Stefan Problems and Numerical Analysis

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Abstract We outline the main contributions of Prof. Enrico Magenes to the analysis and numerical approximation of mathematical models of phase transition processes. Starting from the 1980's, a semigroup approach to Stefan problems, optimal rates of convergence for the nonlinear Chernoff formula, regularity properties of solutions, theoretical and numerical aspects of Stefan models in a concentrated capacity, were investigated by Enrico Magenes. His expertise was fundamental for developing numerical analysis of evolutionary free boundary problems and applications in a modern framework.

1 Stefan Problems and Semigroups: Analysis and Numerical Approximation

Phase transitions occur in many relevant processes in natural sciences and industrial applications. The basic Stefan model represents phase transitions in a rather simplified way by coupling heat diffusion and exchange of latent heat between phases. It has been extensively studied in the last 60 years: the existing literature includes tenths of thousand of papers and a number of meetings has been devoted to this model and its extensions. Following the *International Seminar on Free Boundary Problems* held in Pavia in September–October 1979 [\[33](#page-6-0)], a regular series of *International Symposium on Free Boundary Problems: Theory and Applications* took place in: Montecatini, 1981 [\[23](#page-5-0)]; Maubuisson, 1983 [[5\]](#page-5-1); Irsee, 1987 [[27\]](#page-6-1); Montreal, 1990 [\[11](#page-5-2)]; Toledo, 1993 [\[17](#page-5-3)]; Zakopane, 1995 [[58\]](#page-7-0); Hiraklion, 1997 [[1\]](#page-5-4); Chiba, 1999 [\[31](#page-6-2)]; Trento, 2002 [\[13](#page-5-5)]; Coimbra, 2005 [[25](#page-6-3)]; etc. A series of conferences focusing on numerical methods and applications started with the *Workshop on Generalized Stefan Problems: Analysis and Numerical Methods* held in Pavia in 1995 and took place in: Freiburg, 1995; Lamoura, 1996; Faro, 1996; Berlin, 1996; Ittingen, 1997; Madeira, 1998; Braga, 1998; Hiraklion, 1999; etc.

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Existence, uniqueness, and regularity properties of the solution of Stefan problems were obtained by L. Rubinstein [[79\]](#page-8-0), S. Kamin [[30\]](#page-6-4), O. Oleinik [\[75](#page-8-1)], A. Friedman [\[26](#page-6-5)], D. Kinderlehrer and L. Niremberg [[32\]](#page-6-6), L.A. Caffarelli [[8\]](#page-5-6) and L.C. Evans [\[10](#page-5-7)], E. Di Benedetto [[16\]](#page-5-8), A.M. Meirmanov [\[54](#page-7-1)], A. Damlamian [\[15](#page-5-9)], A. Visintin [\[89](#page-8-2)], M. Niezgodka and I. Pawlow [[57\]](#page-7-2), A. Fasano and M. Primicerio [[20–](#page-5-10)[22\]](#page-5-11), and many others (we refer to the monographs [\[55](#page-7-3), [80](#page-8-3), [91](#page-8-4)[–93](#page-8-5)]; a huge bibliography can be found in [\[83](#page-8-6)]). Numerical analysis and applications were developed by G. Meyer [\[56](#page-7-4)], J. Nitsche [[59\]](#page-7-5), J.F. Ciavaldini [[12\]](#page-5-12), J.W. Jerome and M.E. Rose [[29\]](#page-6-7), C.M. Elliott [[19](#page-5-13)], R.H. Nochetto [\[63](#page-7-6)] among others (see the survey [[86\]](#page-8-7)).

The interest of Enrico Magenes for the Stefan model and its numerical approximation received an impulse during the *International Seminar on Free Boundary Problems* held in Pavia in 1979 and yielded a series of seminars that he delivered at the *V Seminario di Analisi Funzionale e Applicazioni* held in Catania on September 17–24, 1981 (these lecture notes were published in [[34\]](#page-6-8), an interesting overview of the state of the art for the multidimensional two-phase Stefan problem). Enrico Magenes worked on this subject for twenty years, with many original contributions but, more relevantly, by stimulating his students and collaborators with continuous discussions and suggestions.

