Fundamental thermal machines for the thermodynamics of computation

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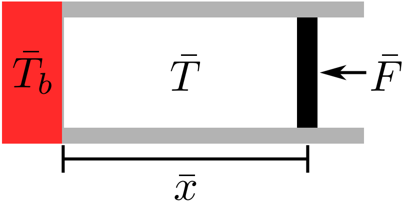
Outline

Gas enclosed by a piston



$\overline{x}$: piston position.
$\overline{T}$: gas temperature.
$\overline{T}_b$: reservoir temperature.
$\overline{F}$: external force.

Question: if the gas-piston system is at equilibrium and $\overline{F}$ or $\overline{T}_b$ change, how do $\overline{T}$ and $\overline{x}$ evolve?

Standard thermodynamics:

- Describes the new final **equilibrium**.
- **No** information on the dynamics.

Gas-Piston equations of Cerino *et al.* PRE 91, 032128

Working hypothesis

- Perfect gas.
- Gas-Piston collisions are elastic.
- Gas-Reservoir collisions sets the gas particle velocities according to the Maxwell-Boltzmann distribution for the reservoir temperature $\overline{T}_b$.
- After each collision the gas temperature $\overline{T} = \sum_i mv^2$ is computed.
- The gas distribution is always a Maxwellian for the temperature $\overline{T}$.
- Averaging Gas-Piston and Gas-Reservoir collisions we get equations for $\overline{x}$ and $\overline{T}$.

Gas-Piston equations of Cerino *et al.* PRE 91, 032128

$$\ddot{\overline{x}} + \frac{\overline{F}}{M} - \frac{\nu N}{\nu+1}\frac{1}{\overline{x}}\,\mathrm{erfc}\left(\sqrt{\frac{m}{2\overline{T}}}\dot{\overline{x}}\right)\left(\dot{\overline{x}}^2 + \frac{\overline{T}}{m}\right) + \frac{\nu N}{\nu+1}\exp\left(-\frac{m\dot{\overline{x}}^2}{2\overline{T}}\right)\frac{\dot{\overline{x}}}{\overline{x}}\sqrt{\frac{2\overline{T}}{\pi m}} = 0,$$

$$\dot{\overline{T}} + \frac{2\dot{\overline{x}}\left[m\dot{\overline{x}}^2 + \overline{T}(1-2\nu)\right]}{\overline{x}(\nu+1)^2}\,\mathrm{erfc}\left(\sqrt{\frac{m}{2\overline{T}}}\dot{\overline{x}}\right) + \sqrt{\frac{2\overline{T}}{\pi m}}\frac{\overline{T}-\overline{T}_b}{\overline{x}}$$
$$+ \frac{2}{\overline{x}(\nu+1)^2}\sqrt{\frac{2m\overline{T}}{\pi}}\left(\frac{2\nu\overline{T}}{m} - \dot{\overline{x}}^2\right)\exp\left(-\frac{m\dot{\overline{x}}^2}{2\overline{T}}\right) = 0,$$

M	piston mass	N	gas particles number
m	gas particle mass	$\overline{F}$	external force
ν	$\frac{m}{M}$	$\overline{T}_b$	reservoir temperature

Problems:

- termodynamic limits $\nu = m/M \to 0,\ N \to \infty$?
- analytic solution?

Dimensionless Gas-Piston Equations

$$\ddot{x} + F + \operatorname{erfc}\left(\frac{\varepsilon\dot{x}}{\sqrt{2T}}\right)\frac{\varepsilon^2\dot{x}^2 + T}{x} + \exp\left(-\frac{\varepsilon^2\dot{x}^2}{2T}\right)\frac{\dot{x}}{x}\sqrt{\frac{2T}{\pi}}\varepsilon = 0,$$

$$\dot{T} - 2\operatorname{erfc}\left(\frac{\varepsilon\dot{x}}{\sqrt{2T}}\right)\frac{\dot{x}}{x}(\varepsilon^2\dot{x}^2 + T) - 2\sqrt{\frac{2T}{\pi}}\varepsilon\frac{\dot{x}^2}{x}\exp\left(-\frac{\varepsilon^2\dot{x}^2}{2T}\right) + \sqrt{\frac{2T}{\pi}}\frac{T - T_b}{\varepsilon x} = 0.$$

