Goal-oriented adaptive methods for a Boltzmann-type equation

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Abstract. The Boltzmann equations is an integro-differential equation posed on a high-dimensional position-velocity space. The complexity of the Boltzmann equation in principle prohibits straightforward approximation by the finite-element method. In many applications of the Boltzmann equation, interest is however restricted to one particular goal functional of the solution. In such cases, significant reduction of the computational complexity can be accomplished by means of goal-adaptive refinement strategies. In this paper, we present a goal-oriented error-estimation and adaptive-refinement procedure for a one-dimensional prototype of the Boltzmann model with a collision term that exhibits the essential complexities and characteristics of higher dimensional Boltzmann models.

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INTRODUCTION

In many fluid-engineering applications, one is interested in *macro-scale* quantities such as a local temperature, heat transfer across a part of a boundary or aggregated mass transfer across a part of the boundary. The Navier-Stokes or Euler equations provide a suitable description of fluids in the continuum regime, i.e., for sufficiently small *Knudsen* numbers. If the continuum assumption is violated, one needs to revert to an alternative description of the flow, e.g., molecular dynamics (MD) or a probabilistic description as provided by the Boltzmann equation. Because macro-scale flow properties depend essentially on ensembles and not on individual molecules, the Boltzmann equation is in principle most suitable for determining macro-scale properties of flows in the transitional molecular/continuum regime; see [1, 2].

The Boltzmann equation specifies the evolution of a *one-particle probability density function* on a high-dimensional position-velocity space, viz., $\mathbb{R}^{2d}$ for d spatial dimensions. Approximation of such a high-dimensional problem requires extremely efficient numerical techniques. Given that practical interest is often restricted to particular quantities, we consider *goal-oriented adaptive* finite-element strategies. Goal-adaptive finite-element strategies provide a (quasi-)optimal computational model for a particular functional. These strategies rely on a-posteriori estimates of the error in the functional, based on the solution of a (linearized) dual problem. The a-posteriori error estimate is subsequently used to construct element-wise refinement indicators to optimally improve the accuracy of the goal functional; see [3, 4] for further details.

In this work we are concerned with goal-adaptive finite-element approximations of a one-dimensional prototype of the Boltzmann equation. We derive the corresponding linearized dual problem and formulate the goal-adaptive refinement strategy. Finally, we present numerical results to illustrate the characteristic properties of the method.

PROBLEM STATEMENT

The Boltzmann model

We consider an open (spatial) interval $\Omega =]0,1[$, a (velocity) interval $\Xi = \mathbb{R}$ and the position-velocity domain $\Sigma = \Omega \times \Xi$. The boundary of Σ, denoted by $\partial\Sigma$, consists of two disjoint parts, Γ_0 and Γ_1, corresponding to $x = 0$ and $x = 1$, respectively. Furthermore, Γ_0 (resp. Γ_1) is composed of an inflow boundary Γ_0^- (resp. Γ_1^-) and and outflow boundary Γ_0^+ (resp. Γ_1^+). Formally denoting by $\mathscr{P}$ the aggregate of all *one-particle probability-density functions* on Σ, the stationary Boltzmann model problem specifies that $f \in \mathscr{P}$ complies with:

$$\begin{aligned} \nabla(f\xi) - Q(f,f) &= 0 \qquad \text{on } \Sigma, \\ f &= f_{\mathrm{B}} \qquad \text{on } \Gamma^-, \end{aligned} \tag{1}$$

where $\Gamma^\pm = \Gamma_0^\pm \cup \Gamma_1^\pm$ and f_{B} is a prescribed function. The *collision term* Q is a bilinear operator from $\mathscr{P} \times \mathscr{P}$ into some dual space, which we assume to coincide with $\mathscr{P}'$.

