Three-way decomposition of the Boltzmann distribution function

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Plan of the talk

- Boltzmann equation
- Motivation
- Three Way Decomposition
- Adaptive Cross Approximation
- Numerical examples

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L. Boltzmann, 1844-1906

Boltzmann equation

$$f_t + (v, \mathrm{grad}_x f) = \frac{1}{Kn} Q(f,f)$$

Distribution function

$$f = f(t,x,v),\ t \geq 0,\ x \in \Omega \subset \mathbb{R}^3, v \in \mathbb{R}^3$$

Collision integral

$$Q(f,f) = \int_{\mathbb{R}^3} \int_{S^2} B(v,w,e)\Big(f(v')f(w') - f(v)f(w)\Big)\, dw\, de$$

$$v' = \frac{1}{2}\Big(v + w + |v-w|\, e\Big)\,,\ w' = \frac{1}{2}\Big(v + w - |v-w|\, e\Big)$$

Boltzmann equation

Collision kernels

Inverse power potentials

$$B(v, w, e) = B(|u|, \mu) = |u|^{1-4/m} g_m(\mu)\,,\ m > 1\,,\ u = v - w$$

Maxwell pseudo–molecules

$$B(|u|, \mu) = g_4(\mu)$$

Variable Hard Spheres model

$$B(|u|, \mu) = C_\lambda |u|^\lambda\,,\ -3 < \lambda \leq 1$$

Hard spheres model

$$B(|u|, \mu) = \frac{d^2}{4}|u|$$

Boltzmann equation

Macroskopic quantities

density

$$\rho(t,x) = \int_{\mathbb{R}^3} f(t,x,v)dv$$

momentum

$$m(t,x) = \int_{\mathbb{R}^3} v\, f(t,x,v)dv$$

flow of momentum

$$M(t,x) = \int_{\mathbb{R}^3} vv^\top f(t,x,v)dv$$

flow of energy

$$r(t,x) = \frac{1}{2}\int_{\mathbb{R}^3} v|v|^2 f(t,x,v)dv$$

Motivation

Gain term of the collision integral

$$Q_+(f,f)(v) = \int\limits_{\mathbb{R}^3}\int\limits_{S^2} B(v,w,e) f(v') f(w')\, de\, dw$$

Discretisation of the $v-$space

$$Q_n = \left\{ v_k = V + h_v\, k,\ \ h_v > 0,\ -n/2+1 \le k_j \le n/2,\ j=1,2,3 \right\}$$

Numerical work for

$$Q_+(f,f)(v_k) \approx \sum_{l \in Q_n} \sum_{m \in ??} B(v_k, w_l, e_m) f(v') f(w')$$

is of the order $O(n^8)$

Motivation

Choise of e_m

$$k' = \frac{1}{2}\left(k + l + |k - l| e_m\right), \; l' = \frac{1}{2}\left(k + l - |k - l| e_m\right)$$

or

$$k' + l' = k + l, \; k' - l' = m \text{ with } m : \; |m|^2 = |k - l|^2, \; e_m = m/|m|$$

Find all solutions $m_1, m_2, m_3 \in \mathbb{Z}$ of the equation

$$m_1^2 + m_2^2 + m_3^2 = K \in \mathbb{N}$$

Additive number theory

- $K = 4^i(8j + 7)$ - no solutions
- $K = 4^i j$ - finite number of solutions
- else - the number of solutions is $O(K^{1/2-\varepsilon})$

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Motivation

Example

$$f_0(v) = \frac{1}{2(2\pi)^{3/2}} \left(e^{-\frac{|v-(2,2,0)^\top|^2}{2}} + e^{-\frac{|v+(-2,0,0)^\top|^2}{2}} \right)$$

