L'CADAME

High Performance Computing &
Machine Learning in Engineering

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Laboratório de Computação de Alto Desempenho e
Aprendizado de Máquina em Engenharia (L'CADAME)

UFRJ

Course

Overview

- Initial Value Problem (IVP)
- Boundary Value Problem (BVP)
- Finite Element Method
- Finite Volume Methos
- Eulerian, Lagrangian and ALE Frameworks
- Modeling Mixtures & Material Behavior
- Spectral Methods
- Direct Numerical Simulation
- Machine Learning

Initial Value Problem

Forward Euler

- Problem definition:

$$\frac{d}{dt}y(t) = f(y,t) \qquad\qquad \dot{y}(t) = \frac{y+t}{y-t}$$

- Taylor expansion:

$$y(t+\Delta t) = y(t) + \Delta t \left.\frac{dy}{dt}\right|_t + O(\Delta t^2)$$

- Define:

$$t \to t_n \qquad t+\Delta t \to t_{n+1}$$
$$y(t) \to y_n \qquad y(t+\Delta t) \to y_{n+1}$$

$$y(t+\Delta t) \approx y_{n+1} = y_n + \Delta t\, f(y_n, t_n)$$

Forward Euler Method

Initial Value Problem

Backward Euler

- Problem definition:

$$\frac{d}{dt}y(t) = f(y,t) \qquad\qquad \dot{y}(t) = \frac{y+t}{y-t}$$

- Taylor expansion:

$$y(t) = y(t+\Delta t) - \Delta t\,\left.\frac{dy}{dt}\right|_{t+\Delta t} + O(\Delta t^2)$$

- Approximation:

$$y(t+\Delta t) \approx y_n = y_{n+1} + \Delta t\, f(y_{n+1}, t_{n+1})$$

Backward Euler Method

Initial Value Problem

Example

- Toy problem:

$$\dot{y}(t) = \frac{y+t}{y-t} \qquad\qquad y(0) = 1$$

- Forward Euler:

$$y_{n+1} = y_n + \Delta t\, f(y_n, t_n)$$

- Solution ($\Delta t = 0.1$):

$$y_0 = 1,$$

$$y(0.1) \approx y_1 = y_0 + \Delta t \times \frac{y_0 + t_0}{y_0 - t_0} = 1 + 0.1 \times \frac{1+0}{1-0} = 1.1$$

$$y(0.2) \approx y_2 = y_1 + \Delta t \times \frac{y_1 + t_1}{y_1 - t_1} = 1.1 + 0.1 \times \frac{1.1+0.1}{1.1-0.1} = 1.22$$

Initial Value Problem

Example

- Toy problem:

$$\dot{y}(t) = \frac{y+t}{y-t} \qquad\qquad y(0) = 1$$

- Backward Euler:

$$y_{n+1} = y_n + \Delta t\, f(y_{n+1}, t_{n+1})$$

- Solution ($\Delta t = 0.1$):

$$y_0 = 1,$$

$$y(0.1) \approx y_1 = y_0 + \Delta t \times \frac{y_1 + t_1}{y_1 - t_1} = 1 + 0.1 \times \frac{y_1 + 0}{y_1 - 0}$$

$$y(0.2) \approx y_2 = y_1 + \Delta t \times \frac{y_2 + t_2}{y_2 - t_2}$$

Initial Value Problem

Error and Order

- Forward Euler (Explicit method):

$$y_{n+1} = y_n + \Delta t\, f(y_n, t_n)$$

- Backward Euler (Implicit Method):

$$y_{n+1} = y_n + \Delta t\, f(y_{n+1}, t_{n+1})$$

- Error:

$$y(t_{n+1}) \neq y_{n+1} \rightarrow e_n = |y(t_n) - y_n|$$

- Order of Method (order *p*):

$$e = O(\Delta t^p)$$

Forward and Backward Euler methods are first order.

- Discrete Solution (finite number of points)

Initial Value Problem

Higher Order Methods

- Forward & Backward Euler:

$$y_{n+1} = y_n + \Delta t\, f(y_n, t_n)$$

$$y_{n+1} = y_n + \Delta t\, f(y_{n+1}, t_{n+1})$$

- Crank–Nicolson Method:

$$y_{n+1} = y_n + \frac{1}{2}\Delta t\big(f(y_n, t_n) + f(y_{n+1}, t_{n+1})\big)$$

- Runge–Kutta Method (RK4):

$$y_{n+1} = y_n + \frac{1}{6}\Delta t(f_1 + 2f_2 + 2f_3 + f_4)$$

$$f_2 = f\left(t + \frac{\Delta t}{2}, y_n + \frac{\Delta t}{2} f_1\right) \qquad f_3 = f\left(t + \frac{\Delta t}{2}, y_n + \frac{\Delta t}{2} f_2\right)$$

Initial Value Problem

Numerical Stability

- Forward Euler:

$$y_{n+1} = y_n + \Delta t\, f(y_n, t_n)$$

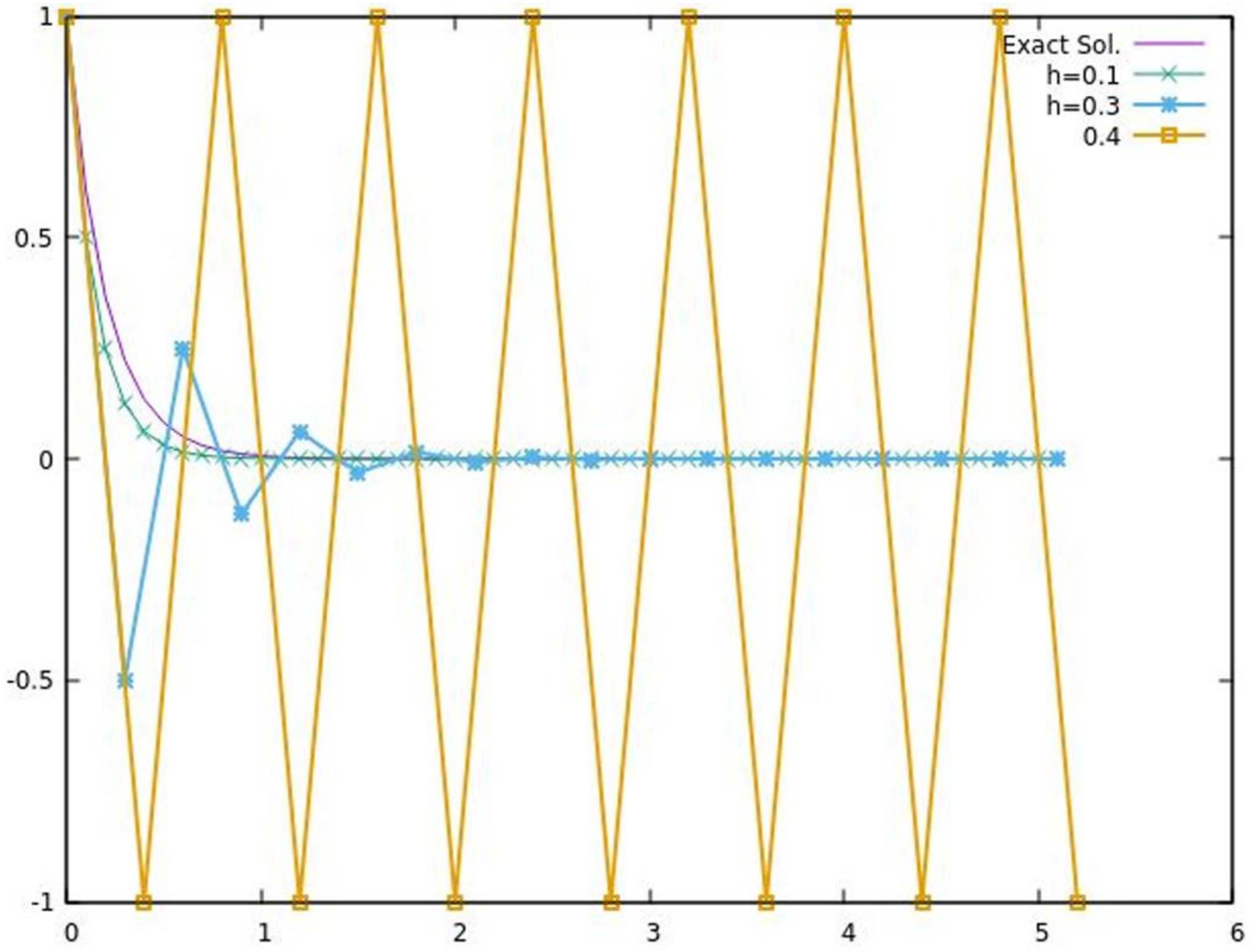
- Toy problem:

$$\frac{dy}{dt} = -5y$$
$$y(0) = 1$$

- Exact Solution:

$$y(t) = e^{-5t}$$

- Region of Stability.



Boundary Value Problem

Introduction

- Model Problem:

$$\frac{d^2u}{dx^2} = f\left(x, u, \frac{du}{dx}\right)$$

- Boundary condition:

$$u(a) = u_a \quad ; \quad u(b) = u_b$$ Dirichlet

$$\left.\frac{du}{dx}\right|_a = \dot{u}_a \quad ; \left.\frac{du}{dx}\right|_b = \dot{u}_b$$ Von Neumann

$$\left.\frac{du}{dx}\right|_a = \alpha_1 u(a) + \beta_1 \quad ; \quad \left.\frac{du}{dx}\right|_b = \alpha_2 u(b) + \beta_2$$ Robin

Boundary Value Problem

Solution Method

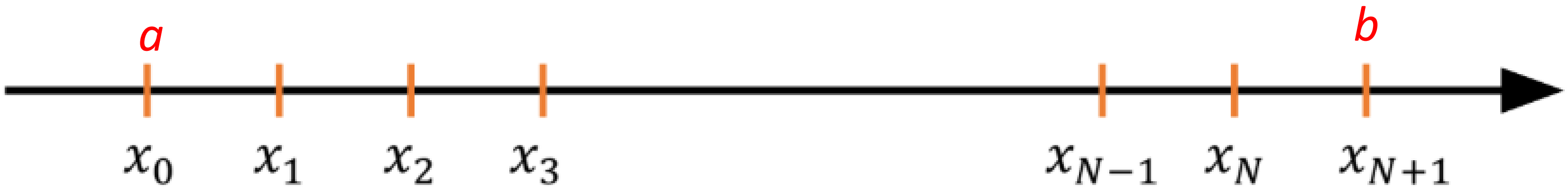
- Model Problem:

$$\frac{d^2u}{dx^2} = f\left(x, u, \frac{du}{dx}\right) \qquad u(a) = u_a \quad ; \quad u(b) = u_b$$

- Approximation (Central Difference):

$$\frac{d^2u}{dx^2} \approx \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2}$$

$$u_{i+1} - 2u_i + u_{i-1} = \Delta x^2\, f\left(x_i, u_i, \left.\frac{du}{dx}\right|_i\right)$$

- Computational Grid
- 

$$x_0 = a \to u(a) = u_0 = u_a$$

$$x_{N+1} = b \to u(b) = u_{N+1} = u_b$$

$$\Delta x = \frac{b-a}{N+1}$$

Boundary Value Problem

Solution Method

- Model Problem:

$$\frac{d^2u}{dx^2} = f\left(x, u, \frac{du}{dx}\right) \qquad u(a) = u_a \quad ; \quad u(b) = u_b$$

- Approximation (Central Difference):

$$\frac{d^2u}{dx^2} \approx \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2}$$

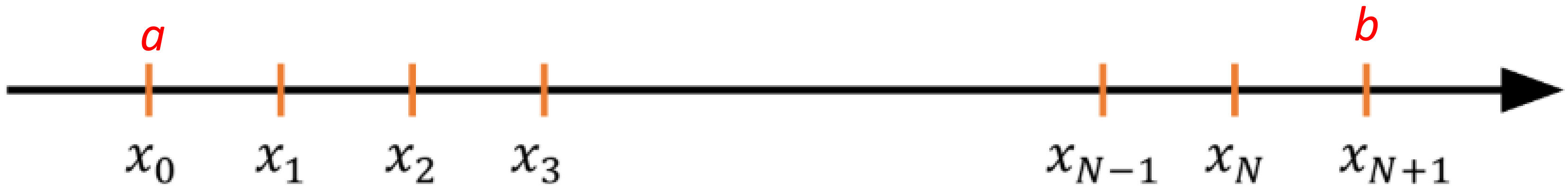
$$u_{i+1} - 2u_i + u_{i-1} = \Delta x^2 \, f\left(x_i, u_i, \left.\frac{du}{dx}\right|_i\right)$$

$$x_0 = a \rightarrow u(a) = u_0 = u_a$$

$$x_{N+1} = b \rightarrow u(b) = u_{N+1} = u_b$$

$$\Delta x = \frac{b-a}{N+1}$$

- Computational Grid

- 

Boundary Value Problem

Solution Method

$$u_{i+1} - 2u_i + u_{i-1} = \Delta x^2 \, f\left(x_i, u_i, \left.\frac{du}{dx}\right|_i\right)$$

- Solution:

$$u_2 - 2u_1 + u_0 = \Delta x^2 f_1$$

$$u_3 - 2u_2 + u_1 = \Delta x^2 f_2$$

$$\vdots$$

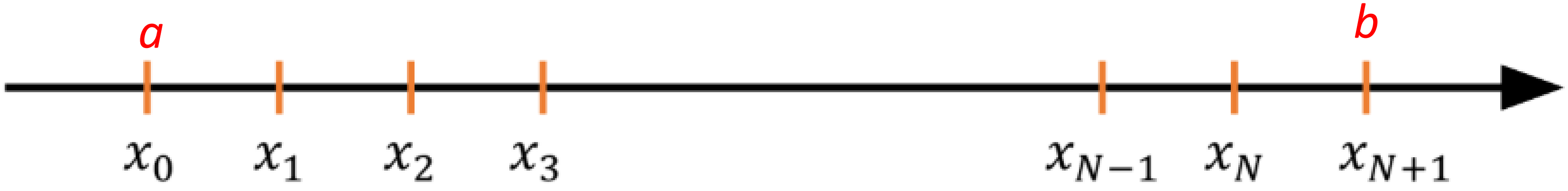
$$u_{N+1} - 2u_N + u_{N-1} = \Delta x^2 f_N$$

$$AU = B$$

$$U = [u_1, u_2, \dots, u_N]^T$$

$$A = \begin{bmatrix} -2 & 1 & 0 & \dots & 0 & 0 \\ 1 & -2 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \dots & \dots & \dots & \dots & 1 & -2 \end{bmatrix}$$

$$B = [L_1 - u_0, L_2, \dots, L_{N-1}, L_N - u_{N+1}]^T$$



Boundary Value Problem

2D Problems

$$\frac{d^2u}{dx^2} + \frac{d^2u}{dy^2} = f(x,y)$$

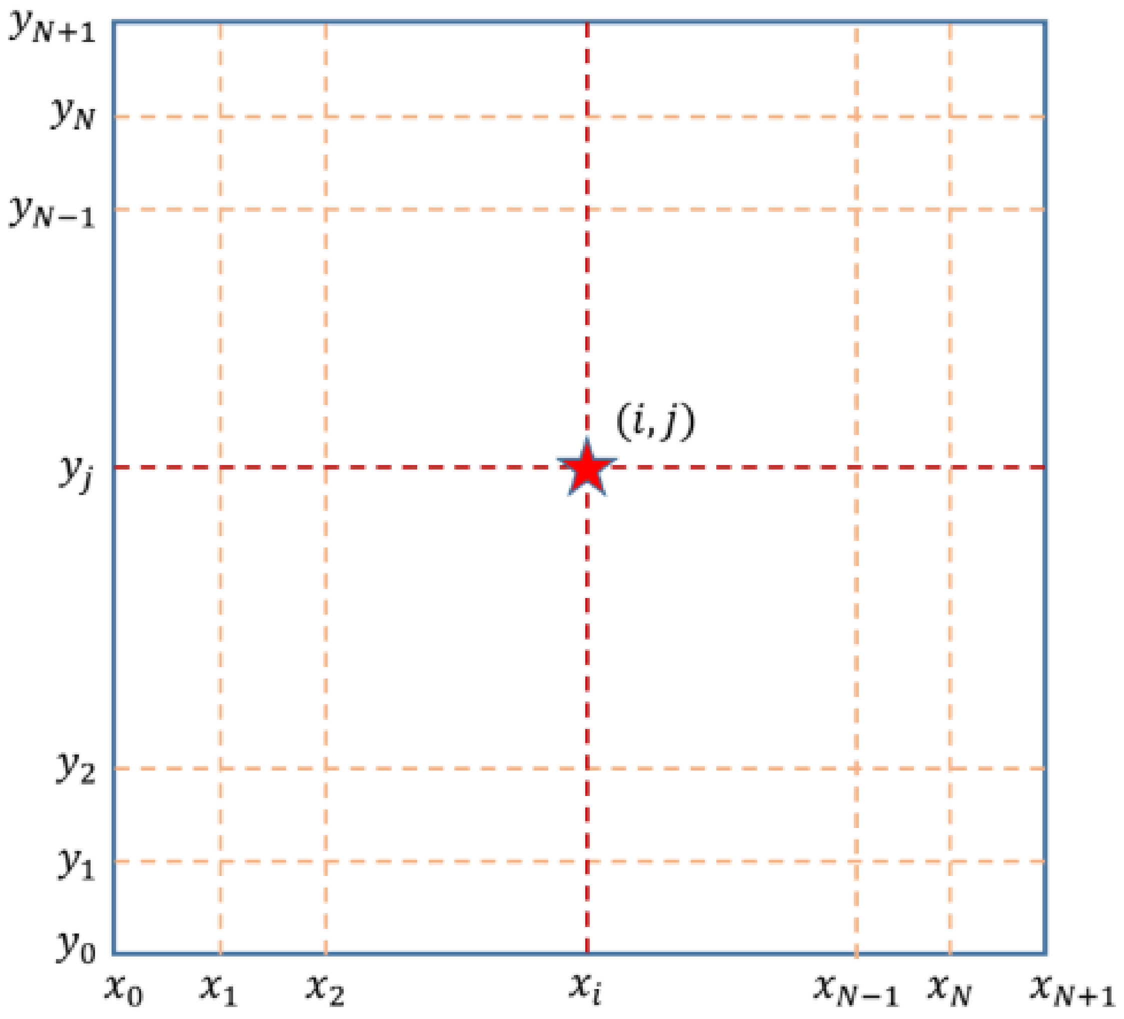
$$u(a,y) = u_a \quad ; \quad u(b,y) = u_b$$

$$u(x,c) = u_c \quad ; \quad u(x,d) = u_d$$

- Solution:

