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On the Development of Godunov Methods and Their Application to Gasdynamics

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We are interested in developing the most accurate numerical models to simulate Gasdynamics of explosions. But we must first recognize that there is no unique way to discretize the partial differential equations (PDEs) of gas dynamics, and also, there is no unique method to integrate the discretized forms of these equations. This has spawned a variety of numerical methods (religions*) that attempt to solve this conundrum, for example:

- Artificial Viscosity method created by the American mathematician John von Neumann
- Flux-Corrected-Transport (FCT) method invented by Dr. Jay Boris, founder of the Laboratory for Computational Physics (LCP) at NRL
- WENO method developed by Professor Stan Osher of UCLA and Professor Bjorn Enquist of U. Texas
- Godunov method by Academician Sergei Konstantinovich Godunov, Professor of the Sobolev Institute of Mathematics, RAS, in Novosibirsk

to name just a few. We believe that the numerical scheme must mimic, as closely as possible, the mathematical properties of the partial differential equations, such as:

1. The governing equations for explosions are the inviscid gas-dynamic conservation laws
2. In strong conservation form, the right-hand-sides of these equations are zero, i.e., there are no viscosity terms in these equations—so there should be no viscosity in the numerical algorithm
3. The system is hyperbolic, with three real characteristics: $\lambda_0 = u$ and $\lambda_{\pm} = u \pm a$
4. Information travels along characteristics; domain of dependence is determined by the Monge cone, thus the numerical stencil must be limited to neighboring cells.
5. Flow fields develop discontinuities (shocks and contact surfaces), so the numerical scheme must be designed to propagate discontinuities
6. The scheme must be “monotone”, i.e., produce results that are devoid of artificially induced numerical oscillations
7. The PDEs must be solved on locally-uniform Eulerian grid patches—thereby eliminating numerical diffusion induced by grid gradients

* We euphemistically call them “religions” because of the intensity that their proponents defend them—similar to religious doctrines.

We believe that the high-order Godunov methods that we have developed, most closely conforms to the above delineated mathematical properties of the governing equations. Hence, we believe in the “Godunov Religion” of numerical methods. Presented here are key papers published in this journey.**

Part 1 describes the development of the high-order Godunov methods and adaptive mesh refinement needed to capture complex features of the flow. It starts with the formulation of this problem as presented by Godunov in his thesis defense [1] at Moscow State University in 1954, and later expounded in his reminiscences of the background to the development of this method [2]. A key element in this theory is summarized in the Godunov Theorem: *Linear numerical schemes for solving partial differential equations, having the property of not generating new extrema (a monotone scheme), can be at most first-order accurate.*

To overcome this limitation, Colella developed a non-linear scheme—the *Piecewise Parabolic Method* (PPM)—to give a second-order in time and fourth-order in space scheme, in smooth regions of the flow [3,4,5]. Bell, Colella and Miller then extended the PPM method to three dimensional flows [6,7,8]. With the integrator optimized, the next step was to improve mesh resolution. This produced the Adaptive Mesh Refinement (AMR) technique of Berger and Colella [9]. AMR was extended to 3 dimensions by Bell et al., [10]. It has recently been extended to run efficiently on exa-scale computers as described by Zhang et al., [11]; it is now called AMReX.

Part 2 describes the validation of these Godunov methods by comparison with experimental data, such as: shock reflections from wedges by Glaz [12] and Kuhl et al., [13,14], blast wave reflections from ideal surfaces by Colella et al., [15], and shear layers by Chien et al., [16].

Part 3 describes the application of these Godunov methods to simulate turbulent mixing and combustion in explosions, such as: turbulent combustion in TNT explosions [17], spherical combustion clouds [18], heterogeneous model of Aluminum particle combustion in explosions [19], and a 3-phase model of turbulent combustion in pyrotechnic explosions [20]. This is followed by an *Appendix* which gives a biography of S. K. Godunov from his web site.

We hope that this anthology will serve as a useful resource for researchers in this field.

** This is not intended to be a comprehensive review of Godunov methods, rather we present selected papers from our research over the last 35 years that directly contributed to the Godunov technology used in applications described in Part 3.

