DETONATION EVOLUTION

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HIGH-SPEED COMBUSTION WORKSHOP
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Two Steps to the Birth of a Detonation

1. Preparation: creation of critical conditions for detonation onset (preconditioning).

    - shock initiation
    - flame acceleration and DDT
    - photochemical initiation
    - injection of a hot, turbulent jet of combustion products into an explosive mixture

    The result, typically, is a hot reactive mixture in a state of nonuniformity.

2. Formation: a local explosion leading to the detonation.

A Detailed Analysis of Stage 2 (Formation)
via
Asymptotics and Numerics

- Hot explosive mixture with a linear temperature gradient.
- Ideal, homogeneous material.
- Depending upon the size of the temperature gradient, there are two distinct pathways to detonation (additional variations exist within them).
- Seminal work by **Zeldovich** *et al*, **Clarke, Lee** *et al*.
- **Khokhlov, Oran and Wheeler**
- Colleagues: **Bdzil, Dold, Hawa, Jackson, Schwendeman, Short, Stewart**.

Plan

- The model.
- Key analytical ideas.
- Numerical simulations.

The Model

- One-dimensional configuration.
- No diffusion.
- Euler, polytropic fluid.
- Only temperature nonuniformities.
- One-step, irreversible, strongly state-sensitive kinetics.

The Model, contd.

Balance Laws

$$\dot{\rho} + \rho \nabla . \mathbf{u} = 0$$

$$\rho \dot{\mathbf{u}} + \nabla p = 0$$

$$\dot{e} + p\dot{v} = 0$$

Constitutive Assumptions

- kinetics $\mathcal{A} \Longrightarrow \mathcal{B}$
- progress variable λ, $0 \leq \lambda \leq 1$
- rate law (Arrhenius kinetics, large activation temperature)

$$\dot{\lambda} = \mathcal{R}(T, \lambda) = k(1-\lambda)\exp(-T_a/T), \quad T_a \gg 1$$

- equation of state

$$e = e(p, v, \lambda) = \frac{pv}{\gamma - 1} - \lambda q$$

- Ideal material

$$pv = RT$$

- sound speed

$$c = \sqrt{\gamma p v}$$

The Model, contd.

Implications of $T_a \gg 1$

Rate equation

$$\dot{\lambda} = k(1-\lambda)\exp(-T_a/T)$$

Scaled with respect to reference $(\lambda = 0,\ T = 1)$ state

$$\dot{\lambda} = (1-\lambda)\exp\left[T_a\left(1-\frac{1}{T}\right)\right]$$

$\underline{1-\frac{1}{T} > 0 \text{ and } O(1)}$

Either reaction completed $(\lambda \sim 1)$ or gradients large

$\underline{1-\frac{1}{T} < 0 \text{ and } O(1)}$

Rate is exponentially small; reaction frozen

$\underline{1-\frac{1}{T} = o(1)}$

$$1-\frac{1}{T} = \frac{1}{T_a}\phi, \quad \text{rate} \ \sim \ (1-\lambda)e^{\phi}$$

Reaction confined to narrow zones of temperature and/or thin layers in space/time

The Model, contd.
Planar, 1-D Geometry

Lagrangian (mass-weighted) coordinate

$$\psi = \int_{x_0(t)}^{x} \rho(\xi, t)\, d\xi$$

$$\left.\frac{\partial F}{\partial x}\right)_t = \rho \left.\frac{\partial F}{\partial \psi}\right)_t, \qquad \left.\frac{\partial F}{\partial t}\right)_x + u \left.\frac{\partial F}{\partial x}\right)_t \equiv \dot{F} = \left.\frac{\partial F}{\partial t}\right)_\psi$$

<u>Reference State</u>

$$p_0,\ v_0,\ T_0,\ c_0 = \sqrt{\gamma p_0 v_0}$$

$$t_0 = \frac{\epsilon}{k}\,\frac{c_p T_0}{q} \exp(T_a/T_0) \ \ \text{(constant-pressure induction time)}$$

$$L_0 = c_0 t_0 \ \ \text{(acoustic length)}$$

$$\epsilon = T_0/T_a \ll 1 \ \ \text{(inverse activation energy)}$$

$$Q = \frac{q}{c_p T_0} \quad \text{(heat-release parameter)}$$

<u>Dimensionless equations</u>

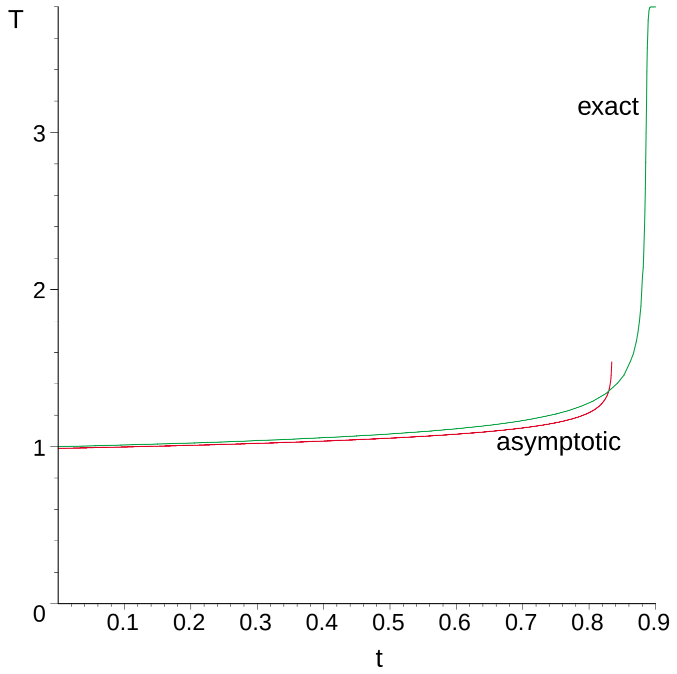
$$v_t - u_\psi = 0, \quad u_t + \frac{1}{\gamma}\, p_\psi = 0, \quad p_t + \frac{\gamma p}{v} v_t = \frac{\gamma \mathcal{R}}{v}, \quad \lambda_t = \frac{1}{Q}\mathcal{R}$$

$$T = pv, \quad \mathcal{R} = \epsilon(1-\lambda)\exp\left[\frac{1}{\epsilon}\left(1 - \frac{1}{T}\right)\right]$$

I. Spatially Uniform Evolution

$$u = 0, \quad v = 1, \quad p = T = 1 + \gamma Q \lambda.$$

$$T'(t) = \frac{\epsilon}{Q}(1 + \gamma Q - T) \exp\left[\frac{1}{\epsilon}\left(1 - \frac{1}{T}\right)\right], \quad T(0) = 1.$$


Evolution of temperature for ε = 1/14, Q = 2, γ = 1.4

In the limit $\epsilon \longrightarrow 0$,

$$T \sim 1 + \epsilon\phi(t), \quad \phi_t = \gamma e^{\phi}, \quad \phi(0) = 0, \quad \phi = -\ln(1 - \gamma t).$$

- Thermal runaway at $t_e \sim 1/\gamma$, onset of vigorous reaction.
- Following runaway, explosion proceeds with exponential rapidity, ending with $\lambda = 1$ and $T = 1 + \gamma Q$.
- Explosion time scale is σ, with $\gamma(t_e - t) = e^{-\sigma/\epsilon}$.

Spatially Uniform Evolution, contd.

- The more general initial condition

  $$T(0) = 1 + \epsilon\phi_0$$

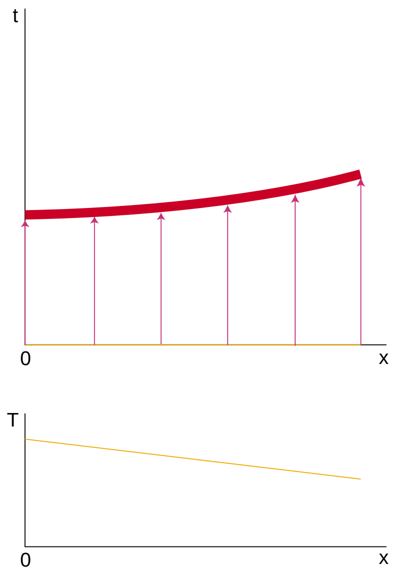
  produces runaway at

  $$t_e \sim \frac{e^{-\phi_0}}{\gamma}.$$

  Order ϵ change in initial condition produces $O(1)$ change in induction time.

- Spatial nonuniformities (in temperature, or other gasdynamic variables) of $O(\epsilon)$ are likely to play an important role in the evolutionary process; such disturbances will have the ability to alter local induction times significantly, and induce significant chemical-gasdynamic coupling.

II. Zeldovich (1980)
Spontaneous Flame and Regime Classification



$$T(x,0) = 1 - \epsilon a x, \quad a > 0, \quad x > 0.$$

Ignoring particle-to-particle communication, local blowup time

$$t_e(x) = \frac{1}{\gamma} \exp\left[\frac{1}{\epsilon}\left(1 - \frac{1}{T(x,0)}\right)\right] \sim \frac{1}{\gamma} e^{ax},$$

leading to a **spontaneous-flame wave speed**

$$W_s = \frac{1}{t_e'(x)} = \frac{\gamma}{a e^{ax}}.$$

Zeldovich's Spontaneous-Flame Hypothesis

1. $W_\mathrm{s} > D_\mathrm{CJ}$.
   - The spontaneous wave is a weak detonation.
   - In the limit of zero nonuniformity, $W_\mathrm{s} \to \infty$, i.e., a constant-volume explosion.
2. $W_\mathrm{s} < D_\mathrm{CJ}$.
   - Combustion of initial portion of the substance results in a shock wave.
   - Conventional detonation may be formed after a transient, with the shock always *ahead of the front*. (Studied numerically in Zeldovich, Librovich, Makhviladze and Sivashinsky, 1970).
3. S (speed of deflagration) $< W_\mathrm{s} \ll c$ (sound speed) $< D_\mathrm{CJ}$.
   - The spontaneous speed W_s is maintained (faster flame, not propagated by diffusion).
   - Pressure disturbances are weak, particle velocities small, induction period not significantly affected. Pressure has sufficient time to equilibrate.
4. $W_\mathrm{s} < S$.
   - Diffusion moves information ahead of the spontaneous wave; normal flame propagation occurs.

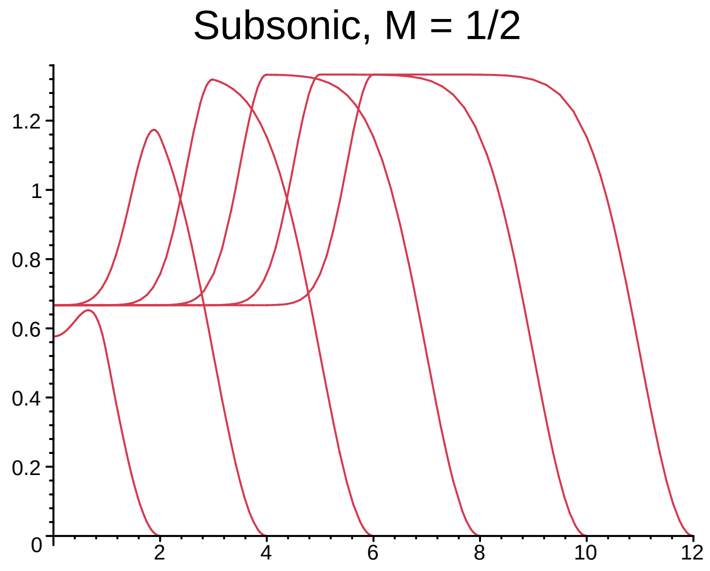
WHAT IS THE PATH TO **CONVENTIONAL, ZND** DETONATION IN THE FIRST TWO SITUATIONS?

