Toward Information Geometric Mechanics

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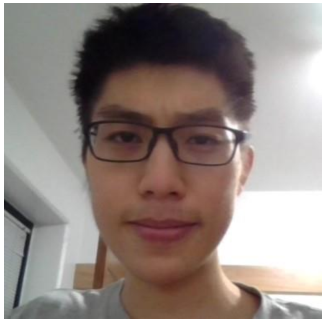
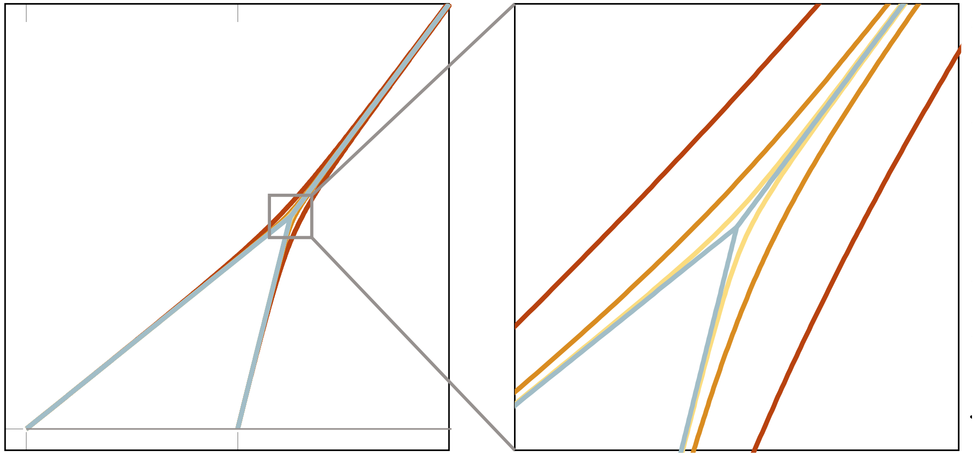
September 2025, MFEM Seminar



Ruijia Cao



Part I: New Methodology

INFORMATION GEOMETRIC REGULARIZATION

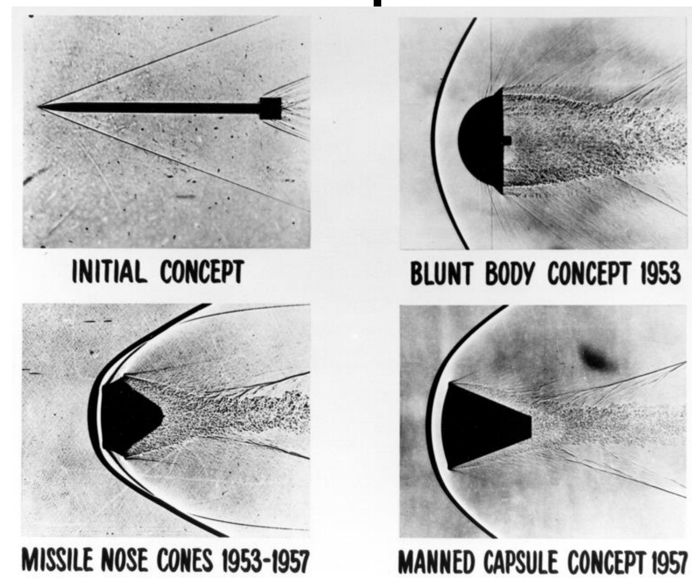
Cao, S, 2023 https://arxiv.org/abs/2308.14127

Shocks in Gas Dynamics

Astrophysics

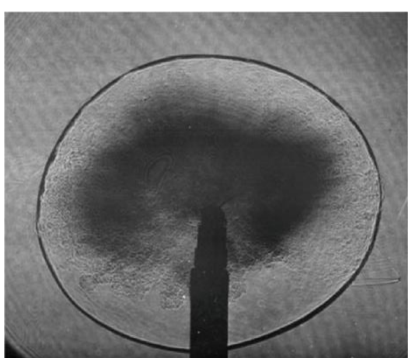
https://www.nasa.gov/image-feature/veil-nebula-supernova-remnant

Aerospace

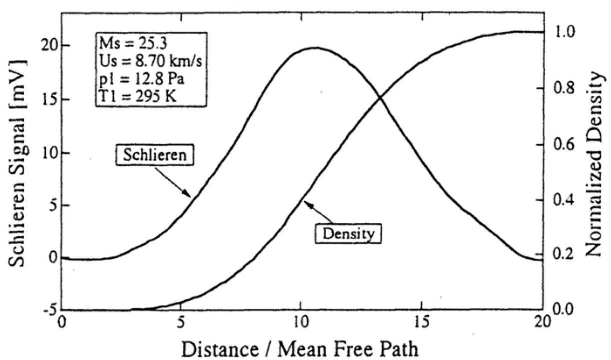


https://en.wikipedia.org/wiki/Atmospheric_entry#/media/File:Blunt_body_reentry_shapes.png

Shocks: jumps in pressure, density, velocity



Takayama, 2019



Koreeda et al., 2019

Microscopically thin, can not resolve in simulation!

Compressible Euler Equations

Model frictionless barotropic gas dynamics

$$\partial_t \begin{pmatrix} \rho \boldsymbol{u} \\ \rho \end{pmatrix} + \mathrm{div} \begin{pmatrix} \rho \boldsymbol{u} \otimes \boldsymbol{u} + P(\rho)\mathbf{I} \\ \rho \boldsymbol{u} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ 0 \end{pmatrix}$$

$\boldsymbol{u}$	Velocity
$\rho \boldsymbol{u}$	Momentum
ρ	Density
$\boldsymbol{f}$	External force
$\boldsymbol{P}(\rho)$	Pressure (increasing function)

Conservation of mass and momentum

Compressible Euler Equations

In one dimension:

$$\partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

Compressible Euler Equations

In one dimension:

$$\partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \underbrace{\begin{pmatrix} \rho u^2 + P(\rho) \\ \rho u \end{pmatrix}}_{\text{Flux of } \begin{pmatrix} \rho u \\ \rho \end{pmatrix}} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

Compressible Euler Equations

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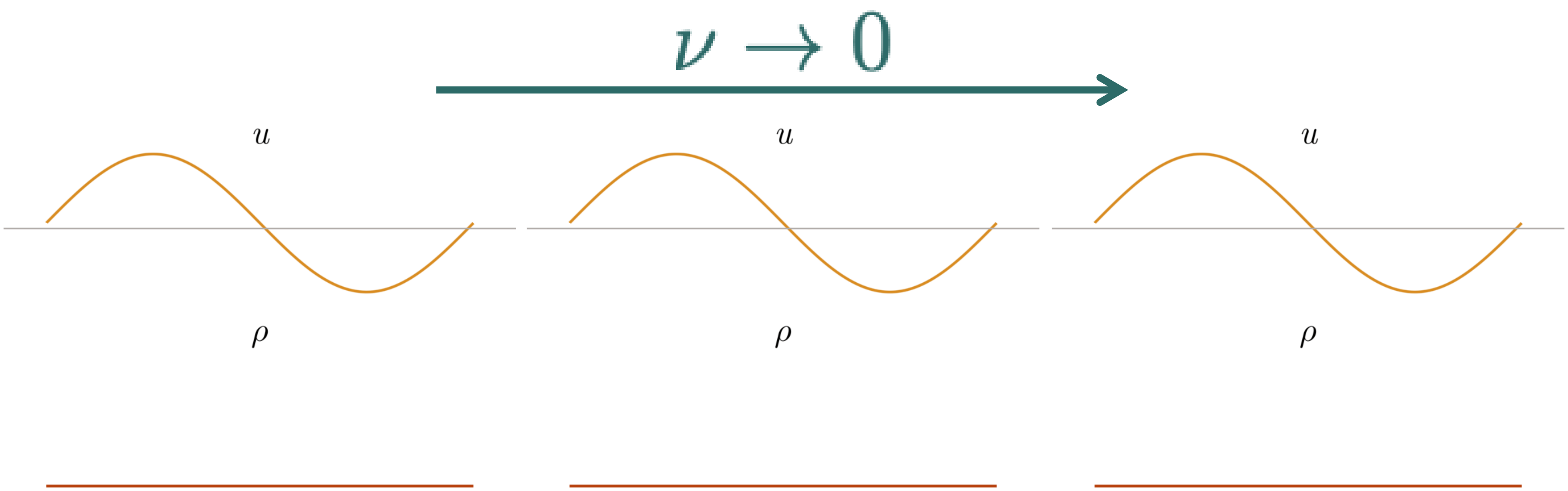
$$\partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \underbrace{\begin{pmatrix} \rho u^2 + P(\rho) \\ \rho u \end{pmatrix}}_{\underbrace{\text{Flux of } \begin{pmatrix} \rho u \\ \rho \end{pmatrix}}_{\text{out minus in}}} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

Vanishing Viscosity Solution

Solution from vanishing viscosity limit $\nu \to 0$

$$\partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) - \nu \partial_x u \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

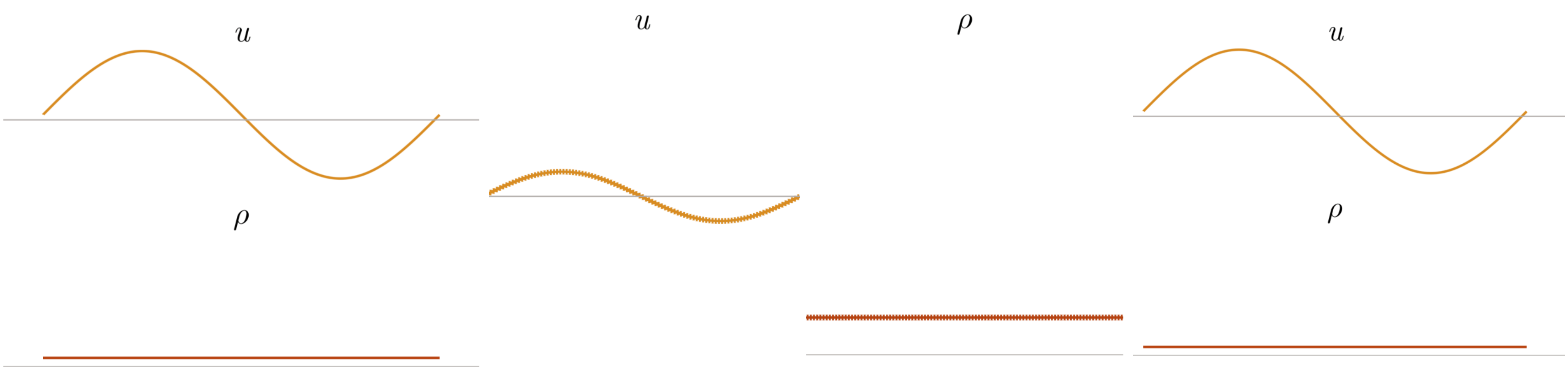


Numerical solution

Choose small ν, use standard methods?

(Near-)discontinuities cause numerics to blow up (Gibbs-Runge Phenomenon)

Larger ν smears out solution over time



Nonlinear Diffusion

$$\partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) - \nu(u,\rho)\partial_x u \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$

Idea: Choose viscosity *adaptively*, at shock

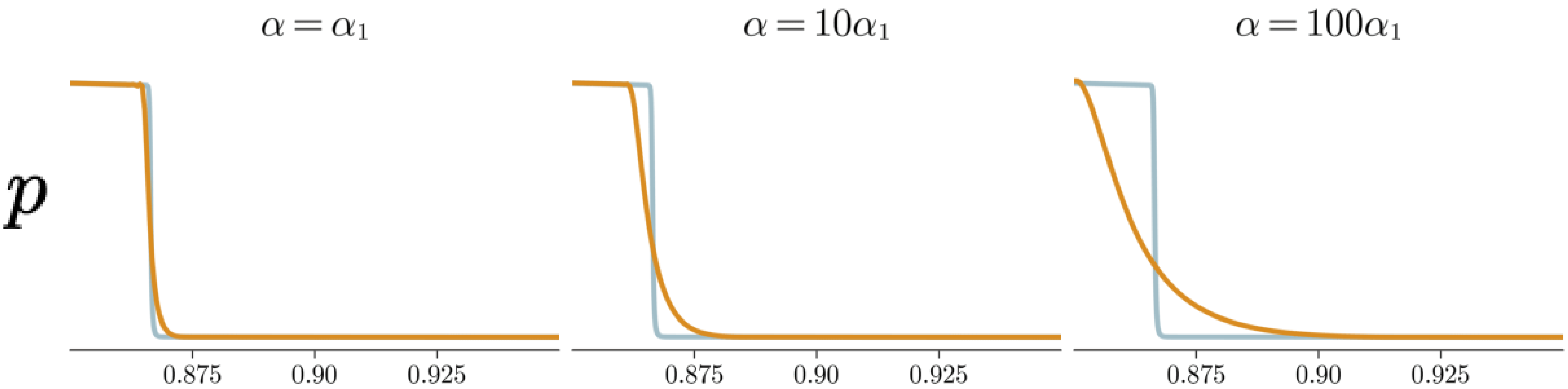
Shock Sensor $\nu(u,\rho)$ needs to detect shocks based on local information.

Try to avoid breakdown and oversmoothing

Von Neumann & Richtmeyer (1950), Dolejvsi et al.(2003), Puppo (2004), Cook & Cabot(2005), Fiorina & Lele (2007), Mane et al. (2009), Barter & Darmofal (2010), Guermond et al. (2011), Bruno et al. (2022)

Localized Artificial Diffusivity

$$\partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) + \alpha \rho (\partial_x u)_- \partial_x u \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}$$



Here: Use local artificial diffusivity following Mani et al. Numerous alternatives exist

Localized Artificial Diffusivity

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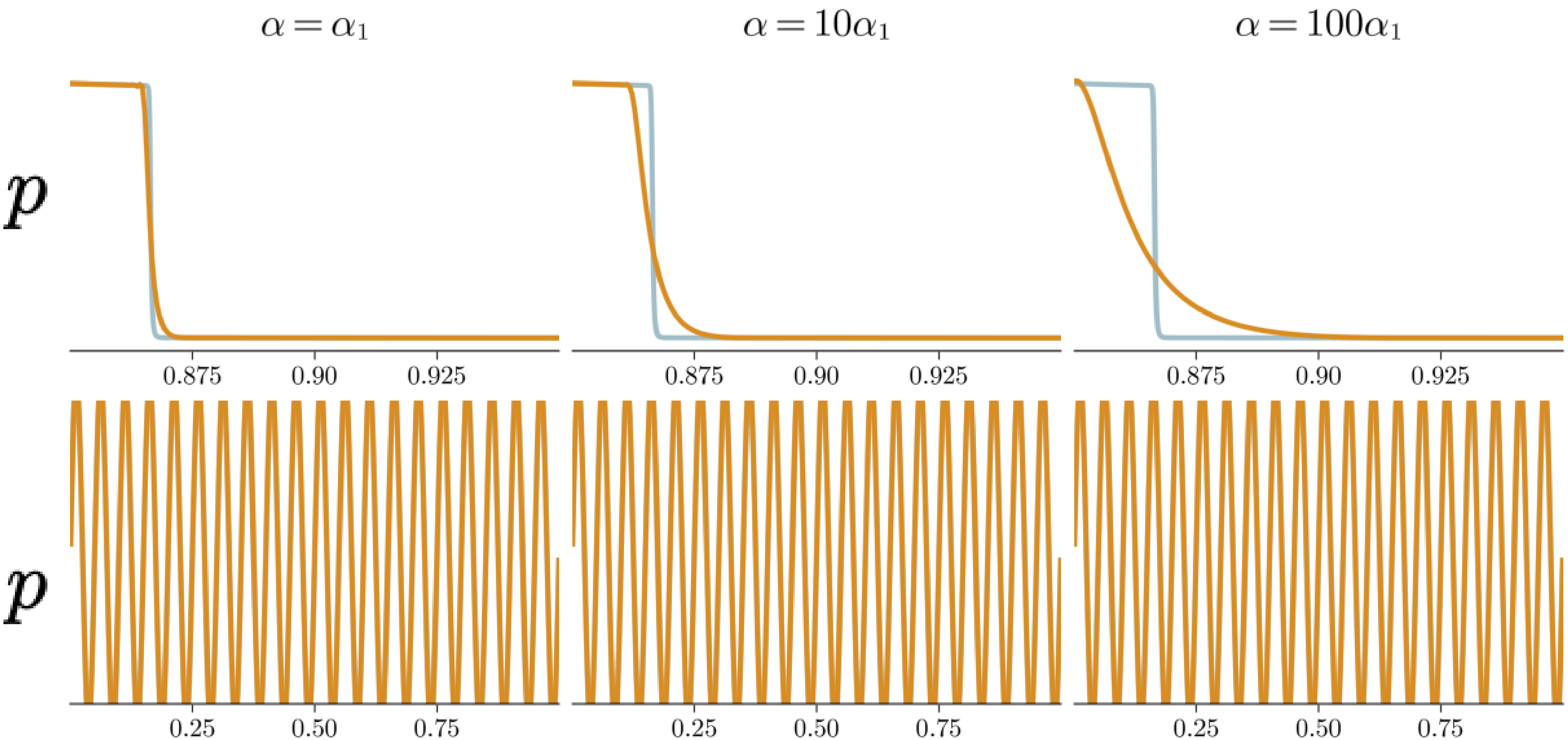


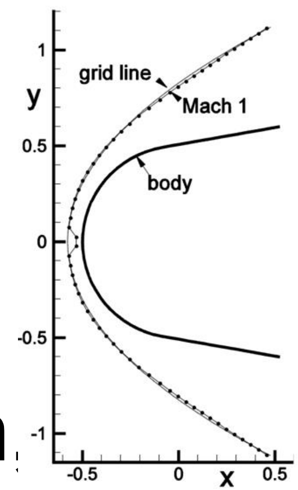
Here: Use local artificial diffusivity following Mani et al. Numerous alternatives exist

Alternative: Nonlinear Numerics

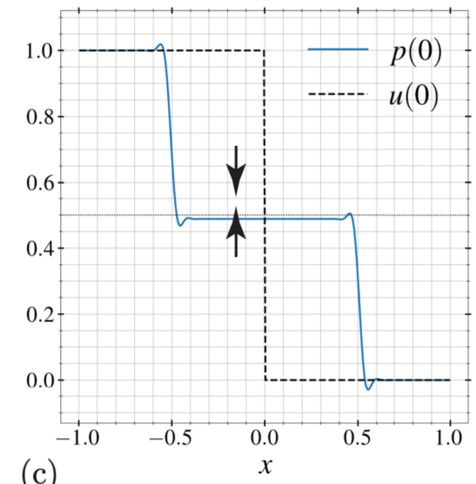
Alternative: Limiters (MUSCL, (W)ENO), Riemann Solvers, Shock tracking.

