

Notes

The following notes might seem disproportionate when compared to the lack of any specific commentary of [18]. This might be justified as follows:

▷ The present article is not easy – but it is at the core of Thom’s work on catastrophes, whose terminology and spirit owe much to the situations considered here. ⁽¹⁾

▷ It is not purely mathematical like [18], and some mathematicians might, like M.C., have difficulties grasping what it is about in treatises of physics. ⁽²⁾

For background on catastrophes, the reader is referred to [47] or [70], [135], respectively in volume II (p. 281) and this volume (p. 35 and 407).

1. Thom generally calls “metabolic models” the fields of “internal” dynamics (M_x, X_x) parametrised by the points x of an “external” space B , also named “control space”. The “internal/external” dialectic is constitutive of the catastrophist models. Thom’s “static models” are those whose internal dynamics are gradient (see section II.A.1 in the sequel of his article). In [47], [70, section 2.7] (and part of the sequel), the fibration over B is trivial, namely, the projection $B \times M \rightarrow B$.

2. $\omega(m)$ denotes the positive limit set of the trajectory starting at $m \in M$.

3. Recall that an ϵ -homeomorphism is a homeomorphism of a metric space that moves each point by less than ϵ .

4. There is a paper by Newhouse and Palis in the proceedings mentioned in the footnote (Academic Press, New York, 1973) but Thom must have referred to S. Newhouse: *Diffeomorphisms with infinitely many sinks*. *Topology* **13** (1974), pp. 9–18. A more recent avatar of Thom’s conjecture is the *Palis conjecture*:

There is a C^r , $r \geq 1$, dense subset V of dynamical systems on any compact manifold that exhibit a finite number of attractors whose basins cover Lebesgue almost all of the manifold. ⁽³⁾

⁽¹⁾ For instance the name *Maxwell set*. We have postponed to Appendix 2 hereafter the discussion of the stratified structure of the functional “Maxwell set” introduced in [72].

⁽²⁾ Hence our Appendix 1, a short “self-contained” introduction to classical thermodynamics.

⁽³⁾ J. Palis: *A global view of dynamics and a conjecture on the denseness of finitude of attractors*, in *Géométrie complexe et systèmes dynamiques* (Orsay, 1995). *Astérisque* **261** (2000), pp. 335–347.

Our (partial) formulation comes from C. Bonatti, L.J. Díaz and M Viana: *Dynamics Beyond Uniform Hyperbolicity*, *Encyclopaedia of Mathematical Sciences* **102**, Springer (2005).

The conjecture does not contradict Newhouse's result asserting the existence of a large set of dynamics with infinitely many sinks, for this set is unlikely to be open. Thom's point is that Newhouse's result prevents the "Thom-Palis" set from being open, which makes the study of "metabolic models" extremely difficult in general.

The fact that attractors can have a complicated internal topology is essential, as this is how Thom proposed to interpret *functions* in Biology and *semiotic content* in semiolinguistics: the unfoldings of the unstabilities of attractors generate the morphologies or the structure (the syntax), whereas the topology of the attractors models the functions or the semiotic contents (semantics).

The list of talks at the Thom Seminar from 1965 on (see the end of this volume) shows his considerable interest in dynamical systems.⁽⁴⁾

5. Read $b \in B$. In the sequel, the points b are also called x .

6. The first definition of a state as a section σ means that some transient instantaneous state $m = \sigma(x) \in M_x$ is selected for *all* $x \in B$.

The definition of the *set-valued* map $\tilde{\sigma}$ is more daring, as it does not exclude "catastrophe points" $x \in B$ at which σ jumps from one attractor basin to another – at such points, the set $\tilde{\sigma}(x)$ is not so obvious.

The "metabolic" models are limits of slow/fast systems with two time scales, where the internal dynamics (in the fibres M_x) are infinitely fast and their evolution with respect to $x \in B$ is infinitely slow in comparison – which raises the problem of equilibrium points of the fibre dynamics, at which everything is infinitely slow. If the instantaneous state $\sigma(x) \in M_x$ lies in the basin of a structurally stable attractor A_x then it is "immediately projected" onto A_x and the internal state $\tilde{\sigma}(x)$ is A_x .

In the sequel (section II.B.), Thom suggests that external dynamics can be generated by "auxiliary couplings".

7. Read $\mathcal{D}(M)$ or $\mathcal{D}(M_b)$ instead of $\mathcal{D}(N)$.

8. Here, F is not an attractor. Attractors are no longer named F , but A .

9. The notation $t > t(x)$ means that one considers a *process*, *i.e.*, a time-dependent path in external space B . "Metabolic" models involve *adiabatic* processes, where the external time t is infinitely slow with respect to the internal time (see note 6).

⁽⁴⁾ Thom [320] acknowledges that Grothendieck's seminar was much more "popular" than his, which nevertheless prompted the renewal of dynamical systems in France.

10. Here U is a neighbourhood of x in B and no longer a neighbourhood of some internal attractor.

11. Physicists definitely call it a *rule*. Though not easily linked to the idea of competing attractors for dynamical systems, it has to do with the *tunnel effect* where a quantum system, lacking energy to “jump”, nevertheless escapes relative minima of the potential to reach its absolute minimum. Despite Thom’s reluctance about Maxwell’s rule, he describes cut-loci [72, this volume p. 125] and even frontiers between tectonic plates [120, 168, this volume p. 357 and 497 respectively] as Maxwell sets. He also suggests [71, p. 80] that Maxwell sets of conflict between four stable regimes appear in the Plateau problem⁽⁵⁾ and in the disposition of cellular walls.⁽⁶⁾ A good introduction to Maxwell sets can be found in [135], this volume p. 407.

12. This very elliptic paragraph requires explanations; apparently, Thom never bothered to detail them because he found them mathematically trivial – which, to some extent, they are, as we shall see in Appendix 2, written in the spirit and with the notation of [72].

