Introduction to Finite Volume Method, Illustris &-TNG Project, & Shock Tube Problem

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Finite Volume Method

Mathematical Basis

Recall the governing equations for fluid mechanics (idea) in 1D situation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0 \rightarrow \text{Continuity}$$
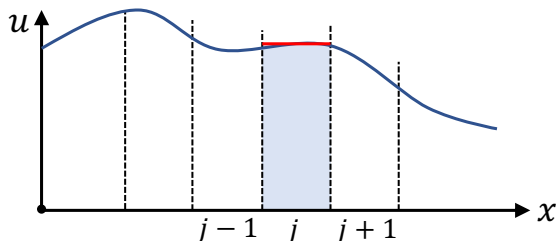
$$\frac{\partial (\rho u)}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0 \rightarrow \text{Momentum}$$

$$\frac{\partial (\rho e_{\text{total}})}{\partial t} + \frac{\partial \left[(\rho e_{\text{total}} + p) u \right]}{\partial x} = 0 \rightarrow \text{Energy}$$

The given equations can be written in the form:

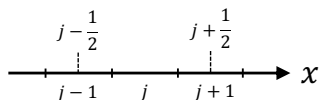$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

where $U = [\rho, \rho u, \rho e_{\text{total}}]^{\text{T}}$, and $F = [\rho u, \rho u^2 + p, (\rho e_{\text{total}} + p) u]^{\text{T}}$.

Consider a distribution function $u(x, t)$, for discretization we apply a grid discretize the axis with N points: $\Delta x = (x_{\max} - x_{\min})/N$. Hence, at time step n, the value at gridpoint j is calculated as the average:

$$u_j^n = u(x_j, t^n) \approx \frac{1}{\Delta t} \int_{(j-\frac{1}{2})\Delta x}^{(j+\frac{1}{2})\Delta x} u(x, n\Delta t) dx$$

This is the application of finite volume method (FVM) for 1D problem.

FVM - *Math. Bas.*

Recall the Euler equation (ideal fluid), we first do the integration.

$$\int \left(\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} \right) dx = 0$$

To obtain the value at gridpoint j, the flux term can be fully discretized.

$$\frac{dU}{dt} \Delta x_j + F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}} = 0$$

Applying a finite difference discretization on the time step n, the Euler equation can be fully discretized as:

$$\frac{U_j^{n+1} - U_j^n}{dt} \Delta x_j + F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}} = 0$$

Finite Volume Method

Applications

I. Geophysics

- Ocean Modelling for Resource Characterization [1]
- Sea Earthquake and Earthquake Tsunami [2]
- Hydrodynamic and ecosystem coupled model and its application to the eutrophication problem [3]

II. Thermodynamics

- Core thermal hydraulics for Industrial Engineering [4]

III. Mantle Dynamics
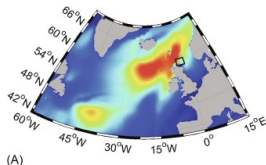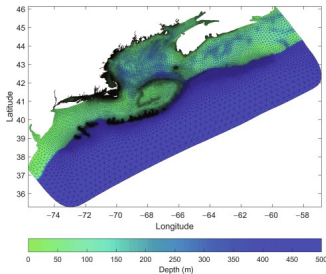
- Numerical Methods for Mantle Convection [5]

[1] https://doi.org/10.1016/B978-0-12-810448-4.00008-2
[2] https://doi.org/10.1016/B978-0-12-812726-1.00005-X
[3] https://doi.org/10.1016/B978-0-444-63536-5.00014-4
[4] https://doi.org/10.1016/B978-0-08-101980-1.00020-X
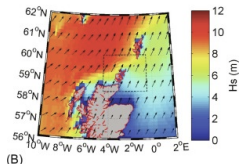[5] https://doi.org/10.1016/B978-044452748-6.00118-8