- x, T, F, T_b are the dimensionless version of $\overline{x}$, $\overline{T}$, $\overline{F}$, $\overline{T_b}$
- $m/M \to 0$ and $N \to \infty$ are already taken;
- $\varepsilon^2 = \frac{Nm}{M}$ is finite;
- standard thermodynamics equilibrium conditions

$$x_{\text{eq}} = \frac{T_b}{F}, \quad \dot{x}_{\text{eq}} = 0, \quad T_{\text{eq}} = T_b.$$

Linear Dimensionless Gas-Piston Equations

- Not too far from the equilibrium
- ε perturbation parameter

$$\ddot{x} + \frac{F^2}{T_b}\left(x - \frac{T_b}{F}\right) + 2\sqrt{\frac{2}{\pi T_b}}\varepsilon F\dot{x} - F\frac{T - T_b}{T_b} = 0$$

$$\dot{T} + 2F\dot{x} + \sqrt{\frac{2}{\pi T_b}}\frac{F}{\varepsilon}(T - T_b) = 0$$

Treated as a third order equation for x coupled with a definition for T

$$\frac{T_b}{F}\dddot{x} + \left[2\frac{\sqrt{T_b}\sqrt{2}\varepsilon}{\sqrt{\pi}} - \frac{T_b\dot{F}}{F^2} + \frac{\dot{T}_b}{F} + \frac{\sqrt{T_b}\sqrt{2}}{\sqrt{\pi}\varepsilon}\right]\ddot{x} + \left[3F + \frac{\sqrt{2}\varepsilon\dot{T}_b}{\sqrt{\pi}\sqrt{T_b}} + 4\frac{F}{\pi}\right]\dot{x}$$

$$+ \left[\dot{F} + \frac{\sqrt{2}F^2}{\sqrt{\pi}\varepsilon\sqrt{T_b}}\right]x - \frac{\sqrt{2}F\sqrt{T_b}}{\sqrt{\pi}\varepsilon} = 0$$

$$T = \frac{T_b}{F}\ddot{x} + 2\sqrt{\frac{2}{\pi}}\sqrt{T_b}\varepsilon\dot{x} + Fx$$

Multiple scales method

$$ODE\left(t, x, \dot{x}, \ddot{x}, \dots, \overset{(n)}{x}, \varepsilon\right) = 0,$$

t independent variable, $x = x(t)$, ε small.

General idea:

1. Conjecture N behaviors with different natural time-scales.
2. Define $N+1$ time functions $(t_0, \dots, t_N)$, $t_i = t_i(\varepsilon, t)$.
   Each t_i isolates a single behaviour with a given time-scale.
3. Expand x and its time derivatives in ODE according to

$$x(t) = \sum_{i=0}^{N} \varepsilon^i x_i(t_0, \dots, t_N) + \mathcal{O}\left(\varepsilon^{N+1}\right), \quad \dot{x} = \sum_{i=0}^{N} \sum_{j=0}^{\infty} \varepsilon^i \frac{\partial x_i}{\partial t_j} \frac{\partial t_j}{\partial t} + \mathcal{O}\left(\varepsilon^{N+1}\right), \quad \dots$$

4. Collect ε coefficients.
5. Transform the ODE in PDEs system.

Multiple scales method

6. Solve the ε^0 equation for x_0.
7. Subs x_0 in the ε^1 equation.
8. Set all the arbitrary functions in x_0 to avoid secular terms in x_1.
9. Solve the ε^1 equation for x_1.
10. Iterate for alle the remaining x_i

At the end of the procedure:

- All the $x_0, \ldots, x_N$ are specified.
- $x_{ap}(t) = \sum_{i=0}^{N-1} \varepsilon^i x_i(t_0, \ldots, t_N) + \mathcal{O}(\varepsilon^N)$ is asymptotic up to $t_N(t, \varepsilon) = \mathcal{O}(1)$.
- Crosscheck on the ansatz on the number of timescales N.

Back to the Linear Dimensionless Gas-Piston Equations

Additional working hypothesis:

- T_b is constant (w.l.o.g. $T_b = 1$)
- F is slowly varying over time $\left(F = F(\varepsilon t)\right)$.

