

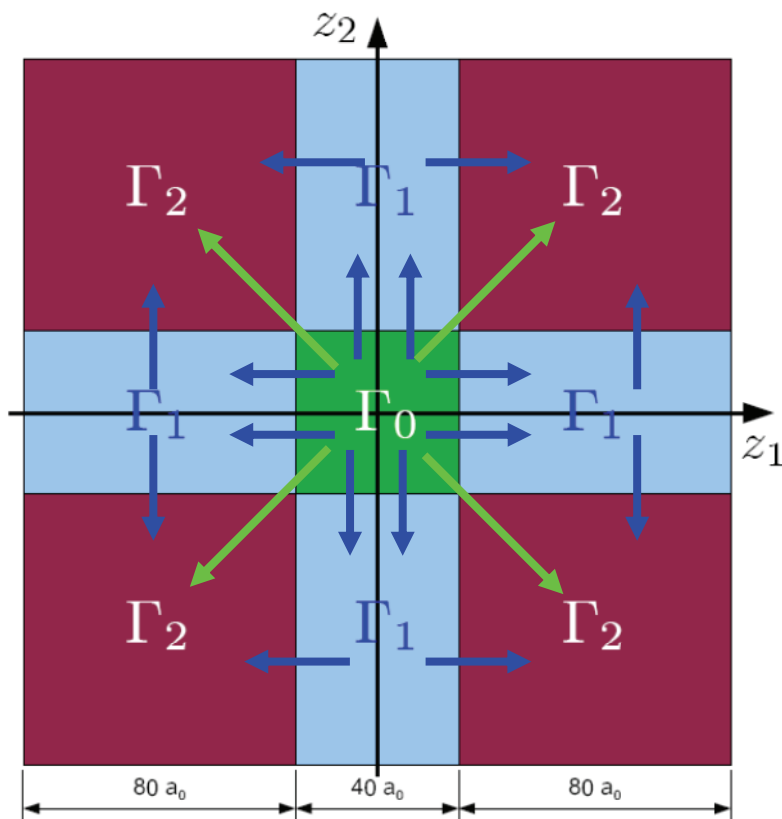
Propagation temporelle & analyse

$$\Psi(\mathbf{R}, z_1, z_2, t + \delta t) = e^{-i [\mathcal{H}_0 + V_{\text{int}}] \delta t / \hbar} \Psi(\mathbf{R}, z_1, z_2, t)$$

$$H_2^{2+} + 2e^- : \Gamma_2 \equiv \{ |z_1| \text{ et } |z_2| > z_A \}$$

$$H_2^+ + e^- : \Gamma_1 \equiv \{ |z_i| < z_A \text{ et } |z_j| > z_A \}_{i,j=1,2}$$

$$H_2 : \Gamma_0 \equiv \{ |z_1| \text{ et } |z_2| \leq z_A \}$$



$z_{max} \sim 100 a_0$ - $R_{max} \sim 12 a_0$
 512 × 512 × 512 points de grille
 $\delta t \sim 1$ as

- (1) Séquentiel
 - (2) Direct
- } ?