Kinetic and Hyperbolic Equations with Applications to Engineering Processes

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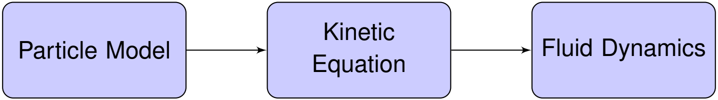
Talk in "Research Modelling Seminar"

Outline

Model Hierarchy: General

- We are interested in *Agent* or *Particle* based dynamics.
- As an intermediate model we establish a *Kinetic Model* of such a process.
- Finally, we go over to a *Fluid Dynamics* model to describe the macroscopic behavior by rescaling the kinetic model.



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Particle Model → Kinetic Equation → Fluid Dynamics

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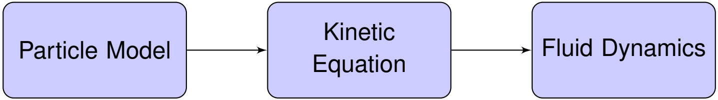

Model Hierarchy: Gas Dynamics

Classical Example: Gas dynamics.

- *Newtonian Dynamic*: free float and *Elastic Collision* of *Hard Spheres* of $N(\in \mathbb{N})$ atoms.
- Boltzmann equation as an mesoscopic kinetic model (featuring a *mean-field*).
- Introducing *Moments* and taking a *Hydrodynamic Limit* to gain a fluid dynamics model e.g. the *Euler Equations of Gas Dynamics*

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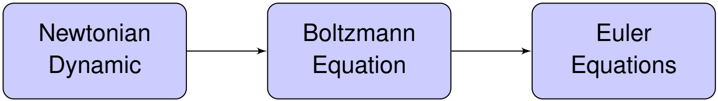

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Gas Dynamics: Pros and Cons of Model Level

- Newtonian dynamic is **physically accurate** but **expansive to compute** (N extremely large).
- Boltzmann equation can be **discretized by less DoF** (DoF$<<N$) but has a **seven dimensional input** (in 3D: position+velocity+time)!
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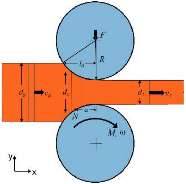
A Steel Rolling Process

Modeling Steel Rolling Processes by fluid-like Differential Equations

A Steel Rolling Process

- We model a single workpiece in a roll mill.
- The model considers the temperature **T** and thickness **g** of the workpiece and their evolution over time.
- We postulate a stochastic "transition" probability of the workpiece to either undergo a deformation process or not (transport of it or change of milling rolls).



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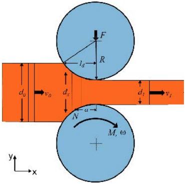

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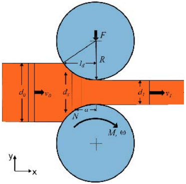

Particle Dynamics 1

- Let τ be a random processing time. We choose

$$P(\tau = s) = \Phi(s).$$

- In case of an rolling event the thickness undergoes the deformation

$$\mathbf{g}(t+\tau) = \mathbf{g}(t) - F(\mathbf{T}(t), \mathbf{g}(t), \tau).$$

- Independent of the event (transport of rolling) we assume a temperature flux

$$\mathbf{T}(t+\tau) = \mathbf{T}(t) - \tau\, c(\mathbf{T}(t)).$$

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Particle Dynamics 2

- We rescale the probability via

$$\omega(\tau) = \frac{\Phi(\tau)}{\int_\tau^\infty \Phi(s)ds}$$

and consider a small time-step $\Delta t > 0$.
[M. Herty, C. Ringhofer, 2001].

- With probability $\omega(\tau(t))\Delta t$ we have (rolling):

$$\begin{aligned} \tau(t+\Delta t) &= 0, \\ \mathbf{g}(t+\Delta t) &= \mathbf{g}(t) - F(\mathbf{T}(t), \mathbf{g}(t), \tau), \\ \mathbf{T}(t+\Delta t) &= \mathbf{T}(t) - \Delta t c(\mathbf{T}(t)), \end{aligned}$$