13. See our Appendix 2, and Appendix 3 for Thom’s paragraph 3. *Bifurcation strata*.

14. This *critical point* in the sense of phase transitions (and not in the geometrical sense) is the point in parameter space Ouv at which the two phases (liquid and gas) become indiscernible, meaning that it is the end of the curve $u < 0, v = 0$ separating them.⁽⁷⁾ These two phases correspond to the competing minima with respect to x of the potential, one of which collides with the local maximum and disappears at the *critical point*. The parameters u, v of the universal unfolding are (local) functions of the “physical” parameters T, P whereas the state variable x is a (local) function of T, P and the volume – somewhat unfortunately also called v , the notation V of our Appendix 1 being used for the potential. . .

15. This “chemical potential” c is the Gibbs free energy, see our Appendix 1.

⁽⁵⁾ With the angles of the barycentric subdivision of the regular tetrahedron (Jean Taylor).

⁽⁶⁾ Which, as observed by d’Arcy Thompson, are surfaces with constant mean curvature like the bubbles in a bottle of shampoo. The angles are again those of the barycentric subdivision of the regular tetrahedron, but no one so far seems to have seen these as Maxwell sets.

⁽⁷⁾ With the notation of Appendix 2 hereafter, this curve is the stratum $\rho_V^{-1}(U_1)$ of the Maxwell set, which Maxwell set is called a *phase diagram* in thermodynamics, see our note 16.

16. For this part, we recall a few classical concepts of thermodynamics, which Thom uses more or less implicitly (see Appendix 1 for a more formal presentation). The macroscopic state of a chemical species like water, assumed at thermodynamic equilibrium, can be described by three state parameters: absolute temperature T (intensive variable⁽⁸⁾ conjugate to the extensive variable S named entropy), pressure P (intensive variable) and volume V (extensive variable conjugate to P). When the system is at equilibrium, these three parameters are related by a *state equation* $\partial_V \Phi(T, P, V) = 0$, defining the *state surface* in (T, P, V) -space—here Φ is a thermodynamic potential, the Gibbs free energy, see Appendix 1.

In general V is considered the internal variable and (T, P) the external one. The catastrophe points at which phase transitions occur form a stratified closed subset of codimension 1 in (T, P) -plane, called a *phase diagram*. It consists of curves along which two phases coexist (transitions “of order 1”, conflict strata of codimension 1) stopping at isolated points (strata of codimension 2): triple points at which three phases coexist (for water, $T = 273.16^\circ \text{K}$ and $P = 0.006 \text{ atm}$) and critical points at which two phases become indiscernible (for water, $T = 647^\circ \text{K}$ et $P = 218 \text{ atm}$). The critical point is called a transition “of order 2”; there, the difference of volume between liquid and gaseous states vanishes and the fluid possesses very special properties such as “critical opalescence” (the density fluctuations become macroscopic and the two phases mix up in a fractal, milky way).

Beyond the critical point there is only one phase, in a “supercritical” state. Thus, in external space (T, P) , there are paths *going around* the critical point and enabling to pass continuously from one phase to the other. This phenomenon plays an essential role in Thom’s ethological models (“confusion of actants”).

At the critical point, the microscopic behaviour of the fluid is so singular that the formalism of dynamical systems may not apply, so physicists use statistical physics instead. However, Thom deals with the problem without leaving dynamical systems.

Classically, near the critical point (T_c, P_c, V_c) , plane sections of the state surface, namely the isotherms ($T = \text{constant}$), the isobars ($P = \text{constant}$) and the isochores ($V = \text{constant}$), show that the projection $(T, P, V) \mapsto (T, P)$, restricted to the state surface, has a cusp singularity at the critical point.

⁽⁸⁾ Independent of the size of the system, whereas extensive ones are additive for subsystems.

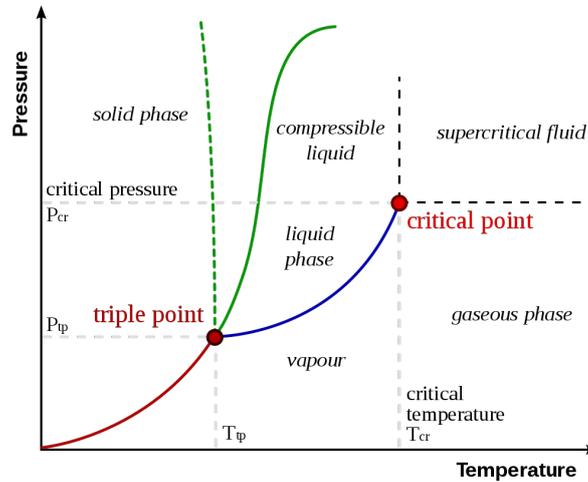


FIGURE 1. The dotted green line represents the (exceptional) case of water

Thus, near (T_c, P_c, V_c) , the critical values of this restricted projection⁽⁹⁾ form a cuspidal curve; if (T, P) lies inside this curve, there are (still locally) three points of the state surface projecting to (T, P) : two local minima of $\Phi_{T,P} : V \mapsto \Phi(T, P, V)$ and a maximum in between. Each minimum corresponds to a phase (here, liquid or vapour) and, according to the Maxwell rule, the line (in blue on Figure 1) along which the corresponding minimal values of Φ are equal separates them neatly. As mentioned by Thom, the phase corresponding to the higher minimum (metastable state) can persist but then the jump to the lower minimum will be more brutal, as it corresponds to a jump of the Gibbs energy Φ .⁽¹⁰⁾ This will never occur on the cusp itself (“perfect delay”), but at most on the *spinodal curve* inside it, where molecular agitation forces the jump.

If Maxwell’s rule holds, the line along which two phases coexist (red, green or blue on Figure 1) is obtained by replacing the isotherms by isotherms with a step, chosen so that the areas A and B in Figure 2 are equal – see Appendix 1.

Figure 3, representing the isobars with step that express Maxwell’s rule (see Appendix 1), shows the gap between V_L and V_G for $P < P_c$.

In this context, the symbol ρ traditionally denotes the molar volume V/n .

⁽⁹⁾ Apparent contour of the state surface in the V -direction, consisting of those (T, P) such that $\partial_V \Phi(T, P, V) = \partial_V^2 \Phi(T, P, V) = 0$ for some V .

⁽¹⁰⁾ Explosions occur if a cup of boiling water is extracted at once from a microwave oven.

