Universität zu Köln

Master Thesis

Astrophysics Institut Cologne

"Modelling turbulent gases with Finite Volume and Discontinuous Galerkin methods "

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submitted by

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Contents

1 Introduction

Turbulent gases are everywhere and play a major role in nature, science and engineering. Consequently, the desire to model resp. simulate fluent media as close to reality as possible has driven many generations of scientists to develop better algorithms.

2 Theory

2.1 Governing equations

Ideal Magneto-Hydrodynamic Equations The magneto-hydrodynamic equations (MHD) are a corner stone of theoretical astrophysics. They model the fluid mechanics of ionized interstellar media in an idealized form. In CGS unit they read as follows.

$$\partial_t \rho + \nabla \cdot (\rho \, \underline{u}) = 0 \tag{1}$$

$$\rho \, \partial_t \underline{u} + \rho(\underline{u} \cdot \nabla)\underline{u} + \nabla p = \frac{\underline{J} \times \underline{B}}{c} + \rho \underline{g} + \underline{F} \tag{2}$$

$$\nabla \times \underline{B} = \frac{4 \, \pi}{c} \underline{J} \tag{3}$$

$$\nabla \times \underline{E} = -\frac{1}{c} \partial_t \underline{B} \tag{4}$$

$$\nabla \cdot \underline{B} = 0 \tag{5}$$

$$\underline{J} = \sigma \left(\underline{E} + \frac{\underline{u} \times \underline{B}}{c} \right) \tag{6}$$

TODO: Explain above equations in detail. Name -> physical meaning ...

We want to keep the simulation simple and do not include electric current ($\sigma = \infty$) and gravity in our model. Hence, $\underline{J} = 0$ and $\underline{g} = 0$. This simplifies above equations to the ideal MHD equations. They are valid for dynamics in interstellar clouds where we have huge spatial dimensions of several parsecs and consequently long crossing times.

TODO: More arguments why ideal MHD equations are valid for ISM simulations

TODO: Insert ideal MHD equations

When we set the initial magnetic field strength to zero $\underline{B} = 0$ no magnetic dynamics come into play and the equations reduces further to the compressible Euler equations.

Compressible Euler Equations The compressible Euler Equations are valid for perfect fluids. We assume no heat conduction ($\mathbb{T}^{i0} = \mathbb{T}^{0i} = 0$), no viscosity ($\mathbb{T}^{ij} = p \mathbb{1}$, $\mu_d = 0$) and no gravity $g = 0$. Within in the comoving frame the *stress-energy tensor* $\mathbb{T}$ reads:

$$\mathbb{T}^{\alpha\beta} = \mathrm{diag}(\rho c^2, p, p, p) = \left(\rho + \frac{p}{c^2} \right) u^\alpha u^\beta + p \, \mathbb{G}^{\alpha\beta} \tag{7}$$

In the flat spacetime the *metric tensor* is set to $\mathbb{G} = \text{diag}(-1, 1, 1, 1)$. The total energy and the number of particles are conserved.

$$\partial_\nu \mathbb{T}^{\mu\nu} = 0 \tag{8}$$

$$\partial_\mu (n\, u^\mu) = 0 \tag{9}$$

Taking the non-relativistic limit, we arrive at the well-known Euler equations in conservative form.

$$\partial_t \rho + \nabla \cdot (\rho\, \underline{u}) = 0 \;\; \text{(mass cons.)} \tag{10}$$

$$\partial_t (\rho\, \underline{u}) + \nabla \cdot (\rho \underline{u} \underline{u}^T) + \nabla p = \underline{F} \;\; \text{(momentum cons.)} \tag{11}$$

$$\partial_t E + \nabla \cdot (\underline{u}\, (E + p)) = 0 \;\; \text{(energy cons.)}, \tag{12}$$

where the total energy E is composed of the internal energy $\mathcal{I}$ and the kinetic energy $\mathcal{K}$.

$$E = \mathcal{I} + \mathcal{K} = \frac{p}{\gamma - 1} + \frac{\rho}{2} u^2 \tag{13}$$

The source term $\underline{F}$ allows us to perpetually inject a force field which gets important in the discussion of driven turbulence later on.

