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Laurent Gosse

Computing Qualitatively Correct Approximations of Balance Laws

Exponential-Fit, Well-Balanced and Asymptotic-Preserving

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To Sonia for all her love and her patience

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Volume 2

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Computing Qualitatively Correct Approximations of Balance Laws

Exponential-Fit, Well-Balanced and Asymptotic-Preserving

Springer

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Preface

I don't see any problem with the math, but this is not a dissertation in economics. We can't give you a Ph.D. in economics for a dissertation that isn't about economics. It's not economics. It's not mathematics. It's not even business administration.

Milton Friedman, about H. Markowitz's manuscript

Balance laws appear in many areas of application, ranging from fluid mechanics modeling, or semi-classical WKB approximations of linear quantum models, to discrete-ordinate reduction of multi-dimensional kinetic equations. These are partial differential equations describing the evolution in time of intensive (or bulk) quantities which are submitted to a physical process involving both convection and another mechanism (reaction, relaxation, or even diffusion). In many situations, such a system of equations stabilizes onto a large-time behavior which is characterized by an accurate balancing between the transport terms and the other ones. Another interesting configuration is the one in which the system contains an independent parameter which variation deeply affects the qualitative behavior of the solutions. We shall therefore speak about qualitatively correct numerical approximations when either (or both) aforementioned distinguished behaviors can be reproduced algorithmically without salient restrictions on the computational grid. Such accurate computations usually result from the use of sophisticate numerical flux functions, which display consistency not only with the convection terms, but with other parts of the equation. Perceiving simultaneously several (if not all) the terms appearing in the partial differential equation helps in preserving at the numerical level desirable qualitative properties, like dissipation of certain norms, respect of positively invariant domains, entropy inequalities or Lyapunov functionals in a robust manner. The objective of the present book is to raise the reader's awareness of how such elaborate flux functions can be built, mainly in a one-dimensional context for hyperbolic systems admitting shock-type solutions and for kinetic equations in the discrete-ordinate approximation as well. An effort will be dedicated to rigorous mathematical derivations and to the analysis of the net gain retrieved from this approach.

In particular, one should often keep in mind that an equilibrium has to be sought between the three edges of the *golden triangle*[1]: observations, modeling and analysis, numerical simulation. While observations are imposed by our surrounding world, modeling can be instead achieved at several levels of complexity. A more intricate

[1] I learnt this nice expression from Prof. Vincent Courtillot.

model can lead to bigger difficulties in terms of mathematical analysis, even if the development of powerful tools in the field of non-linear analysis allowed to successfully resolve delicate problems in terms of existence, uniqueness and stability of appropriate weak solutions (arousing some reflexions[2] about what is called *solving*). Impressive achievements in theoretical analysis don't yield automatically powerful algorithms to simulate efficiently these weak solutions on a computer: concerning balance laws, only Tai-Ping Liu's extension of James Glimm's theorem was actually based on an astute numerical algorithm. One insight in that work was a seemingly simple finite-difference scheme which building block contains a complete time-asymptotic wave pattern, including both convection and source terms. Slightly later, Gary Sod developed a similar processing for convection-diffusion systems, involving again a solver consistent with all the terms. There is an unpleasant fact about increasing the complexity of a physical model: even if mathematical issues can be overcome by means of an elegant theory, usually the level of noise produced by standard approximation algorithms increases too. Second-order accurate numerical schemes which behave nicely on smooth classical solutions can display spurious oscillations when asked to compute discontinuous waves emanating from models endowed with degenerate or vanishing viscosity: the case of the Lax-Wendroff scheme is quite revealing of this type of drawback. Shock solutions are a visual expression of the mathematical fact that no strong dissipation has been kept at the Sobolev level: however dissipation helps when designing algorithms because it smears off part of the numerical truncation errors. *The gain in accuracy when reproducing real-life observations that one obtains by increasing the complexity of a mathematical model must always be vastly superior to the increase of numerical noise resulting from dissipation processes being removed*. There's little doubt that homogeneous systems of conservation laws are somewhat limited when it comes to rendering certain situations: when thinking about large-scale gas dynamics, gravity is an external force which can hardly be bypassed thus leading to the inclusion of source terms on the right-hand side of both momentum and total energy equations. Such terms make the system "less dissipative", therefore more sensitive to truncation errors as new mechanisms appear likely to amplify them. Solvers involving a whole non-interacting, time-asymptotic wave pattern sometimes can help.

