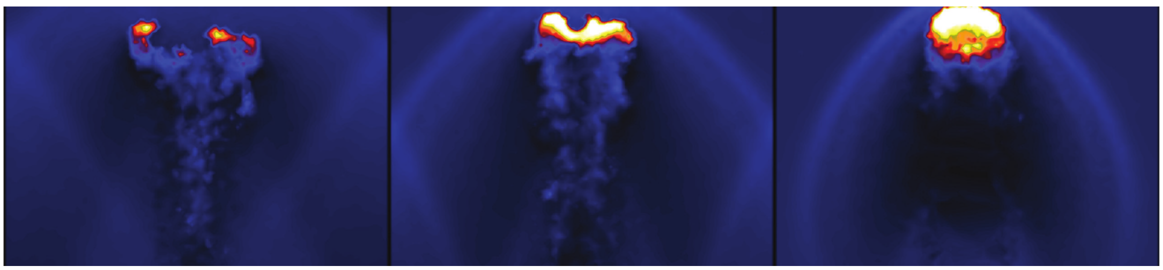
Research Proposal for a Master Thesis in Physics
Verifying the VPH scheme in Galaxy Formation

Sebastian Bustamante Jaramillo



Time evolution of a gas cloud in a supersonic wind using a VPH scheme. Taken from (Heß & Springel, 2010)

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1 General Information

Information of the Student

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Information of the Project

Title	**Verifying the VPH scheme in Galaxy Formation**
Field	Cosmology, Astrophysics, Physical Sciences
Advisor 1	Professor Juan Carlos Munoz-Cuartas. Universidad de Antioquia, Colombia.
University	Universidad de Antioquia, Master of Physics program
Time Frame	2 years

2 Abstract

3 Introduction

As we understand more deeply the physical processes involved in astrophysical phenomena, it becomes necessary to compute complex interactions of a ever increasing number of single components. Some prominent examples include the large-scale Universe, galaxy evolution, stellar interior, star formation and protoplanetary disk dynamics. A common aspect of these examples is that all of them can be regarded basically as a fluid mechanic problem.

Although the development of analytical approaches has demonstrated to be a valuable resource for studying these processes, their increasing complexity makes necessary to invoke numerical solutions as a more feasible alternative. For this purpose, two different families of hydrodynamics solvers has been explored and widely used by the astrophysical community. First, a family of moving-mesh-based techniques (e.g. *Smoothed Particle Hydrodynamics* `SPH` (Lucy, 1977; Gingold & Monaghan, 1977), *Voronoi Particle Hydrodynamics* `VPH` (Heß & Springel, 2010)), and a second family of fixed-mesh-based techniques (e.g. *Adaptive Mesh Refinement* `AMR` (Berger & Colella, 1989)).

Due to the Lagrangian character of moving-mesh methods, techniques like `SPH` are easily implemented on a computer. Furthermore, as the physical system evolves, the mass particles naturally move into higher density regions, providing a self-adjusting spatial resolution. Nevertheless, `SPH` has been shown to produce spurious suppression of fluid instabilities due to its kernel-based density estimator, making it unsuitable to model some of the dynamics accurately. On the other hand, fixed-mesh methods like `AMR` are more efficient for capturing shock dynamics. However, due to the conservative nature of the hydrodynamical equations, a fixed mesh causes a lack of Galilean invariance. Furthermore, the sampling of physical properties over the grid introduces spurious vorticity to the fluid, making this technique poor suitable for studying turbulent flows.

A completely new approach to solve hydrodynamical problems was introduced by Springel (2010a) and implemented into the `AREPO` code. It combines the strengths of `AMR` and `SPH` but overcomes many of their weaknesses, hence it can be though as a mixed technique. `AREPO` uses a moving mesh based on a Voronoi tessellation defined over a set of particles that represents the fluid. The geometry of the mesh resembles very closely that of the point distribution, retaining the self-adaptivity inherent of `SPH` and also keeping a grid to capture shocks like `AMR` does. These features make `AREPO` highly accurate for simulating a wide range of hydrodynamical problems. Nevertheless, there is a price to pay for this accuracy, `AREPO` demands a huge computing time as compared with `SPH` and even `AMR`.

