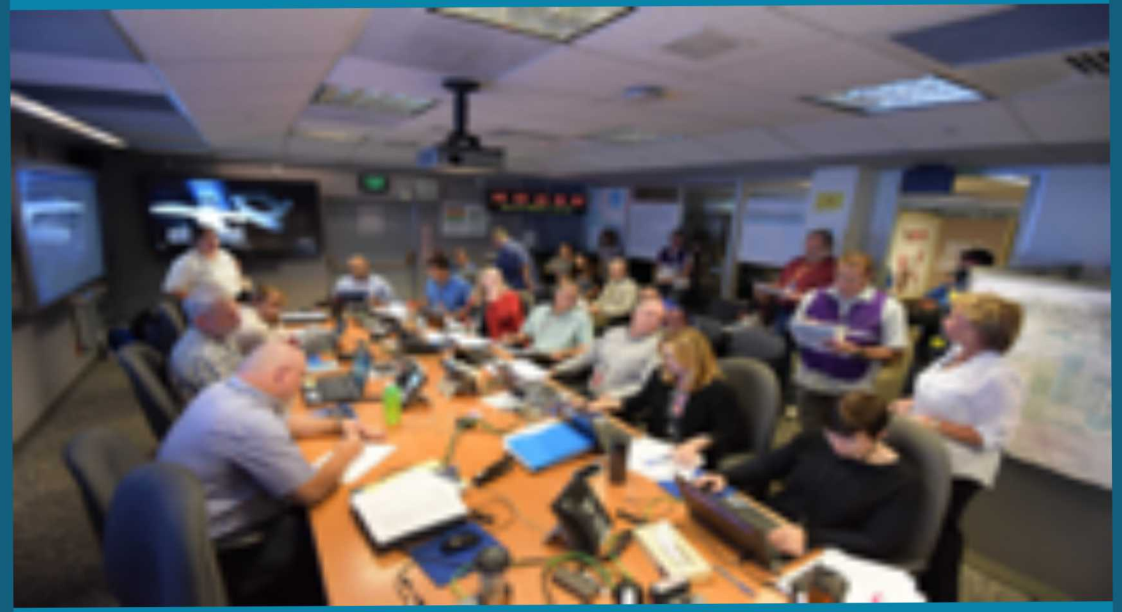
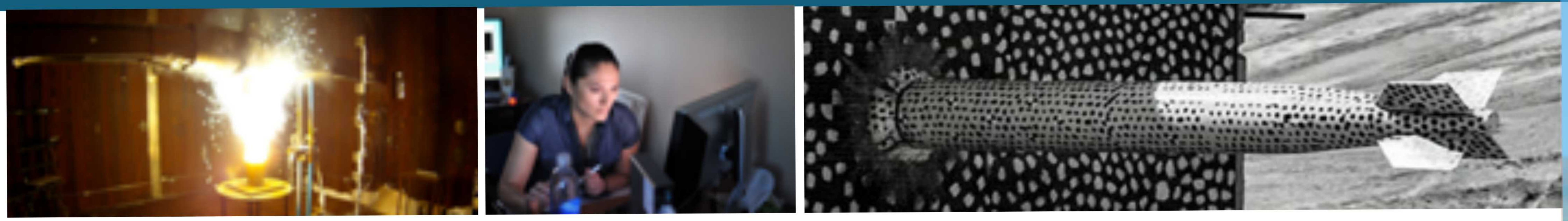
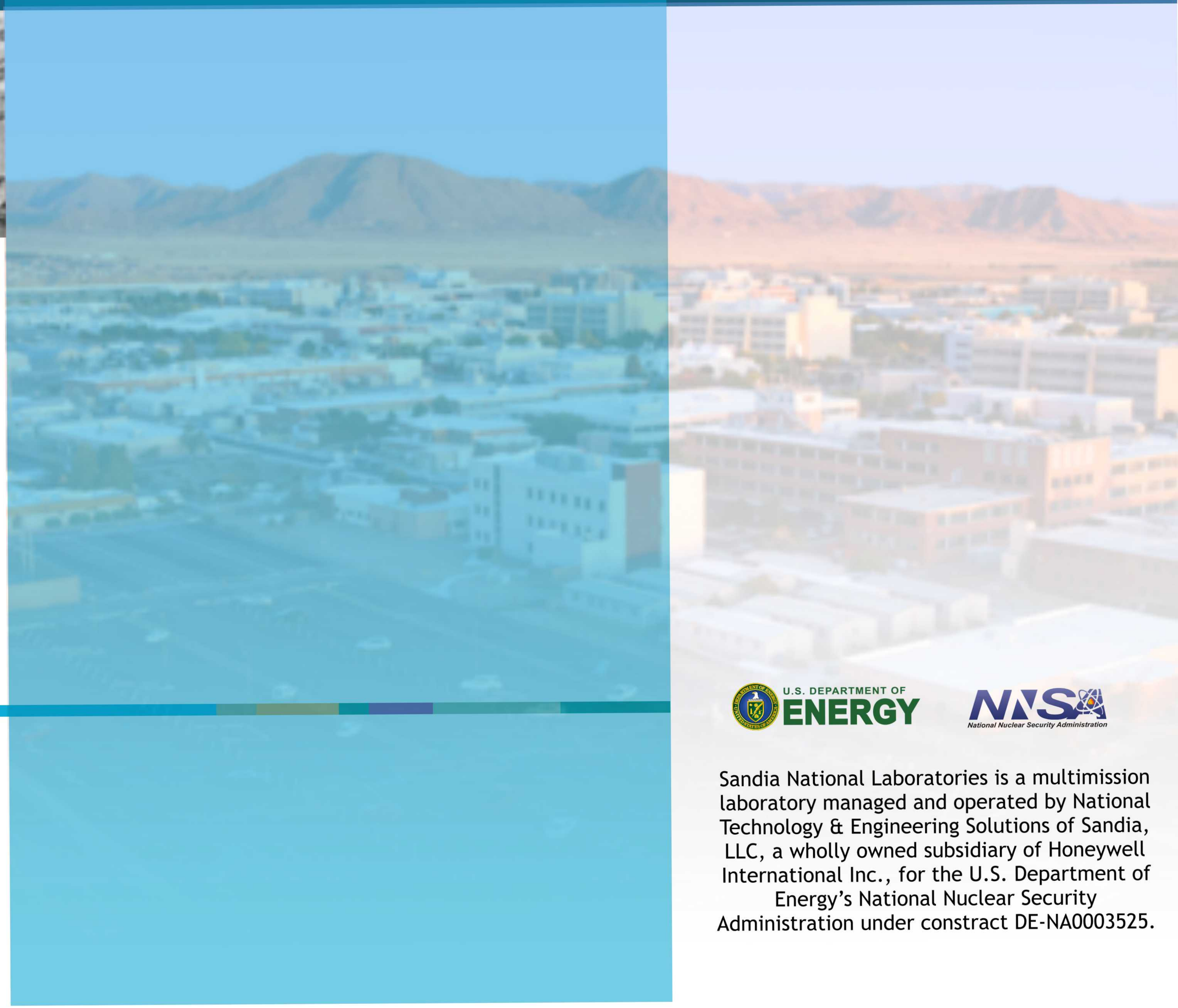
SAND2019-1982C

