La teoría matemática de la difusión y el calor. Grandes figuras y éxitos

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J L Vazquez

Distribution

1 Mathematics, Physics and PDEs

- La magia de las ecuaciones
- 18th century. Le siècle des lumières
- 19th century. Modern times

2 Heat and diffusion

Heat equation

3 Diffusion and the class of Parabolic Equations

- Linear Parabolic Equations
- The heat equation and probability

5 Other equations. Nonlinear, nonlocal, geometric diffusion

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$$u_t = \Delta u$$

La ecuación del calor y la difusión

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Hay magia en una ecuación para quien sabe encontrarla.



Origins of PDEs

• In the 18th century, PDEs appear in the work of Jean Le Rond D'Alembert about string oscillations, around 1746: A set of particles moves together due to *elastic forces*, but every one of the infinitely many *solid elements* has a different motion. This is *Dynamics of Continuous Media*. PDEs are the corresponding mathematical objects. The wave

equation $|u_{tt} = c^2 u_{xx}|$ is one of the first important instances.

The names of Euler and Lagrange also appear.

• Johann and Daniel Bernoulli and then Leonhard Euler lay the foundations of Ideal Fluid Mechanics (1730 to 1750), in Basel and St. Petersburg. This is PDEs of the highest caliber: it is a system, called the Euler equations:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = 0, \qquad \nabla \cdot \mathbf{u} = 0.$$

The system is nonlinear; it does not fit into one of the 3 types that we know today (elliptic, parabolic, hyperbolic); the main pure-mathematics problem is still unsolved (existence of classical solutions for good data; uniqueness of energy solutions). See also the sister system, the *Navier Stokes* equations, in next slide.



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- 1800. The new century confronts revolutions in the concept of heat and energy, electricity and magnetism, and what is space. You may add another revolution, the real fluids, which is still going on.
- All of these fields end up mathematically in PDEs:
 - (i) heat leads to the heat equation, $u_t = \Delta u$, and the merit goes to J. Fourier.

(ii) electricity leads to the Coulomb equation in the Laplace-Poisson form: $-\Delta V = \rho$. This equation also represents gravitation.

(iii) electromagnetic fields are represented by the Maxwell system. The vector potential satisfies a wave equation, the same as D'Alembert's, but vector valued and in several dimensions.



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Other equations. Nonlinear, nonlocal, geometric diffusion

• Our topic today centers on the Heat Equation

$$u_t = \Delta u$$

and the analysis proposed by Fourier, 1807, 1822. Early 19th century.

• The mathematical models of Heat Propagation and Diffusion have made great progress both in theory and application.

They have had a strong influence on several areas of Mathematics: PDEs, Functional Analysis, Probability, and Diff. Geometry. And on / from Physics. Count also Numerics.

• The heat flow analysis is based on two main techniques: -integral representation (convolution with a Gaussian kernel) (this directions leads to SEMIGROUPS)

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- separation into mode and spectral theory



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Fourier analysis

- When we solve the Heat Equation in a bounded domain we go to mode analysis (separation of variables) and then to spectral synthesis (Fourier series)
- Here is the main formula, one of the most useful formulas of Mathematics:

$$u(x,t) = \sum_{i=1}^{\infty} T_i(t)\varphi_i(x)$$

where $T_i(t) = c_i e^{-\lambda_i t}$ and the $\varphi_i(x)$ form the spectral sequence

$$-\Delta \varphi_i = \lambda_i \, \varphi_i, \quad i = 1, 2, \dots$$

• This is the famous linear eigenvalue problem for the Laplace operator. We find in the standard cases $0 \le \lambda_1 \le \lambda_2 \le ... \le \lambda_k \le ...$, and $\lambda_k \to \infty$.

The analysis that follows is the first lesson in Spectral Theory. If Ω is a general domain this is highly nontrivial and important. Spectral theory has enormous scientific applications to diffusion, heat propagation and wave propagation as well as Quantum Mechanics.

