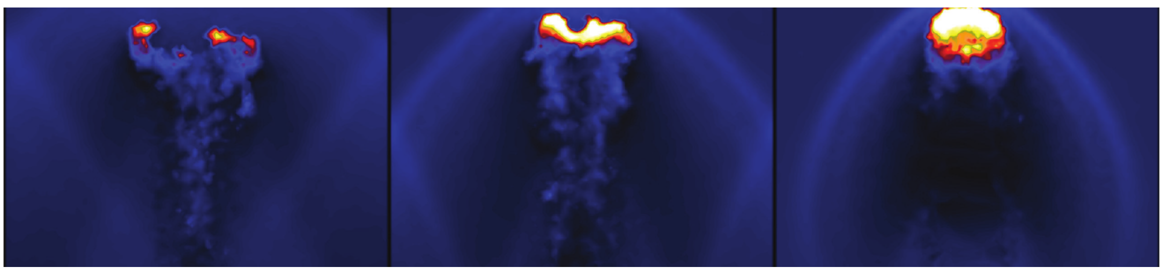
# Research Proposal for a Master Thesis in Physics
## Verifying the VPH scheme in Galaxy Formation

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

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## Information of the Project

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| **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

The complex processes involved in some astrophysical scenarios like galaxy formation, makes necessary the use of numerical approaches for a deeper understanding. We are especially concerned here with hydrodynamical schemes for solving the dynamics of a gas for galaxy formation in a cosmological setup. Two families of hydro-solvers have been widely used in astrophysics, namely a family of Lagrangian methods, where the fluid evolution is followed by means of a set of sampling particles, and a second family of mesh-based methods in which the evolution is performed over a grid. Although these methods describe well several situations, they also exhibit some weaknesses that make them poor suitable for solving full hydrodynamical cosmological simulations. Recently, a new hydro-solver was implemented into the `AREPO` code, in principle solving many of the weaknesses of the classic schemes and exploiting their strengths. Despite of the high accuracy achieved, the price to pay for this is an increased complexity in code development and design, making the reproducibility very hard, in addition to a prohibitive computing time when limited computational resources are available. We shall explore a modification of the *Smoothed Particle Hydrodynamic* `SPH` scheme based on Voronoi tessellations for field estimation, i.e. the *Voronoi Particle Hydrodynamic* `VPH`. This new approach improves greatly the accuracy of classic Lagrangian methods, but keeping a reasonable computing time. We shall compare here the physical accuracy and the computational efficiency of `VPH` with `SPH`and `AREPO`.

# 3 Introduction

As we understand more deeply the physical processes involved in astrophysical phenomena, it becomes necessary to compute complex interactions of an 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 it 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 Lagrangian techniques (e.g. *Smoothed Particle Hydrodynamics* `SPH` (Lucy, 1977; Gingold & Monaghan, 1977), *Voronoi Particle Hydrodynamics* `VPH` (Heß & Springel, 2010)), and a second family of Eulerian techniques (e.g. *Adaptive Mesh Refinement* `AMR` (Berger & Colella, 1989)).

Due to the their Lagrangian character, 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, i.e. an *irregular moving mesh* (`IMM`) technique. 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, `IMM` techniques demand large coding and design work as well as 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 observed in classic SPH as well as retaining the computational efficiency and the simplicity of the implementation 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.

# 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 SPH, AMR and IMM techniques.
- 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 IMM techniques such as the implemented into 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 $\Omega_i$ are the abundance parameters of each specie of matter-energy in the Universe, and where $\Omega_0 = \sum \Omega_i$, $\Omega_m$ is the current abundance of matter (dark+baryon), $\Omega_r$ the abundance of radiation and relativistic matter and finally $\Omega_\Lambda$ is associated to the cosmological constant. This parametrization is very convenient as all of these parameters can be estimated observationally (Planck Collaboration, 2013).