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}$$

$$+ \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = f(x_i, y_j)$$



Finite Element Method

Introduction

- Toy problem:

$$-\frac{d^2u}{dx^2} = f(x) \qquad 0 \leq x \leq 1 \qquad u(0) = u(1) = 0$$

- FE Approximation:

$$u(x) \approx u_h(x) = \sum_{j=0}^{N} c_j \varphi_j(x)$$

- $\varphi_j(x)$ is the base function, which we know beforehand (decision).
- The problem is to find c_j which represents the solution best.

Finite Element Method

Introduction

- Toy problem:

$$-\frac{d^2u}{dx^2} = f(x) \qquad 0 \le x \le 1 \qquad u(0) = u(1) = 0$$

- FE Approximation:

$$u(x) \approx u_h(x) = \sum_{i=0}^{N} c_i \varphi_i(x)$$

- Let's assume that $\varphi_j(x = 0) = 0$ and $\varphi_j(x = 1) = 0$.
- And define residual as:

$$r(x) = \frac{d^2u_h}{dx^2} + f(x) = \sum_{i=0}^{N} c_i \frac{d^2}{dx^2}\varphi_i(x) + f(x) \neq 0$$

Finite Element Method

Introduction

- Approximation

$$r(x) = \frac{d^2 u_h}{dx^2} + f(x) = \sum_{i=0}^{N} c_i \frac{d^2}{dx^2} \varphi_i(x) + f(x) \neq 0$$

- Two paths:

1. Find c_j in a way the $r(x)$ be zero at all grid points (collocation method).
2. Find c_j in a way that

$$\int_0^1 r(x) \varphi_j(x)\, dx = 0 \qquad\qquad j = 1..N$$

Galerkin Method

Finite Element Method

Galerkin Method

- Approximation

$$r(x) = \sum_{i=0}^{N} c_i \frac{d^2}{dx^2}\varphi_j(x) + f(x) \neq 0$$

$$\int_0^1 r(x)\varphi_j(x)\,dx = 0 \qquad\qquad j = 1..N$$

$$\int_0^1 \left[\sum_{i=0}^{N} c_i \frac{d^2}{dx^2}\varphi_i(x) + f(x)\right]\varphi_j(x)\,dx = 0$$

$$\sum_{i=0}^{N} c_i \int_0^1 \left[\frac{d^2}{dx^2}\varphi_i(x)\varphi_j(x)\right] dx + \int_0^1 f(x)\varphi_j(x)dx = 0$$

$$c_1 a_{11} + c_2 a_{12} + \cdots + c_N a_{1N} = b_1$$

$$A\vec{c} = \vec{b}$$

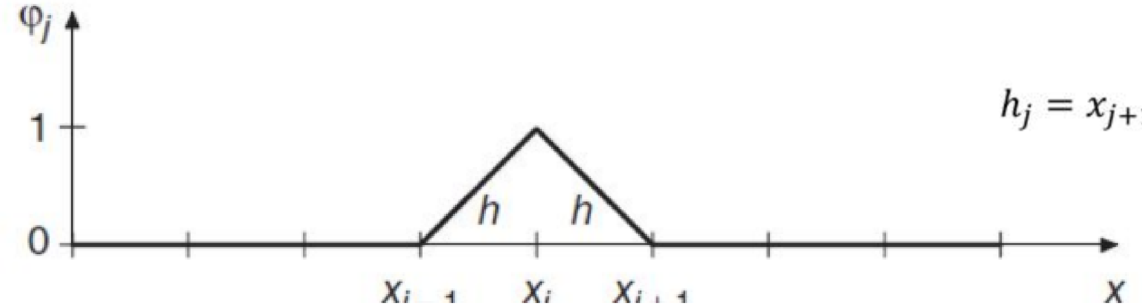
Finite Element Method

Summary

- Continuous solution.
- Different bases (kernels), different accuracies.

$$\phi_j(x) = x^j(x-1)$$

$$\phi_j(x) = \begin{cases} \dfrac{x - x_{j-1}}{x_j - x_{j-1}}, & x_{j-1} \le x \le x_j \\ \dfrac{x_{j+1} - x}{x_{j+1} - x_j}, & x_j \le x \le x_{j+1} \\ 0, & otherwise \end{cases}$$



$$\phi_j(x) = \begin{cases} g_1(\xi_{j-1}(x)), & x_{j-1} \le x \le x_j \\ g_1(1-\xi_j(x)), & x_j \le x \le x_{j+1} \\ 0, & otherwise \end{cases}$$

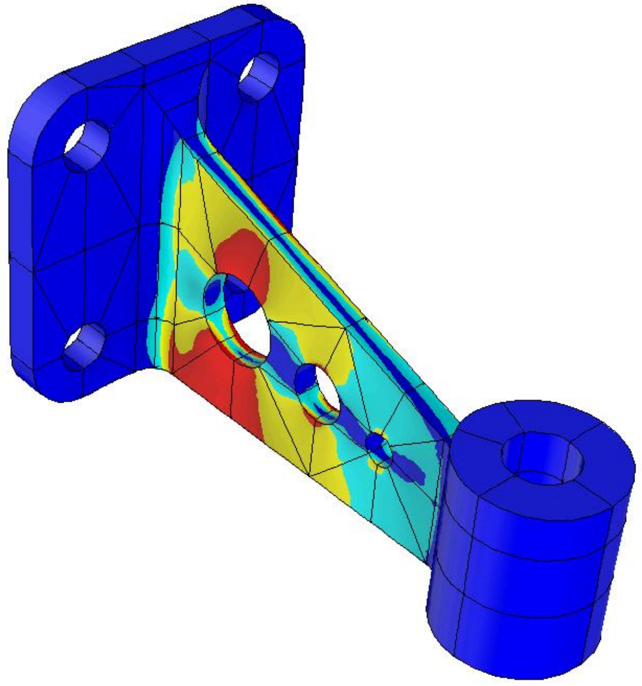
$$\frac{d\phi_j}{dx} = \begin{cases} h_{j-1} g_2(\xi_{j-1}(x)), & x_{j-1} \le x \le x_j \\ -h_j g_2(1-\xi_j(x)), & x_j \le x \le x_{j+1} \\ 0, & otherwise \end{cases}$$

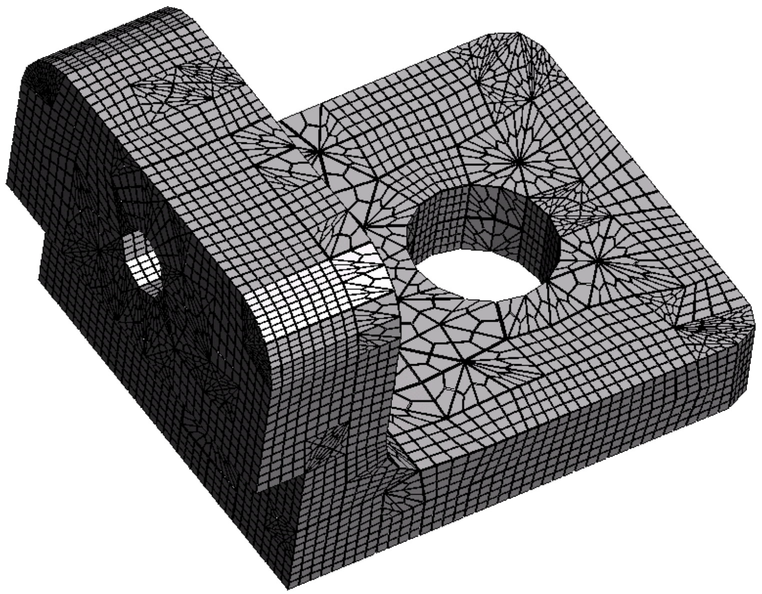
$$h_j = x_{j+1} - x_j, \qquad \xi_j(x) = \frac{x - x_j}{h_j}, \qquad g_1(x) = -2x^3 + 3x^2, \qquad g_2(x) = x^3 - x^2$$

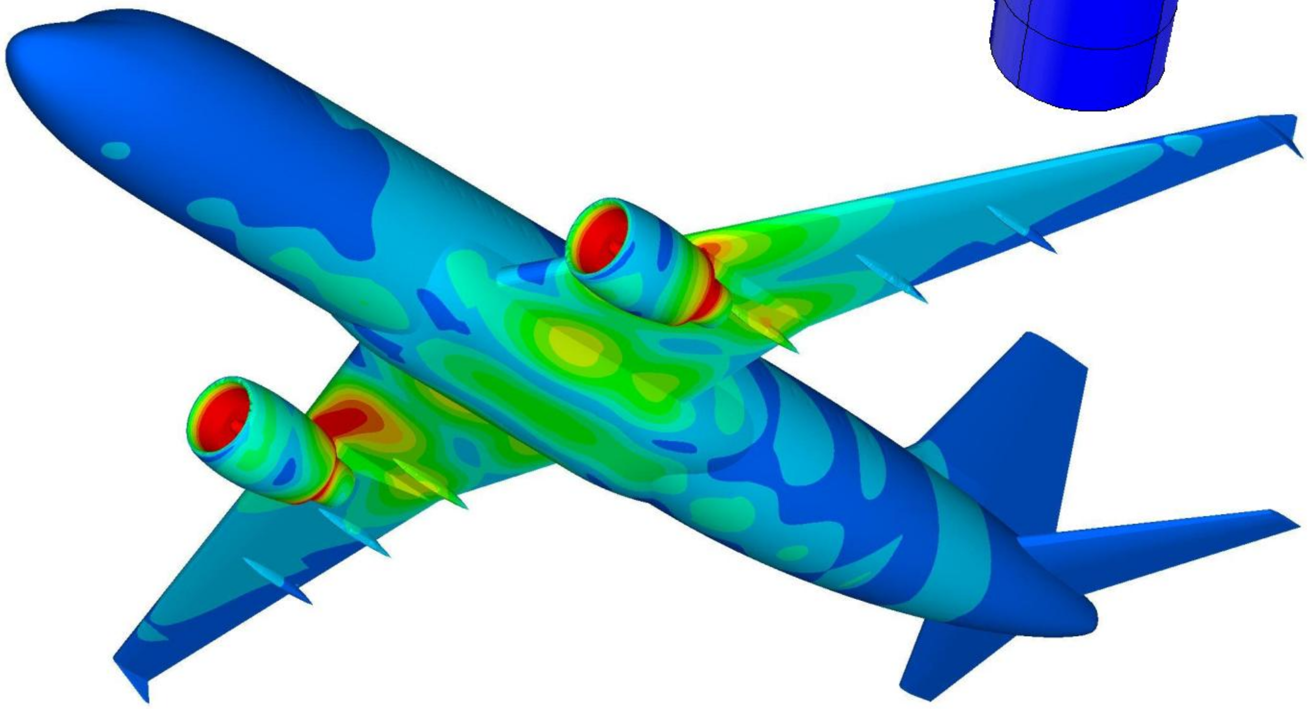
Finite Element Method

Summary

- Complex geometries,
- Different types of computational grid.







Finite Volume Method

Introduction

- Differential equations break down in the presence of discontinuities.
  - Material borders, Shock-waves, Constitutive equations.
- Solving in the integral form can address this issue effectively.

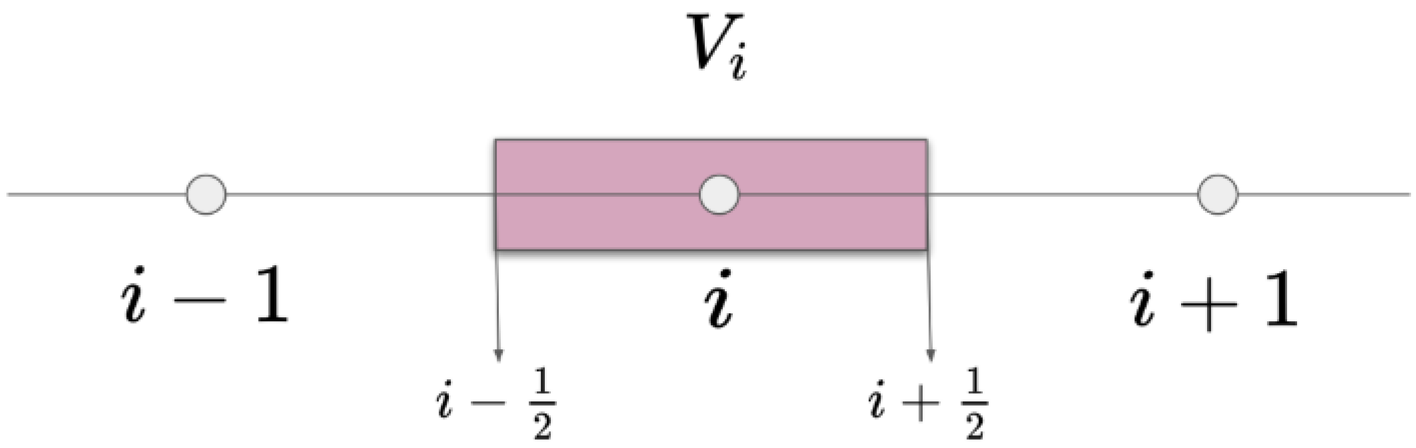
$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0$$

$$\int_{\Omega}\left[\frac{\partial \rho}{\partial t} + \nabla.(\rho u)\right] dV = \int_{\Omega}\frac{\partial \rho}{\partial t} dV + \int_{\partial\Omega}\rho(n.u)\, dS = 0$$

Finite Volume Method

Introduction

- Computational grid in FV method:



- We will track the average value of a quantity in each cell.

$$\overline{u_i}(t_n) = \frac{1}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u(x, t_n)\,dx$$

Finite Volume Method

Introduction

- Toy problem (conservation):

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0$$

$$\int_{V_i} \frac{\partial u}{\partial t}\, dV + \left[f\left(u_{i+\frac{1}{2}}\right) - f\left(u_{i+\frac{1}{2}}\right) \right] = 0$$

$$\frac{\partial}{\partial t} \int_{V_i} u\, dV + \left[f\left(u_{i+\frac{1}{2}}\right) - f\left(u_{i+\frac{1}{2}}\right) \right] = 0$$

$$\Delta x \left(\frac{\partial \bar{u}_i}{\partial t} \right) + \left[f\left(u_{i+\frac{1}{2}}\right) - f\left(u_{i+\frac{1}{2}}\right) \right] = 0$$

$$\frac{\bar{u}_i^{n+1} - \bar{u}_i^{n}}{\Delta t} + \frac{f\left(u_{i+\frac{1}{2}}\right) - f\left(u_{i+\frac{1}{2}}\right)}{\Delta x} = 0$$