Bari, L'Aquila and Rome, August 2012 *Laurent Gosse*

[2] Clément Mouhot, *Que signifie* résoudre *les équations de la physique pour un mathématicien?*

Acknowledgements

> *If you have been successful, you didn't get there on your own… I am always struck by people who think, well it must be because I was just so smart. There are a lot of smart people out there. It must be because I worked harder than anybody else. Let me tell you something, there are a whole bunch of hard working people out there. If you're successful, somebody along the line gave you some help.*
>
> Barack Obama, campaigning in Roanoke, Virginia

Opportunities to make public greetings are fairly rare, so this one is worth an effort for not forgetting anyone. I began to be interested in a professional research career when I graduated from University of Lille (USTL) back in 1992, thanks to a teaching assistant of stochastic processes who spoke to me about this opportunity. Things were different at the time since someone who didn't go through the French *Cursus Honorum* of Grandes Écoles was nonetheless considered able to attend high level courses, in my case the DEA[1] *Analyse non-linéaire Appliquée* at University Paris-IX Dauphine. I remember a tough interview with Claude Kipnis (who sadly succumbed a heart attack less than one year later) who finally decided to give me a chance after warning me that *Si c'est trop difficile, n'hésitez surtout pas à me contacter et on vous changera de DEA* though. Courses were proceeding at an unusual rhythm, different from the one held elsewhere, but teachings by Jean-Pierre Bourguignon, Maria Esteban (*2.45 hours for the written exam, nothing more and no documents*) or Pierre-Louis Lions (*Combien t'as eu chez Lions?* became a recurrent question before Christmas 1992) were really enlightening. I've always been fond of Differential Geometry, but attending the course on Finsler metric by Patrick Foulon made clear to me that I didn't have the level to begin a thesis in this field. Thanks to a recommendation by Grégoire Allaire, I found a financial support to start working on source terms implementation inside a Godunov-type code at the French Atomic Commissary under supervision by both Imad Toumi and Patrick LeTallec. Military Service was still mandatory at the time hence I had to interrupt during 1994/95 and it's been a matter of pure luck I had the authorization to leave the base in order to attend the Ph.D. defense of my friend Alain Zelmanse: Allaire introduced me to Alain-Yves LeRoux who had shocked the audience by saying, *vous mettez un caillou dans un verre d'eau, ça rend instable n'importe quel schéma!* Then he invited me in Bordeaux and that was the beginning of the "well-balanced adventure". My neighbor, Sébastien Clerc was very much interested in this seemingly new stuff, and there's been numerous discussions on how to extend the scalar scheme to systems: we basically discovered the "non-conservative path" inde-

[1] Diplôme d'Études Approfondies, one year before beginning a Ph.D. thesis.

pendently and roughly at the same time. After 35 months, it was time to be granted the Ph.D., and while asking about Postdoc positions at SISSA to Alberto Bressan who came to visit École Polytechnique, I've been answered *Do you know Glimm scheme? A little bit? Well, not this time…* Benoît Perthame, who was referee of my manuscript sent me to IACM, in the beautiful location of Vassilika Vouton close to Heraklion as a 2-year TMR Postdoc, under the supervision of both Georgios Kosioris and Charalambos Makridakis. I had the luck to get money to visit Thanos Tzavaras several times in Madison, WI, where I learnt Compensated Compactness; moreover, Thanos gently took the time to explain how I could re-interpret my non-conservative products within the more rigorous formalism of weak-$\star$ limits (*you strongly need a transversality condition*). Makridakis *you have to respect seniority!* took me into the development of error estimates for scalar conservation laws, at that time I realized that something was very wrong with the "exponential in time" but I was far from having enough skill to cure this defect. Even more humiliating was the experience of being given by Kosioris this Geometric Optics problem to be studied in the framework of Brenier's K-multivalued solutions: I've been finding nothing for more than 2 years, and the best we could produce with my friend François James was a rigorous analysis of the… mono-phase system! After summer 1999 I sadly left windy Crete for a one-year position at L'Aquila under the auspices of Piero Marcati who gave me many advices on the right manner to submit papers (something nobody ever taught me, back in 1995 Ph.D. students hardly published anything). Life in Italy with the Lira was as sweet as life in Crete with the Drachma… Year 1999 went by just getting my Ph.D/Postdoc research material accepted for publication. At some point, I got in touch with Debora Amadori and Graziano Guerra at a CNR conference in Rome: they were presenting results on BV solutions for hyperbolic balance laws with dissipation. Remembering the advice by Tzavaras, *you should try to prove something for systems with your scheme*, I proposed them to study the other case, where source terms aren't sinks, and where transversality (non-resonance) is required. They had the patience to teach me Glimm's interaction estimates and Bressan's stability theory despite I probably was quite disregarding as a student. We finally came up with a rather satisfying result, that Brenier sold short *Quand ça marche avec zéro, ça marche avec une perturbation d'ordre zéro…* Paola Goatin did a fine job in completing this result by means of one-sided estimates too. In 2001, I was granted a temporary position at both the Istituto per le Applicazioni del Calcolo and Università La Sapienza, in Rome where Italo Capuzzo-Dolcetta and Maurizio Falcone gave me back the K-multibranch problem and Roberto Natalini pushed me into studying the Euler-Poisson problem. Suddenly, during winter 2001, I understood how to initialize the K-moment system and recovering both multi-valued phases and intensities passed in a split second from being 'infeasible' to 'so easy'. On the other side, I realized that Euler-Poisson was a tough problem of well-balancing but I couldn't come up with anything interesting (It took me 10 years more, despite giving it a try with Philippe Béchouche too). At the end of june 2001, I was in so much dire straits that hadn't I had close at hand a job offer from Giuseppe Toscani, I would have probably come back to my parents in Nice and left the profession. Basically all the doors were closed in front of me partly because some people were rumoring that all my stuff was fake. Fortunately,