The enthalpy formulation, a fixed domain formulation were the interface or free boundary can be recovered *a posteriori* as level-set of temperature variable, reads in weak or variational form as follows:

$$
\begin{cases}\n\frac{\partial u}{\partial t} - \Delta \beta(u) = 0 & \text{in } \Omega \times (0, T), \\
\beta(u) = 0 & \text{on } \partial \Omega \times (0, T), \\
u(\cdot, 0) = u_0(\cdot) & \text{in } \Omega,\n\end{cases}
$$
\n(1)

where $\Omega \subset \mathbf{R}^d$ and $\beta(s) = (s-1)^+ - s^-$ is the constitutive relation between enthalpy *u* and temperature $\theta = \beta(u)$. Existence and uniqueness of the solution can be proved in suitable functional spaces. The interest of Magenes was focused on the possibility to formulate the Stefan problem [\(1\)](#page-1-0) as an *m*-accretive semigroup of contraction in $L^1(\Omega)$ in the sense of M.G. Crandall and T. Ligget [[14\]](#page-5-14), and Ph. Bénilan [\[3](#page-5-15)], which allows to numerically approximate ([1\)](#page-1-0), either by backward finite differences (here τ denotes the time-step)

$$
U^{n} - U^{n-1} - \tau \Delta \beta (U^{n}) = 0,
$$
\n(2)

or by the nonlinear Chernoff formula, as observed by A.E. Berger, H. Brézis, and J.C.W. Rogers [[4\]](#page-5-16)

$$
\begin{cases} V^n - \tau \Delta V^n = \beta(U^{n-1}), \\ U^n = U^{n-1} - \beta(U^{n-1}) + V^n. \end{cases}
$$
 (3)

In many significant applications, the boundary condition $\beta(u) = 0$ on $\partial\Omega \times (0, T)$ could be replaced by nonlinear flux conditions (e.g. Stefan-Boltzmann law) [[88\]](#page-8-8)

$$
\frac{\partial \beta(u)}{\partial v} + g(\beta(u)) = 0 \quad \text{on } \partial \Omega \times (0, T).
$$

In [[48\]](#page-7-7), Magenes *et al.* extended the semigroup approach to the Stefan problem with nonlinear flux conditions, by proving that the operator $A : w \to -\Delta\beta(w)$ with domain $D(A) = \{w \in L^1(\Omega) : \beta(w) \in L^1(\Omega), \Delta \beta(w) \in L^1(\Omega), \frac{\partial \beta(w)}{\partial v} + g(\beta(w)) = 0\}$ 0 on $\partial\Omega$ } is *m*-accretive in $L^1(\Omega)$, whence the solution exists and is unique in a suitable weak sense. This results was a theoretical step for justifying the convergence properties of the numerical algorithms studied in [[49,](#page-7-8) [84](#page-8-9)].

The backward Euler method [\(2](#page-1-1)) requires the solution of a nonlinear elliptic PDE at each time-step. Combined with a finite element method for spatial approximation and numerical quadrature, it leads to an effective numerical scheme. Stability and *a priori* error estimates under minimal regularity properties on data have been proved in [[65](#page-7-9), [85\]](#page-8-10) (see [[67,](#page-7-10) [68\]](#page-7-11) for *a posteriori* error estimates and an adaptive implementation). On the other hand, the nonlinear Chernoff formula ([3\)](#page-1-2) requires the solution of a linear elliptic PDE at each time step followed by an algebraic correction to recover discrete enthalpy. It turns out that Chernoff is a stable linearization procedure in the spirit of the Laplace-modified forward Galerkin method for non-degenerate parabolic problems introduced by J. Douglas and T. Dupont [\[18](#page-5-17)]. Despite convergence was guaranteed by the theory of nonlinear contraction semigroups in Banach space [[6\]](#page-5-18), error estimates remained open until the paper by Magenes *et al.* [[50\]](#page-7-12). The key argument is a combination of the following three features:

- the use of a variational technique first applied by R.H. Nochetto $[60, 61]$ $[60, 61]$ $[60, 61]$ $[60, 61]$;
- the possibility of dealing with minimal regularity properties $u_0 \,\in L^2(\Omega)$ as shown in $[65]$ $[65]$;
- the relationship between the nonlinear Chernoff formula and the discrete-time scheme studied in [\[87](#page-8-11)] for the approximation of Stefan problems with phase relaxation introduced by A. Visintin [\[90](#page-8-12)].