Classification

Second order equation

- Toy problem (conservation):

$$a\frac{\partial^2 u}{\partial x^2} + 2b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + fu = g(x,y)$$

$b^2 - ac < 0$ Elliptic Equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

$b^2 - ac = 0$ Parabolic Equation

$$\frac{\partial u}{\partial t} = \kappa\frac{\partial^2 u}{\partial x^2}$$

$b^2 - ac > 0$ Hyperbolic Equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial t} = 0$$

Finite Volume Method

Introduction

- Toy problem (conservation):

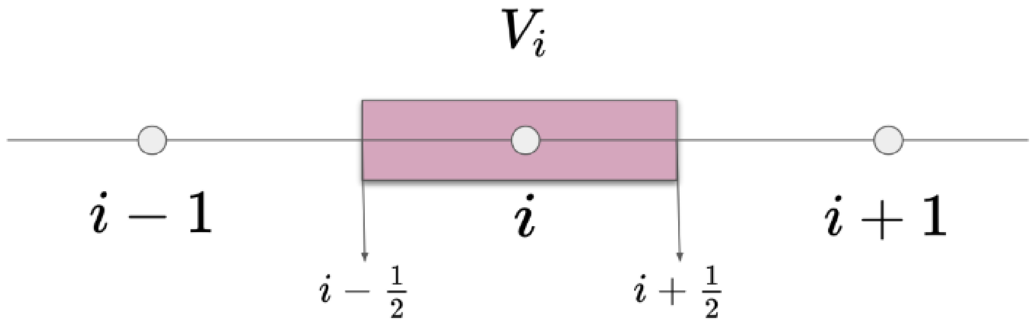
$$\frac{\bar{u}_i^{n+1} - \bar{u}_i^n}{\Delta t} + \frac{f\left(u_{i+\frac{1}{2}}\right) - f\left(u_{i+\frac{1}{2}}\right)}{\Delta x} = 0$$

- Naïve approximation:

$$u_{i+\frac{1}{2}} = \frac{1}{2}\left(\bar{u}_i + \bar{u}_{i+1}\right)$$

- Upwinding:

$$u_{i-\frac{1}{2}} = \bar{u}_{i-1} \qquad\qquad u_{i+\frac{1}{2}} = \bar{u}_i$$



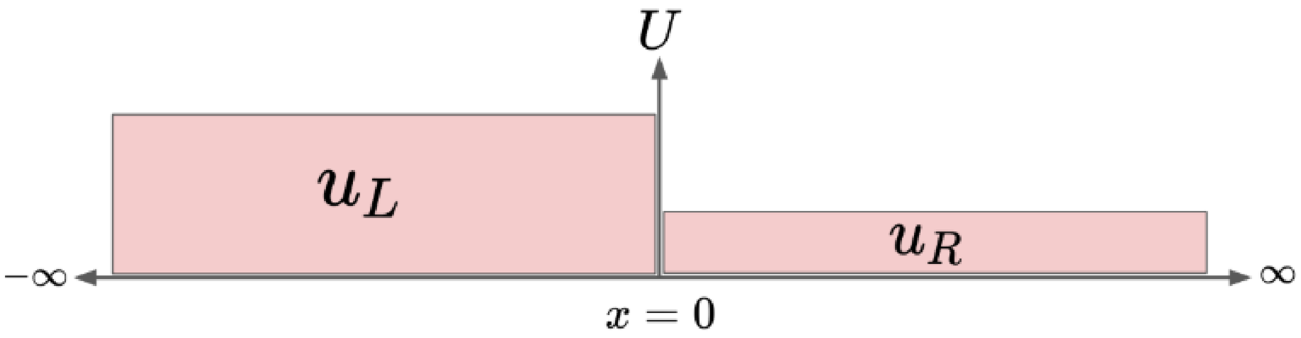
Riemann Problem

Introduction

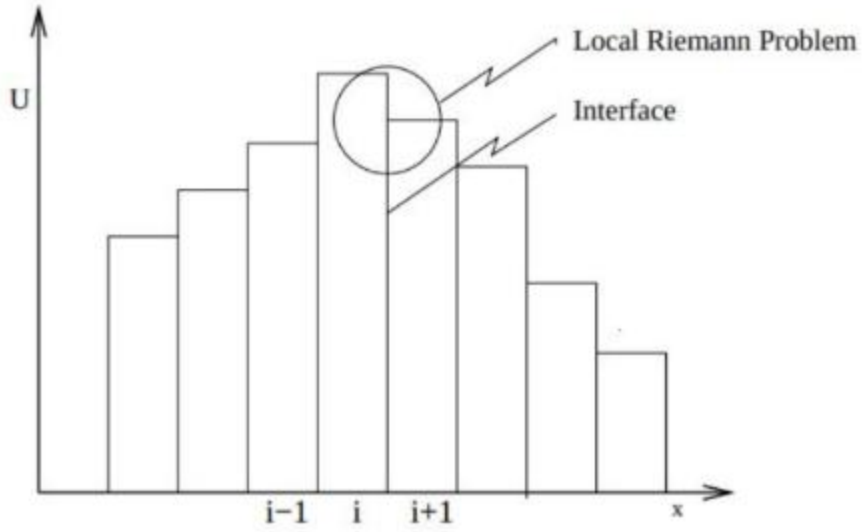
- Toy problem:

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0$$

$$IC: \begin{cases} u(x < 0, t = 0) = u_L \\ u(x \geq 0, t = 0) = u_R \end{cases}$$



- Godunov scheme
  - Exact solution
  - Approximate solution (HLL,HLLE,HLLC,…)



Gas dynamics Equations

Euler Equations

- Euler equation (gas dynamics)

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho \vec{u}) = 0$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla.(\rho \vec{u} \otimes \vec{u}) = \nabla.\sigma$$

$$\frac{\partial \rho e}{\partial t} + \nabla.(\rho e \vec{u}) = \sigma : \dot{\epsilon}$$

- Conservation (mass, momentum and energy),
- Compressible fluid,
- Hyperbolic equation.

Gas dynamics Equations

Navier-Stokes Equation

- Euler equation (gas dynamics)

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho\vec{u}) = 0 \qquad \frac{\partial \rho\vec{u}}{\partial t} + \nabla.(\rho\vec{u}\otimes\vec{u}) = \nabla.\sigma \qquad \frac{\partial \rho e}{\partial t} + \nabla.(\rho e\vec{u}) = \sigma:\dot{\epsilon}$$

- Navier-Stokes equation

$$\nabla.(\vec{u}) = 0$$

$$\frac{\partial \vec{u}}{\partial t} + \nabla.(\vec{u}\otimes\vec{u}) = \frac{1}{\rho}\nabla.\sigma$$

- Incompressible fluid,
- Parabolic equation (elliptic in limit of steady state flow).

$$\sigma = -pI + \tau \quad \rightarrow \quad \frac{\partial \vec{u}}{\partial t} + \nabla.(\vec{u}\otimes\vec{u}) = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla.\tau$$

Gas dynamics Equations

Navier-Stokes Equation

- Navier-Stokes equation

$$\nabla.(\vec{u}) = 0$$

$$\frac{\partial \vec{u}}{\partial t} + \nabla.(\vec{u} \otimes \vec{u}) = -\frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla.\tau$$

- Constitutive Equation (describes the fluid = property of fluid),
- Newtonian fluid

$$\tau = \mu[\nabla u + \nabla u^T] = 2\mu S$$

- Rate-of-strain tensor, $S = \frac{1}{2}[\nabla u + \nabla u^T]$, deformation rate $\dot{\gamma} = \sqrt{2S{:}\,S}$.

$$\frac{\partial \vec{u}}{\partial t} + \nabla.(\vec{u} \otimes \vec{u}) = -\frac{1}{\rho}\nabla p + \nu\,\nabla^2 u$$

Gas dynamics Equations

Navier-Stokes Equation

- Newtonian fluid:

$$\tau = \mu[\nabla u + \nabla u^T] = 2\mu S$$

- Generalized Newtonian Fluid (GNF):

$$\tau = 2\mu(\dot{\gamma})S$$

- Power-law type fluid: $\tau(\dot{\gamma}) = K\dot{\gamma}^n$
- Bingham Fluid:

$$\begin{cases} \tau = \tau_y + \mu\dot{\gamma} & if\ \tau > \tau_y \\ \dot{\gamma} = 0 & if\ \tau < \tau_y \end{cases}$$

- Herschel-Bulkley Fluid:

$$\begin{cases} \tau = \tau_y + K\dot{\gamma}^n & if\ \tau > \tau_y \\ \dot{\gamma} = 0 & if\ \tau < \tau_y \end{cases}$$

