A Unified Continuous State-Space Thermodynamics Framework for Kinetic Fluctuations: Closures, Regularization, and Numerical Paradigms

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This work presents a comprehensive, mathematically rigorous framework for modeling non-equilibrium fluid dynamics by lifting the internal phase-space from a traditional macroscopic description to an invariant continuous state coordinate $s \in [0, \infty)$, which can represent localized peculiar energy spectra, species distributions, or internal molecular states. By transforming cumulative kinetic balances into pure, locally closed 5D partial differential equations, the classical closure problem for non-linear convective transport is analytically eliminated. We establish consistent rheological and thermal closures based on continuous state density distributions and smeared-flux methodologies to handle sharp gradients. To solve the resulting coupled hyper-dimensional system, we introduce a mathematical background tracer matrix regularization technique and propose three distinct numerical paradigms: a deterministic 4D hyper-mesh solver, an Eulerian Stochastic Fields method driven by Wiener processes, and a data-driven Scientific Machine Learning (SciML) surrogate framework.

I. INTRODUCTION AND MATHEMATICAL FRAMEWORK

Consider an arbitrary localized spatial control volume within a non-equilibrium gas flow. Rather than treating the fluid inside this control volume as a homogeneous single-phase continuum, we acknowledge that it comprises a dense ensemble of fluctuating micro-states. To track these internal degrees of freedom, we introduce an invariant continuous state coordinate $s \in [0, \infty)$, which can be physically instantiated as a peculiar energy coordinate ($s \equiv e$), an internal molecular spectrum, or chemical species identities.

By defining the cumulative volume fraction $\Phi(\mathbf{x}, t, s)$ occupied by all fluctuation states up to state level s, the state-specific density $\rho(s, \mathbf{x}, t)$ acts as a localized thermodynamic state function governed by pressure p and temperature T. This formulation allows us to lift the standard three-dimensional spatial domain into a hyper-dimensional 4D space $(\mathbf{x}, s) \in \mathbb{R}^4$.

Within any localized region of this hyperspace, the net change of a fluid property is driven by two uncoupled transport modes: physical convection through spatial coordinates ($\partial/\partial x_i$) and internal conversion (or migration velocity $\dot{s} = ds/dt$) driving continuous phase-space translation along the state coordinate axis. This dual-flux control volume interpretation holds universally for mass, momentum, and enthalpy balances, providing a strict conservative tracking mechanism analogous to the continuous multi-component transport formulations found in advanced reacting flow theories, cf. Kuo [3] and Williams [4]. Since s represents an invariant state coordinate orthogonal to physical space-time, spatial gradients and temporal derivatives commute with the integral bounds via Leibniz's rule ($\nabla s = 0$, $\partial s/\partial t = 0$).

> "For some multicomponent mixtures, where detailed chemical analysis is not feasible, the composition of the mixture may be described by a continuous distribution function."
> — Cotterman, Bender & Prausnitz (1985) [1]

II. GOVERNING TRANSPORT EQUATIONS

Using the Einstein summation convention over repeated spatial indices ($i, j, k = 1, 2, 3$), the coupled mass, momentum, and enthalpy transport laws across the 4D state-hyperspace are formulated below. By directly incorporating the fractional density $\rho(s)$, the fractional integrals display clear linear coupling to the cumulative distribution gradient $\partial\Phi/\partial s$.

A. Cumulative Mass Continuity

The cumulative mass balance tracks the integrated state up to state level s. Ordering density as the primary factor in the kernel, the cumulative integral form is expressed as

$$\frac{\partial}{\partial t}\left(\int_0^s \rho(s')\frac{\partial \Phi}{\partial s'}\,ds'\right) + \frac{\partial}{\partial x_i}\left(\int_0^s \rho(s')u_i(s')\frac{\partial \Phi}{\partial s'}\,ds'\right) + \rho(s)\dot{s}\frac{\partial \Phi}{\partial s} = 0. \tag{1}$$

Differentiating directly with respect to the independent coordinate s yields the uncoupled, pure partial differential equation (PDE) for each specific state fraction

$$\frac{\partial \rho(s)}{\partial t} + \frac{\partial(\rho(s)u_i(s))}{\partial x_i} + \frac{\partial}{\partial s}(\rho(s)\dot{s}) = 0. \tag{2}$$

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B. Cumulative Momentum Conservation

