Chapter 1
Ray-tracing the Ulam way

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1.1 Introduction

Ray-tracing is a well established approach for modelling wave propagation at high frequencies, in which the ray trajectories are defined by a Hamiltonian system of ODEs [Ce01]. An approximation of the wave amplitude is then derived from estimating the density of rays in the neighbourhood of a given evaluation point. An alternative approach is to formulate the ray-tracing model directly in terms of the ray density in phase-space using the Liouville equation. The solutions may then be expressed in integral form using the Frobenius-Perron (F-P) operator, which is a transfer operator transporting the ray density along the trajectories [CvEtAl20]. The classical approach for discretising such operators dates back to 1960 and the work of Stanislaw Ulam [Ul64]. The convergence of the Ulam method has been established

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in some cases, typically in low dimensional settings with continuous densities and hyperbolic dynamics, see for example [Li76, Fr99, BoMu01].

In this chapter we outline some recent work investigating the convergence of the Ulam method for ray tracing in triangular billiards, where the dynamics are parabolic and the flow map contains jump discontinuities. This study builds upon recent work on ray tracing in circular billiards [SlEtAl20], where it was found that a spectral Fourier Galerkin approximation of the F-P operator gave faster convergence rates than would be possible using the Ulam method, and the precise rate depends critically on the regularity of the boundary data driving the problem. However, the rigorous study of polygonal billiards such as the triangle is innately more challenging owing to the presence of vertices. In particular, the momentum component of the boundary flow map, which defines the phase-space coordinates of the ray trajectory at discrete times corresponding to boundary collisions, is discontinuous at the vertices. The presence of these discontinuities necessitates the use of function spaces including discontinuous functions, such as Sobolev spaces of low regularity or spaces of bounded variation [Ke85, Sa00]. A Galerkin projection using a Fourier basis as proposed for circular billiards in [SlEtAl20] and analysed within a Sobolev function space setting is therefore less suited to polygonal billiards, since there is no smoothness of the boundary flow map to exploit. Instead, Ulam-type methods appear to provide a more natural fit owing to their use of discontinuous basis functions that better reflect the properties of the F-P operator here.

In the remainder of this chapter we will first outline a mathematical model for propagating ray densities using transfer operators. We then describe the discretisation of this model using the Ulam method for triangular domains, as well as giving some pointers towards a convergence analysis for this discretisation. Finally, we draw some conclusions from our findings and discuss some related studies where faster convergence rates are plausible.

1.2 Ray-tracing via transfer operators

The transport of densities along a ray trajectory flow map φ^τ through time τ and space $\mathbb{R}^d$ can be formulated in terms of the F-P operator (see, for example, [CvEtAl20]). The action of this operator on a density f may be expressed as

$$\mathscr{L}^\tau f(X) = \int \delta(X - \varphi^\tau(Y)) f(Y)\,\mathrm{d}Y,$$

where X and Y are phase-space coordinates in $\mathbb{R}^{2d}$. Solving such problems when $d > 1$ and for physically relevant systems is often considered intractable due to both high dimensionality and potentially complex geometries [SiEtAl07].

In this work we reformulate the F-P operator as a phase-space boundary integral operator, which is discretised using the Ulam method. We restrict our attention to modelling the propagation of a density f through a convex polygonal domain $\Omega \subset \mathbb{R}^2$. Let us assume that the ray trajectory flow is governed by the Hamiltonian