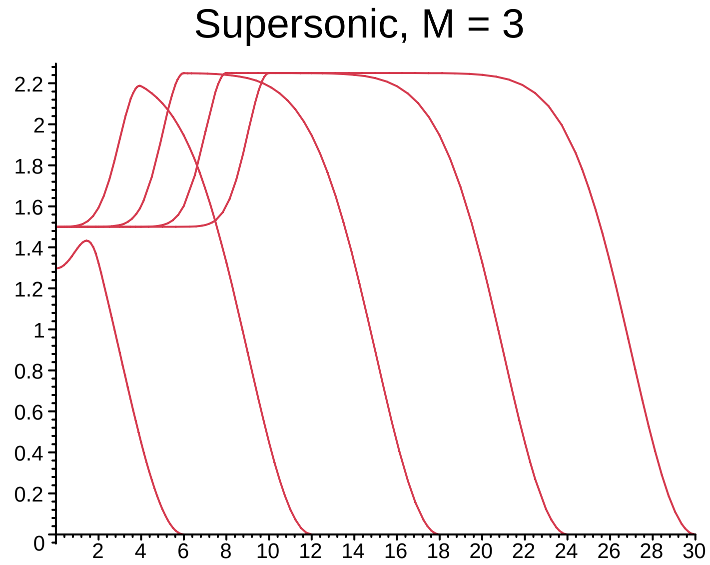
III. Shock Wave Amplification due to Coherent Energy Release (SWACER)

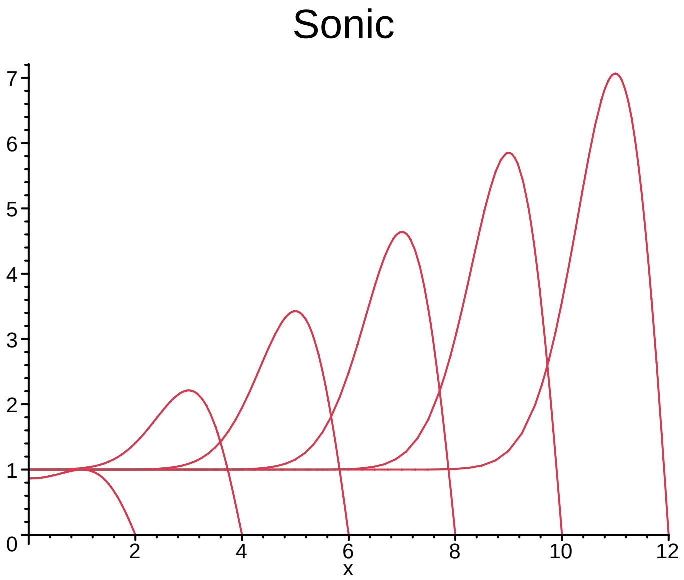
(Addresses Zeldovich's case 2 ($W_\mathrm{s} \le D_\mathrm{CJ}$).

Thiebault, Yoshikawa, Lee (1978), Lee and Moen (1980).

- Amplification of acoustics in an oscillating exothermic environment: Rayleigh's criterion. Compression waves and chemical energy release must synchronize for amplification.
- A linear example: gasdynamical field generated by a moving heat source.







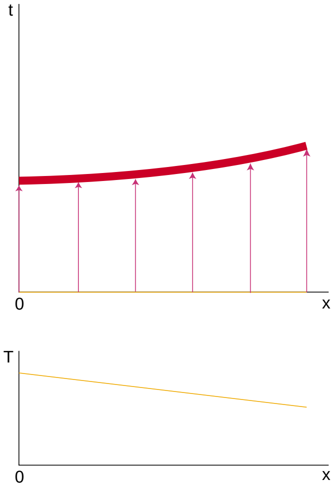
- Maximal amplification at sonic speed. Extension to nonlinear case.

IV. Asymptotic analysis for large activation temperature (JWD, AK)

Early Stage of Evolution

$$v_t - u_\psi = 0, \quad u_t + \frac{1}{\gamma}\, p_\psi = 0, \quad p_t + \frac{\gamma p}{v} v_t = \frac{\gamma \mathcal{R}}{v}, \quad \lambda_t = \frac{1}{Q}\mathcal{R}$$

$$T = pv, \quad \mathcal{R} = \epsilon(1-\lambda)\exp\left[\frac{1}{\epsilon}\left(1 - \frac{1}{T}\right)\right]$$



$$T(x,0) = 1 - \epsilon a x, \quad a > 0, \quad x > 0.$$

Two modes of evolution

- If $a = O(1)$, then temperature drop is $O(\epsilon)$, and induction-time variation $O(1)$, across the region $x = O(1)$.
- If $a \gg 1$, then temperature drop is $O(\epsilon)$, and induction-time variation $O(1)$, only in a thin boundary layer, $x = O(1/a)$. Outside the layer the induction time is exponentially large.

Perturbation (induction) expansion

$$p \sim 1 + \epsilon\gamma P, \;\; T \sim 1 + \epsilon\phi, \;\; v \sim 1 + \epsilon V, \;\; \lambda \sim \epsilon Z/Q, \;\; u \sim \epsilon U.$$

Induction equations

$$\phi_t - (\gamma - 1)P_t = e^{\phi}, \;\; U_t + P_\psi = 0, \;\; V_t - U_\psi = 0, \;\; Z_t = e^{\phi},$$
$$\phi = \gamma P + V.$$

- Generalization of the constant-volume problem.
- Linearized acoustics and weak, but exponentially nonlinear, chemistry.

Initial conditions

$$P = U = Z = 0,$$
$$\phi = -a\psi.$$

Boundary condition

$$U(0, t) = 0.$$

- Solution computed numerically for $a = O(1)$.
- Boundary-layer analysis possible for $a \gg 1$.

Properties of The Induction Solution

(a moderate)

- Inertially confined thermal runaway at hot wall, $\psi = 0$, at $t = \tilde{t}(0)$.

  As $t \to \tilde{t}(0)$,

$$
\begin{aligned}
\phi(0,t) &\sim -\ln[\gamma(\tilde{t}(0) - t)], \\
\gamma P(0,t) &\sim -\ln[\tilde{t}(0) - t], \\
\rho(0,t) &\quad \text{bounded.}
\end{aligned}
$$

  Constant-volume explosion in a thin region at the wall. **Hot spot**. Spatial structure also known.

- For $t > \tilde{t}(0)$, runaway moves into the interior and defines a logarithmic singularity path, $t = \tilde{t}(\psi)$, i.e.,

$$
\phi(\psi, \tilde{t}(\psi)) = \infty.
$$

- The path $\tilde{t}(\psi)$ and its speed (mass flux)

$$
\tilde{D} = \frac{1}{d\tilde{t}/d\psi}
$$

  are determined from a numerical solution of the induction equations.

- In the path-fixed coordinates (ψ, s), where $s = \tilde{t}(\psi) - t$, the induction equations are

$$
\begin{aligned}
\phi_s - (\gamma - 1)P_s &= -e^{\phi}, \\
P_s - \tilde{D}U_s &= -\tilde{D}P_{\psi}, \\
P_s + \tilde{D}^2 V_s &= -\tilde{D}^2 U_{\psi} - \tilde{D}P_{\psi}.
\end{aligned}
$$

As $s \to 0+$, changes across the path dominate, i.e.,

$$\frac{\partial}{\partial \psi} \ll \frac{\partial}{\partial s},$$

$\Longrightarrow$ the quasisteady structure

$$\phi \sim -\ln\left[-\frac{\gamma \tilde{D}^2 - 1}{\tilde{D}^2 - 1} s\right],$$

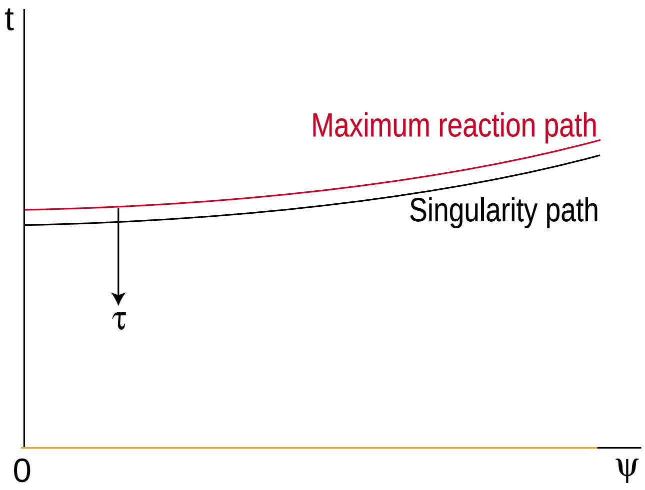
$$P \sim \frac{\tilde{D}^2 \phi - \tilde{b}(\psi)}{\gamma \tilde{D}^2 - 1}, \qquad U \sim \frac{P - \tilde{a}(\psi)}{\gamma \tilde{D}}.$$

- The singularity path is supersonic, $\infty > \tilde{D} > 1$, but decelerates as it advances. Larger the gradient a, the stronger the deceleration. Induction solution breaks down when $\tilde{D}$ reaches 1.
- The singularity path is a first-order approximation to the maximum reaction-rate locus, $t = \hat{t}(\psi)$, $d\hat{t}/d\psi = 1/D$, (cf. constant-volume explosion). Post-induction, this locus defines a supersonic wave of intense reaction: a spontaneous wave or **induction flame**. (Zeldovich Spontaneous Flame, corrected for compressibility.)
- In coordinates (ψ, τ) attached to the maximum reaction-rate locus, where $\tau = \hat{t}(\psi) - t$,

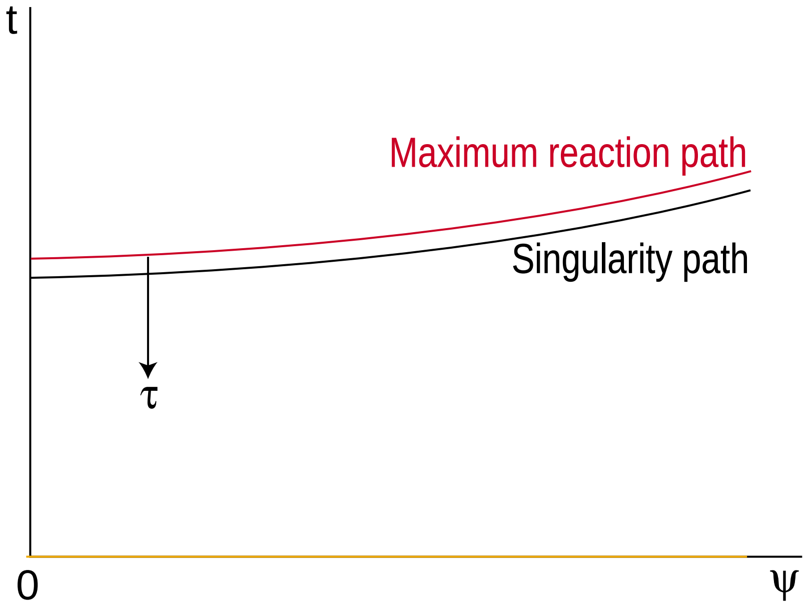
$$\frac{\partial}{\partial \tau} \gg \frac{\partial}{\partial \psi} \text{ exponentially as } \tau \to 0,$$

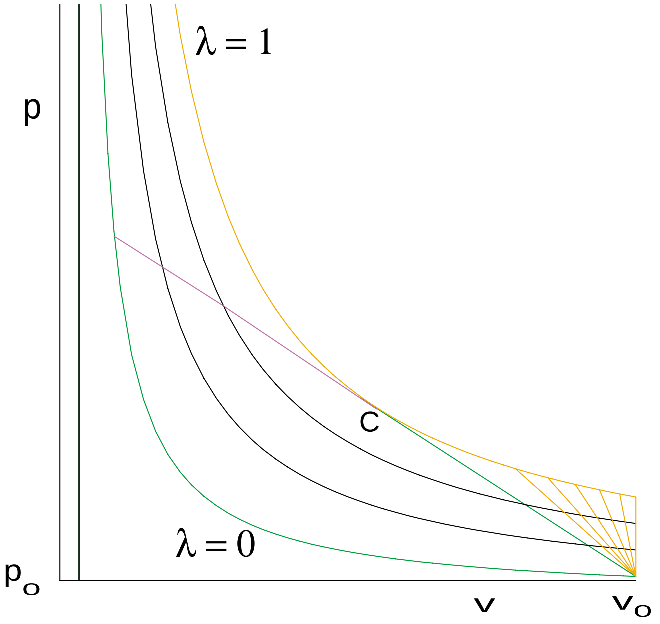
Equations $\Rightarrow$ algebraic statements of conservation to exponentially small errors.

