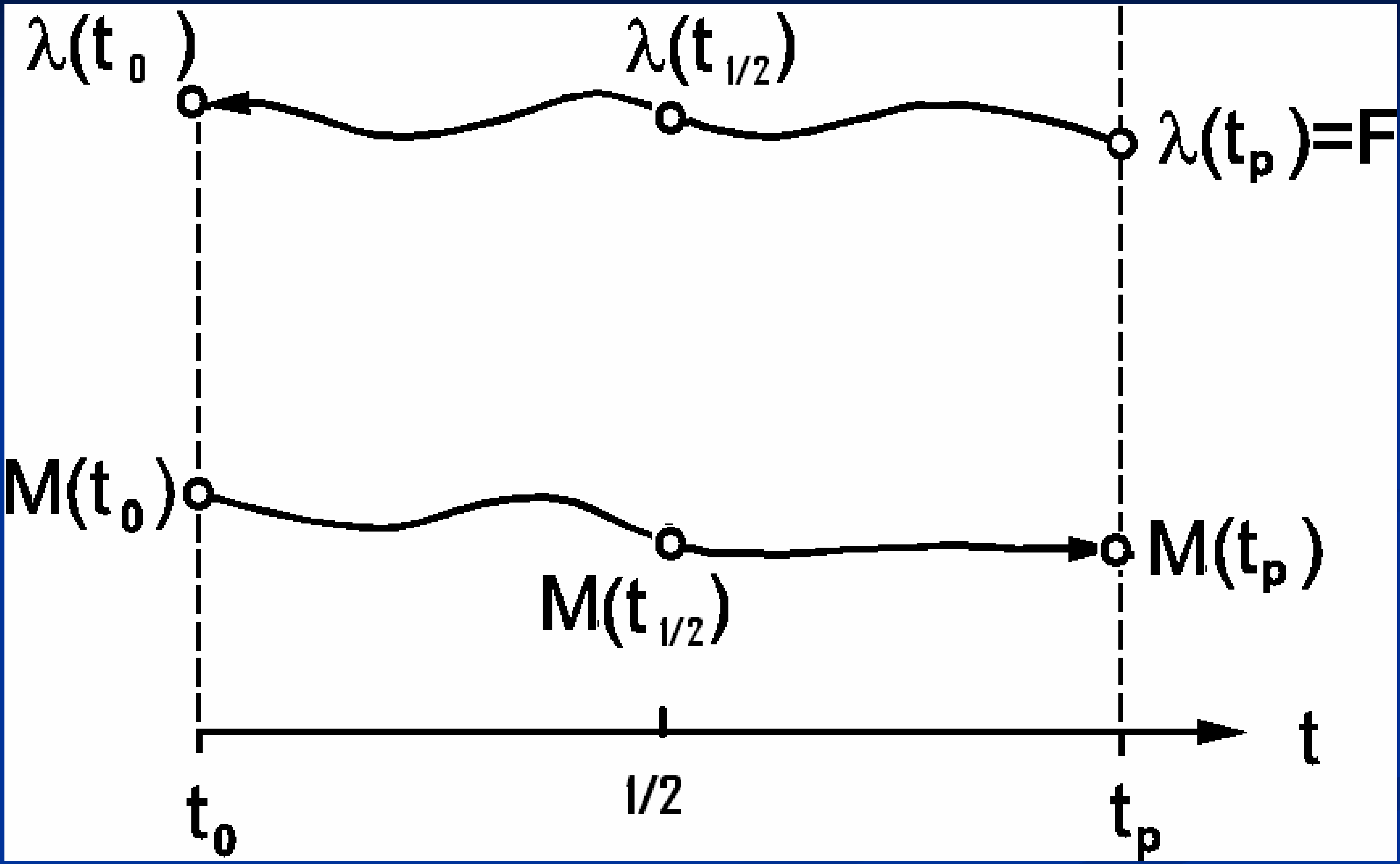
RF field inhomogeneity
A) -10%, **B**) 0%, and **C**) +10%.

SEBOP uses less power.

