Title: Inference Between Continuum Theromechanics and Particle Mechanics via Space-Time Averaging

Date: Aug 10, 2011 04:00 PM

URL: http://pirsa.org/11080077

Abstract:

Inference between Continuum Thermomechanics and Particle Mechanics via Space-time Averaging

Veronica Wallängen

Supervisor: PierGianLuca Porta Mana

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Macroscopic Continuum Thermomechanics

Independent fields:
Mass density $\rho(\mathbf{x}, t)$
Velocity $\mathbf{v}(\mathbf{x}, t)$
Temperature $\theta(\mathbf{x}, t)$

Dependent fields:
Specific internal energy $u(\mathbf{x}, t)$
Heat flow $\mathbf{q}(\mathbf{x}, t)$
Stress $\mathbf{T}(\mathbf{x}, t)$
Specific entropy $s(\mathbf{x}, t)$

Balance laws:

$$\partial_t \rho - \nabla \cdot (\rho \mathbf{v}) = 0$$
$$\nabla \cdot \mathbf{T} + \mathbf{b} - \partial_t(\rho \mathbf{v}) - \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = 0$$
$$\mathbf{T}^T - \mathbf{T} = 0$$
$$\rho \partial_t u + \tfrac{1}{2} \rho \partial_t \mathbf{v}^2 - \nabla \cdot (\mathbf{T}^T \cdot \mathbf{v}) + \nabla \cdot \mathbf{q} -$$
$$- Q - \mathbf{b} \cdot \mathbf{v} = 0$$

Constitutive equations

$$u(\mathbf{x}, t) := \bar{u}[\mathbf{x}, t; \rho(\cdot, \cdot), \mathbf{v}(\cdot, \cdot), \theta(\cdot, \cdot)]$$
$$\mathbf{q}(\mathbf{x}, t) := \bar{\mathbf{q}}[\mathbf{x}, t; \rho(\cdot, \cdot), \mathbf{v}(\cdot, \cdot), \theta(\cdot, \cdot)]$$
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The Clausius-Duhem inequality

$$\rho \partial_t s + \rho \mathbf{v} \cdot \nabla s + \nabla \cdot \left(\frac{\mathbf{q}}{\theta} \right) - \frac{Q}{\theta} \geq 0$$

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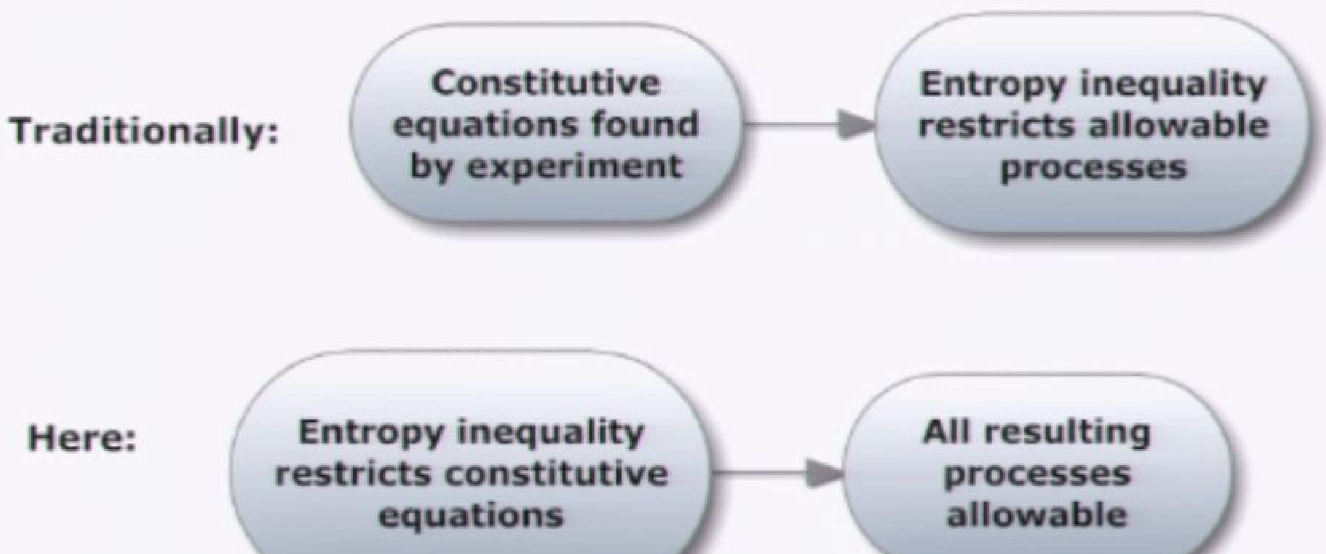

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Macrostate

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Examples:

$$M = \{\rho(\mathbf{x}, t), \mathbf{v}(\mathbf{x}, t), \theta(\mathbf{x}, t) | \forall \mathbf{x}, t_1 \leq t \leq t_0\}$$
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Comparison between the Models

	Macroscopic model	Microscopic model
Independent quantities	$\rho(\mathrm{x,t})$, $\mathbf{v}(\mathrm{x,t})$, $\theta(\mathrm{x,t})$	$\mathrm{x}_i(\mathrm{t})$, $\mathbf{v}_i(\mathrm{t})$
Dependent quantities	$[\mathrm{u}(\mathrm{x,t}),\ \mathbf{q}(\mathrm{x,t}),\ \mathbf{T}(\mathrm{x,t})] = \Xi$	$\mathbf{F}_i(t)$
Balance equations	$\partial_t\rho - \nabla\cdot(\rho\mathbf{v}) = 0$ $\nabla\cdot\mathbf{T} + \mathbf{b} - \partial_t(\rho\mathbf{v}) -$ $-\nabla\cdot(\rho\mathbf{v}\otimes\mathbf{v}) = 0$ $\rho\partial_t u + \frac{1}{2}\rho\partial_t\mathbf{v}^2 - \nabla\cdot(\mathbf{T}^T\cdot\mathbf{v}) +$ $+\nabla\cdot\mathbf{q} - Q - \mathbf{b}\cdot\mathbf{v} = 0$	$\mathbf{F}_i - m_i\ddot{\mathbf{x}}_i = 0$
Constitutive equations	$\Xi(\mathbf{x}, t) = \bar{\Xi}(\mathbf{x}, t; M)$	$\mathbf{F}_i(t) = \bar{\mathbf{F}}_i(t; \{\mathbf{x}_j(\cdot)\})$
State	$M(t; M_0) = \{\rho(\cdot,\cdot), \mathbf{v}(\cdot,\cdot), \theta(\cdot,\cdot)\}$	$\mu[t; \{\mathbf{x}_i(t_0), \mathbf{v}_i(t_0)\}] = \{\mathbf{x}_i(t\|\mu_0), \mathbf{v}_i(t\|\mu_0)\}$

Space-time Averaging

A continuum field can be expressed as a space-time average at position $\mathbf{x}$ and instant t, given a particular microstate μ_0, in the following way

$$y(\mathbf{x}, t|\mu_0) := \sum_{i=1}^{N} \int_{-\infty}^{\infty} y_i(\tau)\phi[\mathbf{x} - \mathbf{x}_i(t|\mu_0), t - \tau]d\tau$$

y_i - molecular quantity associated with point mass P_i

ϕ - normalized weighting function of dimensions $(\text{length})^{-3}(\text{time})^{-1}$ assigning greater contribution to point masses close to $\mathbf{x}$ and times close to t than to those remote therefrom.