Can be more effective, but

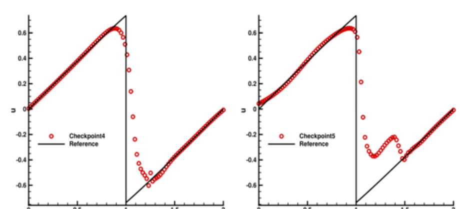
- Numerical artefacts
- Spurious sensitivities
- Restricts discretization, causes technical debt



MacCormack, "The carbuncle CFD problem", 2022



Bodony & Fikl, "Adjoint-based sensitivity of shock-laden flows", 2022



(b) u at $t = 1$ at different epochs (1000, 3000, 5000, 8000 and 11500)

Liu et al., "Discontinuity Computing Using Physics-Informed Neural Networks", 2024

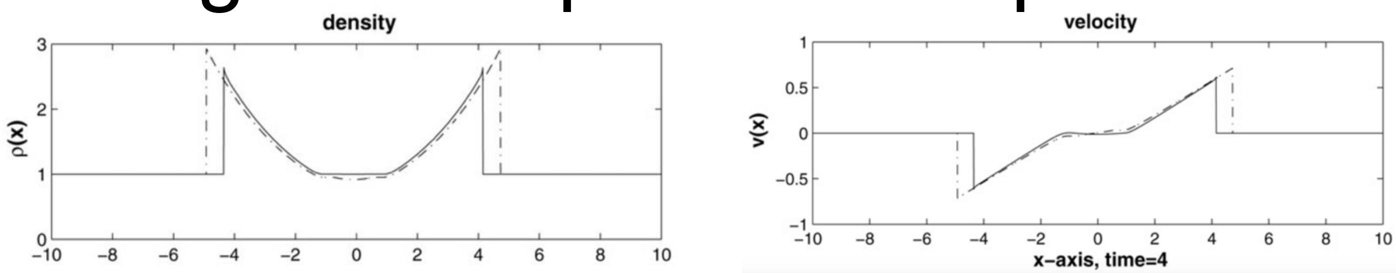
Godunov (1959), Van Leer (1979), Liu et al. (1994), Harten et al. (1997), Shu (1998)

Inviscid PDE regularization?

1. Attempt "Leray Regularization"

Bhat, Fetecau, also Marsden, Mohseni, West, 2003-2009

Wrong shock speed ⇒ not practical

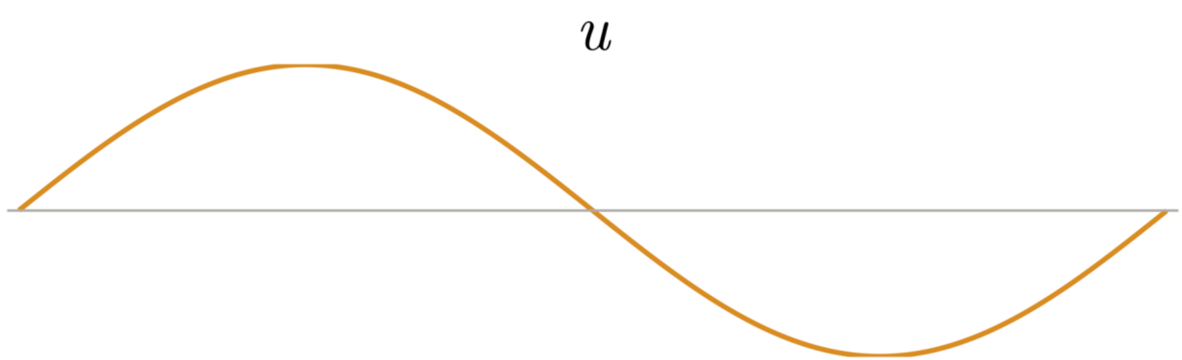


Bhat & Fetecau, "On a regularization of the compressible Euler equations for an isothermal gas", 2009

2. Attempt "Saint-Venant Regularization"

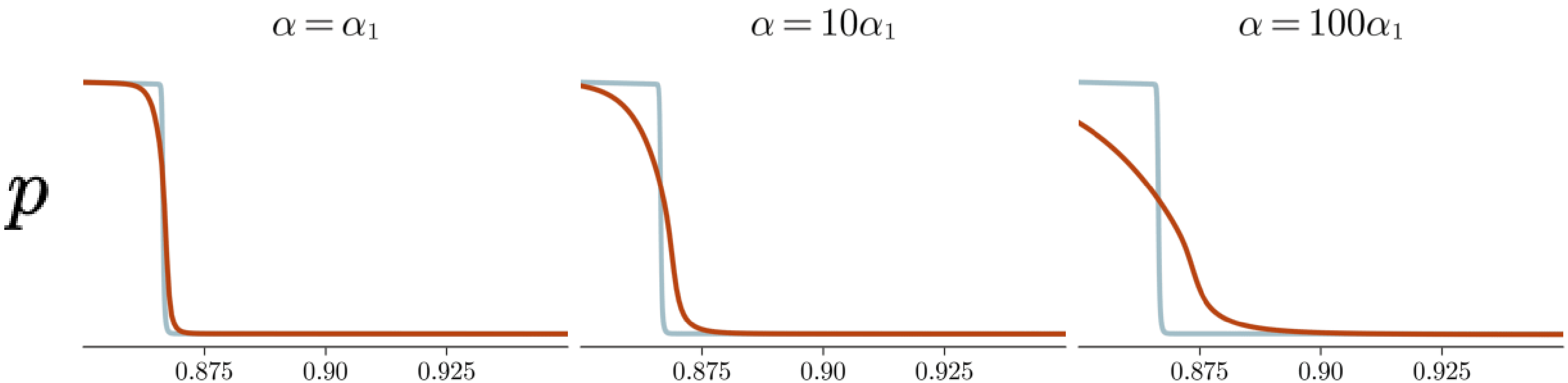
Guelmame, Clamond, and Junca, 2020

Only 1-d, dissipation only in singularities



Information Geometric Reg. (IGR)

$$\begin{cases} \partial_t \begin{pmatrix} \rho \boldsymbol{u} \\ \rho \end{pmatrix} + \operatorname{div} \begin{pmatrix} \rho \boldsymbol{u} \otimes \boldsymbol{u} + (p + \Sigma)\mathbf{I} \\ \rho \boldsymbol{u} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha \operatorname{div}(\rho^{-1}\nabla \Sigma) = \alpha \left(\operatorname{tr}^2\left([\mathrm{D}\boldsymbol{u}]\right) + \operatorname{tr}\left([\mathrm{D}\boldsymbol{u}]^2\right)\right) \end{cases}$$



Cao, S, 2024

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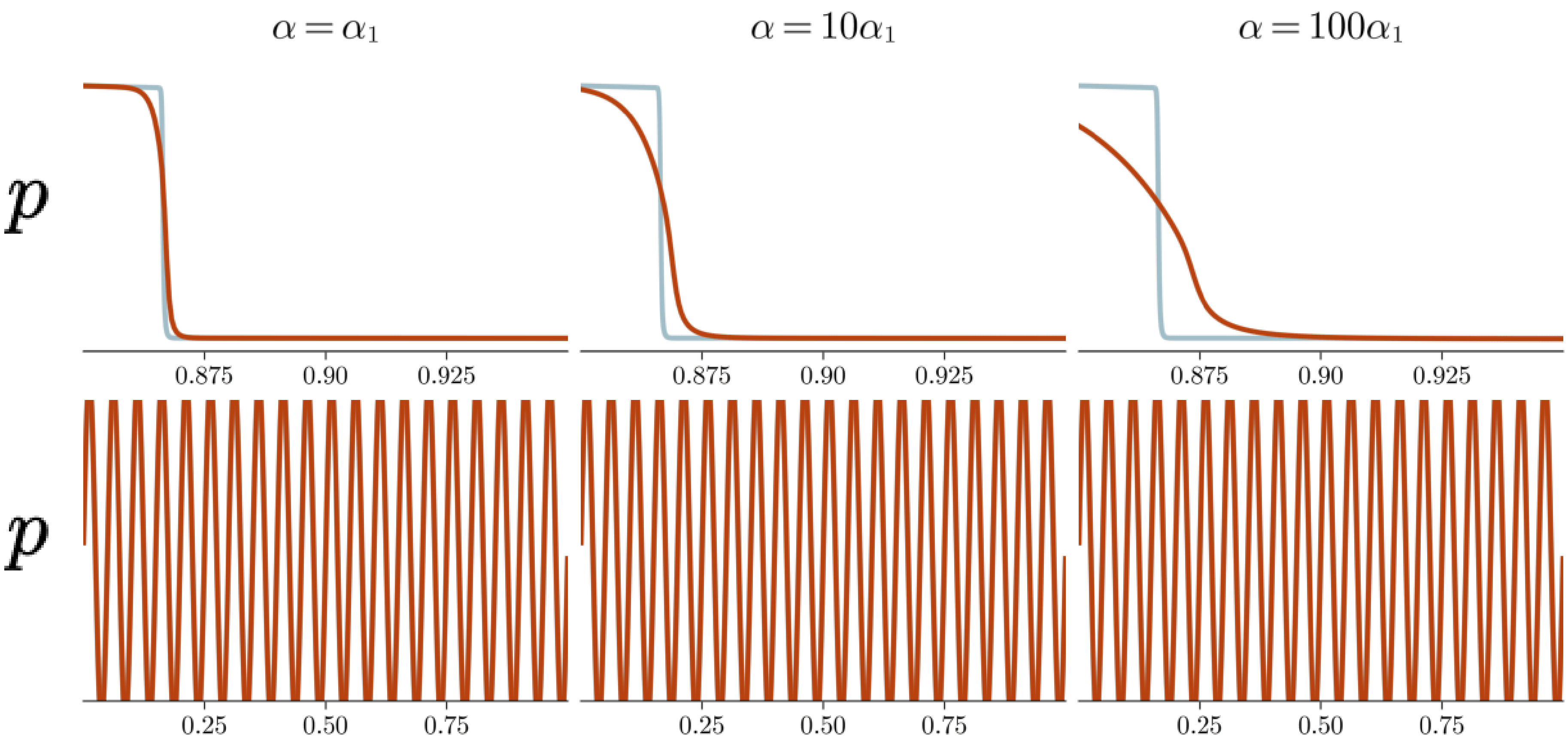
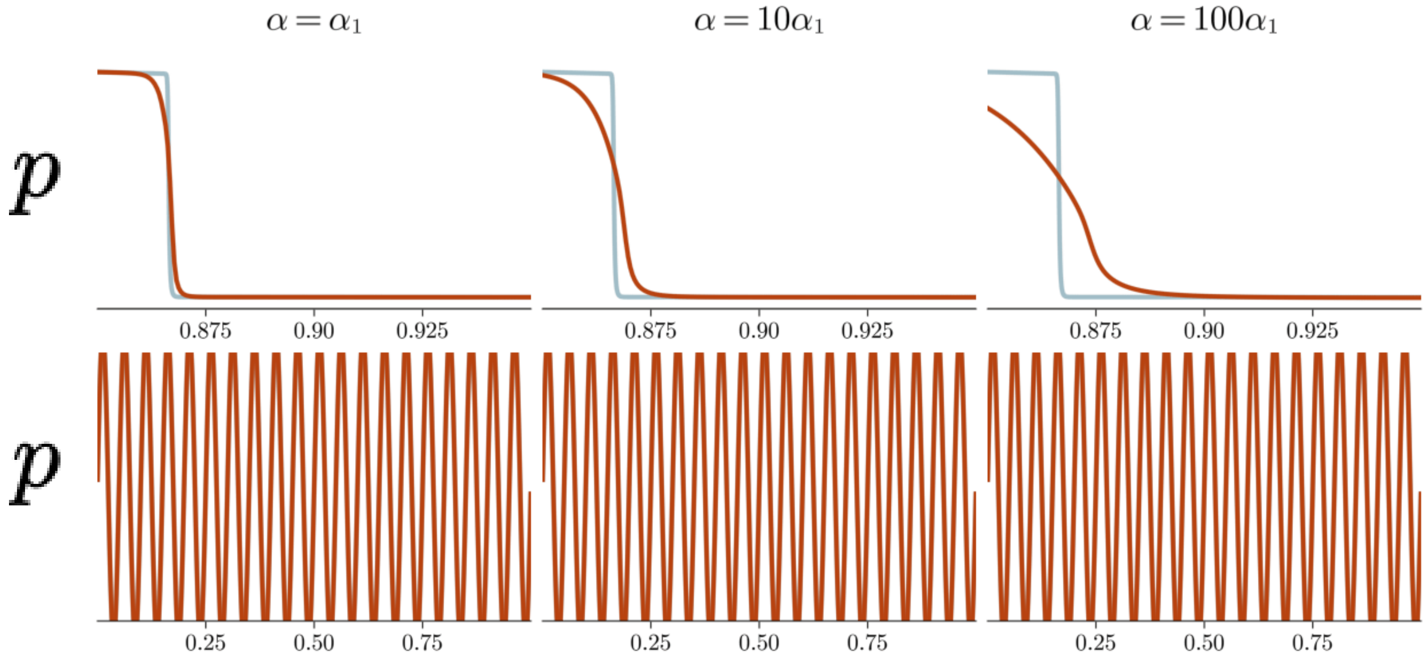
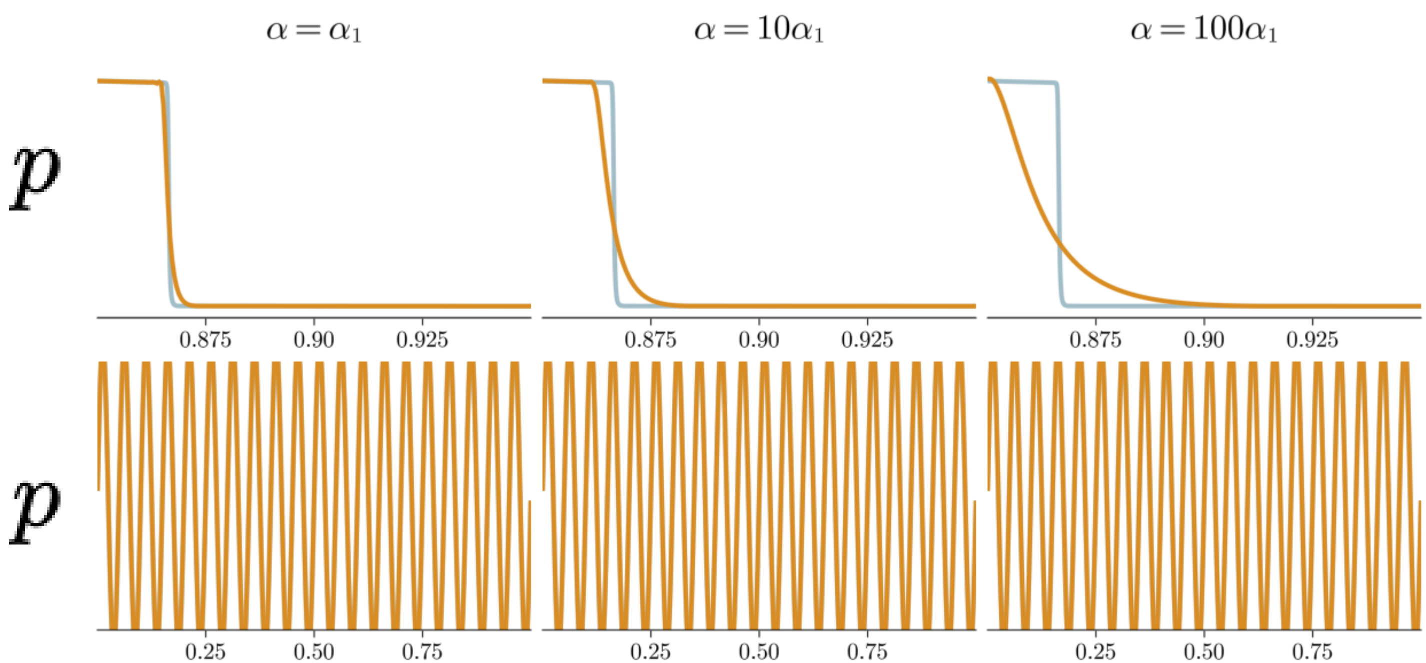



$\alpha = \alpha_1$
$\alpha = 10\alpha_1$
$\alpha = 100\alpha_1$
p
p
0.875
0.90
0.925
0.25
0.50
0.75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p
p
0.875
0.90
0.925
0.25
0.50
0.75

Solution by Particle Tracking

To simplify: set $P \equiv 0$, 1-d

$$\partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 \\ \rho u \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Define family of paths

$$\Phi_t(x) = x + tu(x,0)$$

Obtain solution

$$\begin{pmatrix} u(\Phi_t(x),t) \\ \rho(\Phi_t(x),t) \end{pmatrix} := \begin{pmatrix} u(x,0) \\ (\partial_x \Phi_t(x))^{-1} \end{pmatrix}$$

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Define family of paths

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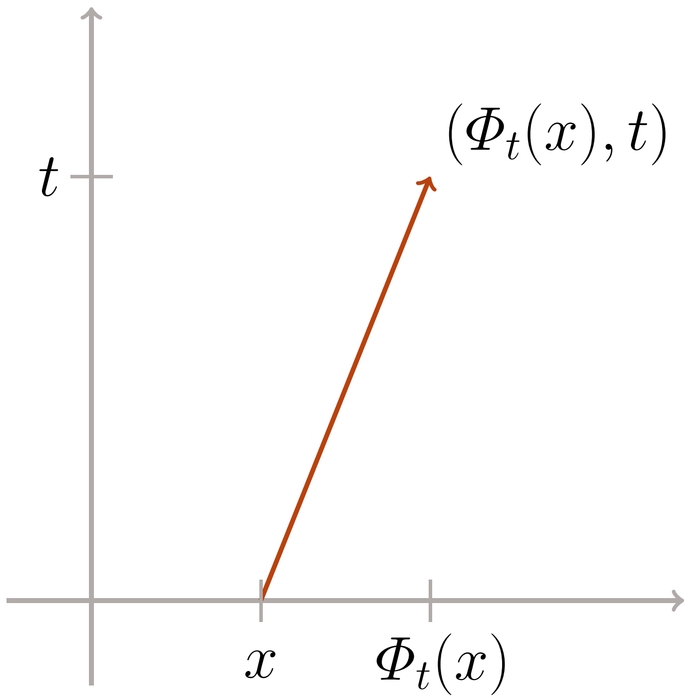