A very interesting alternative was introduced by Heß & Springel (2010), i.e. the *Voronoi Particle Hydrodynamics* `VPH` technique. This approach consists of an implementation of `SPH` with a modified density estimator based on the *Voronoi Tessellation Field Estimator* `VTFE`. The new estimator has demonstrated to improve substantially the spurious suppression of fluid instabilities as well as retaining the computational efficiency of the original formulation.

Finally, galaxy evolution and large-scale structure formation are very rich astrophysical scenarios where a plethora of hydrodynamical processes can be found and studied. In this fashion, cosmological simulations are quite suitable for performing detailed physical and computational comparisons of all above-mentioned techniques. It is especially interesting to quantify the computational performance of the VPH technique in terms of its physical accuracy as compared with the classic approaches and AREPO.

4 Objectives

General Objective

Quantifying the computational performance of the VPH technique in terms of its physical accuracy for a cosmological setup.

Specific Objectives

- Evaluating the physical accuracy provided by VPH for a cosmological setup as compared with AMR, SPH and AREPO.
- Exploring and quantifying the differences between VPH and AMR for describing shock dynamics in specific hydrodynamical instabilities.
- Exploring and quantifying the differences of VPH and SPH for describing turbulent flows.
- Measuring the computational performance of VPH as compared with AREPO.

5 Theoretical Framework

The Cosmological Setup

At very large scales ($\sim h^{-1}$Gpc) the current Universe exhibits a quite homogeneous matter distribution, what is, in fact, a print of its very first stage, that was almost perfectly homogeneous at all scales. Under this considerations, at zero-order the whole Universe can be roughly described through an uniform fluid model, leading, through the Einstein's field equations, to a set of isotropic and homogeneous model better known as Friedmann's solutions (Longair, 2008).

$$H^2(t) = H_0^2 \left[(1-\Omega_0)\frac{1}{a^2} + \Omega_m \frac{1}{a^3} + \Omega_r \frac{1}{a^4} + \Omega_\Lambda \right] \tag{1}$$

where $a(t)$ is the scale factor that quantifies the relative size of the Universe as compared with the current epoch, $H(t)$ is defined as $H = a/\dot{a}$, H_0 is the current Hubble constant and the set

Ω_i are the abundance parameters of each specie in the Universe, namely $\Omega_0 = \sum \Omega_i$, Ω_m is the current abundance of matter (dark+baryon), Ω_r the abundance of radiation and relativistic matter and finally Ω_Λ is associated to the cosmological constant. This parametrization is very convenient as all of these parameters can be estimated observationally (Planck Collaboration, 2013).

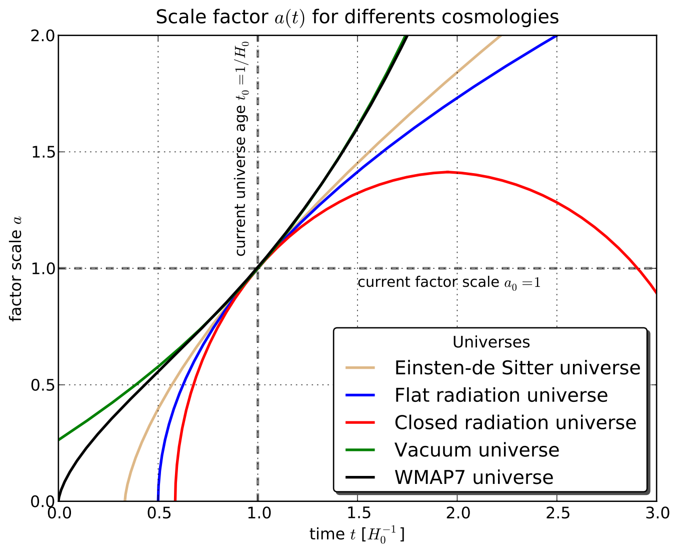

Figure 1: Different solutions to the Friedmann's equation. The WMAP7 solution is consistent with our Universe, where the current epoch is vacuum dominated, corresponding with an accelerated expansion.