FVM - *App.*

Ocean Modelling for Resource Characterization

Finite volume method (FVM), like FEM, is based on an unstructured (e.g. triangular) mesh. Therefore, it is suitable for irregular and complex geometries. FVM has another advantage over FEM for fluid mechanic problems. [1]
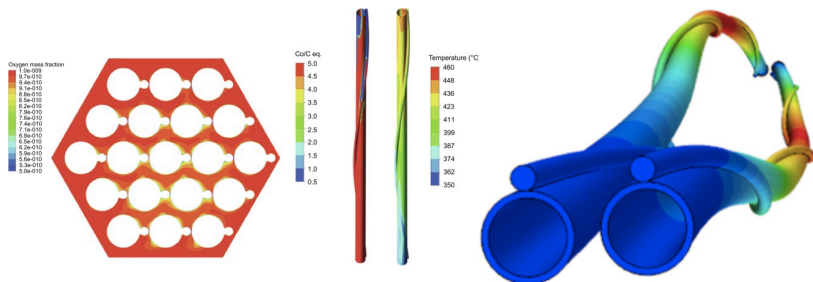
[1] https://doi.org/10.1016/B978-0-12-810448-4.00008-2

[2] https://www.sciencedirect.com/topics/earth-and-planetary-sciences/finite-volume-method

FVM - *App.*

Core thermal hydraulics for Industrial Engineering

CFD is also used to evaluate possible local effects that cannot be derived from one-dimensional system thermal-hydraulic code simulations. [1]

[1] https://doi.org/10.1016/B978-0-08-101980-1.00020-X
[2] https://www.sciencedirect.com/topics/earth-and-planetary-sciences/finite-volume-method

Finite Volume Method

Pros & Cons

Pros

i. Straightforward to implement on non uniform/unstructured grid.

ii. Enforces the right mechanisms for wave propagation.

iii. FVM preserves the overall conservation across the entire domain by maintaining the conservation of mass and momentum on each control volume cell.

Cons

i. Getting high order schemes is a pain, it is extremly cumbersome.

ii. the FVM discretizes the integral form of the equations. It can be shown that is equivalent to use a weak formulation, the only one that can adopted for non regular solutions.

# Illustris Project

Introduction of Illustris Prj.

The Illustris project is an ongoing series of astrophysical simulations originally carried out bt M. Vogelsberger run by an international collaboration of scientists aiming to study the processes of galaxy formation and evolution in the universe with a comprehensive physical model. A followup to the project, **IllustrisTNG**, was presented in 2017.

Introduction of the TNG Prj.