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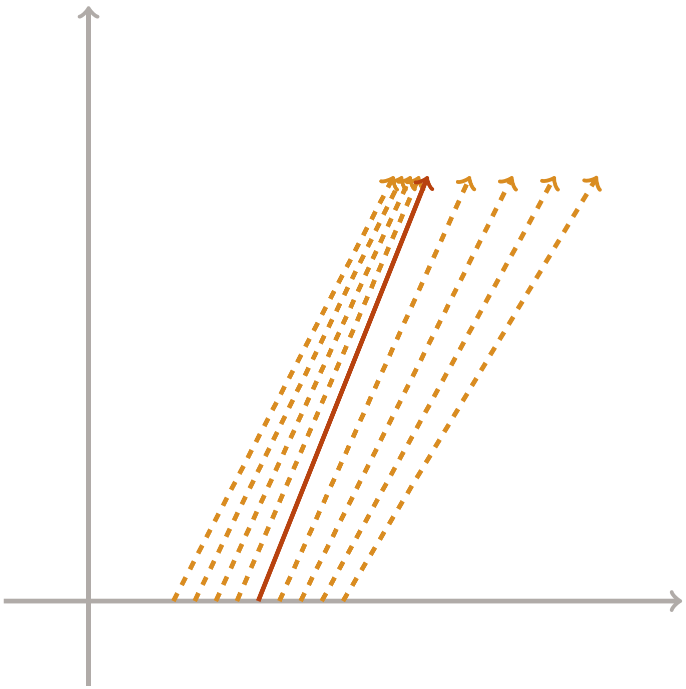

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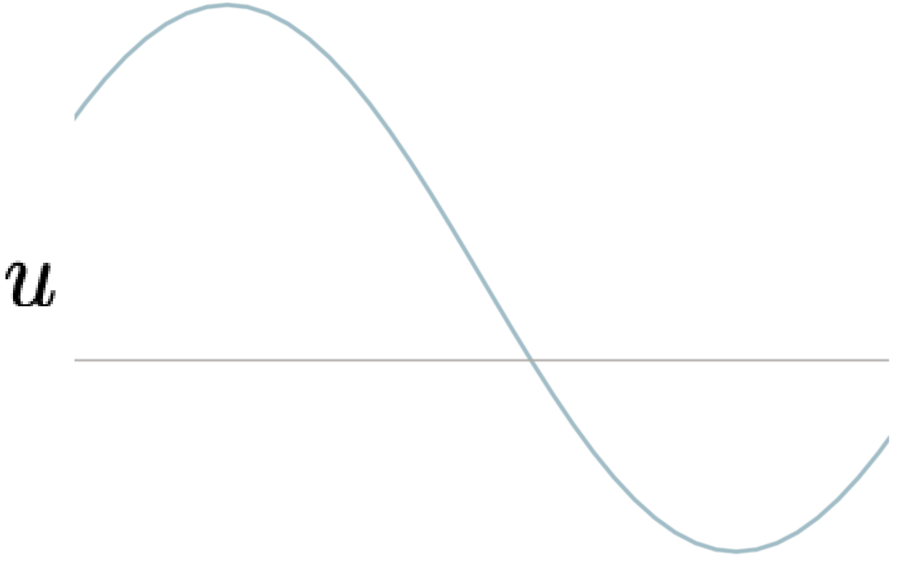
Perspectives on Shocks

I: Particle Collision

Shocks form when trajectories cross.



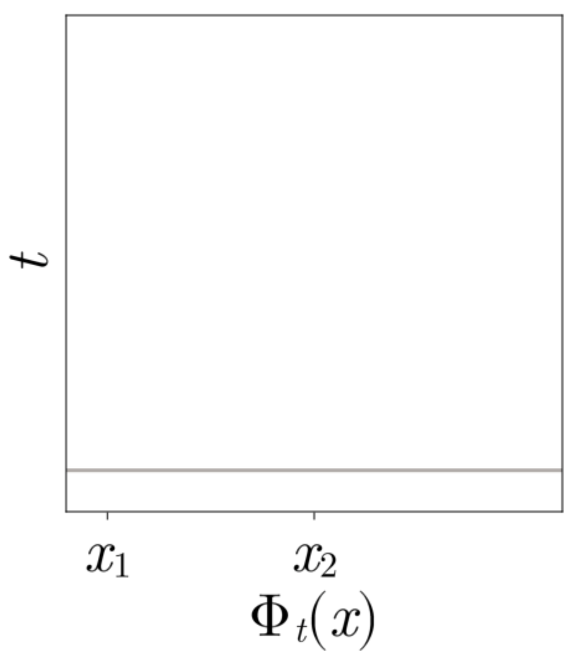
Perspectives on Shocks

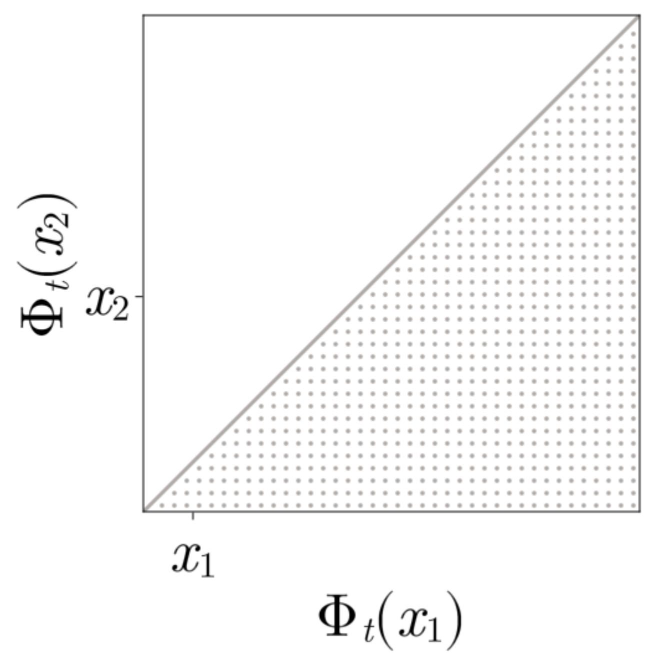
I: Particle Collision

Shocks form when trajectories cross.

II: Boundary

Shocks form when Φ_t hits boundary of diff-eomorphism manifold





Perspectives on Shocks

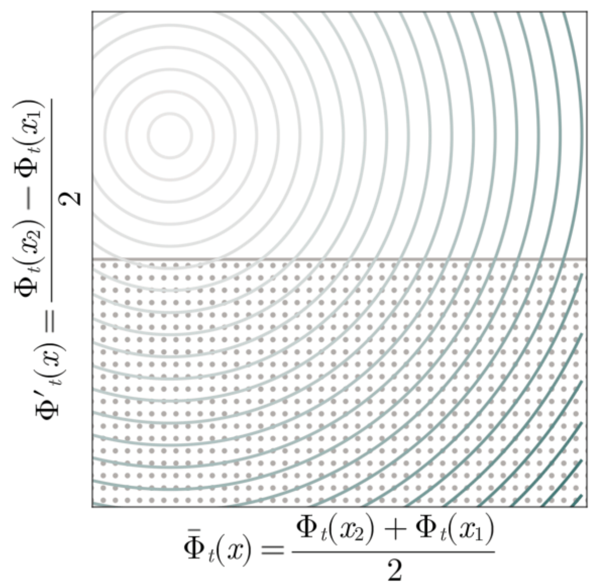
III: Mass collapse

Shocks form when *pushforward* $\rho = \Phi_{\#}\rho_0$ becomes singular

IV: Optimization

Shocks form when constraint activates.

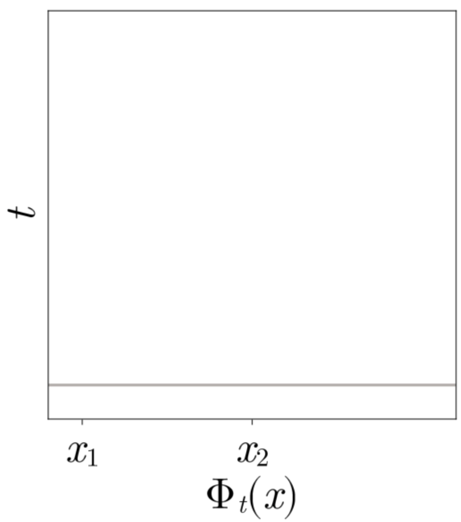
$$\min_{\partial_x \Phi \geq 0} \; -t \int_{\mathbb{R}} u_0(x)\,(\Phi(x) - x)\;\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}} (\Phi(x) - x)^2\;\mathrm{d}x$$



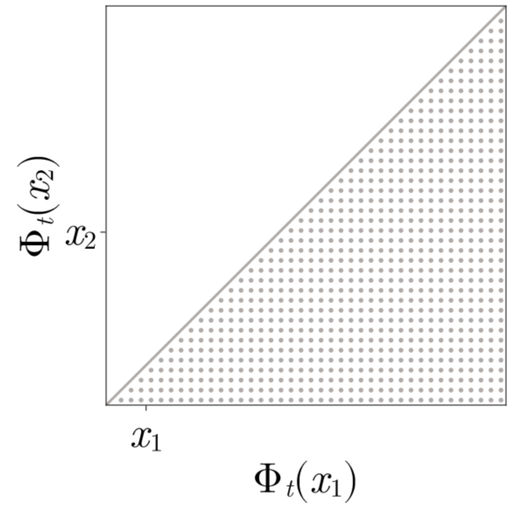
After shock

Vanishing viscosity solutions

merge trajectories

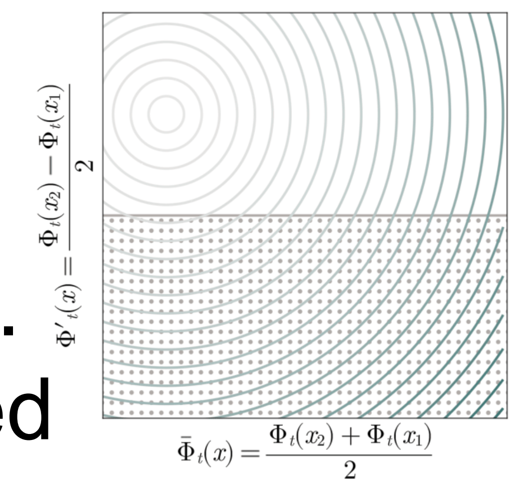


stick to boundary



propagate Diracs

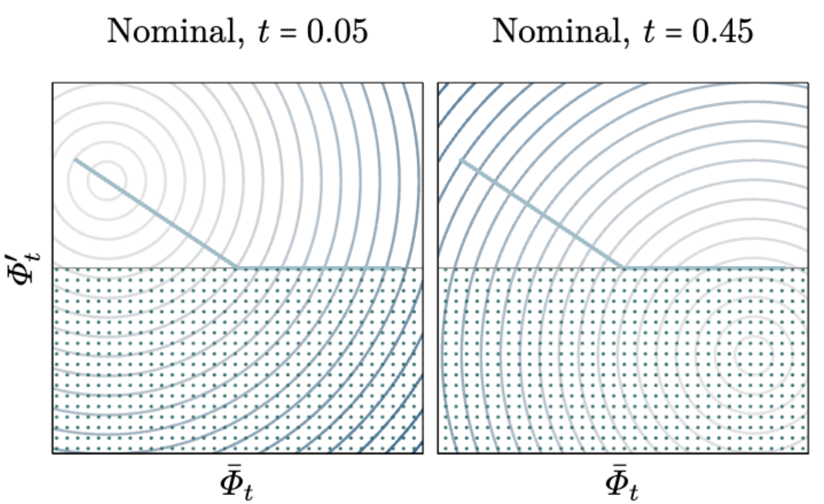
solve ineq. constrained problem



Interior Point Methods for PDEs

Regularize to enforce strict feasibility

$$\min_{\partial_x \Phi \geq 0} -t \int_{\mathbb{R}} u_0(x) \left(\Phi(x) - x\right) \, \mathrm{d}x + \frac{1}{2} \int_{\mathbb{R}} \left(\Phi(x) - x\right)^2 \, \mathrm{d}x$$



Interior Point Methods for PDEs

Regularize to enforce strict feasibility

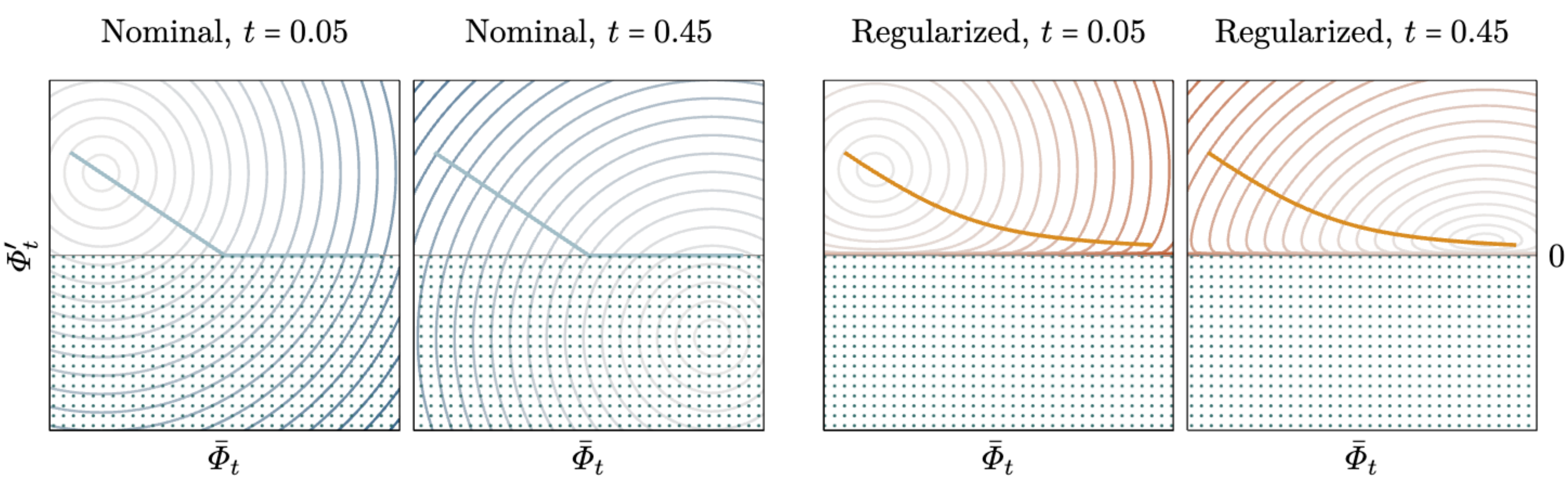
$$\min_{\partial_x \Phi \geq 0} -t \int_{\mathbb{R}} u_0(x)\,(\Phi(x) - x)\;\mathrm{d}x + \underbrace{\psi(\Phi)}_{\text{strictly convex}} - \psi(\mathrm{Id}) - [\mathrm{D}\psi(\mathrm{Id})]\,(\Phi - \mathrm{Id})$$

Nominal problem:

$$\psi_0(\Phi) = \frac{1}{2}\int_{\mathbb{R}} (\Phi(x))^2\;\mathrm{d}x$$

Regularized problem:

$$\psi_\alpha(\Phi) = \psi_0(\Phi) + \alpha \int_{\mathbb{R}} -\log(\partial_x \Phi(x))\;\mathrm{d}x$$

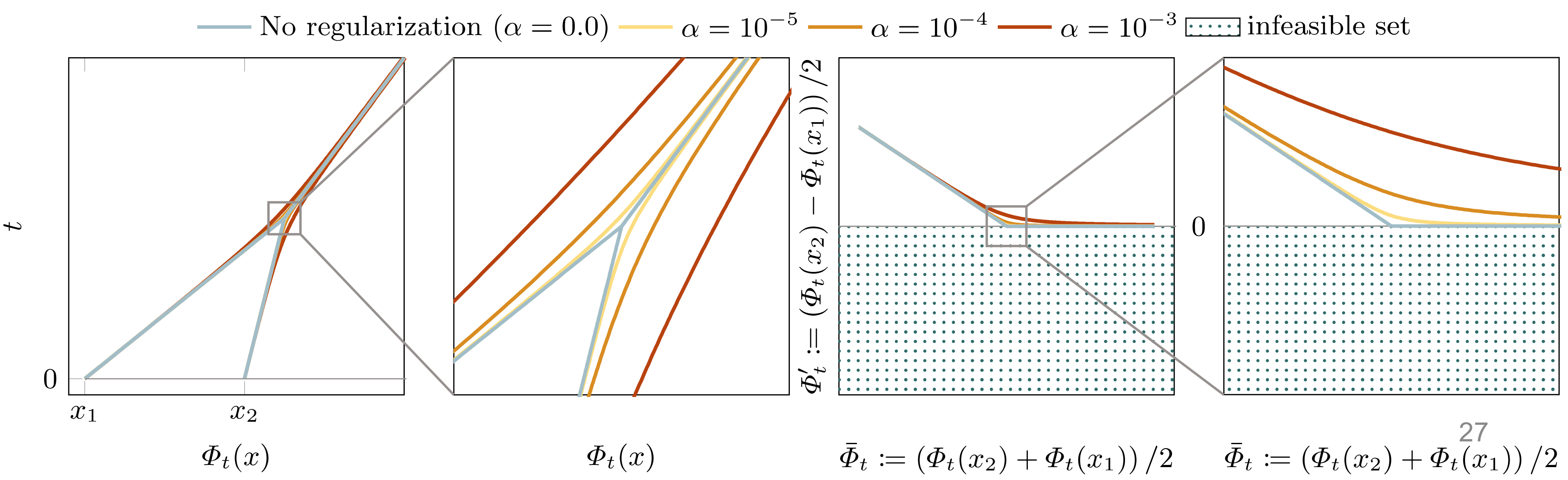


Interior Point Methods for PDEs

Use α to modulate regularization.