[..........Long expression for x_{ap}..........]

[..........Long expression for T_{ap}.........]

Relaxation to equilibrium

- $F = 1$
- $x(t=0) = 1 + x_0,\ \dot{x}(t=0) = \dot{x}_0,\ T(t=0) = 1 + T_0$

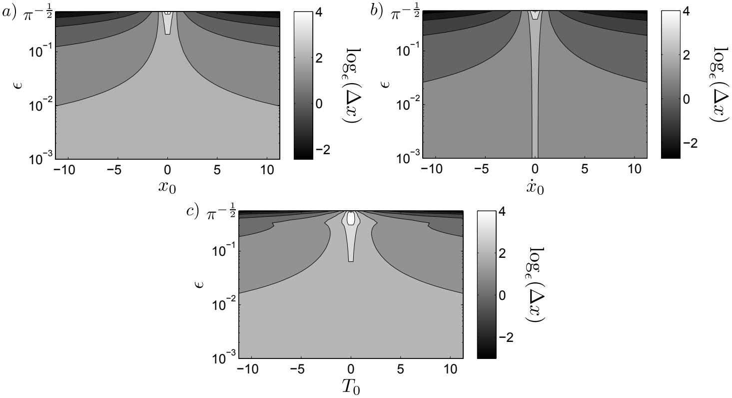
$$x_{ap}(t) = 1 + K_3\varepsilon^2 \exp\left(\sqrt{\tfrac{2}{\pi}}\frac{t}{\varepsilon}(\pi\varepsilon^2 - 1)\right) + \exp\left(-\frac{\varepsilon t(\pi+2)}{\sqrt{2\pi}}\right)\cdot$$
$$\cdot\left[C1\sin(t) + C2\cos(t) + \left(-\frac{t\varepsilon^3}{2}(\varepsilon t\theta^2 - 2\eta)C_1 + \theta t C_2\varepsilon^2 + C_3\varepsilon\right)\sin(t)\right.$$
$$\left.+\left(-\frac{\theta^2 t^2}{2}C_2\varepsilon^4 + (C_2\eta t - C_3 t\theta)\varepsilon^3 + (C_5 - C_1 t\theta)\varepsilon^2\right)\cos(t)\right] + \mathcal{O}\left(\varepsilon^3\right)$$

with

$$\eta = -\tfrac{\sqrt{2\pi}}{4}(\pi + 4), \quad \theta = -\tfrac{(\pi^2 - 4\pi - 4)}{4\pi}$$
$$C_1 = \dot{x}_0, \quad C_2 = x_0, \quad C_3 = \tfrac{(\pi T_0 + \pi x_0 + 2x_0)}{\sqrt{2\pi}}, \quad C_5 = -\tfrac{\pi T_0}{2}, \quad K_3 = \tfrac{\pi T_0}{2}.$$

Relaxation to equilibrium - x_{ap} goodness

- Simulate x numerically
- Compute $\Delta x = \max_{t\in[0,\infty[}(|x - x_{ap}|)$
- Study Δx as function of ε, x_0, $\dot{x}_0$ and T_0



Relaxation to equilibrium - thermodynamics

Analytic expression for the heat exchanged with the reservoir between $t = 0$ and $t = t$

$$
\begin{aligned}
Q_{ap}^{rel}(0,t) =& x(0) - x(t) + \tfrac{\dot{x}^2(0) - \dot{x}^2(t)}{2} + \tfrac{T(0) - T(t)}{2} \\
=& (1 + x_0 - x_{ap}(t)) + \tfrac{\dot{x}_0^2 - \dot{x}_{ap}^2(t)}{2} + \tfrac{1 + T0 - T_{ap}(t)}{2} + \mathcal{O}(\varepsilon),
\end{aligned}
$$

- **New non-equilibrium result**.
- **Analytic** curve of the heat exchanged with the reservoir.