The momentum balance governing the fractional velocity fields $u_i(s)$ is given by

$$\frac{\partial}{\partial t}\left(\int_0^s \rho(s')u_i(s')\frac{\partial \Phi}{\partial s'}\,ds'\right) + \frac{\partial}{\partial x_j}\left(\int_0^s \rho(s')u_i(s')u_j(s')\frac{\partial \Phi}{\partial s'}\,ds'\right) + \rho(s)\dot{s}u_i(s)\frac{\partial \Phi}{\partial s} = -\Phi\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{c,ij}}{\partial x_j}, \tag{3}$$

where $\tau_{c,ij}(s)$ is the cumulative viscous stress tensor. Treating each state fraction as a compressible Newtonian fluid, the cumulative stress based on the integrated dynamic fraction-viscosity $\mu(s,p,T)$ [2, Chap. 5] is

$$\tau_{c,ij}(s,\mathbf{x},t) = \int_0^s \mu(s',p,T)\left(\frac{\partial u_i(s')}{\partial x_j} + \frac{\partial u_j(s')}{\partial x_i} - \frac{2}{3}\frac{\partial u_k(s')}{\partial x_k}\delta_{ij}\right)\frac{\partial \Phi}{\partial s'}\,ds'. \tag{4}$$

C. Rheological Closure and Structural Nature

The expression evaluated in Eq. (4) represents the simplest linear model for momentum diffusion within the continuous hyperspace. However, due to the arbitrary introduction of the continuous state variable s, even this linear formulation inherently incorporates a state-dependent dynamic viscosity $\mu(s,p,T)$. This state dependence reflects the reality that different fluctuation intensities or molecular energy states possess fundamentally distinct localized collision cross-sections and momentum-exchange characteristics.

For complex fluids, non-Newtonian behaviors, or highly dense gases, this linear assumption becomes insufficient. Complex rheological closures would require replacing the linear tensor relation with differential or integral constitutive expressions such as state-specific viscoelastic or shear-thinning formulations, where the dynamic viscosity becomes a non-linear function of both the local state coordinate s and the localized strain-rate.

D. Cumulative Enthalpy Conservation

Following the phase-specific energy balances employed in two-fluid models [5, Chaps. 2, 5, and 9] and structural formulations of reacting continuum mixtures [3, 4], pressure-work and viscous-work terms are formulated here using the fraction-specific velocity $u_i(s)$ rather than the bulk-averaged velocity. The cumulative integral form is given by

$$\frac{\partial}{\partial t}\left(\int_0^s \rho(s')h(s')\frac{\partial \Phi}{\partial s'}\,ds'\right) + \frac{\partial}{\partial x_i}\left(\int_0^s \rho(s')h(s')u_i(s')\frac{\partial \Phi}{\partial s'}\,ds'\right) + \rho(s)\dot{s}h(s)\frac{\partial \Phi}{\partial s} = \int_0^s \left(\frac{\partial p}{\partial t} + u_i(s')\frac{\partial p}{\partial x_i}\right)\frac{\partial \Phi}{\partial s'}\,ds' - \frac{\partial q_{c,i}}{\partial x_i} + \tau_{c,ij}\frac{\partial u_i(s)}{\partial x_j}. \tag{5}$$

E. Differentiated Enthalpy Pure PDE Form

Differentiating the enthalpy equation directly with respect to s yields the uncoupled governing equation

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial(\rho h u_i)}{\partial x_i} + \frac{\partial}{\partial s}(\rho h\dot{s}) = \frac{\partial \Phi}{\partial s}\left(\frac{\partial p}{\partial t} + u_i(s)\frac{\partial p}{\partial x_i}\right) - \frac{\partial q_i}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial s}\frac{\partial u_i(s)}{\partial x_j}, \tag{6}$$

where the localized cumulative heat flux vector is defined as

$$q_{c,i}(s,\mathbf{x},t) = -\left(\int_0^s \lambda(s',p,T)\frac{\partial \Phi}{\partial s'}\,ds'\right)\frac{\partial T}{\partial x_i}. \tag{7}$$

Analogous to the momentum transport, this formulation constitutes the simplest linear model for thermal energy diffusion within the continuous phase-space; capturing highly non-equilibrium or non-Fourier thermal behaviors in complex fluid matrices would necessitate more sophisticated, non-linear closure frameworks where the heat flux vector explicitly depends on localized multi-scale state coupling.

F. Asymptotic Macroscopic Consistency

At the global boundary $s \to \infty$, where $\Phi = 1$ and $\partial\Phi/\partial s = 0$, the exact reduction to the single-phase formulation gives the decomposition [6, Chap. 3, pp. 65–84]

$$\int_0^\infty \rho(s')u_i(s')u_j(s')\frac{\partial \Phi}{\partial s'}\,ds' = \rho_m u_{m,i}u_{m,j} + \int_0^\infty \rho(s')u_{d,i}(s')u_{d,j}(s')\frac{\partial \Phi}{\partial s'}\,ds', \tag{8}$$

where $u_{d,i}(s) = u_i(s) - u_{m,i}$ represents the multi-component algebraic fractional drift velocity, and ρ_m is the bulk mixture density.