• Orthogonality of the modes in L^2 is a fundamental fact of the theory

 $\int \varphi_i(x)\varphi_j(x)\,dx = 0 \quad \text{if} \quad i \neq j$



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The personalities. Fourier

• The originator, Jean-Baptiste Joseph Fourier (Auxerre, 1768- Paris, 1830),



- Fourier accompanied Napoleon Bonaparte on his Egyptian expedition in 1798, In 1801, Napoleon appointed Fourier Prefect of the Department of Isère in Grenoble.
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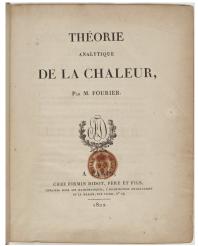
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Fourier's historic book



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- The reference book Théorie Analytique de la Chaleur, (1822). Firmin Didot, Paris. Online version, Ed. Gabay 1988, 637 pgs. It is a historic landmark.
- Fourier contributed (1) the PDE that describes heat, (2) the analysis of functions as sums of sines, (3) dimensional analysis.
- The idea of FOURIER ANALYSIS was proposed in a memoir in 1807 (while at Grenoble) and publication was rejected (paper *On the Propagation of Heat in Solid Bodies*).
- Fourier claimed that every function of a variable, whether continuous or discontinuous, can be expanded in a series of sines of multiples of the variable. This was a matter of debate for many years. Early opponents: Lagrange, Laplace and Poisson. First personality to see the merit: B. Riemann. Early proof that Fourier was right is due to P. L. Dirichlet, 1828. He introduced the Dirichlet Kernel.
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The personalities. Dirichlet

• Johann Peter Gustav Lejeune Dirichlet (1805 - 1859)



• Though German (from Rhineland), Dirichlet decided to go to Paris to study in May 1822.

In 1825 Dirichlet gave a lecture at the Académie which put him in contact with Fourier and Poisson, who raised his interest in theoretical physics, especially Fourier's analytic theory of heat.

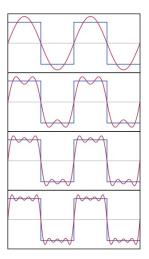
The personalities. Dirichlet II

- Dirichlet made important contributions to
 - number theory (including creating the field of analytic number theory),
 - the theory of Fourier series and other topics in mathematical analysis;
 - study of the Laplace equation and Dirichlet problem

- Dirichlet is credited with being (one of) the first mathematicians to give the modern formal definition of a function: "to any x there corresponds a single finite y". But often he went back to the old idea that a function is a piecewise collection of curves.

At that time confusion was feared in a 'too general' definition of function due to the appearance of 'artificial examples', but the sums of Fourier Series were a very innovative force.

Fourier analysis for discontinuous functions



Approximation of a train of square signals by Fourier series



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Dirichlet's principle

• Principle of Energy minimization t

$$\mathcal{E}[v(x)] = \int_{\Omega} \left(\frac{1}{2} |\nabla v|^2 - vf \right) \, \mathrm{d}x \tag{1}$$

in a domain Ω of the space for differentiable functions (defined in Ω and the boundary) with required boundary condition v = g en $\partial \Omega$.

• Fantasic fact: An easy calculation shows that the minima u(x) of this "variational" problem solve precisely the Laplace-Poisson equation,

$$\Delta u + f = 0.$$

• A modification allows to solve Minimization Problems for the Eigenfunctions

$$\Delta u + \lambda u = 0 \,,$$

using minimization with constraints, called Rayleigh-Ritz method. The eigenvalues are then Lagrange multipliers.



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Figuras del Calor

- The Heat Equation has produced a huge number of concepts, techniques and connections for pure and applied science, for analysts, probabilists, computational people and geometers, for physicists and engineers, and lately in finance and the social sciences.
- Today educated people talk about the Gaussian function, separation of variables, Fourier analysis, spectral decomposition, Dirichlet forms, Maximum Principles, Brownian motion, generation of semigroups, positive operators in Banach spaces, entropy dissipation, ...
- The heat example is generalized into the theory of linear parabolic equations, which is nowadays a basic topic in any advanced study of PDEs. The next step is nonlinear parabolic PDEs.
- In physics the heat equation appears as a diffusion, in probability diffusion is a stochastic process, in geometry there is a heat flow on a Riemannian manifold using the Laplace-Beltrami operator, in functional analysis we find the fractional heat equations that have a probabilistic meaning as Lévy processes, ...