Entropy Stable Discretization of Compressible Flows in Thermochemical Nonequilibrium







PRESENTED BY

Michael A. Hansen, Postdoctoral Appointee

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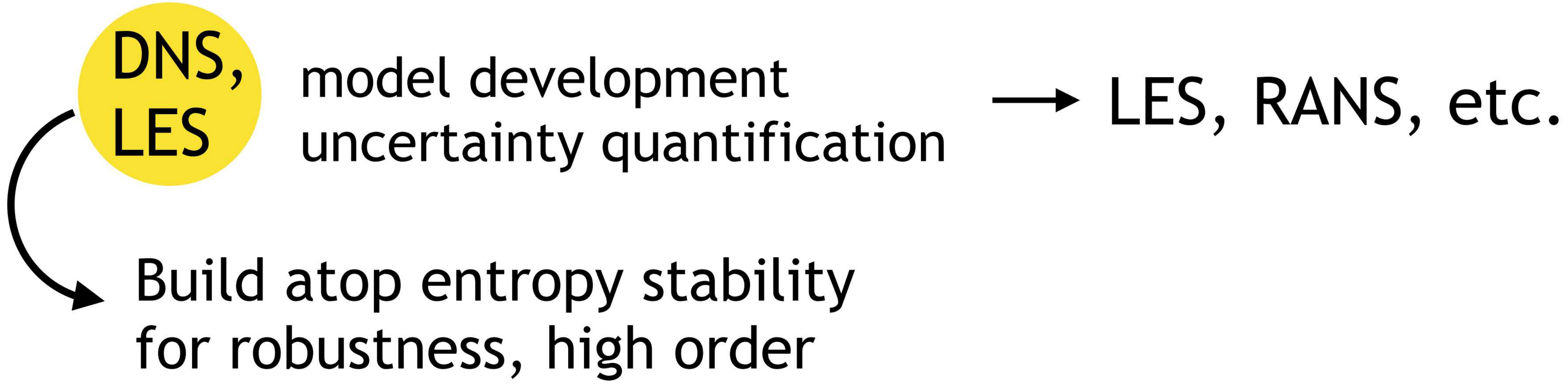
Entropy stability is a beneficial property of numerical methods, which we’ve largely extended to **multicomponent** and **multitemperature** systems

Implies provable nonlinear, integral (L2) stability,
consistency with thermodynamics

- Improved robustness
- Ensures physically-realizable weak solutions
- Less artificial dissipation necessary for stability

High-fidelity simulation of reacting flows is critical due to the cost and difficulty of experimental investigation.


DNS, LES

model development
uncertainty quantification

→ LES, RANS, etc.

Build atop entropy stability
for robustness, high order

continuous stability proofs

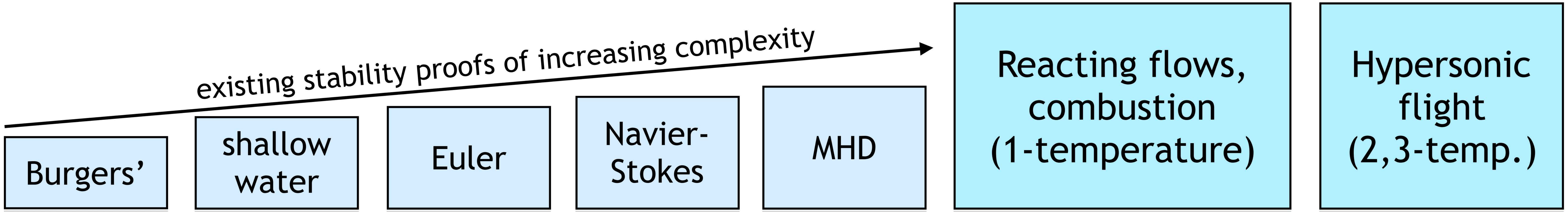
- conditions on constitutive properties
- requirements on mass diffusion model

two-point entropy conservative flux functions

- an automated procedure for conservation form fluxes
- constraints on SBP operators

an issue in boundary conditions

- entropy vars may require extra boundary layer resolution, or a special procedure within the stability proof


existing stability proofs of increasing complexity

Burgers’

shallow water

Euler

Navier-Stokes

MHD

Reacting flows, combustion (1-temperature)

Hypersonic flight (2,3-temp.)

Thermochemical nonequilibrium complicates things greatly

Euler → Navier-Stokes → Reacting flows, combustion (1-temperature) → Hypersonic flight (2,3-temp.)