- Solution is quasisteady, parametrized by D.



- Solution across the wave is monotonic, supersonic, shockless, compressive; **a weak detonation**.
- Descending Rayleigh lines on the pv-plane.

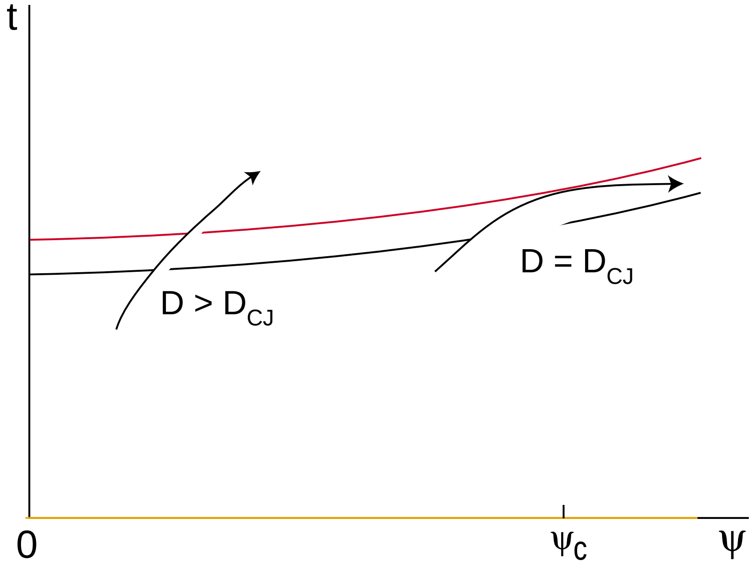

t
Maximum reaction path
Singularity path
τ
0
ψ


λ = 1
p
C
λ = 0
p_o
v
v_o

- Mach number decreases across the wave. A sonic point first appears at the end of the reaction zone, at $\psi = \psi_c$, say, when $\mathcal{R} = 0$.

$$\begin{aligned} \mathcal{A}_c^2 &= 2(\gamma+1)\gamma^2\hat{D}^2\mathcal{B}_c, \\ p_c &= \frac{\mathcal{A}_c}{\gamma+1}, \\ \mu_c &= 1. \end{aligned}$$

- Sonic condition $\Rightarrow D \sim D_{CJ}$. Near CJ, quasisteadiness is lost.



Evolution Near Criticality

New scalings

$$\psi = \psi_c + \delta r \quad \text{and} \quad t = \hat{t}(\psi) - \nu s,$$

$$\nu \ll \delta \ll 1 \;\; \text{and} \;\; \varepsilon \ll 1,$$

$$\nu = \frac{Q}{\epsilon} \exp\left[\frac{1 - T_c}{\epsilon T_c}\right] \ll 1.$$

Full equations

$$\begin{aligned}
P_s + \gamma\alpha^2 \left(\frac{T}{P}\right)_s &= \gamma\rho Q\lambda_s, \\
\frac{D+\alpha}{D}(P_s - \gamma\alpha u_s) + \frac{\nu}{\delta}\alpha(P_r - \gamma\alpha u_r) &= \gamma\rho Q\lambda_s, \\
\frac{D-\alpha}{D}(P_s + \gamma\alpha u_s) - \frac{\nu}{\delta}\alpha(P_r + \gamma\alpha u_r) &= \gamma\rho Q\lambda_s, \\
\lambda_s &= -\frac{\nu\epsilon(1-\lambda)}{Q} \exp\left[\frac{T-1}{\epsilon T}\right].
\end{aligned}$$

($\alpha = \rho c$ is the acoustic impedance.)

Near-critical expansions

$$T \sim T_c + \varepsilon\Gamma, \quad p \sim p_c + \varepsilon\gamma\Theta, \quad u \sim u_c + \varepsilon\,\mathcal{U}, \quad \lambda \sim 1 - \varepsilon^2\eta/\Lambda,$$

$$D = D_c + \delta D_c'\, r + O((\delta r)^2),$$

$$\alpha \sim D_c\left[1 + \varepsilon\left(\frac{\gamma\Theta}{P_c} - \frac{\Gamma}{2T_c}\right)\right], \quad \mu \sim 1 - \varepsilon\frac{\gamma+1}{2P_c}\Theta.$$

Evolution Near Criticality, contd.

Mass

$$\Gamma - \frac{(\gamma-1)T_c}{P_c}\Theta = 0.$$

Backward characteristic

$$\mathcal{U} - \frac{\Theta}{D_c} = 0$$

Forward characteristic

$$L\Theta_r + \Theta\Theta_s = \frac{1}{2}\eta_s$$

Rate

$$\eta_s = \eta e^{\kappa\Gamma}.$$

Parameters

$$g_1 = 2(-D_c')\,\frac{(\gamma D_c^2 - 1)P_c - (\gamma-1)}{\gamma^2(\gamma+1)D_c},$$

$$\Lambda = \frac{2QD_c^2}{\gamma+1}, \quad L = \frac{2P_cD_c}{\gamma+1}\left(\frac{\nu}{\delta\varepsilon}\right), \quad \kappa = \frac{1}{T_c^2}\left(\frac{\varepsilon}{\epsilon}\right), \quad k = \frac{\delta}{\varepsilon^2}.$$

In addition to the prescription that $s = 0$ is the site of maximum reaction rate, the induction solution provides the matching requirement

$$\Theta \sim -\sqrt{\eta - kg_1r} \quad \text{as} \quad s \to \infty.$$

Spatial scale δ and perturbation amplitude ε remain to be chosen.

Evolution Near Criticality, contd.
Stage II: Inviscid, Reactive Burgers Problem

$$\bar{\eta}_z = e^z,$$
$$\Theta_{\bar{r}} + \Theta\Theta_z = \frac{1}{2}\eta_z = \frac{1}{2}e^z,$$
$$\Theta \sim -\sqrt{e^z - \bar{r}} \text{ as } z \longrightarrow \infty.$$

Characteristic form

$$\left.\frac{\partial z}{\partial \bar{r}}\right]_\zeta = \Theta, \quad \text{or} \quad \bar{r} - \zeta + \int_z^\infty \frac{dz}{\Theta} = 0,$$
$$\left.\frac{\partial \Theta}{\partial z}\right]_\zeta = \frac{e^z}{2\Theta},$$

Solution

$$e^z - \Theta^2 = \zeta \;\Rightarrow\; \Theta = \pm\sqrt{e^z - \zeta}.$$

Characteristic

$$\zeta = e^z \sin^2\left(\frac{(\bar{r} - \zeta)\sqrt{\zeta}}{2}\right).$$

Sonic locus

$$\zeta = e^z \;\text{ or }\; (\bar{r} - \zeta)\sqrt{\zeta} = \pi.$$

Evolution Near Criticality
Stage II: Shock Formation, contd.

Implicit solution

$$1-\Theta^2 e^{-z}=\sin^2\left[\frac{1}{2}(\bar{r}-e^z+\Theta^2)\sqrt{e^z-\Theta^2}\right].$$

- Shock forms at first occurence of infinite Θ_z :

$$\zeta_*=2.653658,\quad \bar{r}_*=3\zeta_*-2(3)^{1/3}=5.076205,$$

$$\Theta_*=3^{-1/3}=0.693361.$$

- Shock path $z=Z(\bar{r})$:

$$\frac{dZ}{d\bar{r}}=\frac{1}{2}\left[\Theta(z^+,\bar{r})+\Theta(z^-,\bar{r})\right].$$

  (z^+ : supersonic side, z^- : subsonic side.)

- As the shock moves forward into regions where the reactant concentration is less depleted, both z and $\bar{r}$ become large,

$$\zeta^+\sim\bar{r},\quad\text{and}\quad\zeta^-\sim\frac{4\pi^2}{\bar{r}}.$$

  Correspondingly,

$$\Theta(z^+,\bar{r})\sim -e^{z/2}+\frac{\bar{r}}{2}e^{-z/2}\quad\text{and}\quad\Theta(z^-,\bar{r})\sim e^{z/2}-\frac{2\pi^2}{\bar{r}^2}e^{-z/2}.$$

- Asymptotic forms of the shock locus and shock speed,

$$Z(\bar{r})\sim 4\ln(\bar{r}/4),\qquad Z'(\bar{r})\sim 4/\bar{r}.$$

Shock Growth and Transition to ZND
Post-Burgers Regime

Shock locus

$$t_S(\psi) = \hat{t}(\psi) + \nu\sigma(\epsilon) - \nu Z.$$

Shock speed (mass flux)

$$\frac{1}{D_S} = \frac{1}{D} - \frac{\nu}{\delta}\frac{dZ}{d\bar{r}}.$$

$\Rightarrow$

$$D_s \sim D + \frac{\nu}{\delta} D^2 \frac{dZ}{d\bar{r}} = D + \frac{g_1}{\bar{k}^2} D^2 \nu^{1/3} \frac{dZ}{d\bar{r}}.$$

Induction-flame mass flux

$$D \sim D_c + \delta D_c' \bar{r}.$$

$\Rightarrow$

$$D_s = [D_c + \nu^{2/3}(\bar{k}^2/g_1) D_c' \, \bar{r}] + \nu^{1/3} \frac{D_c^2 g_1}{\bar{k}^2} \, \frac{dZ}{d\bar{r}}.$$

- $D_c' < 0 \Rightarrow D < D_c$ for $\bar{r} > 0$, velocity deficit of order $\nu^{2/3}\bar{r}$.
- Shock travels *faster* than the induction flame, velocity excess of order $\nu^{1/3}/\bar{r}$.
- As $\bar{r}$ increases, velocity deficit grows, velocity excess decays. The two corrections to D_c become comparable, each of order $\nu^{1/2}$, at
$$\bar{r} = O(\nu^{-1/6}), \quad \text{or} \quad \delta\bar{r} = O(\nu^{1/2}).$$

Shock Growth and Transition to ZND
Post-Burgers Regime, contd.

- Perturbation $\varepsilon\Theta$ to the critical pressure p_c, negative ahead of the shock and positive behind, in each case of order $\nu^{1/3}\bar{r}^2$, grows to order unity. Throughout this stage of shock growth, the shock speed undergoes only an $O(\nu^{1/2})$ excursion around the order unity value of D_c.

- Analysis of this stage occurs in two stages: quasisteady Burgers with weakly nonlinear chemistry for $\varepsilon\Theta = O(\epsilon)$ and full, quasisteady equations for $\varepsilon\Theta = O(1)$.

- Speed is determined by requiring smooth passage through the sonic point.

