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Bernard Teissier

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On Thom's interpretation of the Gibbs phase rule

Bernard Teissier

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We give some details on Thom's interpretation of the Gibbs phase rule in the context of versal unfoldings of smooth functions with an algebraically isolated singularity. This hypothesis implies that we may assume, up to a 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 :

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

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 $\mathbf{F}_u : (\mathbf{R}^m \times \mathbf{R}^{\mu-1}, 0) \longrightarrow (\mathbf{R} \times \mathbf{R}^{\mu-1}, 0)$ sending (x, u) to $(F_u(x), u)$. 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 (see [5, §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 : 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 (see [1]). 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 (see [5, §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 gradient vector field), that is, the maximum number of non degenerate 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 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 [6]. Some ideas for a proof can be found in [4], based on the real avatar of the product decomposition theorem for the discriminant of complex miniversal unfoldings of [5, §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 ([3]) 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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B.T.