In the simplest case:

$$\phi = \begin{cases} \frac{1}{V\Delta t}, & \text{if } |\mathbf{x} - \mathbf{x}_i| < r, |t - \tau| < \Delta t \\ 0, & \text{otherwise} \end{cases}$$

Space-time Averaging

Space-time averages for independent continuum fields:

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- **Mass density**

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- **Velocity**

$$\mathbf{v}(\mathbf{x}, t|\mu_0) = \frac{\mathbf{p}}{\rho} := \frac{\sum_{i=1}^{N} \int_{-\infty}^{\infty} m_i \mathbf{v}_i(\mathbf{x}, t|\mu_0) \phi[\mathbf{x} - \mathbf{x}_i(t|\mu_0), t - \tau] d\tau}{\sum_{i=1}^{N} \int_{-\infty}^{\infty} m_i \phi[\mathbf{x} - \mathbf{x}_i(t|\mu_0), t - \tau] d\tau}$$

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- **Temperature**

$$\theta(\mathbf{x}, t|\mu_0) := \frac{2}{3k_B} \frac{\sum_{i=1}^{N} \int_{-\infty}^{\infty} \frac{1}{2} m_i [\mathbf{v}_i(\tau|\mu_0) - \mathbf{v}(\mathbf{x}, \tau|\mu_0)]^2 \phi[\mathbf{x} - \mathbf{x}_i(\tau|\mu_0), t - \tau] d\tau}{\sum_{i}^{N} \int_{-\infty}^{\infty} \phi[\mathbf{x} - \mathbf{x}_i(\tau|\mu_0), t - \tau] \, \mathrm{d}\tau}$$

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$$\mathbf{v}(\mathbf{x}, t|\mu_0) = \frac{\mathbf{p}}{\rho} := \frac{\sum_{i=1}^{N} \int_{-\infty}^{\infty} m_i \mathbf{v}_i(\mathbf{x}, t|\mu_0) \phi[\mathbf{x} - \mathbf{x}_i(t|\mu_0), t - \tau] d\tau}{\sum_{i=1}^{N} \int_{-\infty}^{\infty} m_i \phi[\mathbf{x} - \mathbf{x}_i(t|\mu_0), t - \tau] d\tau}$$

- **Temperature**

$$\theta(\mathbf{x}, t|\mu_0) := \frac{2}{3k_B} \frac{\sum_{i=1}^{N} \int_{-\infty}^{\infty} \frac{1}{2} m_i [\mathbf{v}_i(\tau|\mu_0) - \mathbf{v}(\mathbf{x}, \tau|\mu_0)]^2 \phi[\mathbf{x} - \mathbf{x}_i(\tau|\mu_0), t - \tau] d\tau}{\sum_{i}^{N} \int_{-\infty}^{\infty} \phi[\mathbf{x} - \mathbf{x}_i(\tau|\mu_0), t - \tau]\, \mathrm{d}\tau}$$

Entropy

A specified microstate determines the macrostate

$$\mu_0 \rightarrow M(\mu_0)$$

(Note: The macrostate is not completely defined until we specify the macrostate form)

A specified macrostate determines a set of possible microstates

$$M_0 \rightarrow R(M_0) = \{\mu_0 | M_0\}$$

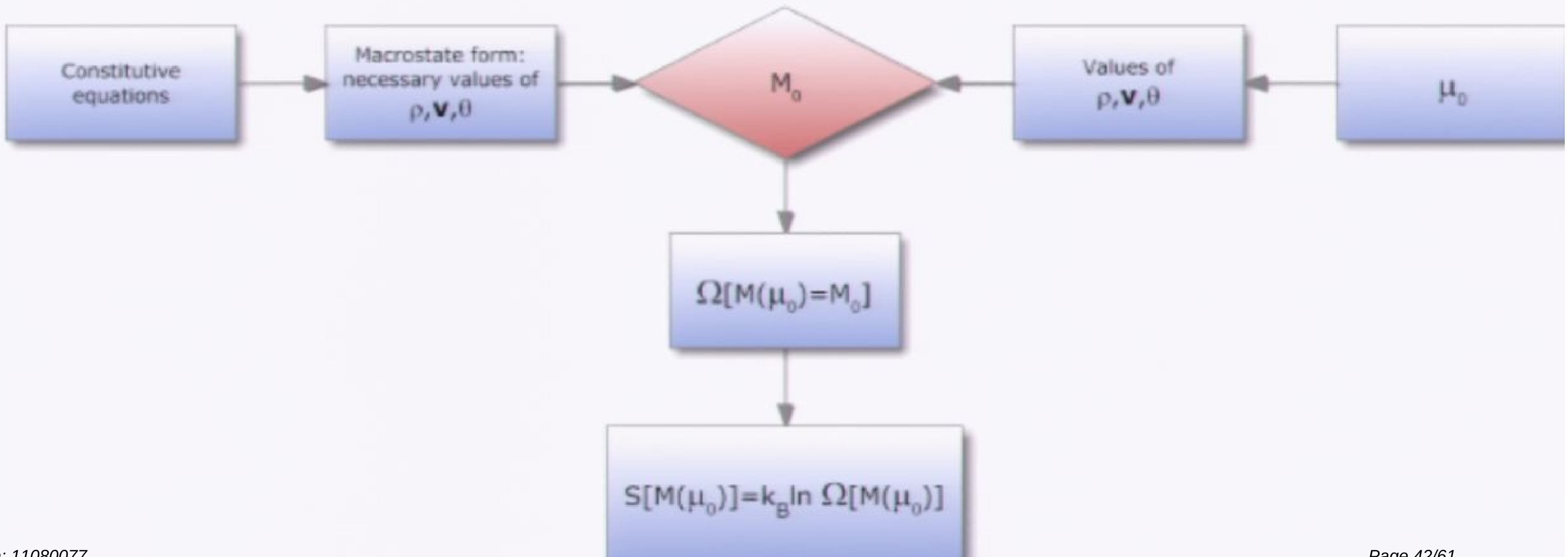
This set corresponds to a region in phase space of volume Ω

Entropy

Boltzmann's entropy formula

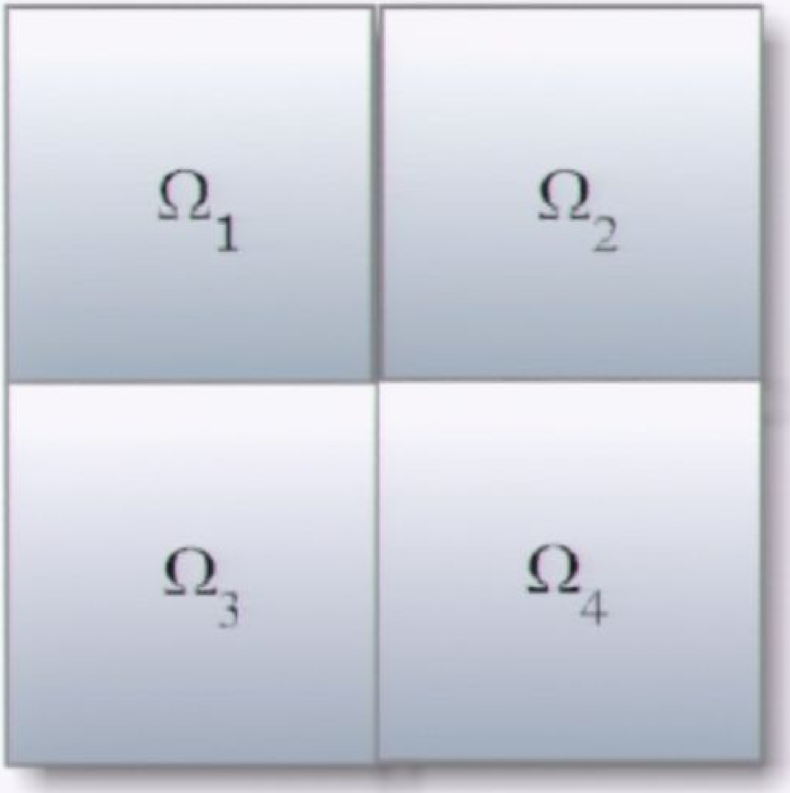
$$S = k_B \ln \Omega$$

- Determining the phase volume Ω requires a specification of the macrostate M_0
- Once such a specification is available we can find the entropy given the microstate of the system