For standard elastic collisions, the collision operator vanishes in 1D. Consequently, the 1D Boltzmann equation with elastic collisions lacks certain essential properties, in particular, weak convergence of solutions to *Maxwell-Boltzmann equilibrium distributions*; see, e.g., [1]. To recover the weak-convergence property, we instead fabricated a 1D Boltzmann equation with *energy-conserving random collisions*. The corresponding collision term can be separated into a gain and a loss term according to $Q(f,h) = \varepsilon^{-1}(G(f,h) - L(f,h))$, where ε denotes the Knudsen number and:

$$\begin{aligned} L(f,h) &= f\,\ell(h) \\ G(f,h) &= \int_{-\infty}^{\xi} \tfrac{1}{2}|\xi-\eta|\,[g^+(f,h)](\xi,\eta)\,\mathrm{d}\eta + \int_{\xi}^{\infty} \tfrac{1}{2}|\xi-\eta|\,[g^-(f,h)](\xi,\eta)\,\mathrm{d}\eta, \end{aligned}$$

with

$$\begin{aligned} [\ell(h)](\xi) &= \int_{-\infty}^{\infty} h(\eta)|\xi-\eta|\,\mathrm{d}\eta \\ [g^\pm(f,h)](\xi,\eta) &= \int_0^\pi f(\pm|\xi,\eta|\cos(\alpha+\tfrac{\pi}{4}))\,h(\pm|\xi,\eta|\sin(\alpha+\tfrac{\pi}{4}))\sin(\alpha)\,\mathrm{d}\alpha \end{aligned}$$

and $|\xi,\eta| = \sqrt{\xi^2+\eta^2}$.

To facilitate the derivation of the dual problem, we condense (1) into the variational formulation: Find $f \in \mathscr{P}$ such that

$$a(f,\varphi) + q(f,f,\varphi) = b(\varphi) \qquad \forall \varphi \in \mathscr{P}, \tag{2}$$

where the bilinear functional a, the trilinear functional q and the linear functional b are defined by

$$\begin{aligned} a(f,\varphi) = -(f,\nabla(\varphi\xi))_\Sigma - (\varphi, f\xi)_{\Gamma_0^+} + (\varphi, f\xi)_{\Gamma_1^+}, \\ q(f,h,\varphi) = -(\varphi, Q(f,h))_\Sigma, \quad b(\varphi) = (\varphi, f_{\mathrm{B}}\xi)_{\Gamma_0^-} - (\varphi, f_{\mathrm{B}}\xi)_{\Gamma_1^-}. \end{aligned}$$

with $(\cdot,\cdot)_\omega$ the standard L^2 inner product on the set ω.

Quantity of interest

Rather than in the solution f itself, we are interested in the value of a goal functional of the solution $J(f)$ with $J \in \mathscr{P}'$. We consider the generic goal functional:

$$J(f) := (f,\psi)_\Sigma - (f\xi,\zeta)_{\Gamma_0^+} + (f\xi,\zeta)_{\Gamma_1^+}. \tag{3}$$

For instance, for $\psi = 0$, $\zeta|_{\Gamma_1^+} = 0$ and $\zeta|_{\Gamma_0^+} = (\cdot)^2$, the functional J represents the energy flux at the outflow boundary Γ_0^+, which is an important quantity in heat-transfer problems. Note that for stationary problems, the total energy flux across the boundary necessarily vanishes.

THE DUAL OF THE BOLTZMANN MODEL

The nonlinear functional $(f,\varphi)\mapsto q(f,f,\varphi)$ is Fréchet differentiable with derivative

$$q(\tilde f,\delta f,\varphi)+q(\delta f,\tilde f,\varphi)=q(\tilde f+\delta f,\tilde f+\delta f,\varphi)-q(\tilde f,\tilde f,\varphi)+O\big(\|\delta f\|^2\big), \tag{4}$$

as $\|\delta f\|\to 0$. At an approximation $\tilde f\in\mathscr{P}$, the linearized dual problem associated with the variational problem (2) and the goal functional J is therefore given by: Find $\gamma\in\mathscr{P}$ such that

$$a(\delta f,\gamma)+q(\tilde f,\delta f,\gamma)+q(\delta f,\tilde f,\gamma)=J(\delta f)\qquad\forall\,\delta f\in\mathscr{P}, \tag{5}$$