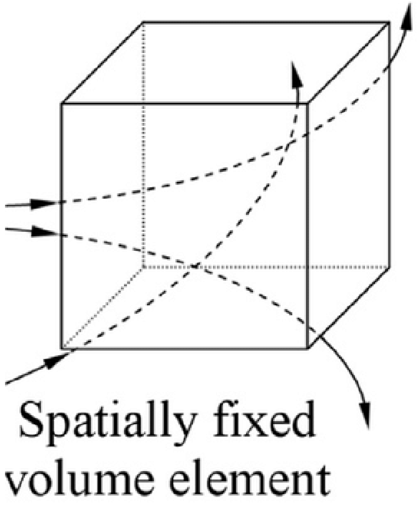
Modeling

$$\tau = \frac{\tau_y + K\dot{\gamma}^n}{\dot{\gamma}} S$$

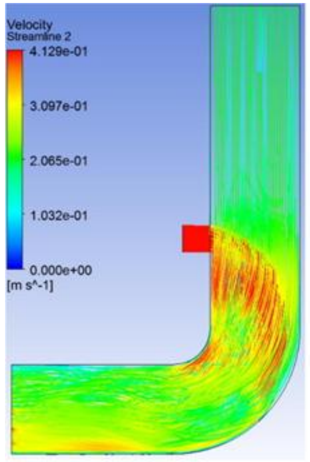
Lagrangian vs Eulerian

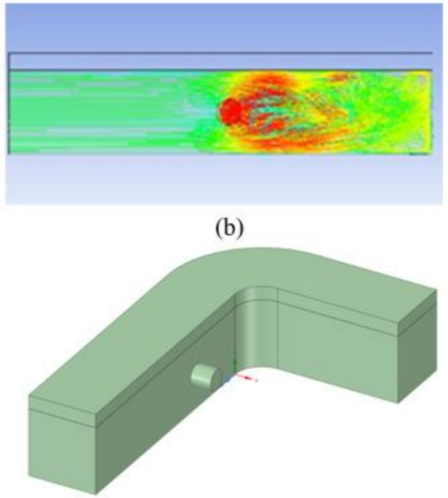
Introduction

Eulerian

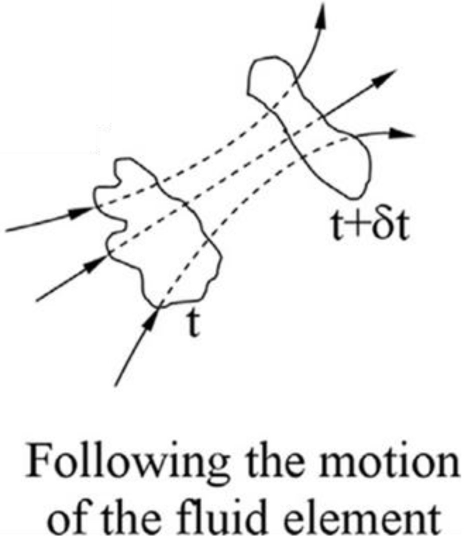


$$\frac{\partial \boxplus}{\partial t} + \nabla.(\boxplus\, \vec{u})$$

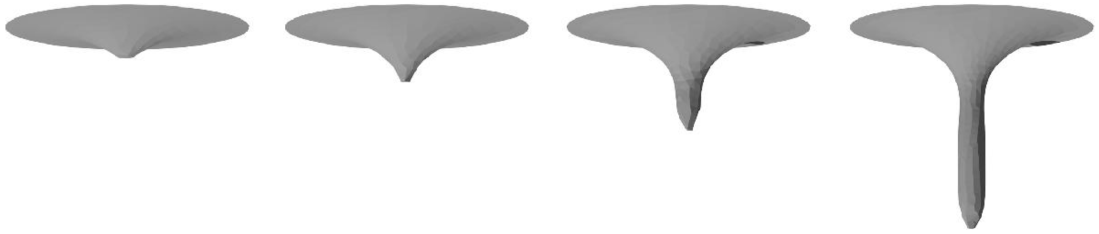




Lagrangian

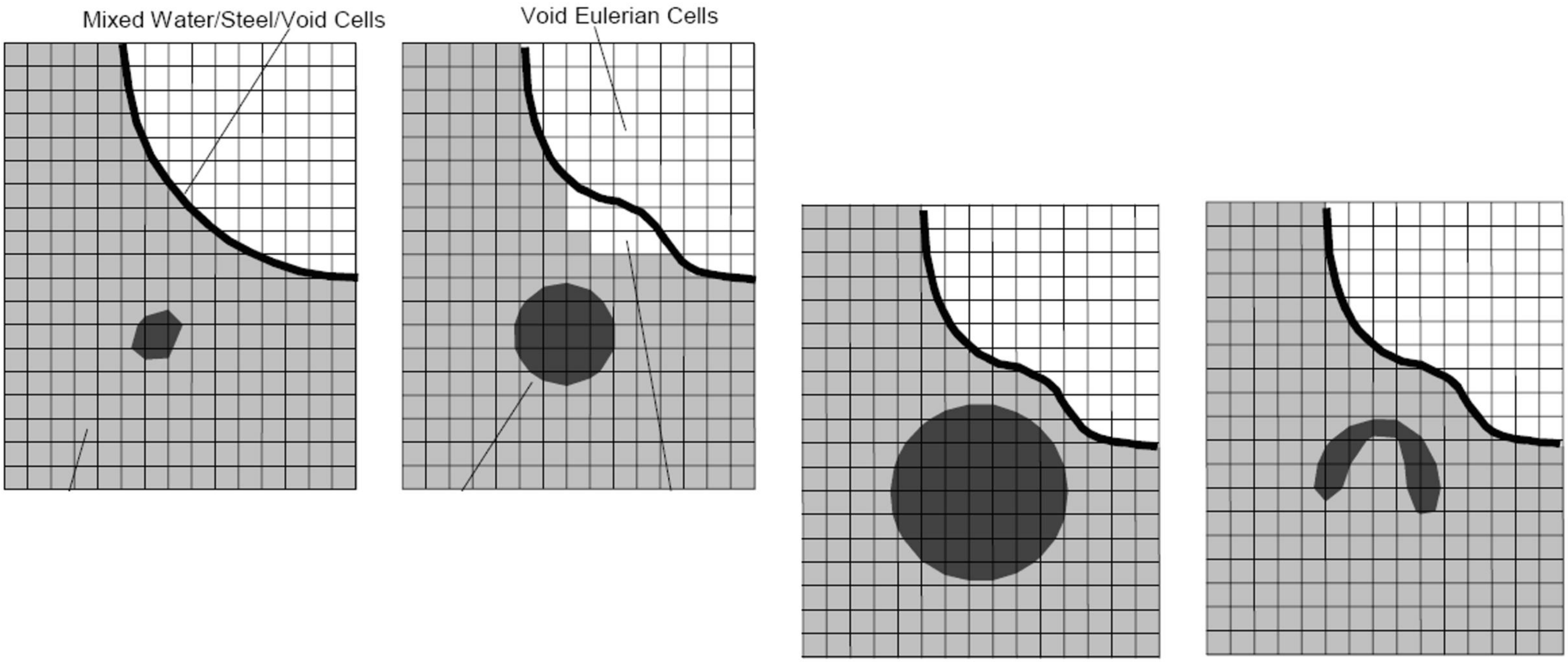


$$\frac{D \boxplus}{D t}$$



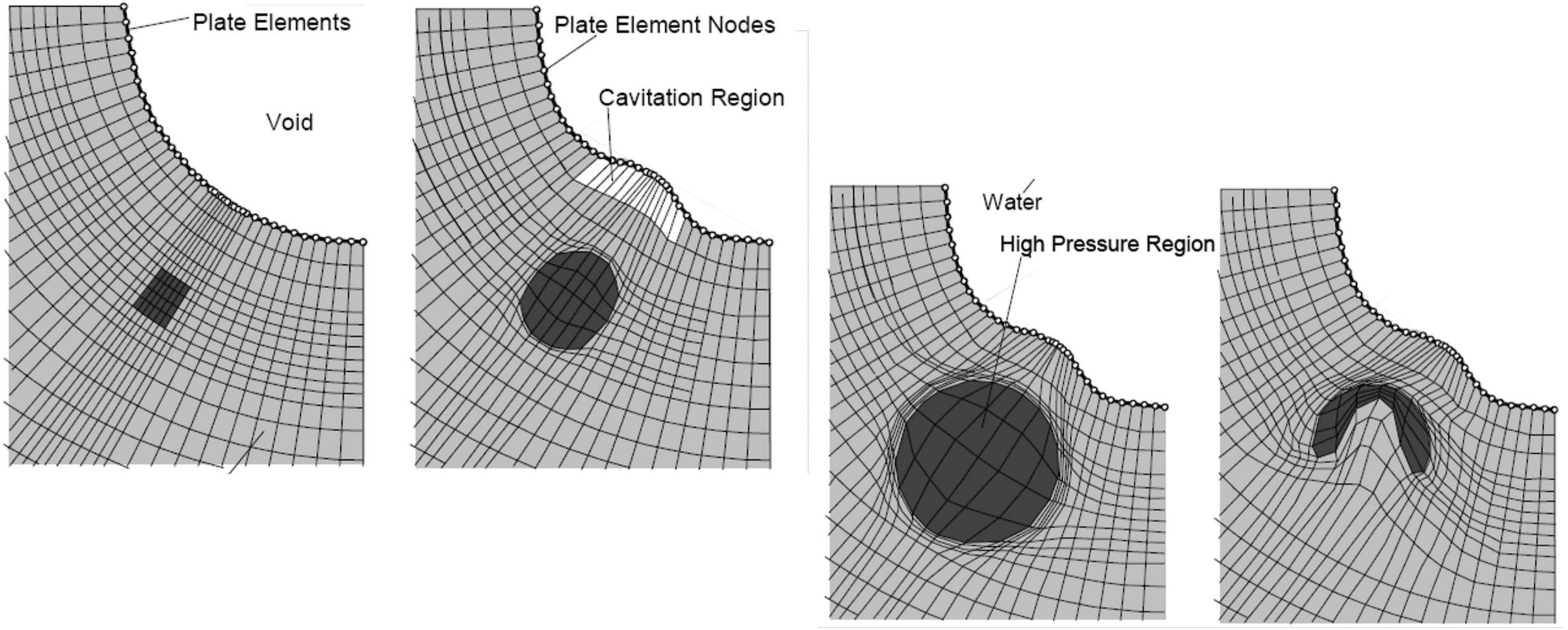
Framework

Eulerian view



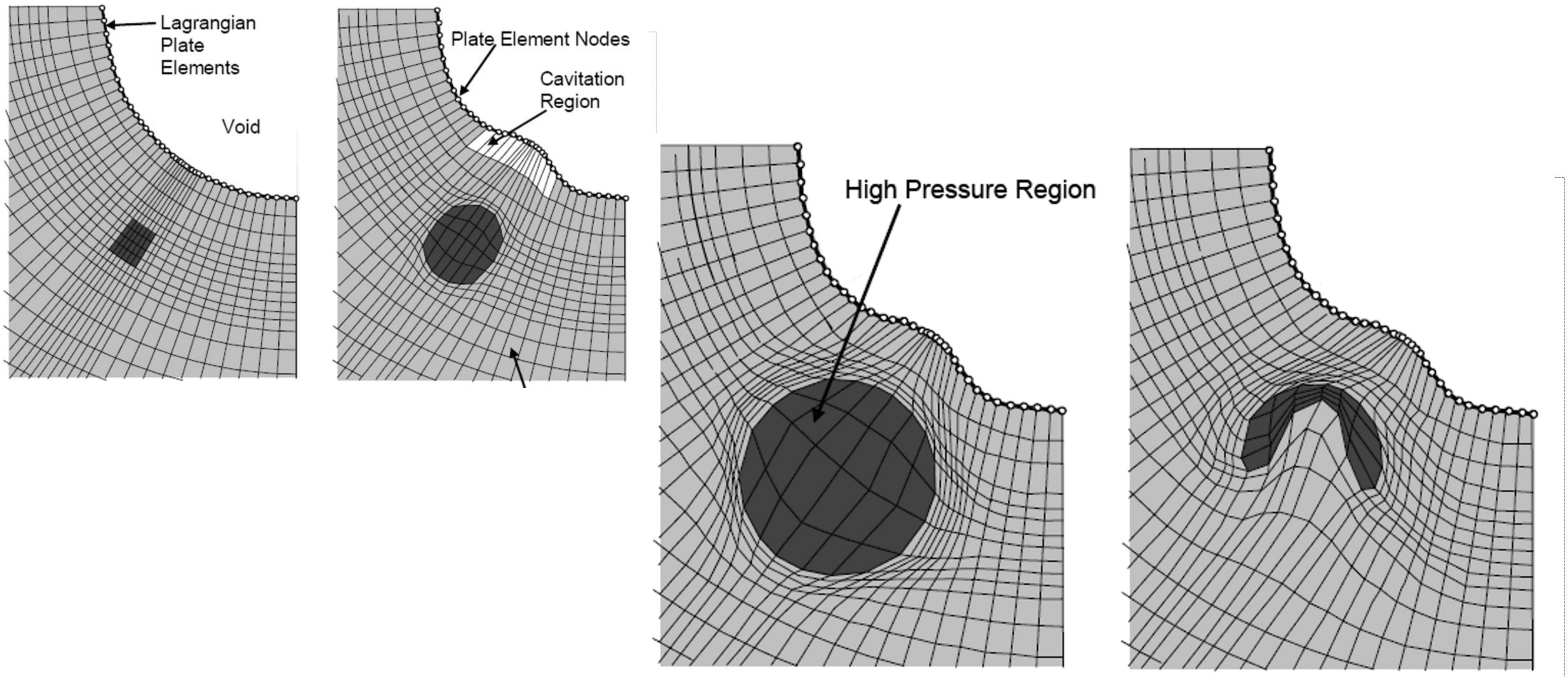
Framework

Lagrangian view



Framework

ALE view



Arbitrary Lagrangian-Eulerian

Formulation

Lagrangian	Eulerian	ALE
$\frac{1}{V}\frac{DV}{Dt} = \nabla.\vec{u}$ $\rho\frac{D\vec{u}}{Dt} = -\nabla p$ $\rho\frac{De}{Dt} = -p\,\nabla.\vec{u}$	$\frac{\partial\rho}{\partial t} + \nabla.(\rho\vec{u}) = 0$ $\frac{\partial\rho\vec{u}}{\partial t} + \nabla.(\rho\vec{u}\otimes\vec{u}) = -\nabla p$ $\frac{\partial\rho e}{\partial t} + \nabla.(\rho e\vec{u}) = -p\nabla.\vec{u}$	$\frac{\partial\rho}{\partial t} + \nabla.\left(\rho(\vec{u} - \vec{u}_g)\right) = 0$ $\frac{\partial\rho\vec{u}}{\partial t} + \nabla.\left(\rho\vec{u}\otimes(\vec{u} - \vec{u}_g)\right) = -\nabla p$ $\frac{\partial\rho e}{\partial t} + \nabla.\left(\rho e(\vec{u} - \vec{u}_g)\right)$ $= -p\nabla.\,\vec{u}$

An extra degree of freedom: $\vec{u}_g$

Arbitrary Lagrangian-Eulerian

Solution Strategy

- Functional Splitting method

$$\frac{\partial \rho\phi}{\partial t} + \nabla.\left(\rho\phi(\vec{u} - \vec{u}_g)\right) = S_\phi$$

Lagrangian

$$\frac{D\rho\phi}{Dt} = S_P$$

Advection

$$\frac{\partial \rho\phi}{\partial t} + \nabla.\left(\rho\phi(\vec{u} - \vec{u}_g)\right) = 0$$

ALE

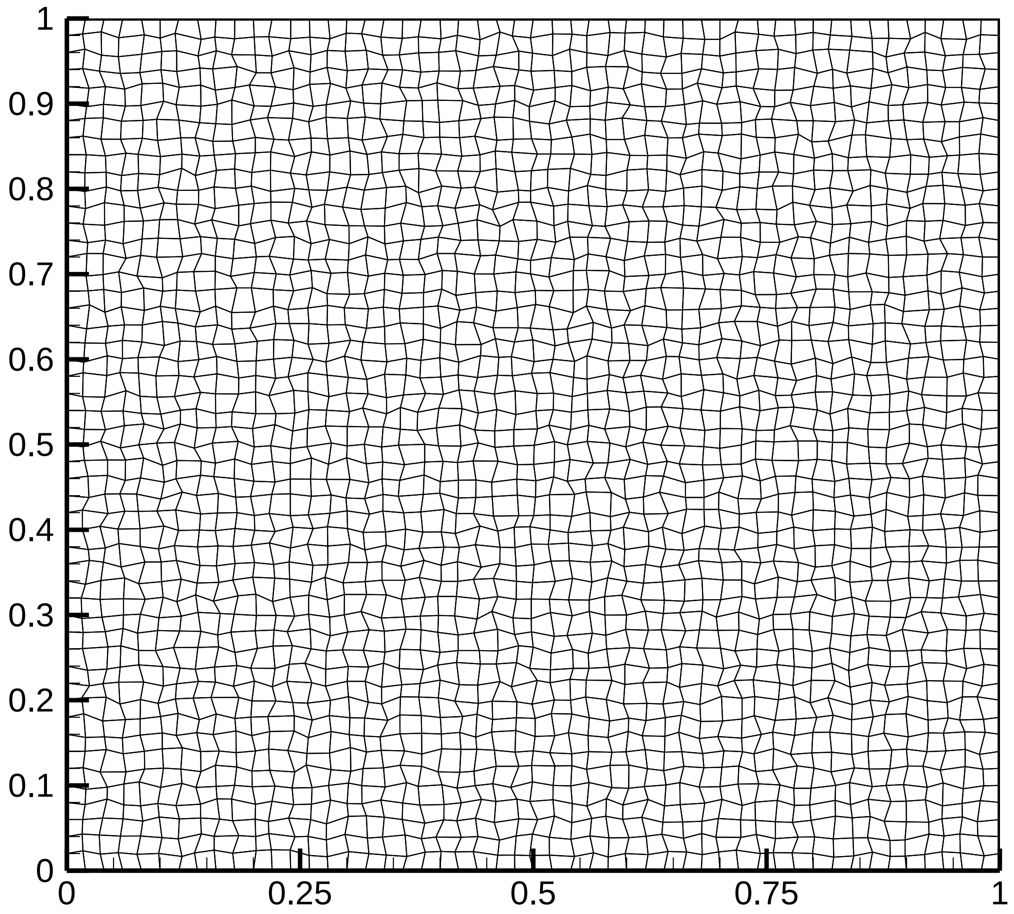
$$\frac{\partial \rho}{\partial t} + \nabla.\left(\rho(\vec{u} - \vec{u}_g)\right) = 0$$

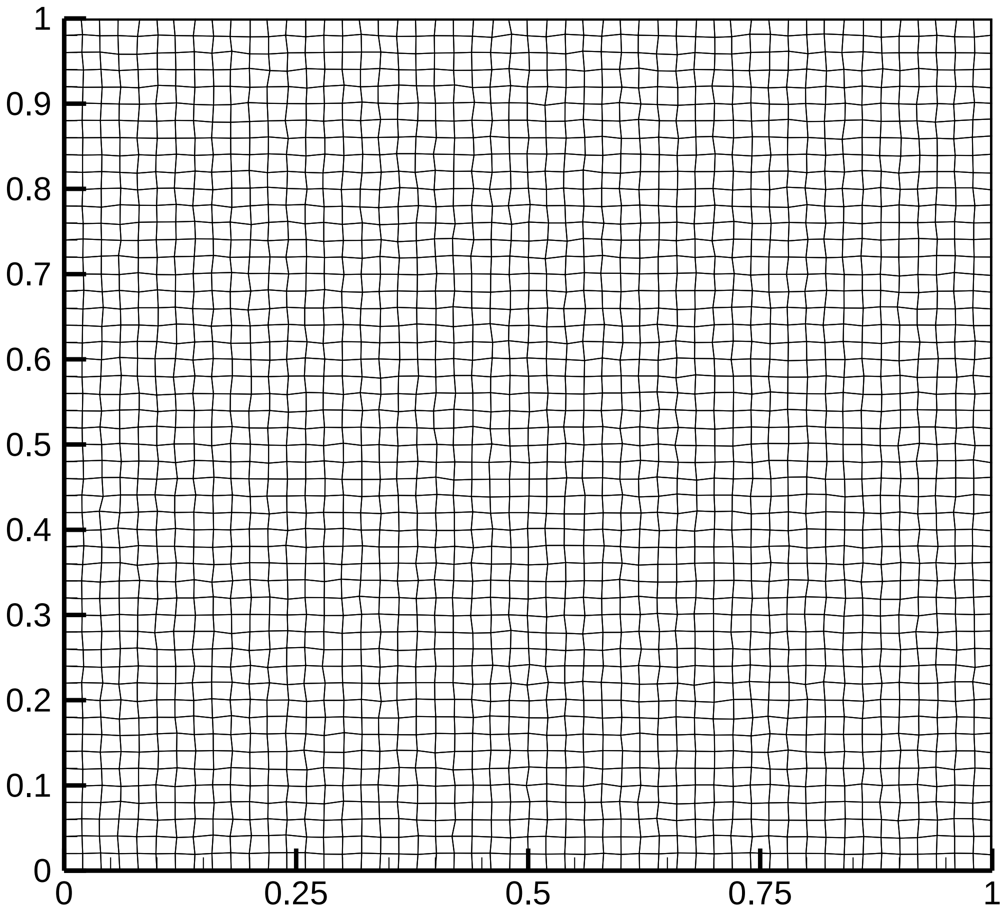
$$\frac{\partial \rho\vec{u}}{\partial t} + \nabla.\left(\rho\vec{u}\otimes(\vec{u} - \vec{u}_g)\right) = -\nabla p$$

$$\frac{\partial \rho e}{\partial t} + \nabla.\left(\rho e(\vec{u} - \vec{u}_g)\right)$$
$$= -p\nabla.\,\vec{u}$$