- And with probability $1 - \omega(\tau(t))\Delta t$ (no rolling):

$$\begin{aligned} \tau(t+\Delta t) &= \tau(t) + \Delta t, \\ \mathbf{g}(t+\Delta t) &= \mathbf{g}(t), \\ \mathbf{T}(t+\Delta t) &= \mathbf{T}(t) - \Delta t c(\mathbf{T}(t)). \end{aligned}$$

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Transition Probability

- As the transition from state $X = (\tau, \mathbf{g}, \mathbf{T})$ to state $X' = (\tau', \mathbf{g}', \mathbf{T}')$ in a time step Δt we have:

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&P(X, X') = \\
&(1 - \omega(\tau')\Delta t) \cdot \delta(\tau - (\tau' + \Delta t)) \cdot \delta(\mathbf{g} - \mathbf{g}') \cdot \delta(\mathbf{T} - (\mathbf{T}' - \Delta t c(\mathbf{T}')) \\
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- Hence, the probability $f(t, X)$ (kinetic model) to be in state X at time t evolves according to

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f(t + \Delta t, X) = \int P(X, X') f(t, X') dX.
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Fluid-like Limit

For reasons of presentation we quickly list the involved steps:

- Scaling frequency ω by $\hat{\omega} = \frac{\omega}{\Delta t}$,
- Taylor expansion w.r.t. Δt and considering resulting first-order dynamics (see Boltzmann limit),
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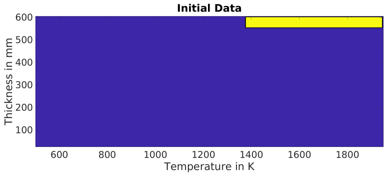
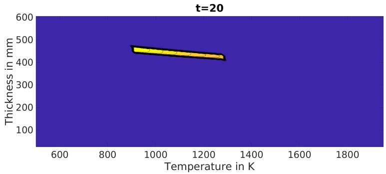
Fluid-like PDE

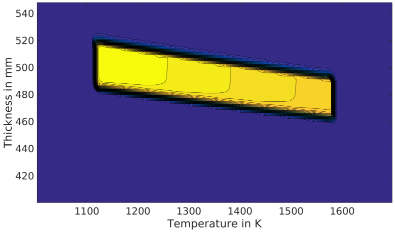
The resulting PDE reads

$$f_t(t,\mathbf{g},\mathbf{T}) = \hat{\omega}(0)\left[\partial_{\mathbf{g}}(F_\tau(\mathbf{T},\mathbf{g},0)f(t,\mathbf{g},\mathbf{T})) + c(\mathbf{T})f_{\mathbf{T}}(t,\mathbf{g},\mathbf{T})\right] + f(t,\mathbf{g},\mathbf{T})(1+\hat{\omega}(0))(c(\mathbf{T})-1).$$

Simulations







Interpretation of Results

- As desired, the resulting dynamics recovers a reduction in thickness and temperature of the initial workpieces,
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Potential Applications

- A credible model would offer the opportunity to predict stochastic quantities of a rolling process e.g. expectation value and variance of thickness,
- This would enable the possibility to control the production precess (choice of applied force),
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Remaining Modeling Steps

To gain a credible model it remains:

- Model $\omega(\cdot)$ after experimental data,
- Implement a higher-order approximation to the temperature flux $c(\cdot)$,
- Discriminate between temperature flux into air and into milling roll,
- **Introduce uncertainties!** on each step (in the particle dynamics) according to experimental data.

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Coupling

Coupling Conditions by high-order Schemes

- We consider a model of flow on graphs.
- A single vertex with n adjacent arcs (which we extend to infinity).
- All arcs are parameterized by $[0,\infty)$, such that the junction is located at $x=0$ (for all arcs).
- We assume the flux $f(\cdot) \in \mathscr{C}^4(\mathbb{R}^2, \mathbb{R}^2)$ and the $u_j(t,x) : \mathbb{R}_0^+ \times \mathbb{R}_0^+$ to be the conserved states on the arcs $j = 1, ..., n$

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Problem Setting

$$\partial_t u_j + \partial_x f(u_j) = 0,\ t \geq 0, x \geq 0, \tag{PDE}$$

$$u_j(0,x) = u_{j,o}(x),\ x \geq 0,$$

$$\Psi(u_1(t,0+),\ldots,u_n(t,0+)) = 0,\ t \geq 0, \tag{CC}$$

where $\Psi : \mathbb{R}^{2n} \to \mathbb{R}^n$ is the (possilbly nonlinear!) coupling condition.
(PDE) are assumed to be strictly hyperbolic.

