$$\textbf{Fluid} = \sum \textbf{particles}$$

A Conservative Numerical Scheme for Hydrostatic Flow in Isentropic Coordinates

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Goal:

construct Hamiltonian model for hydrostatic atmosphere.

Why?

- Investigate how it behaves when weak forcing and friction added.

⇒ Does it produce better climate ensemble forecasts as compared to conventional schemes?

Tasks:

1. Find Hamiltonian description of fluid system,
2. find Hamiltonian discretization.

Pointe:

No general method for Eulerian Hamiltonian discretization.

$\Rightarrow$ will use discretization based on the Hamiltonian
parcel formulation applied to our fluid.
(Bokhove & Oliver, 2006)

Continuum dynamics

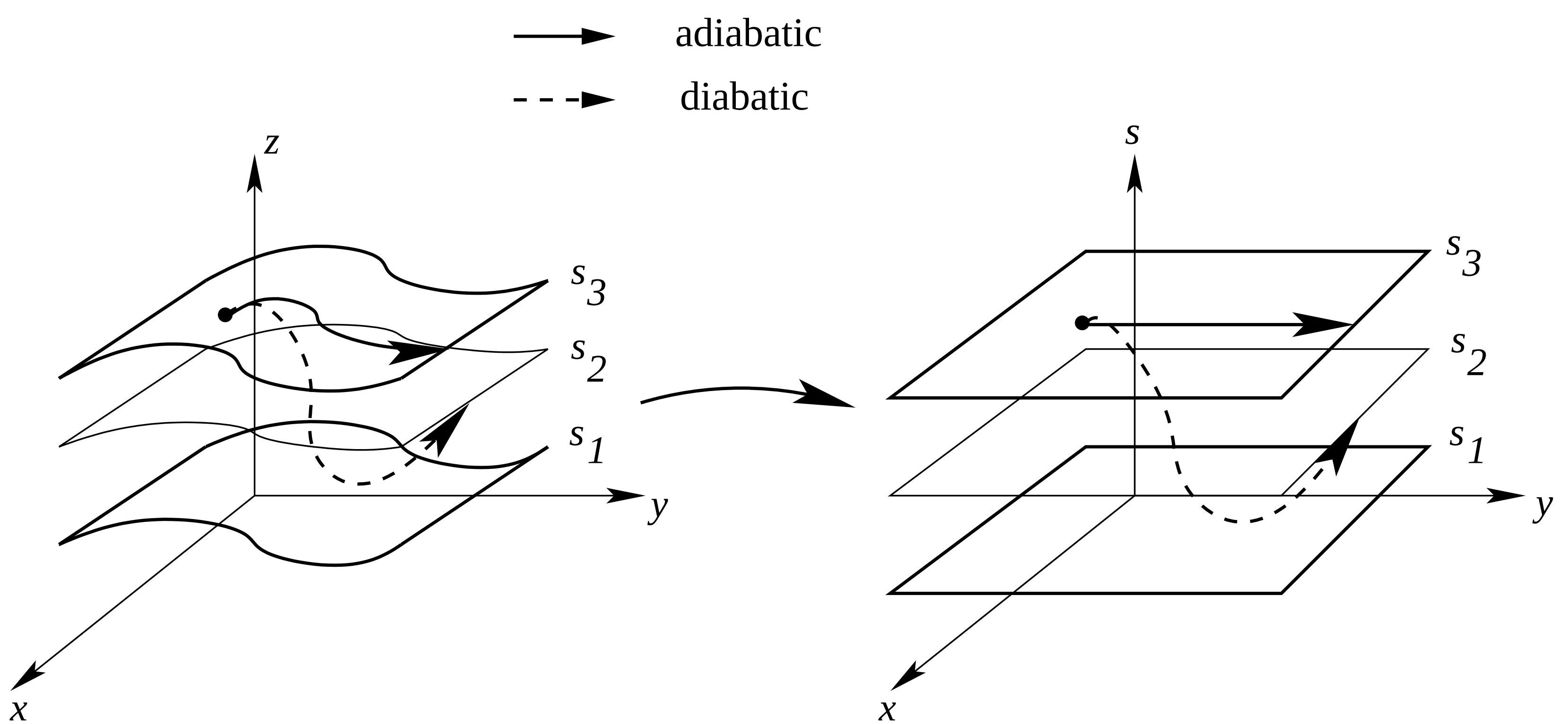
The Eulerian equations

- rotating plane
- hydrostatic balance
- fully compressible
- ideal gas
- statically stable atmosphere → isentropic coordinates (x, y, s)

Why isentropic coordinates?

- flow becomes horizontal → simplifies description
  (except at boundaries...)

Isentropic coordinates



