Guide: GRAPE + CRAB + ADAM with Constraints

1 System Model & Propagation

Hamiltonian (two-level system):

$$H_k = \tfrac{1}{2}\big(\Omega_k \sigma_x + \Delta_k \sigma_z\big), \quad k = 0, \dots, N-1.$$

Discretization: total time $T = N\delta t$, piecewise-constant controls.

$$U_k = e^{-iH_k \delta t}, \quad \rho_{k+1} = U_k \rho_k U_k^\dagger.$$

Sensitivities:

$$\frac{\partial H}{\partial \Omega} = \tfrac{1}{2}\sigma_x, \qquad \frac{\partial H}{\partial \Delta} = \tfrac{1}{2}\sigma_z.$$

2 Objectives

2.1 Terminal Fidelity

$$C_{\text{fid}}^{(1)} = 1 - \mathrm{Tr}[\rho_T \rho_N].$$

Adjoint recursion:

$$\Lambda_N = \rho_T, \qquad \Lambda_k = U_k^\dagger \Lambda_{k+1} U_k.$$

2.2 Adiabatic (Dynamic Path-Tracking)

$$C_{\text{fid}}^{(2)} = 1 - \frac{1}{T}\sum_{k=0}^{N} \delta t \ \mathrm{Tr}[\rho_g(t_k)\rho_k].$$

Adjoint recursion:

$$\Lambda_N = 0, \qquad \Lambda_k = U_k^\dagger \Big(\Lambda_{k+1} + \tfrac{\delta t}{T}\rho_g(t_k)\Big) U_k.$$

2.3 Ensemble Robustness

$$C_{\mathrm{fid}}^{(3)} = \frac{1}{M} \sum_{i,j} w_{i,j}\, C_{\mathrm{fid}}^{(1)}(\alpha_i \Omega,\, \Delta + \delta_j).$$

Each ensemble member has modified controls: $\Omega \to \alpha_i \Omega$, $\Delta \to \Delta + \delta_j$. Gradients are averaged with weights $w_{i,j}$.

3 Constraints

3.1 Power (Fluence) Penalty

$$C_{\mathrm{pow}} = \frac{1}{T} \sum_{k=0}^{N-1} \Omega_k^2\, \delta t, \qquad \frac{\partial C_{\mathrm{pow}}}{\partial \Omega_k} = \frac{2}{T} \Omega_k \delta t.$$

3.2 Positivity Penalty (Smooth)

$$s_k = \frac{\ln(1 + e^{-\kappa \Omega_k})}{\kappa}, \qquad C_{\mathrm{neg}} = \tfrac{1}{2} w_{\mathrm{neg}} \sum_k s_k^2 \delta t,$$

$$\frac{\partial C_{\mathrm{neg}}}{\partial \Omega_k} = -w_{\mathrm{neg}}\, s_k\, \sigma(-\kappa \Omega_k)\, \delta t, \qquad \sigma(x) = \frac{1}{1 + e^{-x}}.$$

4 Total Cost

$$C = C_{\mathrm{fid}} + C_{\mathrm{pow}} + C_{\mathrm{neg}}.$$

5 Slice-wise GRAPE Gradients

$$\frac{\partial C}{\partial \Omega_k} = i \delta t\ \mathrm{Tr}\big[\Lambda_{k+1} [\tfrac{1}{2} \sigma_x, \rho_k]\big] + \frac{\partial C_{\mathrm{pow}}}{\partial \Omega_k} + \frac{\partial C_{\mathrm{neg}}}{\partial \Omega_k},$$

$$\frac{\partial C}{\partial \Delta_k} = i \delta t\ \mathrm{Tr}\big[\Lambda_{k+1} [\tfrac{1}{2} \sigma_z, \rho_k]\big].$$

Ensemble: average over members, with factor α_i on Ω.

6 CRAB Parameterization

$$\Omega = \Omega_0 + B_\Omega c_\Omega, \qquad \Delta = \Delta_0 + B_\Delta c_\Delta.$$

Coefficient gradients:

$$\nabla_{c_\Omega} C = B_\Omega^\top g_\Omega, \qquad \nabla_{c_\Delta} C = B_\Delta^\top g_\Delta.$$

7 ADAM Updates

$$m \leftarrow \beta_1 m + (1 - \beta_1) g_x, \tag{1}$$
$$v \leftarrow \beta_2 v + (1 - \beta_2) g_x \odot g_x, \tag{2}$$
$$\hat{m} \leftarrow m/(1 - \beta_1^t), \quad \hat{v} \leftarrow v/(1 - \beta_2^t), \tag{3}$$
$$x \leftarrow x - \alpha \hat{m}/(\sqrt{\hat{v}} + \varepsilon). \tag{4}$$

8 Unified Optimization Algorithm

1. Initialize CRAB coefficients.
2. Assemble Ω, Δ.
3. Forward propagate ρ_k (single or ensemble).
4. Compute adjoints Λ_k with objective-specific recursion.
5. Compute gradients and add constraint terms.
6. Project to CRAB coefficients ($B^\top$).
7. ADAM update on coefficients.
8. Iterate until convergence.