By denoting $\theta = \beta(u)$ the temperature and $\chi = u - \theta$ the phase variable, the PDE in [\(1](#page-1-0)) reads

$$
\frac{\partial(\theta + \chi)}{\partial t} - \Delta\theta = 0, \quad \chi \in H(\theta), \tag{4}
$$

where *H* stands for the Heaviside graph. Being $\varepsilon > 0$ a time-relaxation parameter, the constitutive relation in [\(4](#page-2-0)) can be approximated with the phase relaxation equation introduced by A. Visintin [[90\]](#page-8-12)

$$
\varepsilon \frac{\partial \chi}{\partial t} + H^{-1}(\chi) \ni \theta. \tag{5}
$$

After coupling this equation (5) (5) with the PDE in (4) (4) , and discretizing in time [\[87](#page-8-11)] we get the following algorithm

$$
\begin{cases} \left(\Theta^n - \Theta^{n-1}\right) + \left(X^n - X^{n-1}\right) - \tau \Delta \Theta^n = 0, \\ \frac{\varepsilon}{\tau} \left(X^n - X^{n-1}\right) + H^{-1} \left(X^n\right) \ni \Theta^{n-1}, \end{cases} \tag{6}
$$

with stability constraint $\tau \leq \varepsilon$. Now it is not difficult to see that this scheme [\(6](#page-2-2)) reduces to [\(3](#page-1-2)) by choosing $\varepsilon = \tau$ and setting $U^n = \Theta^n + X^n$. With the tools above, Magenes *et al.* [[50\]](#page-7-12) completely answered the question of how accurate the nonlinear

Chernoff formula is both for degenerate and non-degenerate parabolic problems. Let $E_{\tau} = ||\theta - \Theta^n||_{L^2(\Omega \times (0,T))}$ be the error for temperature in energy norm, then the following *optimal a priori* error estimates were proved for Stefan problems: $E_{\tau} = O(\tau^{1/4})$ if $u_0 \in L^2(\Omega)$ or $E_{\tau} = O(\tau^{1/2})$ if $u_0 \in D(A) \cap L^{\infty}(\Omega)$.

Combined with a finite element method for spatial approximation, the Chernoff formula ([3\)](#page-1-2) leads to a very efficient numerical algorithm [\[64](#page-7-15), [66\]](#page-7-16) (see [\[69](#page-7-17), [70\]](#page-7-18) for *a posteriori* error estimates and an adaptive implementation). See also [\[28](#page-6-9)] for a refinement of the stabilization parameter in the Chernoff formula.

In a series of papers [[35](#page-6-10)[–38](#page-6-11)] Magenes addressed various extensions of the previous results for the nonlinear Chernoff formula to more general operators and problems, in particular to evolutionary equations on the boundary of a domain. In [\[51](#page-7-19)] Magenes *et al.* proved new regularity results in Nikolskiⁱ spaces for the multidimensional two-phase Stefan problem with general source terms and, as a consequence, error estimates for enthalpy in energy spaces for the implicit Euler algorithm.

2 Stefan Problems in a Concentrated Capacity

The Stefan problems in a *concentrated capacity* [\[24](#page-5-19)] arise in heat diffusion phenomena involving phase changes in two adjoining bodies *Ω* and *Γ* , when assuming that the thermal conductivity along the direction normal to the boundary of *Ω* is much greater than in the others, whence *Γ* can be considered as the boundary of *Ω*. The mathematical model describing phase change process in both bodies reads [\[42](#page-6-12)]:

$$
\begin{cases}\n\frac{\partial u}{\partial t} - \Delta_g \beta(u) = \frac{\partial \beta(u)}{\partial v} & \text{on } \partial \Omega \times (0, T), \\
u(\cdot, 0) = u_0(\cdot) & \text{on } \partial \Omega, \\
\frac{\partial v}{\partial t} - \Delta \gamma(v) = 0 & \text{in } \Omega \times (0, T), \\
v(\cdot, 0) = v_0(\cdot) & \text{in } \Omega, \\
\gamma(v) = \beta(u) & \text{on } \partial \Omega \times (0, T),\n\end{cases} (7)
$$

where Δ_g is the Laplace-Beltrami operator on $\partial\Omega$ with respect to the Riemannian structure *g* inferred by the tangential conductivity, β and γ are the constitutive relations between enthalpies *u* and *v* and temperature $\theta = \beta(u) = \gamma(v)$. Existence and uniqueness of the solution of (7) (7) was proved in suitable functional spaces $[42]$ $[42]$. In a series of papers [\[39](#page-6-13)[–41](#page-6-14), [43](#page-6-15)[–46](#page-6-16)] Magenes addressed the theory of heat conduction with phase change in a concentrated capacity for various operators; see also [[82\]](#page-8-13). The relevance of these models in a number of physical applications motivates their numerical analysis, which was developed in [[47](#page-7-20)]. The implicit Euler scheme reads:

