Application of the MaxEP Principle to Turbulent Fluid Mechanics + Planetary Systems

Mathematical and Statistical Approaches to Climate Modelling and Prediction,
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Advertisements

1. Co-editor (with Valerio Lucarini) of special issue of *Earth System Dynamics* on “Thermodynamics of the Earth system”

2. Will be co-host (with Roddy Dewar) of a “maximum entropy methods workshop”, Canberra, Australia, Sept. 2011

Meeting on maximum entropy and entropy production-related themes:
- theory
- planetary system dynamics (atmosphere, oceans, mantle, biosphere, etc)
- fluid turbulence + convective heat transfer systems
- cosmology / astrophysics / astrobiology
- biological / ecological systems
- solid mechanics (elastic / plastic / viscous deformation + failure)
Contents

1. Concepts
   - introduction to MaxEP
   - overview of Jaynes’ MaxEnt method
   - application to equilibrium systems → minimise Planck potential

2. Analyses of steady-state systems
   - apply MaxEnt → steady-state position (local, global)
   - role of potential $\phi_{st}$

3. Turbulent flow in a pipe
   - role of MaxEP in single and parallel pipes

4. Exoplanets
   - application to “hot Jupiter” planets
Concepts
Maximum Entropy Production (MaxEP) Principle

“A dynamic flow-controlled system seeks a steady state at which there is a maximum rate of production of thermodynamic entropy”

e.g. earth climate system
Application of MaxEP

Earth Climate System
Paltrridge (1975, 1978):
- 10-box (latitudinal) model of atmosphere-ocean system
- atmosphere, oceanic + overall energy balances → many solutions
- choose heat fluxes which maximise entropy production:
Application of MaxEP

Benard cell

\[ \dot{\sigma}_{sys} \]

\[ \text{Ra} \]

Distance from equilibrium

\[ \text{Total} \]

\[ \text{Conduction Only} \]

Ecosystem

\[ \dot{\sigma}_{sys} \]

Entropy production

Distance from equilibrium

Chemical oxidation (thermodynamic mode)

Bacterial growth (dissipative structure)

(Meysman, 2007)

\[ \therefore \text{MaxEP = unifying principle for flow systems of all kinds} \]
Application of MaxEP

Where does MaxEP come from?
When can it be applied?
Analysis of Probabilistic Systems

Consider any system of discrete entities
e.g. atoms / molecules / ions, quantum particles,
biological organisms, transportation units,
economic agents, social actors, humans

- maximise entropy, subject to constraints
→ inferred (“least informative”) description of system

Boltzmann (1877), Planck (1901) MaxProb principle:
- maximise entropy, subject to constraints
→ most probable position of system
Jaynes’ MaxEnt

Consider a type of probabilistic system (of any kind):

Maximise

$$S_\alpha = -\sum_{i=1}^{S} p_i^\alpha \ln \frac{p_i^\alpha}{q_i^\alpha}$$

relative entropy

subject to

$$\sum_{i=1}^{S} p_i^\alpha = 1$$

normalisation constraint

$$\sum_{i=1}^{S} p_i^\alpha f_r^\alpha = \langle f_r^\alpha \rangle, \quad r = 1, \ldots, R$$

moment constraints

Write Lagrangian, extremise $\rightarrow$ most probable realisation:

$$p_i^{\alpha*} = \frac{1}{Z^\alpha} q_i^\alpha e^{-\sum_{r=1}^{R} \lambda_r^{\alpha} f_r^\alpha}$$

Boltzmann distribution

where $\lambda_r^{\alpha}$ = Lagrangian multipliers

$$Z^\alpha = \sum_{i=1}^{S} q_i^\alpha e^{-\sum_{r=1}^{R} \lambda_r^{\alpha} f_r^\alpha} = \text{partition function}$$
Jaynes’ Relations

Maximum entropy:
\[ S^*_{\alpha} = \ln Z^\alpha + \sum_{r=1}^{R} \lambda_r^{\alpha} \langle f_r^{\alpha} \rangle \]

Minimum potential:
\[ \phi^{\alpha} = -\ln Z^\alpha = -S^*_{\alpha} + \sum_{r=1}^{R} \lambda_r^{\alpha} \langle f_r^{\alpha} \rangle \]

