PSE/CAPE paradigm transition towards “La pensée complexe” in a global world under pressure

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June 14, 2022
Acknowledgments

Pr. Xavier Joulia
and
PSI Team at Laboratoire de Génie Chimique

http://lgc.cnrs.fr
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June 14, 2022
Insatiable Humanity

- Exponentially increasing indicators for global socio-economic development and the structure and functioning of the Earth system

The bleak prospect

• Living safely on earth vs exceeding the liveable limits

© Kate Raworth, author of Doughnut Economics: Seven Ways to Think like a 21st Century Economist, 2017
The bleak prospect

- Facts and evidences are gloomy

Environment  Biodiversity  Climate

Waste (the 7th continent)

Land usage shift
The bleak prospect

- Facts and evidences gloomy

Environment | Biodiversity | Climate
---|---|---

The 6th extinction

The 6th extinction
The bleak prospect

• Facts and evidences are gloomy

Environment

- Biodiversity

A barely livable world

Climate

Extreme events

Environment

Biodiversity

Climate

- Climate

- Biodiversity

- Environment

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The bleak prospect

• Facts and evidences are gloomy (more)

We are responsible
We can act!

inequality

inequity

25% of poor people will die before retiring

Humanity

Resources

Energy

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The bleak prospect

- Facts and evidences are gloomy (more)

Humanity

Resources

Energy

thirsty extraction → depletion
The bleak prospect

• Facts and evidences are gloomy (more)

2019:
100 000 000 oil barils / day
15 898 729 m³/day = 4221 olympic swimming pool
5,84 x 10^{14} KJ (1 BEP = 5861520 KJ)

Every day we consume ~2 tsar H-bomba (1954) = ~8000 Hiroshima bombs
The bleak prospect

• And things will get worse!

(a) Global surface temperature change relative to 1850-1900

°C

Business-as-usual scenario
(SSP5-8.5 Shared Socioeconomic Pathways 5 with RCP8.5)

A barely livable world

Will my PSE activity enable my children to grow up happily to a 100 yrs?

- So, I need to shift my paradigm from cartesianism towards ‘La Pensée Complexe’
  - A **methodological shift** in my science
  - An **epistemological shift** in my philosophy of science
  - A **metaphysical shift** in my representation of the world

⇒ No in the business science-as-usual scenario

⇒ 100 years for my children

My grandmother, 100 yrs old

My three daughters, 17, 20, 23
Preliminary

• **Epistemology**
  - The philosophy of knowledge
    - The study of how what constitutes valid knowledge (Piaget)

• **Paradigm**
  - A distinct set of concepts or thought patterns, including theories, research methods, postulates, and standards for what constitutes legitimate contributions to a field
    - Cartesianism (Descartes)
    - Rationalism (Leibnitz)
    - Positivism (Comte)

• **Constructivism**
  - Educational constructivism (Piaget)
  - Pragmatic constructivism (LeMoigne, Avenier, Morin)

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Preliminary

• Audience homework 1:
  – Identify the phases of my transition curve

• Audience homework 2:
  – build your own transition curve via reflexive thinking!
    • Did you also experience these phases over your career?

Elisabeth Kübler Ross 1969
John Fisher 2012
Preliminary

• A thermodynamic homology* for my personal transition curve

  – Helmoltz «free energy» $F \rightarrow$ Acting capability
    
    $dF = dU - T.dS$

    • $U / internal$ energy $\rightarrow$ my resources (knowledge, skills)
    • $T / temperature$ $\rightarrow$ physical & cognitive mobility

  – $S/total$ entropy for an open system

    $dS = dS_i + dS_e$ with $dS_i \geq 0$ (2nd law)

    • $S_i / internal$ entropy $\rightarrow$ degree of disorganization
      $dS_i \geq 0$ (2nd law) $\rightarrow$ learning needs some effort and dissipates energy
    • $S_e / exchanged$ entropy $\rightarrow$ exchanged information (papers, conference, books, thesis)

*Homology: dissimilar reality; similarity at the conceptual level
Early career
1996 – 2011

The world outside? No need to bother as long as Science goes on.

(Descartes is watching me)
The business-as-usual paradigm

- Cartesianism (Descartes)
- Rationalism (Leibnitz)
- Positivism (Comte)

- "Cogito, ergo sum" → reasoning is the source of knowledge
- The world is real and reasoned.