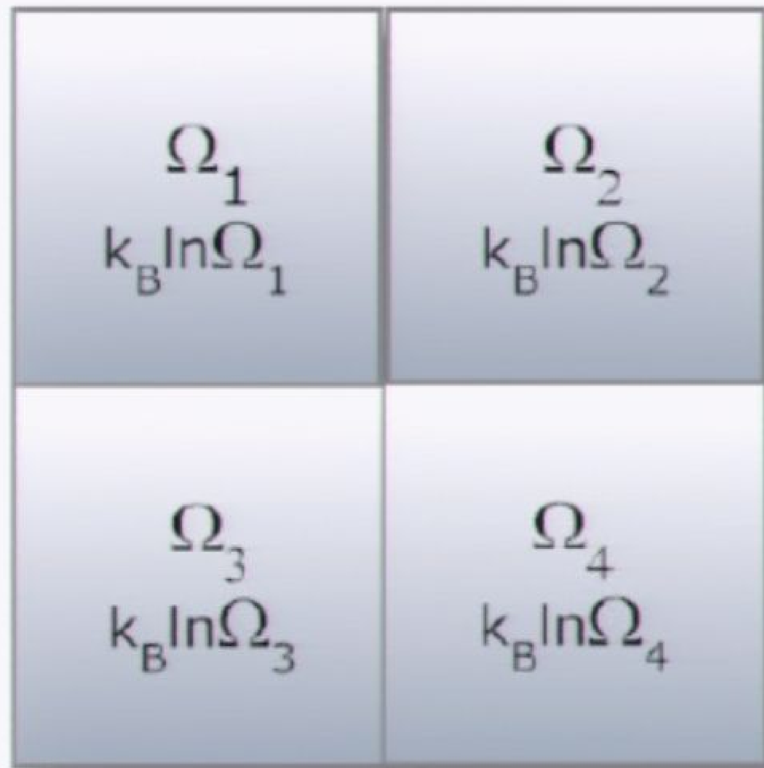
Entropy

- Partition of phase space into regions Ω_i



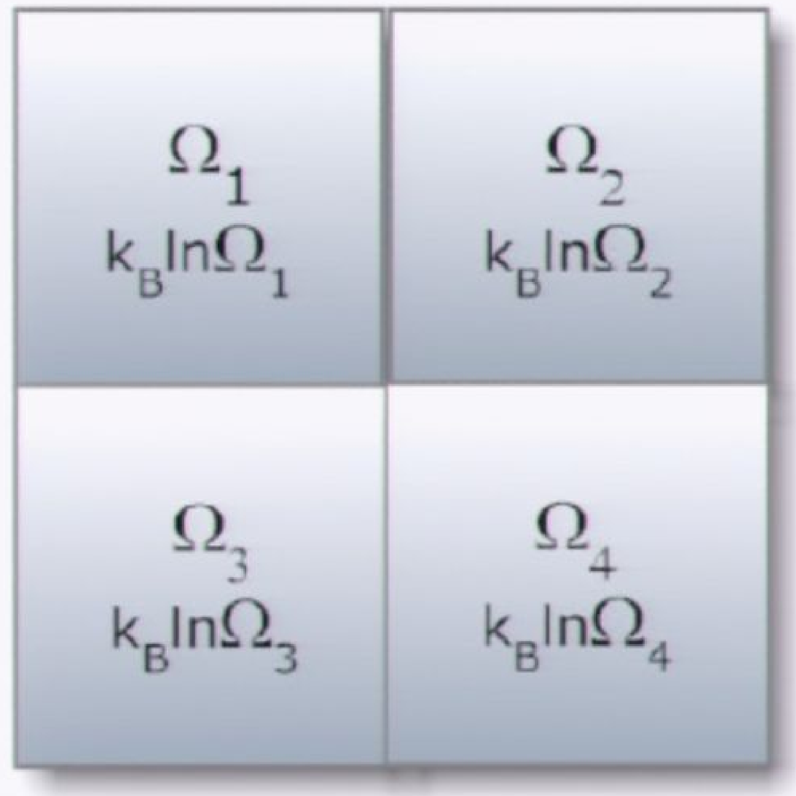
Entropy

- Partition of phase space into regions Ω_i
- To each region we assign a numerical value $k_B \ln \Omega_i$



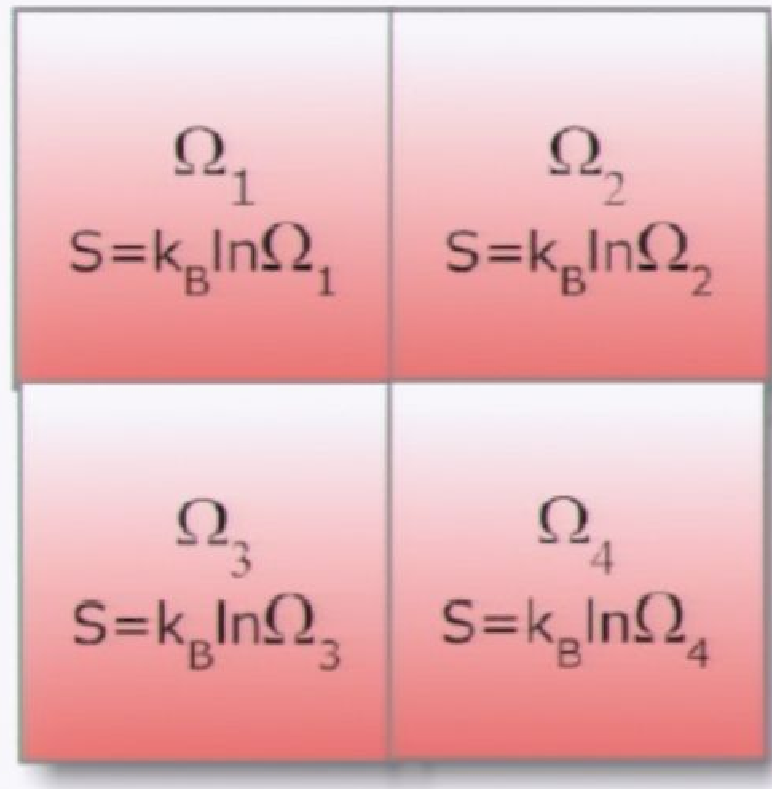
Entropy

- Partition of phase space into regions Ω_i without macrotheory
- To each region we assign a numerical value $k_B \ln \Omega_i$
- Introducing the macrotheory: values of macroscopic variables



Entropy

- Partition of phase space into regions Ω_i without macrotheory
- To each region we assign a numerical value $k_B \ln \Omega_i$
- Introducing the macrotheory: values of macroscopic variables
- Macrostate form$\rightarrow$ **meaningful** partition and entropy!