Transition to ZND structure from quiescent state

Induction

$\Rightarrow$ unsteady, thermal runaway

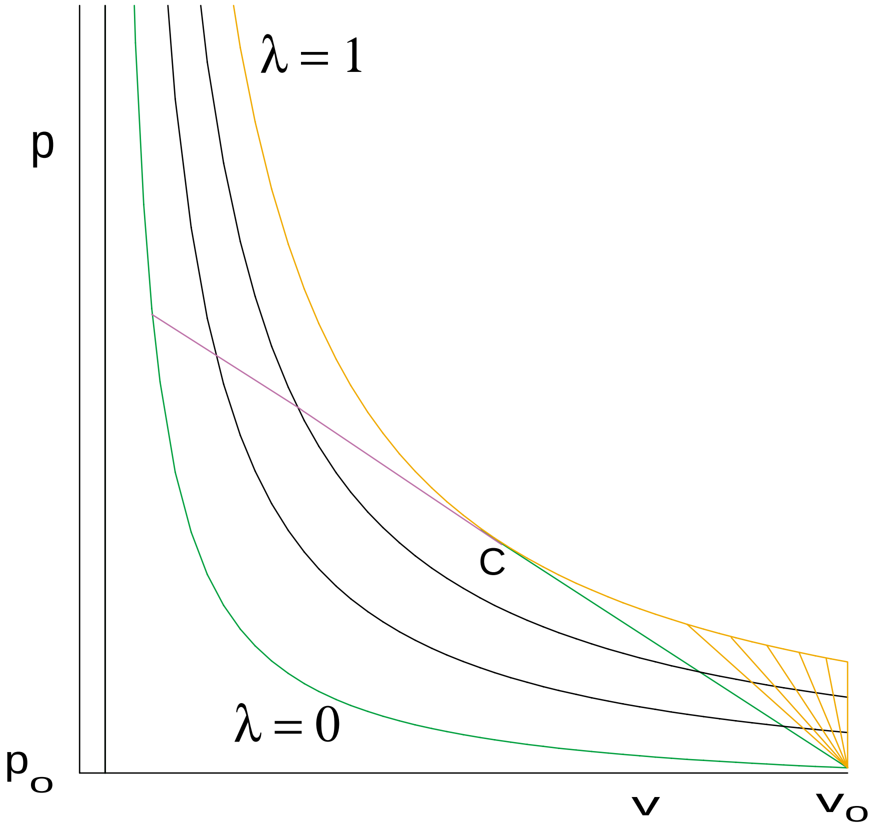
$\Rightarrow$ quasisteady, weak detonation, $D \rightarrow D_{CJ}$

$\Rightarrow$ quasisteady, weakly nonlinear reaction, near-critical

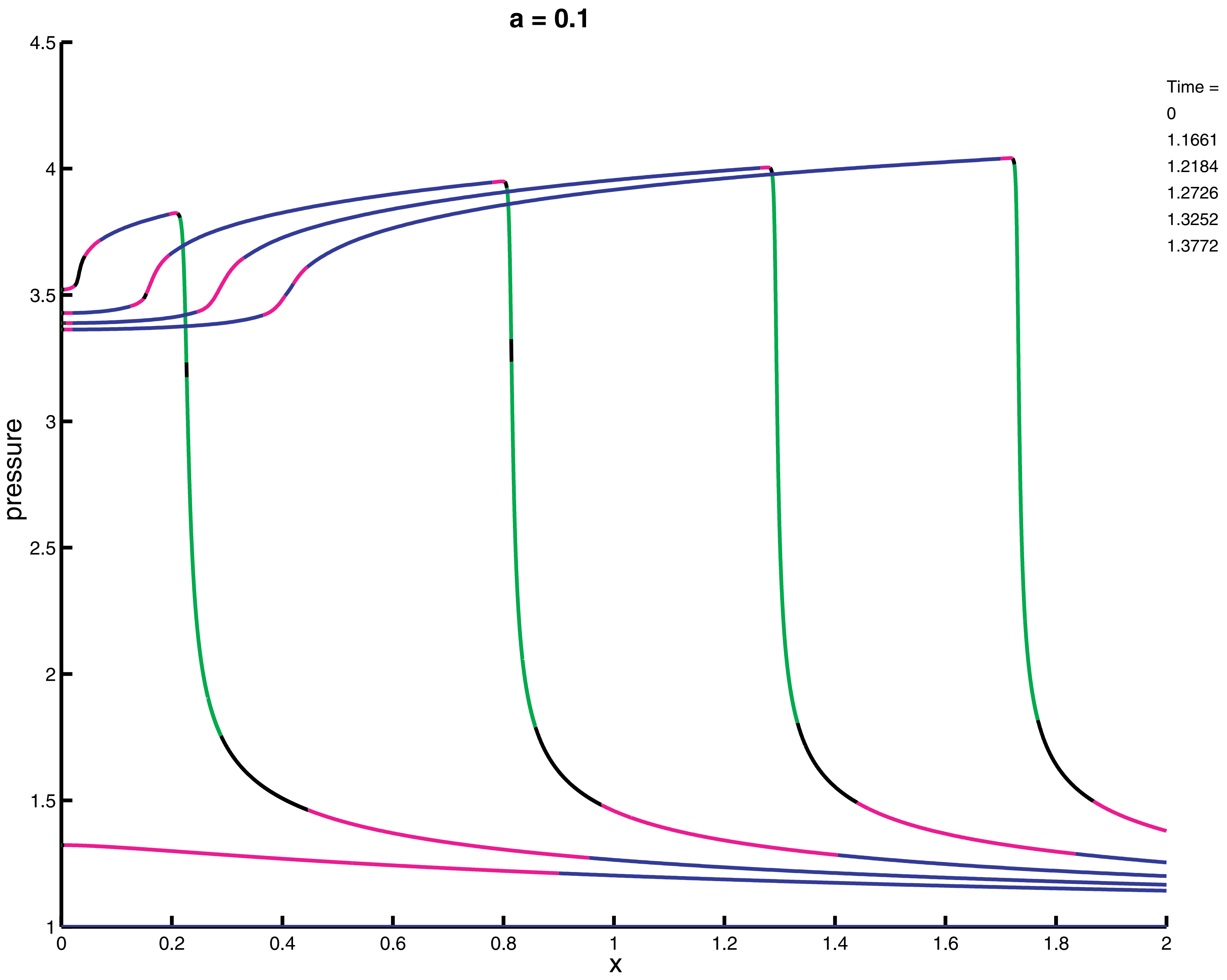
$\Rightarrow$ unsteady Burgers, nonlinear reaction, near-critical

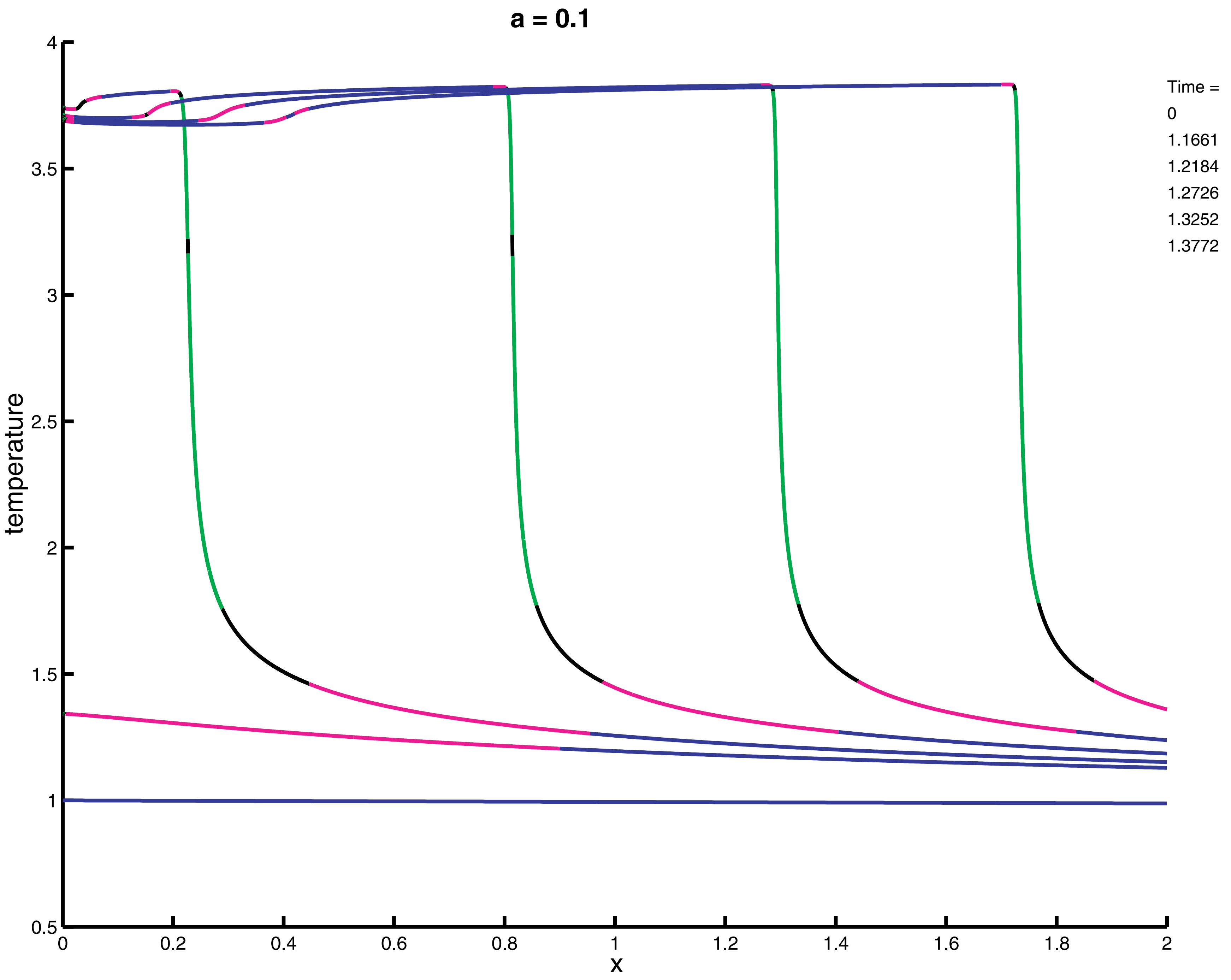
$\Rightarrow$ quasisteady, weakly nonlinear reaction, near-critical

