Combustion dynamics in steady compressible flows

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Outline

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Front propagation

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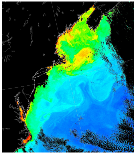
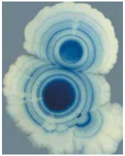
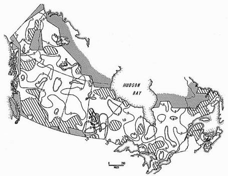


clorophyll/plankton
(O. Naval Research)



bacterial colonies
(Shapiro)



canadian snowshoe hare
(C.H. Smith)

biological
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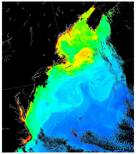

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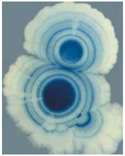

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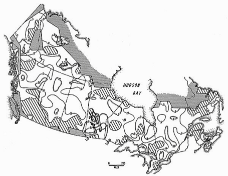

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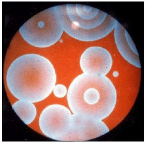
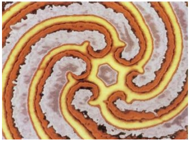


BZ (Winfree)



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chemical
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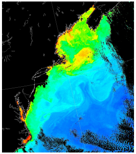
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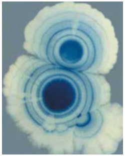
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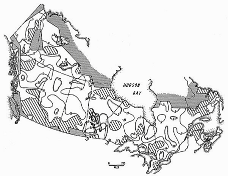

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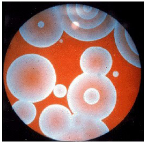
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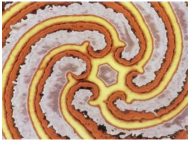
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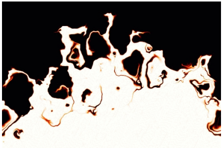

DNS of flames (Vladimirova)


forest fire (USA)


firemen (USA)

flame propagation

[J.D. Murray, “Mathematical biology”, Springer]

Advection-Reaction-Diffusion

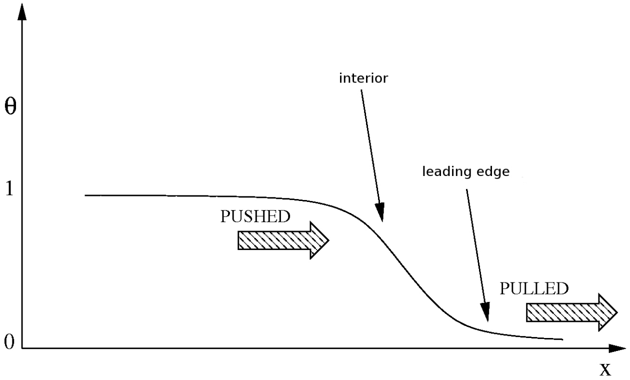
passive limit $\longrightarrow$ **advection-reaction-diffusion** equation
(no back-reaction of reactants on the velocity field)

$$\boxed{\partial_t\theta + \boldsymbol{\nabla}\cdot(\boldsymbol{u}\,\theta) = D_0\nabla^2\theta + \frac{1}{\tau}f(\theta)}$$

- $\theta(\boldsymbol{x}, t) \in [0, 1]$ fractional concentration of products, **normalized temperature**
- $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{x}, t)$ given velocity field
- D_0 molecular diffusivity
- $f(\theta)$ **reaction** term with characteristic time τ

Reaction dynamics

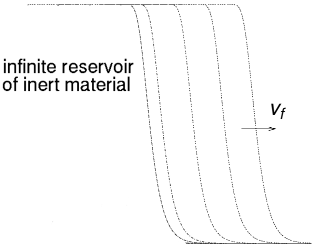
$\boldsymbol{u} = 0 \;\Rightarrow$ travelling-front solutions $\theta(\boldsymbol{x}, t) = \theta(\boldsymbol{x} \pm \boldsymbol{v}_0 t)$



- **pulled** $f(\theta) = \theta(1 - \theta)$ (FKPP - autocatalytic)
- **pushed** $f(\theta) = (1 - \theta)e^{-\frac{\theta_c}{\theta}}$ (Arrhenius)

  $f(\theta) = 0$ for $\theta \leq \theta_c$ (ignition)

The role of advection



enhancement of front propagation speed with respect to the case $\boldsymbol{u} = 0$