- Concepts: Faith in disciplinary science approaches, in truth, in logic
- Principles: objectivity, reductionism, causality, exhaustivity
Classical PSE: excellency and innovation

• 15 thrilling years of conventional PSE/CAPE
  – Quest for numbers & excellency
    • Running for fundings usually as Principal Investigator
      – FR fundings: ANR, ATIP,
      – EU fundings: FP6, FP7, H2020
      – Local fundings
      – Industry-backed fundings
    • Industry driven topics
    • Rewards
    • PhD thesis students
    • MSc students,
    • Publications
    • Conferences
    • Books
    • Patents
    • Software tools

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Classical PSE: excellency and innovation

- **PSE/CAPE fields and approach**
  - Topics
    - Tailored computer aided molecular and solvent design
    - Extractive and azeotropic distillation
    - Hybrid energy production plant
    - Thermodynamic modeling
  - Multiscale
    - Molecules → Aggregates → Fluids → Unit operation → Plant → Supply chain
  - Multiple approaches
    - Conceptual design
    - Simulation
    - Optimization
    - Control
    - Scheduling

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Classical PSE: excellency and innovation

- **PSE/CAPE expertise**
  - Modeling
    - Local transport phenomena (heat, mass, CFD)
    - Global mass & energy balance
    - Phenomenological-driven
    - Data-driven (NN)
  - Numerical methods
    - Molecular simulation
    - PDAE & NLAЕ; steady state (NR) & dynamic (RK4, Gear); simulation
    - Stochastic optimisation (MC, GA)
    - Deterministic optim. (NR, LP, MINLP)
  - Thermodynamics
    - SLE, VLE, SLLE, supercritical
    - EOS, $G^\text{ex}$ models
    - Molecule and mixture property prediction
      - Group Contribution, QSAR,
    - Exergy analysis
    - Nonequilibrium thermodynamics

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• **Acting capability ( \( dF = dU - T \cdot dS \) ) is increased**

- As I gain knowledge and expertise, \( dU > 0 \)
- Conferences, reviews, meetings: \( T \) is quite high
- Entropy change is globally ( \( dS = dS_i + dS_e \) ) \(< 0 \)
  - I spend energy for learning, so \( dS_i > 0 \)
  - I publish, give talk, supervise students, so \( dS_e << 0 \)

\[
dF = ( dU - T \cdot dS ) > 0
\]
**Classical PSE: excellency and innovation**

“design method was validated by batch simulation and experiments”

“Computer time was 5.6s for the 2300 variable problem”

“impurity estimate is 135 ppm, compared to 23 ppm measured”

“the total energy consumption was improved by 23.6%”

“it is the first time a thermodynamic model of two demixing aqueous phases is proposed”

“The solvent property matched the target values within a 5% margin”

• But is this meaningful with respect to global changes?
The bleak prospect is there

- Unsustainable living
The fall... 2011 – 2016

Personal introspection
How am I to cope with the world changing outside?

Professional introspection
Is my PSE work meaningful wrt. the global challenges of our world?

(Descartes is still watching me !)
Should I stick to my paradigm?

• Come-on man, be rational!  
  (Descartes is watching me)

  – Reductionnism: rephrase the global questioning into

    How can I incorporate global challenges in my professional activity?

    How can I incorporate environmental and social issues?

• Come-on man, use a systemic/complex approach!
  – Well, call it « limited complexity »

<table>
<thead>
<tr>
<th>Descartes</th>
<th>limited complexity (complicated)</th>
</tr>
</thead>
<tbody>
<tr>
<td>In short...</td>
<td>Cogito ergo sum</td>
</tr>
<tr>
<td>Approach</td>
<td>causality</td>
</tr>
<tr>
<td>Paradigm &amp; Epistemology</td>
<td>rationalism</td>
</tr>
<tr>
<td>Example</td>
<td>any artefact</td>
</tr>
</tbody>
</table>

Descartes is watching me.