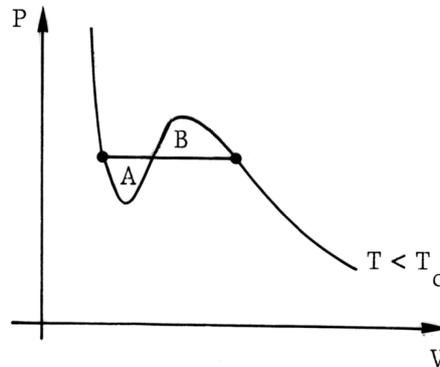


FIGURE 2

The power law in $(T - T_c)^{\frac{1}{2}}$ for V to which Thom refers (in fact $|T - T_c|^{\frac{1}{2}}$ as one considers $T \leq T_c$) tells us that the *critical exponent* of volume is $\frac{1}{2}$. It follows from the hypothesis (introduced by Lev Landau for magnetic transitions of order 2) that the thermodynamic potential (for example G) is still differentiable near the critical point. The dotted parabola in Figure 3 is an illustration (obtained by Landau via Taylor expansions). But Landau's approximation is fundamentally wrong (at least in dimension 2 and 3) for it neglects fluctuations ("mean field" theory) which, on the contrary, become "giant" (macroscopic) at the critical point.

The Fisher law in $(T - T_c)^{\frac{1}{3}}$ to which Thom refers is part of an impressive set of experimental data on critical exponents⁽¹¹⁾ and their scaling laws, at the origin of the theory of second order phase transitions via the *renormalisation group*. This theory, a true revolution in statistical physics and quantum field theory, was set up for phase transitions at the beginning of the 1970's by Kenneth G. Wilson (1971), following a pioneering article of Leo P. Kadanoff (1966) about the Ising model. It is contemporary with Thom's reflections.

17. Read $\frac{1}{2}(\rho_L + \rho_G) = \rho_C(1 + a\Delta T_r)$, where $\Delta T_r = 1 - \frac{T}{T_C}$. The rectilinear diameter law was induced by the physicists L.P. Cailletet and E.O.J. Mathias from their work (initiated in 1866 at the ENS and Sorbonne) on the critical

⁽¹¹⁾ The critical exponents define the laws in powers of $\Delta T = |T - T_c|$ of the main parameters of the system near the critical point, for example (one should adjust signs and constant factors): $(V - V_c) \sim \Delta T^\beta$ and $(P - P_c) \sim (V - V_c)^\delta$. The classical values provided by the Landau model, to which Thom refers, are $\beta = \frac{1}{2}$, $\delta = 3$.

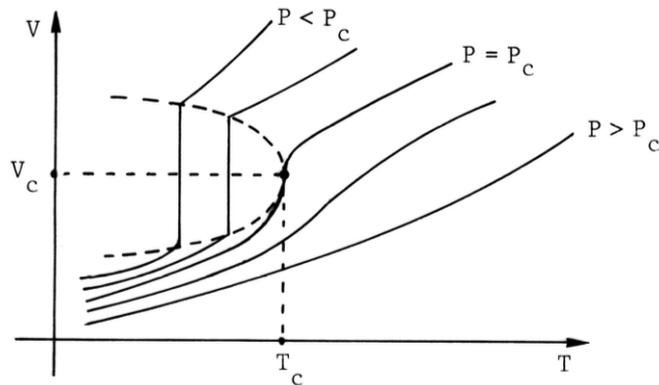


FIGURE 3

points of ethylene, CO_2 , SO_2 , benzene, acetic acid, ether, methanol, *etc.* It avoided the extremely difficult measure of the critical density ρ_C (T_C and P_C are much more accessible). Though only a first order approximation, it turned out to be very useful. The form used by Thom has been obtained by Mathias and H. von Jüptner.

18. This is yet another reference to the experimental results that led to the renormalization group.

19. In Thom's Figure 7, due to the form of f' , the origin should be placed at the maximum.

20. Read s instead of Δ and $f = \frac{1}{4}x^4 - \frac{1}{3}sx^3 + \frac{1}{2}px^2$.

21. The coefficients in the formulae are wrong but the reasoning is not. Read

$s = \frac{3}{2}(c_1 + c_2)$, $p = \frac{1}{2}(c_1^2 + c_2^2 + 4c_1c_2)$, $\lambda = \frac{1}{2}c_1c_2(c_1 + c_2)$, $c_1 + c_2 = \frac{2}{3}s$, hence $p = \frac{2}{9}s^2 + c_1c_2$, $c_1c_2 = p - \frac{2}{9}s^2$, $\lambda = \frac{1}{3}s(p - \frac{2}{9}s^2)$, and

$$(c_1 - c_2)^2 = (c_1 + c_2)^2 - 4c_1c_2 = \frac{4}{9}s^2 - 4(p - \frac{2}{9}s^2) = \frac{4}{3}s^2 - 4p.$$

22. The Clapeyron formula represents the slope of the Maxwell stratum $P_{Max}(T)$ of liquid/gas coexistence, traditionally formulated under the form

$$\frac{dP_{Max}(T)}{dt} = \frac{1}{T} \frac{H_G - H_L}{V_G - V_L},$$

where H is enthalpy (along the Maxwell stratum, before the critical point, the two phases do not have the same enthalpy, hence a transition enthalpy $H_G - H_L$).

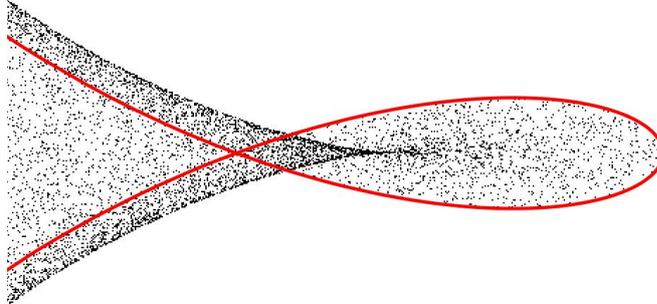


FIGURE 4. The image sent by Michael Berry.