Equation of State If not stated otherwise all simulations follow the *ideal gas law*.

$$p = \frac{c^2}{\gamma}\, \rho = R\, T\, \rho = \frac{R}{c_v} \mathcal{I} = (\gamma - 1) \mathcal{I}, \tag{14}$$

where R is the specific ideal gas constant, T is the gas temperature and $c_v = \frac{\gamma - 1}{R}$ is the specific heat capacity at constant volume. The speed of sound c is a direct consequence of the ideal gas equation.

$$c^2 = \gamma \frac{p}{\rho} := Const_{\text{polytrope}} = C_P \tag{15}$$

During the numerical simulation this equation of state is enforced via the *polytropic process* (sometimes called *polytropic cooling*) at every timestep.

$$p = C_P\, \rho^\Gamma, \tag{16}$$

where the *polytropic exponent* $\Gamma := 1$ which is equivalent to an isothermal process. A thorough derivation can be found in [**?**], p.2-7.

Dimensionless Euler Equations We want to show that the Euler equations are invariant to changes of units. This discussion is useful since most numerical frameworks do not support physical units and rescaled phyiscal quantities avoid truncation errors due to the limits of floating point operations. For this, we choose a characteristic length l_r, a characteristic velocity u_r and a characterstic density ρ_r. Multiplying proper combinations of these constants with the

Euler equations yields

$$[\partial_t \rho + \nabla \cdot (\rho\, \underline{u})] \cdot \frac{l_r}{\rho_r\, u_r} = 0 \tag{17}$$

$$\Big[\partial_t (\rho\, \underline{u}) + \nabla \cdot (\rho \underline{u}\underline{u}^T) + \nabla p - \underline{F}\Big] \cdot \frac{l_r}{\rho_r\, u_r^2} = 0 \tag{18}$$

$$[\partial_t E + \nabla \cdot (\underline{u}\,(E+p))] \cdot \frac{l_r}{\rho_r\, u_r^3} = 0 \tag{19}$$

We simplify and get

$$\partial_{\tilde{t}} \tilde{\rho} + \tilde{\nabla} \cdot (\tilde{\rho}\, \underline{\tilde{u}}) = 0 \tag{20}$$

$$\partial_{\tilde{t}} (\tilde{\rho}\, \underline{\tilde{u}}) + \tilde{\nabla} \cdot (\tilde{\rho} \underline{\tilde{u}}\underline{\tilde{u}}^T) + \tilde{\nabla} \tilde{p} - \underline{\tilde{F}} = 0 \tag{21}$$

$$\partial_{\tilde{t}} \tilde{E} + \tilde{\nabla} \cdot (\underline{\tilde{u}}\,(\tilde{E} + \tilde{p})) = 0, \tag{22}$$

where $t_r = \frac{l_r}{u_r}$ (characteristic time) and

$$\tilde{t} = \frac{t}{t_r},\ \tilde{\rho} = \frac{\rho}{\rho_r},\ \underline{\tilde{u}} = \frac{\underline{u}}{u_r},\ \tilde{\nabla} = l_r\, \nabla,\ \tilde{E} = \frac{E}{\rho_r\, u_r^2},\ \tilde{p} = \frac{p}{\rho_r\, u_r^2},\ \underline{\tilde{F}} = \underline{F}\, \frac{l_r}{\rho_r\, u_r^2}. \tag{23}$$

Conseqently, the dimensionless Euler equations do not change under unit transformation. If not stated otherwise we drop the tilde sign ($\tilde{\cdot}$) and assume always dimensionless quantites from now on.

