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FRACTAL DIMENSION OF ATTRACTORS FOR A STEFAN PROBLEM

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Abstract. For a one-phase free-boundary problem with kinetics, which is known to generate a rich dynamics, we present results of a numerical study of the correlation dimension of the attractor.

1. **Introduction.** It was shown [FRS, FR1] that, in contrast to the classical Stefan problem, the non-equilibrium Stefan problem where the phase transition temperature is related to the interface velocity through the kinetics, exhibits a wide variety of dynamical scenarios. In recent papers [FR3, FR4] we studied one-phase non-equilibrium Stefan problem and proved that it possesses a compact attractor of a finite Hausdorff dimension. The analytical estimate on the dimension produces extremely large values for the dimension.

The situation here is somewhat similar to other well-studied dissipative systems such as, for instance, the Navier-Stokes and the Kuramoto-Sivashinsky equations [T] where, in addition, the estimate of the fractal dimension is strongly dependent on the size of the domain or, for unbounded domains, on the choice of the weighted space [HNZ]. We would like to emphasize the difference between the latter and our problem, whose remarkable feature is that all characteristics of the dynamics are defined by the intrinsic physical parameters only.

At the same time, in [FR2] we demonstrated that a 3×3 pseudo-spectral approximation of the free-boundary problem mimics the infinite-dimensional system very well. These observations suggest that the asymptotic dynamics of the free-boundary problem should be relatively low-dimensional. Below we present numerical evidence in favor of the latter suggestion.

The free-boundary problem is formulated as follows

$$u_t = u_{xx} - \gamma u, \quad -\infty < x < s(t), \tag{1}$$

$$(\partial u/\partial x)|_{x=s(t)} = -V(t),\ g(u|_{x=s(t)}) = V(t),\ u(x,0) = u^0(x). \tag{2}$$

Here $u(x,t)$ is the temperature, $\gamma \geq 0$ is the heat loss coefficient. The two boundary conditions: the Stefan and the kinetics condition overdetermine the problem and allow one to find the free boundary whose position is $s(t)$ and velocity, $V(t) = \dot{s}(t)$.

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The free-boundary problem (1-2) arises naturally as a mathematical model for a variety of exothermic phase transition type processes, such as condensed phase combustion [MS] also known as self-sustained high-temperature synthesis or SHS, solidification with undercooling [L], rapid crystallization in thin films [VW] etc.

2. **Analytical Background.** Existence and uniqueness of bounded classical solutions for the problem (1-2) was established in [FR4]. Next, following [FR4] we briefly describe the necessary prior results on the existence and structure of a compact attractor.

By integrating Green's identity over the domain $\xi < s(\tau)$, $0 < \tau < t$ one can obtain the following representation for the solution:

$$u(x,t) = \int_0^t \widetilde{G}(x, s(\tau), t-\tau)\left[-V(\tau) + U(\tau)V(\tau)\right] d\tau \qquad (3)$$
$$- \int_0^t \frac{\partial \widetilde{G}}{\partial \xi}(x, s(\tau), t-\tau) U(\tau) d\tau + \int_{-\infty}^0 \widetilde{G}(x, \xi, t) u^0(\xi) d\xi$$

Here $\widetilde{G} = e^{-\gamma(t-\tau)}G$ is the fundamental solution of the heat equation with damping, G is the Gaussian kernel

$$G(x,\xi,t-\tau) \equiv G(x,t,\xi,\tau) = \exp\left\{-\frac{(x-\xi)^2}{4(t-\tau)}\right\}\left[4\pi(t-\tau)\right]^{-1/2}.$$

