Learning the Regularisation of a Kinetic 5-Moment Closure

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State $\to f(x,t,c) \geq 0$ — phase-space density (position x, velocity c)

Evolution $\to$ transport + collisions:

$$\partial_t f + c\partial_x f = \frac{1}{\tau}(\mathcal{M}_f - f)$$

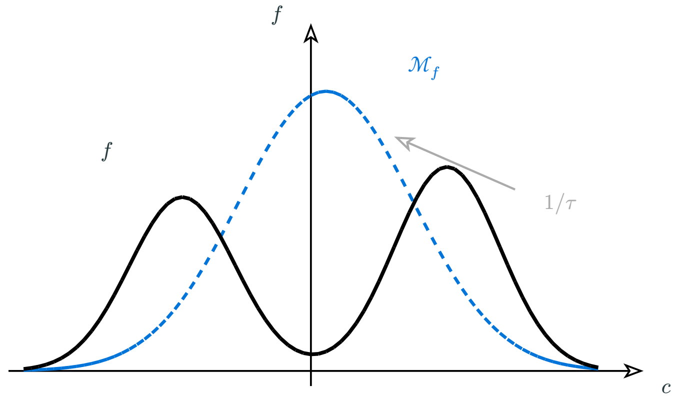
BGK $\to$ relax $f \to \mathcal{M}_f$, rate $1/\tau$:

$$\mathcal{M}_f(c) = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left(-\frac{(c-v)^2}{2\theta}\right)$$

$\mathcal{M}_f \to$ (Maxwellian) function of c only

f/ρ = velocity prob. density
$\to$ macroscopic fields = its low-order moments:

$\rho = \int_{\mathbb{R}} f \, \mathrm{d}c$	$\to$ density	(normalisation)
$v = \rho^{-1} \int_{\mathbb{R}} cf \, \mathrm{d}c$	$\to$ bulk velocity	$(= \mathbb{E}[c]$, mean)
$\theta = \rho^{-1} \int_{\mathbb{R}} (c-v)^2 f \, \mathrm{d}c$	$\to$ temperature	$(= \mathrm{Var}[c]$, variance)



Invariants

$\mathcal{M}_f$, f: same ρ, ρv, $\rho\theta$

$\to \langle (1, c, c^2)(\mathcal{M}_f - f) \rangle = 0$

$\to$ mass, momentum, energy conserved

Knudsen $\mathrm{Kn} \sim \tau$:
$\mathrm{Kn} \ll 1 \to$ fluid (Euler / NS)
$\mathrm{Kn} \sim 1 \to$ rarefied / non-equilibrium

Finite moment list, not all of f $\to$ multiply BGK by c^i, integrate:

$$\partial_t u_i + \partial_x u_{i+1} = \frac{1}{\tau}\big(\langle c^i \mathcal{M}_f\rangle - u_i\big), \quad u_i := \langle c^i f\rangle = \int_{\mathbb{R}} c^i f \,\mathrm{d}c$$

Unclosed

flux of moment i = moment $i+1$

$\to$ $N+1$ equations, $N+2$ unknowns

Conservation

$i = 0, 1, 2$ $\to$ right-hand side $= 0$

($1, c, c^2$ collision invariants)

$\to$ exact mass / momentum / energy laws (closure-free)

Closure

truncate $N = 5$ $\to$ model top flux

$$\hat{S} = u_5 = \hat{S}(u_0, \dots, u_4)$$

Reduction $(5 \to 2)$ $\to$ Galilean (centre at v) + rescale by ρ, θ $\to$ $\hat{S} = \hat{S}\big(\hat{Q}, \hat{R}\big)$

$\hat{Q} = \rho^{-1}\theta^{-\frac{3}{2}} \int_{\mathbb{R}} (c-v)^3 f \,\mathrm{d}c$ $\to$ skewness
$\hat{R} = \rho^{-1}\theta^{-2} \int_{\mathbb{R}} (c-v)^4 f \,\mathrm{d}c$ $\to$ kurtosis

