Analysis and Optimization of Perfectly Matched Layers for the Boltzmann Equation

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Overview

Numerical simulations of problems defined on unbounded domains are challenging due to limited computational resources. When approaching this problem, one is usually forced to truncate the simulation domain and introduce some form of absorbing boundary layer.
We consider the BGK approximation to the Boltzmann equation and study stability and optimization of an absorbing layer developed following the perfectly matched layer (PML) technique. We use ANOVA expansion of multivariate functions to calculate the Total Sensitivity Indices of the parameters. A small set of important parameters is found and minimization techniques are used to choose the optimal parameter values in this set.

Perfectly Matched Layers (PML)

- Introduced by Bérenger in 1994 starting from physical considerations on electromagnetic waves
- Waves entering into the PML are damped out without reflections at the PML interface
- Hagstrom, 2003: new approach based on the modal analysis in Laplace-Fourier space
- Applicable only to *linear* problems
- Key idea: eigenfunctions of the problem outside and inside the PML are the same

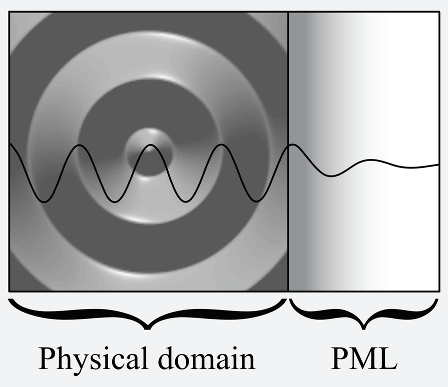


Figure 1: Example of PML.

Bhatnagar-Gross-Krook (BGK) model

- Approximation to the Boltzmann equation

$$\frac{\partial a}{\partial t} + A_1\frac{\partial a}{\partial x_1} + A_2\frac{\partial a}{\partial x_2} = S(a)$$

- Constant coefficient, symmetric hyperbolic system
- *Linear*, some nonlinear terms in $S(a)$: Hagstrom's theory is applicable
- In the case of weakly compressible flows one can recover the isentropic Navier-Stokes equations (NSE)

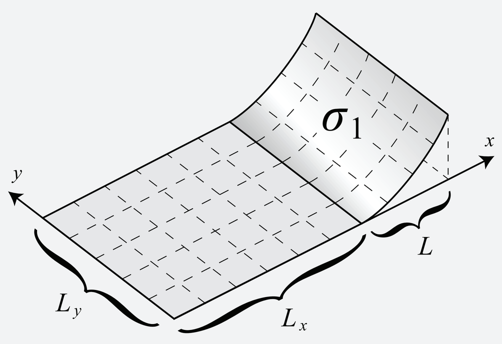
BGK+PML model

- PML for the BGK model proposed by Gao et al. [3]

$$\begin{cases} \dfrac{\partial a}{\partial t} + A_1\left(\dfrac{\partial a}{\partial x_1} + \sigma_1\left(\lambda_0\, a + \omega\right)\right) + A_2\dfrac{\partial a}{\partial x_2} = S(a), \\ \dfrac{\partial \omega}{\partial t} + \alpha_1\dfrac{\partial \omega}{\partial x_2} + (\alpha_0+\sigma_1)\,\omega + \dfrac{\partial a}{\partial x_1} + \lambda_0\,(\alpha_0+\sigma_1)\,a - \lambda_1\dfrac{\partial a}{\partial x_2} = \mathbf{0}. \end{cases}$$