$$\boldsymbol{v} = (u, v, 0)\,,\ \boldsymbol{\nabla} \equiv (\tfrac{\partial}{\partial x}, \tfrac{\partial}{\partial y}, 0).$$

The equations

- momentum eq.

$$\frac{\partial \boldsymbol{v}}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} \boldsymbol{v} + f \boldsymbol{v}^{\perp} + \boldsymbol{\nabla} M = 0 \tag{1}$$

- continuity eq.

$$\frac{\partial \sigma}{\partial t} + \boldsymbol{\nabla} \cdot (\sigma \boldsymbol{v}) = 0 \tag{2}$$

- hydrostatic eq. for ideal gas

$$\sigma = -\frac{p_{00}}{g} \frac{\partial}{\partial s} \left(\left(\frac{\sigma}{\rho_{00} \frac{\partial Z}{\partial s}} \right)^{\frac{c_p}{c_v}} e^{\frac{s - s_{00}}{c_v}} \right) \tag{3}$$

- σ is pseudodensity,
- $M = g\,Z + c_p\,T(\sigma, \frac{\partial Z}{\partial s})$ is the Montgomery potential.

  $\rightarrow$ Closed formulation for $\{\boldsymbol{v}, \sigma, Z\}$.
- $\boldsymbol{v} = \boldsymbol{v}(\boldsymbol{x}, s, t)$
  $\sigma = \sigma(\boldsymbol{x}, s, t)$
  $Z = Z(\boldsymbol{x}, s, t)$

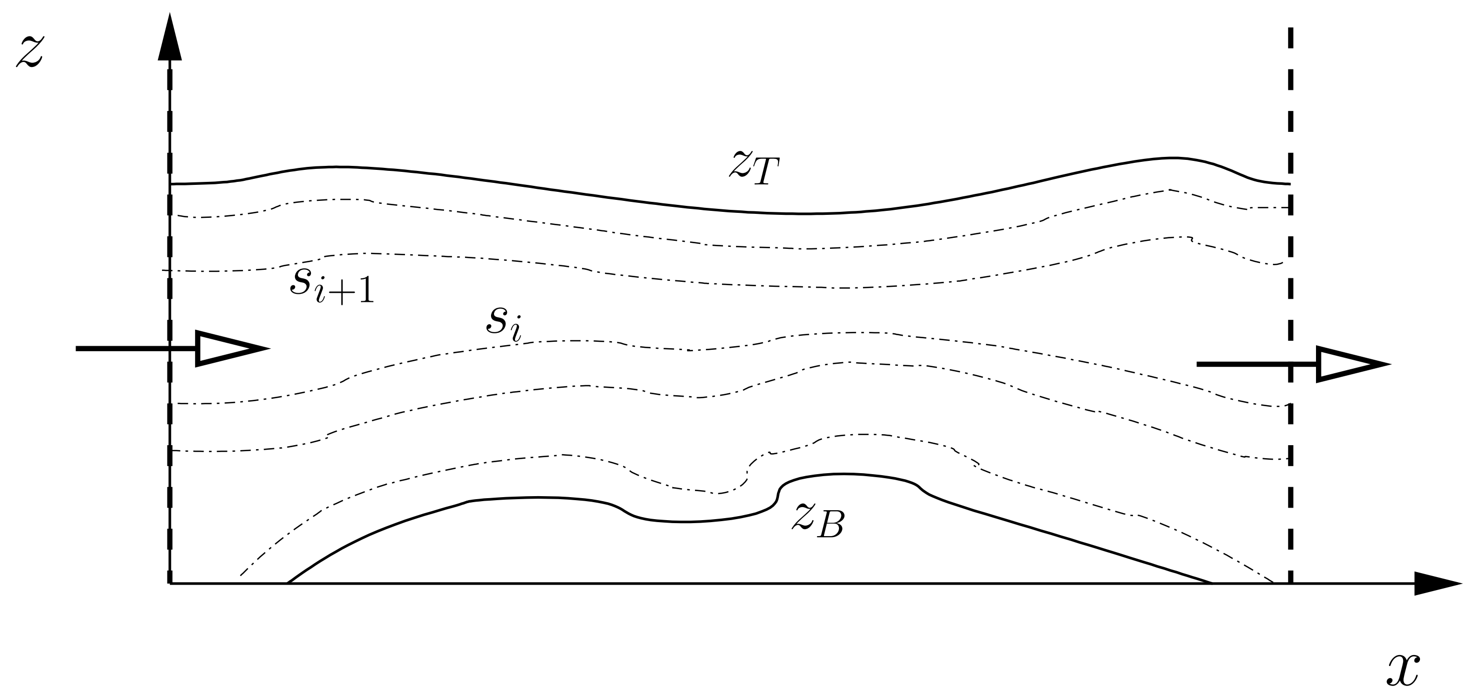
Picture:

Flow can be thought of as being horizontal, where all layers are coupled though eq. (3), which is nonlinear elliptic equation in s only.

Boundaries:

- periodicity in (x, y)
- Z given at bottom (B) and top (T)
- $Z_{B,T}(x, y)$ is isentropic, somewhat restricted...

Flow set-up



The **parcel formulation**

(Bokhove & Oliver, 2006)

- mixed Eulerian-Lagrangian
- fluid is continuum of parcels labelled by $(\boldsymbol{a}, s)$ having horizontal positions $\boldsymbol{X}(t; \boldsymbol{a}, s)$.
  (initially, labels and positions coincide)
- parcels are moving in a Eulerian prescribed potential

Remarks on parcel formulation:

- discretization of this continuum formulation will 'directly' lead to a discrete Hamiltonian scheme: HPM.
- alternative is fully Lagrangian description, which can be discretized into SPH.
- both HPM and SPH require some sort of **smoothing** to maintain accuracy over long-time integrations.
  $\Rightarrow$ Eulerian grid in HPM allows for efficient numerical implementation.

Parcel formulation for the hydrostatic atmosphere

System variables:

- parcel variables: $\boldsymbol{X}(t;\boldsymbol{a},s)$, $\boldsymbol{U}(t;\boldsymbol{a},s)$
- Eulerian variables: $\sigma(\boldsymbol{x},s,t)$, $Z(\boldsymbol{x},s,t)$

Motion of distinguished parcel $(\boldsymbol{A}, S)$ given by

$$\frac{\mathrm{d}\boldsymbol{X}}{\mathrm{d}t} = \boldsymbol{V} = \boldsymbol{\nabla}_{\boldsymbol{V}} H, \tag{4a}$$

$$\frac{\mathrm{d}\boldsymbol{V}}{\mathrm{d}t} = -f\,\boldsymbol{V}^{\perp} - \boldsymbol{\nabla}_{\boldsymbol{X}} M = -f\,\boldsymbol{\nabla}_{\boldsymbol{V}}^{\perp} H - \boldsymbol{\nabla}_{\boldsymbol{X}} H, \tag{4b}$$

with $(\boldsymbol{\nabla}_{\boldsymbol{X}}, \boldsymbol{\nabla}_{\boldsymbol{V}}) \equiv (\frac{\partial}{\partial \boldsymbol{X}}, \frac{\partial}{\partial \boldsymbol{V}})$.