Closure problem $\to$ choose $\hat{S}\big(\hat{Q}, \hat{R}\big)$

The Realizability Domain

Existence $\to \left(\hat{Q}, \hat{R}\right)$ realizable

$\Leftrightarrow \exists$ density $f \geq 0$ on $\mathbb{R}$, moments $\left(1, 0, 1, \hat{Q}, \hat{R}\right)$

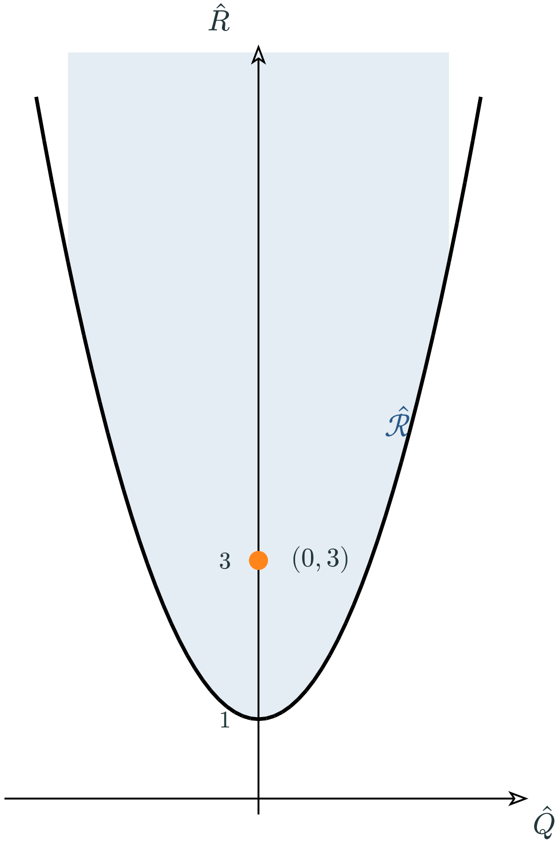
Hamburger moment problem $\to$ such f exists $\Leftrightarrow$ Hankel matrix $\succeq 0$:

$$H = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & \hat{Q} \\ 1 & \hat{Q} & \hat{R} \end{pmatrix}, \quad \det H = \hat{R} - 1 - \hat{Q}^2$$

$$\hat{\mathcal{R}} = \left\{\hat{R} \geq 1 + \hat{Q}^2\right\}$$

$\Leftrightarrow$ kurtosis $\geq 1 + \mathrm{skewness}^2$

Equilibrium $\mathcal{M}_f \to \left(\hat{Q}, \hat{R}\right) = (0, 3)$



Parabola $\hat{R} = 1 + \hat{Q}^2 = \partial\hat{\mathcal{R}}$

equilibrium $(0, 3)$

Coordinate on $\hat{\mathcal{R}}$:

$$\sigma(\hat{Q},\hat{R}) = \sqrt{\left(\frac{\hat{R}-3}{4}\right)^2 + \frac{\hat{Q}^2}{2}} - \frac{\hat{R}-3}{4} \in (0,1]$$