$H(\boldsymbol{r},\boldsymbol{p}) = |\boldsymbol{p}| = 1$ in Ω, where $\boldsymbol{r} \in \Omega$ and $\boldsymbol{p}$ is the momentum coordinate. Let the phase-space P on the boundary of Ω be written $P = \partial\Omega \times (-1,1)$. Then the associated coordinates are given by $X = [s,p] \in P$ with $s \in [0,L)$ parameterising $\partial\Omega$, where L is the total length of the boundary, and $p \in (-1,1)$ parameterising the component of the inward unit vector $\boldsymbol{p}$ tangential to $\partial\Omega$. Next we define $\varphi : P \to P$ to be the boundary flow map, which takes a vector in P and maps it along the Hamiltonian flow defined by H to a vector in P. The propagation of the density f along the map φ is given by a modified F-P operator acting on this map as follows

$$\mathscr{L} f(X) = \int_P \mu(Y)\delta(X - \varphi(Y))f(Y)\mathrm{d}Y. \tag{1.1}$$

The operator $\mathscr{L}$ describes the propagation of f along a trajectory between two points on the boundary of Ω, together with a specular reflection at the arrival point. The term $\mu : P \to (0,1)$ is incorporated to model energy losses at boundary reflections.

The stationary density ρ on P due to an initial boundary distribution ρ_0 on P is the density accumulated in the long time (many iterate) limit. That is

$$\rho(X) = \sum_{n=0}^{\infty} \mathscr{L}^n \rho_0(X), \tag{1.2}$$

where $\mathscr{L}^n$ is the nth iterate of the operator (1.1). Note that the incorporation of the dissipative term μ within (1.1) is necessary for the sum (1.2) to converge. The stationary density ρ may then be obtained as the solution of the following integral equation

$$(I - \mathscr{L})\rho = \rho_0 \tag{1.3}$$

via the standard Neumann series result for (1.2).

1.3 The Ulam method

In this section we restrict our attention to the case when Ω is a triangle. We first outline the implementation of the Ulam method to discretise the integral equation (1.3), before briefly discussing some of the building blocks that we believe will lead to a rigorous convergence analysis of the resulting numerical approximation of the stationary density ρ.

1.3.1 Implementation of the Ulam method

In order to apply the Ulam method to discretise (1.3), we first sub-divide the boundary phase-space $P = [0,L) \times (-1,1)$ into MN rectangles $R_{m,n}$, with $m = 1,2,\ldots,M$

and $n = 1,2,\ldots,N$. We do this by performing an equi-spaced subdivision along the p coordinate with step-size $\Delta p = 2/N$, and along each edge of the triangle $e = 1,2,3$ we perform an equi-spaced subdivision with step-size $\Delta s_e = L_e/M_e$ where $M = M_1 + M_2 + M_3$ and L_e is the length of edge e. The number of sub-intervals on edge e, M_e is defined by first choosing a target number of subdivisions for the whole boundary of length $L = L_1 + L_2 + L_3$ as M^* and then taking $M_e = \text{Round}(M^* L_e/L)$, with Round denoting rounding to the nearest integer.

The stationary density ρ is now approximated by its projection $\mathscr{P}_{MN}\rho$ onto a finite dimensional space of piecewise constant functions of the form

$$\rho(s,p) \approx (\mathscr{P}_{MN}\rho)(s,p) = \sum_{m=1}^{M}\sum_{n=1}^{N} \frac{\rho_{m,n}}{\Delta s_{e(m)}\Delta p}\chi_m(s)\chi_n(p), \tag{1.4}$$

where $\chi_n(p) = 1$ if $2(n-1)/N < p < 2n/N$ and is zero otherwise. Likewise, $\chi_m(s) = 1$ is an indicator for the mth sub-division of the s-coordinate. The index $e(m) = 1$ for $m = 1,2,\ldots,M_1$, $e(m) = 2$ for $m = M_1+1, M_1+2,\ldots,M_1+M_2$ and $e(m) = 3$ for $m = M_1+M_2+1, M_1+M_2+2,\ldots,M$.