Derivatives:
\[ \frac{\partial S^*_{\alpha}}{\partial \langle f_r^{\alpha} \rangle} = \lambda_r^{\alpha} \]
\[ \frac{\partial \phi^{\alpha}}{\partial \lambda_r^{\alpha}} = \langle f_r^{\alpha} \rangle \]

Legendre transf.:
\[ \gamma = g^{-1} \]
for \[ \phi^{\alpha}(\lambda_1^{\alpha}, \lambda_2^{\alpha}, \ldots) \Leftrightarrow S^*_{\alpha}(\langle f_1^{\alpha} \rangle, \langle f_2^{\alpha} \rangle, \ldots) \]
Interpretation

Most systems: **must** consider changes in entropy within + outside system:

\[
d\mathcal{S}_\text{univ} = d\mathcal{S}_\alpha^* + d\mathcal{S}_\text{ext}^* \geq 0
\]

**Generic second law**

But any external change ⇔ changes in constraints and/or multipliers

\[
d\mathcal{S}_\text{ext}^\alpha = -d \sum_{r=1}^{R} \lambda_r \langle f_r^\alpha \rangle = \frac{d\sigma^\alpha}{\kappa}
\]

**Generic entropy production**

\[
\therefore \quad d\phi^\alpha = -d\mathcal{S}_\alpha^* + d \sum_{r=1}^{R} \lambda_r \langle f_r^\alpha \rangle = -d\mathcal{S}_\text{univ} = -d\mathcal{S}_\alpha^* - \frac{d\sigma^\alpha}{\kappa} \leq 0
\]

\[
\therefore \quad \phi^\alpha = \text{generic, dimensionless, free energy concept!}
\]

Minimum \( \phi^\alpha \) → position of maximum \( \alpha \)th entropy of universe

If constraints can vary, **must** minimise \( \phi^\alpha \), **not** maximise \( \mathcal{S}_\alpha^* \)
**e.g.: Thermodynamic Systems**

\[ p_i = \text{joint prob. that entity has particular contents } f_{ri} \]

\[ \text{e.g. energy level, volume level, nos. of particles} \]

Constraints = mean contents of system \( \langle f_r \rangle \)

(a) **Isolated system**
- fixed contents
- entities = molecules
  - (microcanonical ensemble)

(b) **Open (diffusive) system**
- system surrounded by bath
- entities = entire systems
  - (canonical, grand canonical ensembles)

Apply MaxEnt \( \rightarrow \) equilibrium position of system
Thermodynamic System

e.g. \[ \sum_{i=1}^{s} p_i = 1 \] natural constraint
\[ \sum_{i=1}^{s} p_i h_i = \langle H \rangle \] mean enthalpy

Apply MaxEnt (identify \( \lambda_H = 1/kT \) at const. \( P \))

\[ p_i^* = \frac{1}{Z} e^{-\lambda_H h_i} = \frac{1}{Z} e^{-h_i/kT} \]

\[ S^* = k \ln Z + \frac{\langle H \rangle}{T} \]

\[ k \ d\phi_{eq} = d \left( \frac{G}{T} \right) = -dS^* + d\left( \frac{\langle H \rangle}{T} \right) \leq 0 \]

Min \( \phi_{eq} \rightarrow \) interplay between internal & external changes in entropy:

<table>
<thead>
<tr>
<th>Max ( S^* )</th>
<th>Max ( \sigma_{eq} )</th>
<th>Universal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max ( S^* )</td>
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<td>Driven by ( \Delta S^* \geq</td>
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Summary

- Jaynes’ MaxEnt
  → existing equilibrium thermodynamics

- Minimum $\phi_{eq}$ → infer equilibrium position
  - Massieu (1869), Planck (1932):
    - minimise $k\phi_{eq}$ → “Planck potential” in entropy units
  - Gibbs (1875-1878):
    - assume $T$ constant
    - minimise $kT\phi_{eq}$ → “free energy” expressed in energy units
MaxEnt / MaxProb for Systems Analysis

Contention:
MaxEnt / MaxProb method → **dramatic** simplifications to systems analysis
- thermodynamic context ⇒ generic context
- old + new phenomena
- model closure (?)

