High-Order Entropy-Based Moment Closures: A Computational Study of the Optimization Problem

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In the simulation of kinetic systems, moment models are used to create numerically tractable problems by simplifying the description of the state space and by converting the problem to a naturally parallelizable form. Entropy-based moment closures are moment models which retain fundamental properties of the underlying kinetic equations such as hyperbolicity, entropy dissipation, and positivity but require the solution of a constrained, strictly convex optimization problems at each point on a space-time mesh.

The difficulty of this problem for certain moments has been the main obstacle to wide-spread implementation of the method. In this work, we dig in to find out when and why the optimization problem is difficult and address these difficulties.

Our Kinetic Model

For our tests, we model the migration of unit-speed particles that are absorbed by or scattered isotropically off of a background material medium with slab geometry. The particle system is characterized by the non-negative density $F = F(x, \mu, t)$ that is governed by the kinetic equation

$$\partial_t F + \mu \partial_x F + \sigma_t F = \frac{\sigma_s}{2} \langle F \rangle \,, \tag{1}$$

where $\langle \cdot \rangle$ denotes integration over the angle variable $\mu \in [-1, 1]$.

The moments of F with respect to a vector of polynomials $\mu \mapsto \mathbf{m}(\mu) \in \mathbb{R}^{N+1}$ are given by $\langle \mathbf{m} F(x, \cdot, t) \rangle =: \mathbf{u}(x, t)$. The exact evolution of $\mathbf{u}(x, t)$ can be found by multiplying (1) by $\mathbf{m}$ and integrating out μ to get

$$\partial_t \mathbf{u} + \partial_x \langle \mu \mathbf{m} F \rangle + \sigma_t \mathbf{u} = \sigma_s Q \mathbf{u} \,. \tag{2}$$

Entropy-based closures close the moment system by approximating F in (2) by an *ansatz* which solves the constrained, strictly convex optimization problem

$$\min_g \ \langle \eta(g) \rangle \qquad \text{subject to } \langle \mathbf{m} g \rangle = \mathbf{u} \,, \tag{3}$$

where $\eta(z) = z \log z - z$ is the Maxwell-Boltzmann entropy. In our implementation, we solve the unconstrained, finite-dimensional, strictly convex dual problem,

$$\min_{\boldsymbol{\alpha} \in \mathbb{R}^{N+1}} \left\langle \exp(\boldsymbol{\alpha}^T \mathbf{m}) \right\rangle - \boldsymbol{\alpha}^T \mathbf{u} \,. \tag{4}$$

We denote the solution to (4) by $\hat{\boldsymbol{\alpha}}(\mathbf{u})$. The ansatz which solves (3) has the form $G_{\boldsymbol{\alpha}} = \exp(\boldsymbol{\alpha}^T \mathbf{m})$. Substitution of $G_{\hat{\boldsymbol{\alpha}}(\mathbf{u})}$ for F in (2) gives the so-called M_N models.

Addressing the Computational Difficulties

Maintaining realizability

- The optimizer and PDE solver must work together to ensure that the numerical solution of (2) stays in the set of *realizable* moments.

➜ Our optimization enforces the stopping criterion

$$\gamma := \exp\left(\|\hat{\boldsymbol{\alpha}} - \bar{\boldsymbol{\alpha}}\| \max_\mu \|\mathbf{m}\| \right) < 1 + \varepsilon \,. \tag{5}$$

➜ Then with the time-step restriction

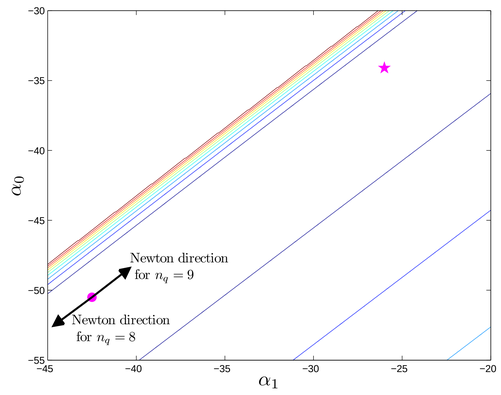
$$\max\{\gamma\} \frac{\Delta t}{\Delta x} \frac{2 + \theta}{2} + \sigma_t \Delta t < 1 \,, \tag{6}$$

the solution maintains realizability.