Arbitrary Lagrangian-Eulerian

Rezoning

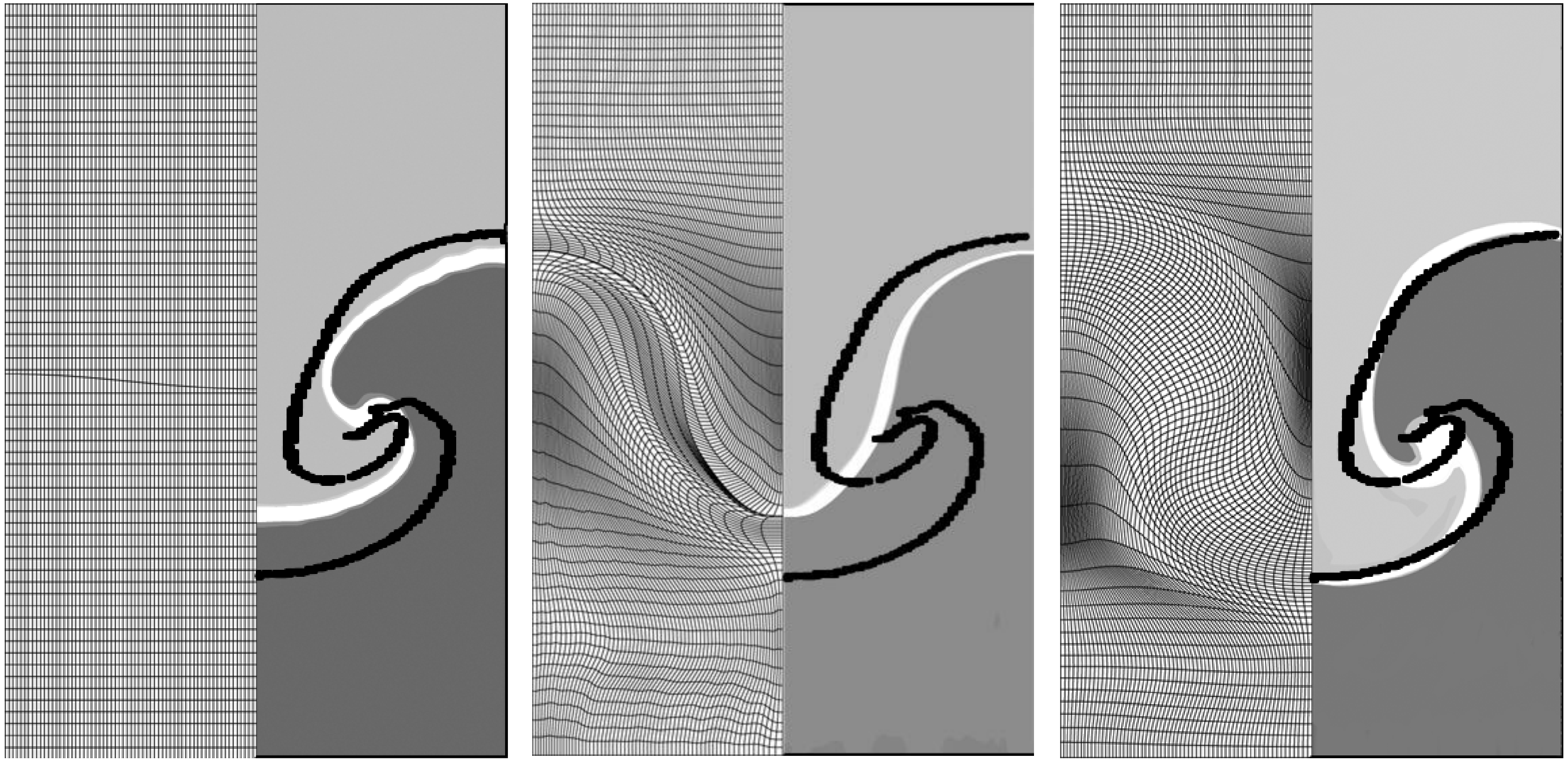




Smoothing computational grid

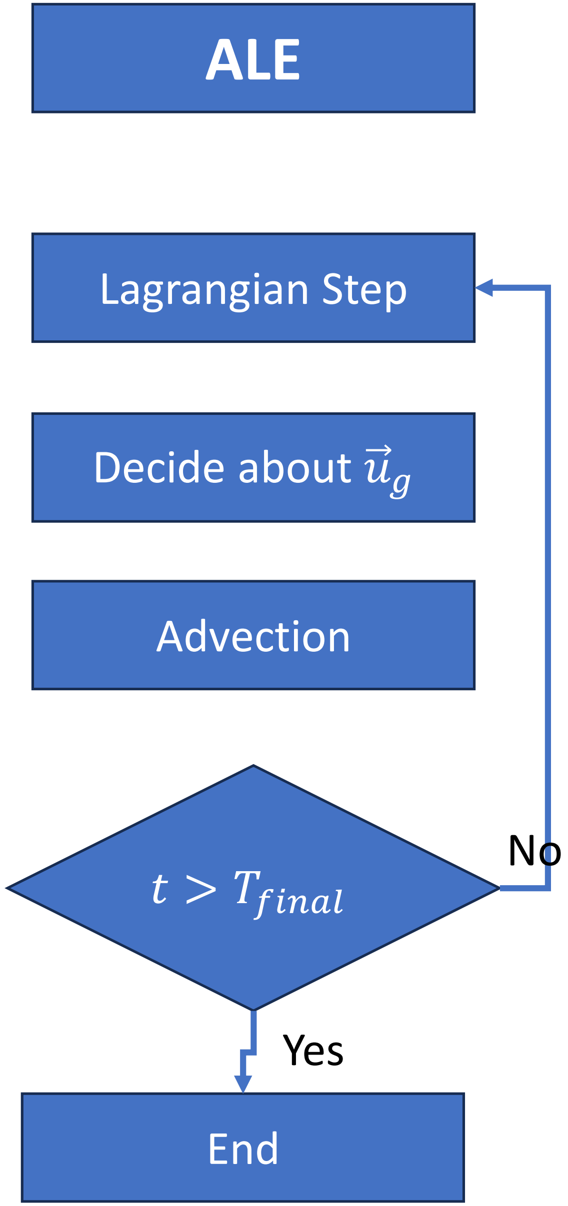
Arbitrary Lagrangian-Eulerian

Solution Strategy



Eulerian   Lagrangian   ALE

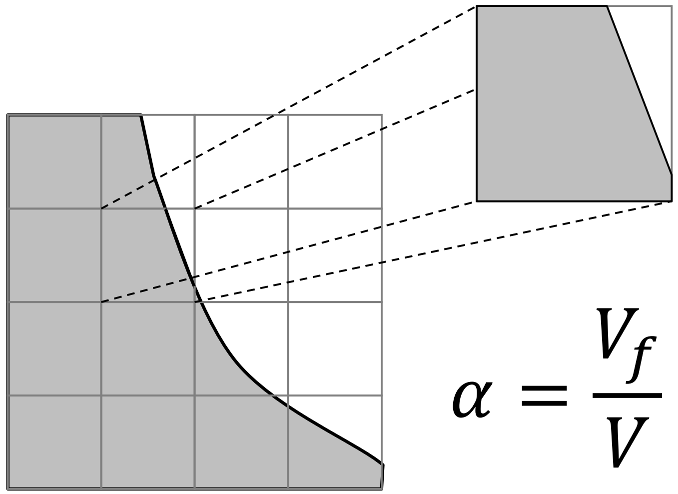
Rayleigh-Taylor Instability



Multi-Material Problems

Solution Strategy

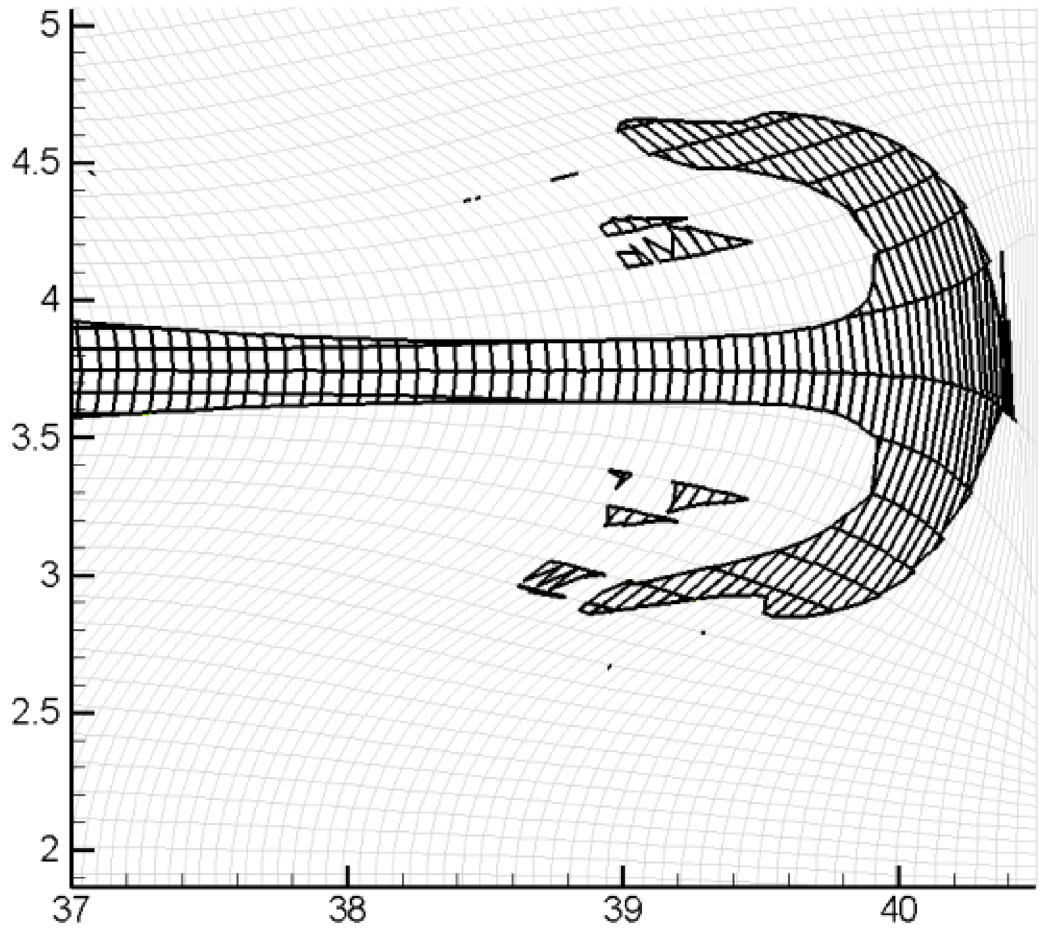
- Fluid mixtures:
  - Miscible fluid mixtures: mix completely, form homogenous mix without any separating layer.
  - Immiscible fluid mixtures: do not mix and instead form distinct separate layers.
- Strategies to model immiscible mixtures:
  - Level set,
  - Interface tracking,
  - Interface Reconstruction (VOF)
    - Advection of VOFs,
    - Reconstruction of interfaces,
    - Mixed cell dynamics.

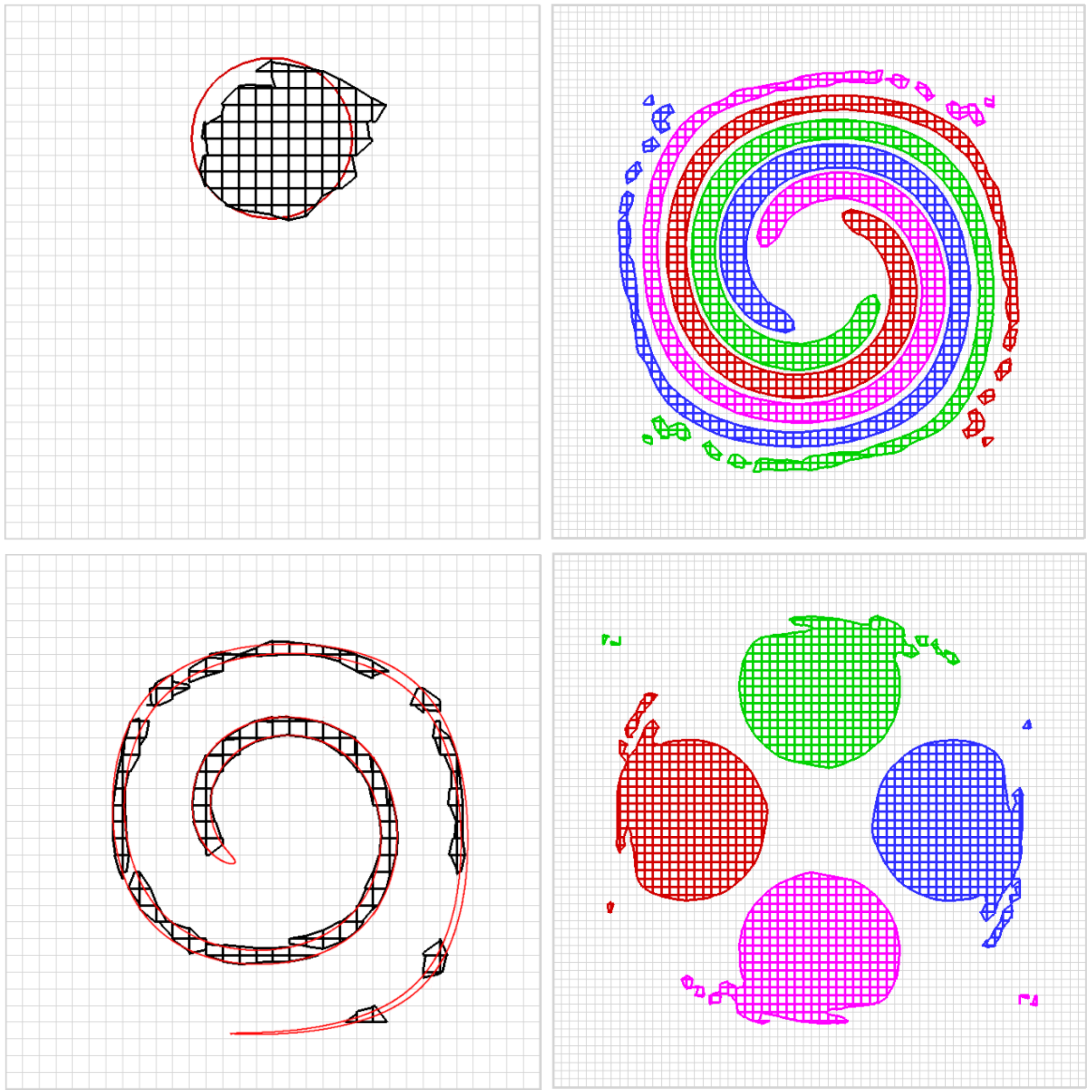


$$\alpha = \frac{V_f}{V}$$

Multi-Material Problems

Volume of fluid





Spectral Methods

Introduction

- Navier-Stokes Equation:

$$\nabla.\vec{u} = 0 \qquad \frac{\partial \vec{u}}{\partial t} + \nabla.(\vec{u} \otimes \vec{u}) = -\frac{1}{\rho}\nabla p + \nu\, \nabla^2 u$$

- Fourier Transform:

$$\hat{u}(k,t) = \int \vec{u}(x,t) e^{-ik.x} dx$$

- Important Property:

$$\mathcal{F}\{f'\}(k) = ik\mathcal{F}\{f\}(k)$$

- Applied to NS Eq.:

$$\frac{\partial \hat{u}}{\partial t} + \widehat{u.\nabla u} = -ik\hat{p} - \nu k^2 \hat{u}$$

Spectral Methods

Introduction

- Navier-Stokes Equation:

$$\nabla . \vec{u} = 0 \qquad\qquad \frac{\partial \vec{u}}{\partial t} + \nabla . (\vec{u} \otimes \vec{u}) = -\frac{1}{\rho} \nabla p + \nu \, \nabla^2 u$$

$$\nabla . \left(\frac{\partial \vec{u}}{\partial t} + \nabla . (\vec{u} \otimes \vec{u}) \right) = \nabla . \left(-\frac{1}{\rho} \nabla p + \nu \, \nabla^2 u \right)$$

$$\nabla . (\vec{u} . \nabla \vec{u}) = \nabla . \left(-\frac{1}{\rho} \nabla p \right)$$

$$\nabla^2 p = \rho \, \nabla . (-\vec{u} . \nabla \vec{u})$$

$$\hat{p} = \frac{i}{k^2} k . \widehat{\vec{u} . \nabla \vec{u}}$$

Spectral Methods

Introduction

- Navier-Stokes Equation:

$$\nabla . \vec{u} = 0$$

$$\frac{\partial \vec{u}}{\partial t} + \nabla . (\vec{u} \otimes \vec{u}) = -\frac{1}{\rho} \nabla p + \nu \, \nabla^2 u$$

- NS in Fourier Space:

$$\frac{\partial \hat{u}}{\partial t} + \widehat{\vec{u} . \nabla \vec{u}} = -ik\hat{p} - \nu k^2 \hat{u}$$

$$\hat{p} = \frac{i}{k^2} k . \widehat{\vec{u} . \nabla \vec{u}}$$

Numerical Implementation

Solution Steps:

1. Initialize velocity field $\vec{u}(x, t = 0)$ in physical space, and transfer it to Fourier space $\hat{u}(k, t = 0)$ using FFT.
2. Compute $\vec{u} . \nabla \vec{u}$ (PS) and transfer it to FS using FFT.
3. Compute $\hat{p}(k, t)$.
4. Solve for velocity $\hat{u}(k, t)$.
5. Transfer $\hat{u}$ to $\vec{u}(x, t)$ (PS) using iFFT.
6. Time advance using RK4.

Spectral Methods

Introduction

- Advantages:
  1. High Accuracy: exponential convergence $E = O(e^{-\alpha N})$,
  2. Efficient in FS: derivatives in FS are simpler,
  3. No numerical dissipation: unlike FD,FV and FE, SM does not introduce artificial dissipation, important in turbulent studies.
- Disadvantages:
  1. Problem in Irregular domains: periodic boundary condition,
  2. Computationally expensive for non-uniform grids,
  3. Cannot handle complex geometries easily.

Direct Numerical Simulation (DNS)

Introduction

- What is DNS?
  - Solving Navier-Stokes equation without any turbulence modeling (LES, RANS).
  - All turbulence scales must be resolved (Large energy-containing to smallest dissipative eddies).