Nevertheless, an uniform fluid model cannot account for the bound structures observed at smaller scales like galaxies and clusters. It is hence necessary to modify the Friedmann's solutions in order to include small perturbations that enable the evolution of such a bound structures at the current time. To do so, the Einstein's equation is linearized as follows (Padmanabhan, 1995):

$$\mathcal{L}(R_{\mu\nu}, \delta R_{\mu\nu}) = \frac{8\pi G}{c^2}(T_{\mu\nu} + \delta T_{\mu\nu}) \tag{2}$$

This approach can be demonstrated to be equivalent to introducing basic Newtonian fluid equations for the matter component.

Continuity equation
$$\frac{\partial \delta}{\partial t} = -\frac{1}{a}\nabla_r \cdot [(1+\delta)\boldsymbol{v}] \tag{3}$$

Euler's equation
$$\frac{\partial \boldsymbol{v}}{\partial t} + \frac{\dot{a}}{a}\boldsymbol{v} + \frac{1}{a}(\boldsymbol{v}\cdot\nabla_r)\boldsymbol{v} = -\frac{\nabla_r P}{a\bar{\rho}(1+\delta)} - \frac{1}{a}\nabla_r \Phi \tag{4}$$

Poisson's equation
$$\nabla_r^2 \Phi = 4\pi G \bar{\rho} a^2 \delta \tag{5}$$

where $\rho = \bar{\rho} + \delta\rho = \bar{\rho}(1+\delta)$ is the matter density, $\boldsymbol{v}$ is the peculiar velocity, $\Phi = \phi + \ddot{a}ar^2/2$ the peculiar gravitational potential, P the fluid pressure and all gradients are evaluated in comoving coordinates.

Assuming an equation of state for an inviscid gas and decomposing the density field into Fourier modes (for a flat universe), we obtain:

$$\frac{d^2\delta_{\boldsymbol{k}}}{dt^2} + 2\frac{\dot{a}}{a}\frac{d\delta_{\boldsymbol{k}}}{dt} = \left[4\pi G\bar{\rho} - \frac{c_s^2}{a^2}k^2\right]\delta_{\boldsymbol{k}} \tag{6}$$

where $\delta_{\boldsymbol{k}}$ are the modes of the density and c_s the velocity of the sound in the medium. For the linear regime, where perturbations are still valid, each mode evolves independently. It is hence possible to assume a general solution of the form $\delta_{\boldsymbol{k}}(t) = \delta_{\boldsymbol{k}}(0)D(t)$, where $t = 0$ is referred to as some suitable time after the epoch of recombination and $D(t)$ is the linear growth function, given by:

$$D(a) = \frac{5}{2}\Omega_m\left[\Omega_m^{4/7} - \Omega_\Lambda + \left(1 + \frac{\Omega_m}{2}\right)\left(1 + \frac{\Omega_\Lambda}{70}\right)\right]^{-1} \tag{7}$$

At this point, it is possible to follow completely the evolution of the Universe in the linear regime. However, when the modes of the density field become large enough $\delta \gg 1$, the assumption of independence is not longer adequate, it is hence necessary to evaluate numerically the evolution in the non-linear regime.

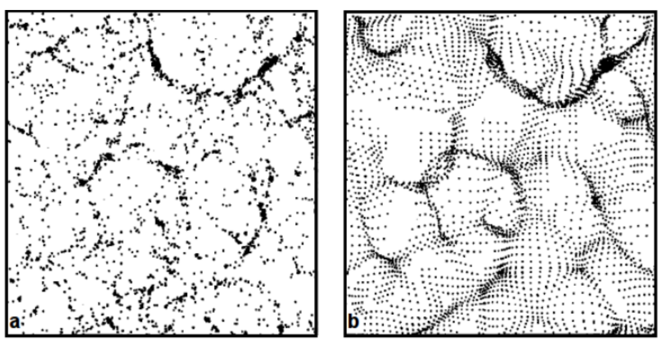

Figure 2: Comparison of the evolution of a density field for a N-body simulation (left) and for the Zel'dovich approximations (right). Taken from Longair (2008).