Finite rate chemistry
High temperatures

Finite rate chemistry
Finite rate molecular relaxation
Extreme T (>5000 K)

admissible
entropy fxns

- Thermodynamic entropy
- Exponential entropies
- ...

heat conduction
only the thermodynamic
entropy is valid

admissible
entropy fxns

- Thermodynamic entropy

\+

Chemical non-equilibrium
solve many (5 to >100)
species equations

Variable heat capacity
thermally perfect gases
ɣ is not constant (T, Y dep.)

Reaction mechanisms
source terms

Mass/heat diffusion
viscous fluxes

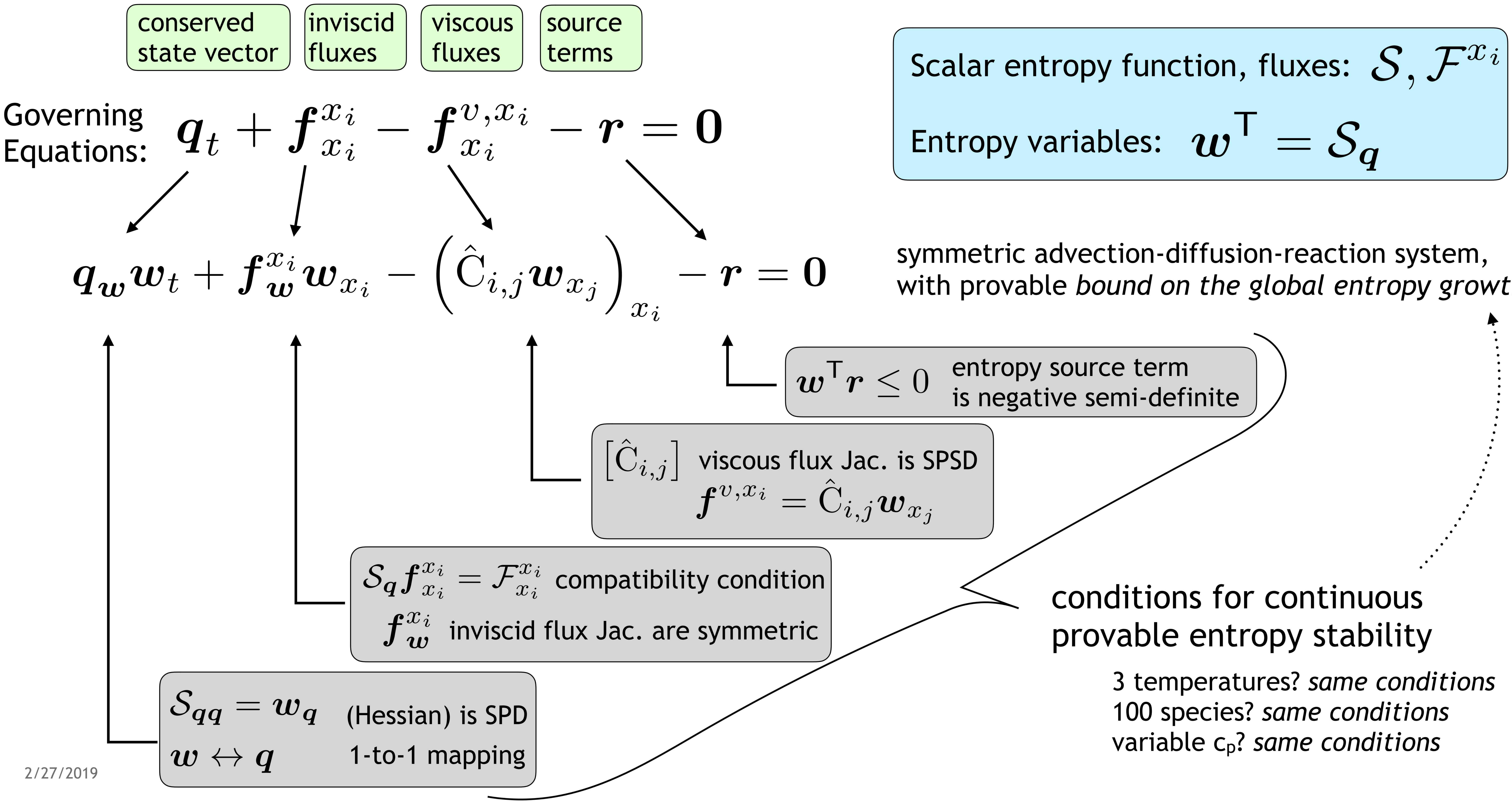
\+

Thermal non-equilibrium
solve multiple energy equations

Thermal relaxation
source terms

Thermochemical nonequilibrium complicates a stability proof

but it doesn't change the fundamental mathematics



conserved state vector

inviscid fluxes

viscous fluxes

source terms

Governing Equations: $\boldsymbol{q}_t + \boldsymbol{f}^{x_i}_{x_i} - \boldsymbol{f}^{v,x_i}_{x_i} - \boldsymbol{r} = \boldsymbol{0}$

$$\boldsymbol{q}_{\boldsymbol{w}} \boldsymbol{w}_t + \boldsymbol{f}^{x_i}_{\boldsymbol{w}} \boldsymbol{w}_{x_i} - \left(\hat{\mathrm{C}}_{i,j} \boldsymbol{w}_{x_j}\right)_{x_i} - \boldsymbol{r} = \boldsymbol{0}$$

$\boldsymbol{w}^{\mathsf{T}} \boldsymbol{r} \leq 0$ entropy source term is negative semi-definite

$\left[\hat{\mathrm{C}}_{i,j}\right]$ viscous flux Jac. is SPSD

$\boldsymbol{f}^{v,x_i} = \hat{\mathrm{C}}_{i,j} \boldsymbol{w}_{x_j}$

$\mathcal{S}_{\boldsymbol{q}} \boldsymbol{f}^{x_i}_{x_i} = \mathcal{F}^{x_i}_{x_i}$ compatibility condition