Part 1: Development

In the Beginning: 1954

1. S. K. Godunov, A difference scheme for numerical computation of discontinuous solution of hydrodynamics equations (first presented in PhD thesis defense 1954) later published in *Math Sb.* **47**, pp. 271-302 (1959)
2. S. K. Godunov, Reminiscences about Difference Schemes, *J. Comp. Phys.* **153**, pp. 6-25 (1999)

High-order Methods: 1984-2002

3. P. Colella and P. Woodward, The Piecewise Parabolic Method (PPM) for gas-dynamical simulations, *J. Comp. Phys.* **54**, pp.174-201 (1984)
4. P. Colella, A direct Eulerian MUSCL scheme for gas dynamics, *SIAM J. Sci. Stat. Comput.* **6** (1), pp. 104-117 (1985)
5. P. Colella and H. M. Glaz, Efficient solution algorithms for the Riemann problem for real gases, *J. Comp. Phys.* **59**, pp. 264-289 (1985)
6. J. B. Bell, P. Colella, J. A. Trangenstein, Higher-order Godunov methods for systems of hyperbolic conservation laws, *J. Comp. Phys.*, **82**, pp. 362-397 (1989).
7. P. Colella, Multidimensional upwind methods for hyperbolic conservation laws, *J. Comp. Phys.* **87**, pp. 171-200 (1990)
8. G. H. Miller, P. Colella, A Conservative three-dimensional Eulerian method for coupled solid-fluid shock capturing, *J. Comp. Phys.* Vol.**183**, pp. 26-82 (2002)

Adaptive Mesh Refinement: 1989-2019

9. M. J. Berger and P. Colella, Local adaptive mesh refinement for shock hydrodynamics. *J. Comp. Phys.* **82** (1), pp. 64–84 (1989).
10. J. B. Bell, M. A. Berger, J. Saltzman and M. Welcome, “Three-dimensional Adaptive Mesh Refinement (AMR) for hyperbolic conservation laws”, *SIAM J. Sci. Stat. Comp.*, **15** (1), pp. 127-138 (1994).
11. W. Zhang, A. Algren, V. Beckner, J. Bell, et al., AMReX: a framework for block-structured adaptive mesh refinement, *Journal of Open Source Software* **4**(37) (2019); to download go to: <https://escholarship.org/uc/item/00j3z3rd>

Part 2: Validation

Shock Reflections from Wedges: 1985-1993

12. H. M. Glaz, P. Colella, I. I. Glass and R. L. Deschambault, A numerical study of oblique shock-wave reflections with experimental comparisons, *Proc. R. Soc. London A* **398**, pp. 117-140 (1985)
13. A. L. Kuhl, R. E. Ferguson, K.-Y. Chien, W. Glowacki, P. Collins, H. Glaz, P. Colella, Turbulent wall jet in a Mach reflection flow, *Dynamics of Detonations and Explosions: Explosion Phenomena*, Edited by A. L Kuhl, J.-C. Leyer, A. A. Borisov, W. A. Sirignano, **134** Prog. Astro. & Aero, AIAA New York, pp. 201-232 (1991)
14. A. L. Kuhl, R. E. Ferguson, K.-Y. Chien, P. Collins, Unstable wall layers created by shock reflections, *Dynamic Aspects of Explosion Phenomena*, Edited by A. L. Kuhl, J.-C. Leyer, A. A. Borisov and W. A. Sirignano, **154** Prog. Astro. & Aero., AIAA New York, pp. 491-515 (1993)

Blast Wave Reflections: 1986

15. P. Colella, R. E. Ferguson, H. M. Glaz, A. L. Kuhl, Mach reflection from an HE-driven blast wave, *Dynamics of Explosions*, Edited by J. R. Bowen, J.-C. Leyer and R. I. Soloukin, **106** Prog. Astro. & Aero., AIAA, New York, pp. 388-421 (1986)

Shear Layers: 1990-1995

16. K.-Y. Chien, R.E. Ferguson, A. L. Kuhl, H. M. Glaz and P. Colella, Inviscid dynamics of two-dimensional shear layers, *Comp. Fluid Dyn.* **5** (1-2), pp. 59-80 (1995); also see A. Kuhl, et al., *Inviscid Dynamics of Unstable Shear Layers*, R & D Associates, Los Angeles CA **RDA-TR-161604-006**, 98 pages (1990).

Part 3: Simulations of Turbulent Combustion in Explosions

17. A. L. Kuhl, J.B. Bell, V.E. Beckner, H. Reichenbach, Gasdynamic model of turbulent combustion in TNT explosions, *Proc. Combustion Institute* **33**, pp. 2177-2185 (2011)
18. A.L. Kuhl, J.B. Bell, V.E. Beckner, K. Balakrishnan, A. J. Aspden, Spherical combustion clouds in explosions, *Shock Waves* **23** (2), pp. 233-249 (2013)
19. A. L. Kuhl, J. B. Bell and V. E. Beckner, Heterogeneous continuum model of Aluminum particle combustion in explosions, *Combustion Explosion & Shock Waves* **46** (4) pp. 433-448 (2010)
20. A. L. Kuhl, D. Grote, A. Almgren and J. B. Bell, Hydrodynamics of pyrotechnic explosions, *16th Int. Detonation Symposium* (in press) 2019.

Appendix: Biography of S. K. Godunov