In order to provide a set of initial conditions for numerical runs, it can be used the Zel'dovich approximation (Zel'dovich, 1970). This approximation allows to follow the evolution of primordial perturbations in the quasi-linear regime ($\delta \sim 1$), what makes it very suitable to tie analytical solutions in the linear regime with numerical solutions in the non-linear regime. Using the Lagrangian frame and taking certain portion of the fluid, its trajectory can be described as follows:

$$\boldsymbol{r}(t, \boldsymbol{q}) = a(t)\left[\boldsymbol{q} + \boldsymbol{\Psi}(\boldsymbol{q}, t)\right] \tag{8}$$

where $\boldsymbol{q}$ is the comoving Lagrangian coordinate when fluid is not perturbed and $\boldsymbol{\Psi}(\boldsymbol{q}, t)$ is the displacement function that accounts for clustering. The displacement function can be approximated as $\boldsymbol{\Psi}(\boldsymbol{q}, t) = D(t)\boldsymbol{\Psi}(\boldsymbol{q})$, where $D(t)$ is the linear growth function (Eq. 7) and $\boldsymbol{\Psi}(\boldsymbol{q})$ is given by:

$$\boldsymbol{\Psi}(\boldsymbol{q}) = \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}\cdot\boldsymbol{q}} \frac{i\boldsymbol{k}}{k^2} \delta_{\boldsymbol{k}}(0) \tag{9}$$

In this same fashion, the perturbed velocity field can be constructed by means of the Zel'dovich approximation. Then, discretizing the fluid, it is obtained a set of positions and velocities $\{\rho_i, \boldsymbol{r}_i, \boldsymbol{v}_i\}$ corresponding with the input initial conditions for some numerical scheme for evolving the non-linear regime, like `SPH`, `VPH`, `AMR`.

Smoothed Particle Hydrodynamics (SPH)

As was previously discussed, the matter component of the Universe can be modelled as an inviscid and collisionless gas that follows the standard fluid equations 3, 4, 5. The objective of any hydrodynamic scheme is then solving these set of equations in a suitable way. One of the classic schemes widely used by the astrophysical community for this task is the Smoothed Particle Hydrodynamics `SPH` as introduced by Lucy (1977) and Gingold & Monaghan (1977).

Kernel Interpolants

The core of `SPH` is the kernel interpolant formalism, where a continuous and smoothed field can be recovered from a discrete set of sampling particles. For any physical field $F(\boldsymbol{r})$ it may be defined a smoothed version $F_s(\boldsymbol{r})$ as

$$F_s(\boldsymbol{r}) = \int_V \boldsymbol{F}(\boldsymbol{r}')W(\boldsymbol{r} - \boldsymbol{r}'; h)d\boldsymbol{r}' \tag{10}$$

where the integral extends over the volume domain and $W(\boldsymbol{r}; h)$ is the kernel interpolant, with h being the smoothing length, which gives the volume associated to the kernel domain.

Several different expressions for the kernel can be used for obtaining the smoothed versions of the fields, where the only conditions to satisfy are normalization $\int W(\boldsymbol{r}; h)d\boldsymbol{r} = 1$ and convergence to the Dirac delta when $h \to 0$. Nevertheless, finite-range kernels like the cubic spline kernel are preferred for their easy computational implementation.

$$W(r; h) \equiv W\left(\frac{r}{2h}\right) = W(q) = \frac{8}{\pi}\begin{cases} 1 - 6q^2 + 6q^3, & 0 \le q \le 1/2, \\ 2(1-q)^3, & 1/2 < q \le 1, \\ 0, & q > 1 \end{cases} \tag{11}$$

If we fix the masses of the sampling particles to be $\{m_i\}_i$, the volume element of each may be approximated as $\Delta\boldsymbol{r}_i = m_i/\rho_i$. The variation of the volume hence relies on the variation of the density. The integral 10 can be then approximated as

$$F_i' \equiv F_s(\boldsymbol{r}_i) \approx \sum_j \frac{m_j}{\rho_j} F_j W(\boldsymbol{r}_i - \boldsymbol{r}_j; h_i) \tag{12}$$

here we use the notation $F_i' = F_s(\boldsymbol{r}_i)$ for the smoothed fields and $F_i = F(\boldsymbol{r}_i)$ for the originals. Although smoothed fields are defined for any position, we are just interested in the positions of the sampling particles $\{r_i\}$. Note that the summation runs over all particles, however, due to the finite-range kernel adopted, it is reduced only to the neighbours inside a sphere of radius $2h$. Hereafter, the smoothing lengths will be taken as adaptive for each particle, what is necessary in order to keep a good precision for high density contrasts occurring in some simulations.