Particles converge, but don't collide!

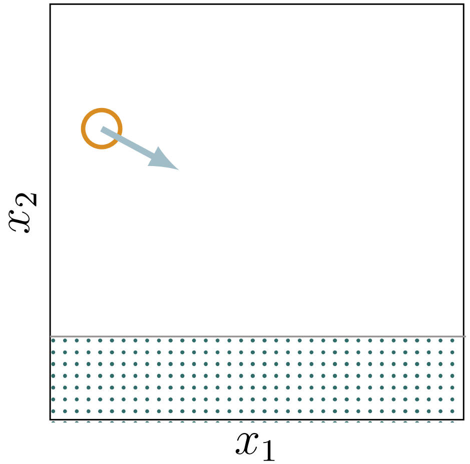
How to extend beyond variational case?



Geometry of Barrier Functions

In differential geometry: Distinguish *points* on manifold and *directions* in tangent space

$\mathrm{Exp}_p(v) :=$ from p, walk in direction v for unit time, return new position



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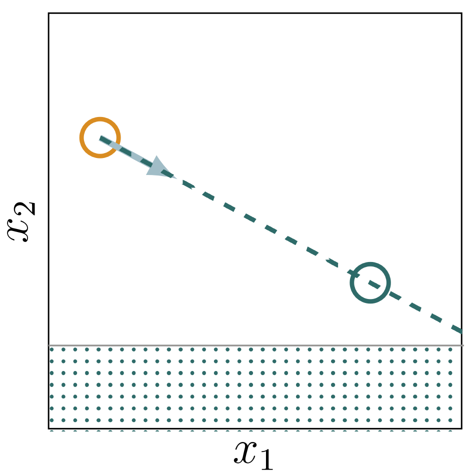
Euclidean: $\mathrm{Exp}_p(v) = p + v$

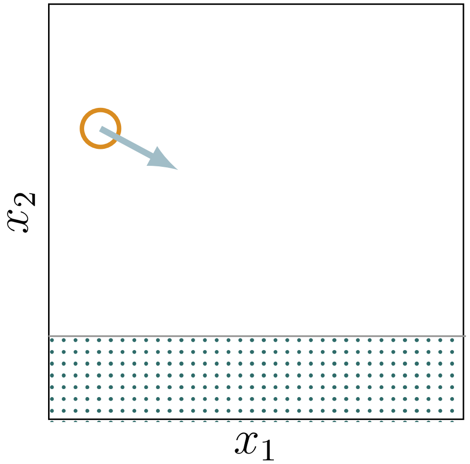


Geometry of Barrier Functions

Barrier function defines *dual* Exp. map

$$\mathrm{Exp}_p^{\psi}(v) := \nabla\psi^{-1}(\nabla\psi(p) + [\mathrm{D}^2\psi(p)]v)$$

Amari & Nagaoka (2000)
Nemirovsky & Yudin (1983)
Amari & Cichocki (2010)
Raskutti & Mukherjee (2013)



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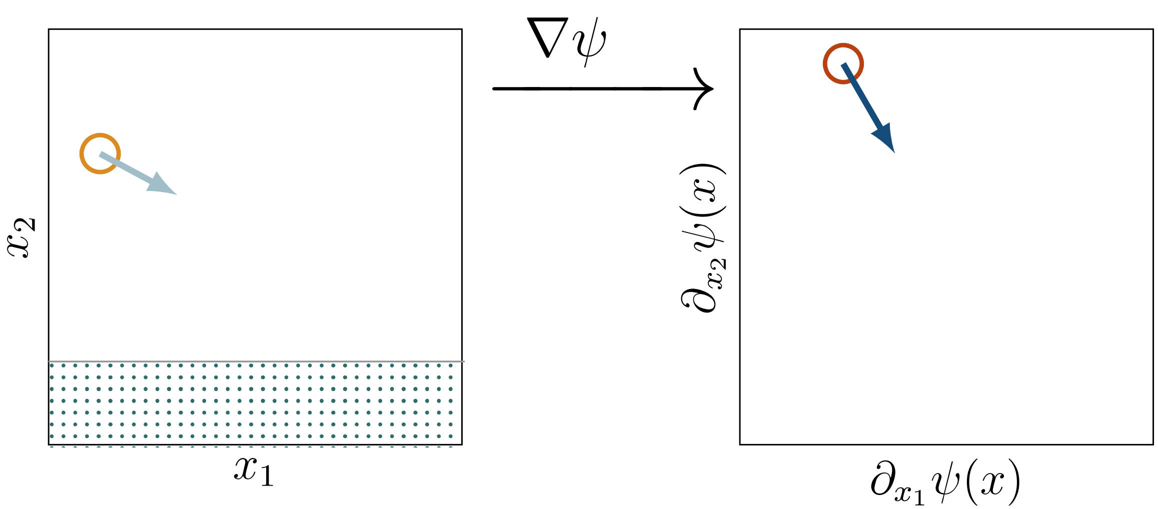

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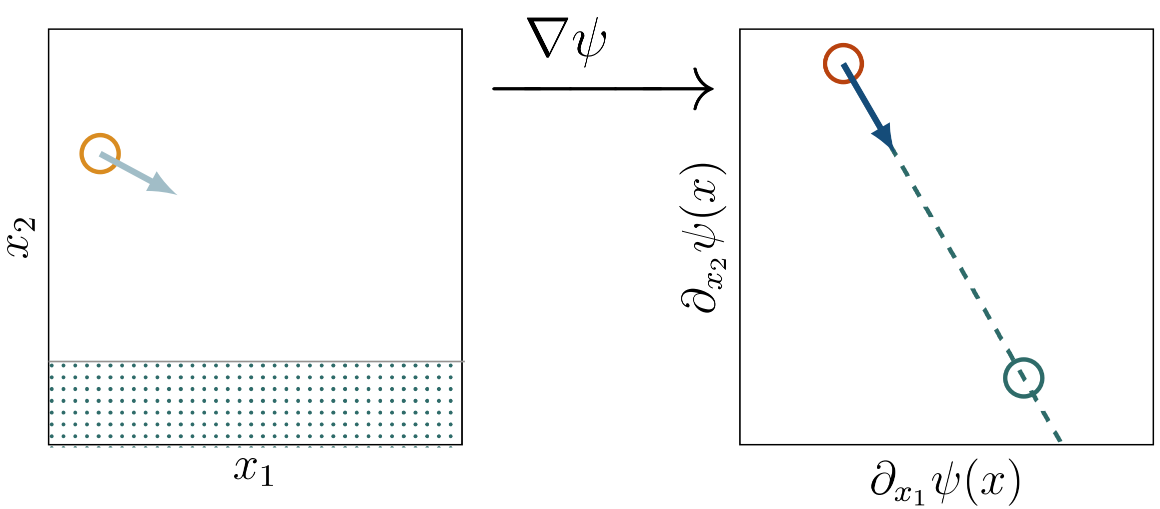

Geometry of Barrier Functions

Barrier function defines *dual* Exp. map

$$\mathrm{Exp}_p^{\psi}(v) := \nabla\psi^{-1}(\nabla\psi(p) + [\mathrm{D}^2\psi(p)]v)$$

Dual straight lines (a.k.a. geodesics) are Euclidean straight lines in $\nabla\psi$-space

Amari & Nagaoka (2000)
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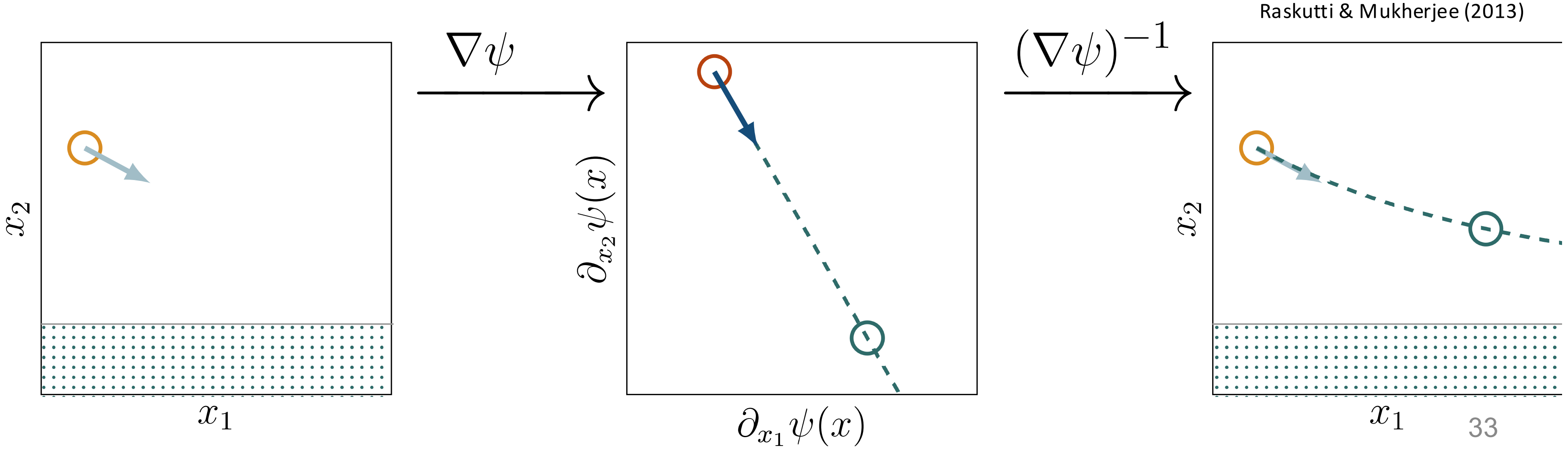
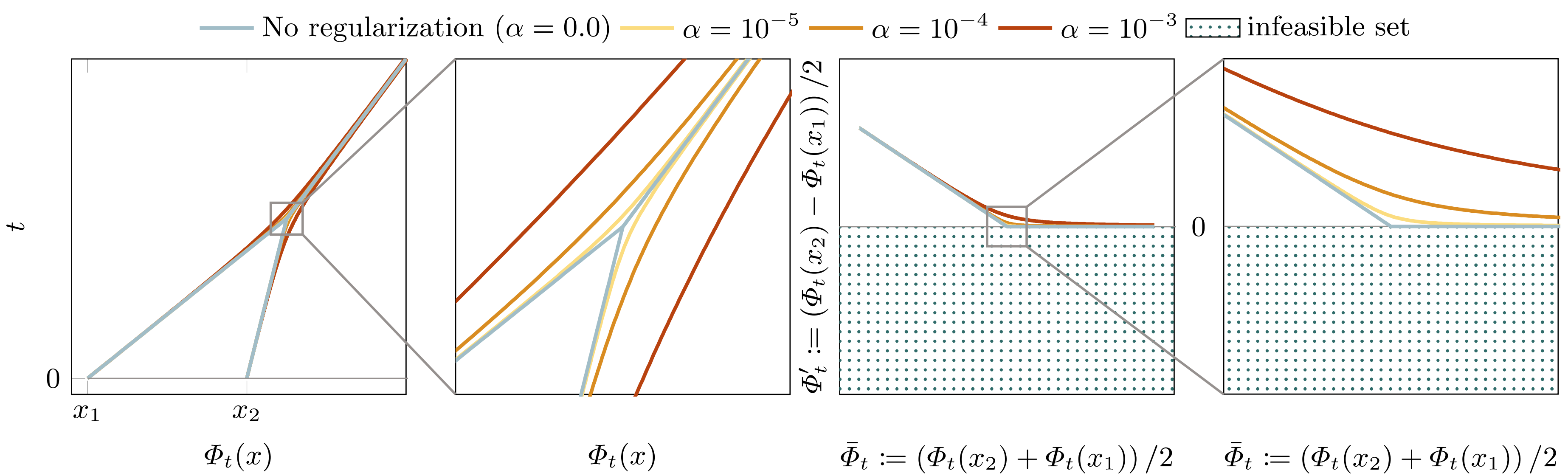


Geometry of Barrier Functions

Solution Paths of IPMs are dual geodesics [Amari 2016], also [Nesterov & Todd, 2002]

Replace characteristics with dual geodesics



The dual equation of motion

Straight lines have the form

$$\varPhi_t = (\nabla\psi)^{-1}\left(\nabla\psi\left(\varPhi_0\right) + t\left[\mathrm{D}^2\psi\left(\varPhi_0\right)\right]\dot{\varPhi}_0\right),$$

yielding

$$\dot{\varPhi}_t = \left[\mathrm{D}^2\psi\left(\varPhi_t\right)\right]^{-1}\left[\mathrm{D}^2\psi\left(\varPhi_0\right)\right]\dot{\varPhi}_0,$$

and the *dual equation of motion*

$$\ddot{\varPhi}_t = -\left[\mathrm{D}^2\psi\left(\varPhi_t\right)\right]^{-1}\left[\mathrm{D}^3\psi\left(\varPhi_t\right)\right]\left(\dot{\varPhi}_t, \dot{\varPhi}_t\right).$$

Time to Compute

$$\left(\frac{(x-1)^2}{2} - \alpha\log(x)\right)''' = \left((x-1) - \alpha\frac{1}{x}\right)'' = \left(1 + \alpha\frac{1}{x^2}\right)' = \left(-\alpha\frac{2}{x^3}\right)$$

and minor wrinkles.

$$[\mathrm{D}\psi(\mathit{\Phi})](U) = \int_{\mathbb{R}} (\mathit{\Phi}(x) - x)U(x)\ \mathrm{d}x + \alpha\int_{\mathbb{R}} -\frac{\partial_x U(x)}{\partial_x \mathit{\Phi}(x)}\ \mathrm{d}x$$

$$\Rightarrow \nabla\psi(\mathit{\Phi}) = \mathit{\Phi} - x + \alpha\partial_x\left(\frac{1}{\partial_x\mathit{\Phi}}\right).$$

$$\left[\mathrm{D}^2\psi(\mathit{\Phi})\right](U,V) = \int_{\mathbb{R}} U(x)\cdot V(x)\ \mathrm{d}x + \alpha\int_{\mathbb{R}} \frac{\partial_x U(x)\cdot\partial_x V(x)}{\left(\partial_x\mathit{\Phi}(x)\right)^2}\ \mathrm{d}x$$

$$\Rightarrow \left[\mathrm{D}^2\psi(\mathit{\Phi})\right] : U \mapsto U - \alpha\cdot\partial_x\left(\frac{\partial_x U}{\left(\partial_x\mathit{\Phi}\right)^2}\right).$$

$$\left[\mathrm{D}^3\psi(\mathit{\Phi})\right](U,V,W) = -2\alpha\int_{\mathbb{R}} \frac{\partial_x U(x)\cdot\partial_x V(x)\cdot\partial_x W(x)}{\left(\partial_x\mathit{\Phi}(x)\right)^3}\ \mathrm{d}x$$

$$\Rightarrow \left[\mathrm{D}^3\psi(\mathit{\Phi},\mathit{\Phi}')\right] :\ (U,V) \mapsto 2\alpha\partial_x\left(\frac{\partial_x U\cdot\partial_x V}{(\partial_x\mathit{\Phi})^3}\right).$$

Time to Compute

Plug into dual equation of motion

$$\ddot{\Phi}_t = -\left[\mathrm{D}^2\psi\left(\Phi_t\right)\right]^{-1}\left[\mathrm{D}^3\psi\left(\Phi_t\right)\right]\left(\dot{\Phi}_t, \dot{\Phi}_t\right)$$

$$= \left(\left(\cdot\right) - \alpha\partial_x\left(\left[\partial_x\Phi_t\right]^{-2}\left[\partial_x(\cdot)\right]\right)\right)^{-1}\left(-2\alpha\partial_x\left(\left[\partial_x\Phi_t\right]^{-3}\left[\partial_x\dot{\Phi}_t\right]^2\right)\right)$$

Defining $\quad u\left(\Phi(x)\right) := \dot{\Phi}(x), \quad \rho(\Phi(x)) := \dfrac{1}{\partial_x\Phi(x)},$

$$\begin{cases} \partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \operatorname{div}\begin{pmatrix} \rho u^2 \qquad\qquad + \Sigma \\ \rho u \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha\partial_x(\rho^{-1}\partial_x\Sigma) = 2\alpha[\partial_x u]^2. \end{cases}$$

Time to Compute

Plug into dual equation of motion

$$\ddot{\Phi}_t = -\left[\mathrm{D}^2\psi\left(\Phi_t\right)\right]^{-1}\left[\mathrm{D}^3\psi\left(\Phi_t\right)\right]\left(\dot{\Phi}_t, \dot{\Phi}_t\right)$$

$$= \left((\cdot) - \alpha\partial_x\left([\partial_x\Phi_t]^{-2}\left[\partial_x(\cdot)\right]\right)\right)^{-1}\left(-2\alpha\partial_x\left([\partial_x\Phi_t]^{-3}[\partial_x\dot{\Phi}_t]^2\right)\right)$$

Defining $$u\left(\Phi(x)\right) := \dot{\Phi}(x), \quad \rho(\Phi(x)) := \frac{1}{\partial_x\Phi(x)},$$

Add external forces & pressure

$$\begin{cases} \partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \mathrm{div}\begin{pmatrix} \rho u^2 + P(\rho) + \Sigma \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha\partial_x(\rho^{-1}\partial_x\Sigma) = 2\alpha[\partial_x u]^2. \end{cases}$$

Extension to Multivariate case

Naïve extension to multivariate Euler

$$\psi(\Phi) = \frac{1}{2}\int_{\mathbb{R}^d} \|\Phi(x) - x\|^2 \mathrm{d}x + \alpha \int_{\mathbb{R}^d} -\log\det(\mathrm{D}\Phi(x))\mathrm{d}x$$

Analog to

linear program → semidefinite program.

But logdet non-convex on general matrices.

Set of diffeomorphisms is not convex!