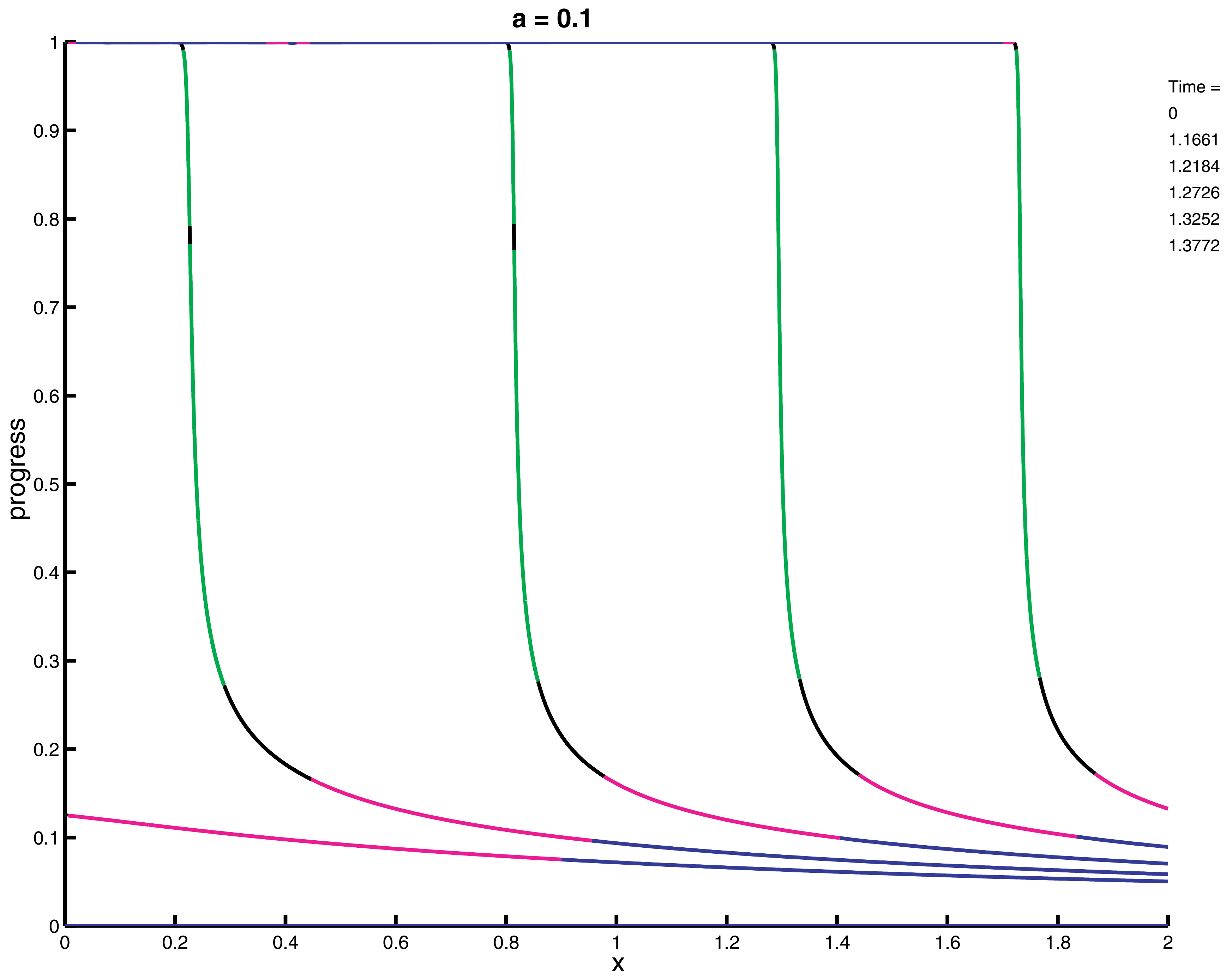
$\Rightarrow$ quasisteady, fully nonlinear, to ZND

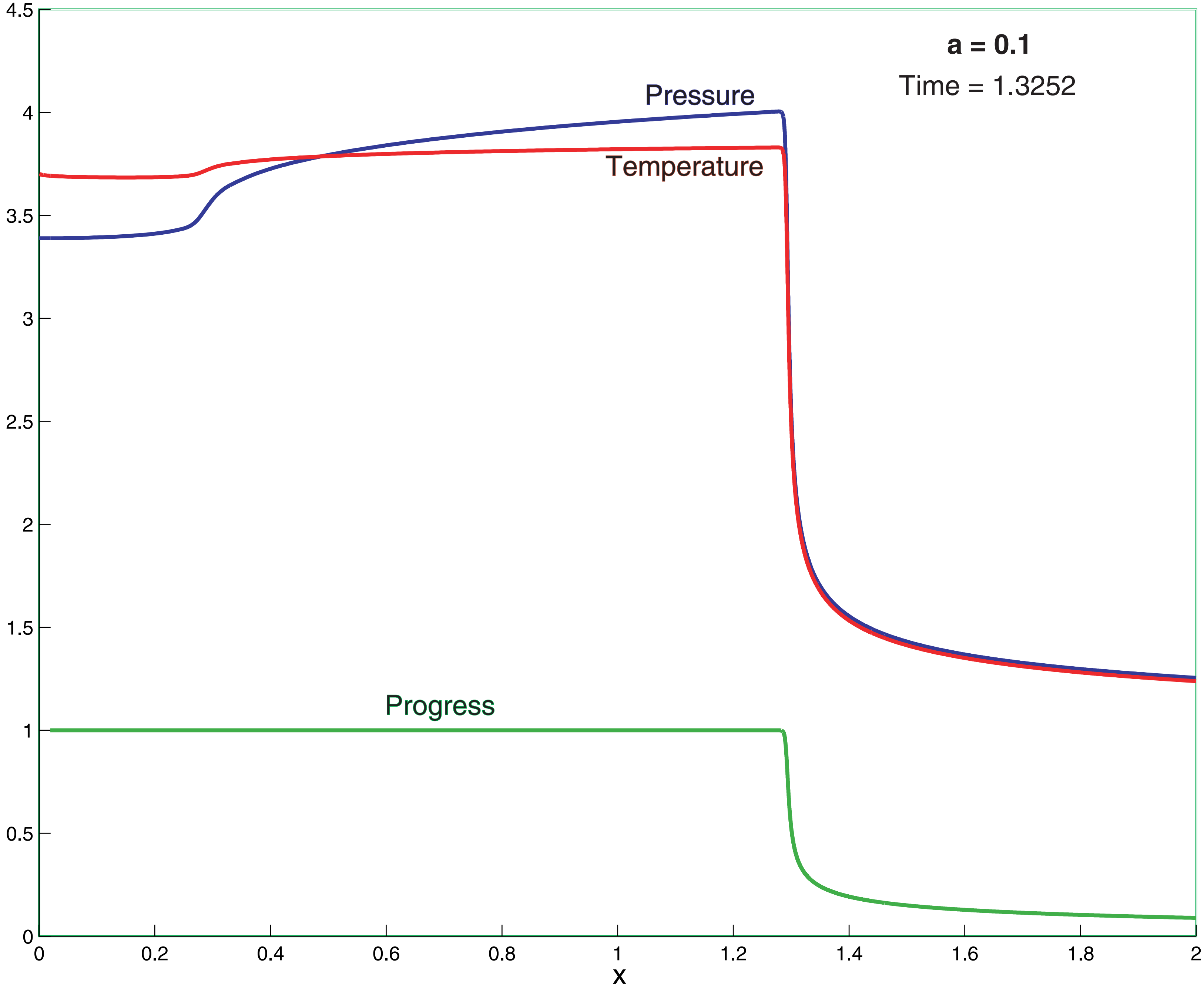


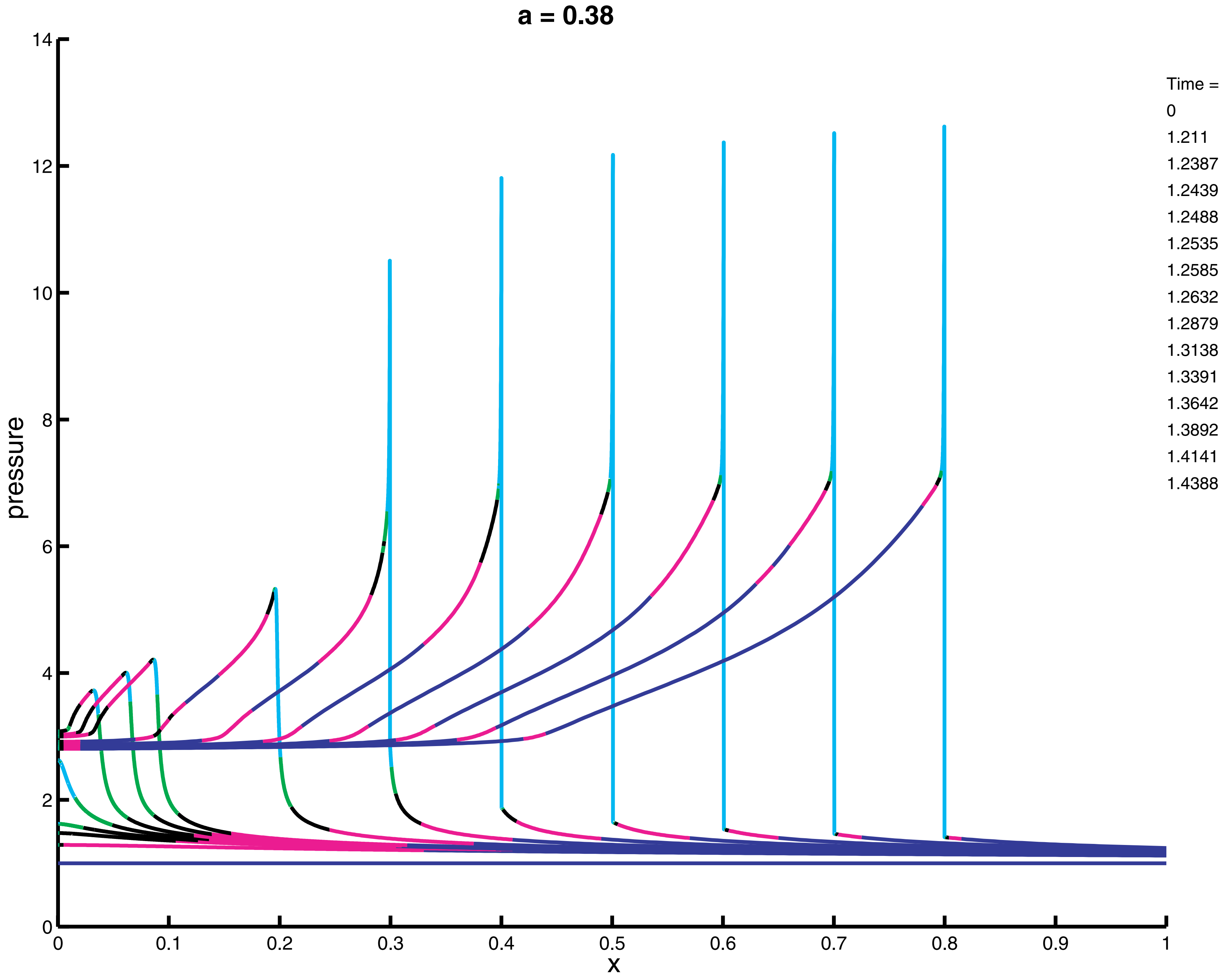
For small a, the region may not be big enough for the CJ state to be reached.