$v_f > v_0$

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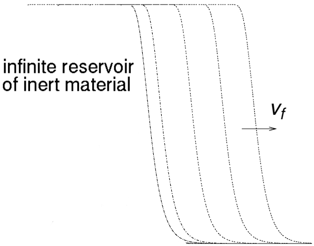

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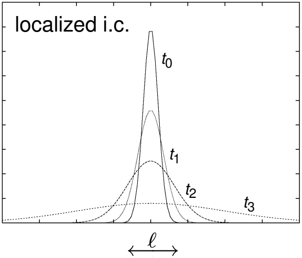

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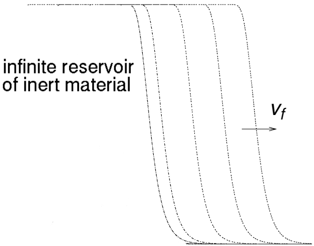

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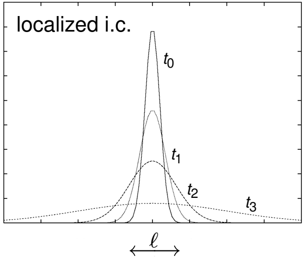

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$\longrightarrow$ what is the **critical size** $\ell_c = \ell_c(U, D_0, \tau, \theta_c)$?

Outline

Localization approximation (1)

1D stationary **compressible** velocity field: $\boxed{u(x) = U_0 \sin\left(\frac{\pi x}{L}\right) \quad (U_0 > 0)}$

the Lagrangian equation $\dot{x} = u(x)$ has...

(S) stable fixed points: $x = \pm L, \pm 3L, \dots, \pm(2n-1)L, \dots$

(U) unstable fixed points: $x = 0, \pm 2L, \dots, \pm 2nL, \dots$

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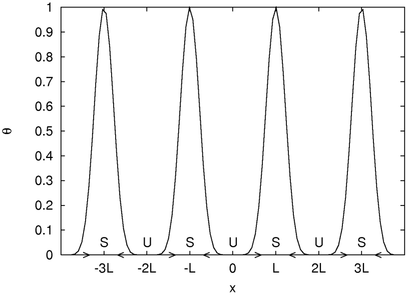

localization of θ around

$x_n = (2n-1)L$

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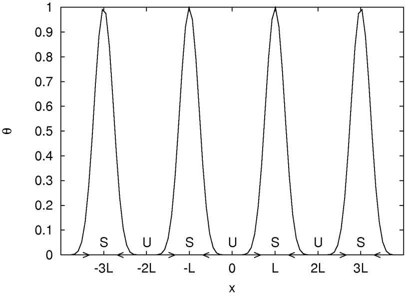

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random walk among these points $\Rightarrow$ lattice model

Localization approximation (2)

we introduce:

$$\theta_n(t) = \int_{x_n-L}^{x_n+L} \theta(x,t)dx = \int_{x_n-\delta}^{x_n+\delta} \theta(x,t)dx \qquad \text{where } \delta \ll L$$

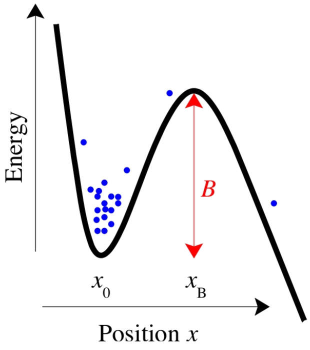
master equation for $\theta_n(t)$:

$$\theta_n(t+\Delta t) = \sum_j P^{(\Delta t)}_{j\to n}\theta_j(t)$$

$$P^{(\Delta t)}_{n\to n} = 1 - 2W\Delta t \qquad P^{(\Delta t)}_{n\to n-1} = P^{(\Delta t)}_{n\to n+1} = W\Delta t$$

$W = W(U_0, D_0)$ Brownian particle's **escape rate**

Kramers formula



$$\partial_t \theta = \partial_x (f'\,\theta) + D_0 \partial_x^2 \theta \qquad \text{FPE}$$

$$f(x) = -\int dx\, u(x) \qquad \text{potential}$$

in the low-noise limit $\frac{D_0}{B} \ll 1$:

$$\boxed{W \equiv r_K = \frac{1}{2\pi}\sqrt{f''(x_0)|f''(x_B)|}\, e^{-\frac{f(x_B)-f(x_0)}{D_0}}}$$

$$f(x) = \frac{U_0 L}{\pi}\cos\left(\frac{\pi x}{L}\right) \qquad B = \frac{2U_0 L}{\pi} \qquad D_0 \to 0$$

$$x_0 = (2n-1)L \quad x_B = (2n+1)L \implies \ln W(U_0, D_0) \sim -\frac{U_0}{D_0}$$