Exact evolution of the moments

$$M(t) = \begin{pmatrix} 5 & -2 & 0 \\ -2 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix} e^{-t/2} + \frac{1}{3} \begin{pmatrix} 8 & 0 & 0 \\ 0 & 11 & 0 \\ 0 & 0 & 8 \end{pmatrix} (1 - e^{-t/2})$$

$$r(t) = \begin{pmatrix} -4 \\ 13 \\ 0 \end{pmatrix} e^{-t/3} + \frac{1}{3} \begin{pmatrix} 0 \\ 43 \\ 0 \end{pmatrix} (1 - e^{-t/3}) - \frac{1}{3} \begin{pmatrix} 12 \\ 4 \\ 0 \end{pmatrix} (e^{-t/2} - e^{-t/3})$$

Motivation

Memory, numerical work and the (formal) accuracy

$$Mem = O(n^3), \quad Op = O(n^7), \quad Acc = O(n^{-1/2})$$

n	M_{11}	M_{22}
4	0.19921	0.19847
8	0.04685	0.09627
16	0.03640	0.08599
32	0.02478	0.06289
64	0.01853	0.04698

A. Bobylev, Rja. 1997

Motivation

Boltzmann collision operator

$$Q_+(f,f)(v) = \mathcal{F}_{y\to v}\Big[\int_{\mathbb{R}^3} T(u,y)\mathcal{F}^{-1}_{z\to y}\big[f(z-u)f(z+u)\big](u,y)\,du\Big](v)$$

$$T(u,y) = 8\int_{S^2} B(2|u|,\mu)e^{-\imath|u|(y,e)}\,de$$

Memory, numerical work and the formal accuracy

$$Mem = O(n^4),\quad Op = 15n^6\ln(n) + O(n^6),\quad Acc = O(n^{-2})$$

VHS-model with $B(|u|,\mu) = C_\lambda |u|^\lambda$

$$T(u,y) = 2^{5+\lambda}\pi C_\lambda |u|^\lambda \mathrm{sinc}(|u|\,|y|)$$

numerical work $Op = n^6/8 + 315/32 n^5\ln(n)$

Motivation

Numerical accuracy

for M_{11}

n	m	error	factor
8	16	0.06785	-
16	32	0.00466	14.5
32	64	0.00135	3.5
64	128	0.00032	4.2

n	m	error	factor
12	24	0.06590	-
24	48	0.00248	26.5
48	96	0.00059	4.2
96	192	0.00014	4.2

Motivation

Numerical accuracy

for r_2

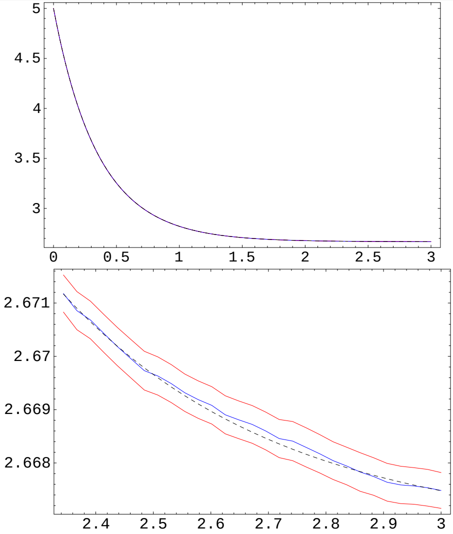
n	m	error	factor
8	16	0.14164	-
16	32	0.00232	61.1
32	64	0.00077	3.0
64	128	0.00018	4.3

n	m	error	factor
12	24	0.15667	-
24	48	0.00137	114
48	96	0.00033	4.1
96	192	0.00008	4.1

I. Ibragimov, Rja. 2002

Hard spheres model

relaxation of M_{11}



Hard spheres model

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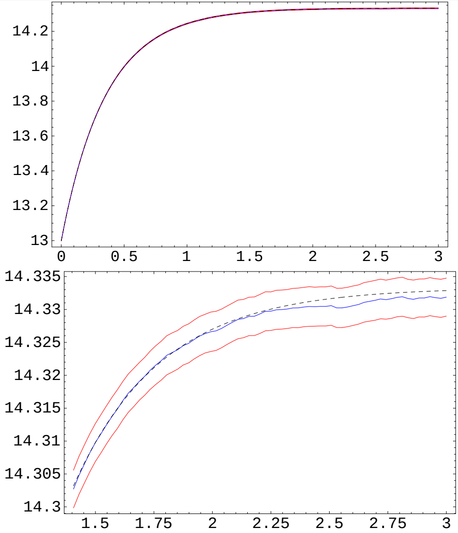