One of the main appealing of the kernel interpolant formalism of `SPH` is the handling of differential operators, where the conditions of continuity and differentiability relies on the kernel rather than the field itself. This is advantageous when dealing with sparse distributions or very rugged fields. So we obtain:

$$\mathcal{D}_i[F_s(\boldsymbol{r}_i)] = \sum_j \frac{m_j}{\rho_j} F_j \mathcal{D}_i[W(\boldsymbol{r}_i - \boldsymbol{r}_j; h_i)] \tag{13}$$

where $\mathcal{D}_i$ is any differential operator evaluated in $\boldsymbol{r}_i$. Note that this expression includes the possibility of h_i as a function of the coordinates, what is the more general case. A very useful expression is the divergence of the velocity field, yielding

$$(\nabla \cdot \boldsymbol{v})_i = \frac{1}{\rho_i} \sum_j m_j (\boldsymbol{v}_j - \boldsymbol{v}_i) \cdot \nabla_i W(\boldsymbol{r}_i - \boldsymbol{r}_j; h_i) \tag{14}$$

where vectorial identities have been used in order to symmetrize the expression.

Equation of Motions

Once discussed the kernel interpolant formalism, we proceed to describe how to get the equations of motions to be solved computationally. The original approach consists in dealing directly with differential operators of the fluid equations 3 4 5 according to the equation 13 (Lucy, 1977; Gingold & Monaghan, 1977). Instead, we will take the approach first proposed by Gingold & Monaghan (1982) and further developed by Springel (2010b). This consists of a variational derivation of the equations of motions by first discretizing the Lagrangian of the system. The main advantage of this derivation is that it retains the conservation laws associated to the Hamiltonian dynamics in a natural fashion.

As demonstrated by Eckart (1960), the hydrodynamic equations can be derived from the Lagrangian

$$\mathcal{L} = \int \rho \left(\frac{v^2}{2} - u \right) dV \tag{15}$$

where u carries with all the interactions of the system. Using the kernel interpolant formalism, we can rewrite this expression as

$$\mathcal{L} = \sum_i \left(\frac{1}{2} m_i v_i^2 - m_i u_i \right) \tag{16}$$

6 Methodology

The proposed project is subject to a M.Sc. study and will cover the following steps:

✓ *First, a bibliographic review of the original papers of the discussed methods will be done. Also a review of previous comparison projects.*

Before carrying out our enterprise in quantifying the performance of `VPH` over cosmological setups, it is necessary to understand deeply the foundations of the classic approaches. At this point, a detailed bibliographic review of the original papers (for `SPH`, `AMR`, `VPH` and `AREPO`) should be done. Although no previous works have been done in comparing thoroughly the performance of `VPH` with other approaches over cosmological setups, there are a plenty of comparison projects for the classic approaches and even `AREPO` over galaxy simulations and commonly used benchmark problems. This literature will have to be reviewed as well.

✓ *Second, a design of the numerical experiments should be done at this point. This includes making cosmological simulations using different techniques and if necessary, constructing and simulating specific benchmark problems.*

As this project will be entirely based on numerical results, computing a set of cosmological simulations as well as some benchmark problems is one of the key steps. For this purpose, we will use some packages like `GADGET` Springel (2005) for `SPH` simulations, `RAMSES` Teyssier (2002) for `AMR` and a modified version of `GADGET` for `VPH`. Other standard benchmark problems will be also simulated, e.g. the sod shock tube, Kelvin-Helmholtz instabilities, a gas cloud in a supersonic wind.