Caveats:
- probabilistic, not deterministic (this is **inference** !)
- discard all unnecessary information (e.g. details of dynamics)
MaxEnt Analyses of Steady-State Flow
Steady-State Flow Systems

(a) **Global** (Dewar, 2003, 2005)
Analyse entire control volume
\[ p_i = \text{joint prob. of instantaneous fluxes } j_{ri}(x) \]
around boundary
Constraints = *mean boundary fluxes* \( \langle j_r \rangle(x) \)
e.g. heat, momentum, nos. of particles

(b) **Local** (Niven, 2009, 2010)
Analyse local infinitesimal area element
\[ p_i = \text{joint prob. of instantaneous fluxes } j_{ri} \]
through element
Constraints = *mean fluxes* \( \langle j_r \rangle \) through element
Apply MaxEnt (different entropy) \( \rightarrow \) *steady-state position* of system
MaxEnt Analysis (Local)
(Niven, PRE 80(2) (2009) 021113; Phil Trans B 365: (2010) 1323-1331)
Consider infinitesimal (or small) area element with
- mean fluxes / rates $\langle j_Q \rangle$, $\langle j_c \rangle$, $\langle \bar{\tau} \rangle$
- instantaneous fluxes / rates $j_{Q,I}$, $\{j_N_c\}$, $\bar{\tau}_J$
Maximise flux entropy $S_{st}^*$ → most probable steady-state description of element:

\[
p_i^* = \frac{1}{Z} q_i \exp\left( -j_{Q,I} \cdot \zeta_Q - \sum_c j_{N_c} \cdot \zeta_c - \bar{\tau}_J : \zeta_{\tau} \right)
\]

\[
S_{st}^* = \ln Z + \langle j_Q \rangle \cdot \zeta_Q + \sum_c \langle j_c \rangle \cdot \zeta_c + \langle \bar{\tau} \rangle : \zeta_{\tau}
\]
where $\zeta_r = $ Lagrangian multipliers

Compare (traditional) calculation (de Groot & Mazur, 1984; Bird et al. 2006)

\[
\hat{\sigma} = \langle j_Q \rangle \cdot \nabla \left( \frac{1}{T} \right) - \sum_c \langle j_c \rangle \cdot \nabla \left( \frac{\mu_c}{M_c T} \right) - \langle \bar{\tau} \rangle : \left( \frac{\nabla v}{T} \right)^T
\]
Since constraints are linearly independent, identify multipliers $\propto$ gradients, hence

$$\hat{\mathcal{H}}_{st}^* = \ln Z - \frac{\hat{\sigma}}{\mathcal{K}}$$

where $\mathcal{K} = \text{constant (units of J K}^{-1} \text{ m}^{-3} \text{ s}^{-1})$

Hence must minimise potential:

$$\phi_{st} = -\ln Z = -\hat{\mathcal{H}}_{st}^* - \frac{\hat{\sigma}}{\mathcal{K}}$$

Again have changes of entropy (here $\hat{\mathcal{H}}_{st}^*$) within and outside the system:

<table>
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Only two of these give a local MaxEP principle!
Conclude:

1. Can derive a local conditional MaxEP principle, based on MaxEnt
2. MaxEP is not universal!
    (c.f. minimum enthalpy principle in thermodynamics)

\[
d\phi_{st} = -d\dot{\mathcal{S}}_{st} - \frac{d\hat{\mathcal{G}}}{\mathcal{K}} \leq 0
\]

\[
d\phi_{eq} = d\frac{G}{kT} = -\frac{dS^*}{k} + d\frac{\langle H \rangle}{kT} \leq 0
\]
MaxEnt Analysis (Global)

(Dewar, 2003, 2005 - reinterpreted)

Consider boundary $\Omega$ of control volume, with:
- mean fluxes / rates $\langle j_Q \rangle(\Omega), \langle j_c \rangle(\Omega), \langle \tilde{\tau} \rangle(\Omega)$
- instantaneous fluxes / rates $j_Q(\Omega), \{j_c\}(\Omega), \tilde{\tau}(\Omega)$