Entropy

Example: Ideal gas

- Constitutive equations

$$\Xi = \hat{\Xi}(\rho, \theta) \quad \text{(No history-dependencies)}$$

- Macrostate

$$M = \{\rho(\mathbf{x}, t), \theta(\mathbf{x}, t) | \forall\, \mathbf{x}, t = t_0\}$$

Specific entropy:

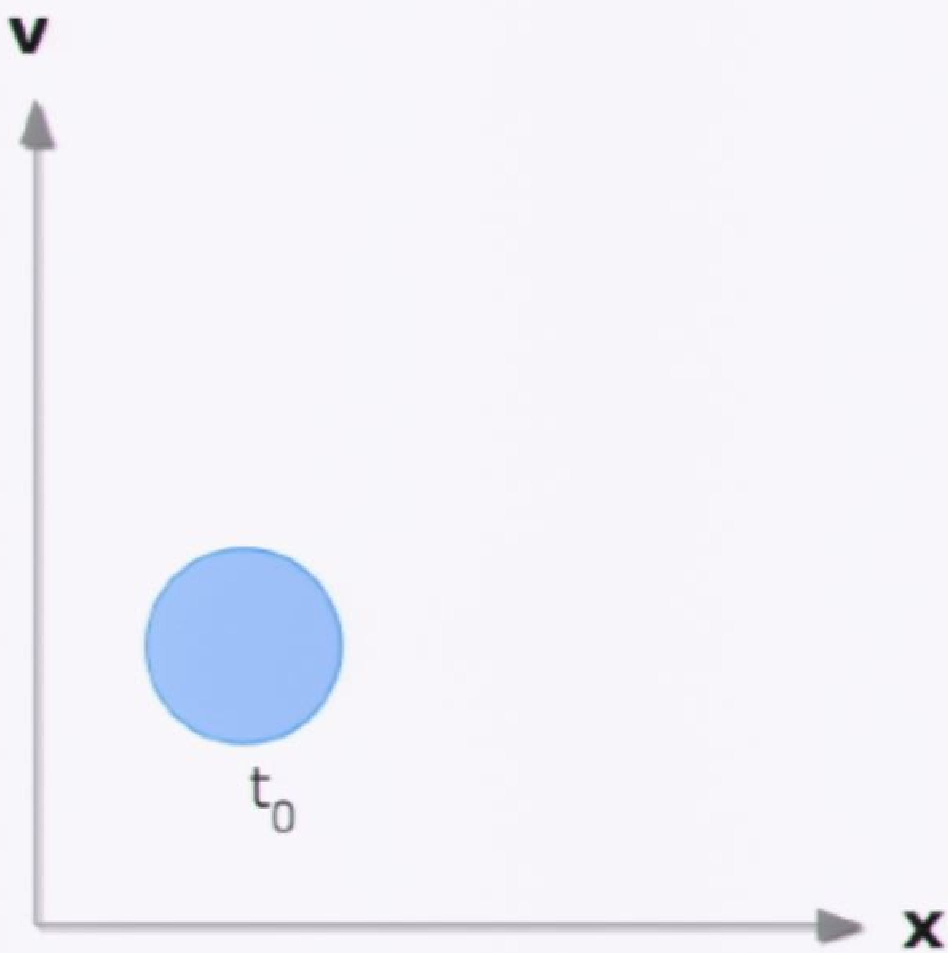
$$s_I d.gas(\rho, \theta) = \frac{k_B}{m} \ln \left[\left(\frac{mN}{\rho} \right)^N \frac{(3\pi m k_B N \theta)^{\frac{3N}{2}}}{(\frac{3N}{2})!} \right] = -\frac{k_B}{m} \ln \rho + \frac{3k_B}{2m} \ln(3k_B\theta) + C$$

Space-time averaged entropy:

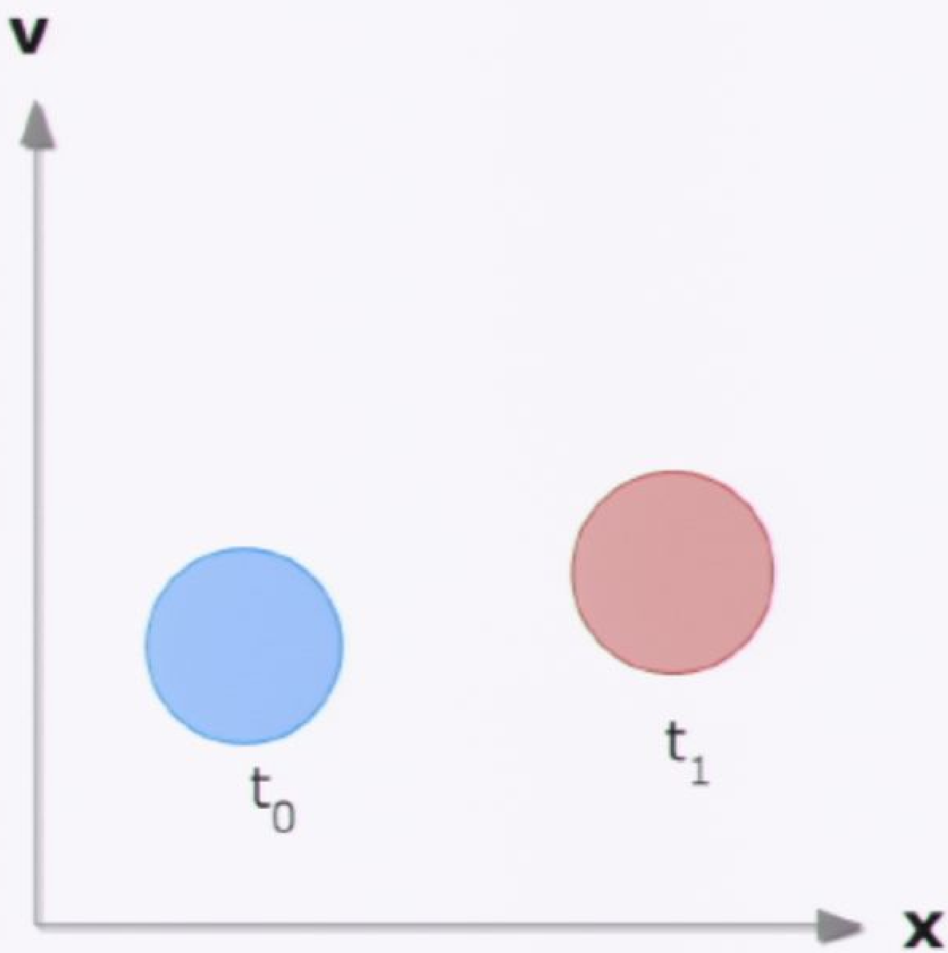
$$s_{Id.gas}(\mathbf{x}, t|\mu_0) := -\frac{k_B}{m} \ln \left(m \sum_i^N \int_{-\infty}^{\infty} \phi[\mathbf{x} - \mathbf{x}_i(t|\mu_0), t - \tau]\, \mathrm{d}\tau \right) +$$

$$+ \frac{3k_B}{2m} \ln \left(m \frac{\sum_{i=1}^N \int_{-\infty}^{\infty} [\mathbf{v}_i(\tau|\mu_0) - \mathbf{v}(\mathbf{x}, \tau|\mu_0)]^2 \phi[\mathbf{x} - \mathbf{x}_i(\tau|\mu_0), t - \tau] d\tau}{\sum_{i=1}^N \int_{-\infty}^{\infty} \phi[\mathbf{x} - \mathbf{x}_i(\tau|\mu_0), t - \tau] d\tau} \right) + C$$