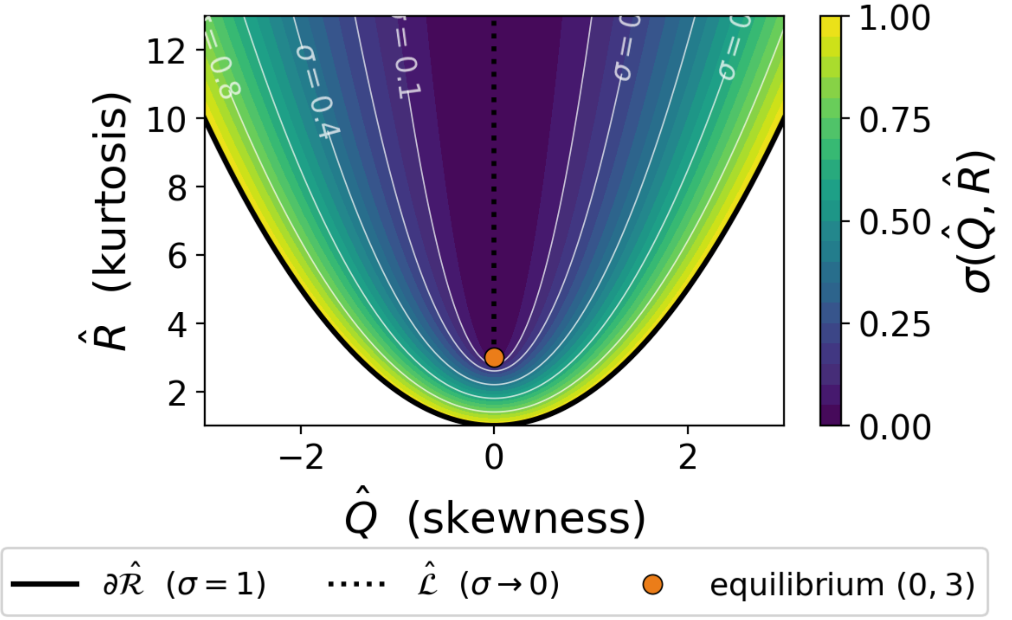
$\sigma = 1 \to$ realizability boundary $\partial\hat{\mathcal{R}}$ ($\hat{R} = 1 + \hat{Q}^2$)

$\sigma \to 0 \to$ Junk line $\hat{\mathcal{L}} = \left\{\hat{Q} = 0, \hat{R} > 3\right\}$

Level sets

$\to$ nested parabolas $\hat{R} = \hat{Q}^2/\sigma + 3 - 2\sigma$

$\to$ natural closure variable: $\hat{S} = \hat{S}(\sigma, \dots)$



σ foliates $\hat{\mathcal{R}}$ from $\partial\hat{\mathcal{R}}$ ($\sigma = 1$) to $\hat{\mathcal{L}}$ ($\sigma \to 0$)

Schaerer–Torrilhon, On Singular Closures for the 5-Moment System in Kinetic Gas Theory, Communications in Computational Physics 17 (2015), Eq. (4.1)

System $\rightarrow$ first-order, 5×5:

$$\partial_t \boldsymbol{u} + J(\boldsymbol{u})\partial_x \boldsymbol{u} = \text{source}, \quad J = \frac{\partial \hat{F}}{\partial \boldsymbol{u}}$$

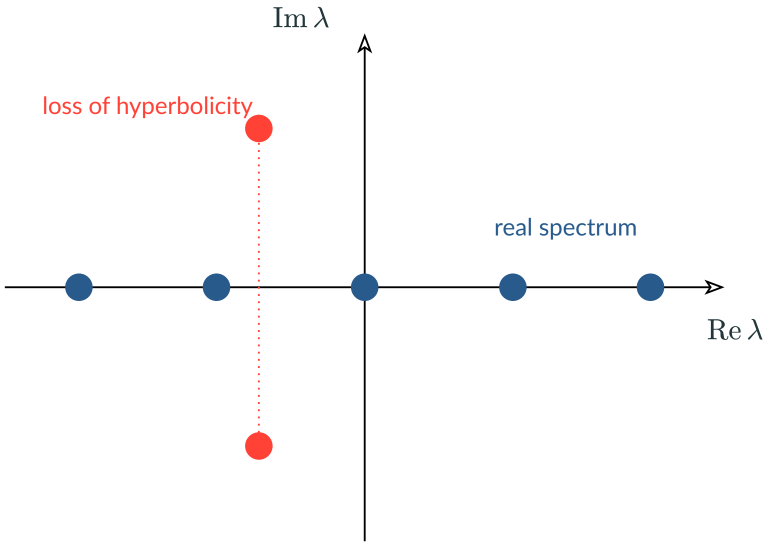
Hyperbolic $\rightarrow J$ real spectrum $+$ diagonalisable