To derive the integro-differential equation associated with (5) and the corresponding boundary conditions, we separate the trilinear form q according to $q=q^{(G)}-q^{(L)}$, corresponding to the partition of Q, and we note that:

$$q^{(L)}(\delta f,\tilde f,\gamma)+q^{(L)}(\tilde f,\delta f,\gamma)=\big(\delta f,\gamma\ell(\tilde f)+\ell(\gamma\tilde f)\big)_\Sigma=:\big(\delta f,L^*(\tilde f,\gamma)\big)_\Sigma.$$

To derive the contribution corresponding to the gain term, we invoke the transformation $(\xi,\eta)=r(\cos\theta,\sin\theta)$ to obtain:

$$\begin{aligned}q^{(G)}(\delta f,\tilde f,\gamma)=&\int_\Omega\int_0^\infty\int_\pi^{2\pi}2^{-1/2}r^2\,\gamma\Big(x,r\cos\Big(\theta+\frac{\pi}{4}\Big)\Big)\,|\sin\theta|\\&\int_0^\pi\delta f\Big(x,r\cos\Big(\alpha+\frac{\pi}{4}\Big)\Big)\,\tilde f(x,r\sin(\alpha+\tfrac{\pi}{4}))\,\sin\alpha\,\mathrm{d}\alpha\,\mathrm{d}\theta\,\mathrm{d}r\,\mathrm{d}x\\+&\int_\Omega\int_0^\infty\int_0^\pi2^{-1/2}r^2\,\gamma\Big(x,r\cos\Big(\theta+\frac{\pi}{4}\Big)\Big)\,|\sin\theta|\\&\int_0^\pi\delta f\Big(x,-r\cos\Big(\alpha+\frac{\pi}{4}\Big)\Big)\,\tilde f(x,-r\sin(\alpha+\tfrac{\pi}{4}))\,\sin\alpha\,\mathrm{d}\alpha\,\mathrm{d}\theta\,\mathrm{d}r\,\mathrm{d}x\end{aligned} \tag{6}$$

Note that (6) admits a change in the order of integration. After a series of tedious manipulations, we then obtain:

$$q^{(G)}(\delta f,\tilde f,\gamma)+q^{(G)}(\tilde f,\delta f,\gamma)=(\delta f,G^*(\tilde f,\gamma))_\Sigma,$$

where

$$[G^*(\tilde f,\gamma)](x,u)=2^{-1}\int_{-\infty}^\infty\tilde f(x,\eta)\,|\xi-\eta|\,\big([g^+(\gamma,1)](x,\eta)+[g^-(\gamma,1)](x,\eta)\big)\,\mathrm{d}\eta$$

The integro-differential equation associated with (5) and the corresponding boundary conditions now follow straightforwardly by identifying like terms:

$$-\nabla(\gamma\xi)-G^*(\tilde f,\gamma)+L^*(\tilde f,\gamma)=\psi\qquad\text{on }\Sigma, \tag{7a}$$

$$\gamma=-\zeta\qquad\text{on }\Gamma^+, \tag{7b}$$

GALERKIN APPROXIMATION AND ADAPTIVITY

Discontinuous Galerkin finite element approximation

To approximate the primal problem (2) and the dual problem (5), we apply a discontinuous Galerkin method (dG). For an elaboration of the dG method, see, e.g., [5]. The velocity domain Ξ is truncated and the corresponding domain $\Sigma=\Omega\times\Xi$ is covered with a regular tessellation $\mathscr{T}$ of disjoint rectangular open element-domains, such that $\Sigma=\mathrm{int}\big(\bigcup_{\sigma\in\mathscr{T}}\overline{\sigma}\big)$. Denoting by $\mathscr{P}_p=\{f\in L^2(\Sigma):f|_\sigma$ is polynomial of degree $\le p$ in both arguments for all $\sigma\in\mathscr{T}\}$ the finite-element approximation space of piecewise tensor-product polynomials of degree p, subordinate to the mesh $\mathscr{T}$, the discontinuous Galerkin approximation of (2) is given by: *find $f_p\in\mathscr{P}_p$ such that*

$$a(f_p,\varphi_p)-q(f_p,f_p,\varphi_p)=b(\varphi_p)\quad\forall\varphi_p\in\mathscr{P}_p. \tag{8}$$