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The heat equation semigroup and Gauss

• We introduce a completely new way of working when heat propagates in free space: representations and kernels. The natural problem is the initial value problem

$$u_t = \Delta u, \qquad u(x,0) = f(x) \tag{2}$$

which is solved by convolution with the evolution version of the *Gaussian function*

$$G(x,t) = (4\pi t)^{-n/2} \exp\left(-|x|^2/4t\right).$$
(3)

Note that *G* has all nice analytical properties for t > 0, but note that $G(x, 0) = \delta(x)$, a Dirac mass.



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Convolution

• The representation formula is a very important object in the History of Mathematics

$$u(x,t) = \int_{\mathbb{R}^n} u_0(y) G_t(x-y) \, dy$$

 G_t works as a parametrized kernel (Green, Gauss). G is one the most beautiful and useful objects of Mathematics.

- The maps S_t : u₀ → u(t) := u₀ * G(·, t) form a continuous semigroup of linear contractions in all L^p spaces 1 ≤ p ≤ ∞.
 (This is pure Functional Analysis, 20th century)
- The solution of linear equations by means of integral representation with a kernel is a very general idea of PDEs, functional analysis and applied mathematics. Kernels are very important but usually they are not explicit. *Big problems arise!*



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Asymptotic convergence to the Gaussian

The main result on the asymptotic behaviour of general integrable solutions of the heat equation consists in proving that they look increasingly like the fundamental solution, Central Limit Theorem. Since this solution goes to zero uniformly with time, the estimate of the convergence has to take into account that fact and compensate for it. This happens by considering a renormalized error that divides the standard error in some norm by the size of the Gaussian solution $G_t(x)$ in the same norm.

Theorem. Let $u_0 \in L^1(\mathbb{R}^n)$ and let $\int u_0(x)dx = M$ be its mass. Then the solution $u(t) = u(\cdot, t)$ of the HE in the whole space ends up by looking like *M* times the fundamental solution $G_t(x)$ in the sense that

$$\lim_{t \to \infty} \|u(t) - MG_t\|_1 \to 0 \tag{4}$$

and also that

$$\lim_{t \to \infty} t^{N/2} \|u(t) - MG_t\|_{\infty} \to 0.$$
⁽⁵⁾

By interpolation we get the convergence result for all L^p norms for all $1 \le p \le \infty$

$$\lim_{t \to \infty} t^{N(p-1)/2p} \|u(t) - MG_t\|_{L^p(\mathbb{R}^n)} \to 0.$$
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 \Rightarrow For proofs you may see my course notes in arxiv, arXiv:1706.10034v2

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Theorem. Let $u_0 \in L^1(\mathbb{R}^n)$ and let $\int u_0(x)dx = M$ be its mass. Then the solution $u(t) = u(\cdot, t)$ of the HE in the whole space ends up by looking like *M* times the fundamental solution $G_t(x)$ in the sense that

$$\lim_{t \to \infty} \|u(t) - MG_t\|_1 \to 0 \tag{4}$$

and also that

$$\lim_{t \to \infty} t^{N/2} \|u(t) - MG_t\|_{\infty} \to 0.$$
⁽⁵⁾

By interpolation we get the convergence result for all L^p norms for all $1 \le p \le \infty$.

$$\lim_{t \to \infty} t^{N(p-1)/2p} \| u(t) - MG_t \|_{L^p(\mathbb{R}^n)} \to 0.$$
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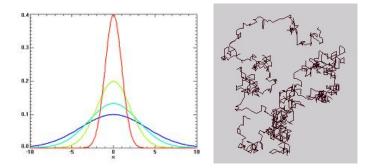
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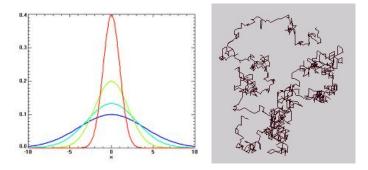
• The comparison of ordered dissipation vs underlying chaos



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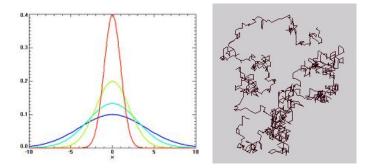
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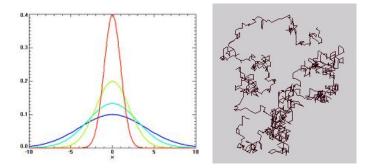
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Outline

Mathematics, Physics and PDEs

- La magia de las ecuaciones
- 18th century. Le siècle des lumières
- 19th century. Modern times

2 Heat and diffusion

• Heat equation

3 Diffusion and the class of Parabolic Equations

• Linear Parabolic Equations

4 The heat equation and probability

5 Other equations. Nonlinear, nonlocal, geometric diffusion

After some years of playing with nonlinear elliptic equations, maximum principles, and compact supports, from 1976 to 1982, I went to the US and devoted most of my mathematical life to Diffusion. But

• what is diffusion in the real world?

