6. Free Boundary Problems and Phase Transitions

Initial and initial-boundary value problems for systems of partial differential equations (PDEs) have functions or, more generally, distributions in the scalar case and vector fields of functions or distributions in the vector-valued case as solutions. Usually, the d-dimensional domain, on which the PDEs are posed, is given and the problem formulation is based on a fixed geometry. Obviously, there have to be compatibilities between the differential operator, particularly its differential order and certain geometric properties, and the side (initial-boundary) conditions and the geometry of the domain on which the problem is posed in order to guarantee well-posedness of the problem under consideration. In particular, for a given differential operator the number of initial-boundary conditions and the geometry of the domain boundary are crucial for solvability, uniqueness and continuous dependence on data.

Free boundary problems for PDEs have a totally different feature, namely that geometric information is an inherent part of the solution. Typically, the solution of a free boundary problem consists of one or more functions or distributions AND a set (the so called free boundary, subset of $\mathbb{R}^d$), on which certain conditions

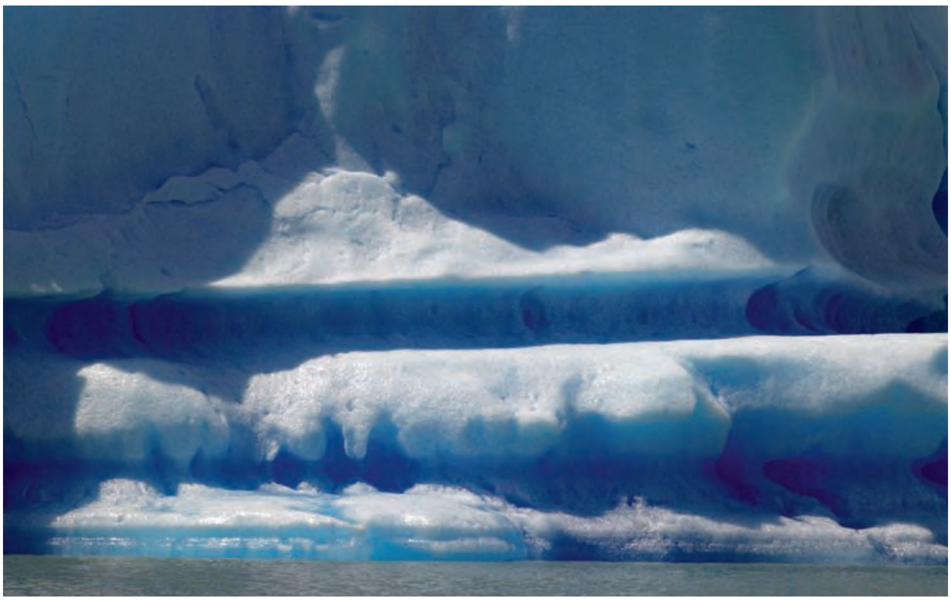

Fig. 6.1. Layered iceberg, Lago Argentino

on the unknown function(s) are prescribed. If we assume for a moment that the free boundary is fixed, then, typically, the problem would be over-determined. So, in fact, the additional conditions are needed to determine the free boundary itself.

Regularity (smoothness) is an important issue in PDE theory. Usually, a certain degree of regularity (differentiability in the classical or weak sense) of the solutions of initial-boundary value problems is necessary to prove their uniqueness, their continuous dependence on the data, to carry out certain scaling limits, as done in singular perturbation theory, and to devise efficient numerical discretisation techniques. For free boundary problems the situation is definitely more complex. Not only the regularity of the unknown functions is important, but also the regularity of the unknown set, the free boundary. Typical questions, which arise, are: does the free boundary have empty topological interior? What are its measure theoretical properties? Is it a (finite union of) smooth manifolds? What is the optimal regularity of the free boundary? In many cases the study of the optimal regularity of the free boundary is of paramount importance for understanding the solution of the free boundary problem under consideration, to prove uniqueness, stability etc.

Obviously, the mathematical literature of free boundary problems is vast, at this point we refer to the book [4] for a review of basic analytical tools and for further references.

To start a more concrete discussion, we consider the maybe best-studied free boundary problem, the so called obstacle problem for the Laplace operator. Let us consider the classical Dirichlet functional

$$D(v) := \frac{1}{2} \int_G |\operatorname{grad} v|^2 dx \,, \tag{6.1}$$

where G is a bounded domain in $\mathbb{R}^d$ with a sufficiently smooth boundary ∂G. Also, let us fix the boundary values of v and, for the moment, the considered class of functions

$$Y := \left\{ v \in H^1(G) \mid v = \psi \quad \text{on} \quad \partial G \right\} \,, \tag{6.2}$$

where ψ is a prescribed function in the Sobolev space $H^1(G)$, which consists of those square integrable functions, defined almost everywhere in G with values in $\mathbb{R}$, which also have a square integrable distributional gradient.