The mathematical formulation presented in Eq. (8) highlights that compressing the fluctuations into a single scalar state coordinate s does not compromise the directional anisotropy of the underlying transport fields. Because the convective transport is managed by the full,

independent components of the vector-valued spectral velocity field $u_i(s)$, normal stress imbalances ($\tau_{xx} \neq \tau_{yy}$) are organically retained during localized shears. This enables the framework to natively map severe anisotropic non-equilibrium behaviors without forcing an unphysical early isotropization of the sub-grid ensembles.

> "... similar in concept to the well-known Krook model but yields the correct Prandtl number of 2/3 for a monatomic gas." – Holway (1966) [7]

This preprint document is a preliminary version of a full-scale physical and mathematical framework intended for future submission to a specialized journal, such as the *Journal of Computational Physics*, the *Journal of Fluid Mechanics*, or *Physics of Fluids*. A high-impact short communication focusing on the core conceptual breakthrough and the proof of anisotropy preservation has been submitted to *Physical Review Letters* [8].

III. NUMERICAL REGULARIZATION AND INDETERMINACY HEALING

A core hazard in continuous state-space tracking emerges when the distribution density vanishes ($\partial\Phi/\partial s \to 0$), leaving sub-intervals unpopulated. Under these conditions, the state-specific velocities $u_i(s)$ become mathematically indeterminate (0/0 form). To heal this singularity, we introduce the asymptotic continuity constraint

$$u_i(s) = u_i(s_1) \quad \forall s < s_1, \tag{9}$$

where s_1 marks the lowest active state threshold. Concurrently, an invariant, non-vanishing background tracer matrix scaled by $\delta \in [10^{-12}, 10^{-8}]$ regularizes the cumulative distribution function according to

$$\Phi_\delta(\mathbf{x}, t, s) = (1-\delta)\Phi(\mathbf{x}, t, s) + \delta \cdot \frac{s}{s_{\max}}, \tag{10}$$

$$\implies \frac{\partial \Phi_\delta}{\partial s} = (1-\delta)\frac{\partial \Phi}{\partial s} + \frac{\delta}{s_{\max}} \geq \frac{\delta}{s_{\max}} > 0. \tag{11}$$

This bounds the linear solver, forcing unpopulated virtual states to relax smoothly toward the bulk velocity $u_{m,i}$ via implicit inter-phase drag without altering active physical mass balances.

IV. ALGORITHMIC SOLVERS FOR LOW-MACH FINITE VOLUME IMPLEMENTATIONS

For low-Mach configurations, pressure-based fractional projection steps compatible with explicit Total Variation Diminishing (TVD) Runge-Kutta time-stepping are introduced.

A. Approach I: Deterministic 4D Hyper-Mesh Solver

The domain is discretized into a rigid multi-dimensional grid $(\mathbf{x}, s) \in \mathbb{R}^4$. High-order numerical quadrature resolves the integrals at every time stage.

Algorithm 1 Deterministic 4D hyper-mesh FVM step

1: Initialize the stage variables with $\Psi^* \leftarrow \Psi^n$.
2: **for** each TVD Runge–Kutta stage $k = 1, \ldots, K$ **do**
3: Evaluate $\rho(s_l)$, $\mu(s_l)$, and $\lambda(s_l)$ subject to the tracer limits.
4: Set $u_i(s_l) \leftarrow u_i(s_1)$ for every unpopulated state below the active threshold.
5: Compute the bulk invariants

$$\rho_m = \sum_l \rho(s_l)\,\Delta\Phi_{\delta,l},$$

$$\rho_m u_{m,i} = \sum_l u_i(s_l)\rho(s_l)\,\Delta\Phi_{\delta,l}.$$

6: Reconstruct $\tilde{\rho}^*$, u_i^*, and h^* at cell faces using TVD van Leer/MUSCL.
7: Solve the pressure Poisson problem

$$\nabla^2 p^{n+1} = \frac{1}{\Delta t}\left[\nabla \cdot u^*_{m,i} + \frac{1}{\rho_m}\sum_l \frac{\partial}{\partial s}\left(\dot{s}\rho(s_l)\frac{\partial \Phi_\delta}{\partial s}\right)_l\right]. \tag{12}$$

8: Project the fraction velocities

$$u_i^k(s_l) = u_i^*(s_l) - \frac{\Delta t}{\rho(s_l)}\frac{\partial p^{n+1}}{\partial x_i}.$$

9: **end for**
10: Advance to t^{n+1} with the TVD Runge–Kutta weighted blend.