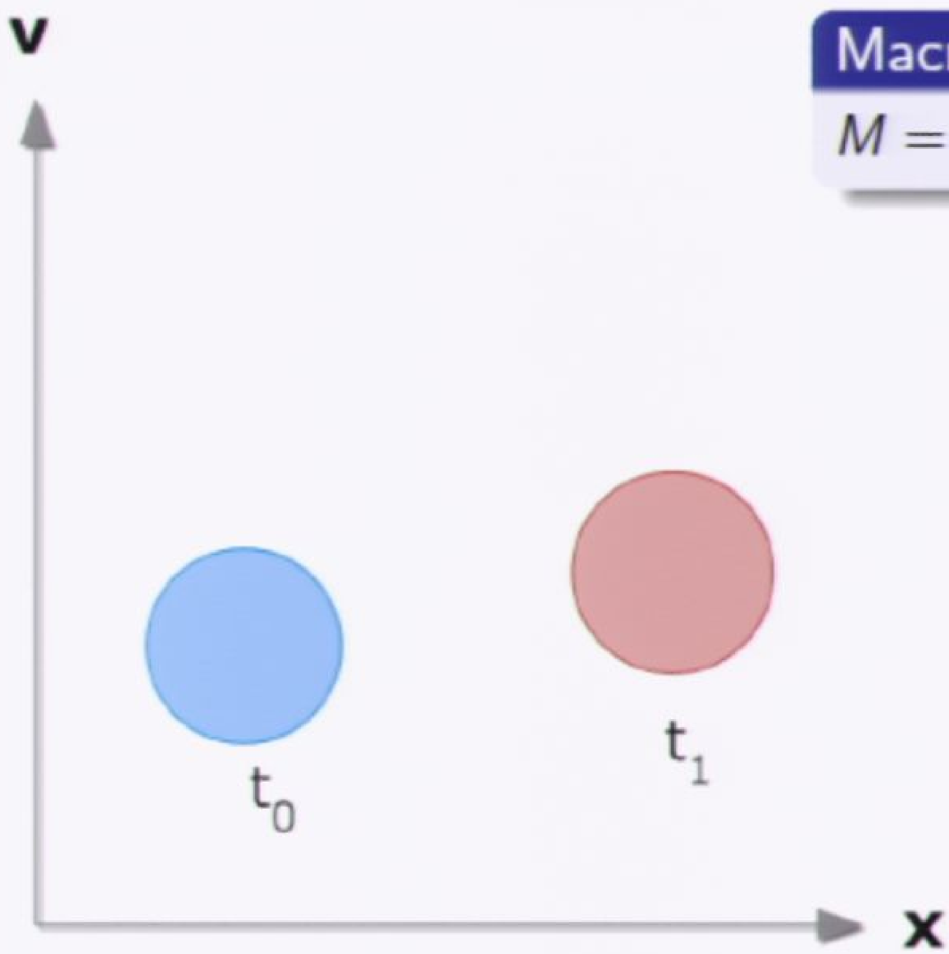
Entropy



Entropy



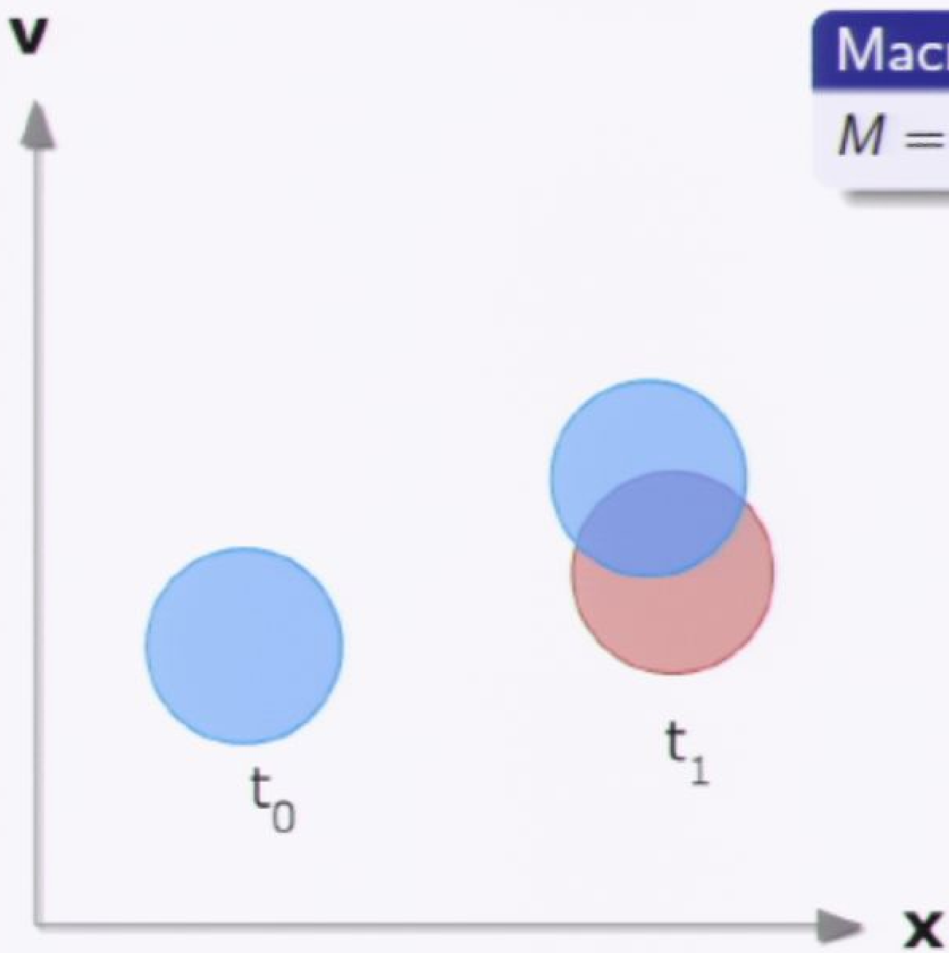
Entropy



Macrostate:

$$M = \{\rho(\mathbf{x}, t), \mathbf{v}(\mathbf{x}, t), \theta(\mathbf{x}, t) | \; \forall \; \mathbf{x}, t = t_0, t_1\}$$

