



# On the Self-Similar approach to solve differential equations

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As one of Lie's group transformations, the self-similar approach offers a powerful tool for solving partial differential equations. Space-time dependent equations are transformed through appropriate transformations into ordinary equations that depend only on a single variable. Consequently, initial condition solvers can be applied to generate numerical solutions for various differential equations, especially those involving moving boundaries, where the boundary equation is often unknown in most real-world problems. In this presentation, we focus on two specific physical problems: expansion and nonlinear structures. Additionally, we will highlight the limitations of the self-similar approach.





## Introduction

## 2 Part I: Expansion

- Modeling
- Differential Equations
- Self-similar approach
- Limitations



- Hillocks Formation
- Experiment vs simulation
- References







https://www.youtube.com/watch?v=OtXOd67TSP0



https://www.youtube.com/watch?v=YpKUhSk2Ff0





#### occurs when a gas encounters open boundaries.



Caused by

- Thermal pressure at the source: rising plume.
- Can be in vacuum or other medium.

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Self-similar approach





#### It is common to different environments as in :

• Nature: pollution, ionosphere penetrated by a comet, ...



https://theplanets.org/hale-bopp-comet-facts/ https://arcnl.nl/news/pulsed-laser-deposition-for-materials-and-surface-science https://www.adaptiiv.com/product/external-beam-radiation-therapy/



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**Expansion Study** 

• Laboratory: pulsed laser deposition, ......



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 Medicine as source of accelerated particles to diagnostic (imaging) or curing (radio-therapy).



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Let us consider the simple case,







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and make the following assumption:

- one dimensional expansion along x-axis
- the number of particles is conserved
- only one species in the gas of mass m and density n



When the expanding front moves, the number of particles remains the dn same, i.e. = 0

However, the density changes with time t and space coordinate x therefore,

and  

$$dn = \frac{\partial n(x,t)}{\partial x} dx + \frac{\partial n(x,t)}{\partial t} dt$$

$$\frac{dn}{dt} = \frac{\partial n(x,t)}{\partial x} \frac{dx}{dt} + \frac{\partial n(x,t)}{\partial t} = 0$$
By setting  

$$v(x,t) = \frac{dx}{dt}, \quad \text{fluid velocity}$$

an

The velocity is different from the velocity of a moving particle with coordinates x because in the case of a fluid, the variable x represents a point within the fluid volume. We cannot track the motion of individual particles that are indiscernible.

The first conservative fluid (gas or liquid) equation corresponds to

$$\frac{\partial n(x,t)}{\partial t} + \frac{\partial n(x,t)v(x,t)}{\partial x} = 0 \qquad (1)$$





Eq.(1) has two unknowns (n(x, t), v(x, t)), additional equation is needed which is obtained by using Newton law

$$\frac{d(m.v)}{dt} = F; \qquad F \text{ is the force exerted on the fluid element}$$

m represents the mass of the fluid element within a fixed volume V:  $\textit{m} = \rho.\textit{V}$ 

If the fluid is incompressible then  $m = \rho V = Constant$ .

$$\frac{d(m.v)}{dt} = \rho V \frac{dv}{dt} = -\frac{dP}{dx};$$

P(x, t) is the thermal pressure exerted on the volume V. But  $\rho = Mn(x, t)$ , M is the molecular mass of the species. The second equation is

$$Mn(x,t)\left[\frac{\partial v(x,t)}{\partial t} + v(x,t).\frac{\partial v(x,t)}{\partial xt}\right] + \frac{\partial p}{\partial x} = 0$$
(2)

Here again, we encounter a new unknown, P(x). We require another equation.

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The set of fluid equations (1-2) can be solved if we add a third equation obtained from physical considerations. For an ideal gas

$$P = nT$$
,  $T$  being the temperature (3)

For an isothermal process T = Constant. Our set of partial differential equations is,

**Closing Equation** 

$$\frac{\partial n(x,t)}{\partial t} + \frac{\partial n(x,t)v(x,t)}{\partial x} = 0 \qquad (1)$$

$$Mn(x,t) \left[ \frac{\partial v(x,t)}{\partial t} + v(x,t) \cdot \frac{\partial v(x,t)}{\partial x} \right] + T \frac{\partial n(x,t)}{\partial x} = 0 \qquad (2)$$

With initial conditions at  $t = t_o$ ,  $n(x, t) = n_o$ ,  $v(x, t) = v_o = 0$ 





There are two types of differential equations:

• Ordinary differential equations (first order with initial condition)

$$\frac{dy(x)}{dx} = f(y(x), x, t), \qquad y(x = x_o) = y_o$$

Partial differential equations (of boundary conditions): contain an unknown function of two or more variables and its partial derivatives with respect to these variables.

## Example

First order equation

$$\frac{\partial U(x,y)}{dx} + \frac{\partial U(x,y)}{dy} = f(u(x,y),x,y)$$

Three Classes of Boundary conditions

- Dirichlet: U(x, y) is know at the boundaries a and b
- 2 Neumann : U'(x, y) is know at the boundaries a and b
- Cauchy: U(x, y) and U'(x, y) are known at the boundaries.





## Frontier equation

When the fluid (gas) expands, the front (frontier) moves. We need the equation  $x_F = f(t)$ . This equation is unknown in most cases.

Any of the boundary conditions doesn't apply in this case. We have to transform the PDE to ODE. For that, the first step is to normalize the governing equations.

Normalization provides

- Dimensionless equations subject to all mathematical operations.
- Rescale the real situation and allow numerical computations.