Since both $U := u(s(\tau),\tau)$ and $V = ds/dt = g(U)$ are determined by the initial conditions, the representation can be thought of as the time evolution of the initial temperature distribution u^0 under the semigroup$T(t)$: $u(t) = T(t)u^0$. We understand the evolution as taking place for the functions on the fixed interval $(-\infty, 0)$. This is equivalent to the introduction of the moving coordinate system attached to the free boundary $x' = x - s(t)$. We split the semigroup operator T into two parts: *the contribution of the free boundary and that of the initial data* $T(t)u^0 = T_1(t)u^0 + T_2(t)u^0$, where

$$T_1(t)u^0 = \int_0^t \widetilde{G}(x, s(\tau), t-\tau)\left[-V(\tau) + U(\tau)V(\tau)\right] d\tau \qquad (4)$$
$$- \int_0^t \frac{\partial \widetilde{G}}{\partial \xi}(x, s(\tau), t-\tau) U(\tau) d\tau$$

$$T_2(t)u^0 = e^{-\gamma t}\int_{-\infty}^0 G(x', \xi - s(t), t) u^0(\xi) d\xi \qquad (5)$$

It can be shown that the contribution from the free boundary exhibits a uniform exponential decay in x and that its spatial derivative is uniformly bounded. This allows us to apply a version of the Arzela-Ascoli theorem and prove that T_1 is uniformly compact. Clearly T_2 decays exponentially in time.

Proposition 1. *Let the metric space X be defined as a ball in the space $C(-\infty, 0]$:*

$$X = \{u \in C(-\infty,0]; \quad ||u|| = \sup|u(x')| \leq N\}$$

where the radius N is large enough. Then:
(i) The semigroup T_2 is uniformly contracting:

$$r_X(t) = \sup_{u^0 \in X} ||T_2(t)u^0|| \to 0 \quad \text{as} \quad t \to \infty.$$

(ii) There exists a constant, R_{abs}, totally determined by the kinetics such that any ball $B_a = \{u \in X; \quad ||u|| \leq R_{abs}\}$ is an absorbing set for the ball B_R with respect to the evolution by T.
(iii). The semigroup $T_1(t)$ is uniformly compact: there exists $t_0 > 0$ such that $\cup_{t \geq t_0} T_1(t)X$ is relatively compact in X.

This yields ([T, Chap. I]) existence of a compact attractor for the dynamics by the semigroup.

Remark 1. The proof of existence of a compact attractor in [FR4] is predicated upon an extra requirement on the kinetic function:

$$-V_0 \leq g \leq -v_0 < 0 \tag{6}$$

The upper bound v_0 corresponds to the "ignition velocity": the model is valid only for moving fronts; this bound can be dropped in the presence of heat losses, $\gamma > 0$. We note that although the lower bound is rather natural and is satisfied for the standard Arrhenius kinetics, *the proof can be carried out even if g has a sublinear growth.*

3. **Rigorous Estimate of Hausdorff Dimension.** Now we briefly describe the main result of [FR5] which presents an estimate on the Hausdorff dimension of the attractor. In [FR5] we studied evolution of the infinitesimal volume along the trajectories in the attractor. We demonstrated that for sufficiently large m that is defined solely by the properties of the kinetics function the m-dimensional volume decays exponentially. We showed that the nonlinear evolution of the volume is well approximated by its linear counterpart. The desired result is ensured by the differentiability with respect to the initial conditions of the semigroup solving the free-boundary problem. This leads to the conclusion that the Hausdorff dimension of the attractor for the solutions of the free boundary problem is finite. In the arguments regarding the Hausdorff dimension of the attractor we followed quite closely the ideas outlined in [T].

Theorem 1. *The Hausdorff dimension of the attractor (functional invariant set) $\mathcal{A}$ is no larger than a constant M defined solely by the kinetics and heat losses,*

$$M \sim cV_0^2/(v_0^2 + 16\gamma/3). \tag{7}$$

The estimate exhibits a transparent and physically natural dependence of the dimension on the heat loss and characteristics of the kinetics which are the defining factors of the dynamics. However, numerical experiments [FR1] demonstrate amazing similarity between dynamical scenarios for different kinetics, and in the absence of the heat losses. Moreover, for standard kinetics (Arrhenius) the estimate in (7) yields rather large upper bounds on the dimension, while the pseudo-spectral ODE reductions of the model [FKRT] suggest substantially lower values. Then a natural question arises: What are the "real-life" values of the fractal dimension and how are they effected by the parameters of the model? In the next section we discuss results of numerical computation of the correlation dimension of the attractor.