23. The following paragraphs are the turning point of the article. Thom introduces the stratum γ of fold bifurcations around the Maxwell stratum and displaces it inside the cusp. Classically, on the side of this separatrix where some phase 1 dominates, the other phase 2 is virtually present, accessible under exceptional experimental conditions until the limit consisting of the spinodal curve, beyond which the minimum m_2 has too small a basin to be physically realisable. It seems that, on the following page, Thom proposes a complementary model in which the spinodal curve would not be merely a narrowing of the classical cusp preserving the critical state, but a deformation of the cusp with a loop whose interior defines physically forbidden states near the critical point.

24. See note 15. The van der Waals state surface is defined by $\partial_v c(T, p, v) = 0$.

25. Replace x by z .

26. The curve to which Thom refers resembles a strophoid. The reference to the cuspidal caustic in “Topological models in biology” (see [52], 1969, vol. II, p. 371) is very interesting. We have asked Sir Michael Berry, a specialist of caustics who was very close to René Thom, to comment on this second curve around the cusp. We thank him for his answer:

“It is not a caustic. In simple language, it is a shadow boundary. It arises because in any experiment the range of the state variables is finite; therefore the additional curve is an edge effect, where the region that is mapped cuts off. In the language of optics, this cutoff is described as a finite pupil. Another source of cutoff is if only the minimum is plotted, rather than all the critical points; this could be relevant for the Riemann-Hugoniot shock, rather than optics.”

“ [Michael Berry has sent us the image of Figure 4] of an optical caustic where the state space (initial wavefront) is restricted by a circular aperture. The red curve is the image of the boundary of the aperture (pupil). It is different from Thom’s image, because the space between the arms of the red curve inside the cusp is filled with light ; in Thom’s case this region is empty, because it is formed only by the minimum-action rays (not saddle and maxima as in optics).”

27. It seems that x means $E - E_c$ in the formula for $S - S_c$ and $\rho - \rho_c$ in the formula for Z . Thom identifies ρ with V and V with E in Clapeyron’s formula. Moreover, Z is identified to the previous $z = d - \bar{h} \dots$

28. With respect to the initial equation $\mu_i = A_i Z^2 + B_i Z^3 + \dots$, notational coherence implies $\mu_G = \frac{\mu_1}{\cos(\theta_1)}$ and $\mu_L = \frac{\mu_2}{\cos(\theta_2)}$, $\frac{K}{4} = K a^2$, $\frac{K'_1}{6} = 2K a b + K_1 a^3$.

29. If L/G means “ L or G ”, Thom writes

$$x_{L/G} = v_{L/G} - v_C \quad \text{and} \quad x_{L/G} = \rho_{L/G} - \rho_C, \quad x_L \leq 0, \quad x_G \geq 0, \quad x_C = 0.$$

In the sequel, he also uses the notation $x_{L/G} = V_{L/G} - V_C$.

30. Read $T = K x_G^3 (1 + \frac{K'_1}{K} x_G^2)$.

31. With T as in Note 30, read

$$\begin{aligned} x_G &= \left(\frac{T}{K}\right)^{\frac{1}{3}} \left(1 - \frac{K'_1}{3K} \left(\frac{T}{K}\right)^{\frac{2}{3}}\right) = \left(\frac{T}{K}\right)^{\frac{1}{3}} - \frac{K'_1}{3K} \frac{T}{K}, \\ x_L &= -\left(\frac{T}{K}\right)^{\frac{1}{3}} \left(1 - \frac{K'_2}{3K} \left(\frac{T}{K}\right)^{\frac{2}{3}}\right) = -\left(\frac{T}{K}\right)^{\frac{1}{3}} + \frac{K'_2}{3K} \frac{T}{K}. \end{aligned}$$

32. The rectilinear diameter law is

$$\frac{1}{2}(\rho_L + \rho_G) = \rho_C(1 + a\Delta T_r)$$

with $\Delta T_r = 1 - T/T_c$ (cf. note 18). Here, $x_{L/G} = \rho_{L/G} - \rho_C$ hence

$$\frac{1}{2}(\rho_L + \rho_G) = \frac{1}{2}(x_L + x_G) + \rho_C = \frac{1}{6K^2}(K'_2 - K'_1)\Delta T_r + \rho_C,$$

which is indeed the law with $a = \frac{1}{6\rho_C K^2}(K'_2 - K'_1)$.

33. Before, A has been denoted K .

34. See note 29.

35. Read x_G or $\rho_G - \rho_C$ but not $x_G - x_C$, as $x_C = 0$.

36. “this would not be easy” is an understatement, as what is involved is the renormalisation group introduced at the time of Thom’s article (cf. note 16).

37. For remarks on these applications to biology, see the comments by Sara Franceschelli and J.P. in volume II, pp. 269 and 343.

M.C. & J.P.

Appendix 1. A mathematical glimpse of classical thermodynamics

The classical thermodynamical description of phase transitions relies on a variational principle. One studies systems⁽¹²⁾ at thermodynamic equilibrium and their variation under reversible infinitesimal transformations, using thermodynamic potentials derived from the *internal energy* U , whose differential during a reversible infinitesimal transformation at equilibrium is $dU = \delta Q + \delta W$ by the first principle of thermodynamics, where δQ is the heat variation and δW the work furnished by the system, neither of which is an exact differential.⁽¹³⁾ By the second principle of thermodynamics, as the transformation is reversible, δQ has an integrating factor, hence $\delta Q = TdS$, where T is the (absolute) temperature and S is called *entropy*. Moreover, $\delta W = -P_{\text{ext}}dV$ (if just the exterior pressure force works); now, the system being at equilibrium, the internal pressure P equilibrates the exterior pressure, hence

$$(1) \quad dU = TdS - PdV.$$

This defines a contact structure on (T, S, P, V, U) -space. Its integral manifolds of maximal dimension (“Legendrian submanifolds”) are known [A] to be surfaces.⁽¹⁴⁾ Near each of its points $(T_0, S_0, P_0, V_0, U_0)$, such a surface \tilde{L} projects to (T, S, P, V) -space as a Lagrangian surface L for the symplectic form $dT \wedge dS + dV \wedge dP$, which Lagrangian surface can *always* [A] be *locally* expressed by means of a real *generating function* of two variables $u(S, V)$, $f(T, V)$, $h(S, P)$ or $g(T, P)$ (defined up to an additive constant which we shall drop),

⁽¹²⁾ Of which we treat only the simplest case, that of a single chemical species, using basic ideas introduced at about the time of this article by the great Soviet mathematician V.I. Arnold [A]—who both much admired and much criticised Thom. Other mathematically understandable references (with very clever reflexions on physics) are [BS], [P].