$\boldsymbol{f}^{x_i}_{\boldsymbol{w}}$ inviscid flux Jac. are symmetric

$\mathcal{S}_{\boldsymbol{q}\boldsymbol{q}} = \boldsymbol{w}_{\boldsymbol{q}}$ (Hessian) is SPD

$\boldsymbol{w} \leftrightarrow \boldsymbol{q}$ 1-to-1 mapping

Scalar entropy function, fluxes: $\mathcal{S}, \mathcal{F}^{x_i}$

Entropy variables: $\boldsymbol{w}^{\mathsf{T}} = \mathcal{S}_{\boldsymbol{q}}$

symmetric advection-diffusion-reaction system, with provable *bound on the global entropy growth rate*

conditions for continuous provable entropy stability

3 temperatures? *same conditions*
100 species? *same conditions*
variable c_p? *same conditions*

Continuous stability proofs for MC, MT exist and place reasonable conditions on physical properties

The entropy of a mixture of ideal gases, with one temperature, is a known result

arbitrary heat capacity

$$s_j = s_j^\circ - R_j \ln\left(\frac{\rho_j^\circ}{\rho_j}\right) + \int_{T^\circ}^{T} \frac{c_{v,j}}{T}\,\mathrm{d}T$$

Negative volumetric total entropy:

$$\mathcal{S} = -\rho s = \sum_{j=1}^{n_c} \rho_j s_j$$

Extending to multitemperature follows classical thermodynamic analysis

partial molar gibbs free energies

entropy variables:

$$\boldsymbol{w} = \mathcal{S}_{\boldsymbol{q}}^{\mathsf{T}} = \frac{1}{T}\begin{pmatrix} \boldsymbol{\mu} - \frac{1}{2}\boldsymbol{v}^{\mathsf{T}}\boldsymbol{v} \\ \boldsymbol{v} \\ -1 \\ 1 - T/T_r \\ 1 - T/T_v \end{pmatrix}$$

ratio of translational/modal temperatures

Convexity

T, rho$_i$, c$_v$ are *strictly positive*

all excited T, c$_v$ are *strictly positive*

Source Terms

chemical reaction mech. consistent with the 2nd law of thermodynamics

Viscous fluxes

Viscosity is nonnegative

Thermal conductivity is nonnegative
Excited modes too

Mass diffusion conditions…

depends on the model!

Strict mass conservation and barodiffusion rule out the provable entropy stability of simple diffusion models

Start from a general formulation

barodiffusion, Soret flux

$$\begin{pmatrix} \boldsymbol{j}^{x_k} \\ \mathfrak{q}^{x_k} \end{pmatrix} = -\begin{bmatrix} \mathrm{A}_1 & \boldsymbol{a}_2 \\ \boldsymbol{a}_3^{\mathsf{T}} & a_4 \end{bmatrix} \begin{pmatrix} \boldsymbol{\rho} \\ T \end{pmatrix}_{x_k}$$

Dufour flux

Phenomenological approach of irreversible thermodynamics is provably stable
(2nd law, Onsager reciprocal relations)

<u>A suitable form</u>

$$j_i = -\rho \mathcal{D}_i \left(d_i - \frac{Y_i}{Y_n} d_n \right)$$

$$j_n = -\sum_i^{n-1} j_i$$

diffusional driving forces

binary/mix-avg diffusion coefficients - ***must be nonnegative***

Conditions on A_1, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$, a_4 from the entropy variable flux Jacobian (symmetry, positive semi-definite)

- Strict mass conservation: $\sum_i j_i^{x_k} = 0$
- At least one of $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ must be nonzero

Fick's Law: $j_i^{x_k} = -\rho D_i (Y_i)_{x_k}$

is not provably stable!

Corrections to conserve mass are not stable either. $j_i^{x_k} = j_{i,(p)}^{x_k} - Y_i \sum_\ell j_{\ell,(p)}^{x_k}$