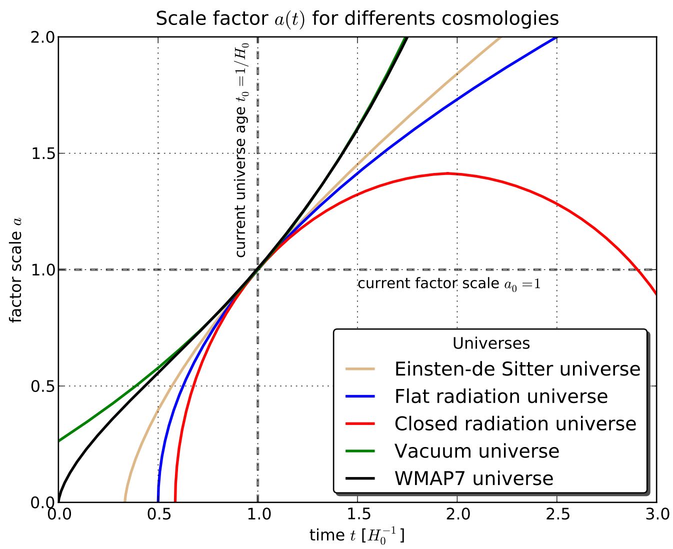


Figure 1: Different solutions to the Friedmann's equation. The WMAP7 solution is consistent with our Universe, where the current epoch is vacuum dominated, corresponding with an accelerated expansion.

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
$$\frac{\partial \boldsymbol{v}}{\partial t} + \frac{\dot{a}}{a}\boldsymbol{v} + \frac{1}{a}\left(\boldsymbol{v}\cdot\nabla_r\right)\boldsymbol{v} = -\frac{\nabla_r P}{a\bar{\rho}(1+\delta)} - \frac{1}{a}\nabla_r \Phi \tag{4}$$

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.

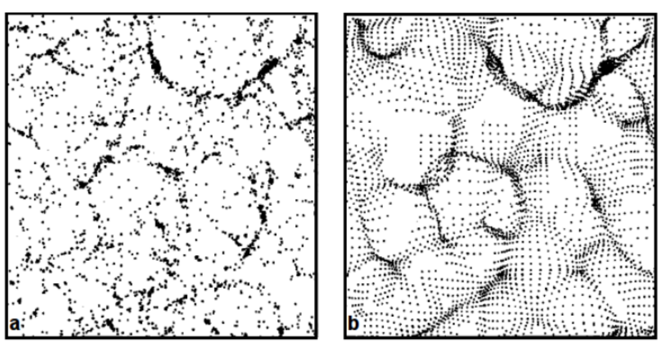


Figure 2: Comparison of the evolution of a density field for a N-body simulation (left) and for the Zel'dovich approximations (right). Taken from Longair (2008).

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 dark matter component of the Universe can be modelled as an inviscid and collisionless gas whereas the baryonic component as a collisional and dissipative gas, both following 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). `SPH` solves the continuous dynamic of the fluid by first discretizing it into parcels, where each of these parcels samples the properties of the fluid. The evolution is reached by solving the equations of motion directly over the moving particle-parcels. Finally, the continuous properties of the gas are recovered by means of interpolation techniques.

### Kernel Interpolants

The core of `SPH` is the kernel interpolant formalism, where a continuous 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, related to the integration volume and 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 compact support and 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 shown in [10] can be then approximated as

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

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 original fields. 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 many astrophysical situations.

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:

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

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

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

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

**Equations of Motion**

Once discussed the kernel interpolant formalism, we proceed to describe how to get the equations of motion 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 motion 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

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

For an inviscid gas, the equation of state is given by

$$u_i(\rho_i) = A_i \frac{\rho_i^{\gamma-1}}{\gamma - 1} = \frac{P_i}{\rho_i} \frac{1}{\gamma - 1} \tag{17}$$

where $\gamma$ is the adiabatic index, $A_i$ the specific entropy and $P_i$ the pressure as evaluated in the $i$th particle. Introducing this expression into the Lagrangian [16], considering the implicit of the smoothing length with the coordinates and applying the Euler-Lagrange equations, it is obtained the equations of motion:

$$\frac{d\boldsymbol{v}_i}{dt} = -\sum_{j=1}^{N} m_j \left[ f_i \frac{P_i}{\rho_i^2} \nabla_i W_{ij}(h_i) + f_j \frac{P_j}{\rho_j^2} \nabla_i W_{ij}(h_j) \right] \tag{18}$$

where the coefficients $f_i$ are defined as:

$$f_i = \left[ 1 + \frac{h_i}{3\rho_i} \frac{\partial \rho_i}{\partial h_i} \right]^{-1}$$

The estimation of the smoothing length of each particle is reached through the implicit differentiation of the expression $\rho_i h_i^3 = const$, what guarantees a mass conservation inside the volume of the kernel.