It is an easy exercise to show that the minimum u of the functional D over the set of functions Y is the unique harmonic function on G assuming the boundary values ψ, i.e. u uniquely solves the boundary value problem:

$$\Delta u = 0 \quad \text{in} \quad G \tag{6.3}$$

$$u = \psi \quad \text{on} \quad \partial G \,. \tag{6.4}$$

The obstacle problem is obtained by a modification of this minimizing procedure. Let $\phi \in H^1(G)$ be another given function, the so called obstacle, and look

Fig. 6.2. An iceberg with a central spire, Lago Argentino

for a mimimizer of the energy functional D, which is in Y AND which nowhere (in the almost everywhere sense) in G stays below the obstacle ϕ. More formally, consider the convex set of functions:

$$X := Y \cap \{v \,|\, v \geq \phi\} \tag{6.5}$$

and find:

$$u := \mathrm{argmin}_{v \in X} D(v) \,. \tag{6.6}$$

Clearly, the obstacle ϕ cannot stay above the function ψ on the boundary of G, i.e. we assume:

$$\phi \leq \psi \quad \text{on} \quad \partial G \,. \tag{6.7}$$

In the two 2-dimensional case the solution of the obstacle problem can be seen as the (small amplitude) displacement of an elastic membrane, fixed at the boundary, minimizing its total energy under the constraint of having to stay above a solid obstacle.

It is actually easy to show that the obstacle problem (6.6) has a unique solution (minimizer) $u \in X$, all the technical mathematical analysis goes into the investigation of the regularity properties of its solution u and of the free boundary defined below.

We define the non-coincidence set N as

$$N := \{x \in G \,|\, u(x) > \phi(x)\}$$

and the coincidence set C

$$C := \{x \in G \,|\, u(x) = \phi(x)\} \;.$$

Then the free boundary F is defined as that part of the topological boundary of N, which lies in G, i.e.

$$F := \partial N \cap G \,,$$

in other words it is the interface between the sets C and N.

It is a simple exercise to derive the Euler–Lagrange equations of the minimisation problem (6.6). We find, assuming sufficient regularity of the minimizer u and of the free boundary F:

$$\Delta u = 0 \quad \text{in} \quad N \,, \quad u = \phi \quad \text{in} \quad C \quad \text{and} \quad -\Delta u \geq 0 \quad \text{in} \quad G \tag{6.8}$$

$$u = \phi \quad \text{and} \quad \mathrm{grad}\, u \cdot n = \mathrm{grad}\, \phi \cdot n \quad \text{on} \quad F \,, \tag{6.9}$$

where n denotes a unit normal vector to F, and finally:

$$u = \psi \quad \text{on} \quad \partial G \,. \tag{6.10}$$

Obviously, when F is a fixed hyper-surface in G, then one of the conditions in (6.9) is redundant and the problem 6.8–6.10 is overdetermined.

In order to illustrate the difficulties of the obstacle problem, set

$$w = u - \phi \,, \quad x \in G \,.$$

Then, denoting $h(x) = -\Delta\phi(x)$, we can rewrite the Euler–Lagrange system (6.8)–(6.10) as

$$\Delta w = h(x) 1_{\{w>0\}} \tag{6.11}$$

$$w = \psi - \phi \quad \text{on} \quad \partial G \,. \tag{6.12}$$

Note that the minimisation of the Dirichlet functional over the set Y defined in (6.2) leads to a simple linear problem while the minimisation over the constrained set X leads to a complicated nonlinear problem, as indicated by the right hand side of (6.11)! Assuming a smooth obstacle we conclude that the right hand side of the semilinear Poisson equation (6.11) is bounded in G, such that by classical interior regularity results of linear uniformly elliptic equations we conclude that the solution w is locally in the Sobolev space $W^{2,p}$ for every $p < \infty$ (which is the space of locally p-integrable functions with locally p-integrable weak second derivatives). By the Sobolev imbedding theorem we conclude that w (and consequently u) is locally in the space $C^{1,\alpha}$ (locally Hölder continuous first derivatives) for every $0 < \alpha < 1$. More cannot be concluded from this simple argument.

From the many results on optimal regularity of the solution of the obstacle problem we cite the review [2], where optimal local regularity for u, i.e. $u \in C^{1,1}$ is shown, if the obstacle is sufficiently smooth. Note that the optimality of this result follows trivially from the fact that Δu jumps from 0 to $\Delta\phi$ on the free boundary F! Moreover, the free boundary has locally finite $(n-1)$-dimensional Hausdorf measure and is locally a $C^{1,\alpha}$ surface, for some α in the open interval $(0, 1)$, except at a 'small' set of singular points, contained in a smooth manifold. Singularities can be excluded by assuming an exterior cone condition. Moreover, if the free boundary is locally Lipschitz continuous, then it is locally as smooth as the data, in particular it is locally analytic, if the data are analytic. We remark that the proof of the optimal regularity of the free boundary requires deep insights into elliptic theory, in particular the celebrated 'monotonicity formula' of Luis Caffarelli[1].