- Needs extremely fine spatial and temporal grids:
  - Very expensive to compute,
  - Time consuming,
- Spatial grid must capture smallest turbulent scale (Kolmogorov size):

$$\eta = \left(\frac{v^3}{\varepsilon}\right)^{\frac{1}{4}}$$

Direct Numerical Simulation (DNS)

Introduction

- Spatial grid must capture smallest turbulent scale (Kolmogorov size):

$$\eta = \left(\frac{v^3}{\varepsilon}\right)^{\frac{1}{4}}$$

- Non-Newtonian fluids: What is the Kolmogorov scales?

$\tau = K\dot{\gamma}^n$ (Power-law type fluid)

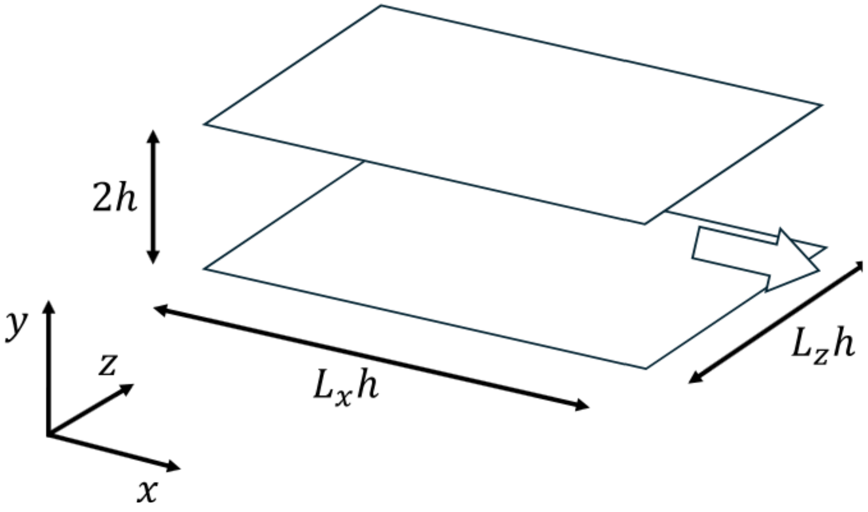
$$\eta \sim \left(\frac{K^3}{\rho^3 \varepsilon^{2-n}}\right)^{\frac{1}{2(n+1)}} \quad ; \quad u_\eta \sim \left(\frac{K\varepsilon^n}{\rho}\right)^{\frac{1}{2(n+1)}} .$$

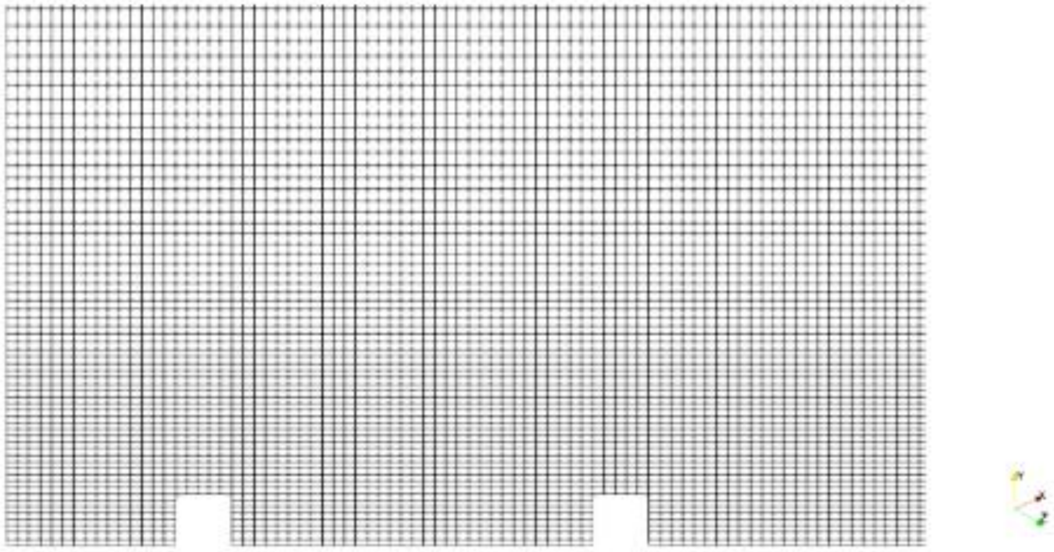
$$\frac{\eta}{L} \sim Re_{n,L}^{-\frac{3}{2(n+1)}} \quad ; \quad \frac{u_\eta}{V_L} \sim Re_{n,L}^{-\frac{1}{2(n+1)}} ,$$

Direct Numerical Simulation (DNS)

Geometry

- Turbulent flow:
  - 2D/3D Isotropic turbulence,
  - 3D Canonical flow (pipe, channel,..)
    - Spectral discretization in period directions,
    - High order finite difference discretization in other directions.

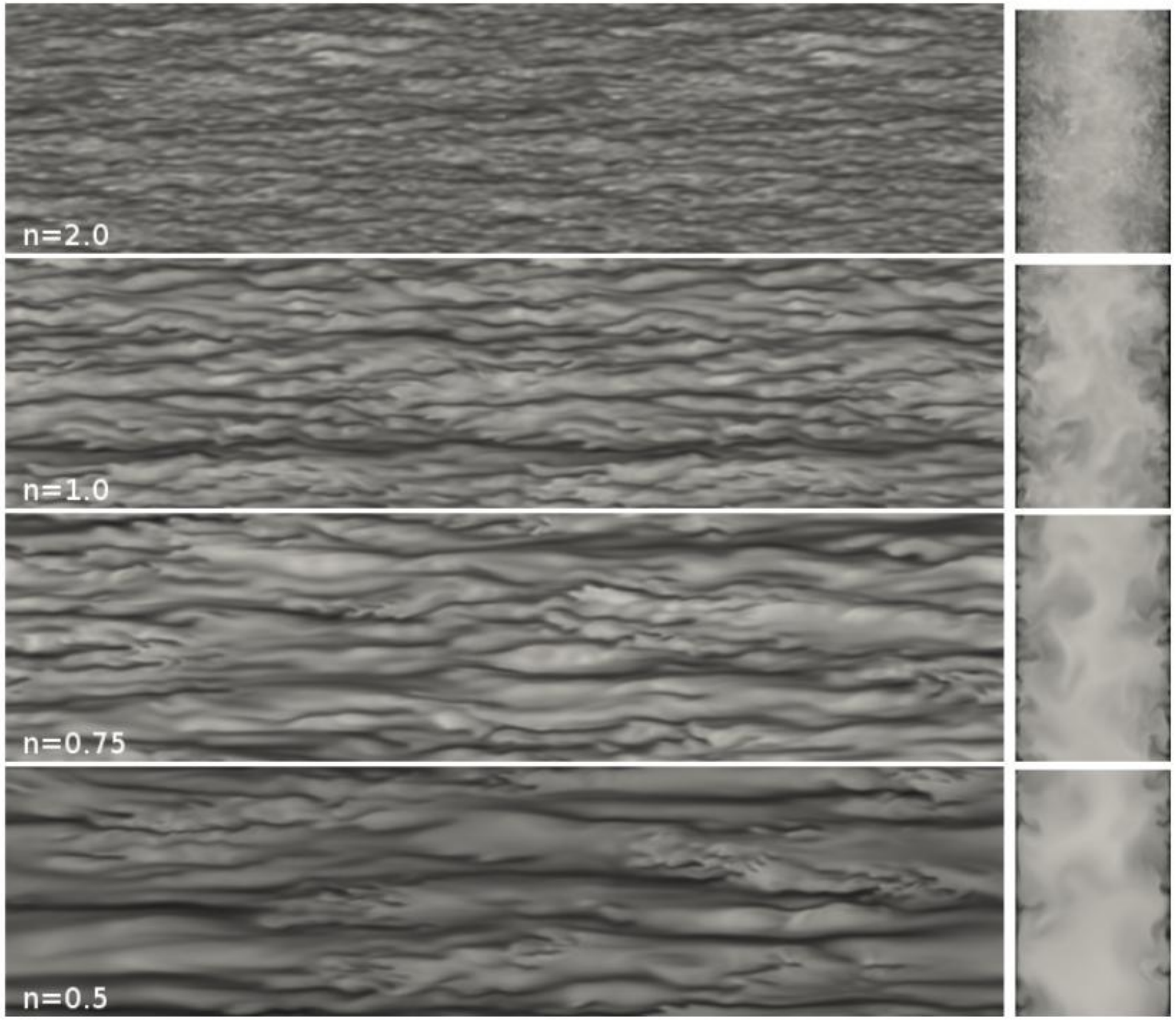




Direct Numerical Simulation (DNS)

Results

- Result of DNS:
  - Instantaneous velocity,
  - In all cells,
  - For many time steps.



Direct Numerical Simulation (DNS)

Simulations

Turbulent flow of non-Newtonian fluids

Power-law fluid
- shear thinning (n=0.75 and 0.5)
- shear thickening (n=2.0)

Channel Flow

$$Re_\tau = 395$$

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June 6, 2024

https://lcadame.github.io/

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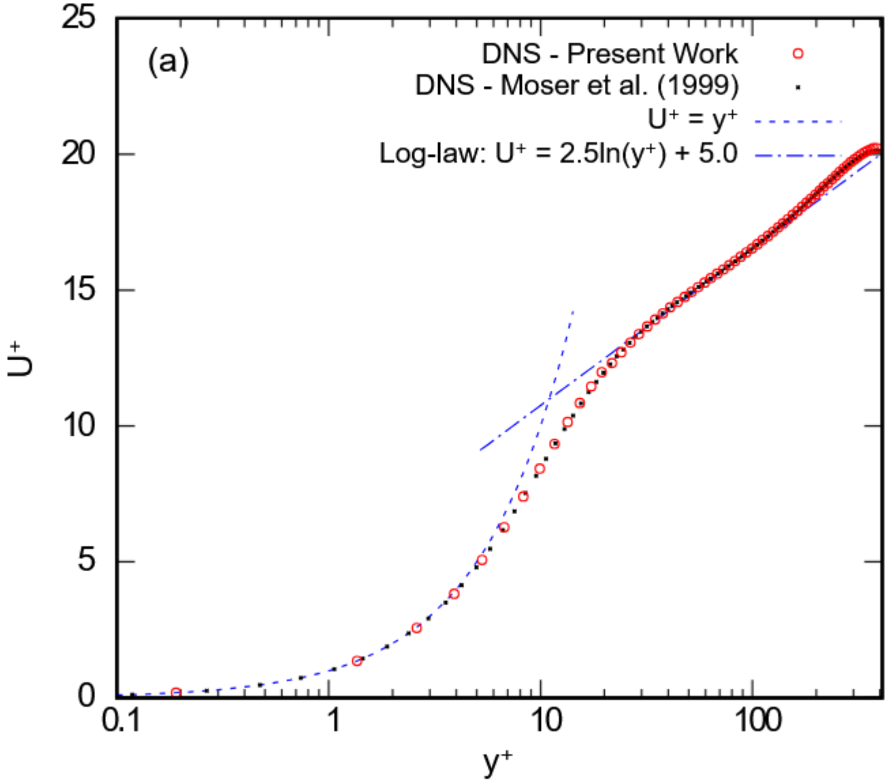
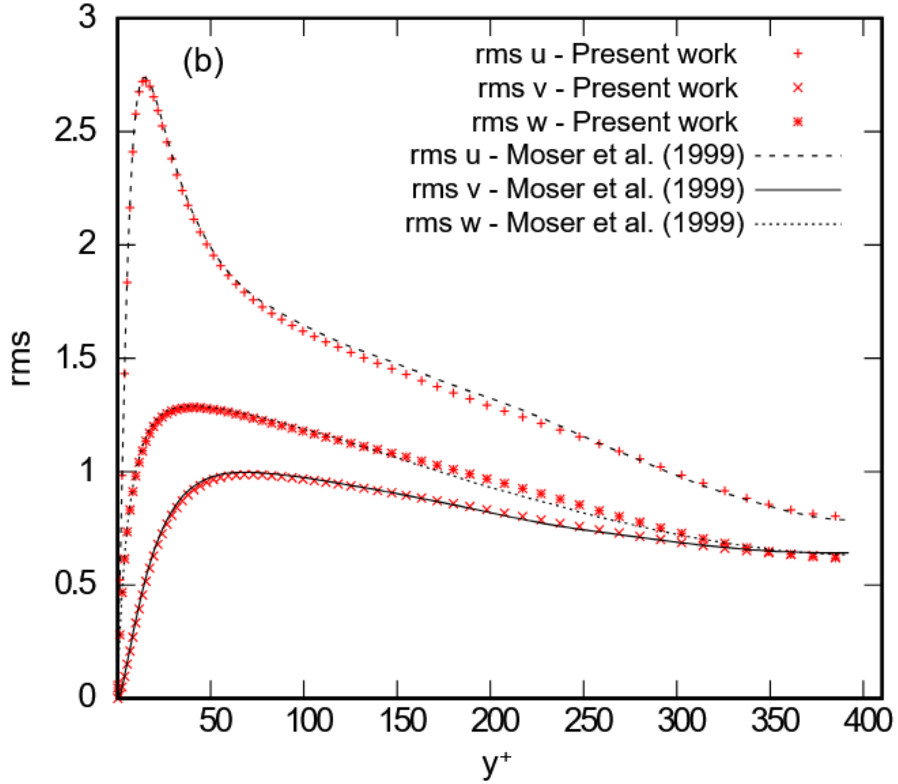
Direct Numerical Simulation (DNS)