Although this equation of motion follows the evolution of an inviscid gas, what is a very approximate description of the matter in a cosmological setup, there are some problematic situations where the approximation is not longer suitable. Namely shock dynamics, where the strict entropy conservation would generate undesirable oscillations. It is hence necessary to introduce a new term that accounts for entropy dissipation in shocks but keeping the inviscid dynamics of the gas elsewhere. This new term, so-called artificial viscosity, is introduced in the form or a extra term in the equation of motion as

$$\left.\frac{d\boldsymbol{v}_i}{dt}\right|_{\text{visc}} = -\sum_{j=1}^{N} m_j \Pi_{ij} \nabla_i \overline{W}_{ij} \tag{19}$$

where $\Pi_{ij}$ is the viscous tensor and $\overline{W}_{ij} = [W_{ij}(h_i) + W_{ij}(h_j)]/2$. Throughout the literature may be found several different parametrizations of the viscous tensor, however the standard parametrization proposed by Monaghan & Gingold (1983) has demonstrated to be very adequate.

$$\Pi_{ij} = \begin{cases} \left[-\alpha c_{ij}\mu_{ij} + \beta\mu_{ij}^2\right]/\rho_{ij} & \text{if} \boldsymbol{v}_{ij}\cdot\boldsymbol{r}_{ij} < 0 \\ 0 & \text{otherwise} \end{cases} \tag{20}$$

with $\mu_{ij}$ defined as

$$\mu_{ij} = \frac{h_{ij}\boldsymbol{v}_{ij}\cdot\boldsymbol{r}_{ij}}{|\boldsymbol{r}_{ij}|^2 + \epsilon h_{ij}^2}$$

where $h_{ij}$, $\rho_{ij}$ and $c_{ij}$ are the arithmetic means of the smoothing length, the density and the sound speed of the $i$th and the $j$th particles respectively. The softening parameter $\epsilon$ is introduced in order to avoid divergence when two particles come very close to each other. The parameters $\alpha$ and $\beta$ quantify the strength of the viscosity term when activated. Usually they are chosen to be $\alpha \approx 0.5 - 1.0$ and $\beta = 2\alpha$.

Note that this viscous term is only activated when two particles come rapidly close to each other, what is caused in most cases by a shock. The entropy generated in this way is always positive definite, accounting for the required dissipation in shocks.

As we are interested in astrophysical applications, it is clear the necessity of coupling self-gravity to the equations of motion derived for `SPH`. Instead of taking the previous approach for the viscous term, we shall couple the self-gravity by first introducing an associated Lagrangian term that will ensure the energy conservation when gravity is included.

$$\mathcal{L}_g = -\frac{G}{2}\sum_{i\neq j} m_i m_j \phi(r_{ij}, \epsilon_j) \tag{21}$$

where the gravitational potential $\Phi(\boldsymbol{r})$ has been defined as $\Phi(\boldsymbol{r}) = G\sum_i m_i\phi(\boldsymbol{r} - \boldsymbol{r}_i, \epsilon_i)$, and $\epsilon_i$ is a softening parameter introduced to prevent singularities. Applying the Euler-Lagrange equations, we obtain the next equation of motion for the gravitation:

$$\left.\frac{d\boldsymbol{v}_i}{dt}\right|_{\text{grav}} = -\sum_j Gm_j \frac{\boldsymbol{r}_{ij}}{r_{ij}} \frac{[\dot{\phi}(\boldsymbol{r}_{ij}, \epsilon_i) + \dot{\phi}(\boldsymbol{r}_{ij}, \epsilon_j)]}{2} - \frac{1}{2} \sum_{j \neq k} G \frac{m_j m_k}{m_i} \frac{\partial \phi(r_{jk}, \epsilon_j)}{\partial \epsilon} \frac{\partial \epsilon_j}{\partial \boldsymbol{r}_i} \tag{22}$$

In this equation we have enabled an adaptive softening length depending on each particle position, this is necessary in order to gain a better numerical convergence. One way of estimating this parameter is to related it directly with the smoothing length of the kernel, i.e. $\epsilon_i = \epsilon_i(h_i)$. It is also noteworthy that these summations run all over the sampling particles as the kernel is not involved, so summations are not restricted only to nearby neighbours. This requires the implementation of sophisticated gravity solvers in order to avoid the prohibitive computing time scaling as $\mathcal{O}(N^2)$. Several gravity solver may be found in the literature, however the `TreeCode` algorithm by Barnes & Hut (1986) scaling as $\mathcal{O}(N \log N)$ has been widely used for this purpose.

Finally, the evolution of the fluid is reached by solving numerically the differential equations leaded by the inviscid, the viscous and the gravitational terms and taking the initial conditions provided by the Zel'dovich approximation. In order to do so, some numerical integration scheme has to be adopted, namely a symplectic integrator or even a time integrator scheme like Runge-Kutta.