A more complex application of free boundary problems arises in the theory of phase transitions. A historically important example of a phase transition is the formation of ice in the polar sea, as originally investigated by the Austrian mathematician Josef Stefan[2] (1835–1893). In the year 1891 Stefan published his

1 *http://www.ma.utexas.edu/users/caffarel/*
2 *http://www-groups.dcs.st-and.ac.uk/~history/Mathematicians/Stefan_Josef.html*

Fig. 6.3. Melting iceberg

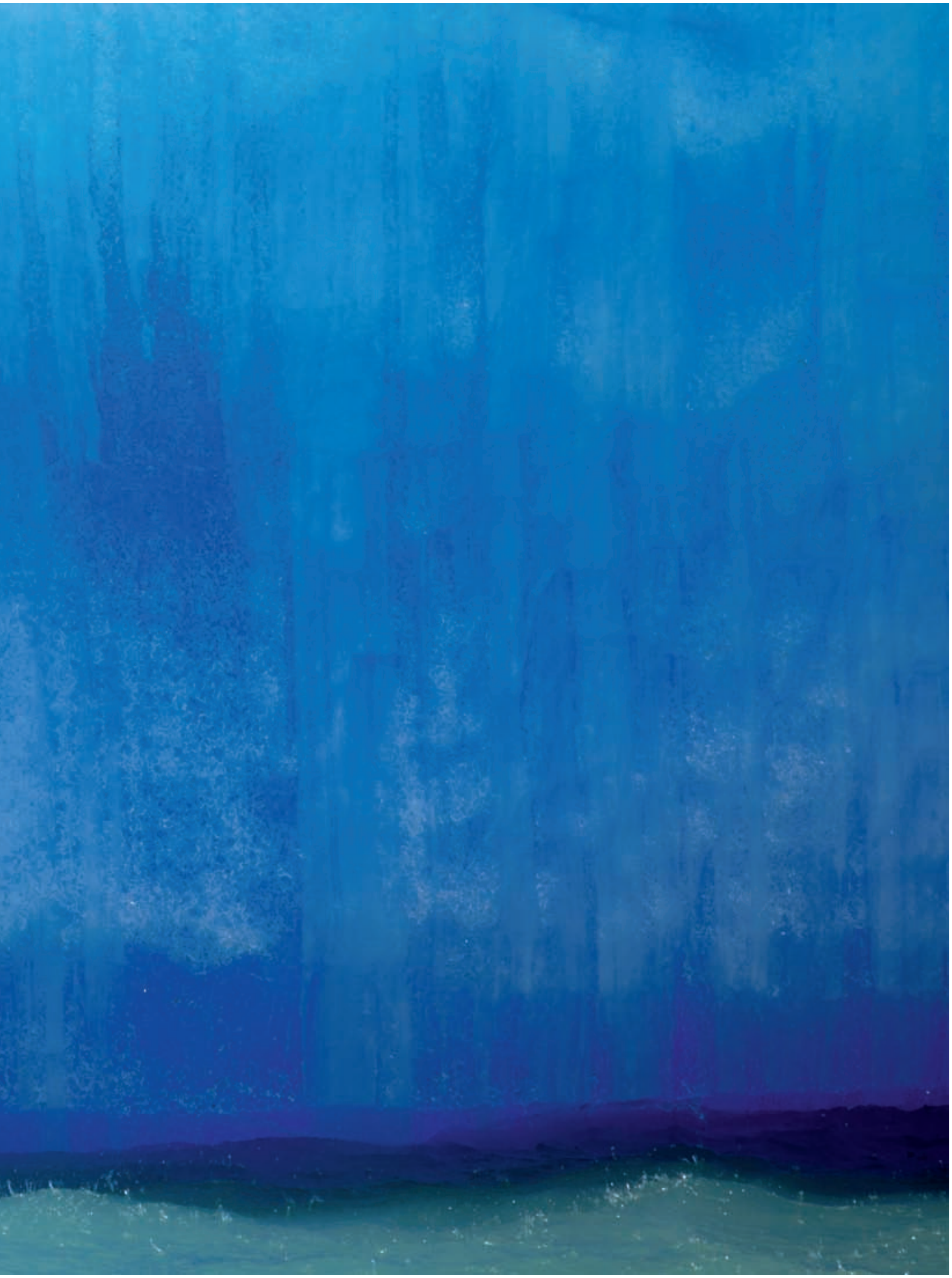

Fig. 6.4. Iceberg, the Stefan boundary hits the fixed boundary (water surface)

seminal paper [7], investigating the ice layer formation in a water-ice phase transition. Interestingly enough, Stefan compared his data, obtained by mathematical modeling, to measurements taken in the quest of the search of a north-west passage [11] through the northern polar sea. In his paper [7] Stefan investigated the non-stationary transport of heat in the ice and formulated a free boundary problem, which is now known as the classical Stefan problem and which has given rise to the modern research area of phase transition modeling by free boundary problems. As a basic reference we refer to [10].

Some of the photographs associated to this chapter show icebergs in lakes of Patagonia. The evolution of their water-ice phase transition free boundary is modeled by the 3-dimensional Stefan problem formulated below.