Accurate integration

- The integral in the objective function of the dual problem (4) must be evaluated by quadrature.
- Near the realizable boundary, the ansatz $G_{\hat{\boldsymbol{\alpha}}(\mathbf{u})}$ approximates atomic distributions—difficult for most quadrature rules!

➜ We implemented an adaptive quadrature.



Level curves of the objective function for an M_1 problem near the boundary of realizability, where n_q is the number of quadruatre points.

Iterative change of polynomial basis

- The Hessian of the dual objective function is given by $H(\boldsymbol{\alpha}) = \left\langle \mathbf{m}\mathbf{m}^T G_{\boldsymbol{\alpha}} \right\rangle$.
- As $\mathbf{u}$ approaches the realizable boundary, the Hessian at the solution $H(\hat{\boldsymbol{\alpha}}(\mathbf{u}))$ approaches singularity.

➜ But in a different polynomial basis, the Hessian is identity:

$$H(\boldsymbol{\alpha}) = \left\langle \mathbf{m}\mathbf{m}^T G_{\boldsymbol{\alpha}} \right\rangle = R^T \underbrace{\left\langle \mathbf{p}\mathbf{p}^T G_{\boldsymbol{\alpha}} \right\rangle}_{=I} R \,. \tag{7}$$

Because H is symmetric positive-definite, we use the Cholesky factorization $H = R^T R$ to define the change of basis $\mathbf{m} = R^T \mathbf{p}$.

➜ The change of basis may be poorly conditioned, so we approach it iteratively by changing basis at every optimization iteration.

Regularization near the boundary of realizability

- For some problems, $\mathbf{u}$ is too close to the realizable boundary to be solved in finite precision.

➜ We construct nearby tractable moments:

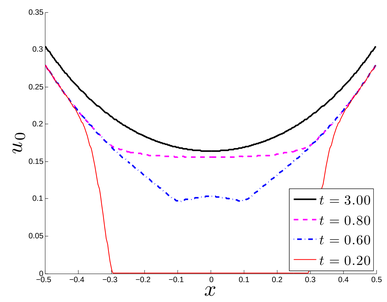
$$\mathbf{v}(r) := (1 - r)\mathbf{u} + r Q \mathbf{u} \,, \tag{8}$$

where $Q\mathbf{u}$ are the moments of the isotropic distribution with the same number of particles.

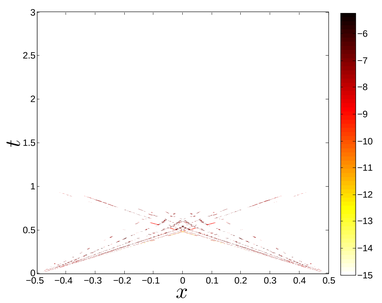
➜ $r \in (0, 1)$ should be chosen as small as possible. Typically, $r \leq 10^{-4}$.

Illustrations

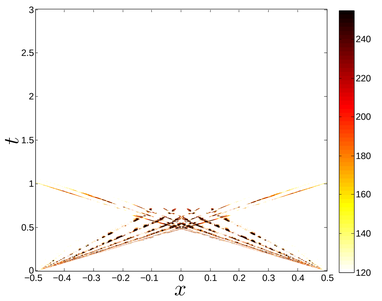
The following figures display some quadrature and optimization details in a 400-cell simulation of a two-beam instability using the M_{15} model.



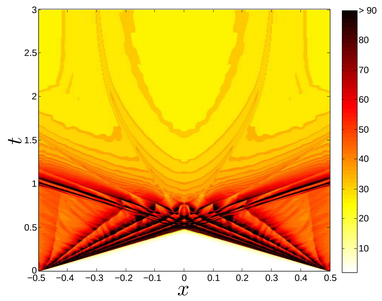
Snapshots of the solution.



$\log_{10} \|\mathbf{u} - \mathbf{v}(r)\|$: *Amount of regularization.*



Number of quadrature points.



Number of optimization iterations.

Conclusions

Our work has detailed the difficulties in solving optimization problems of the form (4) and suggested practical ways to deal with these problems in concert with the numerical solution of the moment model. With our proposed regularization technique, our work has illustrated how to solve the problem up to the limit of finite precision. Our future work will focus on improving the quadrature and incorporating our current progress into partial-moment models, other entropy choices, and higher spatial dimensions.

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