A Galerkin projection of equation (1.3) onto the finite dimensional basis (1.4) may be written in the form

$$(I-T)\boldsymbol{\rho} = \boldsymbol{\rho_0}, \tag{1.5}$$

where I is the $NM \times NM$ identity matrix and T is a matrix with entries

$$\begin{aligned} T_{\alpha,\alpha'} &= \mu \int_P \left(\frac{1}{\Delta s_{e(m')}\Delta p} \int_P \delta(X - \varphi(Y))\chi_{m'}(s')\chi_{n'}(p')dY \right) \chi_m(s)\chi_n(p)dX, \\ &= \frac{\mu}{\Delta s_{e(m')}\Delta p} \int_P \chi_m(\varphi_s(s',p'))\chi_n(\varphi_p(s',p'))\chi_{m'}(s')\chi_{n'}(p')dY, \\ &= \mu \frac{\text{Area}(R_{m',n'} \cap \varphi^{-1}(R_{m,n}))}{\text{Area}(R_{m',n'})}. \end{aligned}$$

In the second line we note that the boundary map φ has been split into its position and momentum components, which are denoted φ_s and φ_p, respectively. In addition, $\text{Area}(R_{m',n'}) = \Delta s_{e(m')}\Delta p$ denotes the area of $R_{m',n'}$, $Y = [s',p']$, $\alpha = m + (n-1)M$ and correspondingly $\alpha' = m' + (n'-1)M$. The vector $\boldsymbol{\rho} = [\rho_\alpha]_{\alpha=1,2,\ldots,MN}$ contains the coefficients $\rho_{m,n} = \rho_\alpha$ from the basis expansion (1.4). The vector $\boldsymbol{\rho}_0$ contains the corresponding coefficients for the expansion of the initial density ρ_0 in the form (1.4). Furthermore, we have assumed that the damping factor μ is constant for simplicity. In the next section we outline a theoretical setting that we believe will lead to rigorous analysis for the convergence of the approximation (1.4) obtained by solving (1.5).

1.3.2 A route toward rigorous analysis

The theory underpinning our analysis stems from the work of Keller in the eighties [Ke85]. We conjecture that a function space setting that remains invariant under the action of $\mathscr{L}$ can be devised using spaces of functions of generalised bounded variation V_ϕ for a particular choice of the map ϕ. In fact V_ϕ are Banach spaces when $\phi : [0,\eta_0] \to [0,\infty)$ is a monotonically increasing map with $\lim_{\eta\downarrow 0}\phi(\eta) = 0$. To define the norm on V_ϕ, we first introduce the *oscillation* of a function f in a set $A \subset \mathbb{R}^2$ as

$$\operatorname{osc}(f,A) = \operatorname{ess\,sup}_{(x,y)\in A\times A}|f(x) - f(y)|.$$

The norm on V_ϕ may then be written as

$$\|f\|_\phi := \|f\|_{L^1} + \sup_{\eta\in(0,\eta_0]} \frac{\int_{\mathbb{R}^2}\operatorname{osc}(f,\mathbb{B}_\eta(x))\mathrm{d}x}{\phi(\eta)},$$

where $\|\cdot\|_{L^1}$ denotes the standard L^1 norm and $\mathbb{B}_\eta(x) \subset \mathbb{R}^2$ is an open ball of radius η and centre x.

Assuming that $\mathscr{L}f \in V_\phi$ for every $f \in V_\phi$, then Lemma 1.11 from [Ke85] provides

$$\|f - \mathscr{P}_{MN}f\|_{L^1} \leqslant \phi(h)\|f\|_\phi,$$

where $h = \sqrt{\Delta s^2 + \Delta p^2}$ and $\Delta s = \max_e\{\Delta s_e\}$. That is, the convergence rate depends critically on ϕ, as does the validity of the assumption $\mathscr{L}f \in V_\phi$. Evidence from numerical experiments typically shows first order convergence, corresponding to $\phi(h) \propto h$. However, the assumption of $\mathscr{L}f \in V_\phi$ would break down in this case owing to the discontinuities in the boundary map φ. We conjecture that instead choosing

$$\phi(h) = |\ln(h)|^{-\beta}$$

with fixed $\beta \in \mathbb{N}$ will provide the necessary assumption of $\mathscr{L}f \in V_\phi$ for every $f \in V_\phi$. The price that we pay for this choice is a rather slower logarithmic convergence rate. We remark that sub-linear convergence of the Ulam method has previously been proved rigorously for piecewise expanding interval maps [BoMu01] and appears to be a realistic starting point for our analysis here.