Therefore, consider a domain $G \in \mathbb{R}^d$ (of course $d = 1, 2$ or 3 for physical reasons but there is no mathematical reason to exclude larger dimensions here), in which the ice-water ensemble is contained. At time $t > 0$ assume that the domain G is divided into 2 subdomains, $G_1(t)$ containing the solid phase (ice) and $G_2(t)$ containing the liquid phase (water). These subdomains shall be separated by a smooth surface $\Gamma(t)$, where the phase transition occurs. $\Gamma(t)$ is the free boundary, an unknown of the Stefan problem. Heat transport is modeled by the linear heat equation:

$$\theta_t = \Delta\theta + f\ , \quad x \in G_1(t) \quad \text{and} \quad x \in G_2(t)\ ,\ t > 0\ , \tag{6.13}$$

where f is a given function describing external heat sources/sinks. Here we assumed that the local mass density, the heat conductivity and the heat capacity at constant volume are equal and constant 1 in both phases. More realistically, piecewise constants can be used for modeling purposes. The parabolic PDE (6.13) has to be supplemented by an initial condition

$$\theta(t = 0) = \theta_0 \quad \text{in} \quad G \tag{6.14}$$

and appropriate boundary conditions at the fixed boundary ∂G. Usually, the temperature is fixed there

$$\theta = \theta_1 \quad \text{on} \quad \partial G \tag{6.15}$$

or the heat flux through the boundary is given:

$$\operatorname{grad}\theta\ .\nu = f_1 \quad \text{on} \quad \partial G\ ,\ t > 0\ . \tag{6.16}$$

Here ν denotes the exterior unit normal to ∂G. Also, mixed Neumann–Dirichlet boundary conditions can be prescribed, corresponding to different types of boundary segments.

Disregarding the phase transition the problem (6.13), (6.14), (6.15) or (6.16) is well-posed. Thus, additional conditions are needed to determine the free boundary. The physically intuitive condition says that the temperature at the free boundary is the constant melting temperature θ_{m} of the solid phase. Obviously

Fig. 6.5. A glimpse on the Stefan boundary under the water surface

Fig. 6.6. Complicated structure of the free boundary and its intersection with the fixed boundary

we can normalize $\theta_{\rm m} = 0$ and regard θ from now on as the difference between the local temperature and the melting temperature:

$$\theta = 0 \quad \text{at} \quad \Gamma(t) . \tag{6.17}$$

Note that the condition (6.17) cannot suffice to determine the free boundary. Fixing $\Gamma(t)$ arbitrarily (in a non-degenerate way) leaves us with two decoupled linear boundary value problems for the heat equation, one in each phase with Dirichlet boundary data on the interface. Both of these problems are uniquely solvable!

The second interface condition, derived from local energy balance [9], reads:

$$Lv_n = [\operatorname{grad}\theta \, .n] , \tag{6.18}$$

where n denotes the unit normal to the interface, [.] stands for the jump across the interface and v_n for the interface velocity in orthogonal direction. L is the latent heat parameter representing the energy needed for a phase change.

When the interface is a regular surface, given by the equation $H(x, t) = 0$, we have

$$v_n = -H_t \operatorname{grad} H \cdot n .$$

In (6.18) we assume that the vector n points into the liquid phase and that the jump is defined by (to get the signs right …):

$$[g] := g|_{\text{fluid}} - g|_{\text{solid}} \quad \text{on} \quad \Gamma(t) \,. \tag{6.19}$$

Note that at time $t = 0$ the interface $\Gamma(t = 0)$ is given by the 0-level set of the initial datum θ_0.

To get more insights we consider the one dimensional single phase Stefan problem, assuming that the temperature in the liquid phase is constant and equal to the melting temperature. Defining u as the difference of the melting temperature and the solid phase temperature (i.e. $u = -\theta > 0$ in the solid phase), we obtain the one-dimensional single phase problem, with interface $x = h(t)$ and fixed (Dirichlet) boundary at $x = 0$:

$$\begin{gathered} u_t = u_{xx} \,, \quad 0 < x < h(t) \\ u(x = 0, t) = \alpha(t) \geq 0 \,, \quad t > 0 \\ u(h(t), t) = 0 \,, \quad t > 0 \\ u(x, t = 0) = u_0(x) \,, \quad 0 < x < h(t) \,, \end{gathered}$$

subject to the Stefan condition:

$$L \frac{dh(t)}{dt} = -u_x(h(t), t) \,, \quad t > 0 \,.$$

This models for example the growth of an ice layer located in the interval $[0, h(t)]$. The Dirichlet boundary $x = 0$ represents the water/ice–air interface, at which the temperature variable is prescribed to be $\alpha(t)$ (below freezing). $x = h(t)$ is the ice-water interface. In order to study the onset and evolution of ice formation we assume $h(0) = 0$, i.e. no ice is present at $t = 0$. Also, external heat sources are excluded and homogeneity in the x_2 and x_3 directions (parallel to the water surface) is assumed in order to obtain a one-dimensional problem. Note that the x-variable denotes the perpendicular coordinate to the water/ice surface, pointing into the water/ice.