⁽¹³⁾ In mathematical language, they are Pfaffian forms, *i.e.*, differential 1-forms.

⁽¹⁴⁾ The macroscopic equilibrium states of a system are defined by the points of such a surface. We assume these surfaces “smooth enough”.

by the formulae

- (2) $T = \partial_S u(S, V), \quad P = -\partial_V u(S, V)$ if L projects well to the (S, V) -plane
 (3) $S = -\partial_T f(T, V), \quad P = -\partial_V f(T, V)$ if L projects well to the (T, V) -plane
 (4) $T = \partial_S h(S, P), \quad V = \partial_P h(S, P)$ if L projects well to the (S, P) -plane.
 (5) $S = -\partial_T g(T, P), \quad V = \partial_P g(T, P)$ if L projects well to the (T, P) -plane

Thus, in case (2), \tilde{L} is locally defined by (1) with $U = u(S, V)$.

To treat the other three cases, it is preferable to make a variable change and replace U by $F = U - TS$ (*Helmholtz free energy*), $H = U + PV$ (*enthalpy*) or $G = H - TS$ (*Gibbs free energy*, alias *free enthalpy*). In these new variables, (1) reads

- (6)
$$dF = -v dT - P dV,$$

 (7)
$$dH = T dS + V dP,$$

 (8)
$$dG = -S dT + V dP,$$

so \tilde{L} is locally defined by (6) with $F = f(T, V)$ in case (3), by (7) with $H = h(S, P)$ in case (4) and by (8) with $G = g(T, P)$ in case (5).

Why define locally the surface \tilde{L} by (8) for some function $G = \Phi(T, P, V)$ and therefore get the *state equation* $\partial_V \Phi(T, P, V) = 0$ (defining the *state surface*)?

▷ This makes local sense only if L projects badly to the (T, P) -plane at (T_0, S_0, P_0, V_0) .

▷ Physically, one is more or less globally [BS] in case (3), as the volume and temperature of the system can be measured and define coordinates on \tilde{L} .

One can then call the additional “vertical” variable v , set (as $G = F + PV$)

$$\Phi(T, P, v) = f(T, v) + Pv$$

and see that (3) is equivalent to the three equations

$$(9) \quad \begin{aligned} S &= -\partial_T \Phi(T, P, v), & \text{that is, } S &= -\partial_T f(T, v) \\ V &= \partial_P \Phi(T, P, v), & \text{that is, } V &= v \\ 0 &= \partial_v \Phi(T, P, v), & \text{that is, } P &= -\partial_V f(T, V) : \end{aligned}$$

one calls Φ a *generating phase of L* ; it becomes a *generating phase of \tilde{L}* if one adds the condition $G = \Phi(T, P, v)$ with $\Phi(T_0, P_0, V_0) = G_0 := U_0 - T_0 S_0 + P_0 V_0$ (adjusting the omitted additive constant). If L projects badly to the (T, P) -plane at (T_0, S_0, P_0, V_0) , the derivative of $(T, V) \mapsto (T, -\partial_V f(T, V))$ is not invertible at (T_0, V_0) , which reads

$$\partial_V^2 f(T_0, V_0) = 0, \quad \text{i.e.,} \quad \partial_v^2 \Phi(T_0, P_0, V_0) = 0 :$$

in words, the critical point V_0 of $v \mapsto \Phi(T_0, P_0, v)$ is *degenerate*.

The “critical point” in note 14 is obtained when moreover $\partial_v^3\Phi(T_0, P_0, V_0) = 0$, *i.e.*, when the projection $(T, P, V) \mapsto (T, P)$, restricted to the state surface, has a singularity at (T_0, P_0, V_0) that is more degenerate than a fold.

Fundamental example: the van der Waals equation (1873)

This is the state equation given by the last line of (9) with

$$\partial_V f(T, V) = \frac{n^2 a}{V^2} - \frac{nRT}{V - nb},$$

where n is the number of moles, a, b, R are positive and f is defined for $T > 0$ and $V > nb$ (so b accounts for the size of moles). The *critical point*, being defined by $\partial_V^2 f(T, V) = \partial_V^3 f(T, V) = 0$, is

$$(T_C, P_C, V_C) := \left(\frac{8a}{27bR}, \frac{a}{27b^2}, 3nb \right).$$

Rewriting the state equation as a polynomial equation of degree 3 in V , one sees that the map $(T, P, V) \mapsto (T, P)$, restricted to the state surface, has a cusp singularity at (T_C, P_C, V_C) .

Of course, the van der Waals equation does not determine L , as it only yields

$$\begin{aligned} \Phi(T, P, v) &= f(T, v) + Pv \\ &= k(T) - \frac{n^2 a}{v} + nRT \ln \frac{1}{v - nb} + Pv, \quad T > 0, P > 0, v > nb \end{aligned}$$

for some function k of temperature. *Whatever k is*, each $\Phi_{T,P} : v \mapsto \Phi(T, P, v)$ “tends to $+\infty$ at infinity”, *i.e.*, when $v \rightarrow nb$ or $v \rightarrow +\infty$, and therefore *has an absolute minimum, reached at points v that do not depend on $k(T)$ —and at which the derivative $\partial_v \Phi(T, P, v)$ of $\Phi_{T,P}$ of course vanishes.*

The *wavefront set* [A] (“Cerf diagram”)

$$\text{WF}(\Phi) = \{ (T, P, \Phi(T, P, v)) : \partial_v \Phi(T, P, v) = 0 \}$$

in (T, P, G) -space is not the graph of a function of (T, P) :⁽¹⁵⁾ in our example, near $(T_C, P_C, \Phi(T_C, P_C, V_C))$, it looks (for all choices of the function k) like the swallowtail discriminant, with the tails of the transversal plane sections $\{T = \text{constant}\}$ upwards.