H is the parcel Hamiltonian,

$$H(\boldsymbol{X}, \boldsymbol{V}, t) = \frac{1}{2}\boldsymbol{V}^2 + M(\boldsymbol{X}, t). \tag{5}$$

- $M(\boldsymbol{X}, t) \equiv M(\boldsymbol{x}, s, t)\big|_{(\boldsymbol{x},s)=(\boldsymbol{X},S)}$

- Remember: Eulerian M found from Eulerian Z and σ.
  $\rightarrow$ Z found from elliptic equation (3), but how to recover σ from parcel data?

- Mass conservation law can be rewritten as

$$\sigma(\mathbf{x}, s, t) = \iint \sigma_0(\boldsymbol{a}, s)\, \delta(\boldsymbol{x} - \boldsymbol{X}(t; \boldsymbol{a}, s))\, d\boldsymbol{a}. \tag{6}$$

  $\rightarrow$ this equation couples all parcels.

Discrete dynamics

Hamiltonian discretization:

The Hamiltonian Particle-Mesh Method (HPM)

(Frank et al., 2002)

- actually introduced before the concept of ’parcel formulation’
  $\rightarrow$ parcel formulation is the continuum analog of HPM

Steps (per isentrope):

i) Fluid decomposed in N particles having fixed finite masses m_k.

ii) Discretize (4) as

$$\frac{\Delta \boldsymbol{X}_k}{\Delta t} = \boldsymbol{V}_k = \boldsymbol{\nabla}_{\boldsymbol{V}_k} \bar{H}_k, \tag{7a}$$

$$\frac{\Delta \boldsymbol{V}_k}{\Delta t} = -f\, \boldsymbol{V}_k^{\perp} - \boldsymbol{\nabla}_{\boldsymbol{X}_k} \bar{M}_k = -f\, \boldsymbol{\nabla}_{\boldsymbol{V}_k}^{\perp} \bar{H}_k - \boldsymbol{\nabla}_{\boldsymbol{X}_k} \bar{H}_k, \tag{7b}$$

with HPM parcel Hamiltonian

$$\bar{H}_k \equiv \bar{H}(\boldsymbol{X}_k, \boldsymbol{V}_k, S, t) = \frac{1}{2} \boldsymbol{V}_k{}^2 + \bar{M}(\boldsymbol{X}_k, S, t).$$

iii) Redistribution of particles induces new density field.
Density on grid found from discretization of (6):

$$\sigma_{ml}(s,t) = \sum_k m_k(s)\,\psi_\lambda(\boldsymbol{x}_{ml} - \boldsymbol{X}_k(t;s))$$

iv) Solve BVP (3) for each gridpoint, leading to $M_{ml}(s,t)$.

v) Reconstruct global M from grid data by discretizing

$$M(\boldsymbol{X},S,t) = \iint M(\boldsymbol{x},S,t)\,\delta(\boldsymbol{X}-\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

$$\Leftrightarrow$$

$$\bar{M}(\boldsymbol{X},S,t) = \sum_{ml} M_{ml}(S,t)\,\psi_\lambda(\boldsymbol{X}-\boldsymbol{x}_{ml})\,\Delta\boldsymbol{x}_{ml} \qquad (8)$$

...still need to discretize in the s-direction.

Vertical discretization: **Finite elements** (FEM)

Why finite elements?
$\rightarrow$ exact **conservation of energy** in the reduced finite element function space

- Hermite FEM basis functions
  $\rightarrow$ solves $Z^h(s)$ and $\partial Z^h/\partial s$ simultaneously.
  $\rightarrow$ $M^h(s)$ will be smooth.