Choice of parameters One consequence of dimensionless units is the free choice of constants. We want to use this feature in choose a sensible set of parameters. Considering the Euler equation in conservative form (10), their functions of space and time

$$\rho = \rho(t,x,y,z),\ \ (\rho \underline{u}) = (\rho \underline{u})(t,x,y,z),\ \ E = E(t,x,y,z) \tag{24}$$

are faced with

$$\gamma := 5/3,\ \ R := 1, \langle \rho \rangle := 1, \langle c \rangle := 1, \tag{25}$$

where we assume a mono-atomic gas without interacting forces. So we derive

$$C_P = \frac{c_0^2}{\gamma} = 3/5 = 0.6,\ \ \langle p \rangle = C_P \cdot \langle \rho \rangle = 0.6,\ \ \langle E \rangle = \frac{\langle p \rangle}{\gamma - 1} = 0.9,\ \ \langle T \rangle = \frac{\langle c \rangle^2}{\gamma\, R} = 0.6 \tag{26}$$

Remark The average sonic mach number $\mathcal{M}$ is consequently equal to the average root-means-square-velocity (rmsv).

$$\mathcal{M} = \frac{\langle \text{rmsv} \rangle}{\langle c \rangle} = \langle \frac{\int_\Omega \sqrt{\underline{u}^2}}{\int_\Omega m} \rangle \tag{27}$$

If not state otherwise, these set of constants define the global state at all times.

2.2 Weak Formulation

In this section we want to derive the *weak formulation* of the governing equations. This establishes the basis for the polynomial formulation which is the core idea of all DG methods. First, the Euler equations get split up into terms resembling the independent one temporal and three spatial dimensions with respect to the linear differential operator.

$$\partial_t \underline{U} + \partial_x \underline{F}(\underline{U}) + \partial_y \underline{G}(\underline{U}) + \partial_z \underline{H}(\underline{U}) + \underline{S} = 0, \tag{28}$$

where

$$\underline{U} = (\rho, \rho u_1, \rho u_2, \rho u_3, E)^T \tag{29}$$

$$\underline{F}(\underline{U}) = (\rho u_1, \rho u_1^2 + p, \rho u_1 u_2, \rho u_1 u_3, u_1(E+p))^T \tag{30}$$

$$\underline{G}(\underline{U}) = (\rho u_2, \rho u_2 u_1, \rho u_2^2 + p, \rho u_2 u_3, u_2(E+p))^T \tag{31}$$

$$\underline{H}(\underline{U}) = (\rho u_3, \rho u_3 u_1, \rho u_3 u_2, \rho u_3^2 + p, u_3(E+p))^T \tag{32}$$

$$\underline{S} = (0, -f_1, -f_2, -f_z, 0)^T \tag{33}$$

Defining a vector-valued test function $\underline{\phi} = (0, .., 0, \phi_i, 0, ..., 0)^T$ $(i \in 1, ..., 5)$, multiplying componentwise with above equation and integrating over the domain Ω we get

$$\int_\Omega \left(\partial_t U_i \, \phi^i + \partial_x F_i(\underline{U}) \, \phi^i + \partial_y G_i(\underline{U}) \, \phi^i + \partial_z H_i(\underline{U}) \, \phi^i + S_i \phi^i \right) d^3x = 0 \tag{34}$$

Integration-by-parts rearranges the integral into a *source term*, *volume term* and *surface term*.

$$\int_\Omega \partial_t U_i \, \psi(x,y,z)^i d^3x + \int_\Omega S_i \psi(x,y,z)^i d^3x = \tag{35}$$

$$\int_{\partial\Omega} \left(F_i(\underline{U}) \, \psi(x,y,z)^i \, n_x + G_i(\underline{U}) \, \psi(x,y,z)^i \, n_z + H_i(\underline{U}) \, \psi(x,y,z)^i \, n_z \right) d^2x,$$

$$- \int_\Omega \left(F_i(\underline{U}) \, \partial_x \psi(x,y,z)^i + G_i(\underline{U}) \, \partial_y \psi(x,y,z)^i + H_i(\underline{U}) \, \partial_z \psi(x,y,z)^i \right) d^3x \tag{36}$$

$$\int_\Omega \partial_t U \, \psi(x,y,z) d^3x + \int_\Omega S \psi(x,y,z) d^3x =$$