Extension to Multivariate case

Idea: Lift to $\mathcal{E} := \left(\mathbf{I} + S\left(\mathbb{R}^d;\mathbb{R}^d\right)\right) \times \left(1 + S\left(\mathbb{R}^d\right)\right)$

$$\psi(\Phi, \Phi') = \frac{1}{2}\int_{\mathbb{R}^d} \|\Phi(x) - x\|^2 \mathrm{d}x + \alpha \int_{\mathbb{R}^d} -\log(\Phi'(x))\mathrm{d}x$$

View diffeomorphisms as submanifold

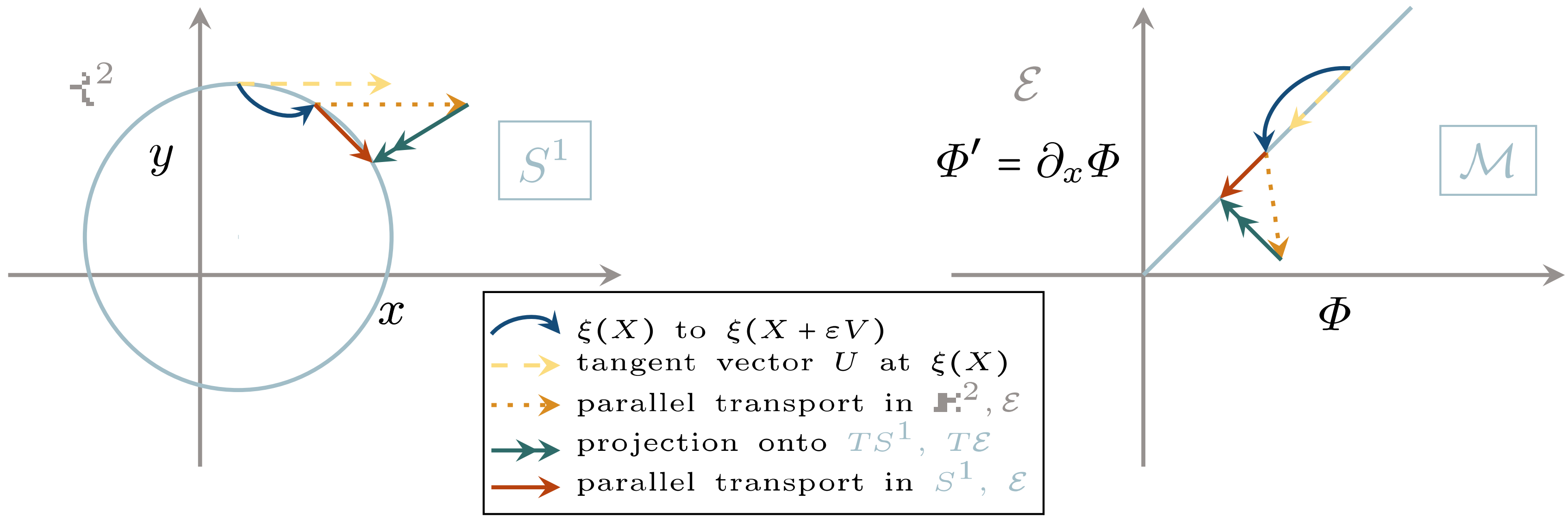
$$\{(\Phi, \Phi') : \Phi' = \det\left(\mathrm{D}\Phi\right)\}$$

with embedding

$$\xi : \Phi \mapsto (\Phi, \det\left(\mathrm{D}\Phi\right))$$

Extension to Multivariate case

Embedding induces exp. on submanifold



$$0 = \ddot{\Phi} + \left([\mathrm{D}\xi(\Phi)]^* \left[\mathrm{D}^2\psi(\xi(\Phi))\right][\mathrm{D}\xi(\Phi)]\right)^{-1} [\mathrm{D}\xi(\Phi)]^* \left[\mathrm{D}^2\psi(\xi(\Phi))\right]$$

$$\left(\left[\mathrm{D}^2\xi(\Phi)\right]\left(\dot{\Phi}, \dot{\Phi}\right) + \left[\mathrm{D}^2\psi(\Phi)\right]^{-1}\left[\mathrm{D}^3\psi(\xi(\Phi))\right]\left([\mathrm{D}\xi(\Phi)]\dot{\Phi}, [\mathrm{D}\xi(\Phi)]\dot{\Phi}\right)\right).$$

Curvature of embedding

Curvature of barrier geometry

Extension to Multivariate case

Re-express as Eulerian conservation law

$$\begin{cases} \partial_t \begin{pmatrix} \rho \boldsymbol{u} \\ \rho \end{pmatrix} + \operatorname{div} \begin{pmatrix} \rho \boldsymbol{u} \otimes \boldsymbol{u} + (P(\rho) + \Sigma)\, \mathbf{I} \\ \rho \boldsymbol{u} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ 0 \end{pmatrix} \\ \rho^{-1} \Sigma - \alpha \operatorname{div}(\rho^{-1} \nabla \Sigma) = \alpha \left(\operatorname{tr}^2 \left([\mathrm{D} \boldsymbol{u}] \right) + \operatorname{tr} \left([\mathrm{D} \boldsymbol{u}]^2 \right) \right) . \end{cases}$$

$$\begin{aligned} 0 = \ddot{\Phi} + \left([\mathrm{D}\xi(\Phi)]^* \left[\mathrm{D}^2 \psi(\xi(\Phi)) \right] [\mathrm{D}\xi(\Phi)] \right)^{-1} [\mathrm{D}\xi(\Phi)]^* \left[\mathrm{D}^2 \psi(\xi(\Phi)) \right] \\ \left(\left[\mathrm{D}^2 \xi(\Phi) \right] \left(\dot{\Phi}, \dot{\Phi} \right) + \left[\mathrm{D}^2 \psi(\Phi) \right]^{-1} \left[\mathrm{D}^3 \psi(\xi(\Phi)) \right] \left([\mathrm{D}\xi(\Phi)] \dot{\Phi}, [\mathrm{D}\xi(\Phi)] \dot{\Phi} \right) \right) . \end{aligned}$$

IGR and diffusion

IGR provides *inviscid* regularization

$$\begin{cases} \partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) + \Sigma \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha \partial_x (\rho^{-1} \partial_x \Sigma) = 2\alpha \big([\partial_x u] \big) \; [\partial_x u]. \end{cases}$$

But squinting *a lot*, reminds of viscous reg.

IGR vs LAD

Example: Localized Artificial Diffusivity (LAD)

[Cook & Cabot 2005, Kawai & Lele 2008, Mani et al. 2009] and others

IGR:

$$\begin{cases} \partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) + \Sigma \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha\partial_x(\rho^{-1}\partial_x\Sigma) = 2\alpha\ [\partial_x u]\ [\partial_x u]. \end{cases}$$

LAD:

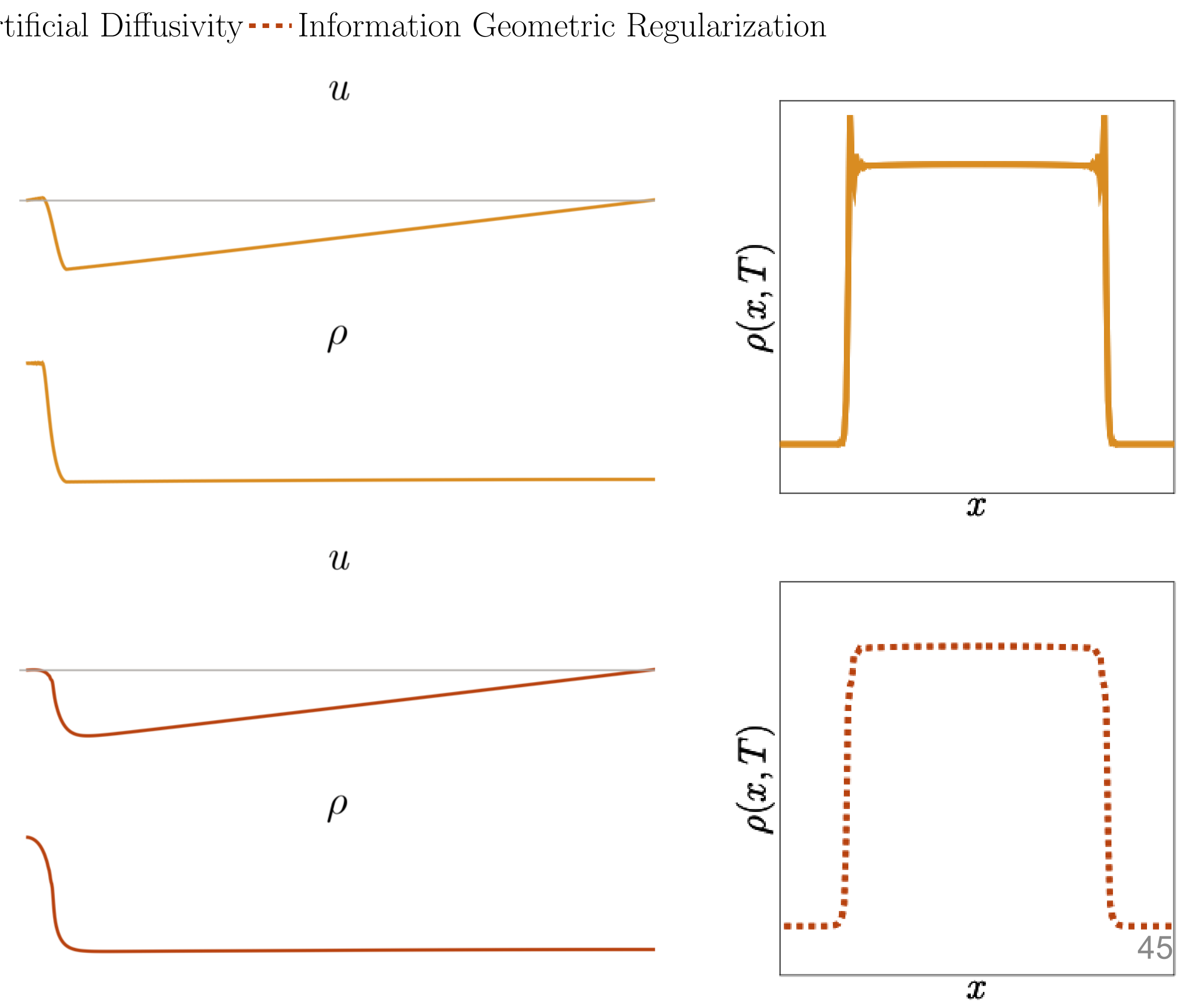
$$\begin{cases} \partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) + \Sigma \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma \cancel{- \alpha\partial_x(\rho^{-1}\partial_x\Sigma)} = 2\alpha\left([\partial_x u]\right)_{-}[\partial_x u]. \end{cases}$$

"Viscosity" nonlocal and nonpositive

Nonlocality reduces oscillation

$$\begin{cases}\partial_t \begin{pmatrix}\rho u\\ \rho\end{pmatrix} + \partial_x \begin{pmatrix}\rho u^2 + P(\rho)+\Sigma \\ \rho u\end{pmatrix} = \begin{pmatrix} f\\ 0\end{pmatrix}\\ \rho^{-1}\Sigma - \alpha\partial_x(\rho^{-1}\partial_x\Sigma) = 2\alpha\ [\partial_x u]\ \ [\partial_x u].\end{cases}$$

$$\begin{cases}\partial_t \begin{pmatrix}\rho u\\ \rho\end{pmatrix} + \partial_x \begin{pmatrix}\rho u^2 + P(\rho)+\Sigma \\ \rho u\end{pmatrix} = \begin{pmatrix} f\\ 0\end{pmatrix}\\ \rho^{-1}\Sigma \cancel{- \alpha\partial_x(\rho^{-1}\partial_x\Sigma)} = 2\alpha\left([\partial_x u]\right)_- [\partial_x u].\end{cases}$$



Nonpositivity reduces dissipation

$$\begin{cases} \partial_t \begin{pmatrix}\rho u\\ \rho\end{pmatrix} + \partial_x \begin{pmatrix}\rho u^2+P(\rho)+\Sigma\\ \rho u\end{pmatrix} = \begin{pmatrix} f\\ 0\end{pmatrix}\\ \rho^{-1}\Sigma - \alpha\partial_x(\rho^{-1}\partial_x\Sigma) = 2\alpha\ [\partial_x u]\ \ [\partial_x u]. \end{cases}$$

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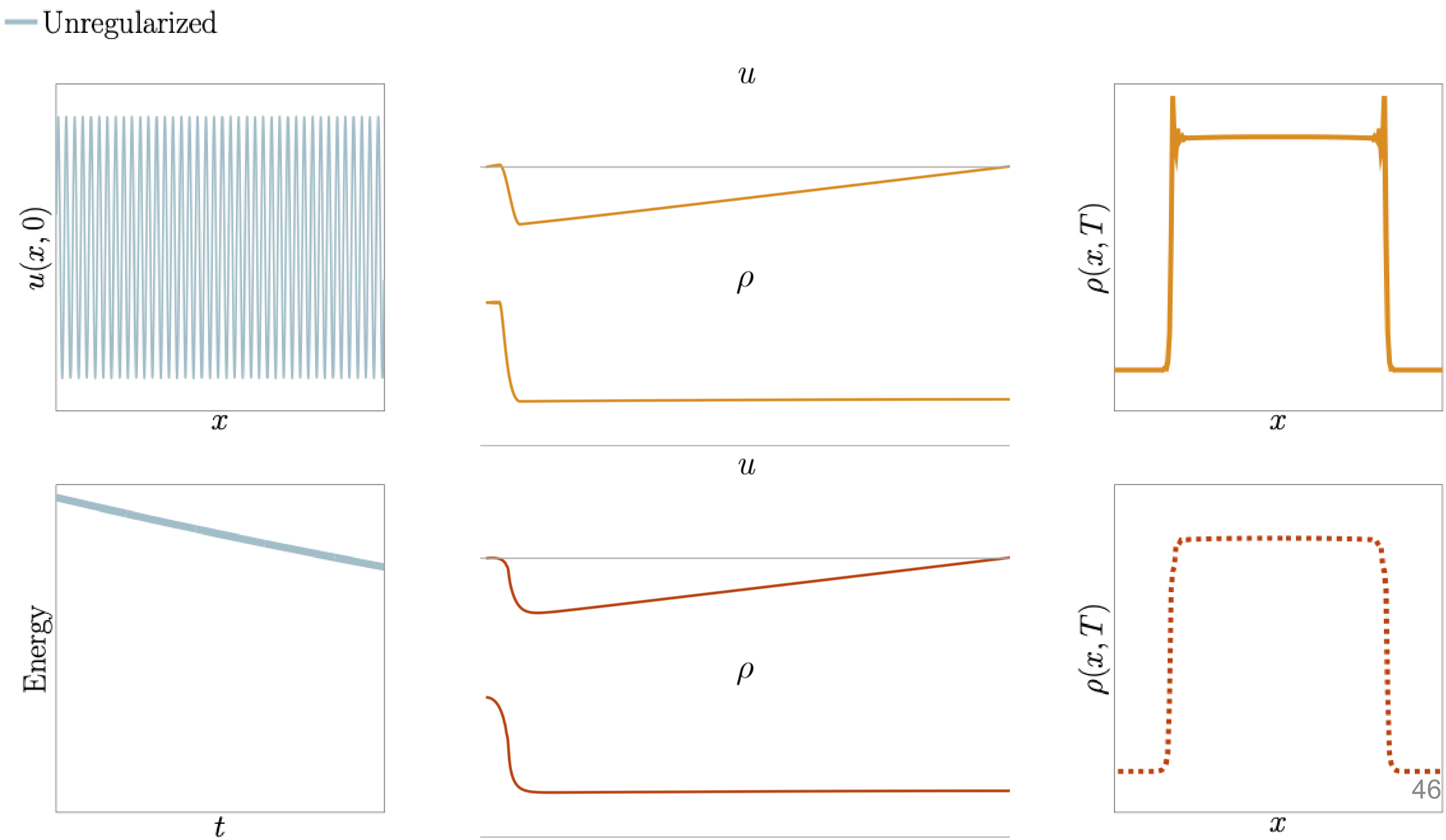

Nonpositivity reduces dissipation

$$\begin{cases} \partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) + \Sigma \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha \partial_x (\rho^{-1} \partial_x \Sigma) = 2\alpha \; [\partial_x u] \;\; [\partial_x u]. \end{cases}$$

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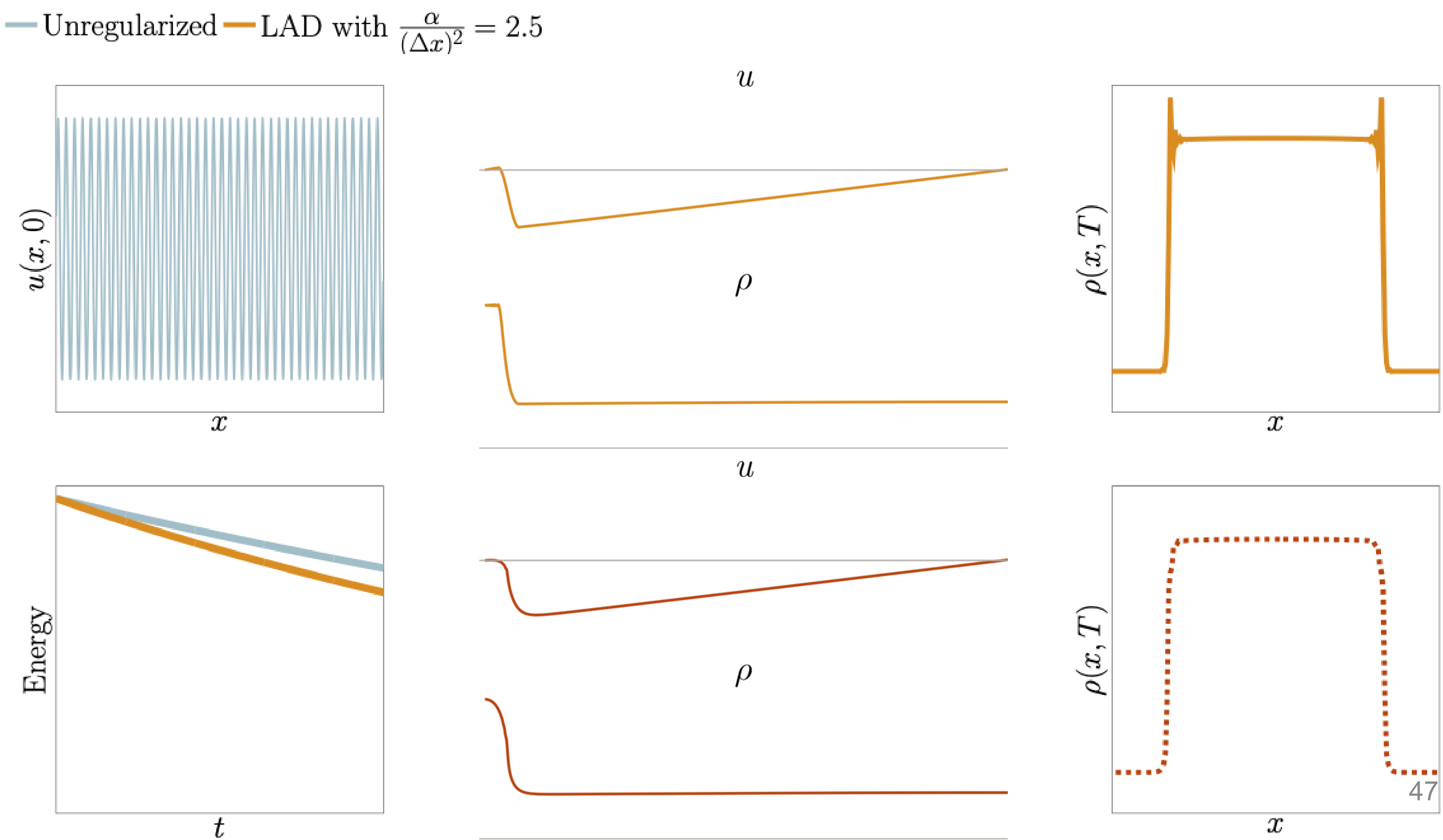