FEM weak formulation of (6) reads:

$$\int \mathsf{w}^h(\boldsymbol{x}, s, t)\, \sigma^h(\boldsymbol{x}, s, t)\, \mathrm{d}s$$

$$= \int \mathsf{w}^h(\boldsymbol{x}, s, t) \int \iint \sigma_0^h(\boldsymbol{A}, S)\, \delta(\boldsymbol{x} - \boldsymbol{X}^h(t; \boldsymbol{A}, S))\, \delta(s - S)\, \mathrm{d}\boldsymbol{A}\, \mathrm{d}S\, \mathrm{d}s$$

$$\equiv \mathsf{w}^h(\boldsymbol{x}, S_j, t) \iint \sigma_{0j}(\boldsymbol{A})\, \delta(\boldsymbol{x} - \boldsymbol{X}_j(t; \boldsymbol{A}))\, \Delta S_j\, \mathrm{d}\boldsymbol{A}.$$

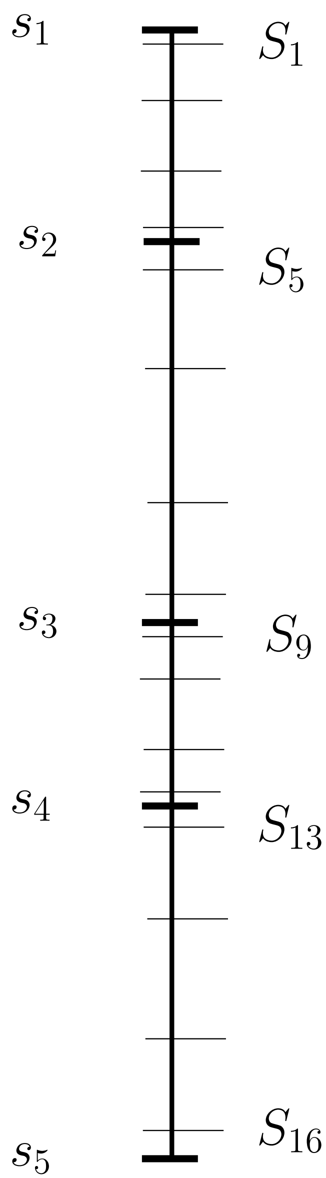
→ we distinguish Eulerian s and Lagrangian S

→ all FEM integrals over Lagrangian S are to be evaluated by (same) quadrature

→ all FEM integrals over Eulerian s have to be solved up to machine precision

Example of FEM discretization:

- 4 Eulerian elements, and
- a four-point Gauss quadrature per element to solve the S-integrals.



Discrete energy expressions

- Discrete kinetic energy - Lagrangian

$$\mathcal{T}(t) = \sum_j \sum_k \frac{1}{2} m_{jk} \, |\boldsymbol{U}_{jk}(t)|^2 \, \Delta S_j .$$

- Discrete potential energy - Eulerian

$$\mathcal{V}(t) = \int_{s_B}^{s_T} \sum_{ml} \left\{ \sigma^h_{ml} \left(c_v \, T(\sigma^h_{ml}, \partial Z^h_{ml}/\partial s) + g \, Z^h_{ml} \right) \right\} \Delta x \, \Delta y \, ds .$$

Properties of HPM-FEM scheme:

- Continuous-time
  - Hamiltonian system of eqs.
  - exact conservation of mass, energy and phase space volume
  - discrete Poisson bracket
- Discrete-time: symplectic time integration
  - exact conservation of mass and phase space volume
  - asymptotic conservation of energy (quadratic)