Well-posed $\Leftrightarrow J$ real-diagonalisable

$\operatorname{Im}\lambda_i \neq 0 \rightarrow$ Hadamard ill-posed $\rightarrow$ modes grow $\sim e^{|\operatorname{Im}\lambda_i|\, kt}$

$$\boxed{\text{hyperbolic} \Leftrightarrow \max_i |\operatorname{Im}\lambda_i(\hat{Q}, \hat{R})| = 0}$$

Characteristic speeds $\rightarrow \lambda_i$ = finite wave speeds



Flux-Jacobian spectrum: on the real axis $\rightarrow$ hyperbolic
conjugate pair off-axis $\rightarrow$ loss of hyperbolicity

Reference Closures: Maximum-Entropy (ME) vs Grad

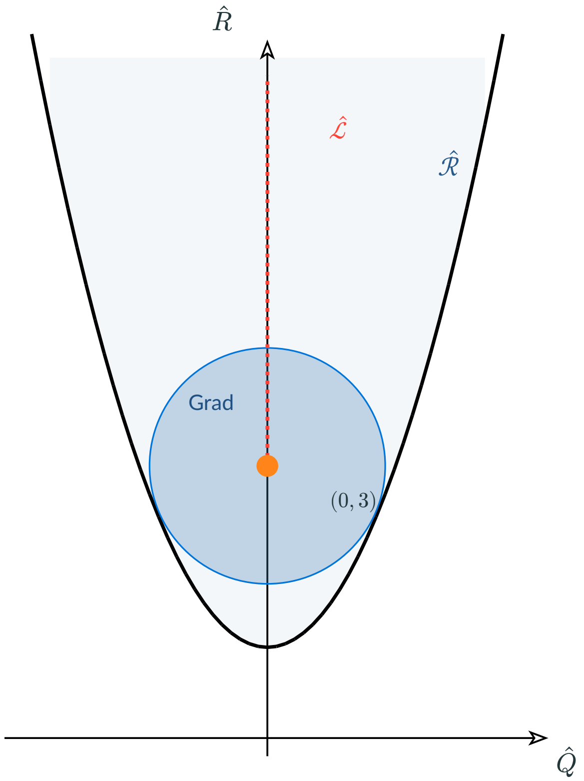
ME-closure $\rightarrow$ entropy-based

$\rightarrow$ symmetric hyperbolic + entropy dissipation (on its domain)
$\rightarrow$ singular on Junk line $\hat{\mathcal{L}}$
$\rightarrow$ per-point entropy maximisation

Grad closure $\rightarrow$ Hermite expansion

$\rightarrow$ closed-form + bounded
$\rightarrow$ hyperbolic only near equilibrium $(0, 3)$

	hyperbolic	bounded $\hat{S}$	closed-form
ME-closure	✓	✗ pole	✗ iterative
Grad closure	✗	✓	✓



blue: Grad hyperbolic near equilibrium, outside: loss of hyperbolicity
red $\hat{\mathcal{L}}$: ME-closure singular

Cai–Fan–Li, Globally Hyperbolic Regularization of Grad's Moment System, Communications on Pure and Applied Mathematics 67 (2014)
Levermore, Moment Closure Hierarchies for Kinetic Theories, Journal of Statistical Physics 83 (1996)

For $\beta \geq 0$: $\hat{S}_\beta\big(\hat{Q},\hat{R}\big) = \hat{Q}\left(10 - 8\sqrt{\sigma} + \frac{\big(2\sigma+\hat{R}-3\big)(1+\beta(1-\sigma))}{\sigma+\beta(1-\sigma)}\right)$