✓ *Third, a thorough analysis of the numerical results will be done.*

Once obtained the numerical results from the performed simulations, a thorough analysis of the physical accuracy of `VPH` as compared with the other techniques will be done for each situation. A computational performance analysis of the `VPH` technique will be also carried out, i.e. computing time, memory and processor usage.

✓ *Fourth, a first-author paper with the main result will be prepared.*

The more relevant results of our project will be prepared as a paper and submitted to some high impact international journal. If possible, a participation in some international event is also included in this step.

✓ *Fifth, a thesis will be written.*

A dissertation for obtaining a M.Sc. in Physics degree will be prepared. A streamlined description of each technique will be included as well as the presentation of the performed simulations and a discussion of all our results and conclusions.

7 Antecedents

Previous activities and projects related with Numerical Cosmology have been successfully carried out within the FACom group, many of these leaded by Prof. Juan Carlos Munoz-Cuartas. This demonstrates the broad research expertise of the supervisor in the topic and the availability of computational resources (computing time, software) required to perform this project satisfactorily.

On the other hand, at the present the student has already some of the fundamental knowledge in Astrophysics and Cosmology required for this investigation. This can be confirmed by his research experience, including a paper (as co-author) published in the ApJL in which the kinematics of the Local Group in a cosmological context was studied, another paper (as co-author) published in the ApJ where the influence of thermal evolution on the magnetic habitability of rocky planets was studied, and some participations in academic congresses. Furthermore, a Bachelors thesis where the preferred place of simulated Local Group-like systems in the cosmic web was studied, also demonstrates the ability of the applicant for handling simulations and massive data, a skill that is necessary for carrying out this project.

Finally, it is worth mentioning the ongoing and already done work related with this project. First, the required codes for performing our simulations are already available (including a modified version of `GADGET` for `VPH`). Some cosmological simulations have been performed as well. Furthermore, part of the toolbox of codes for our analysis has been already developed[1], including basic miscellaneous functions for handling data, plotting point distributions and constructing phase diagrams.

8 Scientific Impact

The matter content of the Universe has been probed to be dominated by the dark matter component (Planck Collaboration, 2013). Accordingly, most of the related numerical work in

[1]You can find some codes and further information of the present stage of the project in this repository `https://github.com/sbustamante/MethodsComparison`

cosmology and galaxy formation has been carried out based on dark matter only simulations. Nevertheless, on smaller (galactic) scales, the effects of baryons become significant. For example, recent hydrodynamical simulations show that filamentary gas accretion in early stages of galaxy evolution is a key physical process; there is evidence that it plays a central role in the formation of discs (Dubois & et al., 2014), determining the alignment of galaxies with respect to the web (Hahn et al., 2010) and fuelling high star formation rates (Dekel et al., 2009).

These results show the importance of modelling baryons by incorporating gas dynamics into cosmological simulations. For this purpose, `AMR` and `SPH` have been widely used by the astrophysical community. However, due to the singular situations where each of those techniques fails, general purpose hydrodynamical simulations cannot be reached by means of them.

The recently developed approach `AREPO` Springel (2010a) has demonstrated to be highly efficient dealing with some of the most critical weaknesses of `AMR` and `SPH`, what makes it a very appealing alternative. However, its demanding computing time also makes it infeasible when computational resources are rather limited. In this direction, our endeavour in quantifying the computational performance and the improved physical accuracy of `VPH` would contribute with valuable insight of this technique as a more feasible option when limited computational resources are available.

9 Expected Results

At the end of the stipulated development time for this project, we hope to have obtained the following results:

- A toolbox of codes to study the performance of hydro-solvers over cosmological setups and over standard benchmark problems in fluid mechanics.
- A set of cosmological simulations computed by using each of the studied techniques.
- A M.Sc. thesis.
- Submitting a first-author paper to an international journal.
- Participating with a poster or an oral presentation in an international event.

10 Schedule

Next it is shown a table with the proposed activities scheduled for each term of the project.

Goals	Term I	Term II	Term III	Term IV
Bibliographic review	X			
Numerical experiments	X	X		
Analysis of results		X	X	
International journal paper			X	
Dissertation				X

Table 1: Terms range from 2014-02 for term I, up to 2016-01 for term IV.

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