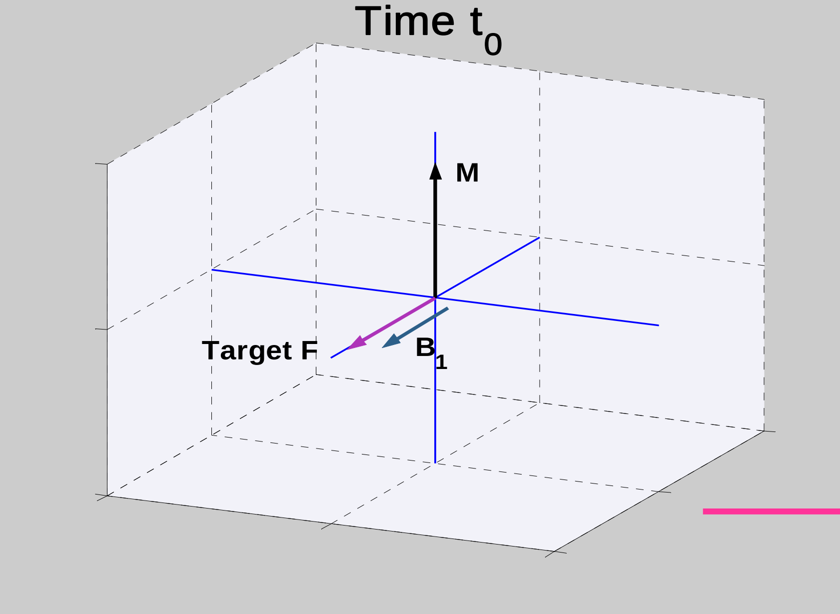


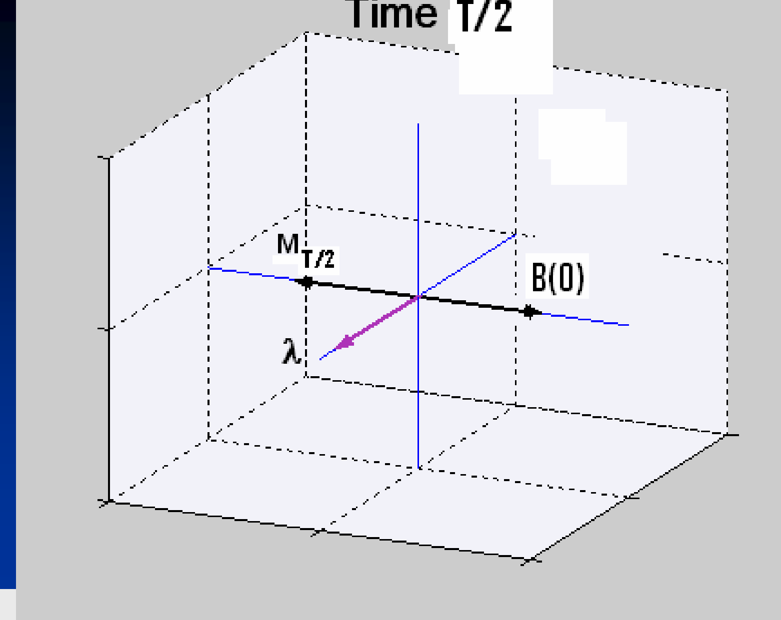


Peak RF (kHz)
14
13
12
11
10
9
8
7
6
-10
-8
-6
-4
-2
0
2
4
6
8
10
Offset (kHz)