(Existence and uniqueness of solution in [R. M. Colombo, M. Herty, and V. Sachers, 2008].)

Transversality condition

Let Ψ fulfill the *transversality condition*

$$\det\Big[D_1\Psi(\hat{u})r_2(\hat{u}_1),\dots,D_n\Psi(\hat{u})r_2(\hat{u}_n)\Big]\neq 0, \tag{TC}$$

where

- $D_j\Psi(\hat{u})=\frac{\partial}{\partial u_j}\Psi(\hat{u})$,
- $\hat{u}\in\mathbb{R}^{2n}$ is a steady state solution to (PDE) (and $\Psi(\hat{u})=0$),
- $Df(\hat{u}_j)$ has a strictly negative $\lambda^1(\hat{u}_j)$ and a strictly positive eigenvalue $\lambda^2(\hat{u}_j)$ with linearly independent (right) eigenvectors $r_1(\hat{u}_j)$ and $r_2(\hat{u}_j)$,
- Corresponding characteristic fields to be either genuine nonlinear or linearly degenerate.

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Finite Volume

- The discretization for each u_i (seperately) is done by a finite volume method, where the cell average $U_{i,j}^m$ of u_j in cell i at time t^m is given by

$$U_{j,i}^m := \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u_j(x, t^m) dx,$$

- Its evolution over Δt follows

$$U_{j,i}^{m+1} = U_{j,i}^m - \frac{1}{\Delta x} \left((\mathscr{F}_j)_{i+\frac{1}{2}} - (\mathscr{F}_j)_{i-\frac{1}{2}} \right). \tag{FVM}$$

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Finite Volume + Coupling

- The flux across the cell interfaces is given by

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- We will use a second order approximation!
- By (CC) we get boundary conditions for (PDE) at $x = 0$!
- The cell average at the first cell $i = 0$ at time t^m is given by the states $u_{j,0}^m$, $j = 1, \ldots, n$. We assume them to be sufficiently close to $\hat{u}_j$ such that (TC) holds.

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$$(\mathscr{F}_j)_{i+\frac{1}{2}} = \int_{t^m}^{t^{m+1}} f\left(u_j\left(x_{i+\frac{1}{2}}, s\right)\right) ds.$$

- We will use a second order approximation!
- By (CC) we get boundary conditions for (PDE) at $x = 0$!
- The cell average at the first cell $i = 0$ at time t^m is given by the states $u^m_{j,0}$, $j = 1, \ldots, n$. We assume them to be sufficiently close to $\hat{u}_j$ such that (TC) holds.

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Characteristic Splitting

- Let $s \to \mathscr{L}_\kappa(u_o, s)$ the κ-th *Lax curve* through the state u_o for $\kappa = 1, 2$.
- We find $(s_1^*, \dots, s_n^*)$ (e.g. using *Newton′s method*) to solve

$$\Psi\left(\mathscr{L}_2(U_{1,0}^m, s_1), \dots, \mathscr{L}_2(U_{n,0}^m, s_n)\right) \stackrel{!}{=} 0$$

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(This is zero order data only!)

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Extend numerical Scheme to Boundary Values (in the Vertex).

Step 0: First order data at x=0

We can now calculate the boundary cell value $U_{j,0}^{m+1}$ at time t^{m+1} by (FVM) for $i = 0$ by using

$$U_{j,-1}^{m} := \mathscr{L}_2\left(U_{j,0}^{m}, s_j^{*}\right). \tag{GC}$$

(Hence, we obtain a first-order approximation to the coupling condition as well as to the solution u_j.)

Step 1: Reconstruction

- Given the cell averages $U_{j,i}^m$ we reconstruct a p.w. linear function $u_j(x, t_m)$ and each cell $\left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}\right]$.

  (This is standard: *MUSCL scheme*.)
- In the first cell $i = 0$ the slope reconstruction will utilize the data gained in (GC) to calculate $\sigma_{j,0}$.