All physical parameters have to be transformed to dimensionless ones

• Density is normalized to  $n_o$ 

$$N(x,t)=\frac{n}{n_o}$$

velocity is normalized to the acoustic speed

$$C_{s} = \sqrt{\frac{T}{M}}; \qquad V(c,t) = \frac{v}{C_{s}}$$
$$\frac{\partial N(x,t)}{\partial t} + C_{s} \frac{\partial N(x,t)V(x,t)}{\partial x} = 0 \qquad (1)$$
$$MN(x,t) \left[ \frac{\partial v(x,t)}{\partial t} + C_{s}^{2}V(x,t) \cdot \frac{\partial V(x,t)}{\partial x} \right] + T \frac{\partial N(x,t)}{\partial x} = 0 \qquad (2)$$

time t and space coordinate x are not normalized yet!





#### PDE are reduced to ordinary ones using the self-similar approach, when:





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- There is no scaling parameter (time or distance).
- The shape is preserved during expansion.



## Self-similar transformation



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## General properties



Let G a group (set of elements with a binary operation that satisfies four axioms: closure, associativity, identity, and inverse)

G is a part of Lie groups if it has a differentiable manifold (different types).

#### Self-similar transformation

is a part of Lie's groups when it has a function F(y) constant con-formally invariant, i.e:

$$F(y) = f(a)F(\widetilde{y})$$

f(a) is any function of the parameter a. When f(a) = 1 the F(y) is absolute constant con-formally invariant.  $\tilde{y}$  being the transformed variable.

### Example

$$G:\begin{cases} x = \tilde{x}/C_{s}t \\ n = n_{o}N, v = C_{s}v \end{cases}; \qquad F: \frac{\partial n(x,t)}{\partial t} + v(x,t).\frac{\partial n(x,t)}{\partial x} = 0 \end{cases}$$



## Initial value problem

Using

$$\frac{\partial}{\partial t} = -\frac{x}{C_s t^2} \frac{\partial}{\partial \widetilde{x}} = -\frac{\widetilde{x}}{t} \frac{\partial}{\partial \widetilde{x}}; \quad \frac{\partial}{\partial x} = \frac{1}{C_s t} \frac{\partial}{\partial \widetilde{x}}$$

The continuity equation can be read as,

$$-\widetilde{x}\frac{\partial N(x,t)}{\partial \widetilde{x}} + \frac{\partial N(x,t)V(x,t)}{\partial \widetilde{x}} = 0 \qquad (1)$$

For the momentum equation one obtains,

$$N(x,t)(V-\widetilde{x})rac{\partial V(x,t)}{\partial \widetilde{x}} - rac{\partial N(x,t)}{\partial \widetilde{x}} = 0$$
 (2)

These equation depends on one variable:  $\stackrel{\sim}{x} = \xi$ . The set od ODE is,

$$(V - \xi)\frac{dN(x, t)}{d\xi} + N(x, t)\frac{dV(x, t)}{d\xi} = 0$$
(1)  
$$N(x, t)(V - \xi)\frac{dV(x, t)}{d\xi} + \frac{dN(x, t)}{d\xi} = 0$$
(2)



From continuity equation we have

$$(V-\xi)^2 \frac{dN(x,t)}{d\xi} = -N(x,t)(V-\xi)\frac{dV(x,t)}{d\xi}$$
 (1)

In equation(2) leads to

$$-(V-\xi)^2 \frac{dN(x,t)}{d\xi} + \frac{dN(x,t)}{d\xi} = 0$$
 (2)

The solution is

$$V = \xi + 1$$
 ( $V_o = 0$ )  
 $N = e^{-\xi}$ 

When  $\xi \to \infty$  the density corresponds to  $N \to 0$  which is an expected results because we have a finite volume

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- The self-similar approach provides an asymptotic solution because it applies when  $t \gg \tau_c$  (a characteristic time).
- As  $V = \xi + 1$  when  $\xi \to \infty$  then  $V \to \infty$ , nonphysical result. When  $N \to 0$ , it doesn't make sens to consider the velocity of a fluid (gas).
- There are myriads of self-similar transformation, to make any conclusion about the appropriate asymptotic solution, one has to compare the given solution with the exact one. Otherwise, physical consideration has to be the only possible criterion for any statement.





We are interested on modeling the formation of nano-structures: Hillocks, rise on some materials (insulators,....).



Figure: Experimental observation of hillocks.

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Figure: Experimental observation of hillocks.

produced by the interaction between highly charged ions (HCI) with surface material.

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## Slow highly charged ions



Highly charged ions are produced in a facility located at *Helmholtz-Zentrum Dresden-Rossendorf (Germany)*, to monitor single highly charged ions interaction with surface materials.



## (See Ayman El-Said works)

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• Slow highly charged ions (HCIs) showed its high effectiveness as promising nanotechnological gentle tool for nano-structures creation in various surfaces.



## Nanotechnology

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- The created nano-features could be controlled by varying ion parameters (mainly charge state) limiting the tailoring to the very top surface layers without modifying the deeper layers, which is unavoidable in case of swift heavy ions.



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Figure: HCI effect on crystals.





- Optoelectronics: such as in ion-beam lithography (IBL) technique, in order to reduces the etching time and enhances the etching depth .
- Semiconductors
- Medical Applications: pinning of bio-molecules to nanostructures for using in drug delivery.



## Experiment vs simulation







## Experiment vs simulation









Figure: The hillocks profile given by the simulation showing changes in the height which depends on the plasma parameters:

 $T_+/T_e = 0.1, n_{-o}/n_o = 0.5$  (solid line),  $T_+/T_e = 0.3, n_{-o}/n_o = 0.5$  (dashed line),  $T_+/T_e = 0.1, n_{-o}/n_o = 0.2$  (dotted) and  $T_+/T_e = 0.3, n_{-o}/n_o = 0.2$  (dashed-dotted). The negative ion to electron temperature ratio is 0.2.





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