Limiting cases

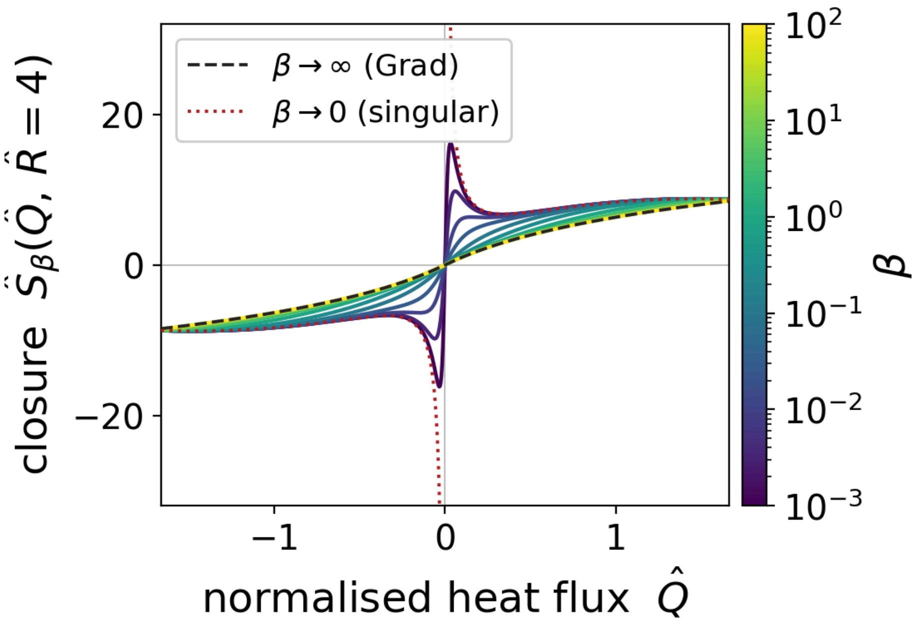
	hyperbolic	bounded $\hat{S}$	closed-form
$\beta = 0$ (ME-closure)	✓	✗ pole	✗ iterative
$\beta \to \infty$ (Grad-type)	✗	✓	✓

$\beta = 0$ Junk-line pole $\hat{S} \sim \big(\hat{R}-3\big)^2/\hat{Q}$

Every $\beta > 0$ $\to$ realizability + Galilean + symmetry
+ boundary (ME-closure on $\partial\hat{\mathcal{R}}$)
+ correct equilibrium slope $\partial_{\hat{Q}}\hat{S} = 10$

Hyperbolicity

$\to \hat{Q} = 0,\ \beta < \frac{3}{2}$ guaranteed for **constant** β only



$\hat{R} = 4$ slice
β (colour): singular $\to$ Grad

Scalar β undetermined $\to$ accuracy $\leftrightarrow$ well-posedness at **opposite limits** ($\beta \to 0$ vs $\beta \to \infty$)

Schaerer–Torrilhon, On Singular Closures for the 5-Moment System in Kinetic Gas Theory, Communications in Computational Physics 17 (2015)

Learned Regularisation: $\beta_\theta\left(\hat{Q}, \hat{R}\right)$

Parametrisation $\rightarrow \beta \rightarrow \beta_\theta\left(\hat{Q}, \hat{R}\right) > 0$, MLP ($\sim 10^3$ params)
softplus $\rightarrow \beta > 0$
MLP input $\left|\hat{Q}\right| \rightarrow \beta_\theta$ even in $\hat{Q} \rightarrow \hat{S}_{\beta_\theta}$ odd in $\hat{Q}$ (exact)

Structural invariants $\rightarrow$ realizability + Galilean + boundary + equilibrium by construction

Learning objective

$$\mathcal{L}(\theta) = \left\|\hat{S}_{\beta_\theta} - \hat{S}_{\text{ref}}\right\|^2 + \gamma \sum_{i=1}^{5} |\operatorname{Im} \lambda_i|$$