λ(t 0)
λ(t 1/2)
λ(t p)=F
M(t 0)
M(t p)
M(t 1/2)
t
t 0
1/2
t p





$$B_1(0) \rightarrow (1/\alpha)\vec{M}_0 \times \vec{\lambda}_0$$

$$M_0 \rightarrow M_{T/2} = \sin(\theta)\hat{x} + \cos(\theta)\hat{z}$$

$$\theta = 2\pi B_1 T/2 = \pi/4B_1 = \pi/(4\alpha)$$

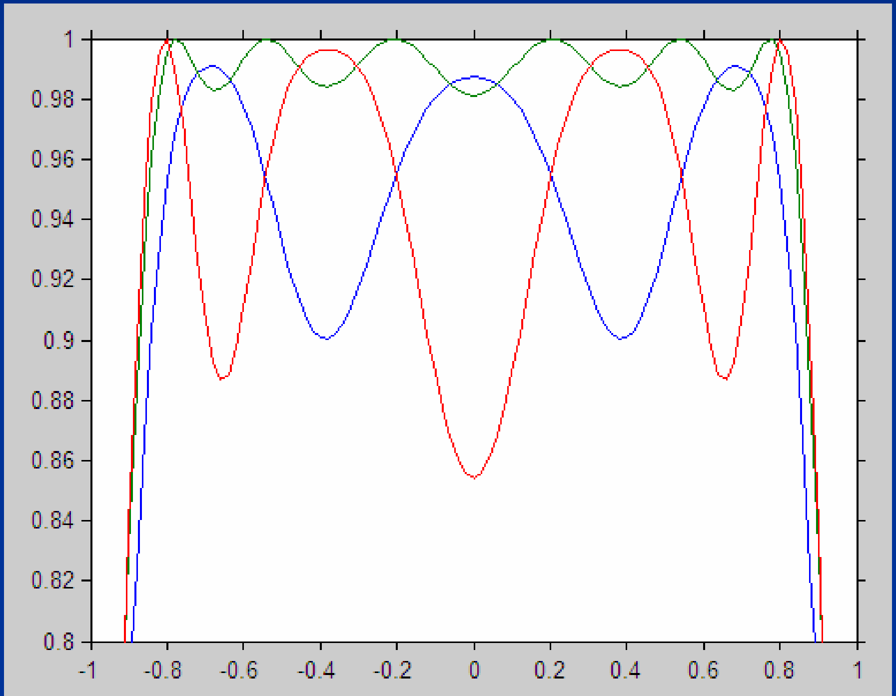
$$B_1(T/2) \rightarrow (1/\alpha)\vec{M}_{T/2} \times \vec{\lambda}_{T/2}$$