## Voronoi Particle Hydrodynamics (VPH)

Although `SPH` is very versatile for a variety of fluid problems and the computational implementation is direct due to its Lagrangian nature, the density estimation based on the kernel interpolant formalism exhibits some problems. Namely `SPH` fails in recovering the total volume, i.e. the sum of all the volume elements of the sampling particles is not equal to the volume of the simulation, and the smoothing of the density field across contact discontinuities generates non-desirable spurious suppressions.

Several modifications of the original formulation of `SPH` have been proposed in order to improve the accuracy. Among them is very interesting the one proposed by Heß & Springel (2010), in which is introduced a new estimative of the density field based on a Voronoi tessellation of the sampling particles. Tessellations techniques have been previously introduced as estimators of physical fields in simulations (see e.g. Delaunay Tessellation Field Estimator DTFE by Schaap & van de Weygaert (2000)) with more accurate results than kernel interpolants of `SPH` (Pelupessy et al., 2003).

Although Delaunay tessellation was first introduced for field estimation, it exhibits some problems that makes it unsuitable for some pathological situations. Due to the definition of a Delaunay triangulation, where no point of the dataset must be inside the circumcircle of any triangle of the tessellation (see Fig. 3), there may be more than a triangulation for a same dataset, besides the volumes of the polyhedra do not change continuously with the

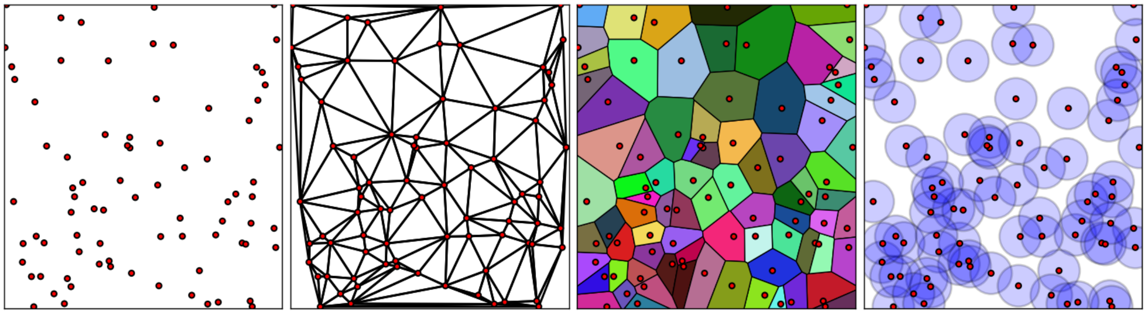

Figure 3: Estimation techniques of the density field. Original dataset (first). Delaunay tessellation (second). Voronoi tessellation (third). Spherical kernel volumes (fourth).

coordinates of the particles as they evolve, generating non-desirable discontinuities in the hydrodynamical equations.

A Voronoi tessellation is defined as a set of adjacent polyhedra outlined by the bisector planes of neighbour points of the dataset (see Fig. 3). This definition makes unique the tessellation associated to a dataset and does not generate discontinuities in the estimations. For these reasons, the Voronoi tessellation is preferable for field estimation in the context of hydrodynamics, as established by Heß & Springel (2010).

**Equations of Motion**

Starting from the discretized Lagrangian [16] and applying Euler-Lagrange variational equations, we obtain:

$$\begin{aligned} m_i \frac{d\boldsymbol{v}_i}{dt} &= -\sum_j m_j \frac{\partial u_j}{\partial \boldsymbol{r}_i} \\ &= -\sum_j m_j \frac{P}{\rho_j^2} \frac{\partial \rho_j}{\partial V_j} \frac{\partial V_j}{\partial \boldsymbol{r}_i} \end{aligned} \tag{23}$$

where has been used the equation of state of an inviscid gas and the variation of the density has been relied on the variation of the volume of the Voronoi polyhedron $V_j$ associated to the $j$th particle. The first derivative term has to be computed through some estimation of the density field, the simplest one and usually adopted is

$$\rho_i = \frac{m_i}{V_i} \tag{24}$$

The evaluation of the second derivative term can be reached by means of a geometric analysis (Serrano & Español, 2001), yielding:

$$\frac{\partial V_j}{\partial \boldsymbol{r}_i} = -A_{ij} \left( \frac{\boldsymbol{c}_{ij}}{R_{ij}} + \frac{\boldsymbol{e}_{ij}}{2} \right) \quad \text{for} \quad i \neq j$$