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Facing the global challenge

• **Come-on man, be rational!** (Descartes is watching me)

  Decision: Let’s drop the personal introspection and keep the professional one
  • How can I incorporate global challenges in my professional activity?
    - Any problem has a **solution**!
    - I need to set **objectives**!
  • **Solution**: incorporate the three pillars of Sustainable Growth: economic, social, environmental in my activity
Facing the global challenge

• Let's do the best I know in classical PSE:

<table>
<thead>
<tr>
<th>Approach</th>
<th>Technique</th>
<th>Limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Modeling</td>
<td>Multiscale modeling</td>
<td>Not trivial to connect local simulation into global model</td>
</tr>
<tr>
<td></td>
<td>Simulation</td>
<td>Dynamic better but harder than static</td>
</tr>
<tr>
<td></td>
<td>Multiobjective optimization</td>
<td></td>
</tr>
<tr>
<td></td>
<td>multiple-criteria decision analysis</td>
<td>Should I weight factors to take a decision?</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Criteria</th>
<th>Key Performance Indicators</th>
<th>Limits</th>
</tr>
</thead>
<tbody>
<tr>
<td>Economics</td>
<td>Cost analysis</td>
<td></td>
</tr>
<tr>
<td>Environment</td>
<td>Environmental Indicators</td>
<td>Complex &amp; uncertain impact assessment</td>
</tr>
<tr>
<td>Social</td>
<td>Job creation</td>
<td></td>
</tr>
</tbody>
</table>
Some examples of a “cartesian complexity”

- Sust. Growth concern at MACRO scale:
  - A framework of sustainable chemical enterprise model and decision-making process
  - Based on Model driven Engineering & multiscale modeling


- Tentative to develop a framework embedding stakeholders and constraints within a pyramidal and rather rigid chemical enterprise perspective
  - Pro: Explicit stakeholders and constraints
  - Pro: dissociating “financial economy” from “sustainable development and society’
  - Cons: Still a mainstream & rigid vision


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Some examples of a “cartesian complexity”

- **Environmental concern at micro-scale:**
  - Computer Aided bio-solvent design
  - Multiple-criteria decision analysis
  - Model driven Engineering
    - UML2. BPMN
    - SBVR, OCL

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Some examples of a “cartesian complexity”

- Social & environmental concern at MACRO scale
  - MO MINLP goal programming - MS modeling of a bioethanol supply chain
  - Biomass seasonability, geographical availability, biomass degradation, process conversion technologies, product demand

- Economics: cost
- Environment impact = Eco-cost LCA method
- Social benefit = job creation
  - Direct & indirect jobs \( \propto \) process plant size
  - Induced jobs: based on geographical location

Some examples of a “cartesian complexity”

- The technosolutionist illusion “A.I will take care of all”
  - Combining data driven & process engineering physics models for new modeling approaches
- “grey box” Hybrid approach

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My entropy sensor

• **Acting capability is decreasing**
  – I still gain knowledge and expertise, \( dU > 0 \)
  – \( T \) remains high as I delve deeper into PSE/CAPE
  – Entropy change is globally \( (dS = dS_i + dS_e) >> 0 \)

  *I’m in a state of cognitive dissonance!*

• My energy is dissipating into states inaccessible for action → entropy is growing
  – I still spend energy for learning, so \( dS_i > 0 \)
  – \( dS_e \sim 0 \) since I struggle to organize my thinking and to devise some professional action compatible with sustainable growth and hopefully global issues.

So, \( dF = (dU - TdS) < 0 \)
Facing the global challenge

• Cartesianism → cartesian systemic complexity:

I do the best I know, but is that enough?

→ No

⇒ So, I need to shift my paradigm

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depressing situation; much like in jail
→ I need to shake the bars of the cage

Shattering & shifting the frame
Bifurcating from cartesianism to ‘La Pensée Complexe’
Bifurcation starts with an insignificant event

- **April 2014: workshop “Acting-Thinking in Complexity”**
  - Important notice: ‘in’ complexity rather than ‘the’ Complexity

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<th>general complexity</th>
<th>subjective complexity</th>
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<tr>
<td>Approach</td>
<td>causality</td>
<td>Thinking ‘the’ complexity</td>
<td>Thinking ‘in’ complexity</td>
<td>Acting-Thinking ‘in’ complexity</td>
</tr>
<tr>
<td>Paradigm &amp; Epistemology</td>
<td>rationalism</td>
<td>constructivism</td>
<td>materialism</td>
<td>subjectivism</td>
</tr>
<tr>
<td>Example</td>
<td>any artefact</td>
<td>a plane</td>
<td>the mobility issue</td>
<td>Should I move?</td>
</tr>
</tbody>
</table>

- **Constructivism:**
  - Knowledge of reality is a human construct using science but also experience, intuition
    » La "pensée complexe" (Morin) "Agir-Penser en complexité" (LeMoigne) Avenier
    - Interdisciplinarity, subjectivity, path dependency, partiality and uncertainty
    - Principles: interrelation, irreductionism, hologrammatism, recursivity, bifurcation, non-linearity, emergence, dialogic, ecology of action, self-organisation, autocriticism, no forecasting...