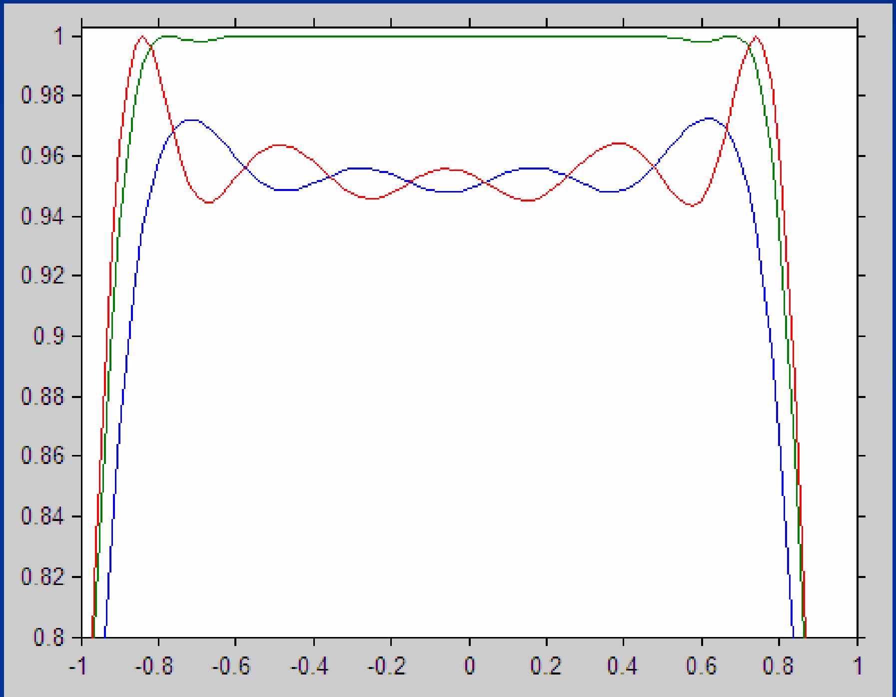
$$= (1/\alpha)\cos(\theta)\hat{y}$$

$$M_{T/2} \rightarrow M_T = \sin(\theta')\hat{x} + \cos(\theta')\hat{z}$$

$$\theta' = \pi/4B_1(T/2) \le \theta \ni [0, \pi/(4\alpha)]$$

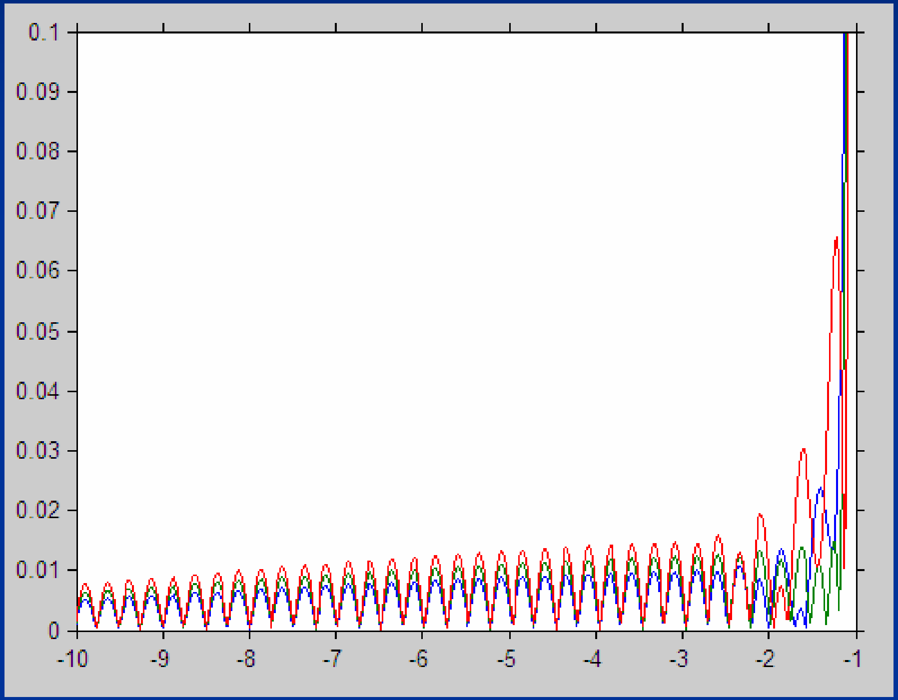
$$\ni [0, \pi/(4\alpha)]$$

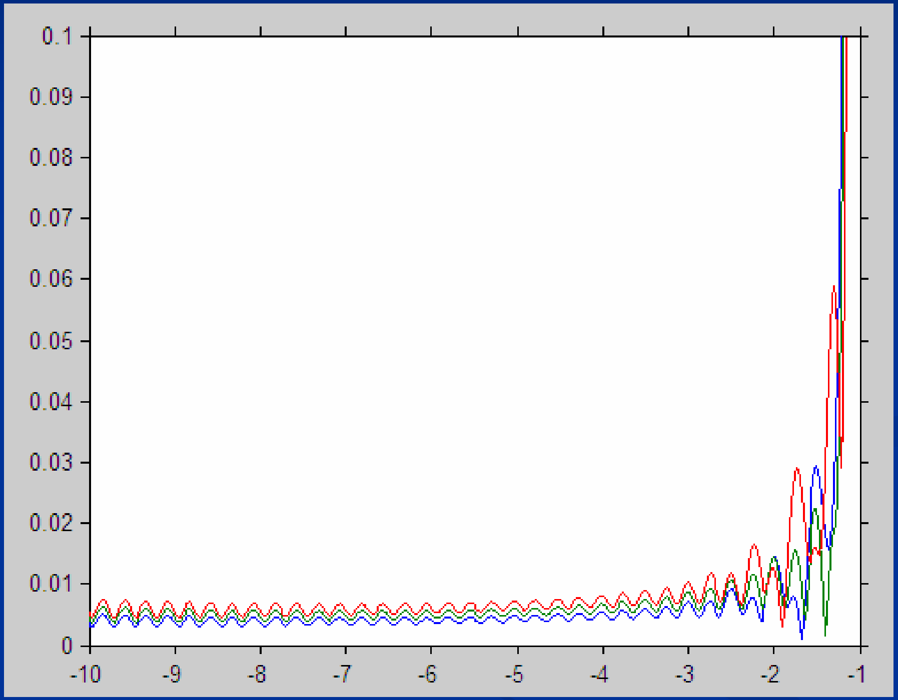