4. **Correlation Dimension.** While the Hausdorff dimension is convenient for analytical estimates, it is highly nontrivial to compute and requires too much storage and CPU time. More convenient computationally is the *correlation dimension.* Although in general $d_{corr} \leq d_{Hausdorff}$, they are usually very close. We follow the now standard procedure for computation of the correlation dimension [GP]. Namely,

consider the set $\{U_i,\ i = 1, ...N\}$ of points on the attractor $U_i = U(T + i\tau)$, where $T \gg 1$. We measure the spatial correlation between the points on the discreet approximation of the attractor with the correlation integral

$$C(l) = \lim_{N\to\infty} \frac{1}{N^2}\{\text{number of pairs with the distance } \rho(U_i, U_j) < l\}$$

If for small l, $C(l)$ scales as l^ν then the correlation exponent ν can be taken as the correlation dimension of the attractor d_{corr}. For practical calculations the frequency of sampling τ, the number k of points in space where the solution is sampled at each time, and the number of samples N are determined empirically. Similarly for low n a better approximation for d_{corr} may be obtained if the distance ρ is not necessarily Euclidean.

To obtain a numerical approximation of the attractors we solve the initial value problem (1)-(2) for sufficiently large time until the asymptotic regime is attained. Obviously the dimension of the attractor should not depend on the choice of initial data, which was confirmed by direct numerical simulations. Problem (1)-(2) was solved in the frame attached to the free boundary on a finite interval $[-L, 0]$ with the Dirichlet condition $u(-L, t) = 0$ simulating the decay of the solution at $-\infty$. According to our observations the results are practically insensitive to the increase in the interval length after $L \sim 10$ (see [FR1] for the details of the numerical algorithm).

To represent different dynamical regimes we use the Arrhenius kinetics

$$V = g(u) := -exp[\alpha(u - 1)/(\sigma + (1 - \sigma)u)], \tag{8}$$

where (in the context of combustion) α is proportional to the activation energy (Zeldovich number), σ is the temperature ratio of the fresh mixture and the product.

Thus, the attractor is represented as a set in $\mathbb{R}^k$, where k is the number of sampling points of temperature profiles. We choose time snapshots of the solution for every 0.4 in the interval of the asymptotic regime ($200 < t < 4200$) and consider them as a discrete approximation of the attractor in $\mathbb{R}^k$. The correlation dimension for this discrete set is evaluated as explained above. As a control experiment we select a periodic asymptotic regime. It is immediately confirmed that $d_{corr} \approx 1$ as one should expect.

In contrast, for $\alpha = 1/0.3261 = 3.0665$, $\sigma = 0.4$ the regime is chaotic as is illustrated in Fig. 1 presenting a series of snapshots of spatial temperature profiles. One can see that in this case $d_{corr} \approx 2.1$ (Fig 2). From our observations it appears that the dimension cannot be much higher than 2.

5. **Concluding Remarks.** The results of numerical estimates of the correlation dimension described in the present paper represent a rather remarkable contrast to the analytical estimate. Indeed, the attracting set for the problem in (1)-(2) turns out to be extremely thin.

Thus, very complex thermo-kinetic oscillations generated by the interaction between the kinetics and the dissipation result in the excitation of just a few modes. Although the numerical dimension is obtained for a finite spatial interval the results, according to our observations, are practically insensitive to the further increase in the interval length. This observation is valid for a variety of kinetic families we experimented with. It should be added that these results were obtained in the absence of damping represented by the heat losses.