It is to be remarked that, in fact, we use a standard modification of the bilinear form a in the dG formulation which includes *upwind fluxes*. For conciseness, this standard modification is not further elaborated. Associated with the primal variational problem (8) is the *residual functional* $r : \mathscr{P} \oplus \mathscr{P}_p \to \mathscr{P}'$,

$$\langle r(f), \cdot \rangle := b(\cdot) - a(f, \cdot) - q(f, f, \cdot)\,. \tag{9}$$

If f solves (2), then $r(f) = 0$. Furthermore, for the solution f_p of (8) we have the *Galerkin orthogonality* relation $\langle r(f_p), \varphi_p \rangle = 0$ for all $\varphi_p \in \mathscr{P}_p$.

Error estimates

For any approximation f_p, we can express the corresponding error in the goal functional up to linearization errors by the duality pairing $\langle r(f_p), \gamma \rangle$. Indeed, we have the chain of identities:

$$\begin{aligned} J(f) - J(f_p) = J(f - f_p) &= a(f - f_p, \gamma) + q(f_p, f - f_p, \gamma) + q(f - f_p, f_p, \gamma) \\ &= a(f, \gamma) + q(f, f, \gamma) - a(f_p, \gamma) - q(f_p, f_p, \gamma) + O(\|f - f_p\|^2) \\ &= b(\gamma) - a(f_p, \gamma) - q(f_p, f_p, \gamma) + O(\|f - f_p\|^2) \\ &= \langle r(f_p), \gamma \rangle + O(\|f - f_p\|^2) = \langle r(f_p), \gamma - \gamma_p \rangle + O(\|f - f_p\|^2), \end{aligned} \tag{10}$$

for all $\gamma_p \in \mathscr{P}_p$. The second and fourth identity in the above chain follow from the dual problem (5) and the primal problem (2), respectively. The final identity holds on account of Galerkin orthogonality. The dual solution γ is in general not computable. A computable error estimate is obtained by replacing γ in the final expression in (10) by dG approximation of the dual solution in $\mathscr{P}_{p+1}$.

Adaptive strategy

To determine element wise error indicators, we consider the following sequence of bounds:

$$|\langle r(f_p), \gamma_{p+1} \rangle| = \Big| \sum_i \langle r(f_p), \psi^i_{p+1} \rangle \hat{\gamma}^i_{p+1} \Big| \leq \sum_{\sigma \in \mathscr{T}} \kappa_\sigma \quad \text{with} \quad \kappa_\sigma = \sum_{i \in \mathscr{I}_\sigma} \big| \langle r(f_p), \psi^i_{p+1} \rangle \big| \, \big| \hat{\gamma}^i_{p+1} \big|,$$

where $\{\psi^i_{p+1}\}$ are the finite-element basis functions of $\mathscr{P}_{p+1}$ and $\hat{\gamma}^i_{p+1}$ are the corresponding coefficients of the approximation to the dual solution. Moreover, $\mathscr{I}_\sigma$ denotes the index set associated with a particular element σ. Based on the error indicators κ_σ, we use a *Dörfler-type strategy* to mark elements with the largest error contributions for refinement, in such a manner that the sum of their error indicators is at least a certain fraction of the total error; see [6].

In this work we restrict ourselves to so-called *h-refinement*, meaning that elements are divided in either x, ξ or both directions. Furthermore, due to the complexity of the collision operator, a semi-local refinement strategy is employed to prevent the occurrence of *hanging nodes*.