Provable entropy stability \=> Mass conservation

✓

continuous stability proofs

- conditions on constitutive properties
- requirements on mass diffusion model

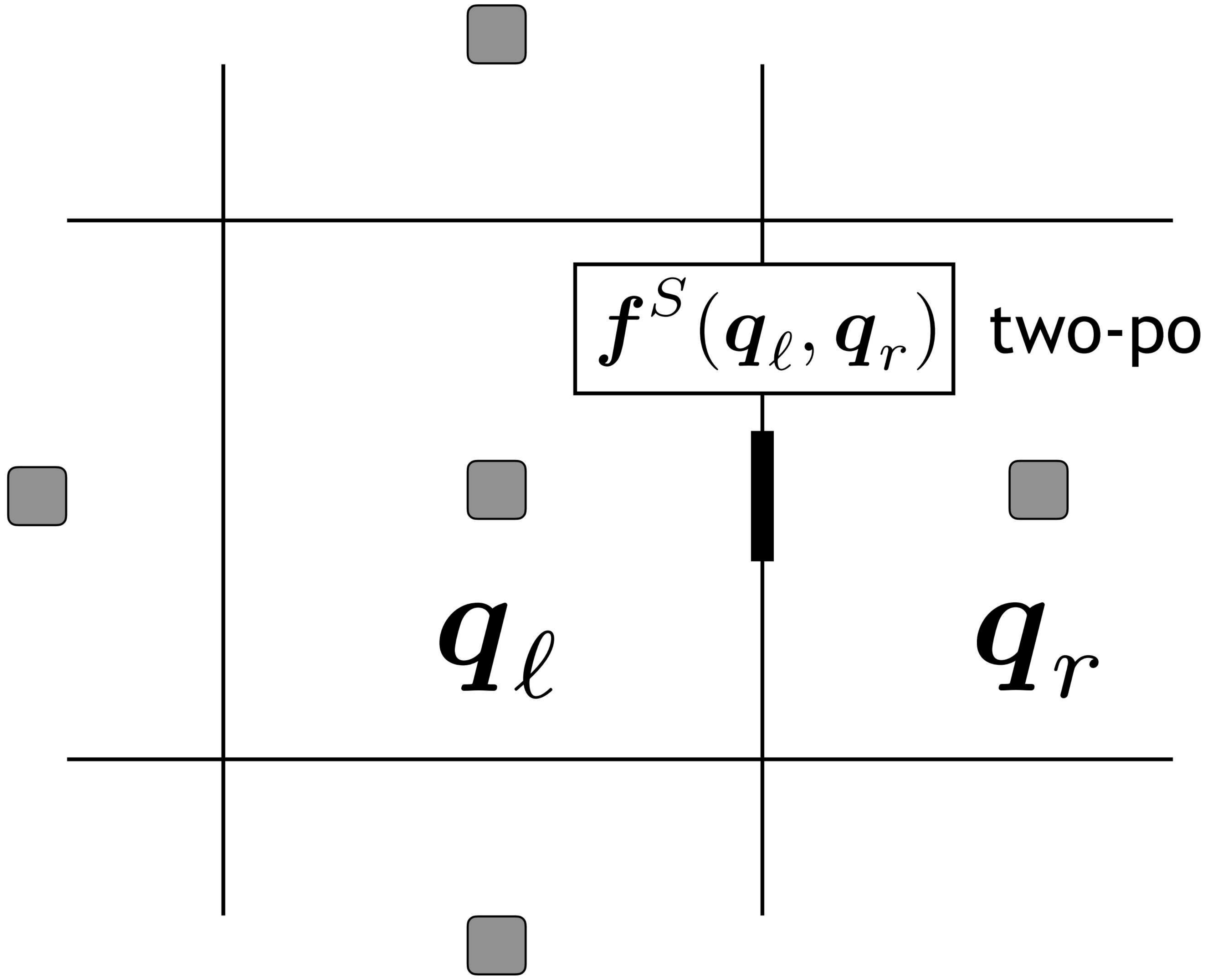
two-point entropy conservative flux functions

- an automated procedure for conservation form fluxes
- constraints on SBP operators

an issue in boundary conditions

- entropy vars may require extra boundary layer resolution, or a special procedure within the stability proof

With appropriate high order summation-by-parts (SBP) operators, global entropy conservation requires a local condition on the flux function



two-point flux function

- consistent: approaches the physical flux

$$\boldsymbol{f}^S(\boldsymbol{q}, \boldsymbol{q}) = \boldsymbol{f}_{\text{phys}}(\boldsymbol{q})$$

- entropy conservative: satisfies the local condition

$$\boxed{(\boldsymbol{f}^S)^\mathsf{T} \underbrace{\Delta \boldsymbol{w}}_{} = \underbrace{\Delta \psi}_{}}$$

jump: $\Delta a = a_r - a_\ell$

entropy potential flux,
$\psi = (\boldsymbol{f}^S)^\mathsf{T} \boldsymbol{w} - \mathcal{F}$

Ensures entropy conservation globally
(entropy flux telescopes to the boundaries)

$$\sum_i \boldsymbol{w}_i^\mathsf{T} (\boldsymbol{f}_{i+1/2} - \boldsymbol{f}_{i-1/2}) = \mathcal{F}_N - \mathcal{F}_0$$

Applies for high-order with special SBP operators

Satisfying the local condition requires “jump expansion” of complex functions

$$\boxed{(\boldsymbol{f}^S)^\mathsf{T}\Delta\boldsymbol{w} = \Delta\psi}$$

Strategy: expand the jump of ***w***, *ψ* in terms of a parameter vector ***z***, then solve for the flux components

Linearity: $\Delta(a+b) = \Delta a + \Delta b$

Product rule: $\Delta(ab) = \bar{b}\Delta a + \bar{a}\Delta b$

arithmetic averages

Chain rule: $\Delta f(g(\ldots)) = \dfrac{\Delta f}{\Delta g}\Delta g$

We quickly run into nonlinear functions with no analytical expansion

$$\Delta \ln a = (???)\Delta a$$

logarithmic average
evaluated with a special series approximation

1-D Euler equations

Ismail & Roe, 2009	Chandrashekar, 2012	Entropy-conservative, NOT consistent!
$z_1 = \sqrt{\rho/p},$	$z_1 = \rho,$	$z_1 = \rho,$
$z_2 = u\sqrt{\rho/p},$	$z_2 = u,$	$z_2 = u,$
$z_3 = \sqrt{\rho p}.$	$z_3 = \dfrac{1}{2RT}.$	$z_3 = T.$

Both are consistent and entropy conservative, but have different properties (e.g. kinetic energy)

Jump expansion is tedious and sensitive to arbitrary choices, made worse by complexity of multicomponent, multitemperature

$$(\boldsymbol{f}^S)^\mathsf{T} \Delta \boldsymbol{w} = \Delta \psi$$

Scalar equation on vector of fluxes.
Many solutions (EC fluxes)

1-D Euler equations

Ismail & Roe, 2009

$$z_1 = \sqrt{\rho/p}, \quad z_2 = u\sqrt{\rho/p}, \quad z_3 = \sqrt{\rho p}.$$

Chandrashekar, 2012

$$z_1 = \rho, \quad z_2 = u, \quad z_3 = \frac{1}{2RT}.$$

Entropy-conservative, NOT consistent!

$$z_1 = \rho, \quad z_2 = u, \quad z_3 = T.$$

Arbitrary simplifications: $\Delta \ln(a/b)$ vs $\Delta(\ln a - \ln b)$

Parameter vector: $\Delta \ln(a\beta)$ vs $\Delta(\ln a + \ln \beta)$

New nonlinear terms from vibrational energy:

$$e_{v,j}(T_v) = \frac{R_j \Theta_j}{\exp(\Theta_j/T_v) - 1} \quad \text{and} \quad \int_{T^\circ}^{T_v} \frac{1}{T_v} \frac{\partial e_{v,j}}{\partial T_v} \mathrm{d}T_v$$