To describe phase transitions, Gibbs proposed to “cut the tails”, that is, extract from $\text{WF}(\Phi)$ the graph of the Lipschitzian function⁽¹⁶⁾

$$(10) \quad \underline{\Phi} : (T, P) \mapsto \min_v \Phi(T, P, v).$$

⁽¹⁵⁾ Obtained by projecting \tilde{L} to (T, P, G) -space, it is readily seen to determine \tilde{L} .

⁽¹⁶⁾ A similar selection procedure, with a max instead of a min—as if we maximized S instead of minimizing G —had been used by Maxwell in electricity (“Maxwell rule”). It plays a central

Except on the Maxwell set (“phase diagram”, independent of k), along which the minimum is not unique, the function $\underline{\Phi}$ is smooth and defines for each (T, P) a single state (a single phase) $S = -\partial_T \underline{\Phi}(T, P)$, $V = \partial_P \underline{\Phi}(T, P)$, $G = \underline{\Phi}(T, P)$.

In the van der Waals model, this phase diagram rightly is a line of *liquid* \mapsto *vapour* transition near its endpoint (T_C, P_C) , but the model does not account for the “triple point” (see Figure 1) at which *three* minima of $\Phi_{T,P}$ should compete.⁽¹⁷⁾

On Figures 2 and 3 in notes 16 and 17

Figure 2 shows an isotherm $P = -\partial_V f(T, V)$ with T constant, on the disputed side $T < T_C$ of the cusp. If P lies between the critical values of the map $V \mapsto -\partial_V f(T, V)$, the local minima of $\Phi_{T,P}$ are reached at the endpoints V_L, V_G of a vertical segment (horizontal in Figure 2) containing the third critical point of $\Phi_{T,P}$. The condition $\Phi_{T,P}(V_L) = \Phi_{T,P}(V_G)$ reads $\int_{V_L}^{V_G} \partial_v \Phi(T, P, v) dv = 0$, that is,

$$P(V_G - V_L) = \int_{V_L}^{V_G} \partial_v (-\partial_v f(T, v)) dv,$$

meaning that the areas A and B are equal.

One can then modify the state surface as follows:

▷ Off the phase diagram W , keep only the point (T, P, V) such that $\Phi_{T,P}$ is minimal at V ; this extracts from the state surface $\partial_V \Phi = 0$ the graph of a function of (T, P) defined on the complement of W (namely, $V = \partial_P \underline{\Phi}(T, P)$ with the notation (10)), hence, for each T , a “cut isotherm”, graph of a function of P except for $(T, P) \in W$.

▷ Then, on W , complete each cut isotherm by the vertical segment (horizontal in Figure 2) joining (T, P, V_L) to (T, P, V_G) .

This yields a continuous surface, of which the “isobars” of Figure 3 are the sections $P = \text{constant}$ – for $P > P_C$, they are just sections of the state surface $\partial_V \Phi = 0$.

role in the theory of weak solutions of Hamilton-Jacobi equations, much developed since the work of Oleinik, Lax, Schaeffer, . . . described by Thom several times in the present volume.

⁽¹⁷⁾ Nevertheless, van der Waals was awarded the Nobel prize in 1910, which shows that a *local* model of phase diagrams near the “critical point” was considered a significant achievement. In Appendix 3 hereafter, B.T. treats the general case of this local situation, providing a more refined (local) version of the Gibbs phase rule than Appendix 2 – physically, as usual, this rule must be somewhere between local and global. To account also for the triple point, J.P. [Pe] sketched a model à la van der Waals based on the butterfly catastrophe, whose organizing center x^6 has more than two parameters in its universal unfolding; one should therefore find a surface (parametrized by T, P) in the space of “universal” parameters.

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Appendix 2. The “interior” of the Maxwell set and the Gibbs phase rule

Given a compact⁽¹⁸⁾ manifold M of dimension n and an integer $r > 1$, the set $\Sigma^r(M)$ of those $(g, x) \in C^r(M, \mathbb{R}) \times M$ such that $d_x g = 0$ is a C^{r-1} submanifold of codimension n .⁽¹⁹⁾ The projection $\Sigma^r(M) \ni (g, x) \mapsto g$ is a local diffeomorphism at (h, a) if and only if the critical point a of h is non-degenerate; then $\Sigma^r(M)$ is the graph of a C^{r-1} implicit function $x = c_{h,a}(g)$ near (h, a) .

It follows easily that the functions $g \in C^r(M, \mathbb{R})$ which reach their absolute minimum only at non-degenerate critical points (“simple minima”) form an open subset U , which is dense since it contains the Morse functions.

As M is compact, every $g \in U$ has a finite number of such simple minima, hence a partition of U into subsets U_k , $k \geq 0$, each of which consists of those $g \in U$ reaching their absolute minimum at precisely $k + 1$ points.

⁽¹⁸⁾ Without boundary. For non-compact manifolds (as in Appendix 1), one should restrict to functions g that tend to $+\infty$ at infinity, meaning that $\{g \leq c\}$ is compact for every $c \in \mathbb{R}$.

⁽¹⁹⁾ Inverse image of the zero section of T^*M under the C^{r-1} submersion $(g, x) \mapsto dg(x)$.

The clearly open “big stratum” U_0 is dense in $C^r(M, \mathbb{R})$, as it contains the dense set of “excellent” Morse functions, those whose values at critical points are all different.

The *Maxwell set* is the closed subset $W = C^r(M, \mathbb{R}) \setminus U_0$.

Its “interior” $\text{int}(W) := U \cap W = \bigcup_{k \geq 1} U_k$ is closed in U and the closure of $\text{int}(W)$ in $C^r(M, \mathbb{R})$ is W . For each integer $\ell \geq 0$, the subset $\bigcup_{k \leq \ell} U_k$ is open (simple minima cannot “explode”), hence $\bigcup_{k > \ell} U_k$ is closed in U .

Stratified structure

The partition $(U_k)_{k \geq 0}$ of U is a stratification, each U_k being a C^r submanifold of codimension k . Thus, $\text{int}(W)$ is a stratified hypersurface.