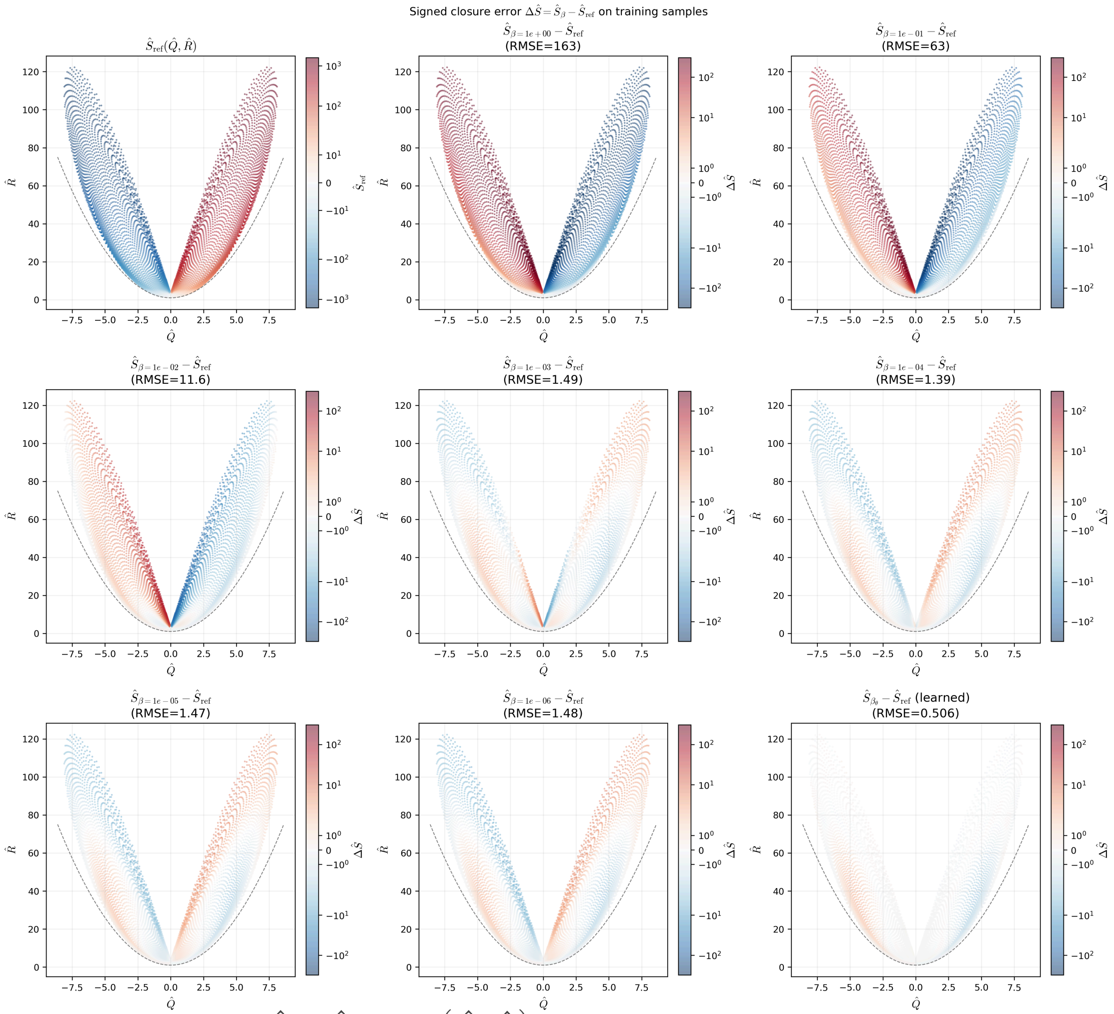
spectral penalty $\gamma \rightarrow$ the natural soft fix; **reported run uses $\gamma = 0$**, and even $\gamma > 0$ fails a-posteriori (see later)

Two evaluation modes:

A-priori — training target
flux MSE + frozen-Jacobian spectrum

A-posteriori — deployment
solver loop: real spectrum + finite?