François Bouchut took the time to check the details in some of my proofs: *Salut, j'ai une question sur ton dernier papier: je comprends que tu consideres toujours des flux monotones, puisque dans le lemme 7 tu demandes en gros* u^0 *positif, et qu'il y a un principe du maximum, puisque* $g(0) = 0$. *Tu me confirmes?* Meanwhile, Toscani took me into kinetic equations, especially in the parabolic scaling: it was hot summer 2001 when we understood that most of the well-balanced non-conservative jump relations could be rewritten in a way to produce a scheme naturally consistent with the limiting diffusion problem. This led to the nowadays well-known "Gosse-Toscani scheme" and its "magic coefficient". Toscani did more: after suggesting me to take on a well-balanced scheme for the Boltzmann equation, *ma io voglio pure una bella equazione per la temperatura!*, which I partly achieved in 2011, he asked me to get involved in what he called "Wasserstein schemes", that now people call Lagrangian schemes for diffusion. Again, it was tough to go into something I knew nothing about … especially that I still didn't have any permanent position at the time (something people who got tenure very quickly never really accept: 'mobility' is the Newspeak word for 'precarious' and hardly means 'exciting adventure'). At the time, TMR postdocs were suffering increasing difficulties for coming back home, and personally, after several years of failure, I had already given up applying in France. An explanation may be that these of European programs were creating a skilled and versatile human offer, rather used to manage risky projects and sharp deadlines, for which any request from the Academics hardly occurred! I had the chance to be offered to join the *sezione di Bari* of the IAC during 2002 (5 years after Ph.D.), just before being invited in the USA by Shi Jin to discuss my multiphase stuff, *everybody can compute a cusp nowadays*, and by Agnès Tourin in Toronto too. Some interest was growing for these uncanny problems and Toscani played again a key role when introducing me to Peter Markowich, end of 2002. Peter gave me a problem which sounded nothing less than impossible to me: performing Geometric Optics for the Schrödinger equation in a crystal modeled by an oscillating potential. I pleaded guilty of being totally ignorant about homogenization, so he gave me a reprint of the famous paper *Homogenization limits and Wigner transforms* which didn't really tranquilize me. Let me just say that performing Bloch homogenization yields a flux function (the "energy band") one doesn't know explicitly: Peter was asking me to do K-multibranch solutions with a flux function nobody knows what it really looks like! It took me many efforts, stimulated by all the *Laurent, any news?* e-mails to come up with a working algorithm, which was to be extended to more complex cases during the years later, thanks to the support offered by Norbert Mauser too, *alors j'ai demandé à Yann Brenier, mais les trucs à Laurent, ça marche ou pas?* Some connections with a mysterious "weak KAM theory" were even stressed by Craig Evans[2]. Unfortunately, I faced an unfair competition against money when the following question was raised: *how do we defend ourselves against someone who says 'in 1d, why bother with analytical-numerical homogenization? just overkill the problem with computer power'*. There was nothing really to reply except that you don't want to kill a fly with a power hammer, or do you? At the time,

[2] See *A survey of partial differential equations methods in weak KAM theory*, Comm. Pure Applied Math. **57** (2004) 445–480.