Results

$$u = \bar{u} + \acute{u}$$
$$\langle u \rangle = \bar{u}$$

Averaging Operator

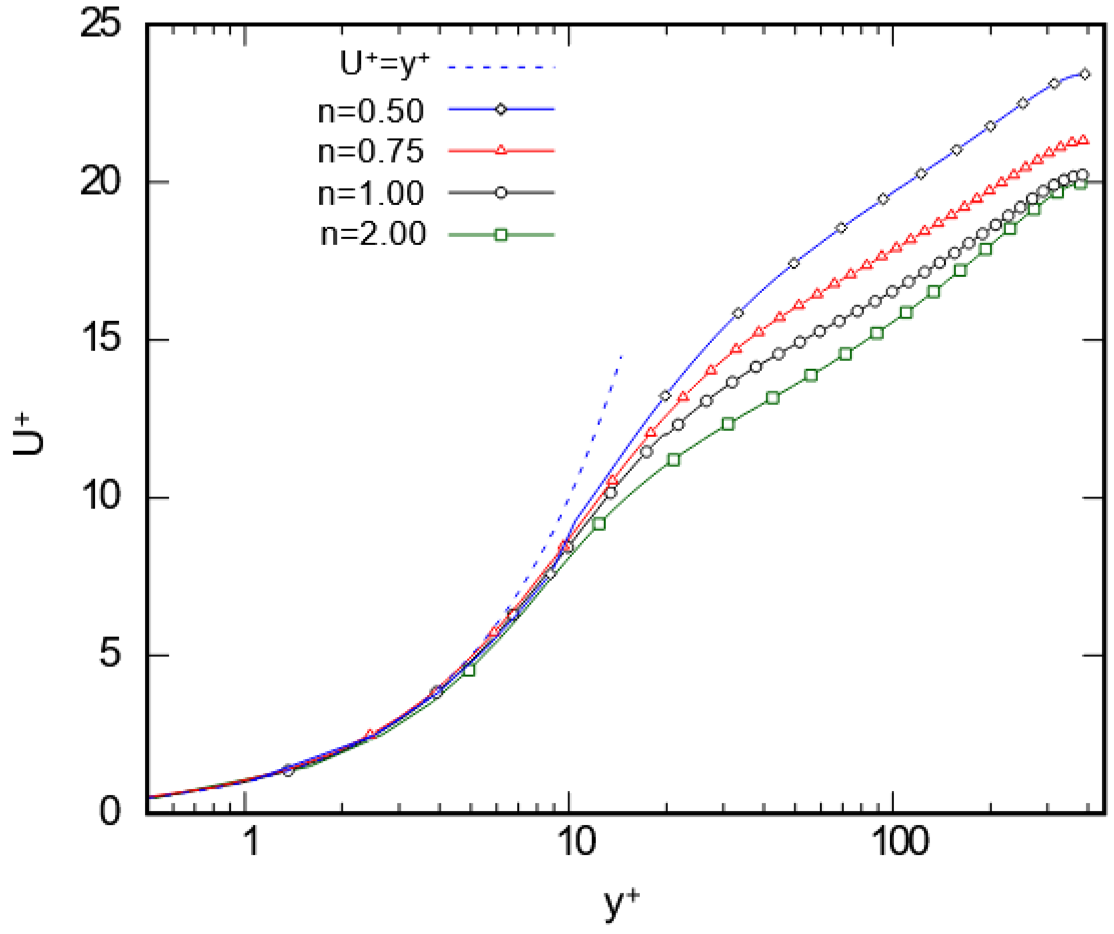


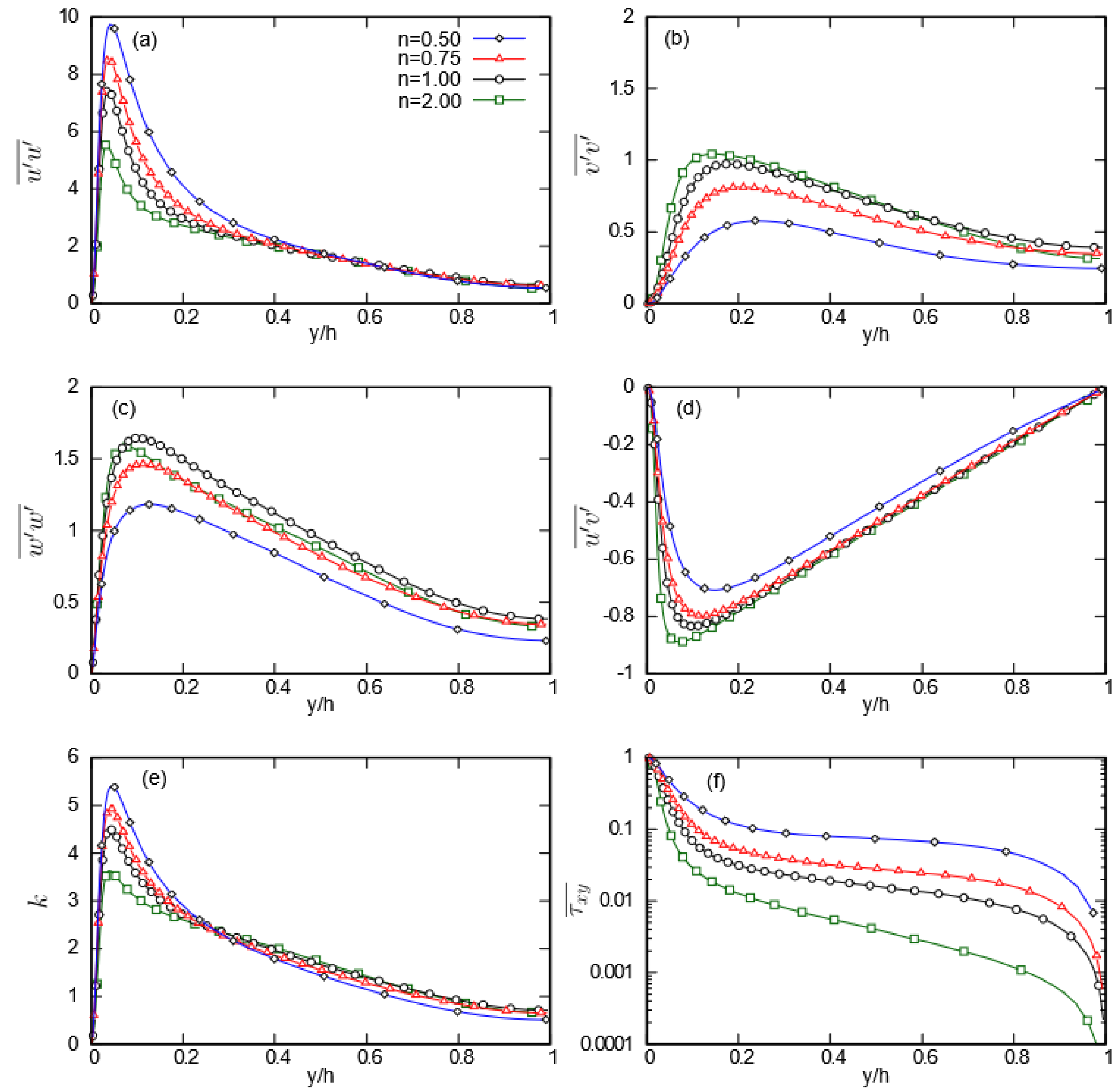


$$u = \bar{u} + \acute{u}$$
$$\langle u \rangle = \bar{u}$$
$$\langle uu \rangle = \langle (\bar{u} + \acute{u}) \times (\bar{u} + \acute{u}) \rangle = \langle \bar{u}^2 + 2\bar{u}\acute{u} + \acute{u}^2 \rangle$$
$$\langle uu \rangle = \langle \bar{u}^2 \rangle + \langle 2\bar{u}\acute{u} \rangle + \langle \acute{u}^2 \rangle = \langle \bar{u}^2 \rangle + \langle \acute{u}^2 \rangle$$

Direct Numerical Simulation (DNS)

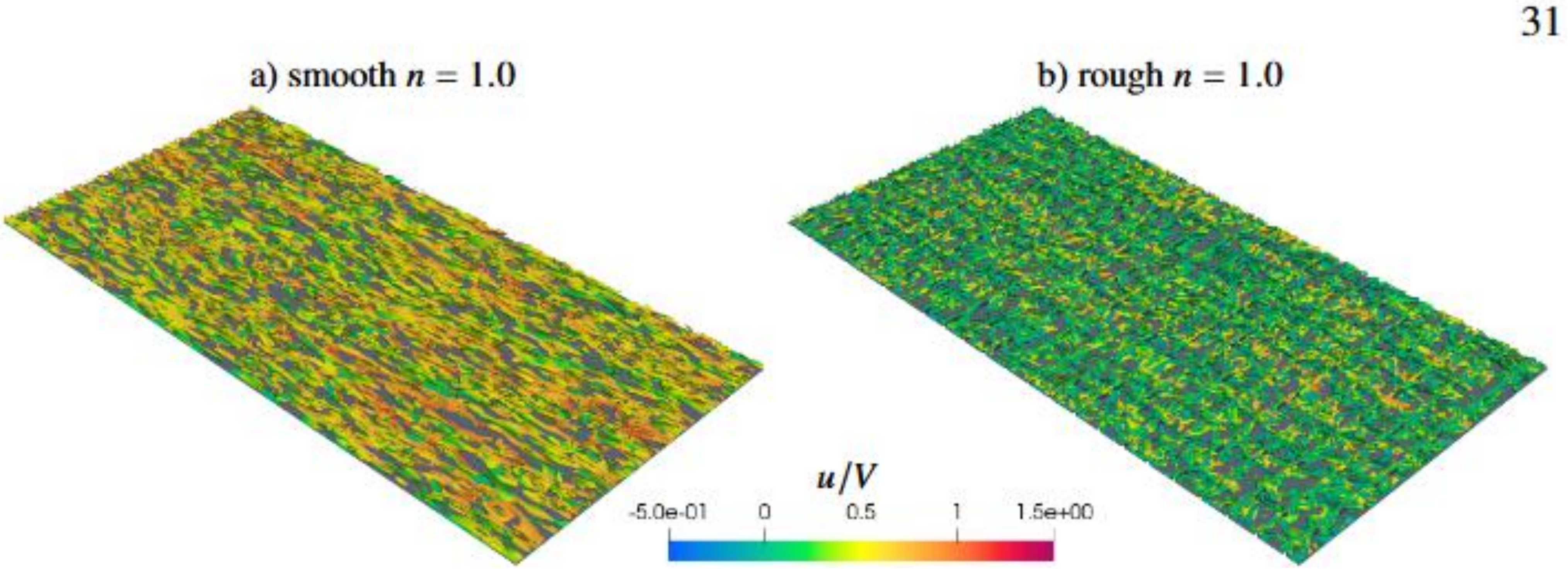
Non-Newtonian fluids

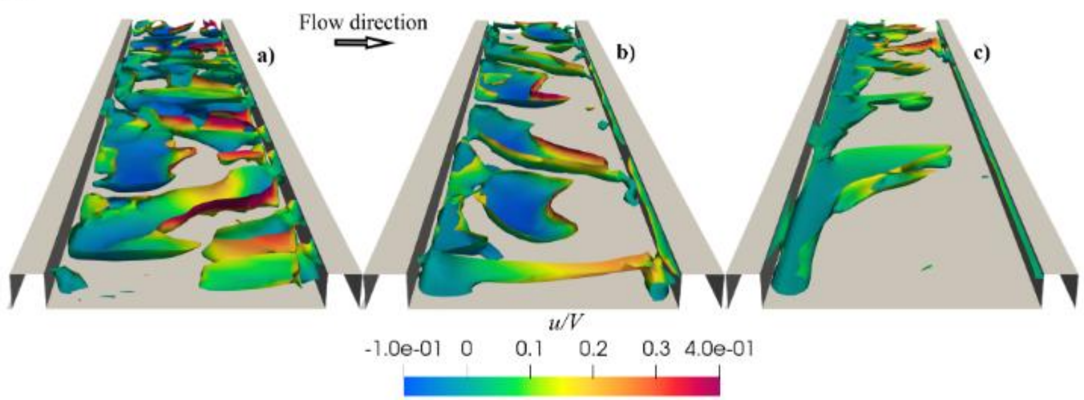




Direct Numerical Simulation (DNS)

Non-Newtonian fluids – rough channel





Integrating Machine Learning with Fluid Simulation

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Kalman Filter

Introduction

- For many practical applications, we don't have proper IC.
  - Atmosphere or ocean current modeling
- But we have some partial observations in time.
  - Satellite weather measurements,
  - Temperature, humidity and … in local stations.
- Usually we start from some IC which make sense,
- The goal is to improve the IC, as soon as a new observations arrive (data assimilation).
  - Observations are not error free,
  - Different observations have different fidelities.

Kalman Filter

Linear model

- Prediction step (numerical simulation with bad IC):

$$\hat{x}_{k|k-1} = A\,\hat{x}_{k-1|k-1} + B\,u_k$$

$$P_{k|k-1} = A\,P_{k-1|k-1}A^T + Q$$

- Update step(correction using new observations):

$$K_k = P_{k|k-1}H^T\left(HP_{k|k-1}H^T + R\right)^{-1}$$

$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_k\left(z_k - H\hat{x}_{k|k-1}\right)$$

$\hat{x}_{k|k-1}$: numerical simulation

z_k: observation

P: covariance matrix

R:observation noise

Ensemble Kalman Filter

Non-linear model

- Prediction step (numerical simulation with bad IC):

$$\hat{x}^i_{k|k-1} = f\left(\hat{x}^i_{k-1|k-1}\right) + W^i_k$$

$$P_{k|k-1} = \mathbb{E}[(X - \bar{X})(X - \bar{X})^T]$$

- Update step(correction using new observations):

$$K_k = P_{k|k-1}\left(P_{k|k-1} + R\right)^{-1}$$

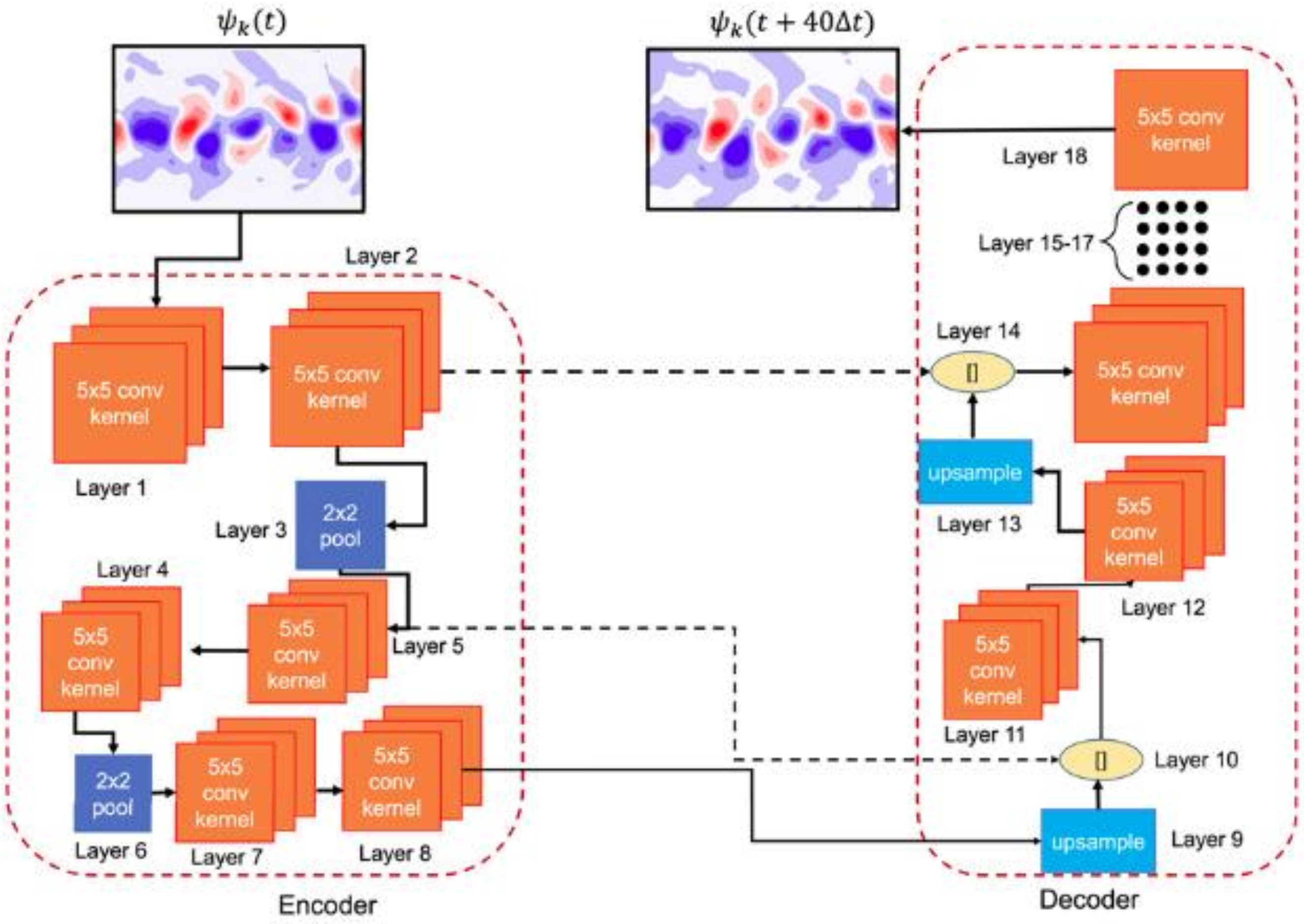
$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_k\left(z_k - \hat{x}_{k|k-1}\right)$$

- Calculating a good $P_{k|k-1}$ needs a large ensemble of numerical simulations, which is very expensive.

Ensemble Kalman Filter

Machine learning to replace numerical integration

- Numerical methods:
  - Expensive,
  - Time marching,
  - High accuracy.
- Machine learning:
  - Long time integration,
  - Cheap,
  - Lower accuracy.



The U-NET model (surrogate) for approximating **X**.