$$\int_{\partial\Omega} \left[F(\underline{U}) \, \psi(x,y,z) \, n_x + G(\underline{U}) \, \psi(x,y,z) \, n_z + H(\underline{U}) \, \psi(x,y,z) \, n_z \right] d^2x, \tag{37}$$

$$- \int_\Omega \left[F(\underline{U}) \, \partial_x \psi(x,y,z) + G(\underline{U}) \, \partial_y \psi(x,y,z) + H(\underline{U}) \, \partial_z \psi(x,y,z) \right] d^3x \tag{38}$$

where $\underline{n} = (n_x, n_y, n_z)^T$ is the outward surface normal to $\partial\Omega$.

2.3 Finite Element Scheme

Solving PDEs numerically comes down to discretizing an original continuous problem. Most approaches consist of in essence three major generally interchangeable modules.

a) Divide the problem domain into adjunct self-contained sub-domains, called elements or cells.

b) Apply an averaging function or polynomial over every sub-domain.

c) Define a flux function through which ever cell communicates with its adjacent neighbors.

REA Algorithm

Briefly, we are going to take a closer look at the class of *Finite Elements* approach where the *Finite Volume* and the *Discontinuous Galerkin* are concrete implementations are. At first the very physical domain Ω is divided into a *mesh* of adjunct self-contained sub-domains Ω_l ($l \in \mathbb{N}$) with concisely defined boundaries. For the rest of this text we omit the element index l. So Ω is now the domain within an element. The unknown solution $\underline{U}$ is replaced by polynomes of order N_p constructed from linear combinations of orthogonal basis functions $\underline{\Psi}^j$.

multi-index

$$U_{\underline{I}}(t,x,y,z) \approx p_{\underline{I}}(t,x,y,z) = \sum_{\underline{J}=0}^{N_p} U_{\underline{I}}^{\underline{J}}(t)\, \Psi^{\underline{I}}(x,y,z) \tag{39}$$

Remark Usally, the polynomes of every element are transformed to a reference space $\hat{\Omega} = [-1,1]^3$ where the actual interpolation takes place. This meassure massively increases efficiency since the basis functions are equal among all elements. For the sake of simplicity this step is ommitted here.

Remembering the general weak formulation of the solution integral, derived in ... The treatment is the same for all five conservative variables of the Euler equation hence we ignore the index i. T

$$\int_\Omega \left(\sum_{j=0}^{N_p} (\partial_t U^j(t))\, \Psi^j(\underline{x}) \right) \phi(\underline{x}) d^3x + \int_\Omega S(t)\, \phi(\underline{x}) d^3x =$$

$$\int_{\partial\Omega} \left[F(t)\, \phi(\underline{x})\, n_x + G(t)\, \phi(\underline{x})\, n_z + H(t)\, \phi(\underline{x})\, n_z \right] d^2x, \tag{40}$$

$$- \int_\Omega \left[\left(\sum_{j=0}^{N_p} F^j(t)\, \Psi^j(\underline{x}) \right) \partial_x \phi(\underline{x}) + \left(\sum_{j=0}^{N_p} G^j(t)\, \Psi^j(\underline{x}) \right) \partial_y \phi(\underline{x}) + \left(\sum_{j=0}^{N_p} H^j(t)\, \Psi^j(\underline{x}) \right) \partial_z \phi(\underline{x}) \right] d^3x$$

If we associate the basis functions $\Psi^{\underline{J}} := L^{\underline{J}}$ and the test functions $\phi := L^{\underline{I}}$ with the LAGRANGE polyonmes of equal order N_p, we can formulate an interpolation and integration scheme (*collocation*) over the domain Ω.

$$l^j(x) = \prod_{k=0, k\neq j}^{p} \frac{x - x_k}{x_j - x_k},\ j = 0, \ldots, p, \tag{41}$$

whith the KRONECKER property $l^j(x_i) = \delta_{ij}$. One gets to three-dimensional formulation via

the *Tensor Product Ansatz*.

$$L^{I}(\underline{x}) = L^{ijk}(x,y,z) = \sum_{i,j,k=0}^{N_p} f^{ijk} \cdot l^i(x) \cdot l^j(y) \cdot l^k(z) \tag{42}$$

Flux Functions Roe, Rusanov, Lax-Wendroff, ES, ...