  We obtain a p.w. linear reconstruction

$$U_j\left(x, t^m\right) = \sigma_{j,i}(x - x_i) + U_{j,i}^m, \qquad x_{i-\frac{1}{2}} \leq x \leq x_{i+\frac{1}{2}},\ i = 0, \dots, \tag{1}$$

  where $\sigma_{j,i}$ is the vector of slopes.
- This way we get distinct values at each interface (in the spatial domain, as well as at the vertex) which we will denote by the values at $x_{i+\frac{1}{2}} \mp$.

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Step 2: Reconstruction at boundary

- Reconstruct for each arc j a piecewise linear function $v_j(t)$ for $t^m \leq t \leq t^{m+1}$ such that

  $$\frac{d}{dt}\Psi(v_1(t), \ldots, v_n(t))|_{t=t^m} = 0.$$

  Let the solution be $(\dot{v}_1, \ldots, \dot{v}_j)$.
  (Solution exists due to (TC).)
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Step 3: Second order flow

Using the *Midpoint rule* for the flux (at the interfaces), Taylor expansion (on $f^{\pm}$) and the p.w. linear reconstruction of u_j we get:

$$
\begin{aligned}
U^m_{j,i-} :=& U^m_{j,i} + \sigma_{j,i}\frac{\Delta x}{2},\ U^m_{j,i+} := U^m_{j,i+1} - \sigma_{j,i+1}\frac{\Delta x}{2},\\
\frac{1}{\Delta x}(\mathscr{F}_j)_{i+\frac{1}{2}} \approx& \frac{\Delta t}{\Delta x}\left[f^{+}\left(U^m_{j,i-} - \frac{\Delta t}{2} Df(U^m_{j,i-})\sigma_{j,i} \right) + \right.\\
& \left. f^{-}\left(U^m_{j,i+} - \frac{\Delta t}{2} Df(U^m_{j,i+})\sigma_{j,i+1} \right) \right],
\end{aligned}
$$

where the flux is splitted as

$$
f(u) = f^{+}(u) + f^{-}(u) := \frac{1}{2}\left(f(u) + au\right) + \frac{1}{2}\left(f(u) - au\right),
$$

with $a = \lambda_{\max}$. [A. Kurganov, E. Tadmor, 2000].

Step 4: Second order flow at boundary

- We need to evaluate the flux at the boundary $(\mathscr{F}_j)_{-\frac{1}{2}}$. By (GC) and Step 2 of the algorithm the characteristic speed of information is non-negative.
- Using the midpoint rule:

$$\begin{aligned}(\mathscr{F}_j)_{-\frac{1}{2}} &= \int_{t^m}^{t^{m+1}} f\left(u_j\left(x_{-\frac{1}{2}}, s\right)\right) ds \\ &\approx \int_{t^m}^{t^{m+1}} f(v_j(s))ds = \Delta t f\left(v_j\left(t^{m+\frac{1}{2}}\right)\right) + \mathscr{O}\left((\Delta t)^3\right).\end{aligned}$$

- Therefore, the boundary flux is given by

$$\frac{1}{\Delta x}(\mathscr{F}_j)_{-\frac{1}{2}} \approx \frac{\Delta t}{\Delta x} f\left(v_j + \frac{\Delta t}{2}\dot{v}_j\right). \tag{BF}$$

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Step 5: Update

Evolve the dynamics according to equation (FVM) for $i = 1, \ldots,$ to obtain the new cell averages at time t^{m+1} and proceed with STEP 1.

Calculate Step 2

- Using the p.w. linear reconstruction

$$u_j\left(x_{-\frac{1}{2}}, t^m\right) = U^m_{j,0} - \frac{\Delta x}{2}\sigma_{j,0}$$

  to get second order accurate boundary values.

- We determine the vector $s = (s_1, \dots, s_n) \in \mathbb{R}^n$ by solving the possibly nonlinear equation:

$$\Psi\left(\mathscr{L}_2\left(U^m_{1,0} - \frac{\Delta x}{2}\sigma_{1,0}, s_1\right), \dots, \mathscr{L}_2\left(U^m_{n,0} - \frac{\Delta x}{2}\sigma_{n,0}, s_n\right)\right) = 0.$$

- Since we want Ψ to hold for $t > t^m$ we solve:

$$\begin{aligned} 0 &= \frac{d}{dt}\Psi(u_1(t,0+), \dots, u_n(t,0+)) \\ &= \sum_{k=1}^{n} D_{u_k}\Psi\left(u_1(t,0+), \dots, u_n(t,0+)\right)\partial_t u_k(t,0+). \end{aligned}$$

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Lemma: Second order CC

Lemma:

Consider a single node with n connected arcs and let t^m be some positive time. Let $\Psi \in C^2(\mathbb{R}^{2n};\mathbb{R}^n)$ and let $\hat{u}_j := U^m_{j,0} - \frac{\Delta x}{2}$ be such that condition (TC) holds true.