The IllustrisTNG project is an ongoing series of large, cosmological magnetohydrodynamical simulations of galaxy formation. TNG aims to illuminate the physical processes that drive galaxy formation: to understand when and how galaxies evolve into the structures that are observed in the night sky, and to make predictions for current and future observational programs.
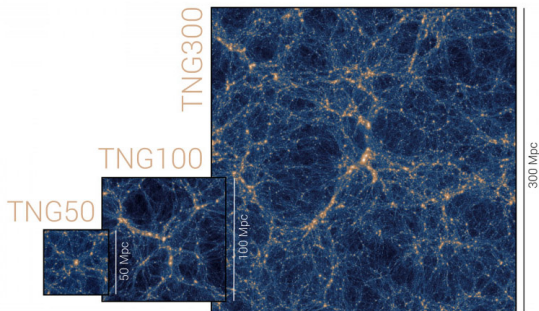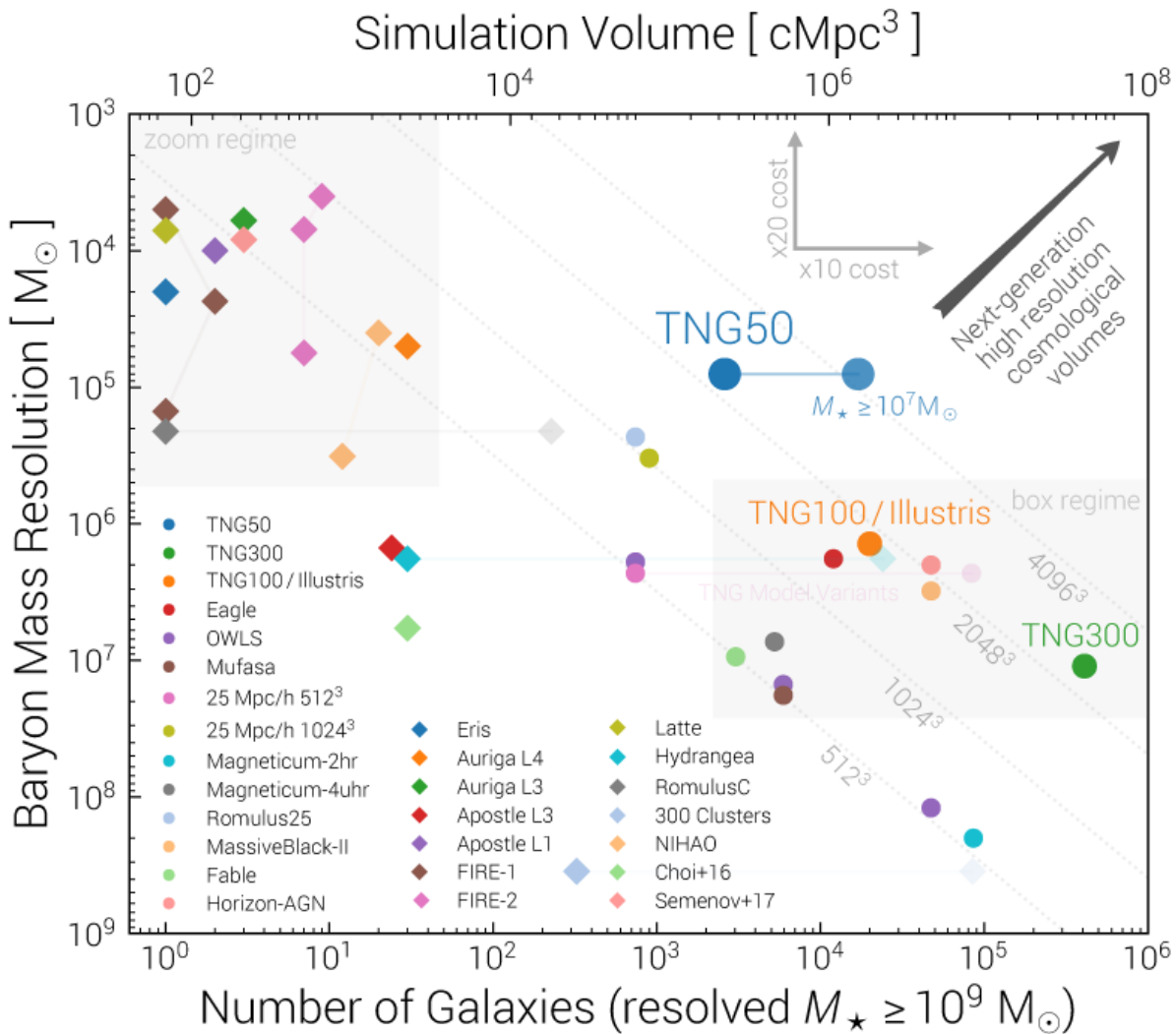
		TNG50	TNG100	TNG300
Volume	$[\mathrm{Mpc}^3]$	51.7^3	110.7^3	302.6^3
L_{box}	$[\mathrm{Mpc}/h]$	35	75	205
N_{GAS}	–	2160^3	1820^3	2500^3
N_{DM}	–	2160^3	1820^3	2500^3
N_{TR}	–	2160^3	2×1820^3	2500^3
m_{baryon}	$[\mathrm{M}_\odot]$	8.5×10^4	1.4×10^6	1.1×10^7
m_{DM}	$[\mathrm{M}_\odot]$	4.5×10^5	7.5×10^6	5.9×10^7
$\epsilon_{\mathrm{gas,min}}$	$[\mathrm{pc}]$	74	185	370
$\epsilon_{\mathrm{DM},\star}$	$[\mathrm{pc}]$	288	740	1480