Entropy



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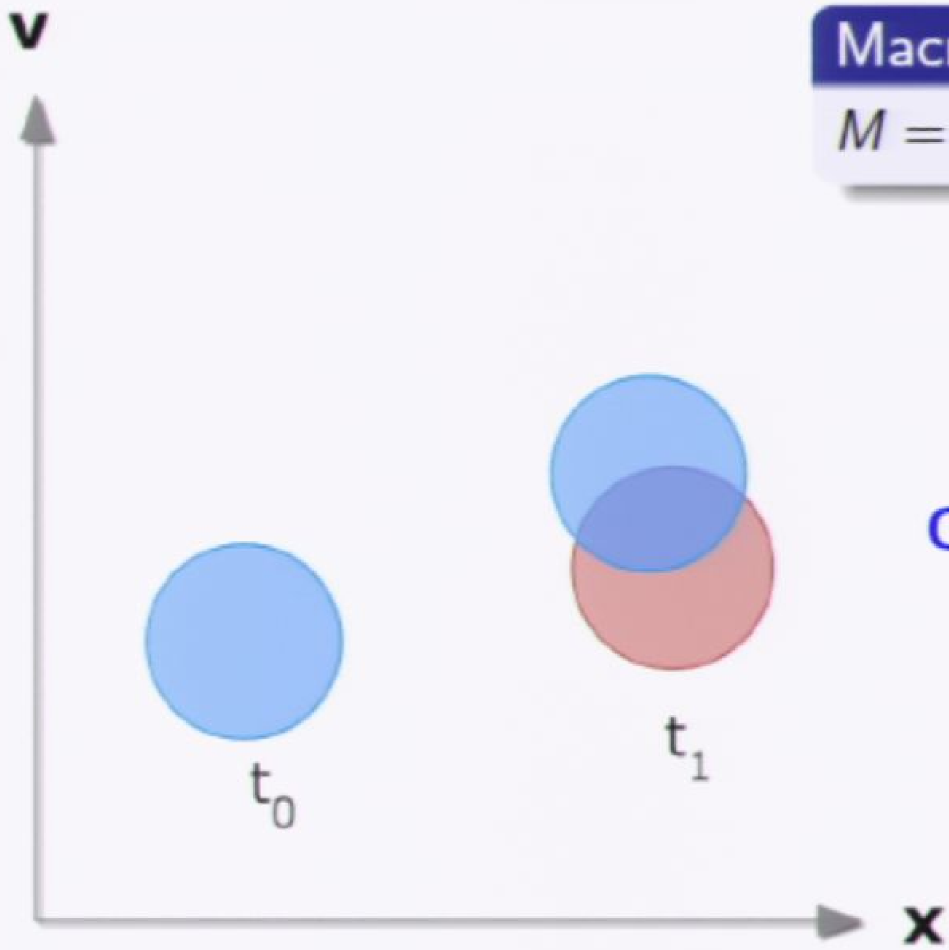
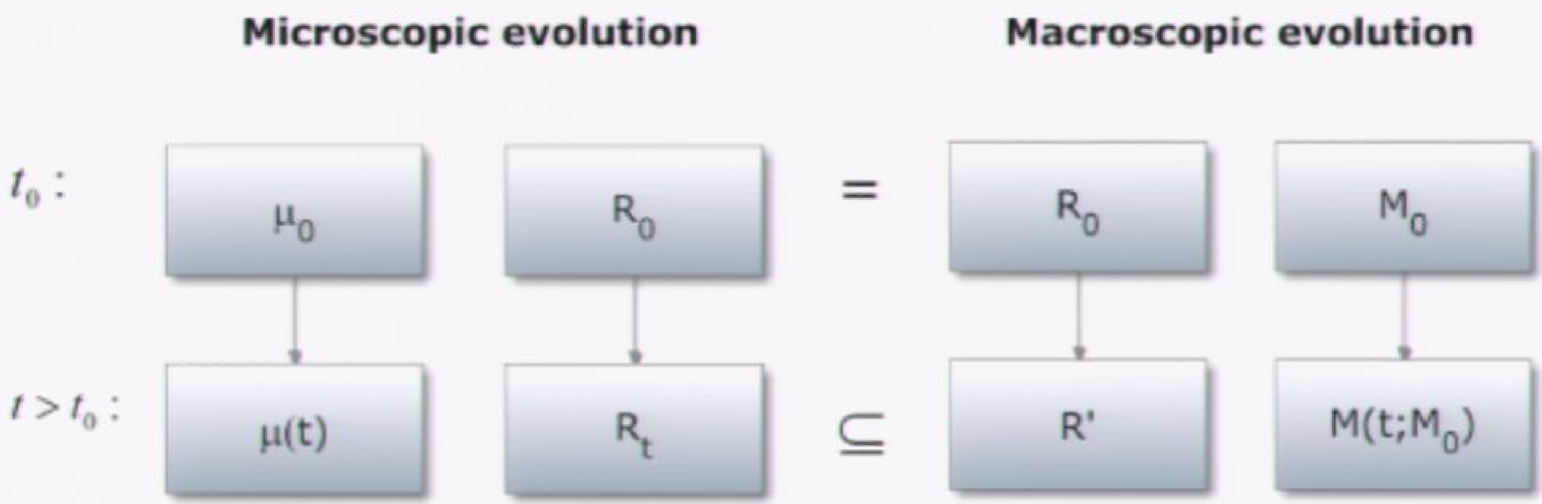


Macrostate:

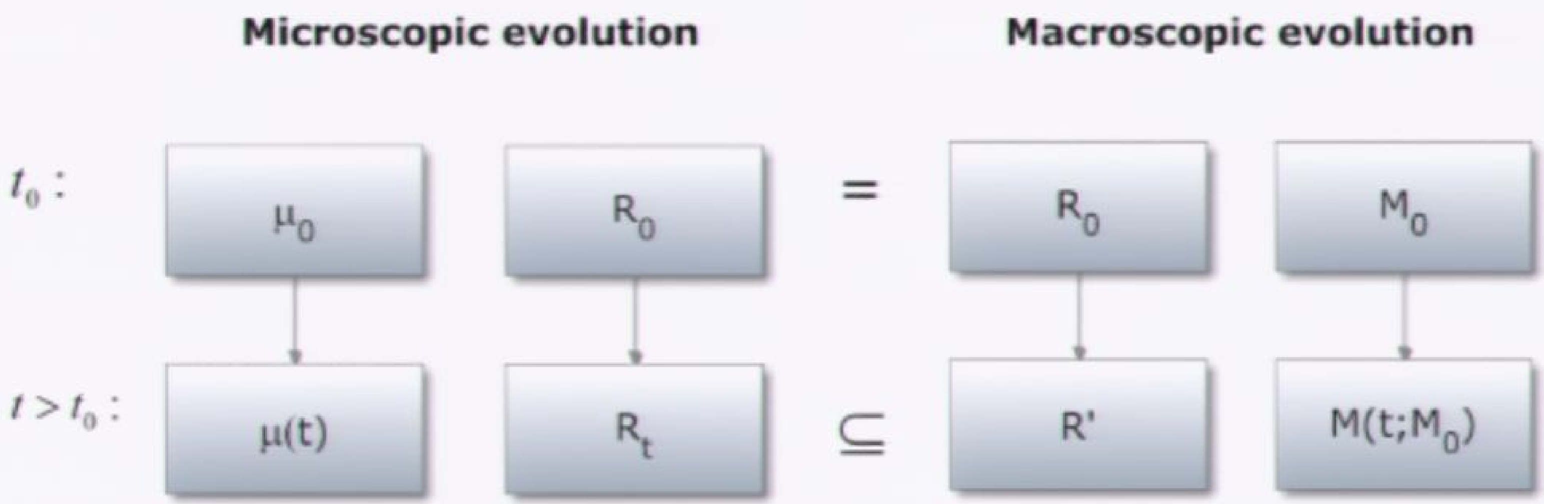
$$M = \{\rho(\mathbf{x}, t), \mathbf{v}(\mathbf{x}, t), \theta(\mathbf{x}, t) | \forall\, \mathbf{x}, t = t_0, t_1\}$$

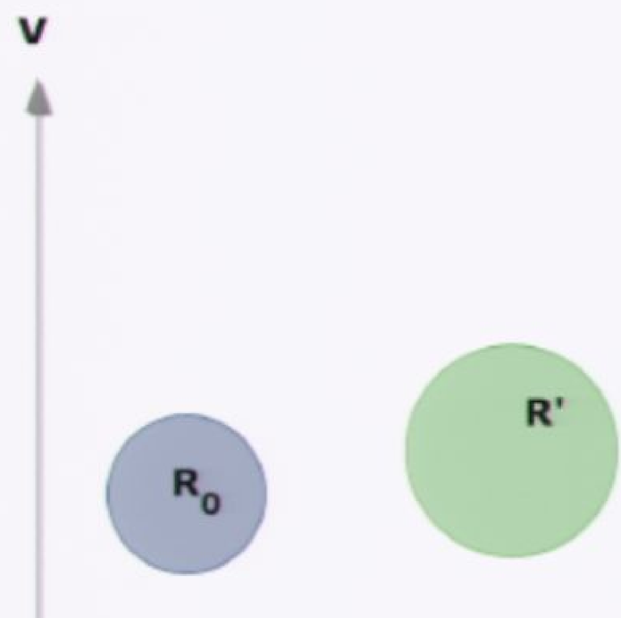
Considering history-dependencies will decrease the entropy!