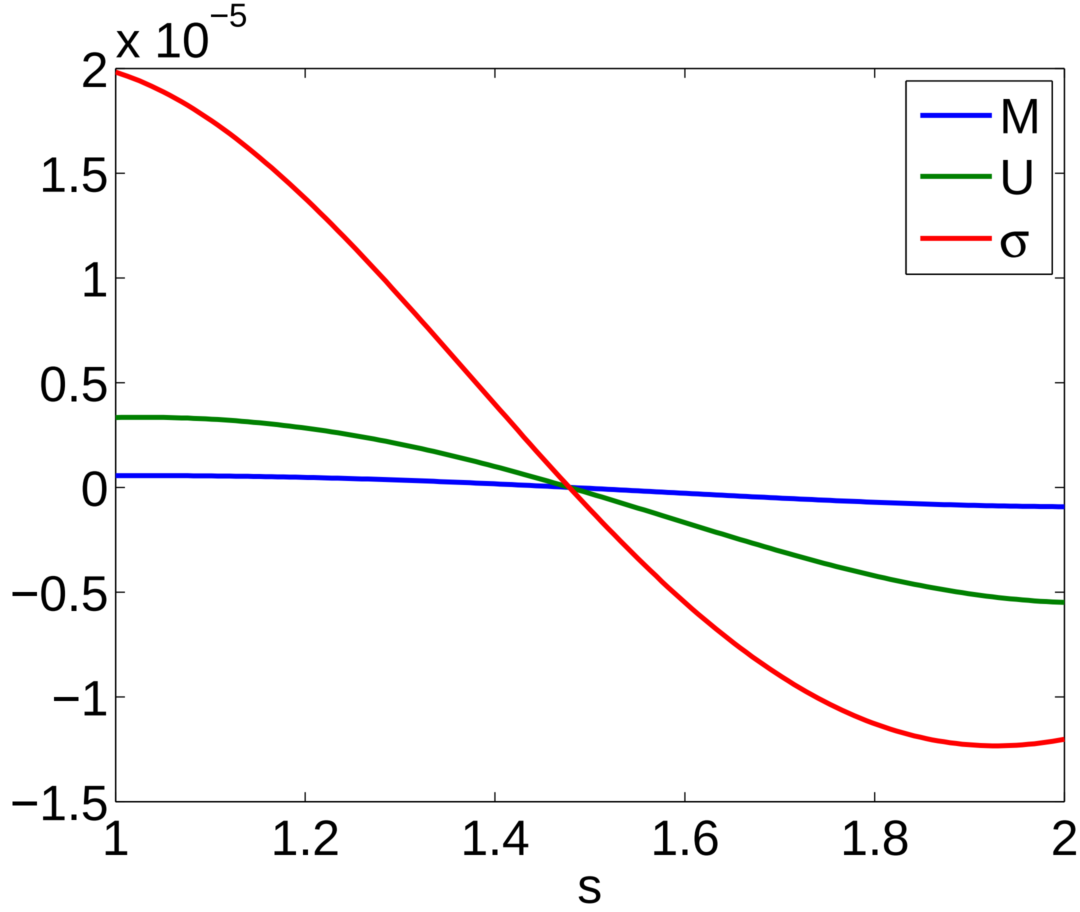
Accuracy of HPM-FEM scheme:

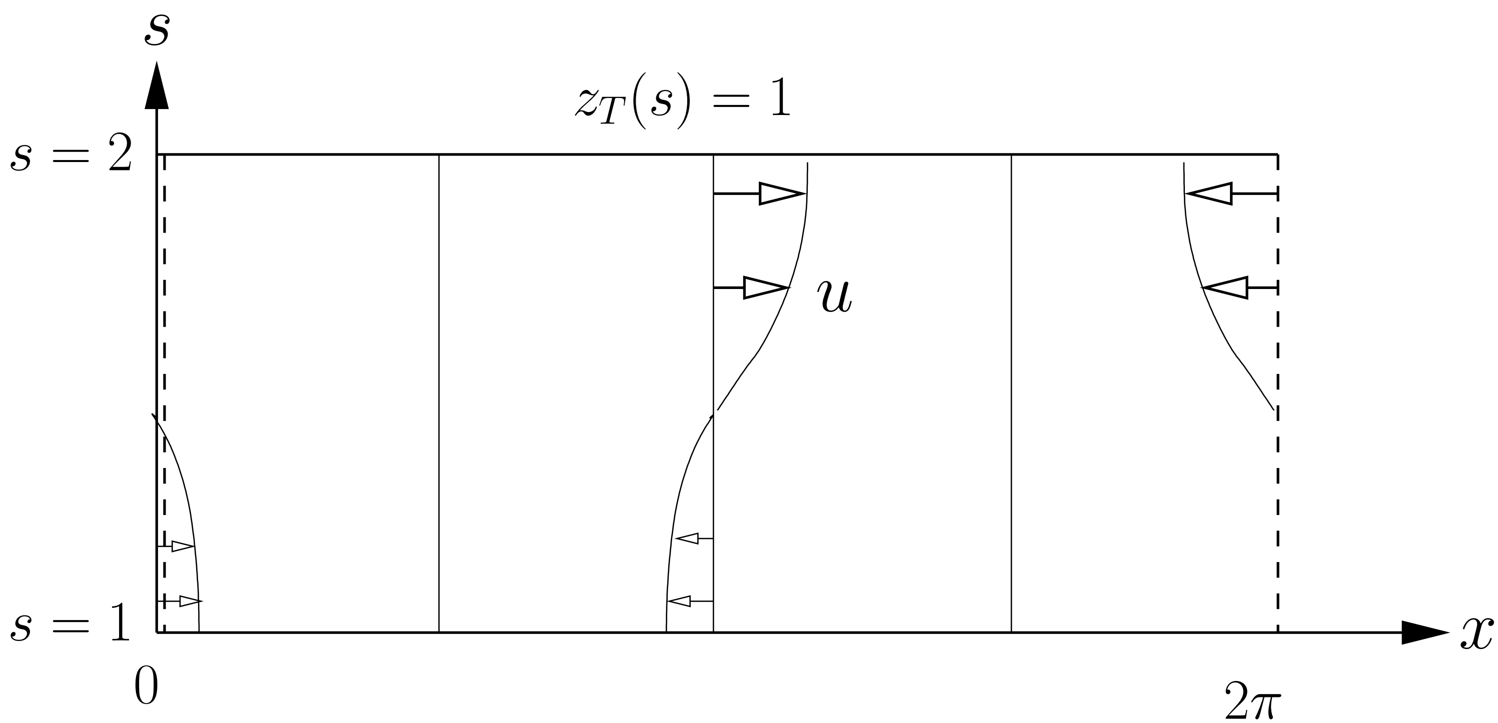
- FEM: up to 4^{th} order,
- HPM: up to 2^{nd} order,
- time integration: 2^{nd} order.

Example 1: normal modes

- nondimensionalized
- static isothermal background
- $f = 0$, 2D-set up (x, s)
- linearize equations ($\epsilon = 10^{-5}$)
- substitute normal modes $u = U(s)\, e^{i(kx - wt)}$ etc.
  $\rightarrow$ Sturm-Liouville system for the amplitudes
- domain $x \in [0, 2\pi[$ and $s \in [1, 2]$
- no topography

Amplitudes of first normal mode:




s
$z_T(s) = 1$
$s = 2$
u
$s = 1$
0
x
2π

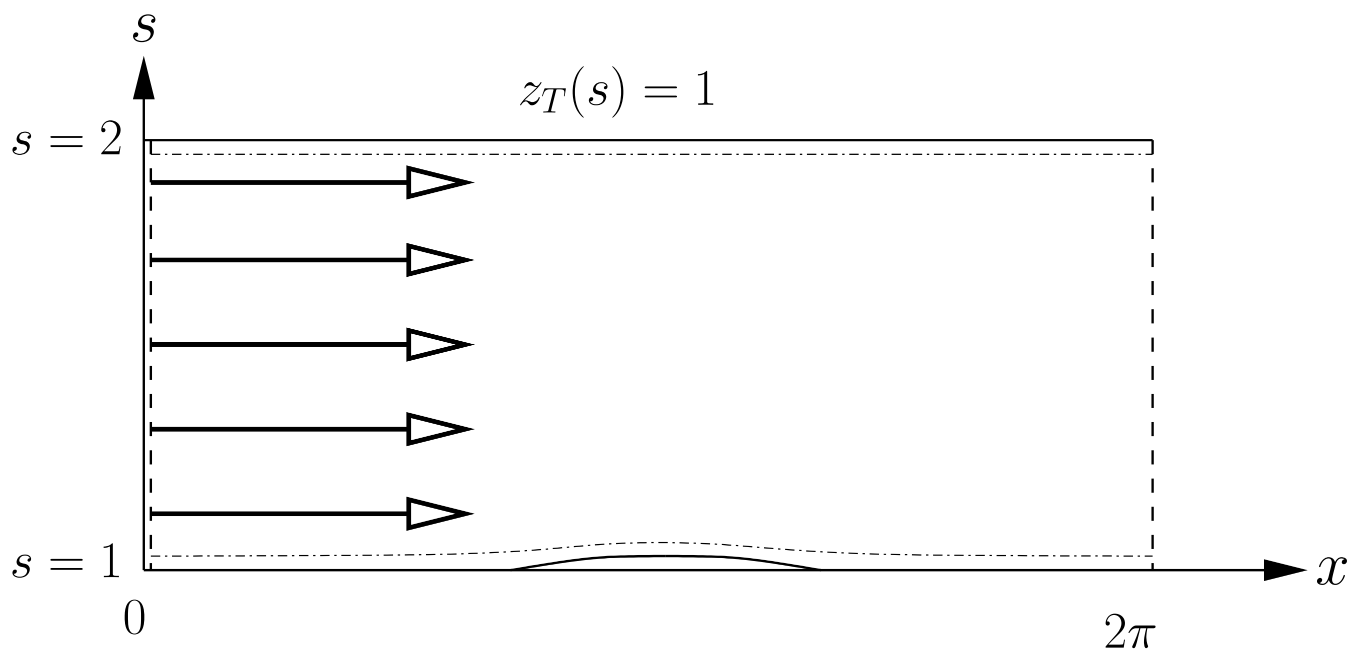
Numerical parameters:

- 40 x-cells,4 particles per cell initially
- 40 s-isentropes, 4-point Gauss quadrature over S
- $\Delta t = 0.0185$, $T = 2$ period

$\Rightarrow$ Can our **nonlinear** code reproduce the linear dynamics?

MOVIE

Example 2: flow over a hill



- nondimensionalized
- $f = 0$, 2D-set up (x, s)
- nonlinear
- stationary
  $\rightarrow$ fluxes independent of x
- small bump (ampl. 0.02) in middle of domain
- onflow $u(s) = 2$
- bottom and top are isentropic

⇒ Can our Lagrangian particle scheme reproduce a Eulerian steady state?

Numerical parameters:

- 100 x-cells, 2 particles per cell initially
- 20 s-isentropes, 4-point Gauss quadrature over S
- $\Delta t = 0.0038$, $T = 10$

MOVIE

Example 3: unsteady flow over a hill

Same set-up as before, except:

- bump amplitude 0.1
- bump rises smoothly in $\Delta t = 2$.

MOVIE

$\rightarrow$ max drift energy after rise: $3.4 \cdot 10^{-7}$.

Conclusion:

Found a conservative numerical scheme for the hydrostatic Euler equations based on HPM in horizontal and Hermite FEM in vertical.

Outlook:

- Further validation of model output from comparisons to pseudospectral-FEM output,
- 3D test case including rotation,
- generalize model to free surface,
- find a way how to handle bottom-intersecting isentropes,
- formulate stabilizer to avoid isentropes to overturn $\sim$ fronts,
- **forcing & friction**.

Questions ??

References

- Bokhove, O., Oliver, M. 2006: Parcel Eulerian-Lagrangian fluid dynamics of rotating geophysical flows. *Proc. R. Soc. Lond.* **A 462**: 2563-2573.
- Frank, J., Gottwald, G., Reich, S. 2002: A Hamiltonian particle-mesh method for the rotating shallow-water equations. *Lecture Notes in Computational Science and Engineering*, vol. **26**. Springer, Heidelberg, 131-142.