Isothermal compression

- $x(t=0)=1$, $\dot{x}(t=0)=0$, $T(t=0)=1$
- Gas compressed in a finite time, then relaxes to equilibrium

$$F=\begin{cases}1 & \text{for } t<0\\ 1+fa\varepsilon t & \text{for } 0\le t\le \dfrac{1}{a\varepsilon}\\ 1+f & \text{for } t>\dfrac{1}{a\varepsilon}.\end{cases}$$

- f is F increment. $\frac{1}{a\varepsilon}$ is the compression duration.

$$x_{ap}(t)=\begin{cases}\frac{1}{fa\varepsilon t+1}+\varepsilon^2\left(-\frac{2a^2f^2}{(fa\varepsilon t+1)^5}+\sqrt{\frac{2}{\pi}}\frac{af(\pi+2)}{(fa\varepsilon t+1)^3}\right)+\mathcal{O}\left(\varepsilon^4\right) & \text{if } t\in[0,\frac{1}{a\varepsilon}]\\ \text{as in relaxation case} & \text{if } t>\frac{1}{a\varepsilon}.\end{cases}$$

Isothermal compression - thermodynamics

Analytic formula for the net heat exchanged with the reservoir during the compression and the following relaxation

$$
\begin{aligned}
Q_{ap}^{lin}(a) =& x(0) - 1 + \frac{\dot{x}^2(0)}{2} + \frac{T(0)-1}{2} + f\ a\ \varepsilon \int_0^{\frac{1}{a\varepsilon}} x(t)\mathrm{d}t \\
=& \ln(1+f) - \frac{2(fa\varepsilon)^2\left[(1+f)^2-\frac{1}{2}\right]\left[(1+f)+\frac{1}{2}\right]}{(1+f)^4} \\
&+ \frac{2fa\varepsilon^2\sqrt{\frac{2}{\pi}}\left[(\pi+\frac{3}{2})(1+f)^2-\frac{\pi+2}{4}\right]}{(1+f)^2} + \mathcal{O}\left(\varepsilon^3\right)
\end{aligned}
$$

- **New result:** analytic expectation value for the heat produced duting an isothermal compression lasting $\frac{1}{a\varepsilon}$.
- **Consistency:** the second principle is satisfied by this formula.

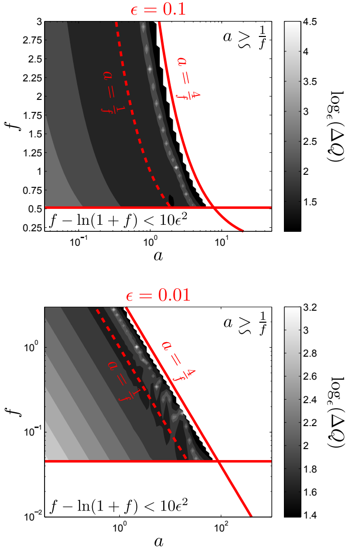
Isothermal compression - thermodynamics

Validity constrains of $Q_{ap}^{lin}(a)$:

- $f > 0$
- $af \lesssim 1$
- $f - \ln(1+f) \gg \varepsilon^2$

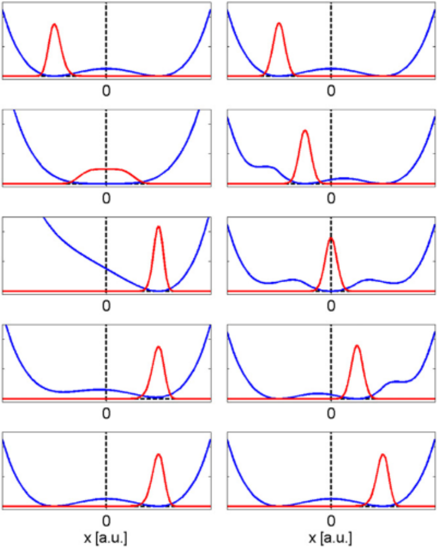
Quality test for $Q_{ap}^{lin}(a)$

- Simulate numerically x
- Compute $\Delta Q = |Q^{lin}(a) - Q_{num}^{lin}(a)|$
- Study ΔQ as function of ε, a ed f
- $\Delta Q = \mathcal{O}(\varepsilon^3)$



Conclusions

- Dimensionless version of the eq. from PRE 91, 032128.
- Application of the multiple scales method to the Linear Gas-Piston Equations.
- Analytic formulas on the thermodynamic of non-equilibrium processes.
- Thermodynamic cycles with the “slow expansion” approach.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