A-Priori: β_θ vs Constant β



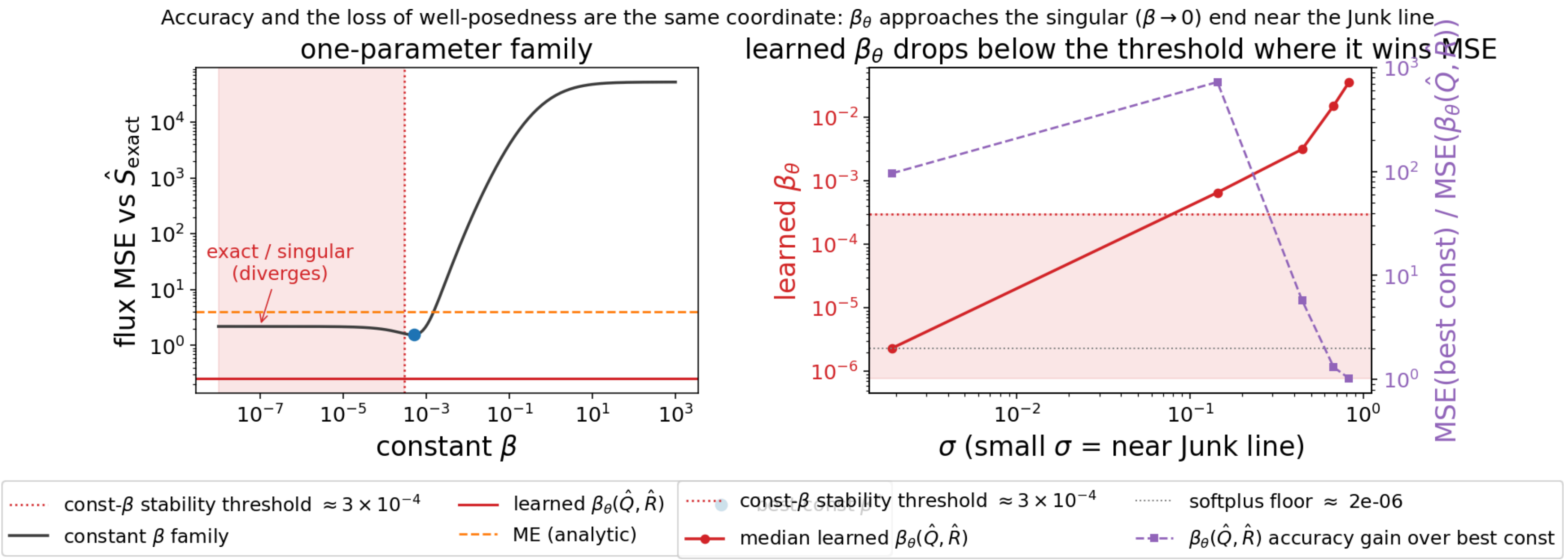
$|\hat{S} - \hat{S}_{\text{ref}}|$ on $(\hat{Q}, \hat{R})$ - common colour scale

β_θ picks the **best β at each σ** — the family's **lower envelope**
floor $\sim 10^{-6}$ at small σ

Error map $\to$ each fixed β has a high-error region
$\beta_\theta \to$ low error across the domain

Accuracy $\to$ flux MSE $\mathbf{0.26}$ vs
best constant β $\mathbf{1.54}$ $(6\times)$, gain near $\hat{\mathcal{L}}$

Data — 1D BGK two-stream, $\text{Kn} = 1$
initial data $v_0 \in [0.5, 8] \to 22.5\text{k}$ samples $(\hat{Q}, \hat{R}) \mapsto \hat{S}_{\text{ref}}$



left: constant-β MSE vs β + threshold β_{crit} right: $\beta_\theta(\sigma) < \beta_{\text{crit}}$ where MSE gain peaks ($\sim 700\times$)

Constant β ($\nabla\beta \equiv 0$), $\beta < \beta_{\text{crit}} \approx 3 \times 10^{-4}$:

- realizability loss: $\theta \to 0$ (vacuum) $\Rightarrow \hat{R} \to \infty$
- solver divergence
- learned $\beta_\theta \to 10^{-6} \ll \beta_{\text{crit}}$ near $\hat{\mathcal{L}}$