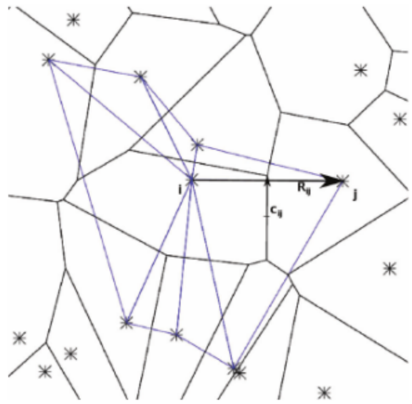


Figure 4: It is sketched how to evaluate the dependence of the volume of a Voronoi cell on the coordinates of neighbour particles (asterisks). Vectors $\boldsymbol{c}_{ij}$ and $\boldsymbol{e}_{ij}$ needed to calculate the derivative are also sketched. Taken from Heß & Springel (2010).

$$\frac{\partial V_j}{\partial \boldsymbol{r}_i} \;=\; -\sum_{k\neq j} \frac{\partial V_k}{\boldsymbol{r}_i} \quad \text{for} \quad i = j \tag{25}$$

where $\boldsymbol{e}_{ij} = (\boldsymbol{r}_j - \boldsymbol{r}_i)/R_{ij}$ is a unitary vector pointing from the $i$th particle to the $j$th neighbour, $A_{ij}$ is the area of the Voronoi face between the cells $i$ and $j$, and $\boldsymbol{c}_{ij}$ is defined as sketched in Fig. 4. The expression when $i = j$ is obtained by invoking volume conservation.

Finally, the equation of motion for an inviscid gas is given by

$$m_i \frac{d\boldsymbol{v}_i}{dt} = -\sum_{i\neq j}^{N} A_{ij} \left[ (P_i + P_j)\frac{\boldsymbol{e}_{ij}}{2} + (P_j - P_i)\frac{\boldsymbol{c}_{ij}}{R_{ij}} \right] \tag{26}$$

where the right hand term has been explicitly symmetrized. It is noteworthy that the summation only runs over neighbour cells as the area of the face $A_{ij}$ vanishes for non-abutted cells. Unlike kernel interpolants, where the number of contributing terms of the summation depends on the user-defined smoothing length of the kernel, Voronoi tessellations restricts naturally this number, depending only on the number of faces of the Voronoi cell.

Although the Voronoi tessellation estimator improves greatly the efficiency of `SPH`, it is still required to use a viscous term in order to account for shock dynamics. As the expression [19] for `SPH` involves the kernel interpolant, it is necessary to introduce a new form of the viscous term that can work with `VPH`. Here we adopt the parametrization of Heß & Springel (2010), yielding:

$$m_i \frac{d\boldsymbol{v}_i}{dt}\bigg|_{\text{visc}} = -\sum_{j=1}^{N} A_{ij}\rho_{ij}^2 \Pi_{ij} \frac{\boldsymbol{e}_{ij}}{2} \tag{27}$$

$\rho_{ij}$ is the arithmetic mean of the densities of the $i$th and the $j$th particles and the viscous tensor is given by:

$$\Pi_{ij} = \begin{cases} \left[-\alpha c_{ij} w_{ij} + \beta w_{ij}^2\right] / \rho_{ij} & \text{if} \boldsymbol{v}_{ij} \cdot \boldsymbol{r}_{ij} < 0 \\ 0 & \text{otherwise} \end{cases} \tag{28}$$

where $w_{ij}$ is the projected pairwise velocity defined as

$$w_{ij} = \frac{\boldsymbol{v}_{ij} \cdot \boldsymbol{r}_{ij}}{|\boldsymbol{r}_{ij}|}$$

Note that this definition of the viscous tensor is exactly equal to the adopted for SPH, but changing $\mu_{ij}$ for $w_{ij}$ as the parameter $\mu_{ij}$ depends on the smoothing length of the kernel. The parameters $\alpha$ and $\beta$ are chosen like SPH, i.e. $\alpha \sim 0.5 - 1.0$ and $\beta = 2\alpha$.

Finally, for the self-gravity term, note that Eqs. [21] and [22] do not involve the kernel at all, and the summation runs all over the sampling particles. This implies that this term remains equal for VPH, and the same gravity solver techniques previously discussed for SPH are equally applicable here.

# 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 Previous Experience

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 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.

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

- 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.

| **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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