Maximise global flux entropy $S_\Omega \to$ most probable steady-state:

$$p_i^* = \frac{1}{Z_\Omega} q_i \exp \int_{\Omega} \left( -j_Q \cdot \eta_Q - \sum_c j_c \cdot \eta_c - \tilde{\tau} : \eta_\tau \right) dA$$

$$S^*_\Omega = \ln Z_\Omega + \int_{\Omega} \left( \langle j_Q \rangle \cdot \eta_Q + \sum_c \langle j_c \rangle \cdot \eta_c + \langle \tilde{\tau} \rangle : \eta_\tau \right) dA,$$

Compare:

$$\dot{S}_\Omega = \int_{\Omega} \left( \langle j_Q \rangle \cdot \frac{1}{T} - \sum_c \langle j_c \rangle \cdot \frac{\mu_c}{M_c T} - \langle \tilde{\tau} \rangle : \frac{v^T}{T} \right) dA$$

$\eta_r$ = Lagrangian multipliers
Identify multipliers \( \propto \) intensive variables along boundary, hence

\[
\hat{s}_\Omega^* = \ln Z_\Omega - \frac{\dot{\sigma}_\Omega}{\kappa}
\]

where \( \kappa = \text{constant (units of J K}^{-1} \text{s}^{-1}) \)

Hence must minimise potential:

\[
\phi_\Omega = -\ln Z_\Omega = -\hat{s}_\Omega^* - \frac{\dot{\sigma}_\Omega}{\kappa}
\]

Again have changes of entropy \((\hat{s}_\Omega)\) within and outside the system

\(\rightarrow\) global MaxEP principle in some cases

**Unresolved questions**

1. How are global and local MaxEP connected?

2. What does a mean mean?
   - in fact “steady state” is anything but steady!
Turbulent Flow in a Pipe
Turbulent Flow in a Pipe


Head loss (friction loss) = pressure loss per unit weight

\[ H_L = \frac{fL}{2gD} \frac{U|U|}{L} \]

Reynolds number:

\[ |Re| = \frac{\rho D |U|}{\mu} \]

Laminar: \( f_{lam} = \frac{64}{|Re|} \)

Turbulent: empirical only!

Smooth: \( \frac{1}{\sqrt{f}} = 2.0 \log_{10}(Re\sqrt{f}) - 0.8 \)

Fully rough: \( \frac{1}{\sqrt{f}} = 2.0 \log_{10}\left(\frac{D}{\varepsilon}\right) - 1.14 \)

General

\[ \frac{1}{\sqrt{f}} - 2\log_{10}\left(\frac{D}{\varepsilon}\right) = 1.14 - 2.0 \log_{10}\left(1 + \frac{9.28}{\text{Re}\left(\frac{D}{\varepsilon}\right)^{\frac{1}{2}}\sqrt{f}}\right) \]

\( f \) = Darcy friction factor

\( g \) = gravitational accel.

\( D \) = pipe diameter

\( L \) = pipe length

\( U \) = mean velocity

\( \rho \) = density

\( \mu \) = viscosity

\( \varepsilon \) = surface roughness
Moody diagram:
Power law: \[ H_L = XQ|Q|^{\alpha-1} \]

with \( X \) = function of pipe and fluid properties (and flow)
\( Q \) = volumetric flow rate
\( 1 \leq \alpha \leq 2 \) indicates flow regime

Entropy production:
\[
\frac{P_L}{\rho g} = \frac{\dot{\sigma}T}{\rho g} = |H_L Q| = |XQ^{\alpha+1}| \geq 0
\]

Dimensionless form:
\[
gamma = \frac{4\dot{\sigma}T}{\pi d\mu g L} = \left| \frac{H_L}{L} \right| \text{Re} = \frac{1}{2} f \left| \text{Re} \right|^3 \geq 0
\]

where \( \text{Ga} = \frac{\rho^2 gD^3}{\mu^2} \) = Galileo number
Plot:
Plot:

Benard cell

Ecosystem

Chemical oxidation (thermodynamic mode)
Bacterial growth (dissipative structure)
Flow in Parallel Pipes
(Flow Constraint)

Laws:
1. Conservation of mass (fluid): \( Q - Q_1 - Q_2 = 0 \)
2. Head losses the same: \( H_{L1} = H_{L2} \)
   \[ \therefore X_1 Q_1 |Q_1|^{\alpha_1 - 1} = X_2 Q_2 |Q_2|^{\alpha_2 - 1} \]

