# Modeling Expansion of Particle Clouds

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## 1 Introduction

Given initial positions and velocities of particles in a cloud, we derive a similarity solution for the expansion of the particle in a vacuum. The conservation laws admit an inertial solution where $u \sim r$ at a fixed time. In this case the similarity solution is $u = u_s \xi$, where the similarity variable is $\xi = r / r_s = r / u_s t$, and $u_s$ denotes the expansion velocity of the cloud boundary. This can be used to predict the inertial expansion of the particle cloud. The analytic solution can be used to compute the L2 norm of numerical simulations of such cloud expansions.

## 2 Similarity Solution

We consider the dispersion of a spherical cloud of particles in a vacuum, where $\nabla p = 0$. Under such circumstances the momentum equation acquires the form:

$$\partial_t u_r + u_r \cdot \partial_r u_r = 0 \tag{1}$$

This equation admits an inertial solution (Stanyukovich, 1960)[1], (Kuhl & Seizew, 1981)[2]:

$$r / t \tag{2}$$

that satisfies the PDE Eq. (1), that is: $-\frac{r}{t^2} + \frac{r}{t}\frac{1}{t} = 0$. Next, we assume that the boundary of the particle cloud expands at a constant radial velocity: $u_s$. In this case, cloud radius and time are linked by the relation:

$$r_s = u_s \cdot t_s \tag{3}$$

[1] K. P. Stanyukovich, *Unsteady Motion of Continuous Media*, Pergamon Press, London, 1960, 749 pp. (*vid. esp.* § 63. Expansion of Gaseous Sphere in a Vacuum, pp. 498-501 & Eq. 63:13).

[2] A. L. Kuhl and M. R. Seizew TNT explosions in a hard vacuum, *Gasdynamics of Detonations and Explosions, Progress in Astronautics and Aeronautics* **75** (ed. R. Bowen, N. Manson, A. Oppenheim, & R. Soloukhin), AIAA, 1981, pp. 227-241.

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This allows us to construct a similarity variable:

$$\xi \equiv r / r_s \tag{4}$$

and a similarity solution:

$$\boxed{U \equiv u / u_s = f(\xi) = \xi} \tag{5}$$

that is consistent with the inertial solution Eq. (2). The solution is depicted in Fig. 1. One can see that the velocity profile within the spherical cloud of particles varies linearly with radius, and equals $u_s$ on the boundary.

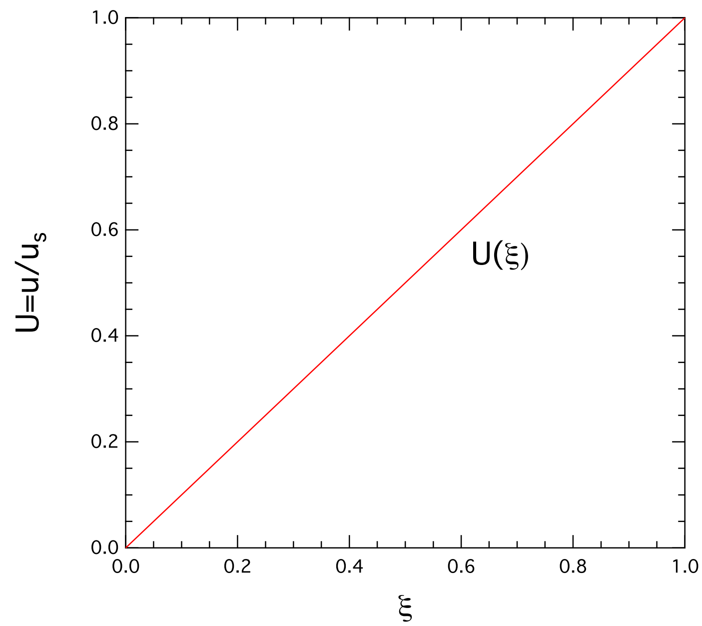


Figure 1. Similarity solution for inertial flow.