Complexity:

species entropies, energies, entropy variables, etc. are all nontrivial
- modal energy forms (translational, vibrational, etc.)
- polynomial forms (NASA/JANAF)

Writing a library atop SageMath has largely automated the derivation of entropy conservative flux functions for complex systems

$$\boxed{(\boldsymbol{f}^S)^{\mathsf{T}}\Delta\boldsymbol{w} = \Delta\psi}$$

***poblano*: library atop SageMath**
- builds expressions into an abstract syntax tree
- calculates jump expansions recursively
- setup and solution of the linear system for **f**^{S}
- verify consistency
- reproduces fluxes of earlier work for Euler eqns

$$\Delta\boldsymbol{w} = \mathrm{H}\Delta\boldsymbol{\mathcal{Z}}$$

$$\Delta\psi = \boldsymbol{g}^{\mathsf{T}}\Delta\boldsymbol{\mathcal{Z}}$$

$$\boxed{\boldsymbol{f}^S = (\mathrm{H}^{\mathsf{T}})^{-1}\boldsymbol{g}}$$

This always produces an EC flux function
(HT is nonsingular for convex parameter vec.)

poblano has facilitated EC fluxes for:

1 temperature, n species
- calorically perfect
- modal energy decomposition (**aero**)
- NASA polynomials (**combustion**)

Thermally perfect, 2 and 3 temperatures, n species

Some 'highlights'

Fluxes are affordable, direct functions - no phase space integration

Species mass fluxes need the logarithmic average, $f_i^{S,n} = \widehat{\rho}_i\overline{v}^n$

We've introduced a cheap '**exponential average**'
for expansion of nonlinear vibrational energy terms

directly analogous to the log avg for the Euler eqns

✓ **continuous stability proofs**

- conditions on constitutive properties
- requirements on mass diffusion model

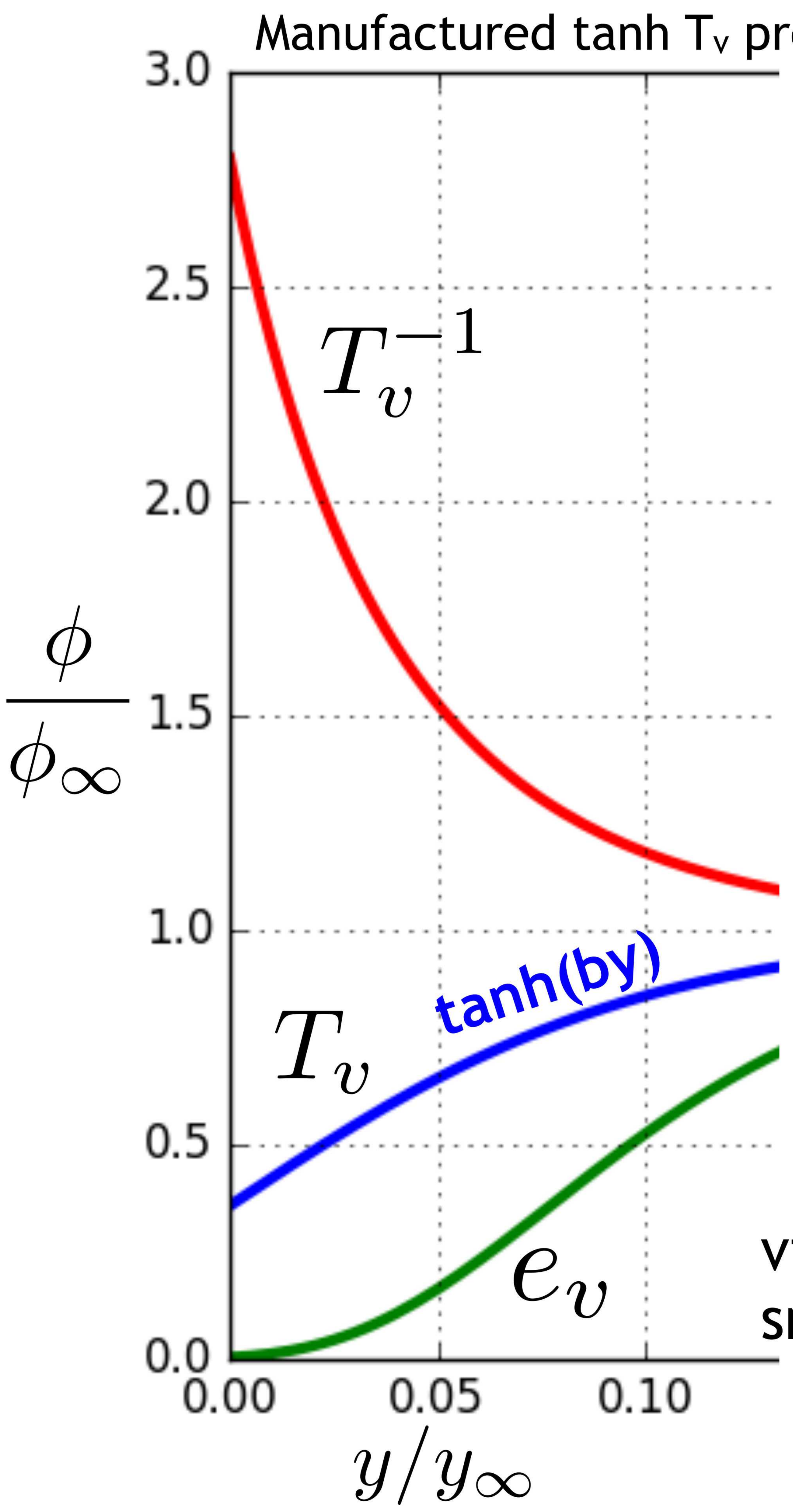
✓ **two-point entropy conservative flux functions**

- an automated procedure for conservation form fluxes
- constraints on SBP operators