Illustris Project

Hydro Methods Applications

As in Illustris, we follow the coupled dynamics of DM and gas with the robust, accurate, and efficient quasi-Lagrangian code AREPO. In this approach, an unstructured Voronoi tessellation of the simulation volume allows for dynamic and adaptive spatial discretization, where a set of mesh generating points are moved along with the gas flow. "

Illustris Prj. - *Hydro. App.*
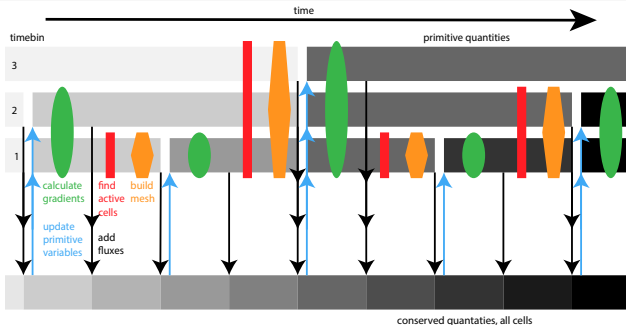
To solve the equations of (magneto)hydrodynamics, Arepo uses a second-order accurate finite-volume discretization. To this end, volume-averaged primitive variables ρ, u and B are stored as properties of the cell at its center. "
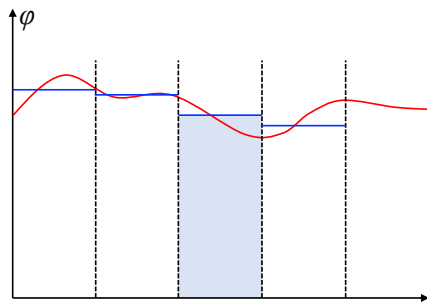
The discretization step for second order scheme can be written as :

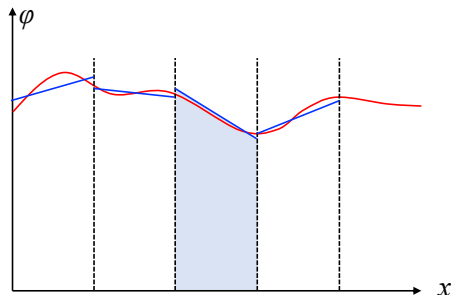$$\rho^{n+1} = \rho^n - \frac{1}{2}\Delta t(\rho^n\nabla \cdot u + u \cdot \nabla\rho^n)$$

$$u^{n+1} = u^n - \frac{1}{2}\Delta t\left(u^n\nabla \cdot u^n + \frac{1}{\rho}\nabla p\right)$$

$$p^{n+1} = p^n - \frac{1}{2}\Delta t(\gamma p\nabla \cdot u + u \cdot \nabla p)$$

Schematic for the first and second order time step discretization on finite volume method to a given function $\phi(x)$, where ϕ could be u, p, ρ, etc.

1st Order FVM

2nd Order FVM

Problem Formulation

Recall the Euler equation in the explicit conservation form:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

where $U = [\rho, \rho u, \rho e_{\text{total}}]^{\text{T}}$, and $F = [\rho u, \rho u^2 + p, (\rho e_{\text{total}} + p)u]^{\text{T}}$. The equation can be written as:

$$\frac{\partial U}{\partial t} + J\frac{\partial U}{\partial x} = 0$$

where J is the Jacobian matrix, which can be diagonized as:
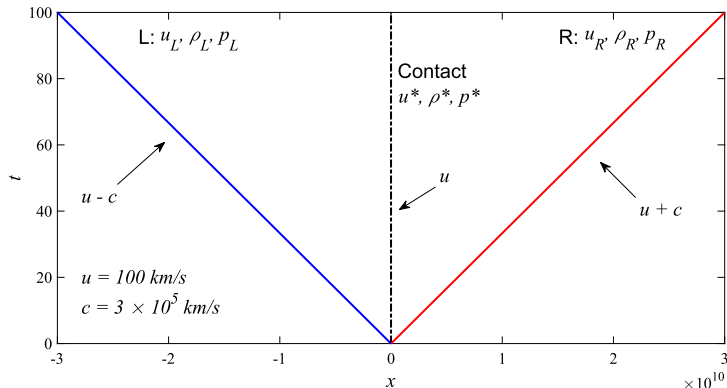
$$J = S^{-1}\Lambda S$$