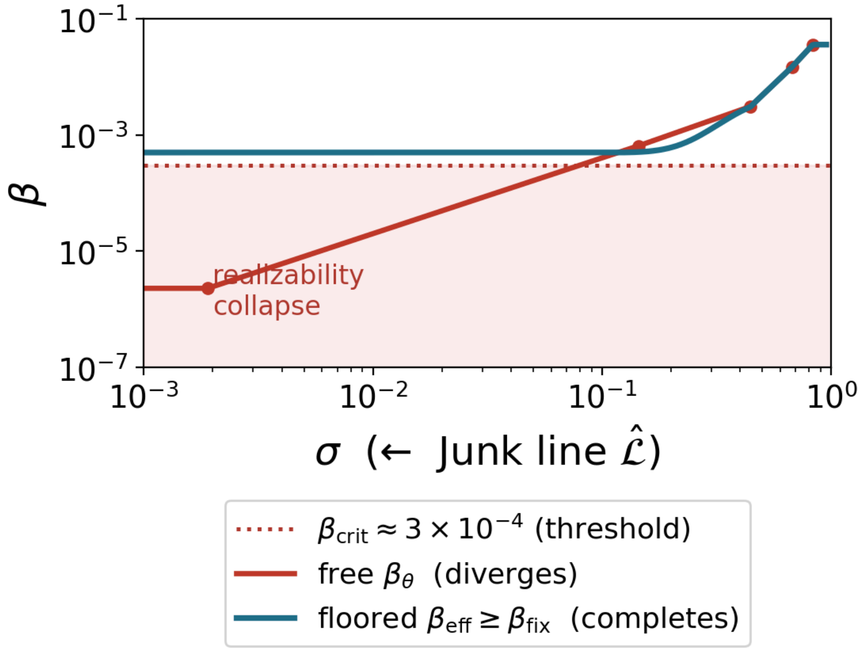
accuracy gain $\Leftrightarrow \beta < \beta_{\text{crit}} \to$ mechanism: **realizability loss**, not loss of hyperbolicity

$$\boxed{\beta_{\text{eff}}\left(\hat{Q},\hat{R}\right) = w(\sigma)\ \beta_{\text{fix}} + (1-w(\sigma))\ \beta_\theta\left(\hat{Q},\hat{R}\right)}$$

Convex weight $w(\sigma) \in [0,1]$ $\rightarrow C^2$-function
$w = 1$ at $\hat{\mathcal{L}}$ ($\sigma \rightarrow 0$) $\rightarrow \beta \equiv \beta_{\text{fix}} \approx 5\times10^{-4}$ (**enforced**)
$w = 0$ far ($\sigma \geq \sigma_{\text{free}}$) $\rightarrow$ free β_θ
structural, not a soft penalty

β near $\hat{\mathcal{L}}$	flux MSE ↓	solver
free β_θ (no β_{fix})	0.256	**diverges**
β_{fix} learned	0.428	**diverges**
β_{fix} **imposed** $= 5\times10^{-4}$	0.429	**completes**
best constant β	1.543	completes

Learned β_{fix} $\rightarrow$ training drives $\beta_{\text{fix}} < \beta_{\text{crit}}$ $\rightarrow$ collapse
$\rightarrow \beta_{\text{fix}}$ must be **imposed**, not learned



β_{eff}: constrained to β_{fix} near $\hat{\mathcal{L}}$, free β_θ away
free β_θ alone $\rightarrow$ realizability collapse

Take-Aways

β-closure

- scalar β: ME-closure (singular) $\leftrightarrow$ Grad closure (bounded)

Tension

- accuracy gain $\Leftrightarrow$ $\beta < \beta_{\text{crit}}$ $\Leftrightarrow$ realizability loss

Result

- σ-windowed constraint $\beta = \beta_{\text{fix}} > \beta_{\text{crit}}$ near $\hat{\mathcal{L}}$
- MSE $3.6\times <$ best constant β, well-posed (shock completes)

Open

- **Structural by construction** $\rightarrow$ entropy / Lagrange-multiplier surrogate $\rightarrow$ realizability + hyperbolicity intrinsic
- **Multi-Kn** $\beta_\theta\left(\hat{Q}, \hat{R}, \mathrm{Kn}\right)$ — direct-flux closure with stronger prior