Populations diffuse, substances (like particles in a solvent) diffuse, heat propagates, electrons and ions diffuse, the momentum of a viscous (Newtonian) fluid diffuses (linearly), there is diffusion in the markets, ...

• how to explain it with mathematics?

• A main question is: how much of it can be explained with linear models, how much is essentially nonlinear?

• The stationary states of diffusion belong to an important world, elliptic equations. Elliptic equations, linear and nonlinear, have many relatives: diffusion, fluid mechanics, waves of all types, quantum mechanics, ... The Laplacian Δ is the King of Differential Operators.



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Linear heat flows

Until well into the 20th century diffusion was almost exclusively heat equation, a part of the classical theory of PDEs. From 1822 until 1950 the heat equation has motivated

(i) Fourier analysis decomposition of functions (and set theory),

(ii) development of other linear equations \implies Theory of Parabolic Equations

$$u_t = \sum a_{ij}\partial_i\partial_j u + \sum b_i\partial_i u + cu + f$$

Note: (a_{ij}) must be a positive matrix (there must be dissipation in the system).

Main inventions in the Parabolic Theory:

(1) a_{ij}, b_i, c, f regular \Rightarrow Maximum Principles, Schauder estimates, Harnack inequalities; C^{α} spaces (Hölder); potential theory; generation of semigroups.

(2) coefficients only continuous or bounded $\Rightarrow W^{2,p}$ estimates, Calderón-Zygmund theory, weak solutions; Sobolev spaces.



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The random walk and the heat equation I

• We take a random walk on a regular 1D mesh of site distance *h* and we take the time increments of size τ .

The probabilities of reach site x_i and time t_j are u_i^j . IN numerics take a bound L = Nh and $T = M\tau$, and keep L, T fixed

There a recursion law based on conditional probabilities for Markov processes:

$$u_i^{j+1} = \frac{1}{2}u_{i-1}^j + \frac{1}{2}u_{i+1}^j$$

(equal probability of jumping to nearest neighbour).

- The problem can be solved and the u_i^j can be calculated step by step in time starting from an initial probability u_i^0 , which usually is the Dirac delta.
- The calculation looks hopeless for many nodes and time divisions. This is where differential calculus finds the simple harmony in an apparent chaos.



Random walk and the heat equation II

• The calculation looks hopeless for many nodes and time divisions. Actually, it is very easy if you take the limits when $N, M \to \infty$ so that $h, \tau \to 0$

$$\frac{1}{\tau}(u_i^{j+1} - u_i^j) = \frac{h^2}{2\tau} \frac{u_{i-1}^j + u_{i+1}^j - 2u_i^j}{h^2}$$

Let now $h, \tau \rightarrow 0$ and we get in the limit the diffusion equation

$$\partial_t u = D \,\partial_x^2 u$$

but only if the compatibility condition holds,

$$\exists \lim_{h,\tau \to 0} \frac{h^2}{2\tau} = D$$

This is the explanation of Brownian motion and the Comp. Cond. is called Brownian scaling: $\Delta x^2 \sim \Delta t$.

Heat Equation, Diffusion and Stochastic Processes

- At the beginning of the 20th century, a selected group of great mathematicians (Markov, Bachelier, Einstein, Smoluchowski, Wiener, Levy, Kolmogorov) looked at the limit of the discrete RW (which is a Discrete Stochastic Process, DSP), and used the existence of the limit probabilities (i.e., the Gaussian solution of the HE is used as Markov transition function) to build a Continuous-in time Stochastic Process, the Wiener Process which is the mathematical realization of the intuitive Brownian motion.
- There are enormous technicalities to (rigorously) define the Wiener process on a set of continuous paths, but this is the core of the courses in SP. It is not true that the typical Brownian path is NOT Lipschtiz, the optimal regularity is $C^{1/2}$ a.s.
- The next step is to invent the Stochastic Differential Equation (SDE) based on the correct sense of derivative and integral, which is the Ito calculus. Here is the end equation

$$dX = bdt + \sigma dW$$

where *bdt* is the deterministic drift term, *dW* is Wiener's process, and $D = 1/2\sigma^2$ the diffusion coefficient.