Ensemble Kalman Filter

Numerical + Machine Learning

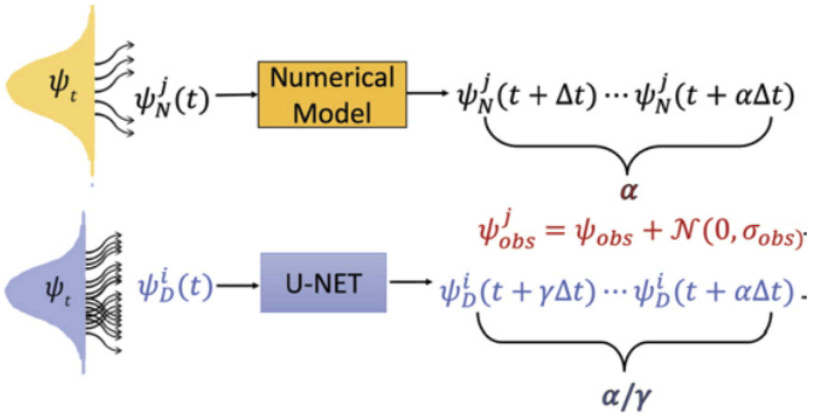
Filter

$$\hat{x}^i_{k|k-1} = f\left(\hat{x}^i_{k-1|k-1}\right) + W^i_k$$

$$P_{k|k-1} = \mathbb{E}[(X-\bar{X})(X-\bar{X})^T]$$

$$K_k = P_{k|k-1}\left(P_{k|k-1}+R\right)^{-1}$$

$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_k\left(z_k - \hat{x}_{k|k-1}\right)$$



Ensemble Kalman Filter U-NET model (surrogate) for approximating **X**.

$$P_D = \mathbb{E}\left[\left(\psi^i_D(t+\alpha\Delta t) - \bar{\psi}(t+\alpha)\right)\left(\psi^i_D(t+\alpha\Delta t) - \bar{\psi}(t+\alpha\Delta t)^T\right)\right]$$

$$K_D = P_D(P_D + \sigma_{\text{obs}} I)^{-1}$$

$$\psi^j_a = \psi^j_N(t+\alpha\Delta t) - K_D\left(\psi_{\text{obs}} - \psi^j_N(t+\alpha\Delta t)\right)$$

Ensemble Kalman Filter

Results

Data Assimilation and Machine Learning

Ensemble Kalman Filter

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June 18, 2024

Laboratório de Computação de Alto Desempenho e Aprendizado de Máquina em Engenharia (L'CADAME)

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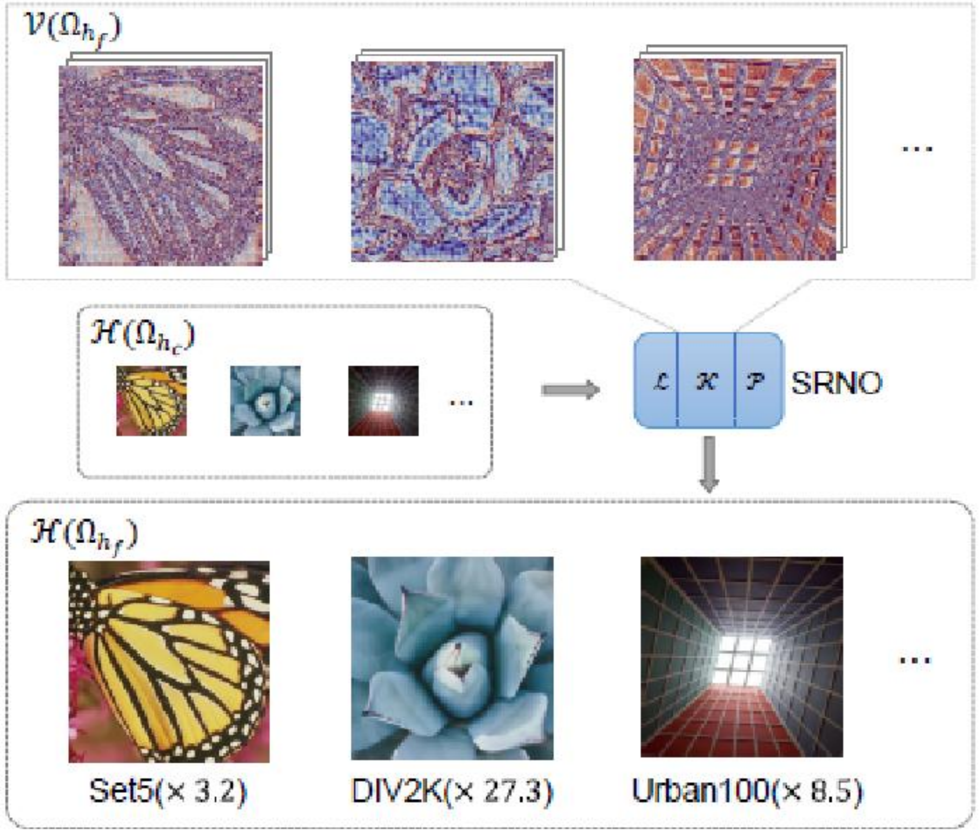
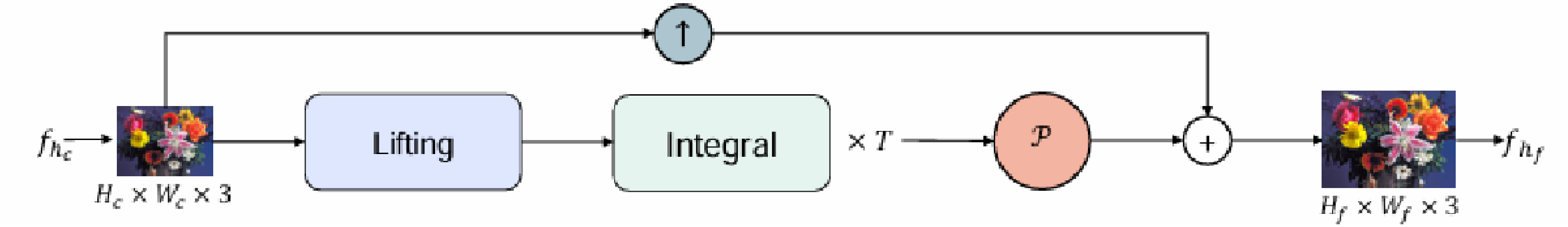
Super-Resolution

Introduction

- Super-resolution: low resolution image to high quality image using machine learning.
- Idea: perform fast low resolution simulations and using ML to improve the quality of the results.
- Goal: recover the missing features in low res simulations.

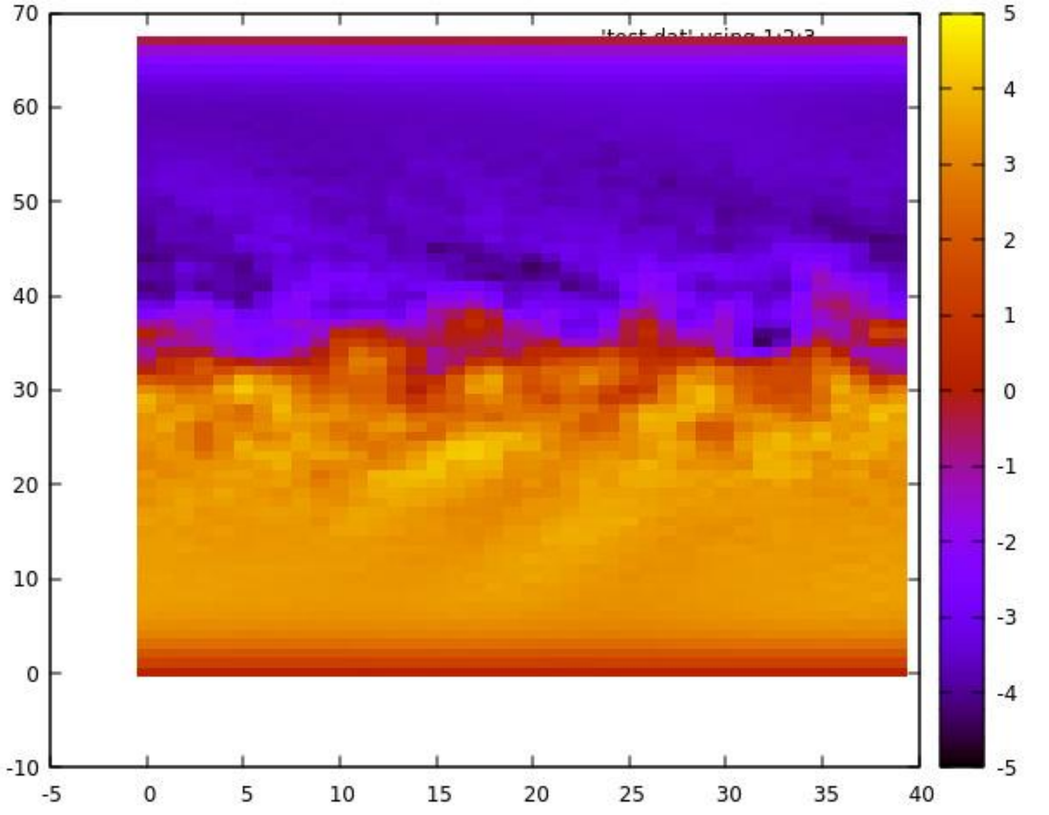




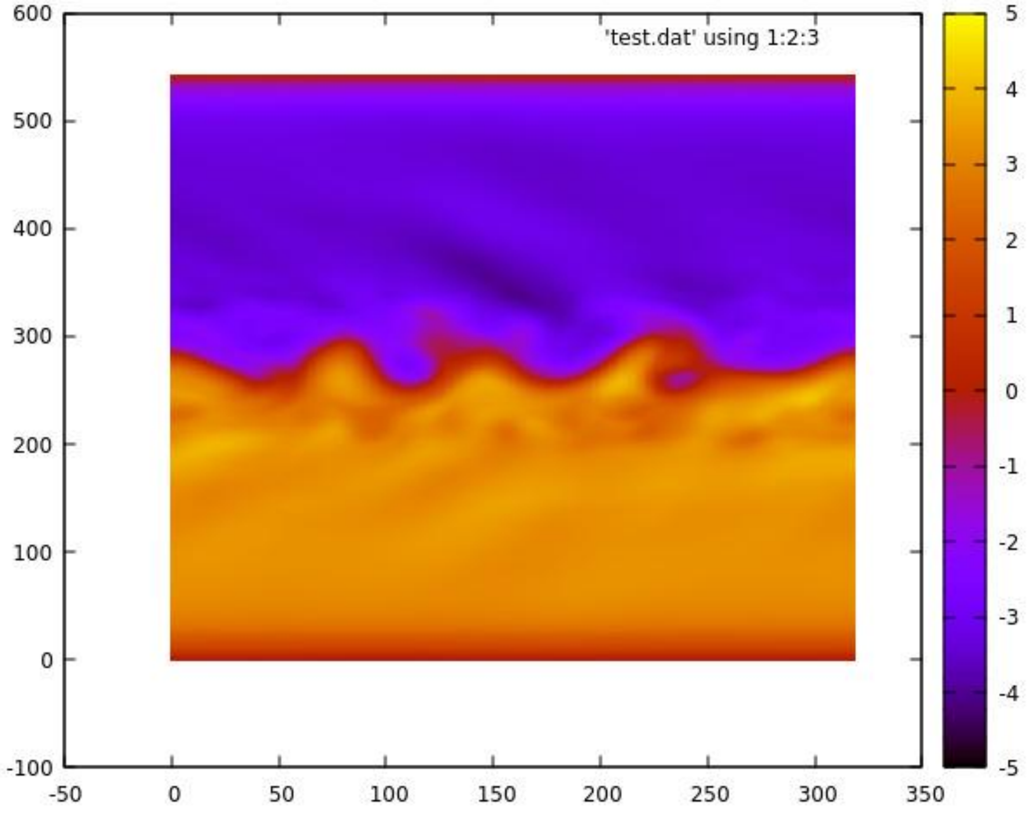
SRNO architecture.

Super-Resolution

Results



Low Res. Numerical Simulations

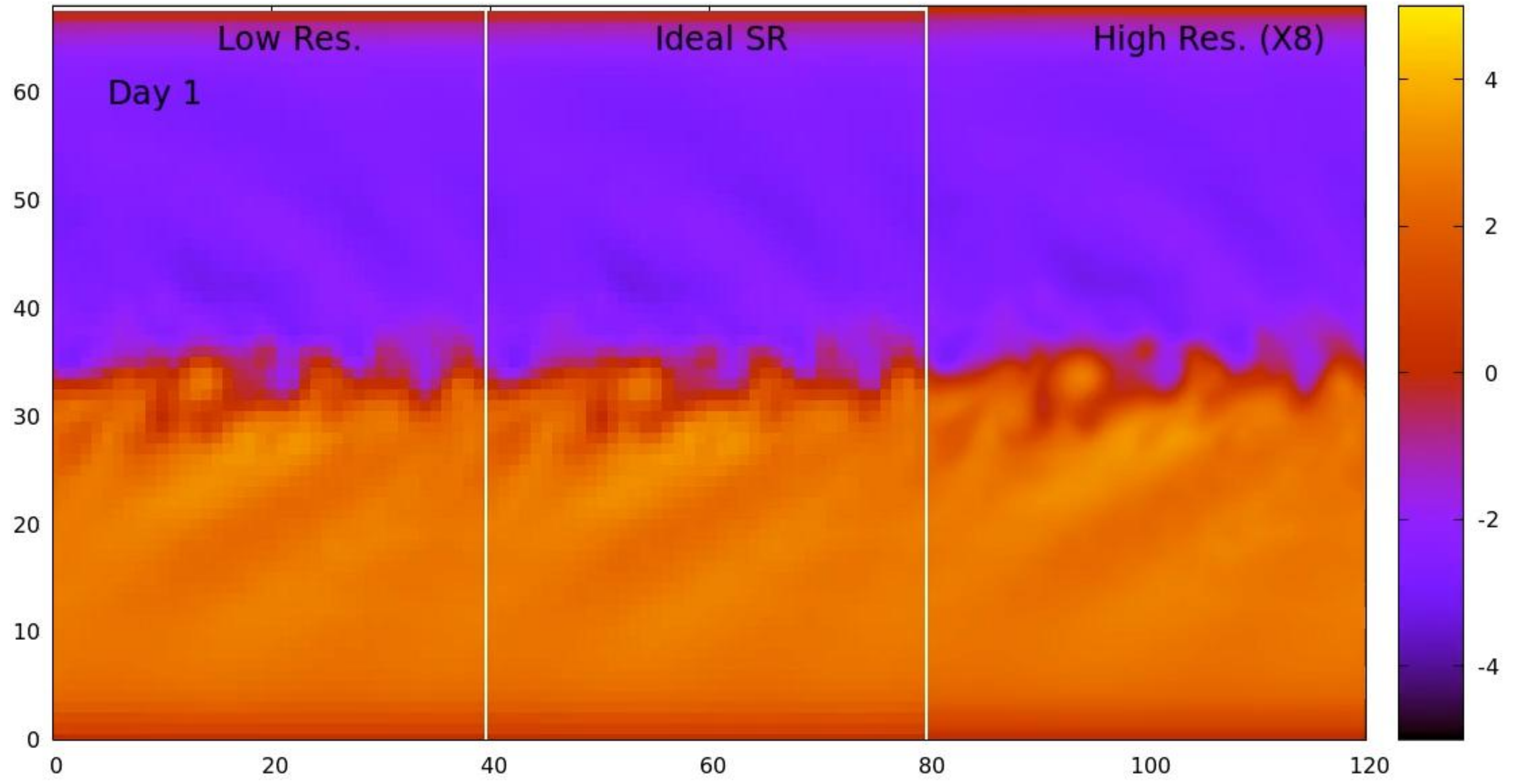


High Res. Super-Resolution

Super-Resolution

Results

- Low res simulations lose accuracy in time,
- Some fine features does not appear in low res simulations.



Pipeline

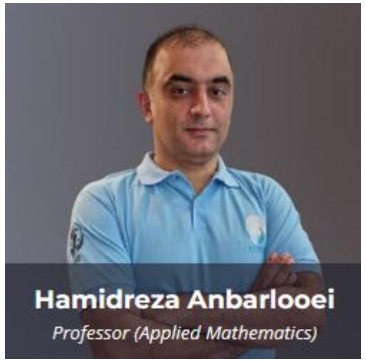
1- Low res. Simulation for a period of time,

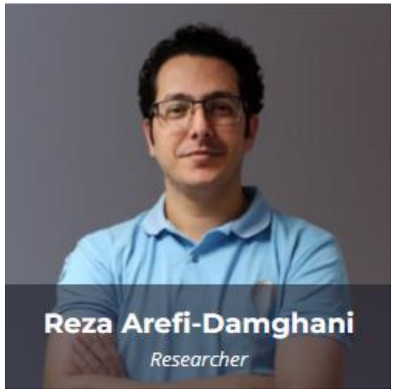
2- One high res. reconstruction,

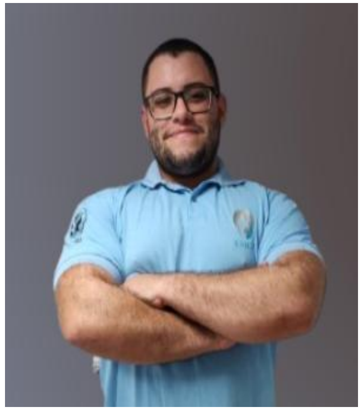
3- Down grading the high res. Data to produce IC for low res. simulation

L’CADAME

Team







L’CADAME

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Thank You!

For your time and attention.

Feel free to reach out for any questions or further discussion.

Contact Information: hamidreza@im.ufrj.br

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