Then, for $v_j(t)$ as in the the previous construction, the coupling condition is satisfied up to second order in time

$$\Psi\left(v_1(t),\dots,v_n(t)\right) = \mathscr{O}\left((t-t^m)^2\right).$$

Application: Gas Dynamics

Conservation Law + CC

- We will connect two arcs $j = 1, 2$.
- We consider isothermal Euler equations, where the conservation law reads:

$$\partial_t \begin{pmatrix} \rho_j \\ q_j \end{pmatrix} + \partial_x \begin{pmatrix} q_j \\ a^2 \rho_j + \frac{q_j^2}{\rho_j} \end{pmatrix} = 0,\ a > 0 \quad \left(U = \begin{pmatrix} \rho \\ q \end{pmatrix} \right).$$

- $\Psi^1(U_1(t,0+), U_2(t,0+)) = q_1(t,0+) + q_2(t,0+)$ and
- $\Psi^2(U_1(t,0+), U_2(t,0+)) = \left(a^2 \rho_2(t,0+) + \frac{q_2^2(t,0+)}{\rho_2(t,0+)} \right) + \left(a^2 \rho_1(t,0+) + \frac{q_1^2(t,0+)}{\rho_1(t,0+)} \right).$

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Solving Step2

- For subsonical states U_j we have $\lambda_j^1 < 0$ and $\lambda_j^2 > 0$.
- For small $t - t^m$ we use the decomposition
  $U_j(t^m, 0+) = v_j^1(t) r_j^1(v(t^m)) + v_j^2(t) r_j^2(v(t^m)) = R_j \begin{pmatrix} v_j^1(t) \\ v_j^2(t) \end{pmatrix} = R_j V_j(t).$
- $v_j^i(t) = v_j^i + (t - t^m)\dot{v}_j^i$. We know v_j^i from (GC) and $\dot{v}_j^1$.
- $\dot{v}_j^1 = -\lambda_1 \partial_x \left(R^{-1} U_j(t^m, 0+)\right)^1 = -\lambda_1 \left(R^{-1} \begin{pmatrix} \sigma_{j,0}^1 \\ \sigma_{j,0}^2 \end{pmatrix}\right)^1.$

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Linearize of Influx: $\dot{v}_j^2$

- Linearize Ψ:

$$
\begin{aligned}
0 &= \frac{d}{dt}\Psi(U_1(t^m,0+),U_2(t,0+))\\
&= \frac{d}{dt}\Psi(V_1(t),V_2(t))\,|_{t=t^m}\\
&= -\sum_{j=1}^{2} D_{V_j}\Psi(V_1(t),V_2(t))Df(V_j)\begin{pmatrix}\dot{v}_j^1\\ \dot{v}_j^2\end{pmatrix}.
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- $\Rightarrow$ $\dot{v}_j^2$ $\Rightarrow$ $V_j(t)$ which we will use to calculate the fluxes at $x=0$.

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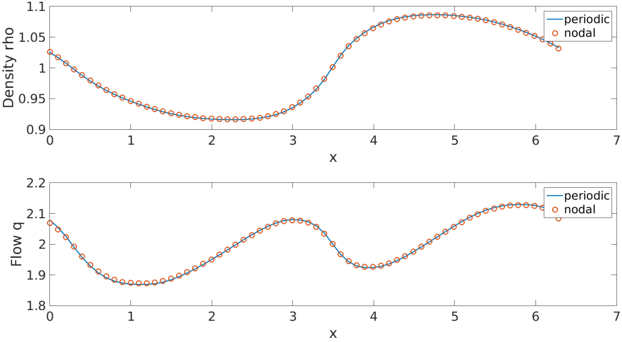
Plot Periodic vs. Coupled

- Initial data: $\rho(x)_0 = 0.1\cos(x) + 1$, $q(x)_0 = 0.05\cos(x) + 2$, final time $T = 0.3$.
- Plot of solutions U_p (periodic) and U_c (coupled).