Have 2 equations in 2 unknowns \( \rightarrow \) deterministic
Consider “minimum EP” principle (a la Prigogine):

\[
\min \frac{P_L}{\rho g} = \min \frac{\dot{\sigma} T}{\rho g} = \min \sum_j |H_{Lj}Q_j|
\]

Can prove that this “minEP” principle gives (known) steady state
BUT - requires power law pipes of constant \( \alpha \)

AND - no dependence on \( T \)
\( \rightarrow \) really a minimum power principle

Still have Paltridge MaxEP principle \( \rightarrow \) selects laminar or turbulent flow
Simultaneous effects:

- Locus of non-steady-state turbulent points
- Locus of non-steady-state laminar points

Graph showing:
- Steady-state laminar solution
- Steady-state turbulent solution

Axes:
- \( \frac{\dot{T}}{\rho g} (10^{-8} \text{ m}^4 \text{ s}^{-1}) \)
- \( |Re_{\text{tot}}| / 10^3 \)
- \( |Re_1| / 10^3 \)
Flow in Parallel Pipes
(Head Constraint)

Laws:
1. Head losses the same: \[ \Delta H = H_{L1} = H_{L2} \]
   \[ \therefore X_1 Q_1 |Q_1|^{\alpha_1 - 1} = X_2 Q_2 |Q_2|^{\alpha_2 - 1} \]
2. Heat = work:
   \[ W = \rho g \Delta H \parallel Q_1 + Q_2 = \rho g (|H_{L1} Q_1| + |H_{L2} Q_2|) \]

Again have 2 equations in 2 unknowns → deterministic
Consider “maximum EP” principle (a la Županović):

\[
\max \frac{P_L}{\rho g} = \max \frac{\sigma T}{\rho g} = \max \sum_j |H_{Lj}Q_j|
\]

Can prove that this “maxEP” principle gives (known) steady state
BUT - requires power law pipes of constant \( \alpha \)
AND - no dependence on \( T \)
\( \rightarrow \) really a maximum power principle

Still have the Paltridge principle, but now inverted as MinEP principle \( \rightarrow \)
selects laminar or turbulent flow
Simultaneous effects:

- steady-state laminar solution
- steady-state turbulent solution
- locus of non-steady-state laminar points
- locus of non-steady-state turbulent points
Summary:

Although based on empirical equations, can infer:

1. Single pipe (constant flow rate):
   - Paltridge MaxEP principle \(\rightarrow\) selects laminar or turbulent flow

2. Parallel pipes (total flow rate constraint)
   - Paltridge MaxEP principle \(\rightarrow\) selects laminar or turbulent flow
   - (trivial) MinEP or min. power principle \(\rightarrow\) choose steady state from non-steady state flows

3. Parallel pipes (total head constraint)
   - (inverted) Paltridge MinEP principle \(\rightarrow\) selects laminar or turbulent flow
   - (trivial) MaxEP or min. power principle \(\rightarrow\) choose steady state from non-steady state flows

Planetary Climate Systems

MaxEP Models
- since Paltridge (1975), many $n$-box MaxEP models of climate systems on rocky planets, incl. surface-atmosphere and (sometimes) ocean interactions
- reasonable success (planetary scale): Earth, Titan, Mars
- much less success: Venus

Gas Giants
- no (?) surface interactions \( \therefore \) need different model
- extrasolar planets:
  - many new types (tidally locked “hot Jupiters”; “hot Neptunes”, super-Earths/Venuses)
- data much more sparse
  (intensities not location-specific)

(e.g. HD189733b, Knutson et al. 2007)
Conclusions
Conclusions

1. Concepts
   - introduction to MaxEP
   - MaxEnt algorithm $\rightarrow$ minimise potential function $\phi$
   - application to equilibrium systems $\rightarrow$ use of Planck potential

2. Analysis of steady-state systems
   - apply MaxEnt $\rightarrow$ steady-state position (local, global)
   - minimise potential $\phi_{st}$ $\rightarrow$ conditional MaxEP principle

3. Turbulent flow in a pipe
   - single pipe: laminar-turbulent transition due to MaxEP
   - parallel pipes
     - const. $Q$: Paltridge MaxEP + (trivial) min. power
     - const. $\Delta H$: inverted Paltridge MinEP + (trivial) max power

4. Exoplanets
   - upper atmospheric MaxEP model
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