We remark that this problem was already stated by Stefan in his original paper [7] and that he found an explicit solution for

α = const. The solution reads (see also [11]):

$$h(t) = 2\mu\sqrt{t}$$

$$u(x, t) = \alpha \frac{\int_{\sigma(x,t)}^{\mu} \exp(-z^2) dz}{\int_0^{\mu} \exp(-z^2) dz} \,, \quad 0 < x < h(t)$$

where

$$\sigma(x, t) = \frac{x}{2\sqrt{t}}$$

Fig. 6.7. A glacier flowing into Lago Argentino from the southern ice field

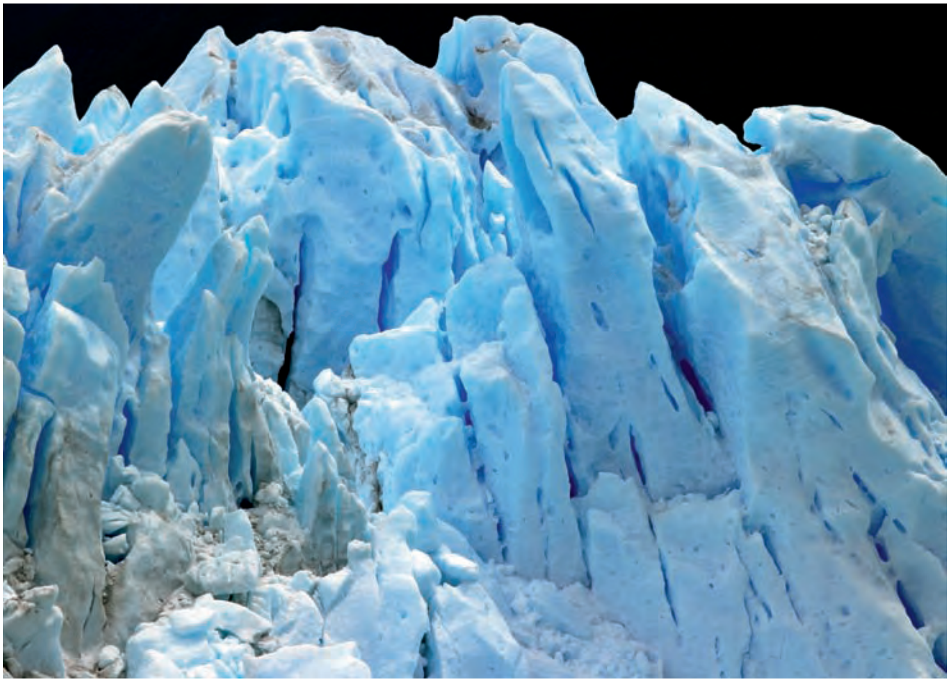

Fig. 6.8. Penitentes

and μ solves a transcendental equation:

$$\mu \exp(\mu^2) \int_0^\mu \exp(-z^2) dz = \frac{\mu}{2L} .$$

Note that the thickness of the ice layer behaves like $\sqrt{t}$. Stefan found coincidence of this theoretical result with the experimental data available to him.

There is a convenient reformulation of the Stefan problem in terms of a degenerate parabolic equation, making use of the enthalpy formulation of heat flow. The physical enthalpy e is related to the temperature θ by

$$\theta = \beta(e) , \tag{6.20}$$

where

$$\begin{aligned} \beta(e) &= e + \frac{L}{2} , && \text{for} \quad e < 0 \\ \beta(e) &= 0 , && \text{for} \quad -\frac{L}{2} < e < \frac{L}{2} \\ \beta(e) &= e - \frac{L}{2} , && \text{for} \quad e > 0 \end{aligned} \tag{6.21}$$