1.4 Conclusions and outlook

We have introduced a ray-tracing model for the propagation of phase-space densities through convex polygonal domains, which was expressed in terms of a damped F-P operator $\mathscr{L}$ for the boundary flow map φ. The stationary density ρ may be obtained from the solution of a second-kind Fredholm equation (1.5). We discussed the discretisation of (1.5), and consequently the damped F-P operator $\mathscr{L}$, using the Ulam method. Some ideas were then proposed regarding how one may prove the convergence of the solution obtained via this discretisation to the solution of the original problem. We only expect to obtain sub-linear convergence rates and the reason for this slow convergence can be directly linked to the lack of regularity of the boundary map φ for the triangle, or indeed any convex polygon.

We note that there are a number of settings in which one can realistically hope for faster convergence of discretisation schemes for estimating ρ, such as for domains with smooth boundaries. This was explored further in [SlEtAl20], where rigorous convergence estimates were established for circular billiards using a Fourier basis approximation of ρ and more general smooth domains were investigated numerically. A further case that may yield faster convergence rates is that of stochastically smoothed F-P operators, which describe uncertain ray dynamics [ChTa14]. A significant advantage in this case is that the transfer operator is compact meaning one can draw upon a considerably wider body of supporting theory as discussed in [BaCh18].

References

[Ce01] Červený, V.: *Seismic ray theory*, Cambridge University Press, Cambridge, UK (2001).

[CvEtAl20] Cvitanović, P., Artuso, R., Mainieri, R., Tanner, G., and Vattay, G.: *Chaos: Classical and Quantum*, `ChaosBook.org`, Niels Bohr Institute, Copenhagen, Denmark, (2012).

[Ul64] Ulam, S.: *Problems in Modern Mathematics*, Wiley, New York, NY (1964).

[Li76] Li, T-Y.: Finite approximation for the Frobenius–Perron operator. A solution to Ulam's conjecture. *J. Approx. Theory*, **17**, 177–186 (1976).

[Fr99] Froyland, G.: Ulam's method for random interval maps. *Nonlinearity*, **12**, 1029–1052 (1999).

[BoMu01] Bose, C., and Murray, R.: The exact rate of approximation in Ulam's method. *Discrete and Continuous Dynamical Systems*, **7**(1), 219–235 (2001).

[SlEtAl20] Slipantschuk, J., Richter, M., Chappell, D.J. , Tanner, G. , Just, W. and Bandtlow, O.F.: Transfer operator approach to ray-tracing in circular domains. *Nonlinearity*, **33**, 5773–5790 (2020).

[Ke85] Keller, G:. Generalized bounded variation and applications to piecewise monotonic transformations. *Z. Wahrscheinlichkeitstheorie verw Gebiete* **69**(3), 461-–478 (1985).

[Sa00] Saussol, B.: Absolutely continuous invariant measures for multidimensional expanding maps. *Isr. J. Math.* **116**, 223–248 (2000).

[SiEtAl07] Siltanen, S., Lokki, T., Kiminki, S. and Savioja, L.: The room acoustic rendering equation. *J. Acoust. Soc. Amer.* **122**, 1624–1635 (2007).

[ChTa14] Chappell, D.J. and Tanner, G.: A boundary integral formalism for stochastic ray tracing in billiards. *Chaos* **24**(4), 043147 (2014).

[BaCh18] Bajars, J. and Chappell, D.J.: A boundary integral method for modelling vibroacoustic energy distributions in uncertain built up structures. *J. Comp. Phys.* **373**, 130–147 (2018).