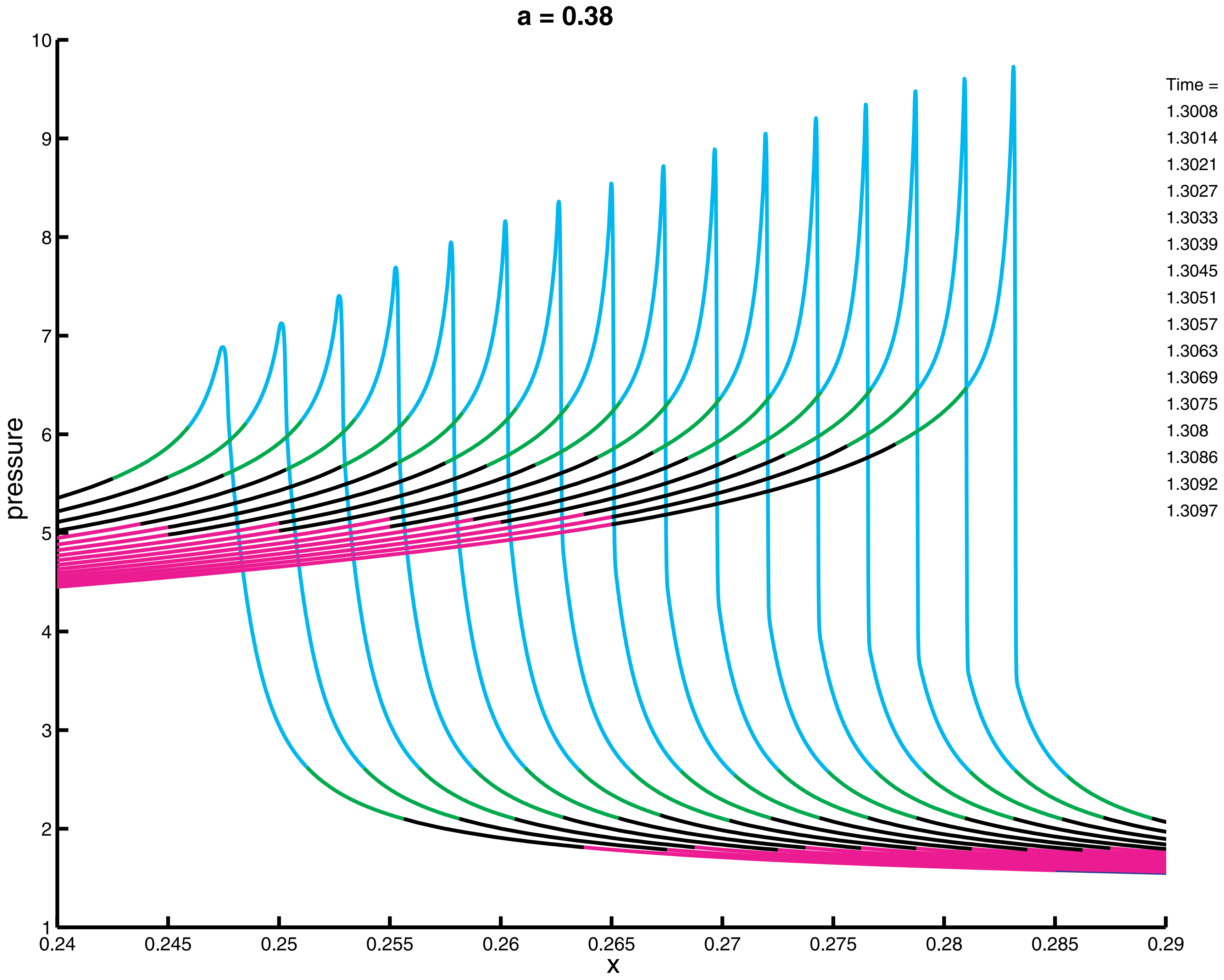

a = 0.1
4.5
4
3.5
3
2.5
2
1.5
1
pressure
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
x
Time =
0
1.1661
1.2184
1.2726
1.3252
1.3772

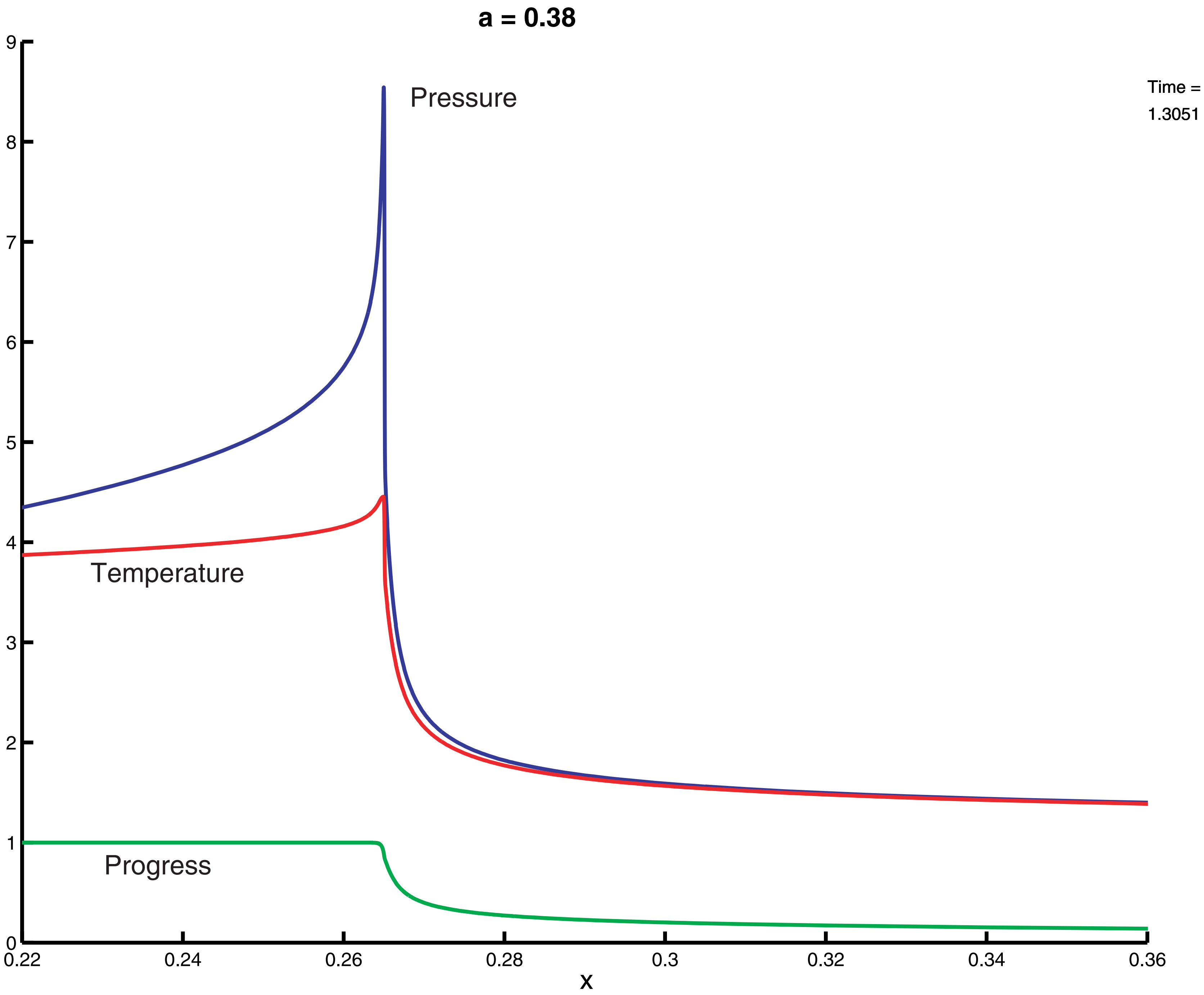

a = 0.1
temperature
x
4
3.5
3
2.5
2
1.5
1
0.5
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
Time =
0
1.1661
1.2184
1.2726
1.3252
1.3772


a = 0.1
progress
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
Time =
0
1.1661
1.2184
1.2726
1.3252
1.3772


a = 0.1
Time = 1.3252
Pressure
Temperature
Progress
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
x

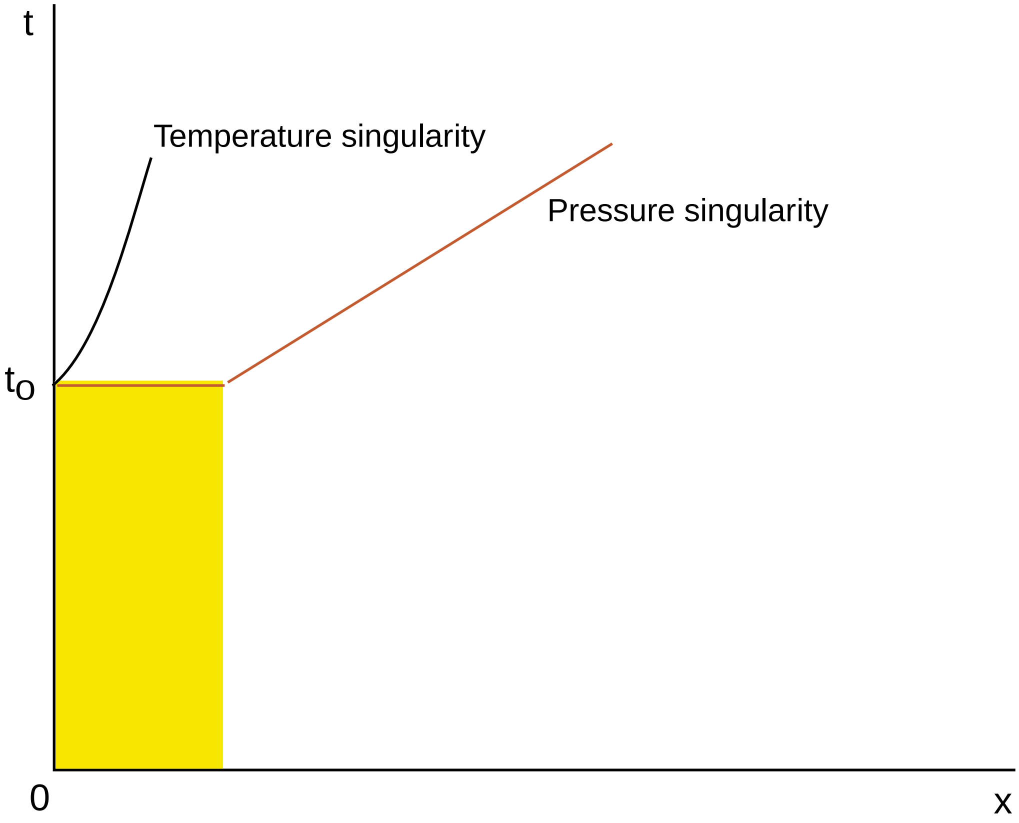

a = 0.38
pressure
x
0
2
4
6
8
10
12
14
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Time =
0
1.211
1.2387
1.2439
1.2488
1.2535
1.2585
1.2632
1.2879
1.3138
1.3391
1.3642
1.3892
1.4141
1.4388