it seemed that many "level set" people were willing to and the hype around Bloch homogenization was on its way down. I started a collaboration with Rémi Carles thanks to several invitations in CMAF, Lisbon, coming from Joao-Paolo Dias: we sought numerical hints on the high frequency limits of nonlinear Schödinger equations by using the time-splitting FFT scheme partly developed by Markowich. As I personally already had some doubts about its reliability for computing Bloch-type problems, some more low quality outcome convinced me that something was wrong with it, and probably Peter felt offended for that. The situation got later clarified[3] but the connection with him remained irremediably damaged. I felt things as unfinished because a major piece was missing: when setting up Brenier's ideas, one has to go back and forth from moment variables to Riemann invariants. This he could do for $K = 2$, my talented friend Olof Runborg did for $K = 3,4$ in his Ph.D. thesis, but how to solve for arbitrary K as the Jacobian is the ugly Vandermonde matrix? I finally realized that this was an inverse problem for which a strange 'Korobov-Sklyar' algorithm existed: very quickly, Olof cracked it and produced a simple and stable version we could insert inside the numerical fluxes (the "Gosse-Runborg algorithm"). Numerical simulations with $K = 5,7$ and even $K = 11$ became possible along with a complete justification. Brenier went long, but not leveraged, *c'est bien que ça revive, ces machins-là*. After taking some sort of sabbatical in experimenting on a completely different field, trying to trade on the markets by means of signal processing extrapolation tools (not so bad, thank you) during 2007/09, I came back into more conventional research when I casually rediscovered the beautiful *Caseology* formalism, which resulted possible partly because of the spectacular performances of internet search engines. This allowed to extend the old Gosse-Toscani scheme toward virtually any linear kinetic equation: numerous e-mail discussions happened between Christophe Buet and myself, as his experience in the field was precious for me to understand in which way pushing. At the end of the day, I must thank Nicola Bellomo who offered me to write a draft that some people accepted to read carefully and amend: Debora Amadori, Thierry Gallouët and Roberto Natalini read first Chapters, Christophe Buet commented on kinetic parts, Ansgar Jüngel looked at parts dealing with semiconductor models. Besides, Yann Brenier, Vincent Calvez, and Albert Cohen were so nice to give me some very worthy unpublished material.

[3] See page 183 of Jin S., Markowich P., Sparber C.: Acta Numerica **20**, 211–289 (2011).

Acronyms

ADO	Analytical Discrete-Ordinate
AP	Asymptotic-Preserving
BGK	Bhatnaghar-Gross-Krook
BV	Banach space of integrable functions with bounded variation
BVP	Boundary Value Problem
CFL	Courant-Friedrichs-Lewy
FD	Finite Differences
FFT	Fast Fourier Transform
FP	Fokker-Planck
FS	Fractional Steps
FV	Finite Volumes (or Box scheme)
FVS	Flux Vector Splitting
GNL	Genuinely Non-Linear
HLL	Harten-Lax-Van Leer
IMEX	IMplicit-EXplicit
IVP	Initial Value Problem
LD	Linearly Degenerate
NC	Non-conservative
NSP	Navier-Stokes-Poisson
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
PS	Perthame-Siméoni
RH	Rankine-Hugoniot
RK	Runge-Kutta
RT	Radiative Transfer
SW	Shallow Water
TS	Time-Splitting
TV	Total Variation
WB	Well-balanced
WKB	Wentzel-Kramers-Brillouin
WFT	Wave-Front Tracking

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Chapter 1
Introduction and Chronological Perspective

> *There is a theory which states that if ever anyone discovers exactly what the Universe is for and why it is here, it will instantly disappear and be replaced by something even more bizarre and inexplicable. There is another theory which states that this has already happened.*
>
> Douglas Adams, The Hitchhiker's Guide to the Galaxy

This introductory chapter aims at positioning the book's primary topics according to both a scientific and an historic context; loosely speaking, the objective here is more trying to unify seemingly different sectors in numerical analysis rather than being very specific (this will come later on). In particular, one can figure out the main ideas exposed in the sequel by examining very classical computations which trace back to 1960–70, namely the passage from finite differences to exponentially-fitted schemes for transient convection-diffusion equations. In some sense, well-balanced schemes are but an extension of these methods for hyperbolic problems: the link being provided by both the finite volumes discretization (what was formerly called the "box scheme") and the exact solving of the steady-state equations in order to compute the numerical fluxes at each interface of the computational grid. A point of crucial importance is the following (quoting [61, p. 159]):

> Choosing a computational representation is just as important as choosing a mathematical model to describe the system, or choosing the algorithms to implement that model. For example, the choice of either an Eulerian or Lagrangian representation is important because this choice constrains the type of numerical algorithms and gridding methods that can be used.

This type of choice we shall very few discuss hereafter: let's just emphasize the enormous numerical issues which are simply annihilated when choosing a Lagrangian "stringy" representation of 1D gravitational Navier-Stokes-Poisson in Chapter 7. No algorithmic magic can fully recover a bad representation choice.

1.1 The Leap from Crank-Nicolson to Scharfetter-Gummel

1.1.1 Limitations for Gradients Computed with Finite Differences

Let us fix at once a uniform Cartesian computational grid determined by Δx and Δt, its positive characteristic parameters: the indexes $j \in \mathbb{Z}$, $n \in \mathbb{N}$ refer to the space, time axes respectively thus $x_j = j\Delta x$ and $t^n = n\Delta t$. An equation which was considered of

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