B. Approach II: Eulerian Stochastic Fields Method

Following the stochastic-fields formulation of Valiño [9] and its subsequent application by Jones and Navarro-Martinez [10], the continuous spectrum is resolved by an ensemble of N_f stochastic fields driving independent multi-dimensional Wiener processes $dW_j^n = \zeta_j^n\sqrt{\Delta t}$ where $\zeta \sim \mathcal{N}(0,1)$.

> "The source terms [...]appear in closed form and are direct solutions of the chemistry ODE system for the n-th field." — Breda et al. (2021) [11, p. 448]

Algorithm 2: Eulerian Stochastic Fields Low-Mach Solver

1. Sample independent Gaussian random numbers ζ_j^n globally per field $n \in [1, N_f]$.

2. Loop over explicit TVD Runge-Kutta stages $k = 1 \ldots K$:

(a) Advance the stochastic scalars with the closed transport source $\dot{s}$

$$\xi_n^* = \xi_n^{k-1} + \Delta t[\text{Conv} + \text{Diff} + \dot{s}(\xi_n^{k-1})] + \sqrt{2D_{\text{sgs}}}\frac{\partial \xi_n^{k-1}}{\partial x_j}\zeta_j^n\sqrt{\Delta t}. \quad (13)$$

(b) Apply tracer regularization and phase boundary mapping ($s < s_1$) using the asymptotic constraint.

(c) Map the sub-grid PDF using $\rho_m = \frac{1}{N_f}\sum_n \rho(\xi_n^*)$ and $u_{m,i} = \frac{1}{N_f}\sum_n u_i(\xi_n^*)$.

(d) Solve the ensemble-averaged low-Mach Pressure Poisson Equation for p^{n+1}.

(e) Apply localized pressure gradient correction to project the field velocity distribution.

3. Apply temporal sliding-window smoothing over ΔN_t steps to damp statistical Wiener noise.

C. Approach III: Data-Driven SciML Surrogates

An offline deep neural network (DNN) maps local thermodynamic states and compositional shape moments α to pre-integrated non-local cumulative transport components through the surrogate relation [12]

$$\mathcal{F}\text{ML}: p(\mathbf{x},t), T(\mathbf{x},t), s, \alpha \longrightarrow \rho_m, \rho_m u_m, \tau c, ij, q_{c,i}. \quad (14)$$

The global asymptotic boundary conditions verified at $s \to \infty$ are embedded in the loss function of the Physics-Informed Neural Network (PINN) through the hard regularizing constraint [13]

$$\mathcal{L}\text{total} = \mathcal{L}\text{data} + \gamma|\mathcal{F}\text{ML}(s \to \infty) - \Psi\text{mixture}|_2^2. \quad (15)$$

V. COMPARATIVE DISCUSSION AND APPLICABILITY MATRIX

TABLE I. Numerical Applicability Matrix for Continuous Kinetic Space Transport.

Paradigm	**Complexity / Regime**	**CPU Cost / Bottleneck**
Approach I	Low ($N_s \leq 10$) Laminar	High ($\mathcal{O}(N^4)$) Grid scaling
Approach II	High (Polyd.) Turbulent	Moderate Stat. noise
Approach III	Stiff / Non-Lin. Industrial	Extr. low Training / data

VI. CONCLUSIONS AND PARADIGM SHIFTS

This work establishes a mathematically uncoupled hyper-dimensional formulation that fundamentally redefines the traditional modeling hurdles of non-equilibrium flows. By mapping localized fluctuation kinetics onto an invariant continuous state coordinate s and formulating the governing laws via pure 5D partial differential equations, we execute a radical paradigm shift. In classical Reynolds-averaged or filtered continuum frameworks, the primary closure challenge lies within the highly nonlinear convective transport terms (e.g., the Reynolds stress tensor or subgrid-scale convective fluxes). In our continuous state-space framework, this convective closure problem is analytically eliminated because the state-specific velocity fields are tracked independently across the hyperspace.

Consequently, the physical and mathematical closure challenge is shifted entirely to the state-space diffusion, cross-property conduction, and localized relaxation terms. Within this new paradigm, the critical modeling frontier centers on closing the localized diffusion terms where the gradients of the cumulative velocities interact across unpopulated or sharply bounded regions of the continuous spectrum. Managing these interfaces requires robust regularization techniques—such as the background tracer matrix introduced here—to prevent numerical indeterminacy. This shifting of the closure challenge from physical convection to hyper-dimensional diffusion opens an alternative path for high-fidelity non-equilibrium fluid dynamics, providing an organic mechanism to preserve transport anisotropies without early numerical isotropization.

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