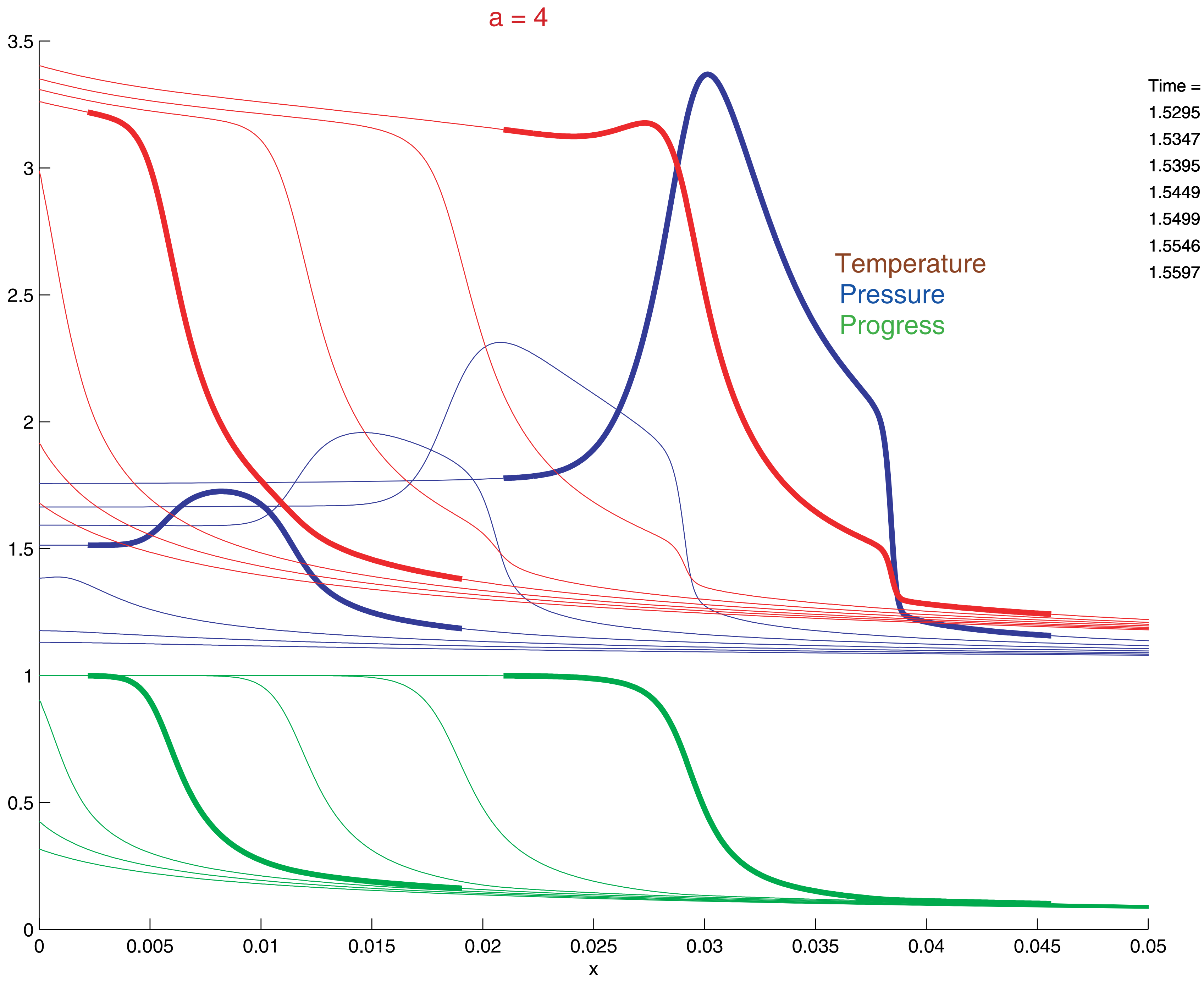

a = 0.38
pressure
x
10
9
8
7
6
5
4
3
2
1
0.24
0.245
0.25
0.255
0.26
0.265
0.27
0.275
0.28
0.285
0.29
Time =
1.3008
1.3014
1.3021
1.3027
1.3033
1.3039
1.3045
1.3051
1.3057
1.3063
1.3069
1.3075
1.308
1.3086
1.3092
1.3097


a = 0.38
Time =
1.3051
Pressure
Temperature
Progress
9
8
7
6
5
4
3
2
1
0
0.22
0.24
0.26
0.28
0.3
0.32
0.34
0.36
x