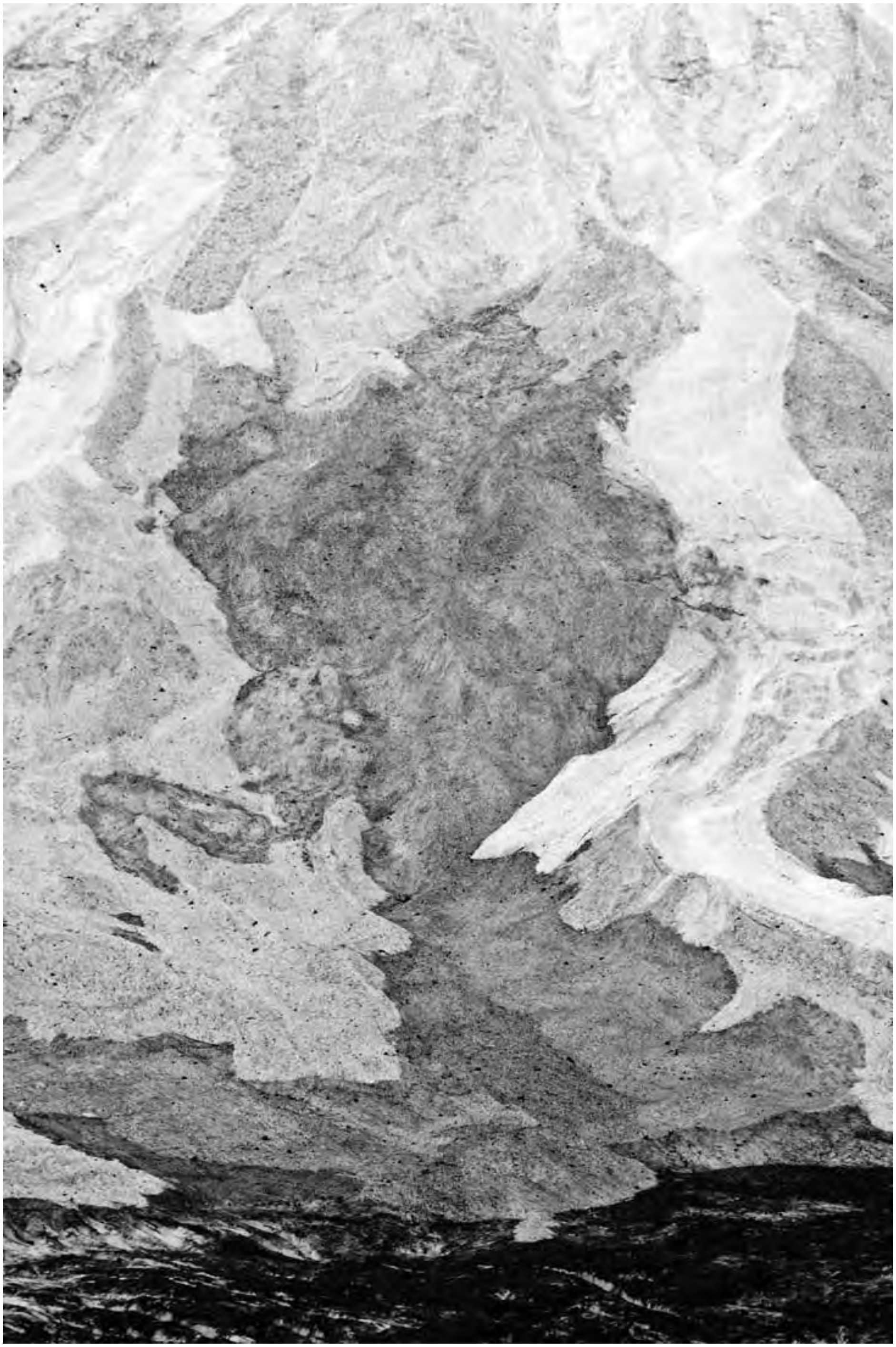

Fig. 6.9. Glacier in Chilean Patagonia

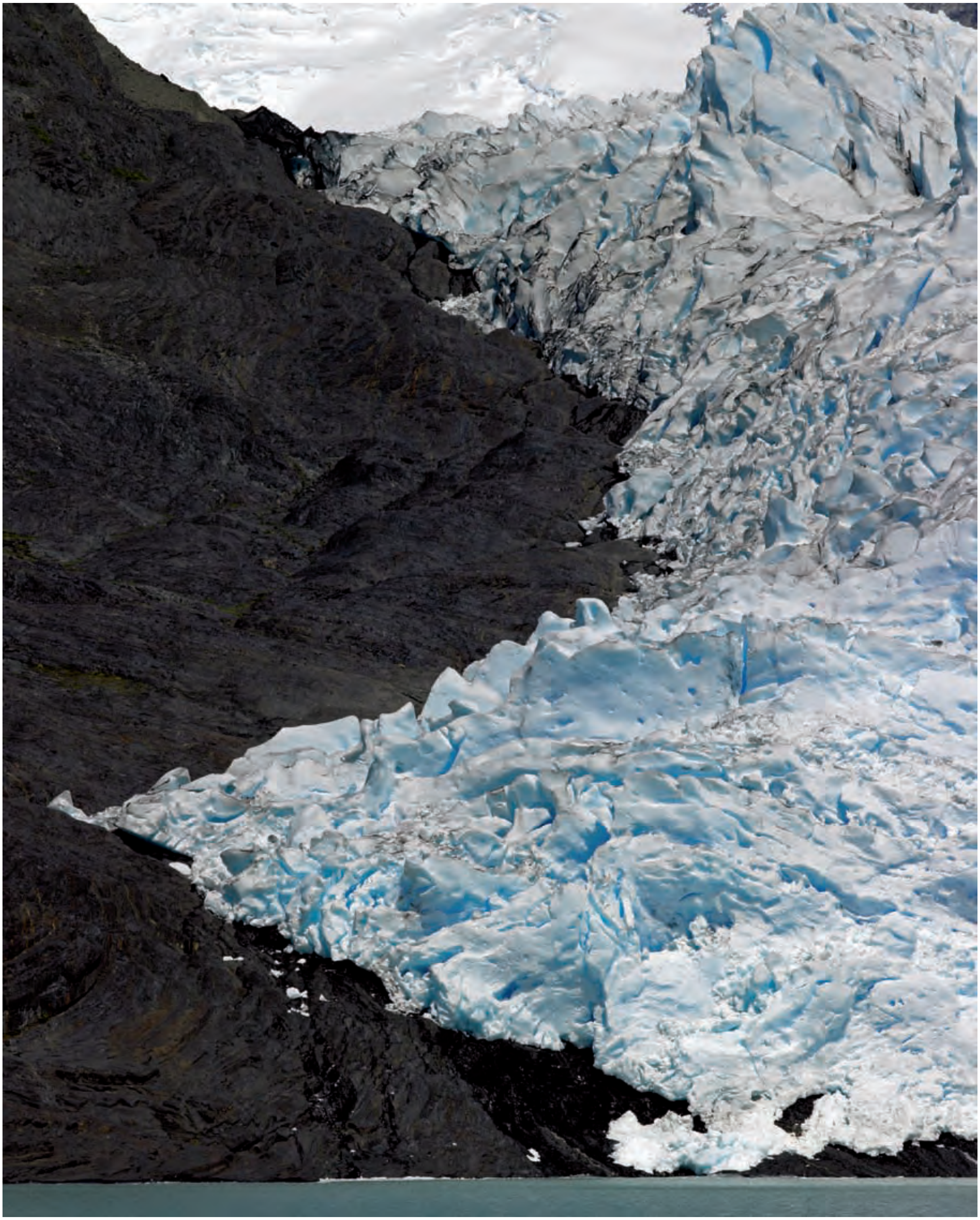

Fig. 6.10. Free boundary of glacier flow, Patagonia