NUMERICAL EXPERIMENT

To illustrate the potential of goal-adaptive methods for the Boltzmann equation, we consider a test case in which the solution corresponds to the equilibrium distribution $f_{\text{eq}}(x, \xi) = (2\pi)^{-1/2} \exp(\xi^2/2)$, and we compare results obtained by uniform mesh-refinement and goal-adaptive mesh-refinement in terms of the error in the goal functional versus the number of degrees of freedom N_{dofs}. We provide the Boltzmann equation with the boundary conditions $f_{\text{B}} = f_{\text{eq}}(0, \cdot)$ at Γ_0^- and specular reflection at Γ_1, viz., $f(1, -\xi) = f(1, \xi)$ for $\xi \in \mathbb{R}_+$. Furthermore, we consider two distinct goal functionals, corresponding to a boundary flux at Γ_0^+, i.e., referring to (3), we set $\psi = 0$, $\zeta|_{\Gamma_1^+} = 0$ and

$$\zeta|_{\Gamma_0^+}(\xi) = \cos(\xi) - 1 \quad \text{and} \quad \zeta|_{\Gamma_0^+}(\xi) = \begin{cases} \cos(\xi) - 1 & -\pi/2 < \xi < 0 \\ 0 & \text{otherwise} \end{cases}, \tag{11}$$

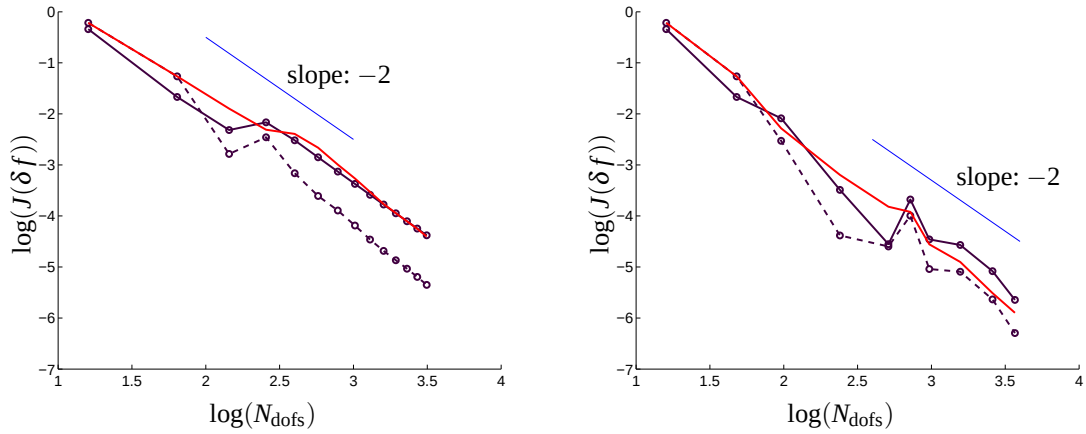

FIGURE 1. Convergence of the error (continuous), error estimate (dashed) and the upper bound $\sum_{\sigma\in\mathscr{T}}\kappa_\sigma$ of the error estimate (red continuous) for goal functional I for uniform mesh refinement (*left*) and goal-adaptive mesh refinement (*right*).