Indeed, given $k \geq 1$ and $h \in U_k$, denoting by a_0, \dots, a_k its minima, one defines a C^r local submersion⁽²⁰⁾

$$\pi_h : (U, h) \longrightarrow \mathbb{R}^{k+1}, \quad \pi_h(g) := (g(c_{h,a_0}(g)), \dots, g(c_{h,a_k}(g))).$$

Near h , the subset U_k clearly is the inverse image under π_h of the “small diagonal”

$$S_{k,k} := \{(b_0, \dots, b_k) : b_0 = \dots = b_k\},$$

a line which contains $\pi_h(h) = (h(a_j))_{0 \leq j \leq k}$. Thus, U_k is a C^r submanifold of codimension k .

Near h , for $0 < \ell < k$, the submanifold U_ℓ is the inverse image under π_h of

$$S_{k,\ell} := \bigcup_{0 \leq i_0 < \dots < i_\ell \leq k} \{(b_0, \dots, b_k) : b_{i_0} = \dots = b_{i_\ell} < b_j \text{ for all other } j \text{'s}\};$$

likewise, near h , the open subset U_0 is the inverse image under π_h of

$$S_{k,0} = \bigcup_{0 \leq i \leq k} S_{k,0,i}, \quad \text{where } S_{k,0,i} = \{(b_0, \dots, b_k) : b_j > b_i \text{ for } j \neq i\}.$$

The “first derived barycentric subdivision of the simplex”

The stratification $(S_{k,\ell})_{0 \leq \ell \leq k}$ of \mathbb{R}^{k+1} , being invariant under translation in the direction $S_{k,k}$,⁽²¹⁾ is determined by its transversal structure, that of its intersection with the hyperplane $H_k = \{(b_0, \dots, b_k) : b_0 + \dots + b_k = 1\}$. The *first derived barycentric subdivision of the simplex* mentioned by Thom

⁽²⁰⁾ It is not just C^{r-1} like each c_{h,a_j} : indeed, as $d_{c_{h,a_j}(g)}g = 0$ by definition, the differential $d_g \pi_h : \delta g \mapsto (\delta g(c_{h,a_\ell}(g)))_{0 \leq \ell \leq k}$ is a C^{r-1} function of g . To see that π_h is a local submersion, note that a section of $d_h \pi : g \mapsto (g(a_0), \dots, g(a_k))$ is $(y_0, \dots, y_k) \mapsto \sum y_j \theta_j$ if the smooth functions θ_j on M verify $\theta_0(a_0) = \dots = \theta_k(a_k) = 1$ and have mutually disjoint supports.

⁽²¹⁾ This corresponds to the fact each U_k is invariant under the translations $g \mapsto g + c$, $c \in \mathbb{R}$ (one is considering *potentials*).

is the stratification $(\sigma_{k,\ell})_{0 \leq \ell \leq k} := (S_{k,\ell} \cap \sigma_k)_{0 \leq \ell \leq k}$ of the standard k -simplex $\sigma_k = H_k \cap \mathbb{R}_+^{k+1}$.

Thus, near $h \in U_k$, the stratification (U_j) of U is the inverse image of $(\sigma_{k,\ell})_{0 \leq \ell \leq k}$ under the local submersion $p_h : (U, h) \rightarrow (\sigma_k, \sigma_{k,k})$ obtained by composing π_h with the projection of \mathbb{R}^{k+1} onto H_k in the direction $S_{k,k}$.

The Gibbs phase rule à la Thom

Since $S_{k,0}$ has $k + 1$ components $S_{k,0,i}$, $0 \leq i \leq k$, for every submanifold $N \ni h$ of $C^r(M, \mathbb{R})$ intersecting U_k transversally at h , the germ of $N \cap U_0$ at h has $k + 1$ components (“phases”), inverse images of the $S_{k,0,i}$ ’s under the submersion germ $\pi_h|_N$.⁽²²⁾

By the Thom-Mather transversality lemma, for each separable k -dimensional manifold B , $k \geq 0$, the smooth⁽²³⁾ real functions $V : (b, x) \mapsto V_b(x)$ on $B \times M$ such that $\rho_V : b \mapsto V_b$ is transversal to the stratified hypersurface $\text{int}(W)$ (i.e., to each U_j with $j \geq 1$) form a residual subset \mathcal{R} . Thus, for $V \in \mathcal{R}$, there are at most $k + 1$ local components of $\rho_V^{-1}(U_0)$ (“phases”) near each $b \in \rho_V^{-1}(U) -$ and indeed $k + 1$ for $V_b \in U_k$.

M.C.

Appendix 3. Bifurcations and Gibbs phase rule

We give some details on Thom’s interpretation of the Gibbs phase rule in the context of versal unfoldings of smooth functions f with an algebraically isolated minimum at 0. This hypothesis implies that we may assume, up to a local diffeomorphism, that the function is a polynomial. We keep most notations of page 96 of the paper, and write a (mini-)versal C^∞ unfolding as :

$$F_u = f + \sum_{i=1}^{\mu-1} u_i g_i,$$

⁽²²⁾ Assuming the number of chemical species to be $c = 1$, the phase rule $v = c + p - \varphi$ is verified by the number of phases $\varphi = k + 1$, the number $p = \dim N$ of “intensive parameters” and the “variance” $v = p - k = \dim(U_k \cap N)$.

For instance, at a triple point, $v = 0$ (the point has codimension 2 in (T, P) plane), $c = 1$ (e.g., water), $p = 2$ (temperature T and pressure P), $\varphi = 3$ and indeed $0 = 1 + 2 - 3$. Along the coexistence line of two phases, the value of one of the intensive variables T or P determines that of the other and $v = 1 = 1 + 2 - 2$.

⁽²³⁾ And even C^s with $s > k$ (and $s > r$), a condition that might still be too strong. The transversality argument works for competing non-degenerate local minima as in thermodynamics.

where the functions g_i are polynomials whose images, together with 1, form a basis of the quotient algebra

$$\mathbf{R}\{x_1, \dots, x_m\}/(f_{x_1}, \dots, f_{x_m})$$

as a vector space over \mathbf{R} . We denote the number of internal variables by m to avoid confusion with Thom's notation. The dimension ν of the parameter space of the versal unfolding is the Milnor number minus one, and not the Milnor number.