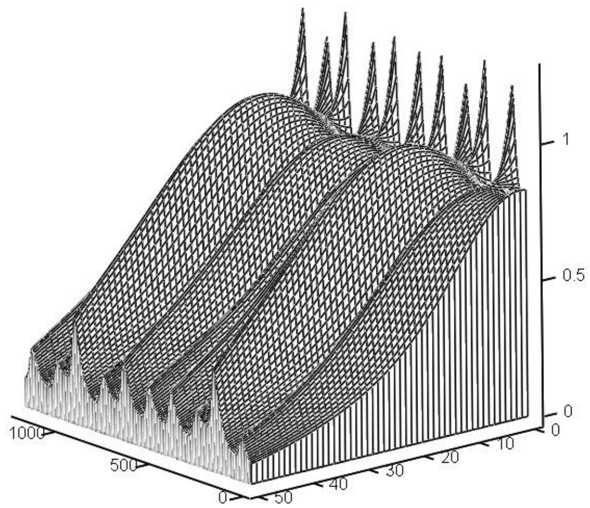

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FIGURE 1. Time history $0 < t < 1000$ for chaotic dynamics $u(x, t)$ vs. x, t.

We should emphasize again that for our problem, all characteristics of the dynamics including the Hausdorff dimension are defined by the intrinsic physical parameters only. Our results presented above suggest that the chaos generated by the one-phase non-equilibrium Stefan problem is low-dimensional.

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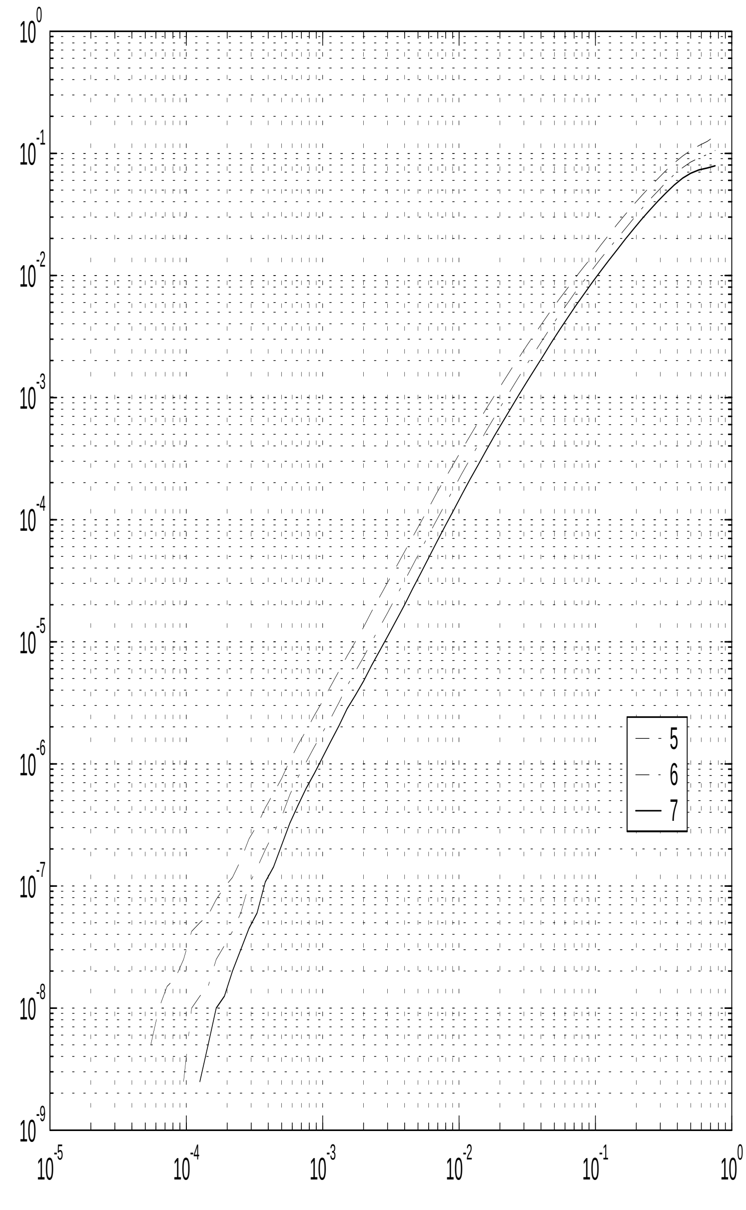

FIGURE 2. Correlation integral for 5-, 6- and 7-point samples.

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