The eigenvalue matrix takes the form $\rightarrow \Lambda = \begin{pmatrix} u - c & 0 & 0 \\ 0 & u & 0 \\ 0 & 0 & u + c \end{pmatrix}$

Shock Tube Prob. - *Prob. Form.*

	$t = 0$	
ρ_L, u_L, p_L		ρ_R, u_R, p_R
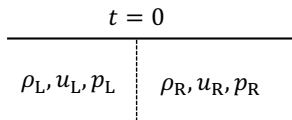
The Riemann solver can be applied on the initial conditions:

$$(u^*, \rho^*, p^*) = \mathrm{Riemann}(u_L, \rho_L, p_L, u_R, \rho_R, p_R)$$

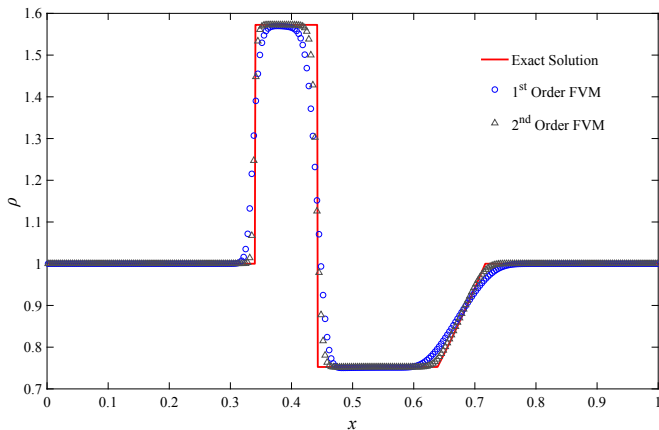# Shock Tube Problem

Parameters & Initial Conditions

Problem I

- Cell Numbers = 300
- Step Numbers = 200
- Time Steps = 0.001
- $\rho_L = 1.0, \rho_R = 1.0$
- $u_L = 0, u_R = 0$
- $p_L = 0.7, p_R = 0.2$
- @ t = 0.2

Problem II

- Cell Numbers = 200
- Step Numbers = 200
- Time Steps = 0.001
- $\rho_L = 1.0, \rho_R = 0.3$
- $u_L = 0, u_R = 0$
- $p_L = 1, p_R = 0.1$
- @ t = 0.2

https://github.com/bwvdnbro/python_finite_volume_solver

Results - Problem I

Density distribution of shock tube @ t = 0.2.
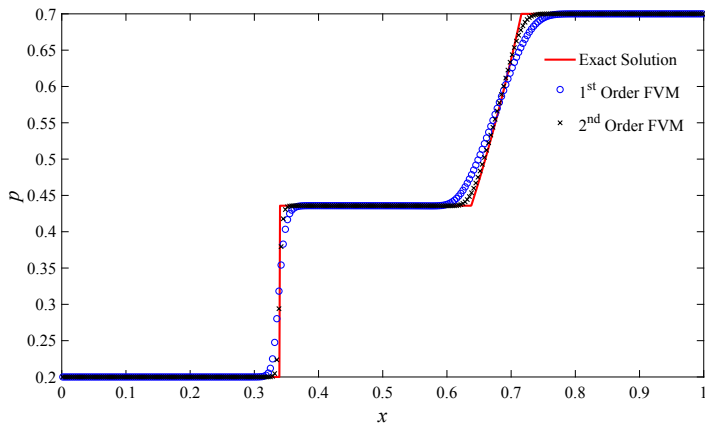
Shock Tube Problem