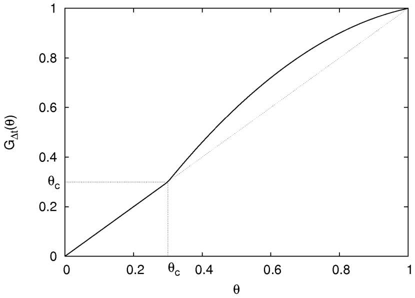
[H. Risken “The Fokker-Planck equation”, Springer; J.P. Sethna “Entropy, order parameters, and complexity”, OUP]

Reactive map

In presence of **reaction**: $\theta_n(t+\Delta t) = G_{\Delta t}\left(\sum_j P^{(\Delta t)}_{j\to n}\theta_j(t)\right)$

For the **ignition-type** nonlinearity:

$$G_{\Delta t}(\theta) = \begin{cases} \theta & 0 \le \theta \le \theta_c \\ \theta + (\theta-\theta_c)(1-\theta)\dfrac{\Delta t}{\tau} & \theta_c < \theta \le 1 \end{cases}$$



threshold value: $\theta \le \theta_c \Rightarrow$ no reaction

[Mancinelli et al., Physica D 185, 175 (2003)]

Outline

Simulation settings

Numerical integration of the lattice reactive model with:

- lattice spacing $\Delta x = 1$
- lattice size $L_x \leq 4 \cdot 10^4$
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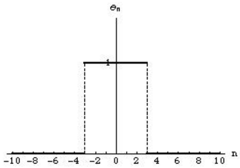

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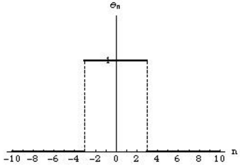


Analysis:

- $Q(t) = \sum_{n=-\infty}^{+\infty} \theta_n(t)$ total burnt area (ideal fronts)
- $v_f(t) = \frac{1}{\Delta t} \sum_{n=-\infty}^{+\infty} [\theta_n(t + \Delta t) - \theta_n(t)]$ front speed

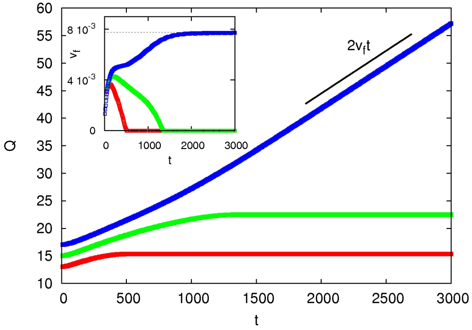
Quenching phenomena

propagation $\Longrightarrow$ $Q(t) \simeq 2v_f t$ for large t

$\theta_c = 0.6$

$W = 0.1$

$\tau = 50$



$\ell = 18$

$\ell = 16$

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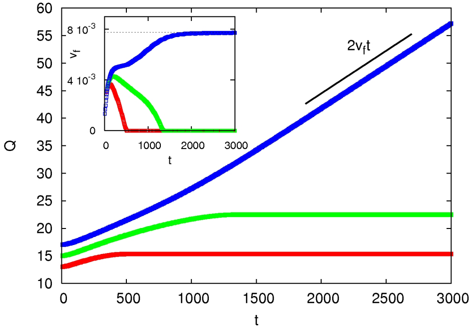

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This way it is possible to determine a **critical length** ℓ_c separating the two regimes:

$$\begin{array}{llll} \ell < \ell_c & \Rightarrow & \theta(x, t \to \infty) \to 0 & \text{quenching} \\ \ell > \ell_c & \Rightarrow & \theta(x, t \to \infty) \to 1 & \text{propagation} \end{array}$$

Dimensional scaling

relevant parameters: τ, W, θ_c

Measure of the critical size ℓ_c:

(A) $\tau =$ const, W variable

(B) $W =$ const, τ variable

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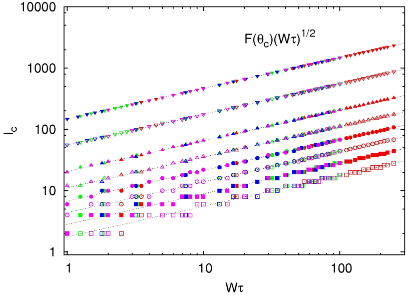
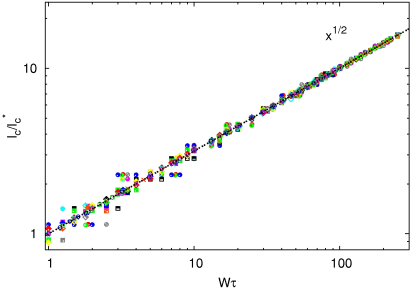
$$\boxed{\ell_c = F(\theta_c)\sqrt{W\tau}}$$