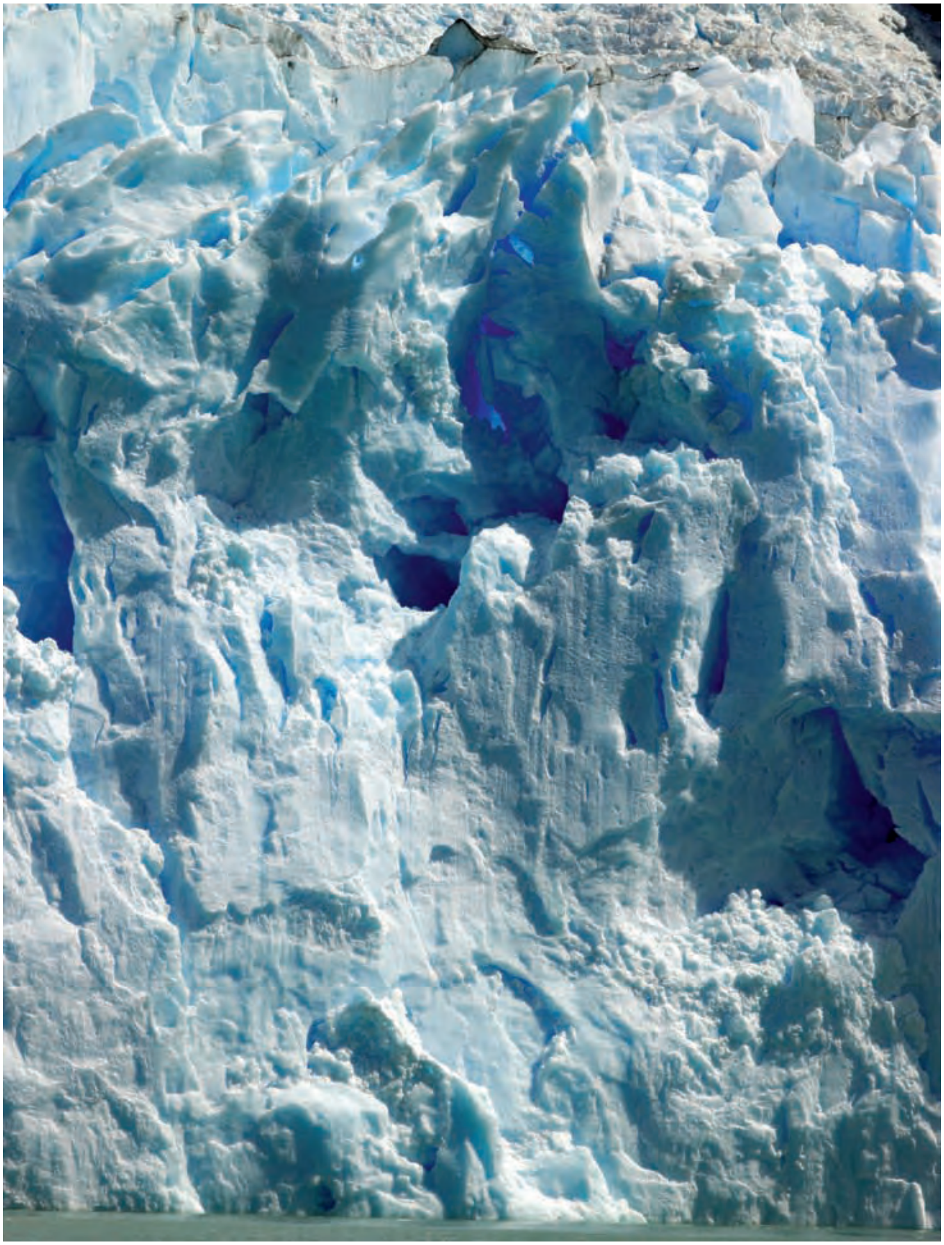

Fig. 6.11. A glacier front entering Lago Argentino

(see [9]). Now consider the degenerate parabolic PDE for the enthalpy:

$$e_t = \Delta\beta(e) + f\ , \quad x \in G\ ,\ t > 0 \tag{6.22}$$

subject to an initial condition

$$e(t = 0) = e_0 \tag{6.23}$$

which is such that $\theta_0 = \beta(e_0)$. Note that the temperature can be calculated uniquely from the enthalpy but not the other way around! Also we prescribe appropriate boundary conditions of Dirichlet or Neumann type (in correspondence to the boundary conditions (6.15)) on the fixed boundary ∂G:

$$e = e_1 \quad \text{on} \quad \partial G\ ,\ t > 0 \tag{6.24}$$

where, again, e_1 is such that $\theta_1 = \beta(e_1)$, or, resp.

$$\operatorname{grad} e.\nu = f_1 \quad \text{on} \quad \partial G\ ,\ t > 0\ . \tag{6.25}$$

It is a simple exercise in distributional calculus to show that a smooth solution e of (6.22)–(6.25), which is such that its 0-level set is a smooth surface in G for $t > 0$, gives a smooth solution θ of the Stefan problem (6.13)–(6.18), simply by defining the temperature $\theta = \beta(e)$ and the free boundary $\Gamma(t)$ as the 0-level set of $e(\cdot, t)$. The nice feature of the nonlinear initial-boundary value problem for the degenerate parabolic equation (6.22) is the fact that the phase transition boundary $\Gamma(t)$ does not appear explicitely. This allows for somewhat simpler analytical and numerical approaches.

For a collection of analytical results and references on the Stefan problem and its variants we refer to [8].

Comments on the Images 6.1–6.8 The Images 6.1–6.7 show icebergs in Patagonian lakes. Clearly, the free Stefan boundary is not visible itself, since it is the ice-water phase transition under the water surface. In Image 6.5 and in Image 6.6 we get a glimpse of it, though … What we see on the other images is – at least in part – the intersection of the free (Stefan) boundary with the fixed boundary (water surface). Note that about 7/8 of the mass of a typical iceberg is under water[3]!

Also the air-ice interface of icebergs, which is very well visible in most of the Images 6.1–6.7 is determined by a free boundary problem, however, of much more complicated nature than the Stefan Problem determining the ice-water phase transition. Clearly, various mechanisms enter in the formation of the above-water surface of an iceberg: the formation process of the iceberg itself (mostly through calving from a glacier) giving the initial condition, the wind pattern, erosion by waves, ablation (through solar radiation), melting …[4].

[3] *http://www.wordplay.com/tourism/icebergs*
[4] *http://www.wordplay.com/tourism/icebergs*

For a mathematical model of ablation see [1], where an integro-differential equation for the snow/ice surface is derived, based on the heat equation with a self-consistent source term accounting for ablation through solar radiation. We remark that in this reference the flow of melt water along the surface and refreezing effects are neglected (the paper deals with glacier surface modeling), which are important in iceberg surface modeling. In reference [1] it is argued that the derived nonlinear model, which takes into account surface light scattering, is able to describe typical glacier surface structures like penitents (resembling a procession of monks in robes), as can be seen in the Image 6.8.

Comments on the Images 6.9–6.11 For most macroscopic modeling purposes the flow of glaciers and ice fields is assumed to be slow and incompressible, taking into account a specific relationship between the strain tensor and the ice viscosity [6]. Assuming isothermal flow and shallow ice, a time-dependent highly nonlinear version of the obstacle roblem, based on a quasilinear diffusion equation for the local height (over ground) of the ice is obtained, known as a classical model of glaciology (see [6] for a physical derivation and references). The free boundary is represented by the edge of the glacier or ice field (the obstacle is the ground level surface!). In its most simple form, assuming 2-dimensional flow of an ice sheet over its bed surface $z = H(x)$, with small variations in x and uniform in the second spatial coordinate y, the model reads:

$$h_t = \left(\frac{(h-H)^5 h_x^3}{5} - u_b(x,t)(h-H) \right)_x + a(x,t) \quad \text{on} \quad \{h(x,t) > H(x)\} \ .$$

The unknown h denotes the height over ground, assuming uniformity of the flow in y, and u_b the given sliding velocity in x direction. Clearly, the cross-section of the ice sheet at time t is the set in the (x,z)-plane, where $H(x) < z < h(x,t)$. The flow is assumed to be driven by gravity, caused by the variation of the weight of the ice depending on its height, and by sliding at the ice-bed interface. For realistic glacier modeling large variations of the bed $z = H$ have to be taken into account to describe mountain slopes, e.g. by tilting the geometry. We remark that this problem becomes particularly interesting when source terms $a = a(x,t)$ are present, e.g. modeling snowfall on the glacier or ablation by solar rays. A mathematical analysis of properties of the free boundary (in one space dimension) can be found in [3]. We refer to [5] for an excellent account of glacier physics.

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[6] can be downloaded from *http://www.dmf.bs.unicatt.it/cgi-bin/preprintserv/paolini/Pao02A*