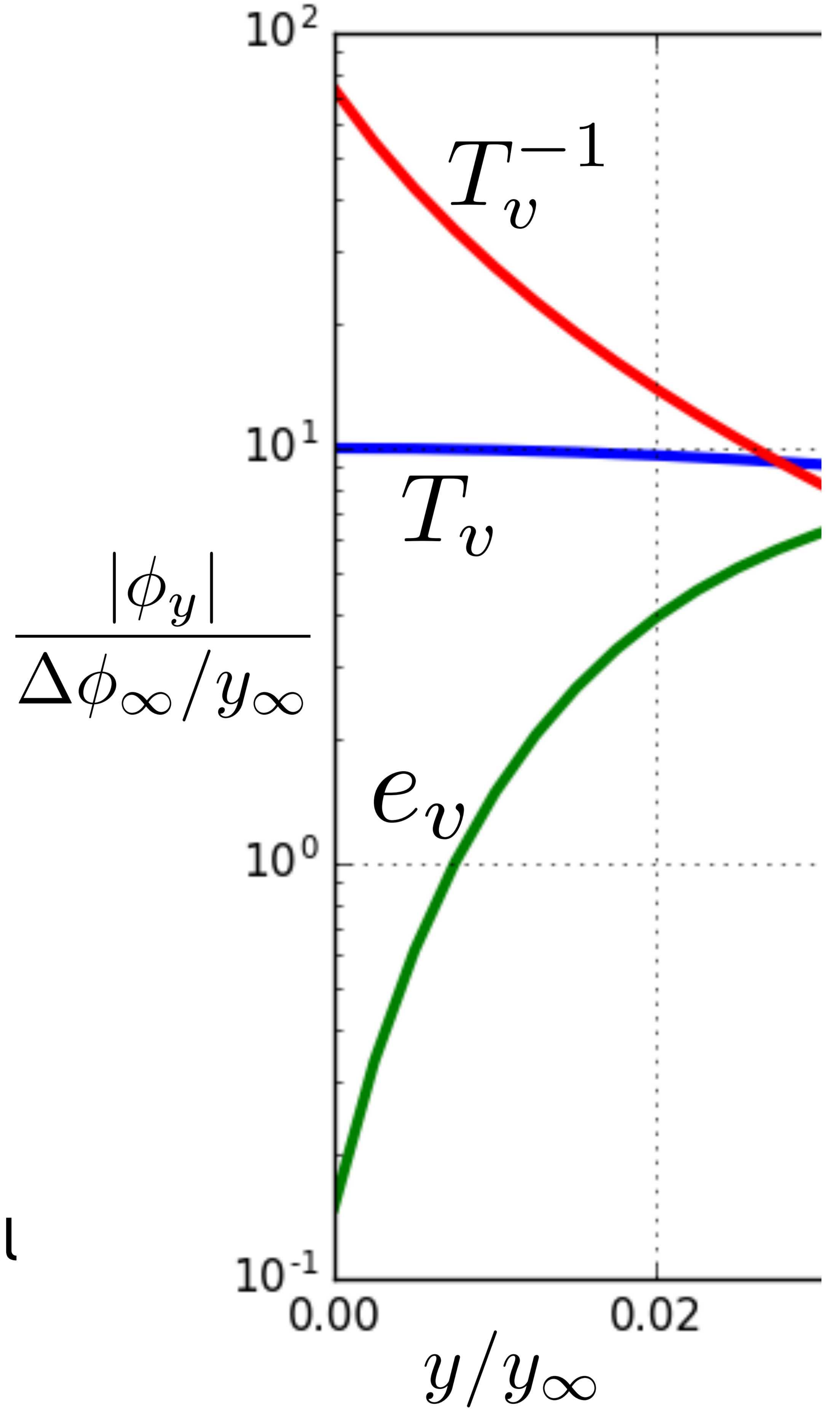
an issue in boundary conditions

- entropy vars may require extra boundary layer resolution, or a special procedure within the stability proof

Computing viscous fluxes with entropy variable gradients gives provable stability, but their large gradients in boundary layers can lead to BC flux errors