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The link. Kolmogorov's Equations

• **History.** In 1931 A. N. Kolmogorov started working with continuous-time Markov chains. More precisely, he studied the transition probability density

$$p(x,s;y,t) = P(X_t^{x,s} \in dy)$$

The same year he introduced TWO very important partial differential equations. These equations are known under the names the Kolmogorov backward equation and the Kolmogorov forward equation. Both equations are parabolic differential equations for the probability density function of some stochastic process of the diffusion form

$$dX_t = bdt + \sigma dW.$$

• The names, forward and backward, come from the fact that the equations are diffusion equations that has to be solved in a certain direction, forward or backward.

• Forward:

$$\partial_t p = L_f p, \quad L_f(p) := -\partial_y(bu) + \frac{1}{2}\partial_{yy}^2(\sigma^2 p)$$

Backward:

$$\partial_s p + L_b p = 0, \quad L_b p := b \partial_x u + \frac{1}{2} \sigma^2 \partial_{xx}^2 p.$$

They are dual equations. KFE needs initial conditions, for KBE final conditions.

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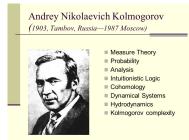
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Kolmogorov I

- Kolmogorov is considered the greatest mathematician in the history of Russia and also one of best mathematicians in the 20th century. He was a man of many interests and with his creativity and sharp intellect he was able to contribute to many different areas of mathematics.
- In 1922, Kolmogorov gained international recognition for constructing a Fourier series that diverges almost everywhere. At this time he decided to devote his life to mathematics.



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Kolmogorov II

He was incredibly brilliant. Here is a written comment on him:

"Most mathematicians prove what they can. Kolmogorov was of those who prove what they want".

- Probability theory was one of Kolmogorov's main interests. He put probability theory in the category of rigorous mathematics. Before Kolmogorov one could doubt the results in probability the same way one would doubt the correctness of a model. Kolmogorov changed all of this by building a rigorous foundation for probability theory to stand on. Not only did he build the foundation he also contributed with advanced results to the field.
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$$u_t + (-\Delta)^s u = 0, \quad (-\Delta)^s u = c \int \frac{u(x) - u(y)}{|x - y|^{n+2s}} dy$$

Here 0 < s < 1 is the fractional exponent. Related to fractional stochastic processes, ther now famous Lévy processes.

• The method works for equations evolving on manifolds. This is a challenging connection with differential geometry. Diffusion uses the Laplace-Beltrami operator

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$$u_t = L_{LB}u, \qquad L_{LB}u = \frac{1}{\sqrt{|g|}}\partial_i \left(g^{ij}\sqrt{|g|}\partial_j u\right)$$

• It has been an intense effort. The work related to our research is reported in the survey paper of a CIME summer course in Italy

♡ The mathematical theories of diffusion. Nonlinear and fractional diffusion, by J. L. Vázquez. CIME Summer Course 2016. Springer Lecture Notes in Mathematics, 2017.



• Since 2007: fractional heat equation and fractional porous medium equations, ...

$$u_t + (-\Delta)^s u = 0, \quad (-\Delta)^s u = c \int \frac{u(x) - u(y)}{|x - y|^{n+2s}} dy$$

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 2017.



Books as proof of progress



2006



Avec of Factors Carolio - Manaed et Pine Avec of Factor - Cuespoe Manadore Tan Laiv Viceore Diffusions and Interactions: New Methods and Directions Cetraro, Italy 2016 Mattee Benforte - Gabriele Grillo Editors

Lecture Notes in Mathematics 2186

2016



J L Vazquez

2007

Final comment

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There are many more connections to explore, more windows to open

Though many important problems have been solved for the main models, many important problems are still open.

Buena suerte, amigos!



Esto es todo por hoy, solo la punta del iceberg

Gracias por su atención



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J L Vazquez

Figuras del Calor

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