Thus we have a map germ

$$\mathbf{F}_u: (\mathbf{R}^m \times \mathbf{R}^{\mu-1}, 0) \longrightarrow (\mathbf{R} \times \mathbf{R}^{\mu-1}, 0), \quad (x, u) \longmapsto (F_u(x), u).$$

We denote by u_0 a coordinate on \mathbf{R} .

The *discriminant* $D_{\mathbf{F}_u}$ of the map \mathbf{F}_u is the image of its critical locus $C_{\mathbf{F}_u}$. It is a semialgebraic hypersurface in $\mathbf{R} \times \mathbf{R}^{\mu-1}$. It is known [T2, §5] that $C_{\mathbf{F}_u}$ is non singular and the map $C_{\mathbf{F}_u} \rightarrow D_{\mathbf{F}_u}$ is finite.

The singular locus of $D_{\mathbf{F}_u}$ is of codimension one and its image $\Delta_{\mathbf{F}_u}$ in $\mathbf{R}^{\mu-1}$ by the second projection $\mathbf{R} \times \mathbf{R}^{\mu-1} \rightarrow \mathbf{R}^{\mu-1}$ is a semialgebraic hypersurface containing the bifurcation locus Σ and the conflict strata. Indeed, a point u is in $\mathbf{R}^{\mu-1} \setminus \Delta_{\mathbf{F}_u}$ if and only if the function F_u is an excellent Morse function in a suitable neighborhood of 0 in \mathbf{R}^m . In particular the Maxwell set, which corresponds to functions F_u attaining at least twice their absolute minimum, is contained in $\Delta_{\mathbf{F}_u}$ because it is the image of a singular stratum of $D_{\mathbf{F}_u}$.

The map \mathbf{F}_u is a stable map-germ and as such can be Thom-stratified [GWPL, Chapter 4, §2]: there exist finite partitions of the source and target into semialgebraic non singular strata such that :

- ▷ The restriction of \mathbf{F}_u to a stratum of the source is a submersion onto a stratum of the target ;
- ▷ The Thom isotopy theorem is valid : the topological type of the germ of \mathbf{F}_u at a point of a stratum of the source depends only on the stratum.

It is not clear in which cases there exists such a stratification which is minimal in some sense, since already minimal Whitney stratifications do not exist in general for semialgebraic sets [BT]. However, the statement we are interested in concerns the largest possible dimension of the stratum of the origin in such a stratification.

Let us denote by T_0 the stratum in $\mathbf{R} \times \mathbf{R}^{\mu-1}$ containing the origin.

The discriminant hypersurface $D_{\mathbf{F}_u}$ has a very special geometry [T2, §5], in particular all limit directions of its tangent hyperplanes at smooth points tending to the origin are the hyperplane $u_0 = 0$. This implies that the images

in $\mathbf{R}^{\mu-1}$ by the second projection $\mathbf{R} \times \mathbf{R}^{\mu-1} \rightarrow \mathbf{R}^{\mu-1}$ of the strata in $\mathbf{R} \times \mathbf{R}^{\mu-1}$ form a stratification and the map from T_0 to its image $T'_0 \subset \mathbf{R}^{\mu-1}$ is an isomorphism. Let $S_0 \subset \mathbf{R}^m \times \mathbf{R}^{\mu-1}$ be the stratum of the origin at the source; it is contained in the critical locus and so is a finite submersion onto its image T'_0 so that the maps $S_0 \rightarrow T_0 \rightarrow T'_0$ are algebraic diffeomorphisms. Thus, as a point u moves in T'_0 , the corresponding functions F_u have a unique critical point at which their germs are all topologically equivalent. From the viewpoint of catastrophe theory the parameters corresponding to coordinates on T'_0 are not significant and the number p_f of significant parameters is the minimum codimension of the stratum $T'_0 \subset \mathbf{R}^{\mu-1}$ in a Thom stratification of \mathbf{F}_u .

On the other hand, the maximum number of stable attractors (for the opposite of the gradient vector field), that is, the maximum number of non degenerate local minima of a function F_u which can appear represents the number of phases which can coexist in the sense that the system can make a transition from one to an other.

Let us denote by ϕ_f the maximum number of local minima which a function F_u in a versal unfolding of f can present (in a suitable neighborhood of 0). They have to be non degenerate.

A rather coarse form of the classical Gibbs phase rule states that the number ϕ of coexisting phases in a thermodynamical system is at most equal to the number of parameters of the system plus one : $\phi \leq p + 1$. In our model, this translates as :

$$\phi_f \leq p_f + 1 = \text{codim}_{\mathbf{R}^{\mu-1}} T'_0 + 1 = \text{codim}_{\mathbf{R} \times \mathbf{R}^{\mu-1}} T_0.$$

See also [77]. Some ideas for a proof can be found in [T1], based on the real avatar of the product decomposition theorem for the discriminant of complex miniversal unfoldings of [T2, §5]. Let $\delta_{\mathbf{R}}(\mathbf{F}_u)$ denote the maximum number of singular points that can be found in a fiber of a function F_u , in a suitable neighborhood of 0 in \mathbf{R}^m and for u in a small neighborhood of 0 in $\mathbf{R}^{\mu-1}$. By the product decomposition theorem this corresponds to points in $D_{\mathbf{F}_u}$ where this hypersurface is locally the union of $\delta_{\mathbf{R}}(\mathbf{F}_u)$ non singular hypersurfaces in general position. The locus of such points is of codimension $\delta_{\mathbf{R}}(\mathbf{F}_u)$ in $\mathbf{R} \times \mathbf{R}^{\mu-1}$ and since the topology of the situation is constant along T_0 and this configuration of non singular hypersurfaces is topologically invariant on $D_{\mathbf{F}_u}$ (again a consequence of the product decomposition theorem), this locus must contain T_0 in its closure, so that

$$\delta_{\mathbf{R}}(\mathbf{F}_u) \leq \text{codim}_{\mathbf{R} \times \mathbf{R}^{\mu-1}} T_0.$$

The next step is to prove that $\phi_f \leq \delta_{\mathbf{R}}(\mathbf{F}_u)$. This should follow (the argument is not complete) from a Smale-type argument [CG] asserting that since the ϕ_f minima of one of the F_u have the same index they can be moved to the same level by a perturbation of that function small enough to be represented in \mathbf{F}_u .

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