SLR (left) and OC (right) passband

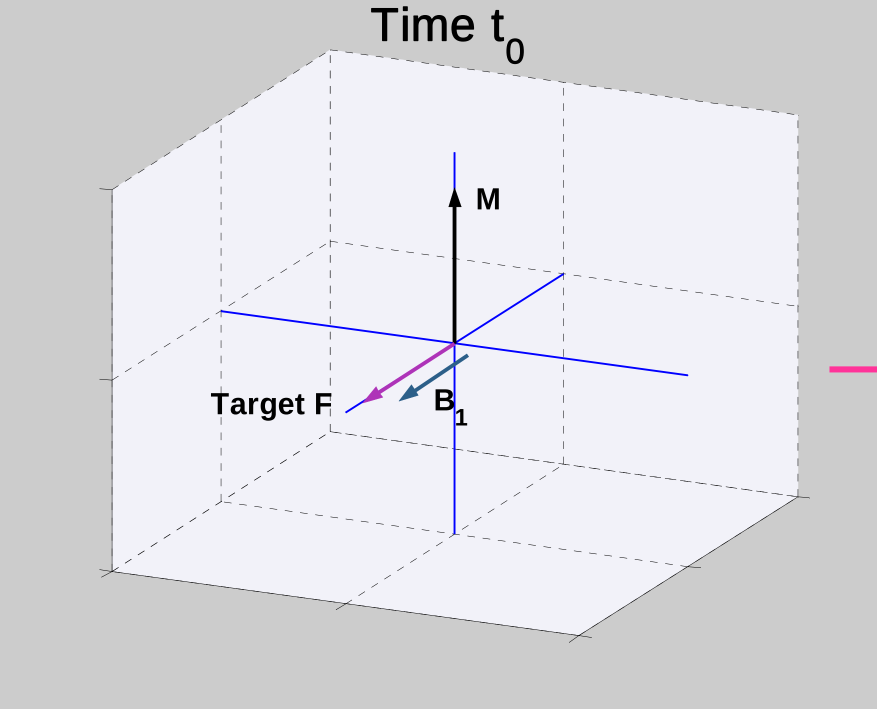
Ideal RF (green) Ideal + 20% (red) Ideal – 20% (blue)



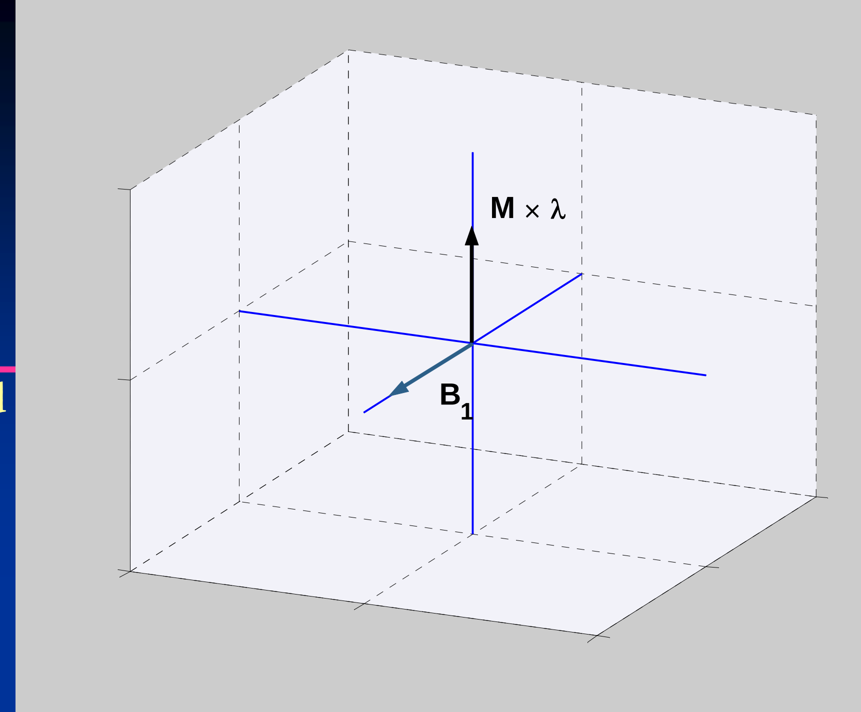


SLR (left) and OC (right) stopband

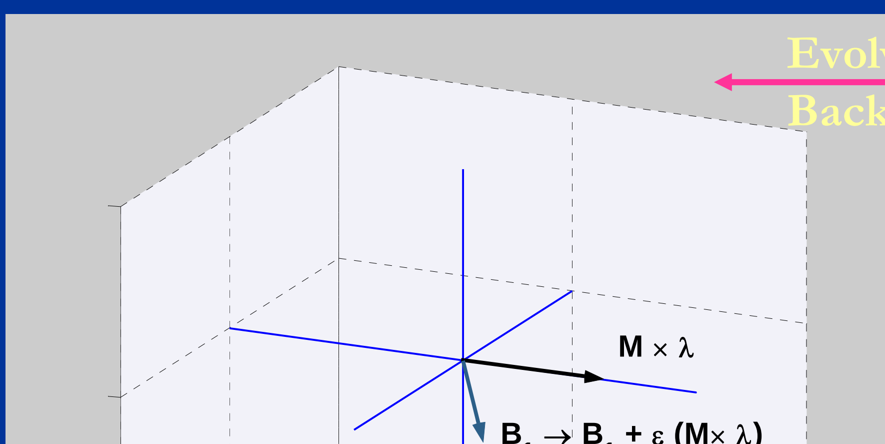
Ideal RF (green) Ideal + 20% (red) Ideal – 20% (blue)