- Other similar approach:
  - The “School of Palo Alto” on systemic and relational approach

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Rising at last! the paradigm shift

Confidence in the future
Acting – thinking in complexity

Morin  LeMoigne  Avenier

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Three necessary shifts

1. **A metaphysical shift**
   - Like every living creature, I walk in a changing world along a path towards the ever farer horizon

2. **An epistemological shift**
   - Pragmatic constructivism of LeMoigne & Avenier
     - **Concepts:**
       - Interdisciplinarity, subjectivity, path dependency, partiality, uncertainty, experiential learning
     - **Principles of La Pensée Complexe:**
       - Interrelation, irredutionism, hologrammatism, recursivity, bifurcation, non-linearity, emergence, dialogic, ecology of action, self-organisation, autocriticism, no forecasting...
Three necessary shifts

3. **A methodological shift**

   - Experiential learning whenever possible and a new research focus
   - Study socio-ecological transitions
     - Setting a dynamic perspective on complex ecosystems evolution
practicing *in complexity: making connections*

- Exploring non-financial economic theories
  - micro
    - ....
  - Meso
    - Geels’ MLP: A multilevel perspective on transition pathways in sociotechnical regimes.
  - MACRO
    - N. Georgescu Roegen: “The entropy law and the economic process” / “tomorrow, degrowth”
(non financial) economical theories

• Meso scale: Geels’ multilevel perspective on transition pathways in sociotechnical regimes.
  – Multi-actor networks
  – Multi-level perspective
    • Niche → where innovation starts
    • Regime → where activity is operant
    • Landscape → surrounding context
  – 5 transition pathways
    • Transformation
    • Reconfiguration
    • Technological substitution
    • De-alignment
    • Re-alignment

F.W. GEELS, Causality and explanation in socio-technical transitions research: Mobilising epistemological insights from the wider social sciences. Res. Policy, 51, 2022
(non financial) economical theories

- **MACRO scale: Nicholas Georgescu-Roegen**
  - 1971: The entropy law and the economic process
    - In french: Demain la décroissance = "tomorrow, de-growth"
  - His theoretical claims:
    - Physical limits on earth resources impact the economic process
    - Any economic process is an open system as in irreversible thermodynamics
    - According Thermodynamics’ second law, sustainable economic process means that degrowth is desirable
  - A leading contributor of bioeconomics
    - based on describing economic activity via ‘flow-fund’ (+stock) approach
    - quite analog to mass and energy balances!

\[
\begin{bmatrix}
Q(t); R(t); I(t); M(t); W(t); L(t); K(t); H(t) \end{bmatrix}_0
\]

avec, pour les fonds, \(L\) : la terre; \(K\) : le capital; \(H\) : les hommes et, pour les flux, \(Q\) : la quantité de produit; \(R\) : ressources naturelles; \(I\) : inputs intermédiaires; \(M\) : maintenance du capital; \(W\) : les déchets.

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(non financial) economical theories

• MACRO scale: Prospective scenarios
  – Macro-economy prospective simulation
    • (sequel from fund – flow modeling)
      – The 1985’ ATHEMA model for the prospective analysis of territorial economy by Ph. Courrege
        » Physical economy model based on fund – flow description at the local scale
        » activity described following the NAF and NACE economy activity classification
        » A LP framework solved with GAMS over a 20 year time horizon scenarios
  – Design of Hybrid renewable energy systems
    – MILP framework solved with ILog

practicing in complexity: making connections

• Exploring social theories of change
  
  – Micro
    • Individual behavior is what matters and they aggregate to make society
  
  – Meso
    • Clustering mechanism:
      – Groups express values and devise rules in which individual trajectory evolve
        » Cursus, social class, ...
    • Lockdown mechanism:
      – Cluster interacts, power relations, self organized system
    • Inertia mechanism:
      – Path dependency; regulations and norms; technology, infrastructure
  
  – MACRO
    • Society / large number scale behavior
      – Social entropy theories of disorder
Some examples for tackling social issue