vibrational energy smooths at the wall



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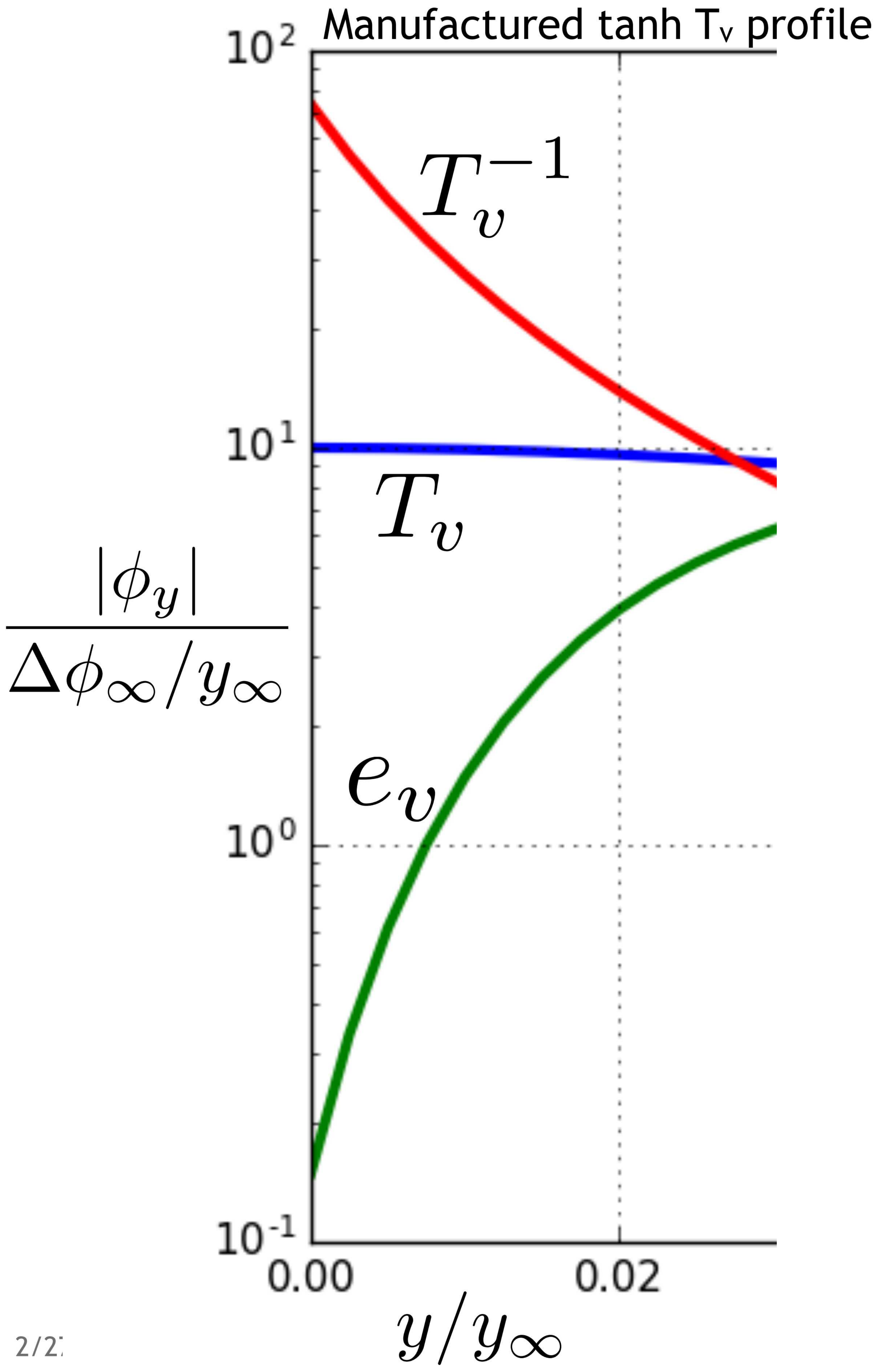

Nonequilibrium effects can demand the most boundary layer resolution

Recent findings motivate the use of vibrational energy in the gradient calculation, instead of vib. temperature.

$$\mathbf{q}_{bc} = \overset{\text{intuitive form}}{\boxed{-\kappa_v \nabla T_v}} = \underset{\text{Least resolution required}}{\overset{\text{‘optimal’ form}}{\boxed{-\frac{\kappa_v}{c_{v,v}} \nabla e_v}}} \underset{\text{MOST resolution required}}{\overset{\text{entropy var. form}}{\boxed{= T_v^2 \kappa_v \nabla T_v^{-1}}}}$$

Isothermal wall - use temp or energy at in the wall-normal gradient

- use a comparison approach,
  blend more accurate (less resolution) and more stable fluxes

We’ve extended continuous and semi-discrete entropy stability to multicomponent, multitemperature systems

<u>Thanks to my collaborators</u>
Travis C. Fisher, SNL
Mark Carpenter, NASA

continuous stability proofs

- straightforward constitutive property conditions
- mass diffusion model must be strictly conservative and include barometric diffusion

Simple Fick’s law, $j_i=-\rho D_i \partial Y_i$, is not provably stable

Provable entropy stability \=> conservation of mass

two-point entropy conservative flux functions

- automated jump expansion and linear system formulation led to affordable fluxes for a variety of MC, MT systems

Derived affordable fluxes for MC, MT systems

Need a new ‘exponential average’ for vibrational energy

Simplified, efficient forms exist for NASA polynomials

an issue in boundary conditions

- entropy vars may require extra boundary layer resolution, or a special procedure within the stability proof

Comparison approach to avoid overresolution required by the entropy variables

supplemental slides

Calorically perfect, n species, 1 temperature flux function

$$f_i^{S,n} = \widehat{\rho}_i \overline{v}^n$$

species mass fluxes
- log avg of species density
- arithmetic avg of velocity

$$f_{\mathrm{mom}}^{S,n} = \overline{\boldsymbol{v}} f_{\mathrm{mass}}^{S,n} + p^* \boldsymbol{n}$$

momentum fluxes
- total mass flux appears
- consistent approx. of pressure

$$f_e^{S,n} = \sum_{i=1}^{n_c} f_i^{S,n} e_i^* + p^* \overline{v}^n + \left(\overline{\boldsymbol{v}}^{\mathsf{T}} \overline{\boldsymbol{v}} - \frac{\overline{\boldsymbol{v}^{\mathsf{T}} \boldsymbol{v}}}{2} \right) f_{\mathrm{mass}}^{S,n}$$

energy flux
- consistent approx. of total enthalpy
- log avg of inverse temperature

$$\Delta e_{f,1}^{\circ} + \frac{3 + 2\nu_i}{2} R_i \left(\frac{1}{\widehat{\mathcal{Z}}_T} - T^{\circ} \right)$$

Exponential average series expansion

Comparison with arbitrary precision numerics shows
double precision accuracy up to jump(T) = 10 K at T = 3000 K
(shock, flame front)

$$\frac{\Delta \exp(ax)}{\Delta x} = \frac{a}{[x]_{\exp}} = a \exp(ax) \left(1 + \delta \left(\frac{1}{2} + \delta \left(\frac{1}{6} + \delta \left(\frac{1}{24} + \delta \frac{1}{120}\right)\right)\right)\right), \quad \delta = a\Delta x$$

New nonlinear terms from vibrational energy:

$$e_{v,j}(T_v) = \frac{R_j \Theta_j}{\exp(\Theta_j / T_v) - 1} \qquad \text{and} \qquad \int_{T^\circ}^{T_v} \frac{1}{T_v} \frac{\partial e_{v,j}}{\partial T_v} \mathrm{d}T_v$$