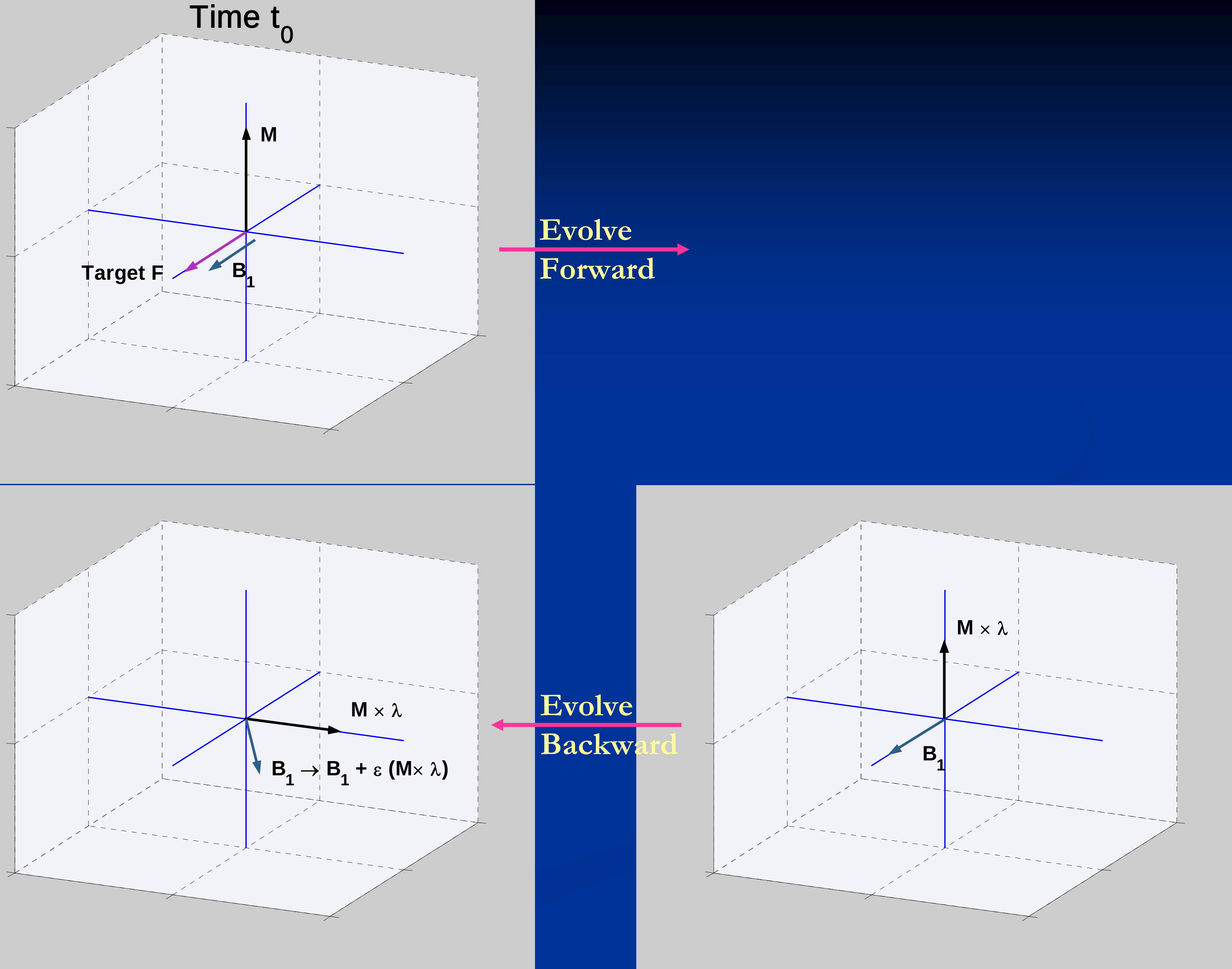


Evolve
Forward

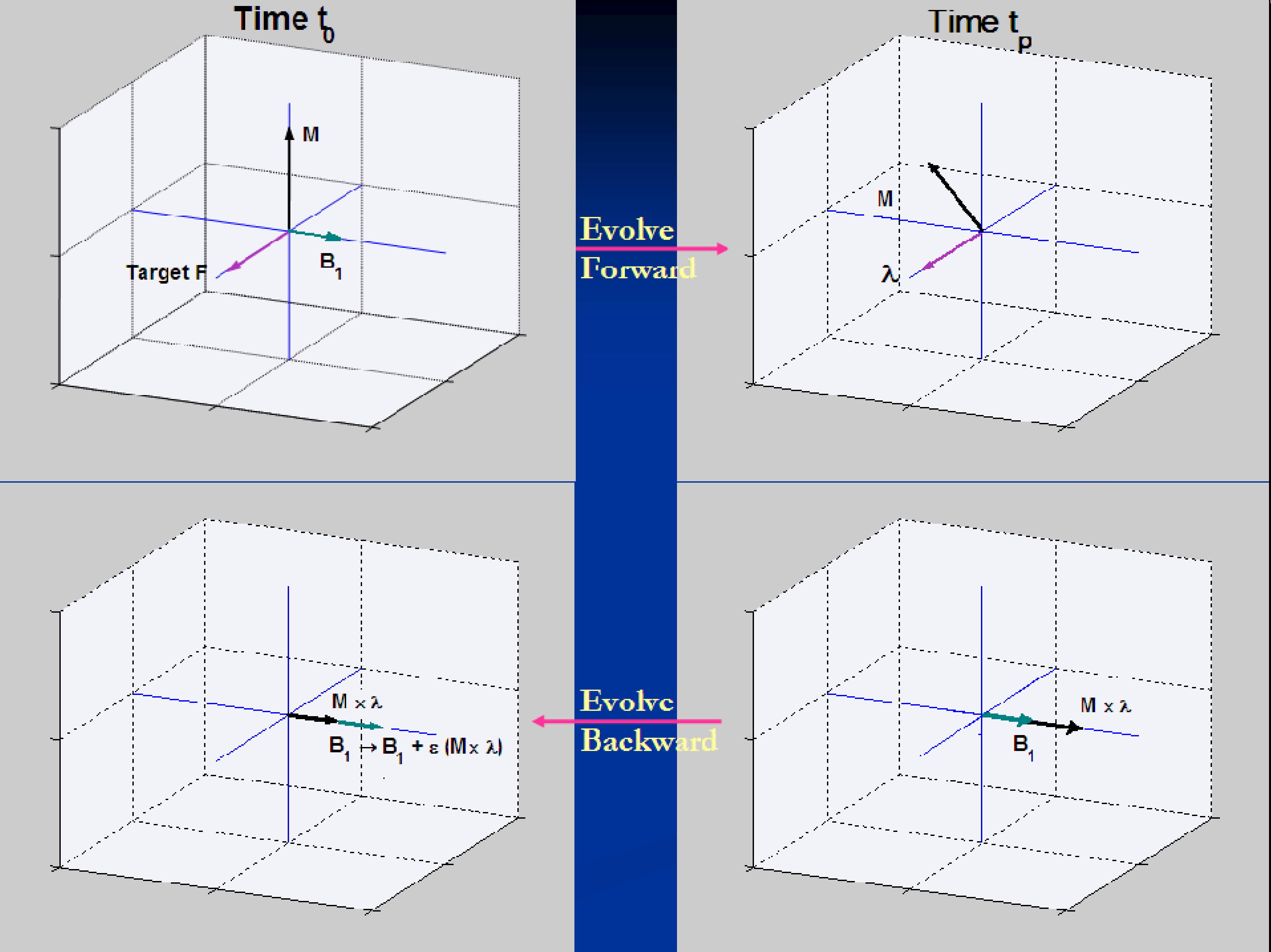


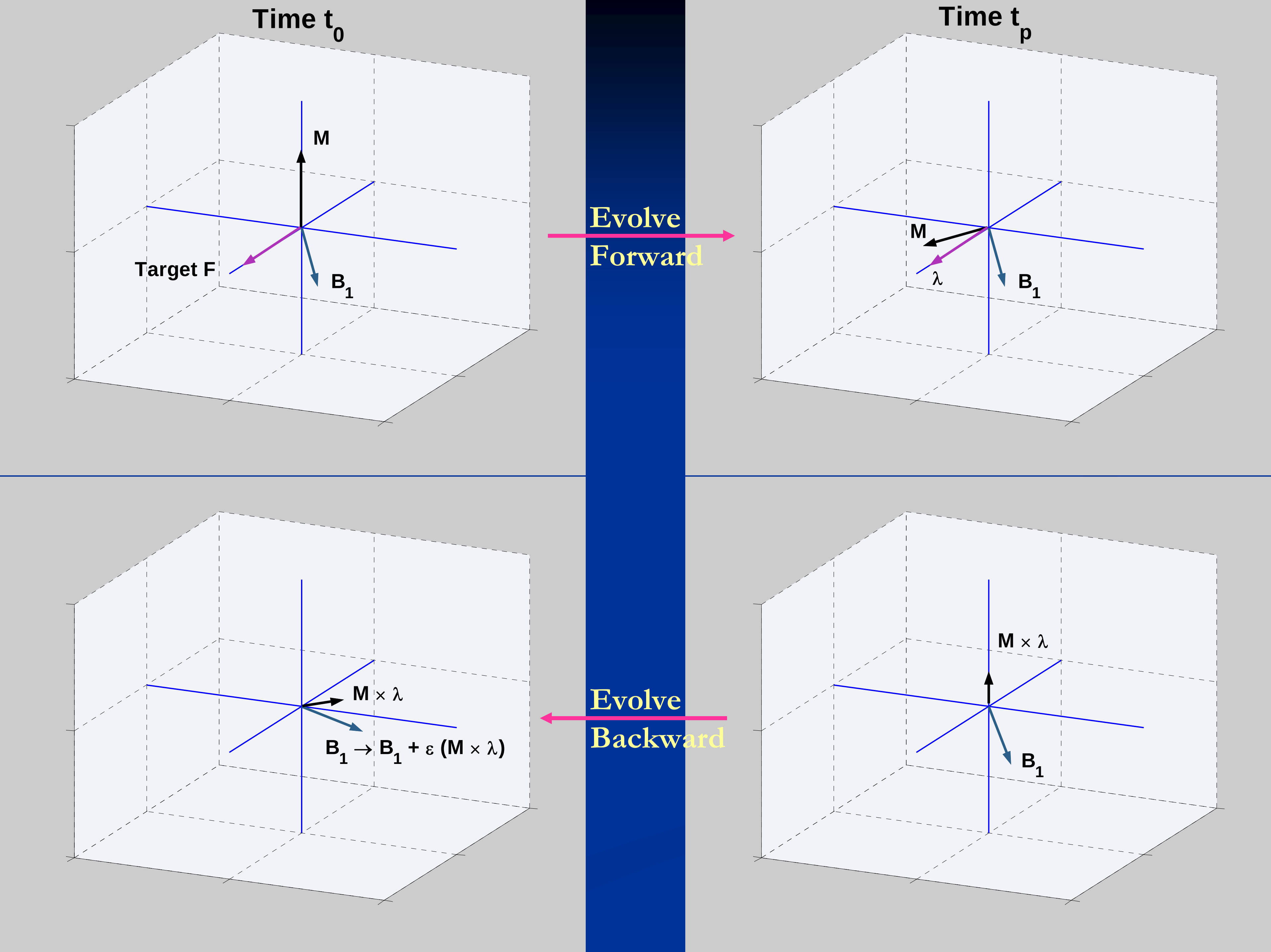
Evolve
Backward





Time t_0
M
Target F
B_1
Evolve
Forward
$M \times \lambda$
B_1
Evolve
Backward
$M \times \lambda$
$B_1 \rightarrow B_1 + \varepsilon\,(M \times \lambda)$


Time t_0
M
Target F
B_1
Evolve
Forward
Time t_p
M
λ
Evolve
Backward
M × λ
$B_1 \mapsto B_1 + \varepsilon\,(M \times \lambda)$
M × λ
B_1



Time t_0
M
Target F
B_1
Evolve
Forward
Time t_p
M
λ
B_1
M × λ
$B_1 \rightarrow B_1 + \varepsilon (M \times \lambda)$
Evolve
Backward
M × λ
B_1