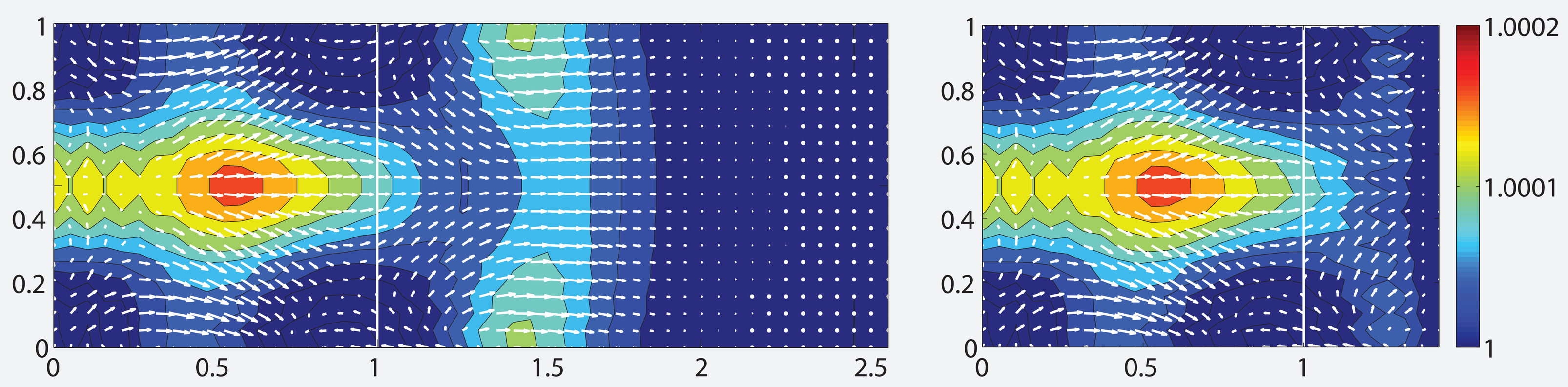
- Parameters $\alpha_0, \alpha_1, \lambda_0, \lambda_1$, whose role we seek to understand
- Shape of damping function $\sigma_1(x)$:

$$\sigma_1(x) = C\left(\frac{x-x_0}{L}\right)^{\beta}, \quad C \simeq (\Delta t)^{-1}.$$



Implementation

- 4th-order finite differences in space and 4th-order Runge-Kutta in time



(a) Simulation without the PML. (b) Simulation with the PML.
Figure 2: Density distribution and velocity field at $t = 1.00$.

Stability analysis through energy decay

- BGK+PML model in matrix form

$$\begin{cases} \dfrac{\partial \boldsymbol{u}}{\partial t} = P\boldsymbol{u}, \\ \boldsymbol{u}(x_1,x_2,t=0) = \boldsymbol{f}(x_1,x_2), \end{cases} \xrightarrow{\text{Fourier Transform}} \begin{cases} \dfrac{\mathrm{d}\hat{\boldsymbol{u}}}{\mathrm{d}t} = \hat{P}\hat{\boldsymbol{u}}, \\ \hat{\boldsymbol{u}}(k_1,k_2,t=0) = \hat{\boldsymbol{f}}(k_1,k_2), \end{cases}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\hat{\boldsymbol{u}}\|^2 = \hat{\boldsymbol{u}}^*(\hat{P}+\hat{P}^*)\hat{\boldsymbol{u}} \Rightarrow \hat{P}+\hat{P}^* \leq 0 \Rightarrow \boxed{\lambda_0 \geq 0, \quad \alpha_0 \geq -\sigma_1.}$$

Stability analysis through continued fractions

- Appelö et al. [1] studied the sign of the eigenvalues of $\hat{P}$ by means of

Theorem – Frank (1946)

Consider any polynomial $q(z)$ of degree n. Let D be a real number and define the polynomials Q_0 and Q_1 with real coefficients by

$$q(\mathrm{i}D) \equiv \mathrm{i}^n[Q_0(D) + \mathrm{i}Q_1(D)].$$

Then there is a continued fraction

$$\frac{Q_1(D)}{Q_0(D)} = \cfrac{1}{c_1D + d_1 - \cfrac{1}{c_2D + d_2 - \cfrac{1}{c_3D + d_3 - \cdots - \cfrac{1}{c_{n_r}D + d_{n_r}}}}}$$

with $c_j \neq 0$ and $n_r \leq n$. The number of roots of $q(z)$ with positive (negative) real part equals the number of positive (negative) c_j. Moreover, there are $n - n_r$ roots on the imaginary axis.