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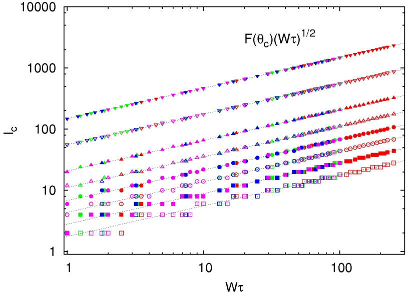

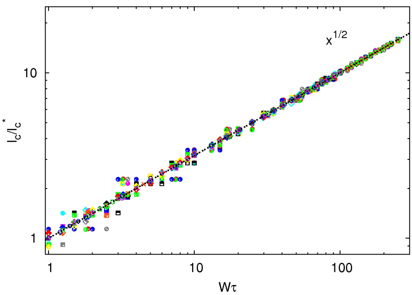

Continuum limit: $L_x \gg \Delta x = 1 \Rightarrow$ pure reaction-diffusion with $D = W\Delta x^2 = W$

$$W \equiv D, \tau, \theta_c \Rightarrow [\ell_c] = [D\tau]^{1/2}[F(\theta_c)] = [W\tau]^{1/2}$$

Dependence on the threshold concentration (1)

ansatz based on the physical hypothesis:

(i) $F(\theta_c) \geq 0$ monotonically increasing with $\theta_c \in [0, 1]$

(ii) $F(\theta_c) \to 0$ when $\theta_c \to 0$

(iii) $F(\theta_c) \to \infty$ when $\theta_c \to 1$

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$$\Rightarrow F(z) = a_0 + \frac{a_{-1}}{1-z} + \frac{a_{-2}}{(1-z)^2} + ... = \sum_{k=0}^{\infty} \frac{a_{-k}}{(1-z)^k} \qquad \text{Laurent exp. (z=1)}$$

from the numerics...

$\lim_{z \to 1}(1-z)^\alpha F(z) = 0$ for $\alpha \geq 3 \implies F(z) = a_0 + \frac{a_{-1}}{1-z} + \frac{a_{-2}}{(1-z)^2}$

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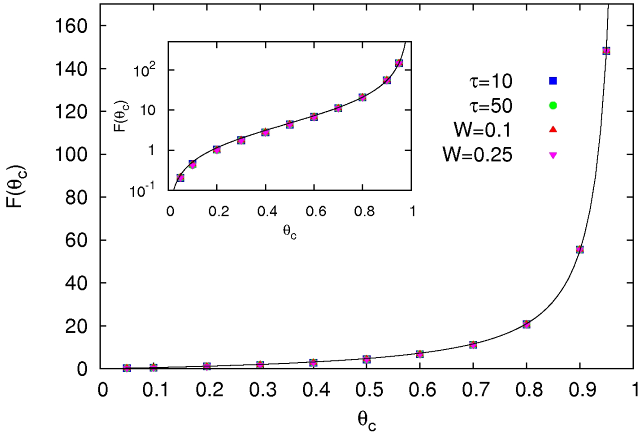
$$\text{imposing (ii): } F(z=0) = 0 \Longrightarrow \boxed{F(z) = a_0 \tfrac{z}{1-z}\left(1 + \tfrac{a_{-2}}{a_0}\tfrac{1}{1-z}\right)}$$

Dependence on the threshold concentration (2)

$$F(z) = a_0 \frac{z}{1-z}\left(1 + \frac{a_{-2}}{a_0}\frac{1}{1-z}\right)$$



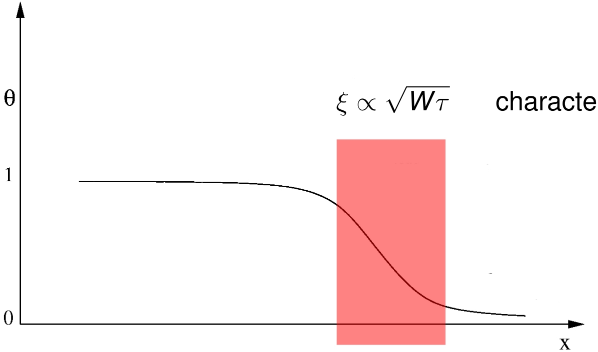
$a_0 \simeq 4.39$

$a_{-2} \simeq 0.17$

experiments A ($\tau = 10$, $\tau = 50$) and B ($W = 0.1$, $W = 0.25$)