Nonpositivity reduces dissipation

$$\begin{cases} \partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) + \Sigma \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha\partial_x(\rho^{-1}\partial_x\Sigma) = 2\alpha \; [\partial_x u] \quad [\partial_x u]. \end{cases}$$

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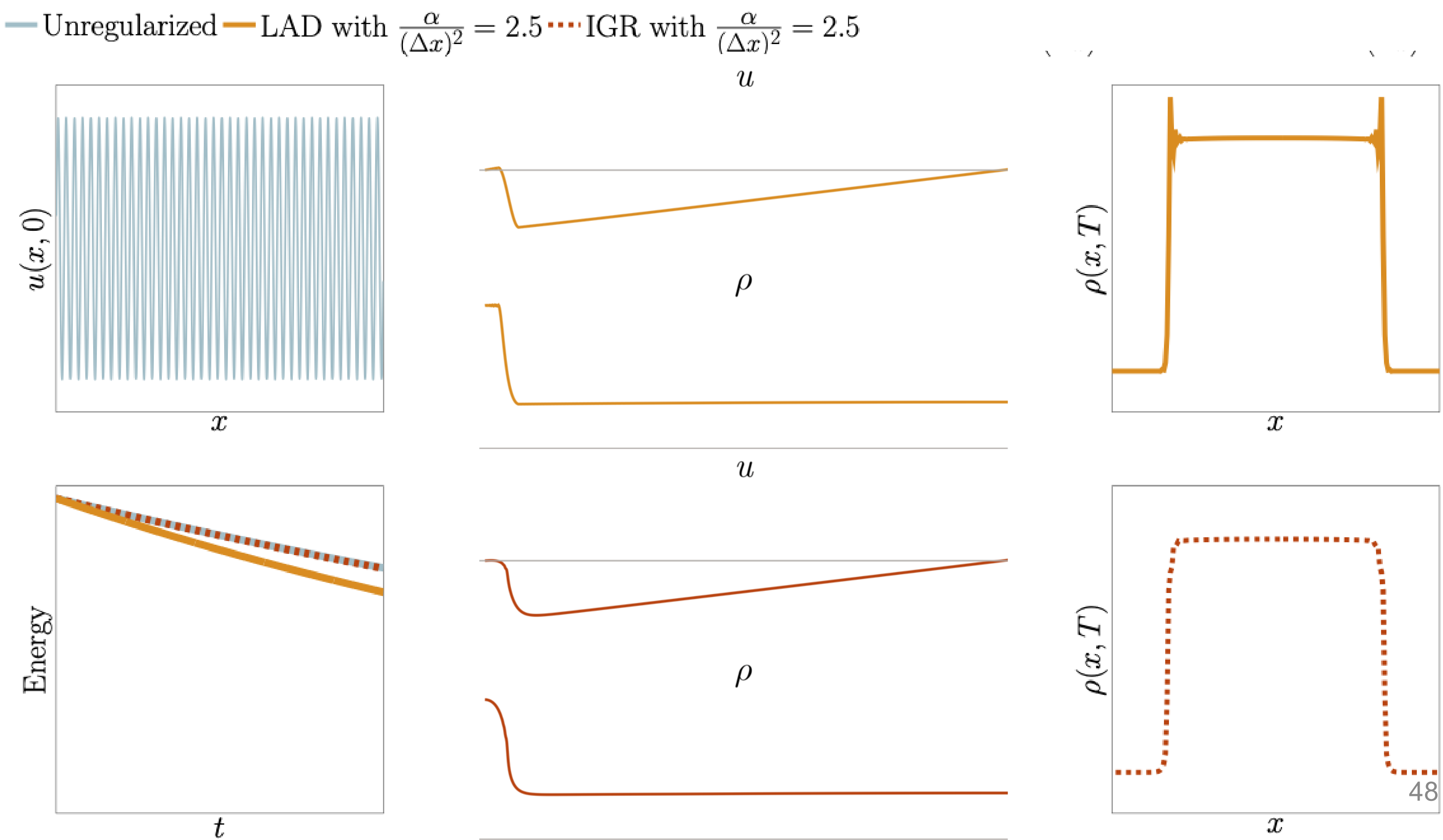

Nonpositivity reduces dissipation

$$\begin{cases} \partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) + \Sigma \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha \partial_x(\rho^{-1}\partial_x \Sigma) = 2\alpha \ [\partial_x u] \ \ [\partial_x u]. \end{cases}$$

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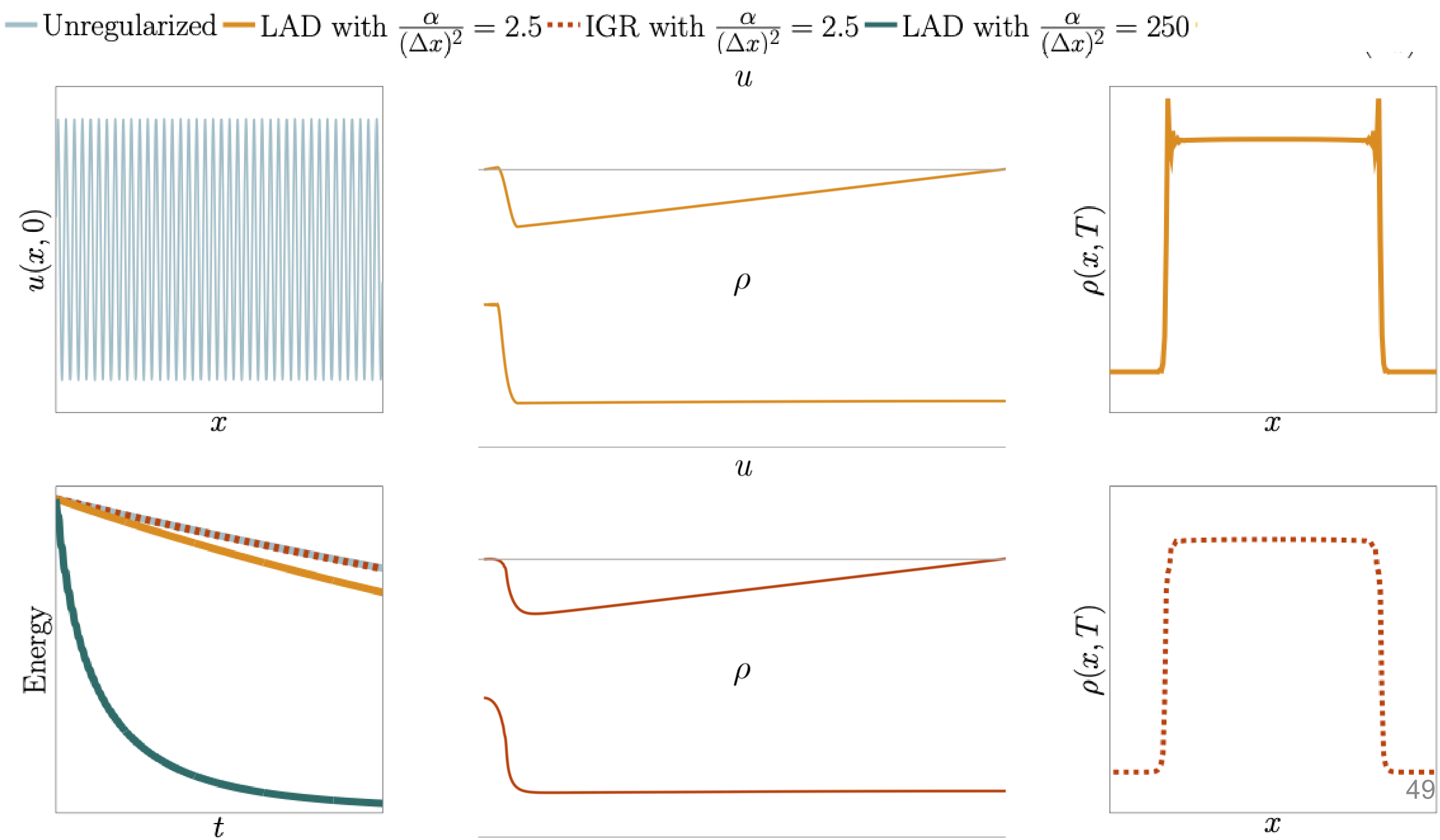

Nonpositivity reduces dissipation

$$\begin{cases} \partial_t \begin{pmatrix} \rho u \\ \rho \end{pmatrix} + \partial_x \begin{pmatrix} \rho u^2 + P(\rho) + \Sigma \\ \rho u \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha\partial_x(\rho^{-1}\partial_x \Sigma) = 2\alpha \; [\partial_x u] \; [\partial_x u]. \end{cases}$$

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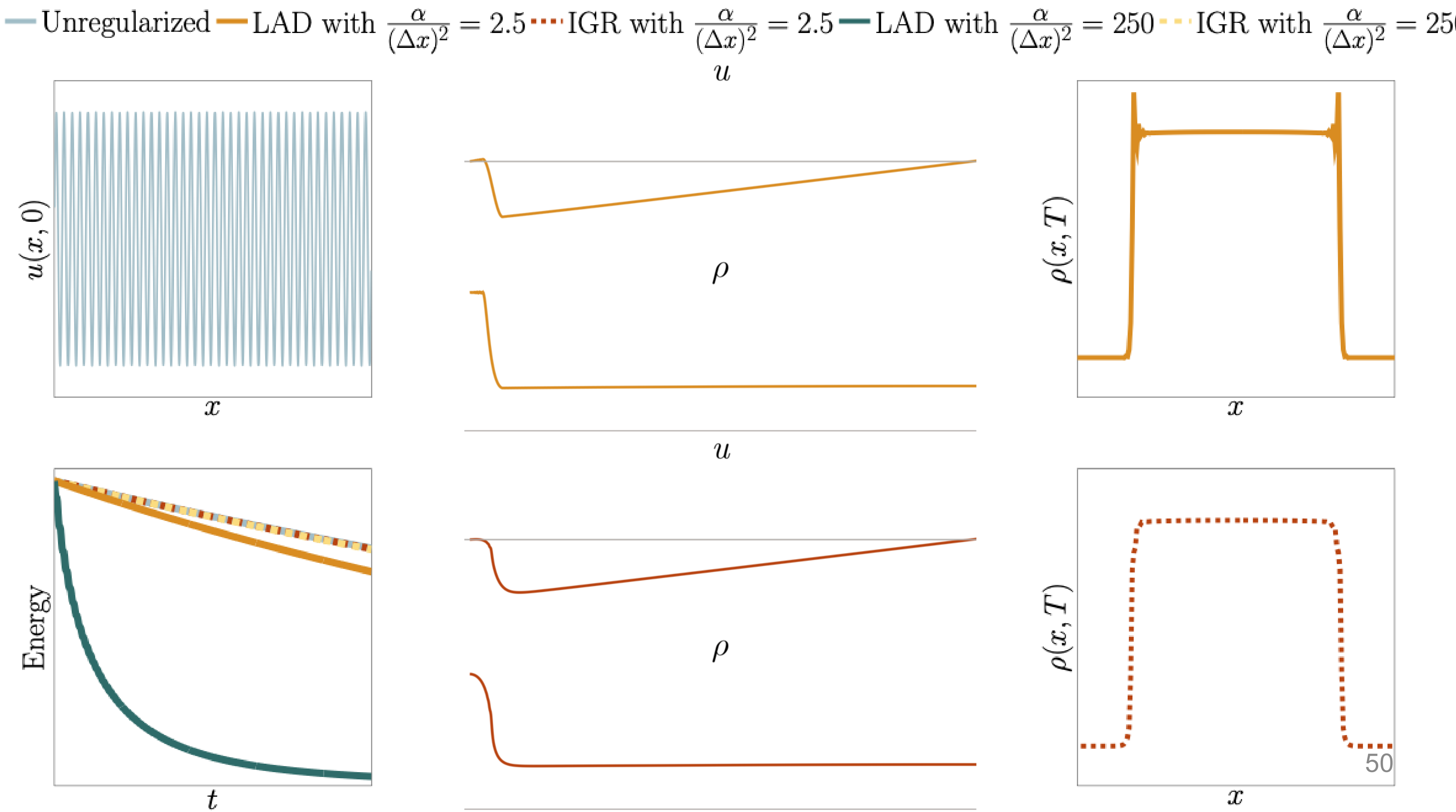

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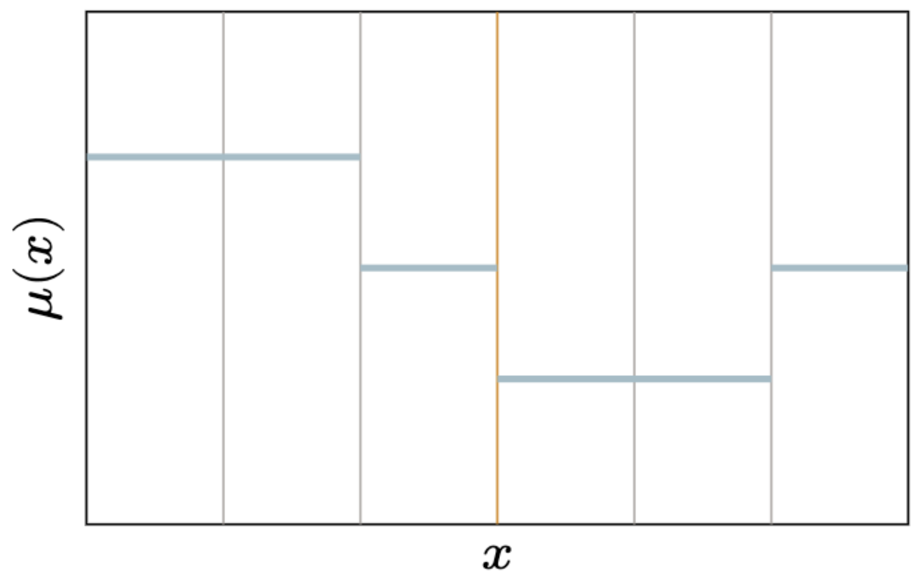
Part II: Practical Applications

EXASCALE APPLICATIONS OF INFORMATION GEOMETRIC REGULARIZATION

R. Budiardjia
Oak Ridge

Finite Volume Methods

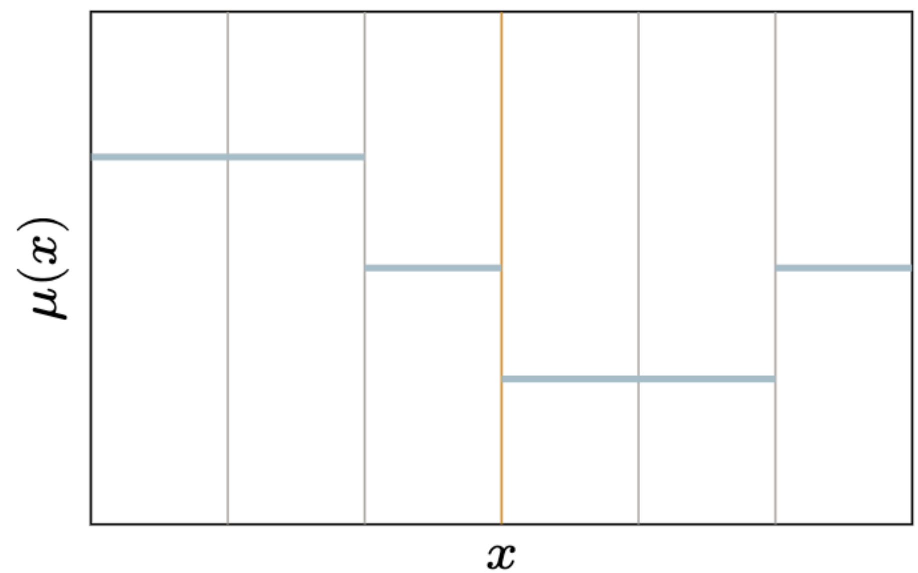
Keep track of cell averages of soln.



Finite Volume Methods

Keep track of cell averages of soln.