Reproducibility



Reproducibility





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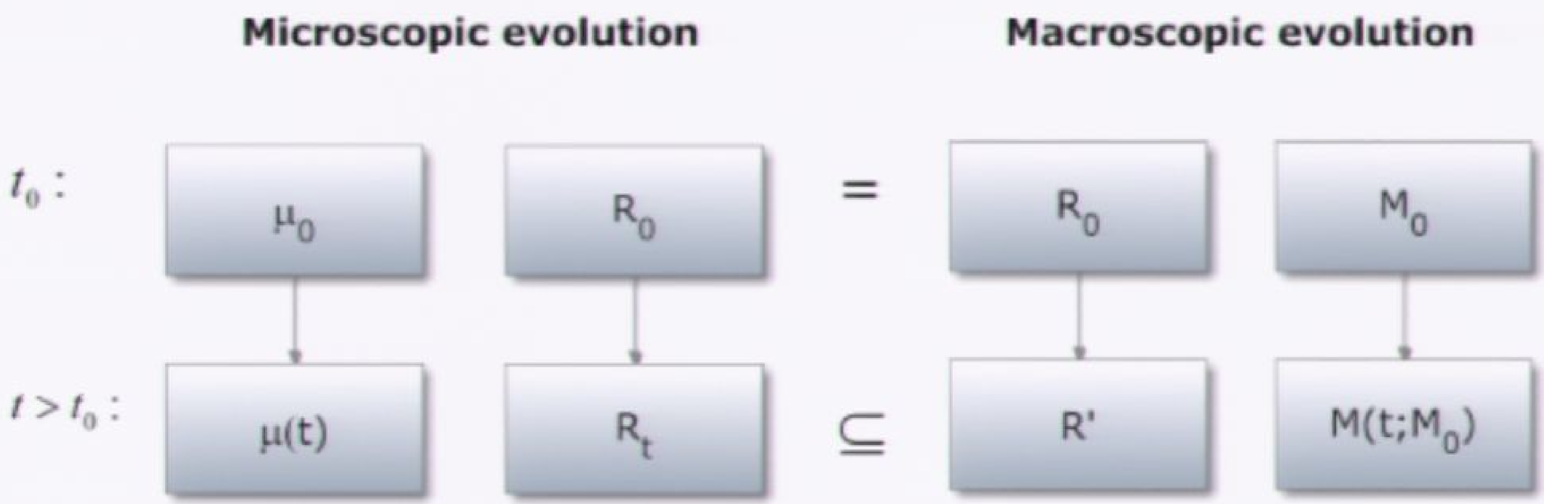
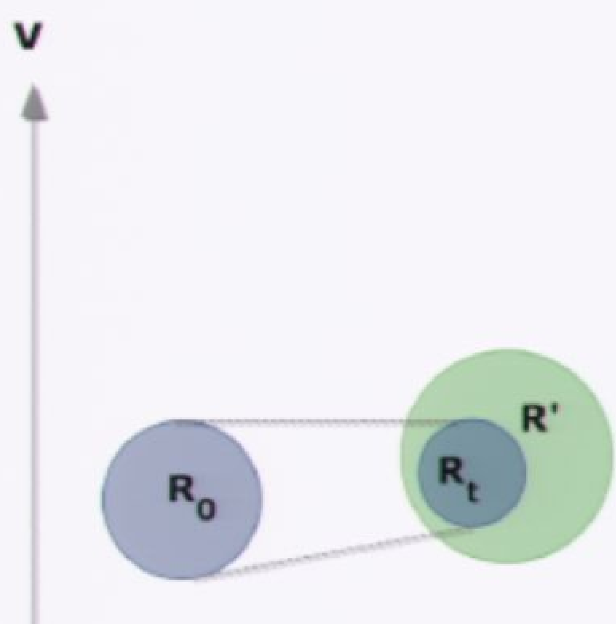
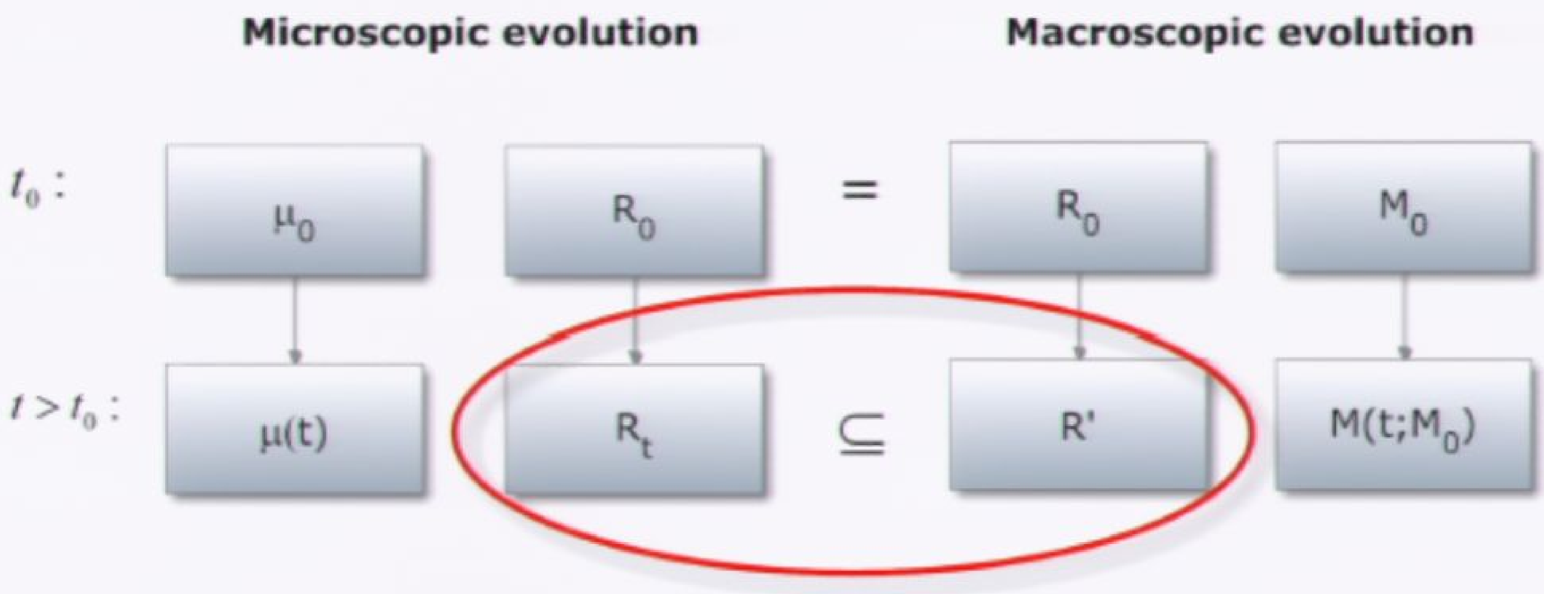
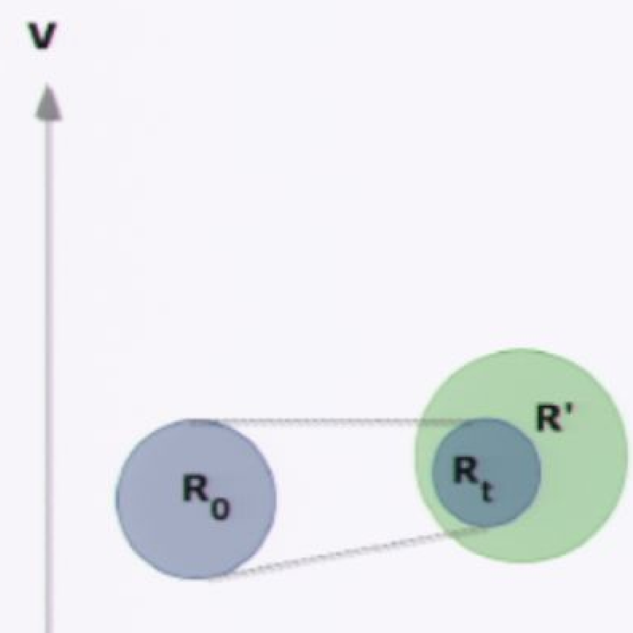