$$
\begin{cases}\n\beta(U^n) = \gamma(V^n) & \text{on } \partial\Omega, \\
\int_{\partial\Omega} (U^n - U^{n-1})\varphi + \tau (d\beta(U^n), d\varphi)_g \\
+ \int_{\Omega} (V^n - V^{n-1})\eta + \tau \int_{\Omega} \nabla \gamma(V^n) \cdot \nabla \varphi = 0 \quad \forall \varphi.\n\end{cases}
$$
\n(8)

The linear scheme based on the nonlinear Chernoff formula reads:

$$
\begin{cases}\n\Xi^n = \Theta^n & \text{on } \partial\Omega, \\
\int_{\partial\Omega} \Xi^n \varphi + \tau (d\Xi^n, d\varphi)_g + \int_{\Omega} \Theta^n \eta + \tau \int_{\Omega} \nabla \Theta^n \cdot \nabla \varphi \\
= \int_{\partial\Omega} \beta (U^{n-1}) \varphi + \int_{\Omega} \gamma (V^{n-1}) \varphi \quad \forall \varphi, \\
U^n = U^{n-1} - \beta (U^{n-1}) + \Xi^n & \text{on } \partial\Omega, \\
V^n = V^{n-1} - \gamma (V^{n-1}) + \Theta^n & \text{in } \Omega.\n\end{cases}
$$
\n(9)

Both algorithms [\(8](#page-3-1)) and [\(9](#page-4-0)) are well posed. The latter is linear in the unknowns \mathbb{Z}^n and Θ^n , the nonlinearity reducing to pointwise corrections for U^n and V^n , whence it is expected to be more efficient than (8) (8) from a numerical viewpoint. Stability and error estimates in the natural energy spaces were proved for both schemes in [\[47\]](#page-7-20).

3 Approximation of Interfaces, Adaptivity and Applications

Optimality of error estimates for the proposed algorithms was one of the main aspects attracting Magenes' interest; in this direction let me mention [[74\]](#page-8-14), where R.H. Nochetto *et al.* proved *optimal a posteriori* error estimates for variable time-step discretizations of nonlinear evolution equations; see also [[81\]](#page-8-15).

Thanks to stimulating discussions with E. Magenes, C. Baiocchi, F. Brezzi, and L.A. Caffarelli, [[2,](#page-5-20) [7,](#page-5-21) [9\]](#page-5-22) convergence and accuracy estimates for the approximation of the free boundary of parabolic phase-change problems under suitable condition of non-degeneracy at the interface were proved [\[62,](#page-7-21) [78\]](#page-8-16).

The intense interest of Enrico Magenes for the numerical approximation of phase-change models and their applications involved the Istituto di Analisi Numerica of the CNR in Pavia and his collaborators in various national and international projects focused on phase transition problems; I will mention, e.g., the European projects "Phase Transition Problems" (1986–1988), "Mathematical Treatment of Free Boundary Problems" (1993–1996), "Phase Transition and Surface Tension" (1995–1997), "Viscosity Solutions and their Applications" (1998–2000). Within the framework of the national projects of the CNR "Software: Ricerche di Base e Applicazioni; Software Matematico" (1986–1987) and "Sistemi Informatici e Calcolo Parallelo: Calcolo Scientifico per Grandi Sistemi" (1988–1993), a computational code for solving general parabolic free boundary problems with the finite elements algorithms studied above was implemented [\[77](#page-8-17)]; some interesting collaborations took place with Himont (Ferrara), a leading factory in polymer production [\[52\]](#page-7-22), and Istituto Ortopedico Rizzoli (Bologna) [\[53](#page-7-23)].

Numerical approximation of geometric motion of interfaces, a first step for the approximation of more complex phase transitions problems including surface tension effects, was addressed by R.H. Nochetto *et al.* [[71–](#page-8-18)[73](#page-8-19), [76](#page-8-20)], also thanks to helpful discussions and suggestions of E. De Giorgi, L.A. Caffarelli, A. Visintin, and Magenes himself.

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