Compute left/right reconstruction

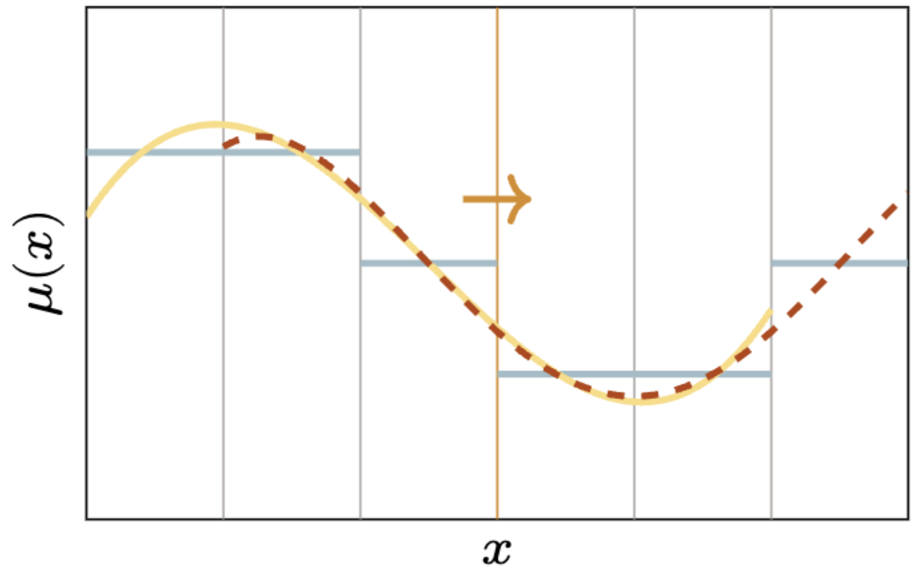


Finite Volume Methods

Keep track of cell averages of soln.

Compute left/right reconstruction

Compute flux through interface

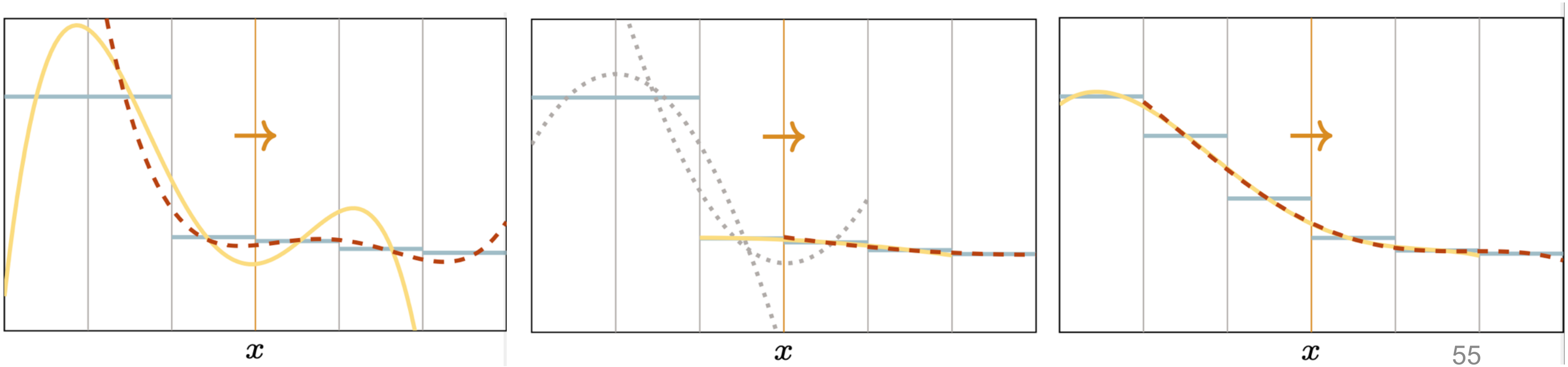


Shocks and Oscillations

Discontinuities cause oscillations

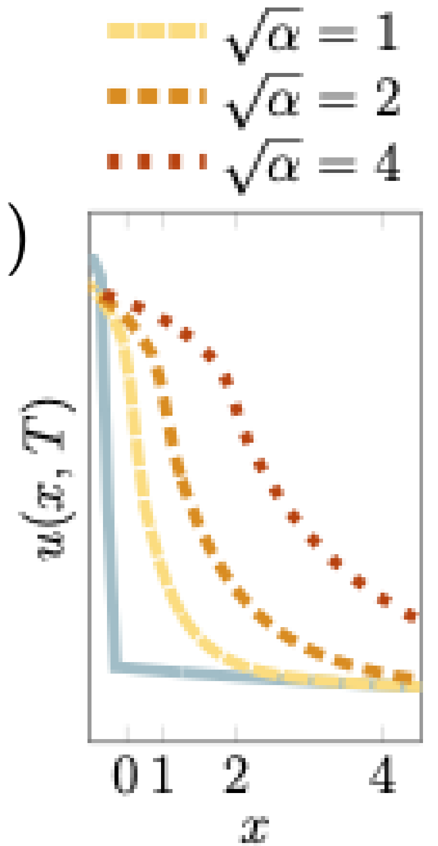
Common remedy: (W)ENO type limiters

With IGR, can use standard reconstruction



But is it not too costly?

$$\begin{cases} \partial_t \begin{pmatrix} \rho \boldsymbol{u} \\ \rho \end{pmatrix} + \operatorname{div} \begin{pmatrix} \rho \boldsymbol{u} \otimes \boldsymbol{u} + (p + \Sigma)\mathbf{I} \\ \rho \boldsymbol{u} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ 0 \end{pmatrix} \\ \rho^{-1}\Sigma - \alpha \operatorname{div}(\rho^{-1}\nabla\Sigma) = \alpha \left(\operatorname{tr}^2([\mathrm{D}\boldsymbol{u}]) + \operatorname{tr}([\mathrm{D}\boldsymbol{u}]^2)\right) \end{cases}$$



Computing flux needs solving for Σ

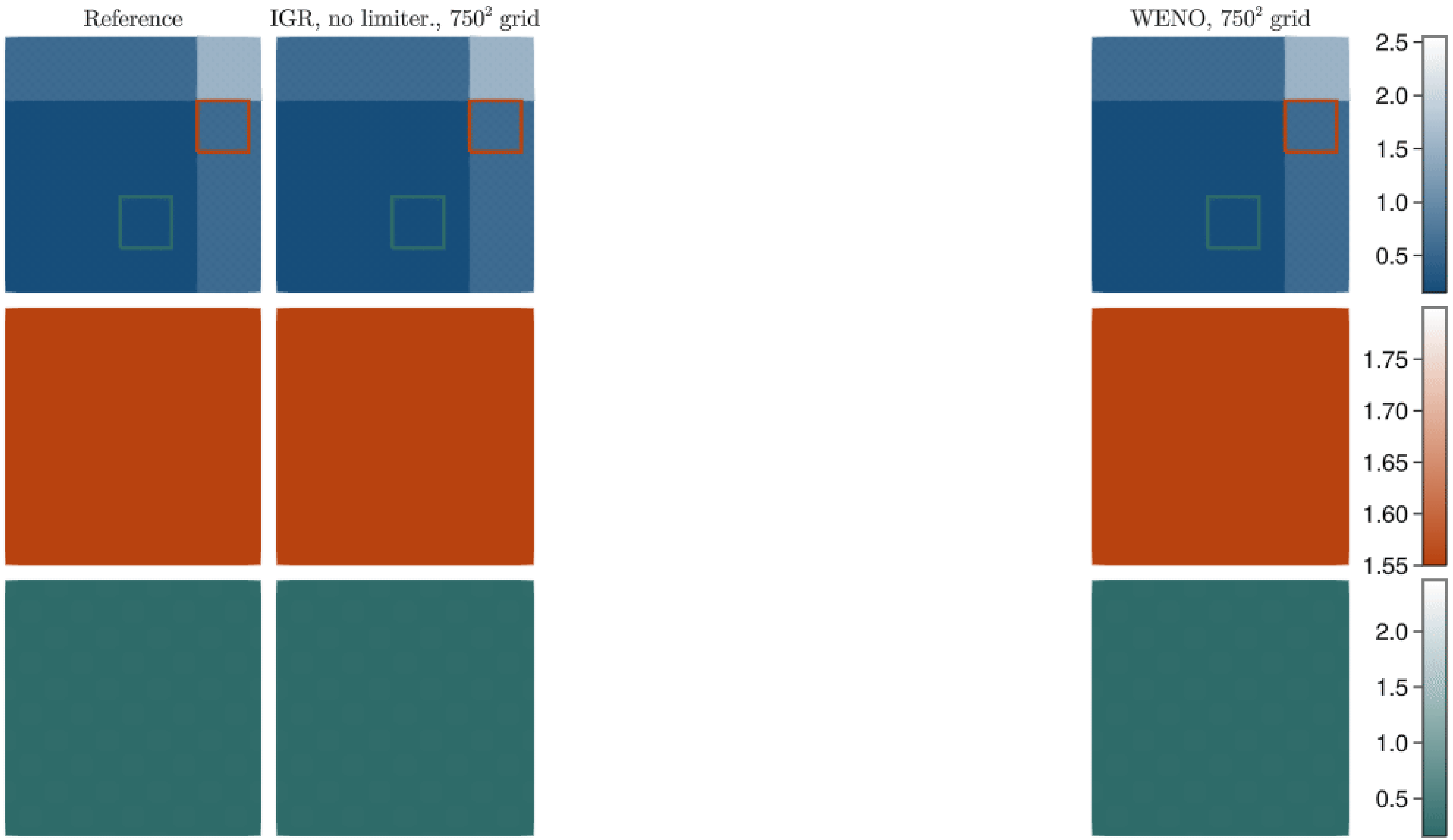
Elliptic Pb., But shock width is $\sqrt{\alpha}$

Choose $\sqrt{\alpha} \propto$ mesh width
⇒ system is well-cond.

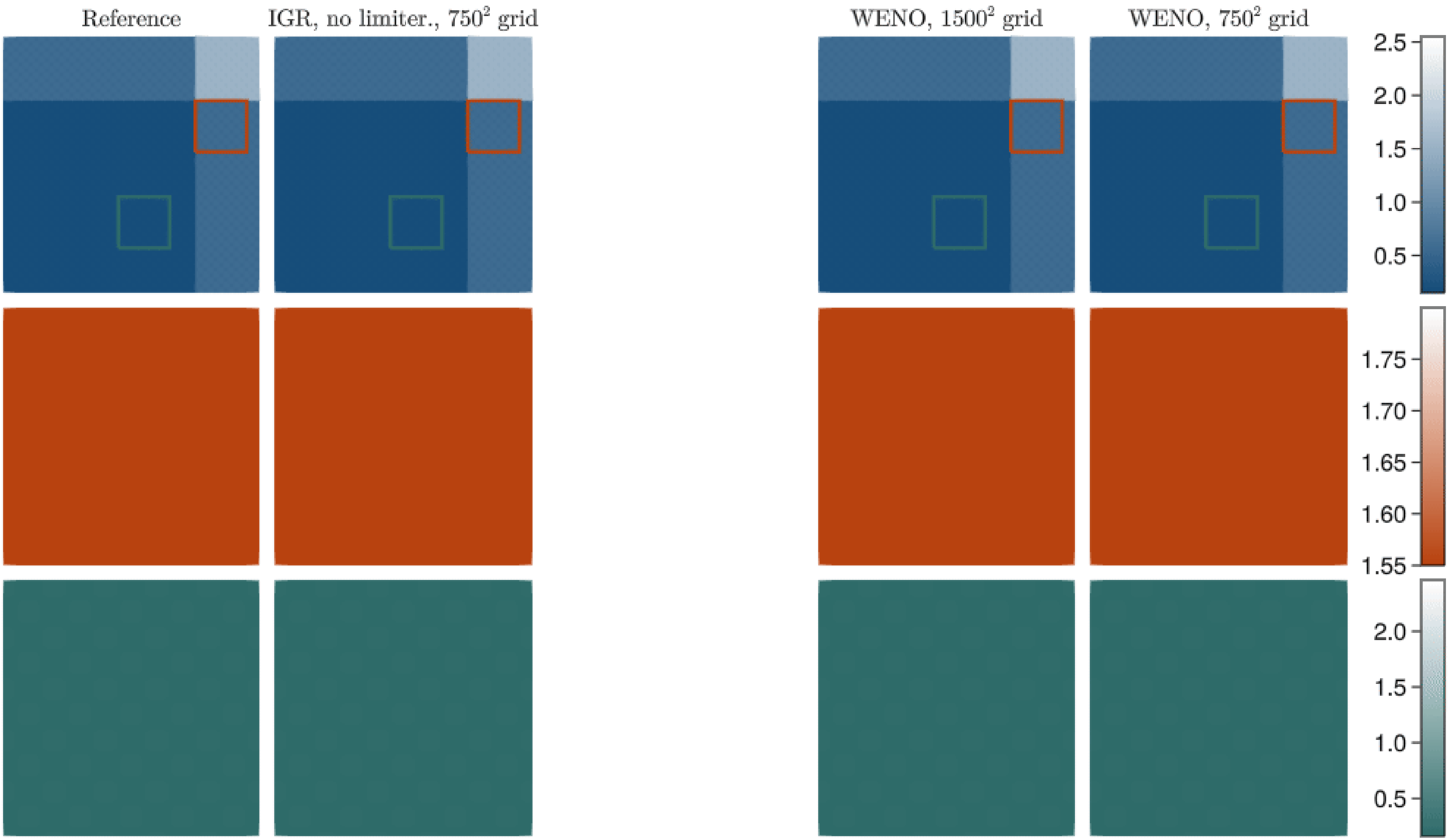
Two Jacobi iters suffice, negligible cost

Beyond Barotropic: Add Σ to pressure

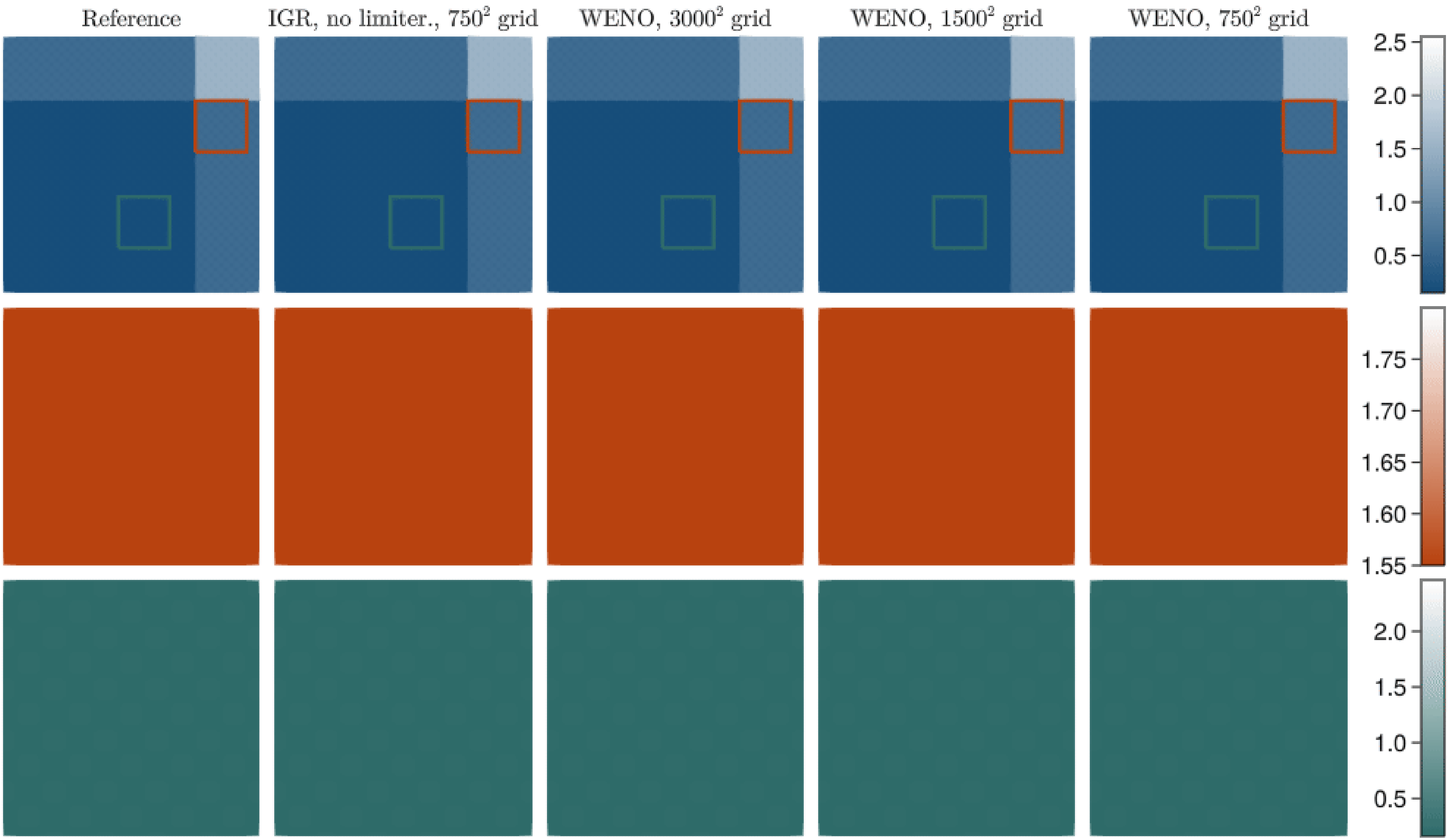
Riemann pb. with entropy wave



Riemann pb. with entropy wave



Riemann pb. with entropy wave



Application at Exascale

Collaborative effort to achieve largest ever compressible CFD simulation

Integrate IGR into MFC code developed by Bryngelson group

Simulate back heating in multi-engine rockets

Simulating many-engine spacecraft: Exceeding 1 quadrillion degrees of freedom via information geometric regularization

Benjamin Wilfong*, Anand Radhakrishnan*, Henry Le Berre*, Daniel J. Vickers*, Tanush Prathi*, Nikolaos Tselepidis†, Benedikt Dorschner†, Reuben Budiardja‡, Brian Cornille§, Stephen Abbott¶, Florian Schäfer‖, Spencer H. Bryngelson*

Application at Exascale

Removing Riemann Solvers + Limiters enables 20x problem size and 4x speedup.

Further size improvements through unified memory and mixed precision computation

First CFD simulation with >1 quadrillion dofs

2025 Gordon Bell Prize Finalist

Information Geom. Reg.

Exp^{ψ} extends IPMs from opt. to dynamics

On prob. simplex Δ_{n-1}, define neg-entropy

$$\psi(x) := -\sum_{i=1}^{n} x_i \log(x_i)$$

Exp^{ψ} is the only exp. map on Δ_{n-1} invariant under sufficient statistics, geodesically complete, and flat! [Chentsov 1972]

Geometries of samples and distributions

Log determinant is neg.