## 3 Particle Cloud

We consider a 3-D Cartesian grid lattice: $R_{ijk} = \{x_i, y_j, z_k\}$ with a uniform mesh spacing: $\Delta x_i = \Delta y_j = \Delta z_k = 1$. We assume the cloud is composed of spherical particles of diameter $d_0 = 1$, initially located on the grid lattice points:

$$P_{ijk} = \{x_i, y_j, z_k\} \tag{6}$$

Note that initially the particles are touching each other. From this lattice one can construct a sphere (S) or spherical shell (SS) of particles by enforcing the following conditions:

* *Sphere:* $1 \le r_i / d_0 \le 100$ (100 radial particles in sphere) (S)
* *Spherical Shell:* $95 \le r_i / d_0 \le 100$ (5 radial particles in shell) (SS)

In other words, we accept the particles that satisfy (S) or (SS) and reject particles that violate (S) or (SS). We call this the initial particle cloud: $P_{ijk}^0$ with particles at $\{ijk\}$ locations that satisfy (S) or (SS). Assume that the velocity of the particles satisfy the similarity solution of Eq. (5). Then their velocities are:

$$\mathbf{U}_{ijk}^0 = (r_{ijk} / r_s^0)\,\hat{\mathbf{i}}_{ijk} \quad \text{where} \quad r_{ijk} = \sqrt{x_i^2 + y_j^2 + z_k^2} \;\; \& \;\; \hat{\mathbf{i}}_{ijk} = \mathbf{r}_{ijk} / |\mathbf{r}_{ijk}| \tag{7}$$

How the particles have acquired this velocity field comes from other physics modeling that is beyond the scope of this manuscript.

At some later time: $t_s^n$, the cloud will have expanded to radius: $r_s^n = u_s t_s^n$. At this time the particles will be located at:

$$\mathbf{r}_{ijk}^n(t^n) = \xi_{ijk}\, r_s^n\, \hat{\mathbf{i}}_{ijk} = \xi_{ijk}\, u_s\, t_s^n\, \hat{\mathbf{i}}_{ijk} \tag{8}$$

with velocities:

$$\mathbf{U}_{ijk}^n(t^n) = (r_{ijk}^n / r_s^n)\,\hat{\mathbf{i}}_{ijk} = \xi_{ijk}\hat{\mathbf{i}}_{ijk} \tag{9}$$

Thereby satisfying the similarity solution $U(\xi) = \xi$ of Eq. (3). Note that particle positions dilate linearly with time.

## 4 Kinetic Energy

Using the similarity solution, the kinetic energy of the particle system may be calculated:

$$\begin{aligned} KE &= \int_0^{r_s} 0.5\,\rho u^2\, 4\pi r^2 dr = 2\pi\rho_0 u_s^2 r_s^3 \int_0^1 U^2 \xi^2\, d\xi \\ &= 2\pi\rho_0 r_s^3 u_s^2 \int_0^1 \xi^4\, d\xi = \left(\frac{4\pi}{3} r_s^3 \rho_0\right)\frac{3}{10} u_s^2 \end{aligned} \tag{10}$$

$$\boxed{KE = 0.3\, M_0 u_s^2} \tag{11}$$

## 5 Discrete Lagrangian Particle (DLP) Model

The similarity solution for the particle cloud, Eq. (8)-(9), models the particle expansion in a vacuum. If the particle cloud expansion occurs in an atmosphere, then the particles are subject to both drag and gravity along with heating from convective heat transfer and combustion with air. The particle system then obeys the conservation laws for Discrete Lagrangian Particles (DLP):

| | | | |
|---|---|---|---|
| *Position:* | $\dot{\mathbf{x}}_p(t) = \mathbf{v}_p(t)$ | for all particles $p$ | (12) |
| *Momentum:* | $m_p(t)\dot{\mathbf{v}}_p(t) = \mathbf{D}_P(\mathbf{x}_p) + m_p(t)\mathbf{g}$ | for all particles $p$ | (13) |
| *Energy:* | $m_p(t)\dot{e}_p(t) = Q_P(\mathbf{x}_P)$ where $e_i = c_s T_i$ | for all particles $p$ | (14) |
| *Mass:* | $\dot{m}_p(t) = -\dot{s}_p(\mathbf{x}_p(t))$ | for all particles $p$ | (15) |

*Drag:* $$\mathbf{D}_p(\mathbf{x}_p) = \frac{1}{4} 0.5\rho[\mathbf{u}(\mathbf{x}_p) - \mathbf{v}_p(\mathbf{x}_p)]\left|\mathbf{u}(\mathbf{x}_p) - \mathbf{v}_p(\mathbf{x}_p)\right|\pi d_p^2 C_D \tag{16}$$

*Drag Coefficient:* $$C_D \equiv \frac{Force}{0.5\rho u^2 A} = 0.48 + 28\, Re^{-0.85} \tag{17}$$

*Heat Transfer*: $$Q_p(\mathbf{x}_p) = \pi d_p \mu C_d Pr^{-1}(T - T_p(\mathbf{x}_p))\, Nu \tag{18}$$