- **MACRO scale**: Establishment of collaborative networks
  - how to increase acting capability?
- A model-driven engineering approach combined with thermodynamic analogy

**Context** is described by state variables
- **opening** (Temperature) presence of competitors, partners, clients and informational/physical connections, [ability to a move]
- **easiness** (Pressure) legal, cultural and financial frame [constraint to a move]
- **widthness** (Volume) market size. [size]

Goal: to go to liquid state where ‘stakeholders are neither frozen (solid) nor in chaos (gas); to gain acting capability

Virial EOS: \( PV/(nRT) = 1 + B(n/V) + C(n/V)^2 \ldots \)
Some examples for tackling social issue

• **Meso scale: The Maelia® Integrated Assessment and Modelling platform**
  
  – Modelling the social-ecological systems at the farmer scale.
    
    • A multi-agent platform
    
    • For assessing the environmental, economic and social impacts of agricultural activities, transformation and recycling of biomass, natural resource management strategies (e.g. water) and global (demography, dynamics of land cover and climate) changes.


http://maelia-platform.inra.fr/
Some examples for tackling social issue

- **micro scale: Soclab: a framework simulating power games in social organizations**
  - based on Le Crozier & Friedberg's sociology of organized action / theory of actor-network
    - Postulate: organizational phenomena are constructed by individual activities and behavior

- **A Model-driven engineering approach**

- **Modeling of “how stakeholder’s capability is impacted by the +/- variation of each factor”**
  - e.g. increase river flow by opening dam lock makes farmers happy

- **Multiagent modeling for playing the social game of power relationships**
  - e.g. managing river resource
    - *What is the best compromise (overall capability)?*
    - *Which actors win? Loose?*
    - *What is the acting capability of each actor?*

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My grandmother, 100 yrs old

Conclusion: The new HORIZON – EUROPE
Some examples on the horizon

• From a business-as-usual approach
Some examples on the horizon

• Towards a participative co-building and evaluation

A. ROTH, participative decision process. 2020

LGC

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Some examples on the horizon

- Towards a participative co-building and evaluation


Some examples on the horizon

• Mixing viewpoints
  – Farms: architecture
  – Farmer: stakeholder-oriented
  – Farming: dynamic process oriented

• Taking care of regulations
  – The five square diagram of activity
• Acting capability is increasing again!
  – I still gain knowledge and expertise, \( dU > 0 \)
  – \( T \) remains high as I explore new disciplines
    • Macroeconomy
    • Social entropy theories
  – Entropy change is globally ( \( dS = dSi + dSe \) ) < 0
    • I’ve made peace with myself
      – I still spend energy for learning, so \( dSi > 0 \)
      – \( dSe < 0 \) since I have found new ways to disseminate knowledge, to conduct research....

So, \( dF = (dU - T.dS) > 0 \)
Guidelines & Conditions of change

• Be bold! think & act
  – Practice “acting-thinking in complexity”
    • Connect, link, join, relate
    • Question the question
      – Reformulate the problem to be explored
      – Investigate contexts of any subject
      – Reveal implicits and untold
    • Pay attention to weak signals and feedback to adjust your progress along the path
    • Value the path more than the “expected result” so as to reach a ‘satisfactory result’
      – Do it with other people
      – Accept uncertainty
      – Accept contradiction
      – Redefine ways, means and ends
      – Bifurcate if necessary

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Guidelines & Conditions of change

- **Shift!**
  - **Metaphysical shift**
    - Reassess your relationship within the current world
  - **Epistemological shift**
    - Shift from cartesianism to pragmatic constructivism
  - **Methodological shift**
    - Act on what is meaningful
      - Act on what matters for you and for the socio-ecological transitions
    - **Look-up**
      - Drop excellency, h-factor as the ruling mark
      - Shift from economy-first towards more environment and social
      - Value alternative ways of evaluating research activity
  - Build a collective environment favorable for change
    - Discuss with colleagues and family
      » *Join academic activist groups*
    - Practice with human beings, not just with computers:
      » *Interdisciplinarity, low-profile on your expertise*
      » *Participative science with non-expert stakeholders*
As I walk along the uncertain path ahead, I’m confident that research approach embedded in La pensée Complexe is heading towards truely sustainable solutions meaningful for me
A moving path towards future

Confident and resolute

Backpack checklist

- Knowledge, methods & tools
- Paradigm « La Pensée complexe »
- A novel metaphysic (world perception)

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