Reproducibility





The Second Law of Thermodynamics

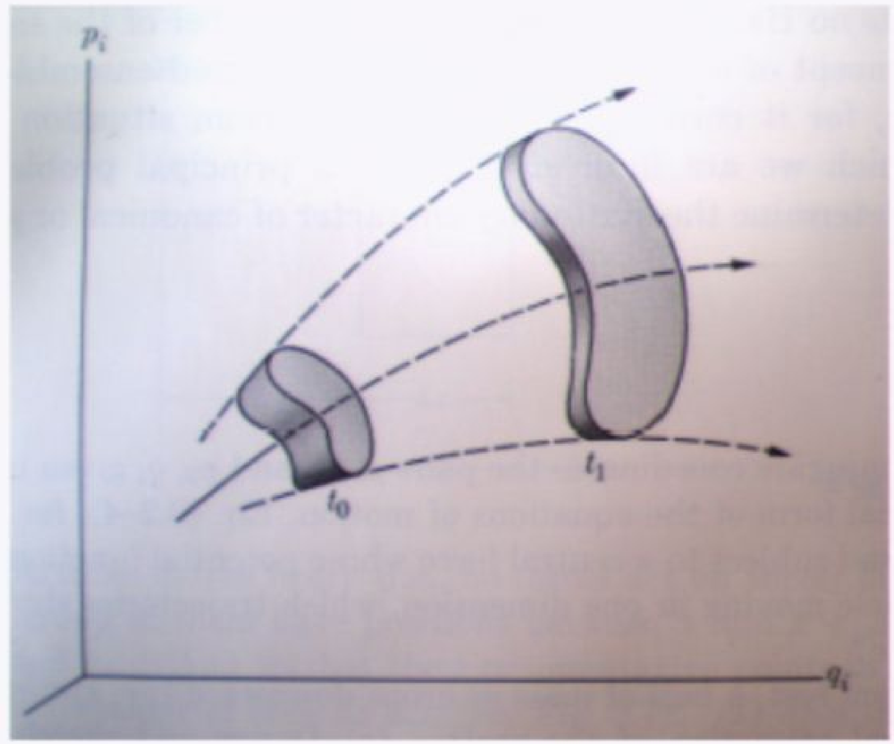
Microscopically:

Liouville's theorem

$$\rightarrow \Omega_{R_0} = \Omega_{R_t}$$

Macroscopically:

$$\Omega_{R_0} \leq \Omega_{R'}$$



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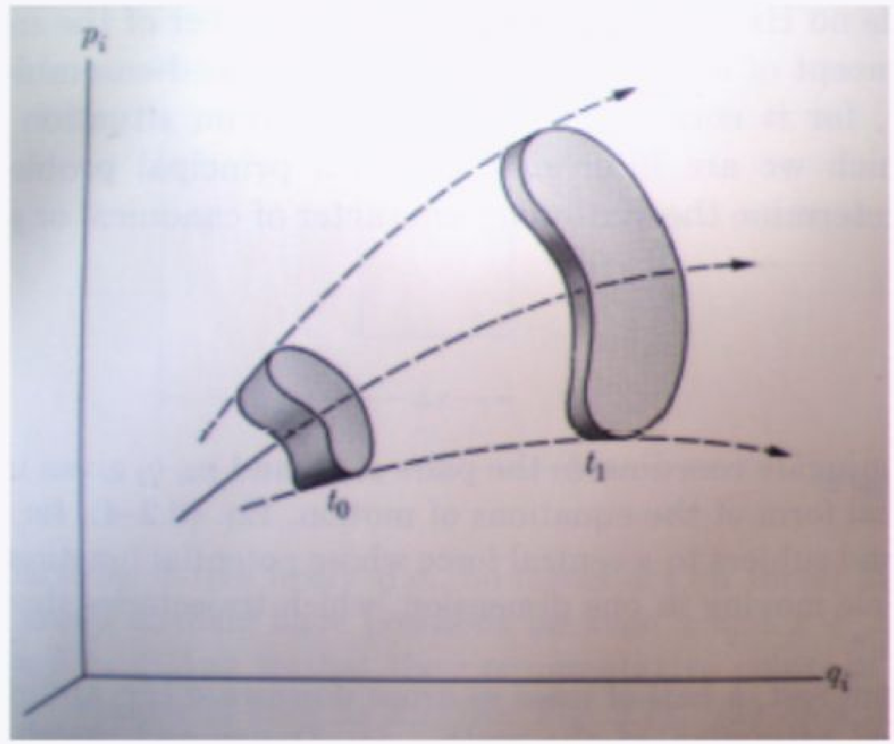


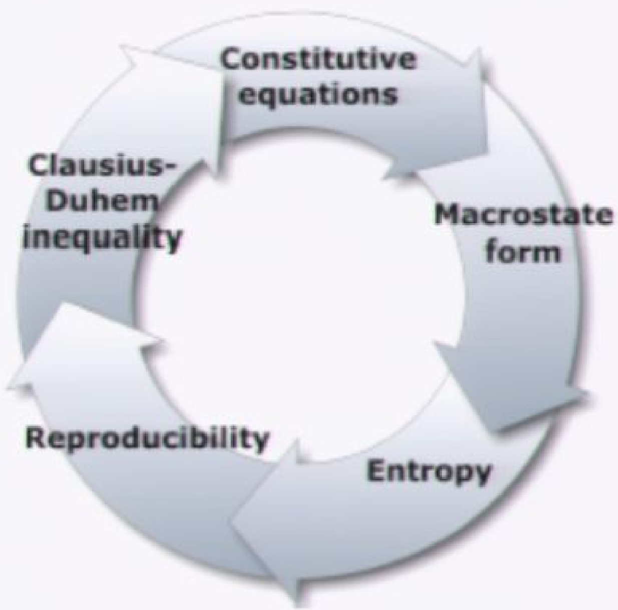
The second law follows from the reproducibility requirement

Conclusions

- Entropy cannot be defined *a priori*, i.e. before the macrostate is completely specified.
- Relation between the role of the Clausius-Duhem inequality in restricting the constitutive equations and the way that states have to evolve in phase space in order to ensure reproducible behaviour.

$$\mu_0 \rightarrow \rho, \mathbf{v}, \theta, u, \mathbf{q}, \mathbf{T}$$

$$\mu_0 + \text{macrostate form} \rightarrow s$$



- The second law must be a restriction on constitutive equations rather than on processes.

No constitutive equations → **No macrostate form** → **No entropy**

No entropy → **No reproducibility** → **No macrocopic theory!**

Thank you!

Reproducibility