*Nusselt Coefficient:* $$Nu = 2 + 0.6\, Pr^{1/3}\sqrt{Re} \tag{19}$$

*Burning Rate* (empirical): $$\dot{s}_p = c\, d_p^2 \tag{20}$$

## 6 Solution for a Quiescent Atmosphere

Assume a quiescent atmosphere where $\rho_a = 1.2\, mg/cc, u_a = 0, T_a = 300K$ with $\mathbf{g} = 0$. Then the momentum equation for a particle takes the form:

$$\begin{aligned} m_p \dot{\mathbf{v}}_p &= -0.5\rho_a \mathbf{v}_p^2 A C_D \\ \frac{4}{3}\pi r_p^3 \rho_p \dot{\mathbf{v}}_p &= -0.5\rho_a \mathbf{v}_p^2 \pi r_p^2 C_d \\ \dot{\mathbf{v}}_p &= -\frac{\rho_a}{\rho_p}\frac{3C_D}{8r_p}\mathbf{v}_p^2 \end{aligned} \tag{21}$$

that is $$\dot{\mathbf{v}}_p = -K\,\mathbf{v}_p^2 \quad \text{where} \quad K = constant = \frac{\rho_a}{\rho_p}\frac{3C_D}{4d_p} \tag{22}$$

This is an ordinary differential equation that specifies the temporal evolution of the particle velocity subject to drag. The solution of (52.) is

*Drag Solution:* $$\mathbf{v}_p(t) = \frac{-K\,\mathrm{v}_p^0\,\hat{\mathbf{i}}_p}{(t_0 - t)\mathrm{v}_p^0 + 1} \tag{23}$$ [3]

Next consider the expansion of the particle cloud in a vacuum with gravity **g**. The momentum equation takes the form

$$m_p(t)\dot{\mathbf{v}}_p(t) = m_p(t)\mathbf{g} \tag{24}$$

*Gravity Solution:* $$\mathbf{v}_p(t) = \mathbf{v}_p^0 + \hat{\mathbf{i}}_p \cdot \mathbf{g}\, t \tag{25}$$

*Complete Solution:* $$\boxed{\mathbf{v}_p(t) = \frac{-K\,\mathrm{v}_p^0\,\hat{\mathbf{i}}_p}{1 - (t - t_0)\mathrm{v}_p^0} + \hat{\mathbf{i}}_p \cdot \mathbf{g}\, t} \tag{26}$$

[3] The ODE y' = y $^2$ has the solution: $y(x) = y_0 / [(x-x_0)\, y_0+1]$; see *Ordinary Differential Equations*, Wikipedia.org

## 7 Integration Scheme

The DLP model equations are integrated with a 2nd order Runge-Kutta (RK2) method:

*Position:* $$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + [\mathbf{v}_p]^{n+1/2} \Delta t^n \tag{27}$$

*Velocity:* $$\mathbf{v}_p^{n+1} = \mathbf{v}_p^n + [\mathbf{D}_p / m_p + \mathbf{g}]^{n+1/2} \Delta t^n \tag{28}$$

*Energy:* $$e_p^{n+1} = e_p^n + [Q_P / m_p]^{n+1/2} \Delta t^n \tag{29}$$

*Mass:* $$m_p^{n+1} = m_p^n - [\dot{s}_p]^{n+1/2} \Delta t^n \tag{30}$$

Assume initial conditions at $r_0, t_0$:

$$\mathbf{x}_p(t_0) = \xi_p u_s t_0 \hat{\mathbf{i}}_p \tag{31}$$

$$\mathbf{v}_p(t_0) = \xi_p u_s \hat{\mathbf{i}}_p \tag{32}$$

then the numerical solution is given by integrating eqs. (6.1)-(6.3), assuming no particle burning. The accuracy of the integration scheme may be checked by computing the *L2 Norms* of the solution:

$$\left|\mathbf{e}_x(t^n)\right| = \sqrt{\sum_p \left|\mathbf{x}_p^n - \mathbf{x}_p(t^n)\right|^2} \tag{33}$$

$$\left|\mathbf{e}_v(t^n)\right| = \sqrt{\sum_p \left|\mathbf{v}_p^n - \mathbf{v}_p(t^n)\right|^2} \tag{34}$$

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## References

1. K. P. Stanyukovich, *Unsteady Motion of Continuous Media*, Pergamon Press, London, 1960, 749 pp. (*vid. esp.* § 63. Expansion of Gaseous Sphere in a Vacuum, pp. 498-501 & Eq. 63:13).

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3. *Ordinary Differential Equations*, Wikipedia.org:
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