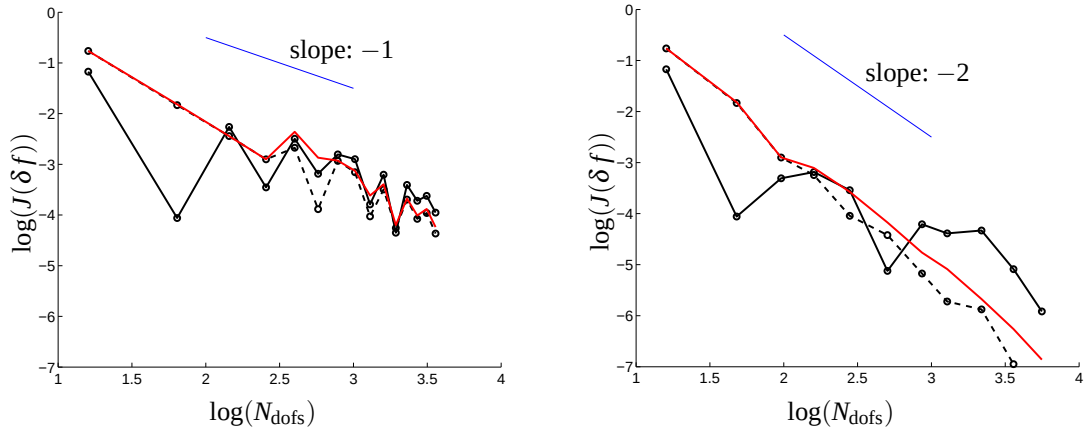

FIGURE 2. Convergence of the error (continuous), error estimate (dashed) and the upper bound $\sum_{\sigma\in\mathscr{T}}\kappa_\sigma$ of the error estimate (red continuous) for goal functional II for uniform mesh refinement (*left*) and goal-adaptive mesh refinement (*right*).

for goal functionals I and II, respectively. Noting that $\zeta|_{\Gamma_0^+}$ appears as boundary data in the dual problem (7), we infer that goal functional I yields a smooth dual solution, while goal functional II yields a non-smooth dual solution.

We consider linear dG approximations, i.e., $p=1$. Figures 1 and 2 present convergence results for goal functional I and goal functional II, respectively, for uniform refinement (*left panel*) and goal-adaptive refinement (*right panel*). Figure 1 shows that both uniform and adaptive refinement converge with optimal order (in this case, $p+1$) if the dual solution is smooth. Figure 2 illustrates that uniform refinement leads to suboptimal convergence if the goal functional engenders a non-smooth dual solution. The goal-adaptive refinement procedure restores the optimal convergence behavior, by effectively refining the finite element mesh in the vicinity of the discontinuity in the dual solution; see also the adaptively refined meshes in Figure 3. The symmetry of the mesh with respect to $\xi=0$ has been imposed to avoid mesh irregularity (hanging nodes) due to the specular-reflection boundary condition at Γ_1.

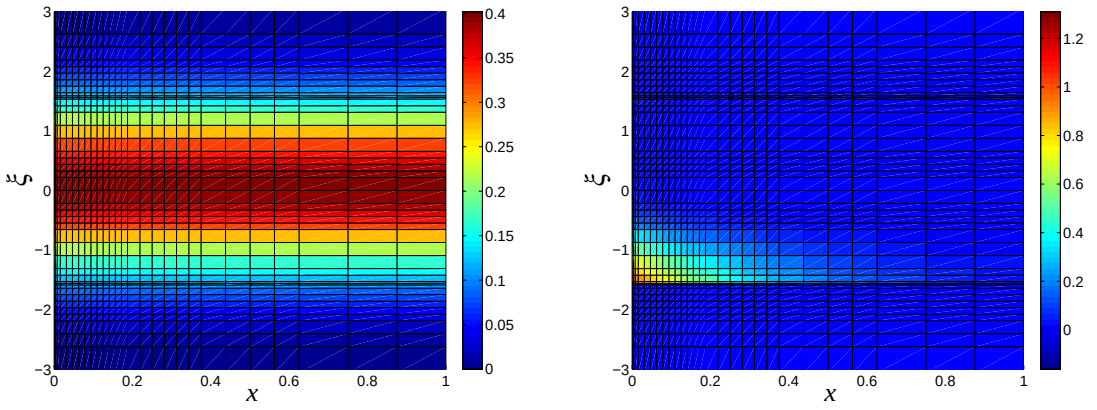

FIGURE 3. Primal solution (left) and dual solution (right) on the adaptively refined finite element mesh for goal functional II, which generates a discontinuity in the dual solution on Γ_0^+ at $\xi = -\pi/2$.

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