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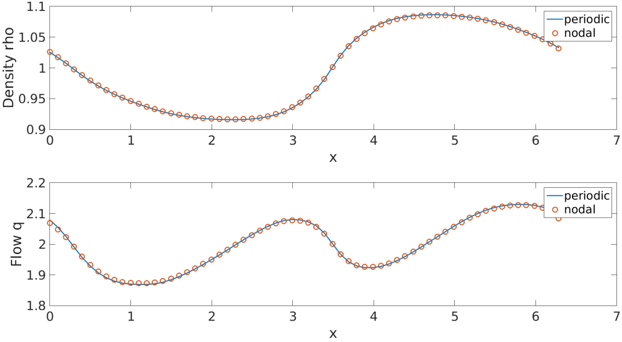

Table of Error

N_k	L^1 ρ	L^1 q	Rate ρ	Rate q
2^5	8.8259	7.1826	/	/
2^6	10.4556	8.6067	1.6297	1.4242
2^7	12.1436	10.3566	1.6880	1.7499
2^8	13.8907	12.1301	1.7471	1.7735
2^9	15.6996	13.9506	1.8089	1.8205
2^{10}	17.5927	15.8745	1.8931	1.9239
2^{11}	19.5538	17.8503	1.9611	1.9758
2^{12}	21.5445	19.8373	1.9907	1.9870

Table: L^1 convergence of the periodic boundary to the nodal coupled method.

Y-Junction: Setup

- Consider $n = 3$ (arcs); spatial domain $x \in [0,2]$,
- Neumann boundary conditions (outflowing) at $x = 2$,
- Coupling conditions: Conservation of mass and conservation of flow (as in the previous example),
- The initial data:
  For the first arc, $j = 1$, we set

$$\rho_1(x,0) = \begin{cases} -x^3 + \frac{3}{2}x^2 + 1 & x \in [0,1) \\ \frac{3}{2} & x \in [1,2] \end{cases} \text{ and } q_1(x,0) = \begin{cases} -x^3 + \frac{3}{2}x^2 & x \in [0,1) \\ \frac{1}{2} & x \in [1,2] \end{cases}.$$

  For the second and the third arcs, $j = 2,3$, we set

$$q_j(x,0) \equiv 0 \text{ and } \rho_j(x,0) \equiv 1.$$

- We have: $\Psi(U_1(x,0), U_2(x,0), U_3(x,0)) = (0,0,0)^\top$.

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  For the second and the third arcs, $j = 2,3$, we set

$$q_j(x,0) \equiv 0 \text{ and } \rho_j(x,0) \equiv 1.$$

- We have: $\Psi(U_1(x,0), U_2(x,0), U_3(x,0)) = (0,0,0)^\top$.

Y-Junction: Setup

- Consider $n = 3$ (arcs); spatial domain $x \in [0,2]$,
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Y-Junction: Plots ρ

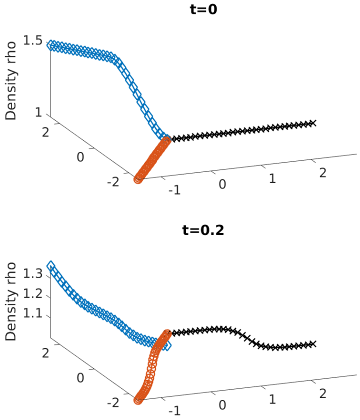

Figure: Evolution of the density ρ. Arcs: $\diamond$ $j = 1$, $\circ$ $j = 2$, $\times$ $j = 3$.

Y-Junction: Plots q

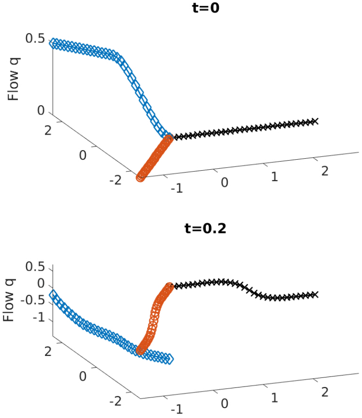

Figure: Evolution of the flow q. Arcs: $\diamond$ $j = 1$, $\circ$ $j = 2$, $\times$ $j = 3$.

References

Thank you!

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