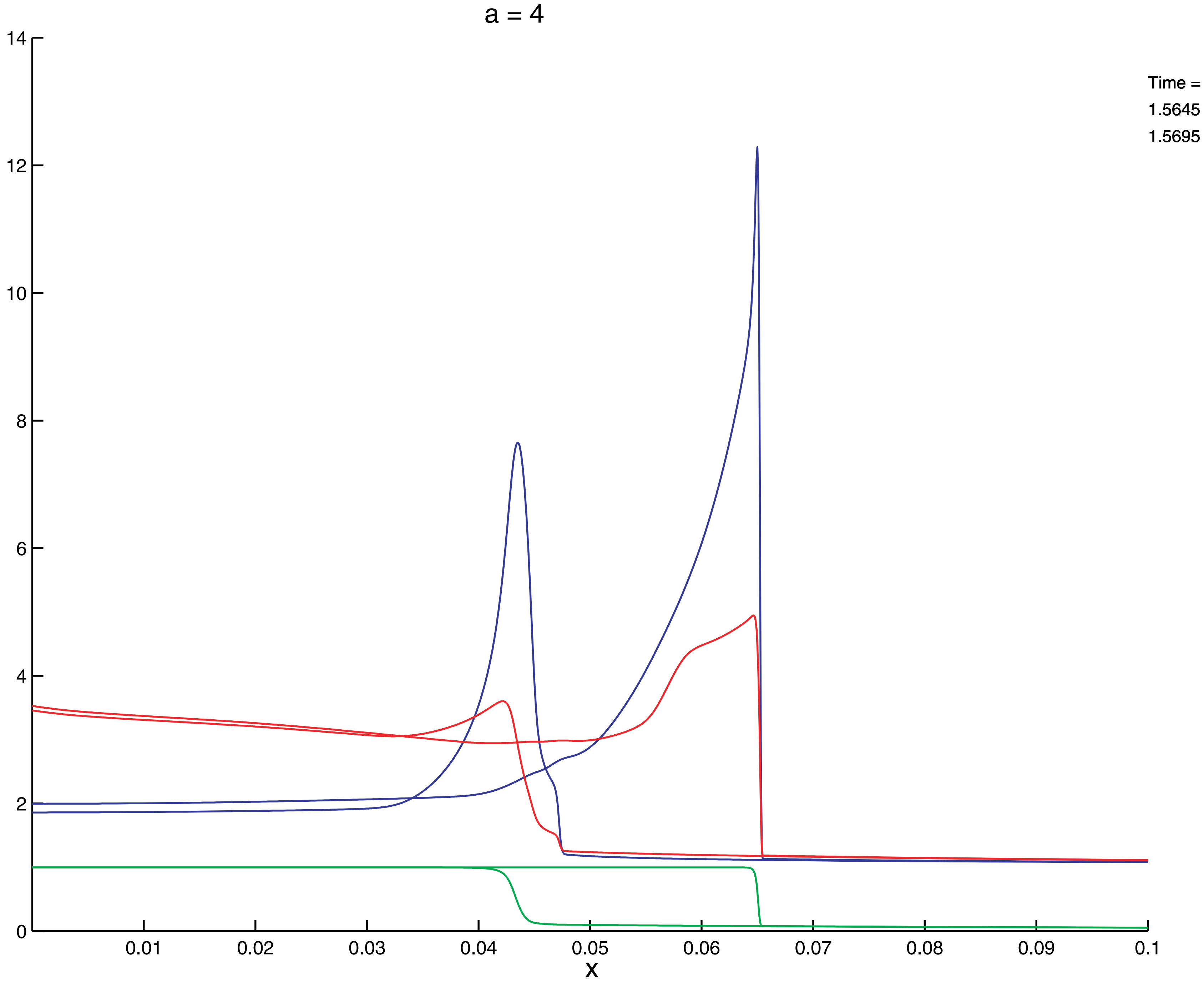
Scenario for Larger Gradients

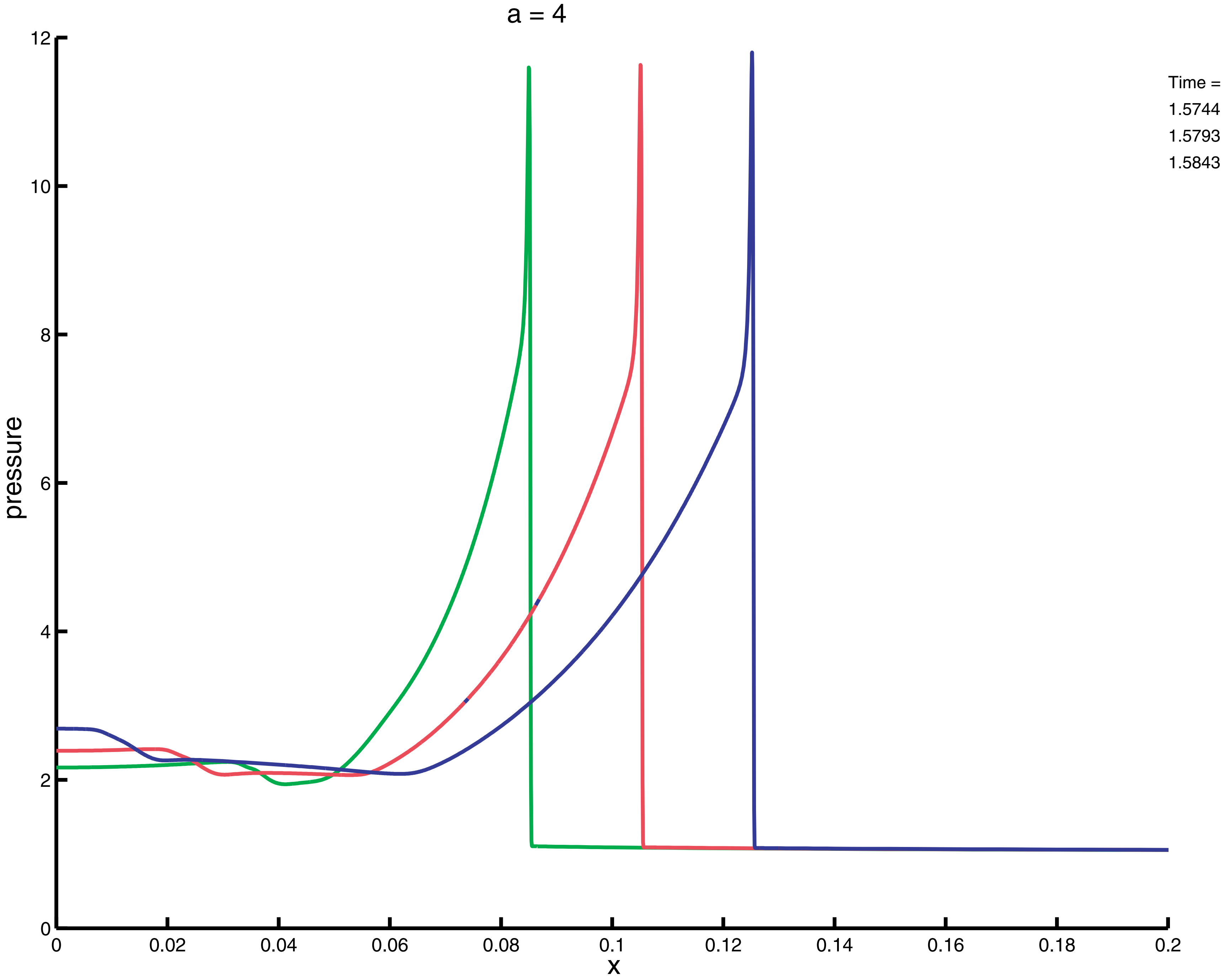
$a \gg 1$

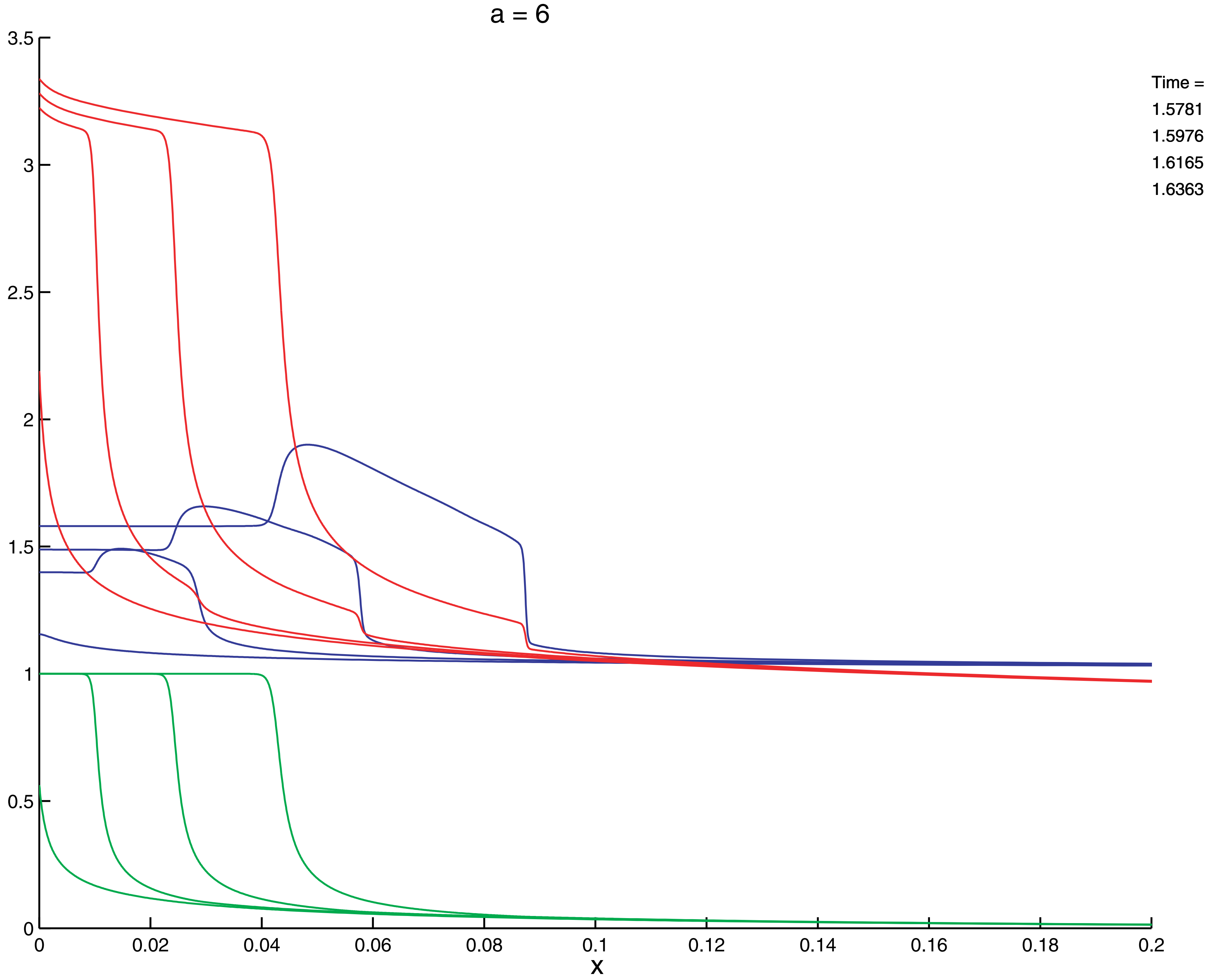


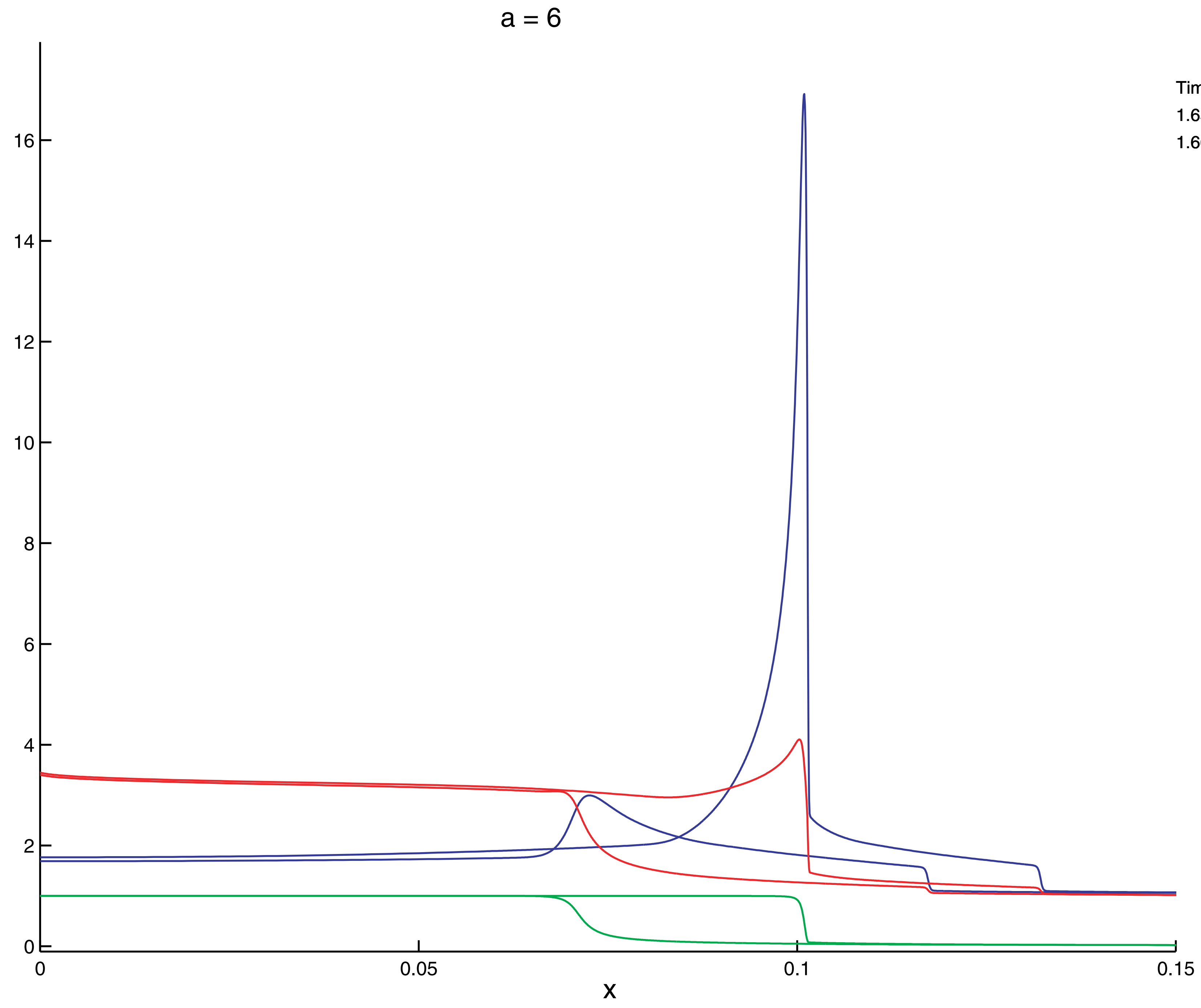


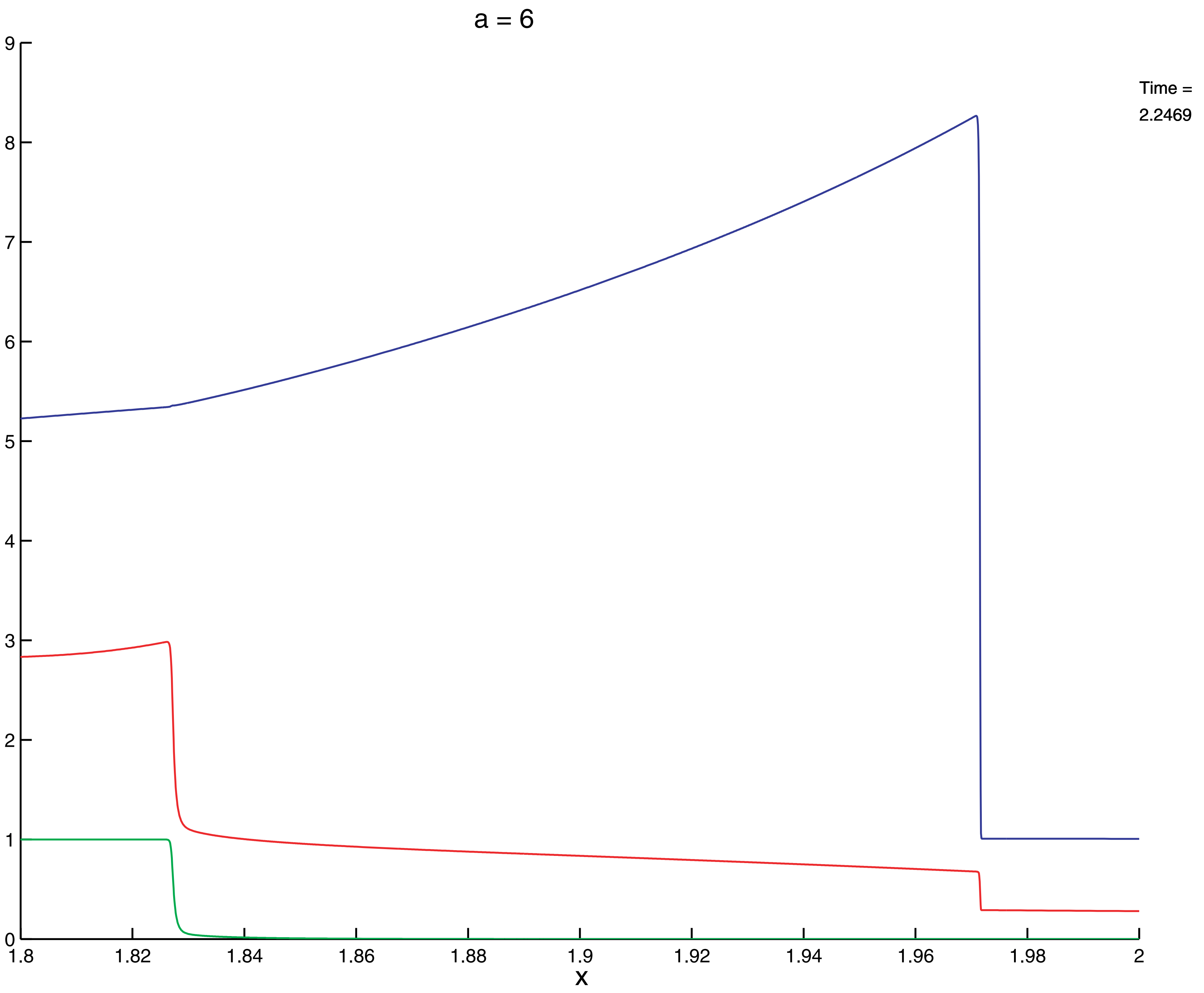
a = 4
3.5
3
2.5
2
1.5
1
0.5
0
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
0.04
0.045
0.05
x
Time =
1.5295
1.5347
1.5395
1.5449
1.5499
1.5546
1.5597
Temperature
Pressure
Progress


a = 4
Time =
1.5645
1.5695
0
2
4
6
8
10
12
14
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
x


a = 4
Time =
1.5744
1.5793
1.5843
pressure
x
0
2
4
6
8
10
12
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2


a = 6
Time =
1.5781
1.5976
1.6165
1.6363
3.5
3
2.5
2
1.5
1
0.5
0
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
x


a = 6
Time =
1.6563
1.6662
16
14
12
10
8
6
4
2
0
0
0.05
0.1
0.15
x


a = 6
Time =
2.2469
9
8
7
6
5
4
3
2
1
0
1.8
1.82
1.84
1.86
1.88
1.9
1.92
1.94
1.96
1.98
2
x

Properties of Sample Explosive

$$\begin{aligned}
Q &= 2,\\
\gamma &= 1.4,\\
\epsilon &= 1/16,\\
p_e &= 3.8,\\
T_e &= 3.8,\\
p_c &= 7.13,\\
T_c &= 4.42,\\
D_c &= 4.01,\\
p_n &= 13.27,\\
T_n &= 3.17.
\end{aligned}$$

Conclusions

- Nonuniformities are essential to provoke a detonation in a hot, reactive medium. Preconditioning is the key.
- An $O(\epsilon)$ gradient in temperature provides enough nonuniformity.
- Evolution begins with a localized explosion.
- A small gradient (on the ϵ scale) involves a broad induction domain, produces a localized constant-volume explosion, followed by a decelerating weak detonation which, in due course, transits to a CJ wave.
- A moderate gradient reduces the run to detonation.
- A moderately large gradient confines induction initially to a narrow domain, in which a (nearly) constant-pressure explosion occurs. The pressure pulse leaves the induction domain, amplifies into a weak shock, and additional chemical-gasdynamic coupling leads to detonation. (SWACER mechanism, and variations thereof.) Run-to-detonation distances are shorter.
- Very large gradients produce a very narrow initial induction region and hence a very weak shock; too weak to produce a detonation.