Front thickness

$\theta(x < 0, t_0) = 1$ (reservoir of burnt material) $\Rightarrow$ front propagation



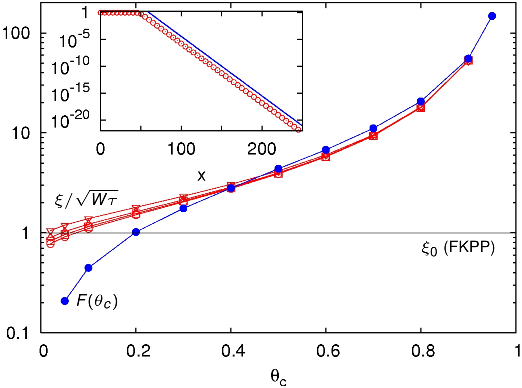
$\xi \propto \sqrt{W\tau}$ characteristic front width

FKPP: $\theta(x,t) \sim e^{-\frac{x - v_0 t}{\xi_0}}$ for $x \gtrsim v_0 t$

where $v_0 = 2\sqrt{D_0/\tau}$ and $\xi_0 = \sqrt{D_0 \tau}$

Different length scales

in the present case: $\theta(x,t) \propto e^{-\dfrac{x - v_f t}{\xi}} \Rightarrow$ measure of ξ



$\ell_c \neq \xi \Rightarrow$ quenching is not simply related to usual features of the front

Outline

Conclusions

We studied the quenching phenomenon of ignition-type reaction dynamics in a steady compressible flow.

1. Localization approximation $\Rightarrow$ lattice model and efficient numerical implementation.
2. Single critical length-scale ℓ_c: $\begin{cases} \ell < \ell_c \Rightarrow \theta(x, t \to \infty) \to 0 & \text{quenching} \\ \ell > \ell_c \Rightarrow \theta(x, t \to \infty) \to 1 & \text{propagation} \end{cases}$
3. Dimensional scaling: $\ell_c = F(\theta_c)\sqrt{W\tau}$, with $F(\theta_c)$ characterized by a pole of order $\alpha = 2$ in $\theta_c = 1$.
4. Agreement with results in different configurations: pure reaction-diffusion systems [Zlatoš 2005], and reactive transport systems in two-dimensional incompressible velocity fields [Constantin et al. 2001,2003].

Comparisons

$2D$ ARD system with $\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$ and $\tau \gg \tau_A$

a) shear flow (U) $\Rightarrow \ell_c \sim U$
b) cellular flow (U) $\Rightarrow \ell_c \sim U^{1/4}$

[Constantin et al., Commun. Pure Appl. Math. 54, 1320 (2001); Vladimiriova et al., Combust. Theory Model. 7, 487 (2003)]

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b) cellular flow (U) $\Rightarrow \ell_c \sim U^{1/4}$

... we observe $\quad \ell_c \sim \sqrt{W\tau}\,; \quad W = W(U_0)$

$$\tau \gg \tau_A \implies \partial_t \theta = D^{eff} \nabla^2 \theta + \frac{1}{\tau} f(\theta)\,; \quad D^{eff} = D^{eff}(U)$$

[Constantin et al., Commun. Pure Appl. Math. 54, 1320 (2001); Vladimiriova et al., Combust. Theory Model. 7, 487 (2003)]

Comparisons

$2D$ ARD system with $\nabla \cdot \boldsymbol{u} = 0$ and $\tau \gg \tau_A$

a) shear flow (U) $\Rightarrow \ell_c \sim U \;\sim \sqrt{D^{eff}\tau}$

b) cellular flow (U) $\Rightarrow \ell_c \sim U^{1/4} \;\sim \sqrt{D^{eff}\tau}$

... we observe $\quad \ell_c \sim \sqrt{W\tau}\,; \quad W = W(U_0)$

$$\tau \gg \tau_A \implies \partial_t \theta = D^{eff} \nabla^2 \theta + \frac{1}{\tau} f(\theta)\,; \quad D^{eff} = D^{eff}(U)$$

a) shear flow $D^{eff} \sim U^2$

b) cellular flow $D^{eff} \sim U^{1/2}$

[Constantin et al., Commun. Pure Appl. Math. 54, 1320 (2001); Vladimiriova et al., Combust. Theory Model. 7, 487 (2003)]