2.4 Turbulences

Turbulences are very common phenomena in nature. They can be desired as well as unsoliceted. In astrophysics turbulence are suspected to play a major role in star formation in interstellar clouds. Hence, a good understanding of the underlying mechanics is crucial in order to model them correctly in numerical simulations. While turbulences in incompressible media has been thoroughly studied in the past, there is still an on-going debate about what additional dynamics compressibility brings especially in supersonic setups where shocks emerge.

Say something about fluctuation property around mean see Hydrodynamic and MHD Turbulent Flows Chapter 1

Energy Cascade see Kolmogorov-Burgers Model for Star-forming Turbulence - inertial range -> Kolmogorov scaling since large scales - dissipative range -> Burgers scale - theoretical ground

see SCALING RELATIONS OF SUPERSONIC TURBULENCE IN STAR-FORMING MOLECULAR CLOUDS - numerical validation of theory in above paper

Density and Velocity Distribution - skewness, log, log-log scale ...

2.5 Global Quantities

Mach Number $\mathcal{M}$

$$\mathcal{M} = \sqrt{\frac{\int_\Omega \rho \, \underline{u}^2 \, d\Omega}{\int_\Omega \rho \, d\Omega}} \tag{43}$$

Total Kinetic Energy $\mathcal{K}$

$$\mathcal{K} = \frac{\int_\Omega \frac{\rho}{2} \, \underline{u}^2 \, d\Omega}{\int_\Omega \rho \, d\Omega} \tag{44}$$

Kinetic Energy Dissipation Rate ϵ

$$\epsilon = -\frac{d\mathcal{K}}{dt} \tag{45}$$

$$(\underline{\underline{S}})_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \lambda \delta_{ij} \frac{\partial u_k}{\partial x_k} \tag{46}$$

Bulk viscosity coefficient $\lambda := 2/3$

$$\epsilon_1 = 2\,\frac{\mu}{\rho_0\,\Omega}\,\int_\Omega \underline{\underline{S}} : \underline{\underline{S}}\,d\Omega \tag{47}$$

$$\epsilon_2 = 2\,\frac{\mu_v}{\rho_0\,\Omega}\,\int_\Omega (\nabla\cdot\underline{u})^2\,d\Omega \tag{48}$$

$$\epsilon_3 = -\frac{1}{\rho_0\,\Omega}\,\int_\Omega p\,\nabla\cdot\underline{u}\,d\Omega \tag{49}$$

Total Enstrophy $\mathcal{E}$

$$\underline{\omega} = \nabla\times\underline{u} \tag{50}$$

$$\mathcal{E} = \frac{\int_\Omega \frac{\rho}{2}\,\underline{\omega}^2 d\Omega}{\int_\Omega \rho\,d\Omega} \tag{51}$$

For subsonic mach numbers:

$$\epsilon \approx 2\frac{\mu}{\rho_0}\,\mathcal{E} \tag{52}$$

Reynolds Number

$$R = \frac{\rho_0\,V_0\,L}{\mu} \tag{53}$$

Adiabatic Constant

$$\gamma = \frac{c_p}{c_v} \tag{54}$$

Prandtl Number

$$Pr = \frac{\mu\,c_p}{\kappa_H} \tag{55}$$

Kinetic Dissipation

2.6 Local Quantities

2.7 Turbulent Forcing

Inducing natural looking turbulence with the desired properties is not a trivial task. One commonly used method is by exploiting the intermittent behaviour of random walks, in particular the Ornstein-Uhlenbeck process.

It has the advantage of being replicable but irregular at the same time.