Shannon entropy of ρ

$$\int_{\mathbb{R}^d} \log\det([\mathrm{D}\Phi](x))\ \mathrm{d}x = \int_{\mathbb{R}^d} \log\det([\mathrm{D}\Phi]\circ\Phi^{-1}(x))\det([\mathrm{D}\Phi]^{-1}]\circ\Phi^{-1}(x))\ \mathrm{d}x = -\int_{\mathbb{R}^d} \rho(x)\log(\rho(x))\ \mathrm{d}x$$

$||\phi||_{L^2}^2$: Particle geometry, Wasserstein geodesic

Logdet: Information geometry, dual geodesic

IGR combines the two. Appropriate for *statistical estimator* of *physical truth*!

Benamou and Brenier (2000) Cuturi (2013)

Information Geometric Mechanics

"Ground truth:" Boltzmann equation

$$\partial_t p_t(x,v) + v \cdot \nabla_x p_t(x,v) = \mathcal{C}(p_t)(x,v)$$

Euler eqn. = Gaussian ansatz for Boltzmann

[Levermore 1996]

$$p(x,v) = \rho(x)\mathcal{N}\left(v | u(x), \theta(x)\right)$$

For constant θ, logdet of IGR is its entropy

Information Geometric Mechanics

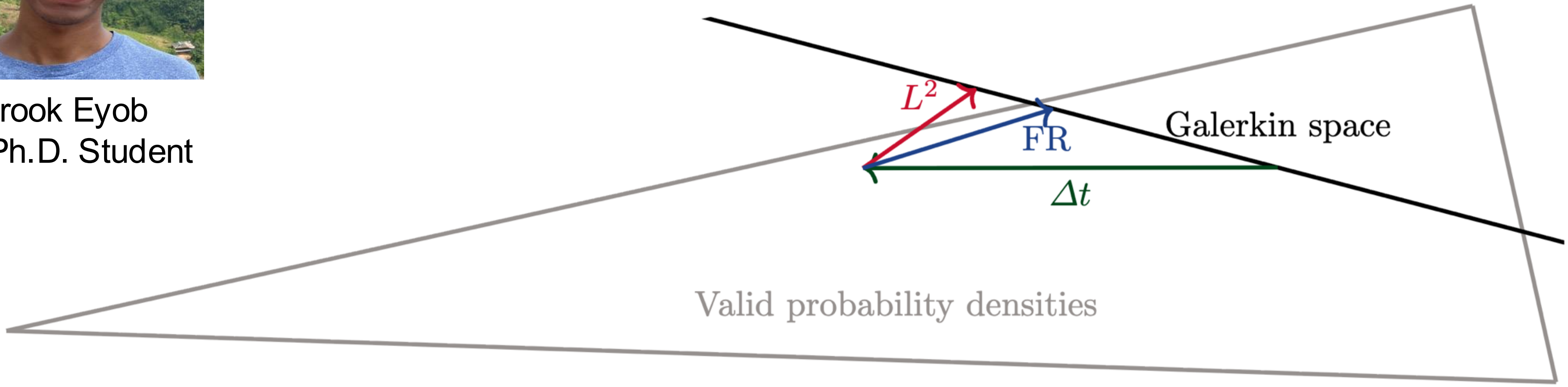
Common: PDE sols. describe *representative volumes*, subject to geometry of *particles*

Instead: View as describing *parameters of prob. dists.*, subject to information geometry

IGR is only the first step!

- Maximum likelihood discretization
- Kinetic effects, Plasmas, Solids
- Interaction with model uncertainties
- Reduced order modeling across scales

Brook Eyob
GT Ph.D. Student



Part III:

MAXIMUM LIKELIHOOD DISCRETIZATION

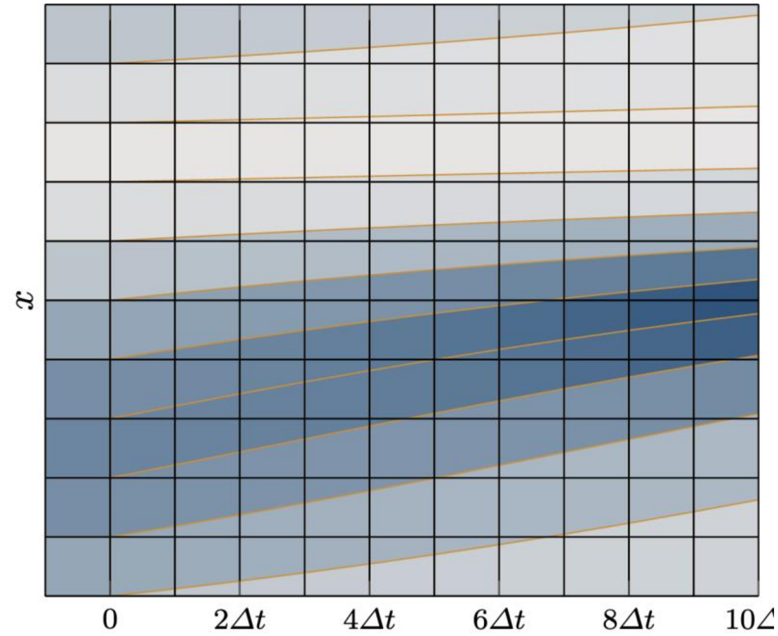
Solving Transport

Consider mass transport $\partial_t \rho_t + \mathrm{div}(\rho_t \boldsymbol{u}_t) = 0$

Galerkin ansatz: $$\hat{\rho}(\boldsymbol{x}, t) = \sum_{i=1}^{m} r_i(t) \varphi_i(\boldsymbol{x}) \in V$$

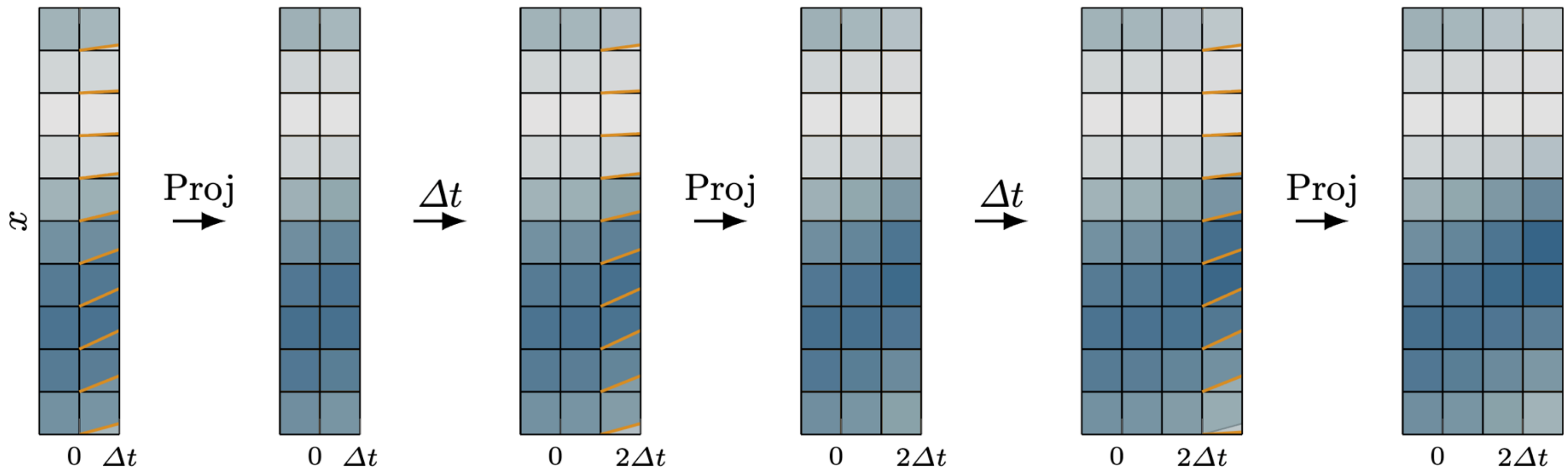
But solution leaves ansatz space over time:

Need to project back!



Eyob and S (2025), *arXiv:2505.10713*

Maximum Likelihood Discretization



Standard approach: L^2 projection

$$\int \hat{\sigma}\,\dot{\hat{\rho}}_t \,\mathrm{d}\boldsymbol{x} + \int \hat{\sigma}\,\mathrm{div}\left(\hat{\rho}_t \boldsymbol{u}_t\right)\,\mathrm{d}\boldsymbol{x} = 0,\ \forall \hat{\sigma} \in V.$$

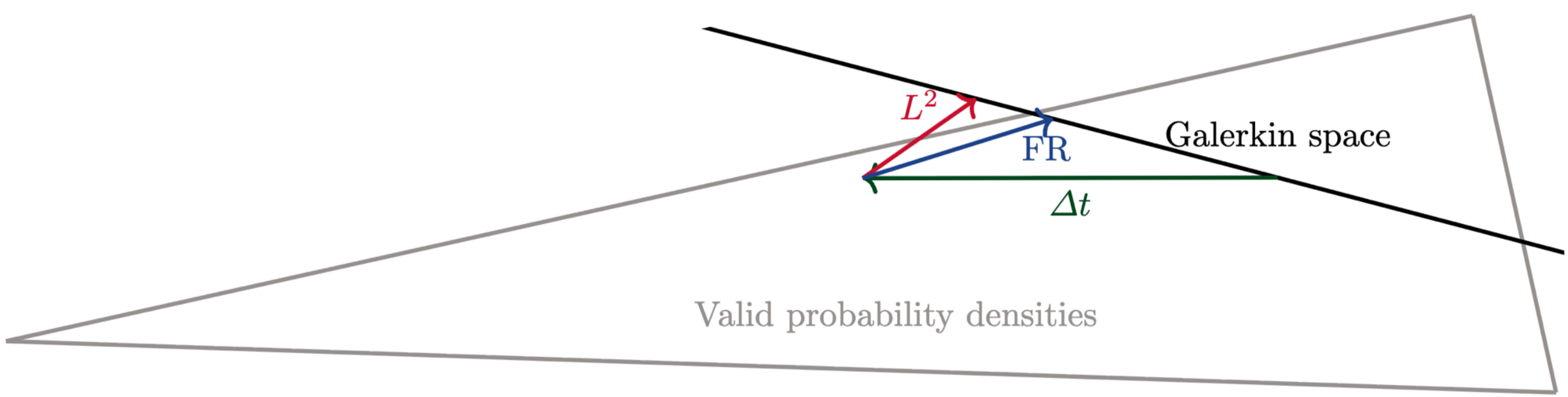
Method of moment for estimating $\dot{\hat{\rho}}$ from advected particles. Prone to loss of $\hat{\rho} \geq 0$

Instead: Use Maximum Likelihood

$$\boldsymbol{r}(t+\delta_t) = \arg\max_{\hat{\boldsymbol{r}} \in \mathbb{R}^m} \begin{cases} \int_{\boldsymbol{x}\in\Omega} \log\left(\frac{\mathrm{d}P_{\hat{\boldsymbol{r}}}}{\mathrm{d}P_{\boldsymbol{r}(t),\delta_t \boldsymbol{u}_t}}(\boldsymbol{x})\right) \mathrm{d}P_{\boldsymbol{r}(t),\delta_t \boldsymbol{u}_t}, & \text{if } P_{\boldsymbol{r}(t),\delta_t \boldsymbol{u}_t} \ll P_{\hat{\boldsymbol{r}}}, \\ -\infty, & \text{else.} \end{cases}$$

Results in Fisher-Rao projection

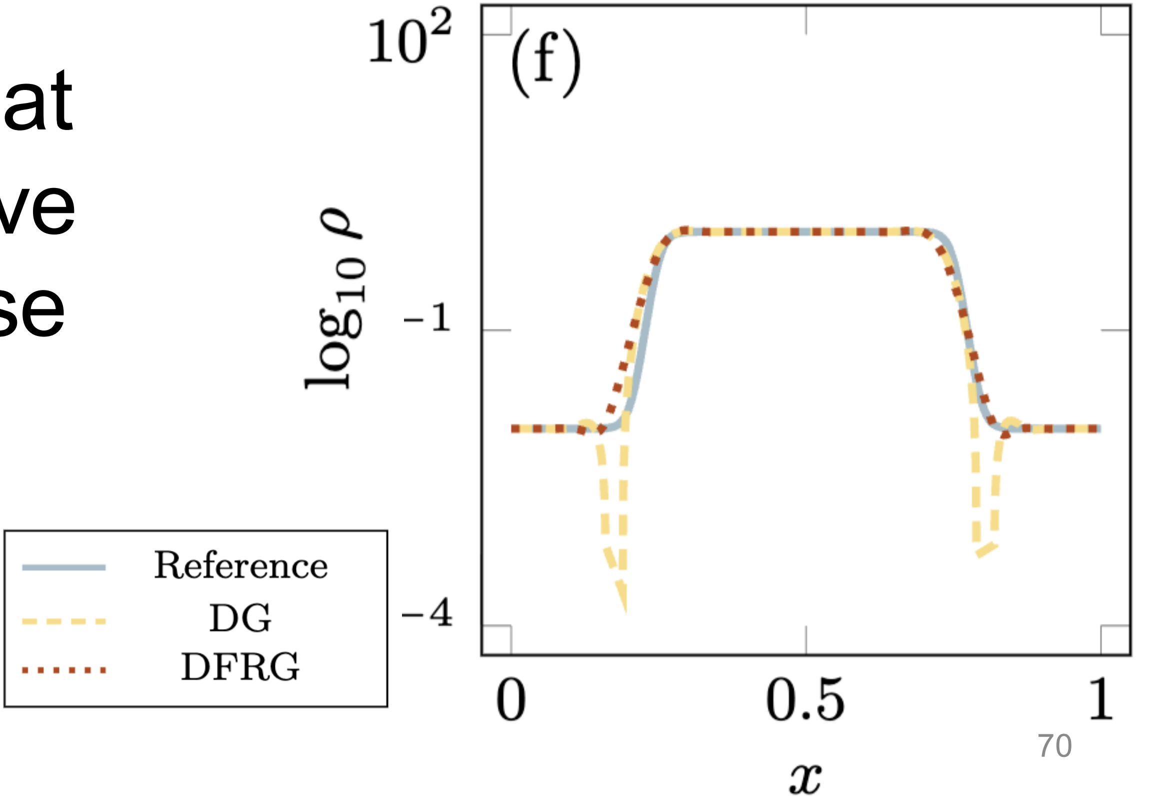
$$\int \frac{\hat{\sigma}\dot{\hat{\rho}}}{\hat{\rho}}\, \mathrm{d}\boldsymbol{x} + \int \frac{\hat{\sigma}\,\mathrm{div}\left(\hat{\rho}\boldsymbol{u}_t\right)}{\hat{\rho}}\, \mathrm{d}\boldsymbol{x} = 0, \ \forall \hat{\sigma} \in V$$



Relative Accuracy

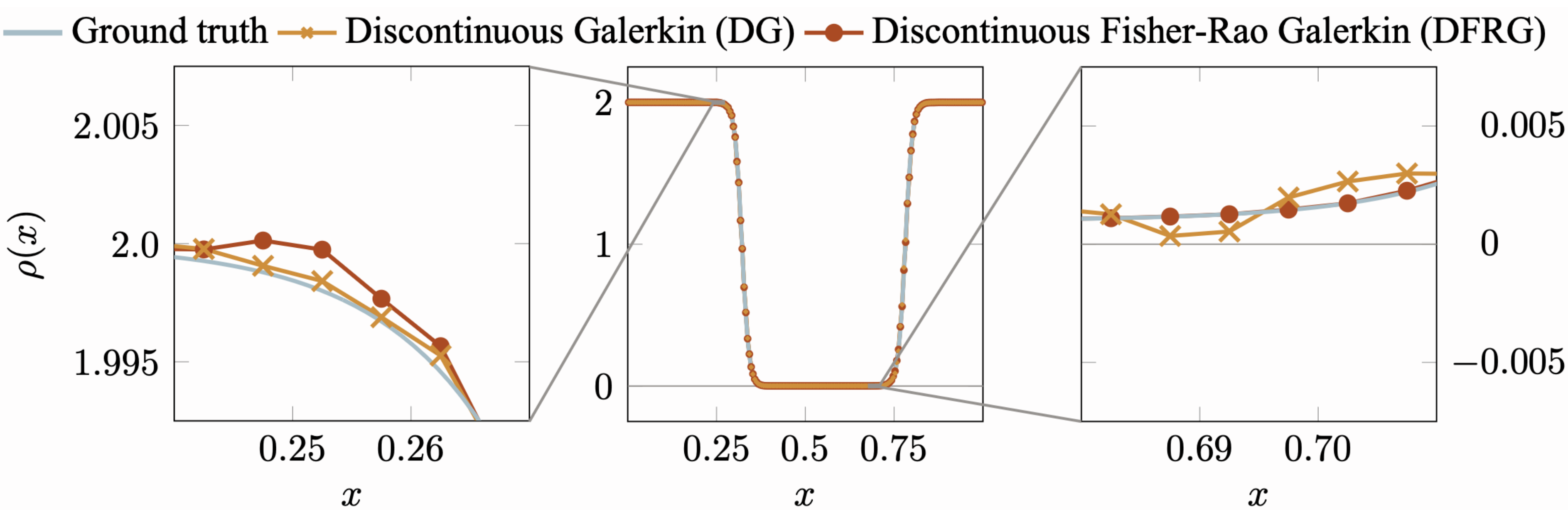
Positivity preserving, conservative, global error bounds in KL-divergence.

Especially good at preserving relative accuracy, promise for reactions



Integration in Euler Equation

Extreme temperature gradients can lead to vanishing density, causing blow-up of sim.



CIGMO

THE CENTER FOR INFORMATION GEOMETRIC MECHANICS AND OPTIMIZATION

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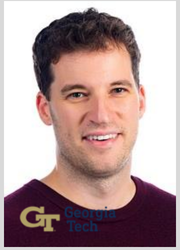

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https://www.firehouse.com/apparatus/article/21082328/does-vehicle-color-play-a-role-in-apparatus-safety

Part 4:

BACKUP SLIDES