Results - Problem I

Velocity distribution of shock tube @ t = 0.2.
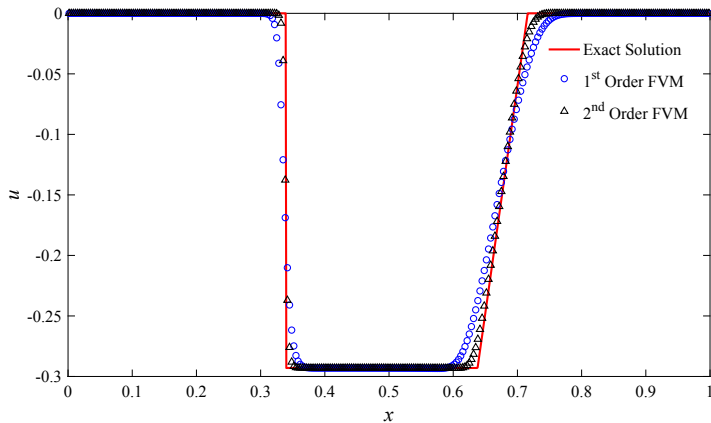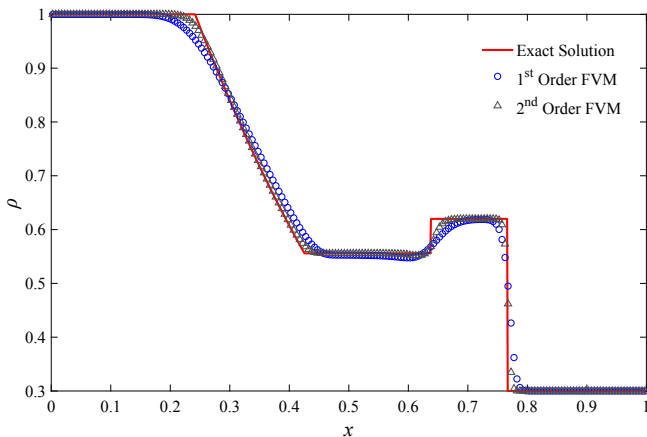
Shock Tube Problem

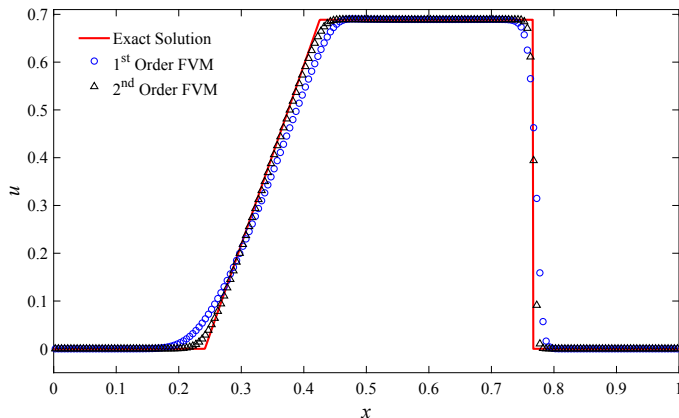## Results - Problem I

Pressure distribution of shock tube @ t = 0.2.

Shock Tube Problem

Results - Problem II

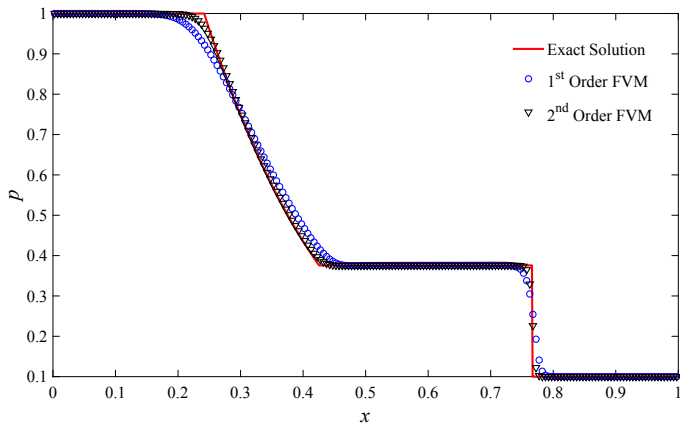Density distribution of shock tube @ t = 0.2.

Shock Tube Problem

Results - Problem II

Velocity distribution of shock tube @ t = 0.2.

Results - Problem II

Pressure distribution of shock tube @ t = 0.2.

Thanks for Listening!

Any Questions...?