Following [**?**] we formulate

$$d\hat{\mathbf{f}}(\mathbf{k},t) = \frac{3}{\sqrt{1-2\zeta+3\zeta^2}} \left[-\hat{\mathbf{f}}(\mathbf{k},t)\frac{dt}{T} + F_0 \left(\frac{2\sigma^2(\mathbf{k})}{T} \right)^{1/2} \mathbf{P}_\zeta(\mathbf{k}) \cdot d\mathbf{W}_t \right] \tag{56}$$

$$(P_{ij})(\mathbf{k}) = \zeta\, P_{ij}^{\perp}(\mathbf{k}) + (1-\zeta) P_{ij}^{\parallel} = \zeta\, \delta_{ij} + (1-2\,\zeta)\frac{k_i k_j}{k^2} \tag{57}$$

$$\tag{58}$$

This acceleration field in fourier space allows us to precisely specify at which spatial scales we want to apply the forcing as well as the ratio of compressive and solenoidal modes.

The projection parameter $\zeta \in [0,1]$ sets the relative contribution of compressible and solenoidal injection rates. If not stated otherwise ζ is set to 0.5. Turning time T and base forcing F_0 depend on the general simulation setup.

2.8 Shock Capturing

In hypersonic simulations the solver has to deal with strong shocks in an accurate and robust manner. The utilized shock capturing strategy consists of two parts: sensoring and capturing.

2.8.1 Sensoring

Many shock sensors have been developed. Within FLEXIfollowing indicators are available.

Jameson [?]

Ducros [?]

Persson [?]

Based on the PERSSON indicator we develop a *smoothness* sensor. The basic idea is to find a meassure for the variance of the highest frequencies in modal space of the polynome.

First we express the solution of order p within each eleement in terms of an orthogonal basis as

$$u = \sum_{i=1}^{N(p)} u_i \psi_i, \tag{59}$$

where $N(p)$ is the total number of terms in the expansion and ψ_i are the LEGENDRE basis functions. Now we only consider the terms up to order $p-1$, that is

$$\hat{u} = \sum_{i=1}^{N(p)} u_i \psi_i, \tag{60}$$

Whithin each element Ω we define the following *smoothness* indicator

$$s = \log_{10} \frac{\langle u-\hat{u}, u-\hat{u} \rangle}{\langle u, u \rangle}, \tag{61}$$

where $\langle \cdot, \cdot \rangle$ is the standard inner product in $L_2(\Omega)$.

The smaller the indicator s, the smoother is the approximating solution. By setting a specific threshold for s one can decide when to switch between DG and FV mode. This procedure is done at every timestep hence the elements in FV mode should follow along the shock waves throughout the domain.

2.8.2 Capturing

Entropy Stable Flux [?]

Local Finite Volume

Split Schemes See [?] for further details.

Artificial Viscosity ...

$$\frac{\partial \underline{U}}{\partial t} + \nabla \cdot \underline{F} = \nabla \cdot (\epsilon \nabla U) \tag{62}$$

The amount of viscosity varies for each element depending on the current shock strength. We have to consider two cases.

If the element is in FV mode the AV is set quadratic proportional to the maximal RMS v_{rmsv} within the element.

$$\epsilon = \epsilon_0 \cdot \max(v_{rmsv})^2 \tag{63}$$

This step is necessary for FV schemes who do not handle strong shocks via their flux schemes.

In case of DG mode the amount of AV is based on the *Persson Indicator* introduced above.

$$\epsilon = \begin{cases} 0 & \text{if} \quad s < s_0 - \kappa \\ \epsilon_0 & \text{if} \quad s > s_0 + \kappa \\ \frac{\epsilon_0}{2}\left(1 + \sin \frac{\pi(s-s_0)}{2\kappa}\right) & \text{else} \end{cases} \tag{64}$$

The parameters ϵ_0 and κ are chosen empirically. Since we do not have any natural viscosity the artifical one must be as small as possible; just enough for diffusing velocity spikes in the presence of shocks. Typical values are around $\epsilon_0 \propto 10^{-10}$.

3 Numerical Setup

3.1 FLASH framework

3.2 FLEXI framework

3.3 Grids and Meshes

Periodic Box