- The characteristic polynomial $p(z)$ of the symbol $\hat{P}$ factorizes as:

$$p(z) = z^2\left(z + \alpha_0 + \mathrm{i}k_2\alpha_1 + \sigma_1\right)^2 \mu_4(z)\,\nu_4(z),$$

- First coefficient in the continued fraction expansion of $\mu_4(z)$:

$$c_1 = -\frac{1}{2(\alpha_0+\sigma_1)} \Rightarrow \boxed{\alpha_0 > -\sigma_1.}$$

- Second coefficient:

$$c_2 = \text{very complicated!} \xrightarrow{\text{Assuming } \sigma_1 \to 0} \boxed{\lambda_0 = \lambda_1 = 0.}$$

ANOVA expansion of multivariate functions

- The ANOVA expansion allows to rewrite a multivariate function $g(\boldsymbol{\alpha})$, with $\boldsymbol{\alpha} = \alpha_1, \ldots, \alpha_p$, as:

$$g(\boldsymbol{\alpha}) = g_0 + \sum_{\mathcal{T}\subseteq\mathcal{P}} g_{\mathcal{T}}(\boldsymbol{\alpha}_{\mathcal{T}}).$$

- In our case g is an error functional of the solution to the BGK+PML
- From the $g_{\mathcal{T}}(\boldsymbol{\alpha}_{\mathcal{T}})$ it is possible to define the Total Sensitivity Index (TSI) of a parameter α_i, which measures the combined sensitivity of all terms that depend on α_i [2]. These TSIs tell us which parameters are most important, and represent the final goal of the ANOVA expansion.
- Central ingredient: multivariate numerical integration, here implemented with product rules with Gauss-Legendre quadrature, $(G_n)^p$

Results of the ANOVA analysis

Cubature type	α_0	α_1	β	L
$(G_2)^4$	0.1638	0.2474	0.2775	0.9312
$(G_3)^4$	0.1635	0.1916	0.2879	0.9385

Table 1: TSIs for the parameters α_0, α_1, β and L, using $g(\alpha_0, \alpha_1, \beta, L)$.

α_0	α_1	β	L
2.7561	2.7361	3.3077	0.6717
2.5493	2.0772	3.8463	0.5505
0.4991	0.4749	3.8877	0.4222
0.2551	0.0609	3.9325	0.4133

Table 2: Four sets of optimal values for the parameters α_0, α_1, β and L, obtained by minimizing $g(\alpha_0, \alpha_1, \beta, L)$.

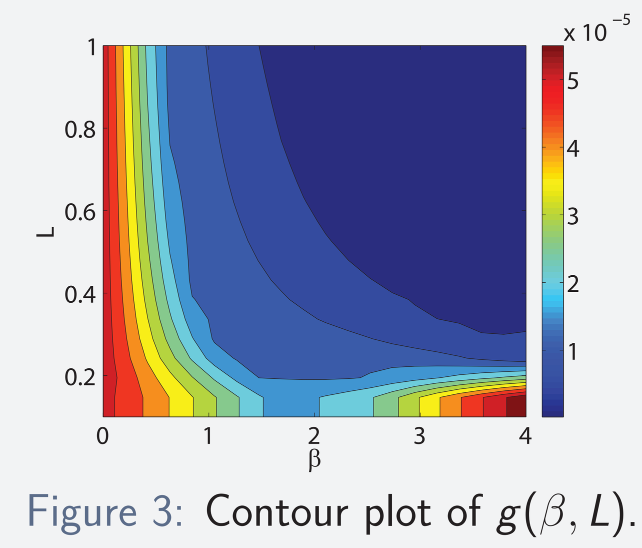


Figure 3: Contour plot of $g(\beta, L)$.

Future work

- Explore the influence of initial conditions and boundary conditions
- Coupling the BGK+PML model with the Navier-Stokes equations, solving the former in the PML and the latter in the physical domain

Essential references

[1] D. Appelö, T. Hagstrom, and G. Kreiss, *Perfectly Matched Layers for Hyperbolic Problems: General Formulation, Well-Posedness and Stability*, SIAM Journal on Applied Mathematics, 67 (2006), pp. 1–23.

[2] Z. Gao and J. S. Hesthaven, *Efficient Solution of Ordinary Differential Equations with High-Dimensional Parametrized Uncertainty*, Communications in Computational Physics, 10 (2011), pp. 253–278.

[3] Z. Gao, J. S. Hesthaven, and T. Warburton, *Efficient Absorbing Layers for Weakly Compressible Flows*.