Motivation

Degenerated Function

$$f(t,v) = \sum_{k=1}^{r(t)} \beta_k(t) \prod_{\ell=1}^{3} f_k^{(\ell)}\left(t, v^{(\ell)}\right), \quad v = \left(v^{(1)}, v^{(2)}, v^{(3)}\right)^\top$$

Discretisation

$$F(t) = \left(f_j(t)\right)_{j \in C_n}, \quad f_j(t) = \sum_{k=1}^{r(t)} \beta_k(t) \prod_{\ell=1}^{3} f_k^{(\ell)}\left(t, v_j^{(\ell)}\right), \quad j \in C_n$$

Memory requirements, FFT

$$Mem = \mathcal{O}(n), \quad Op(FFT) : 125 n^3 \ln n \longrightarrow 15\, r\, n \ln n$$

Low Rank Tensor $\|F - F_\varepsilon\|_F \leq \varepsilon \|F\|_F, \quad \|F\|_F = \sqrt{\sum_{j \in C_n} \left(f_j\right)^2}$

Motivation

Maxwell Distribution, $r = 1$

$$f_M(v) = \rho_0 \prod_{\ell=1}^{3} \frac{1}{(2\pi\, T_0)^{1/2}}\, e^{-\frac{\left(v^{(\ell)} - V_0^{(\ell)}\right)^2}{2\,T_0}}$$

BKW Solution, $r = 3$

$$f(t,v) = \frac{\rho_0}{(2\pi\, T_0)^{3/2}} (\beta(t)+1)^{3/2} \left(1 + \beta(t)\left(\frac{\beta(t)+1}{2\,T_0}|v|^2 - \frac{3}{2}\right)\right) e^{-\frac{\beta(t)+1}{2\,T_0}|v|^2}$$

with

$$\beta(t) = \frac{\beta_0\, e^{-\rho_0\, t/6}}{1 + \beta_0\left(1 - e^{-\rho_0\, t/6}\right)}$$

Motivation

Maxwell Distribution, $r = 1$

$$f_M(v) = \rho_0 \prod_{\ell=1}^{3} \frac{1}{(2\pi T_0)^{1/2}} e^{-\frac{\left(v^{(\ell)} - V_0^{(\ell)}\right)^2}{2T_0}}$$

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with

$$\beta(t) = \frac{\beta_0 \, e^{-\rho_0 t/6}}{1 + \beta_0 \left(1 - e^{-\rho_0 t/6}\right)}$$

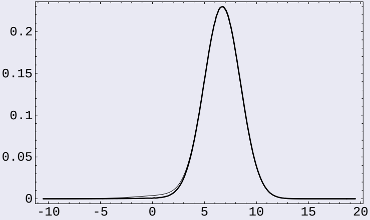
Motivation

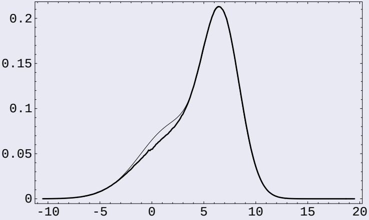
Mott-Smith model, $r = 2$

$$f_{MS}(x,v) = a(x)\, f_{M_-}(v) + (1 - a(x))\, f_{M_+}(v)\,,\; 0 \le a(x) \le 1\,,\; x \in \mathbb{R}$$

with

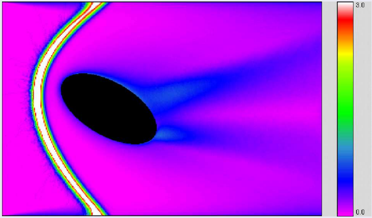
$$a(x) = \frac{e^{\beta(x - x_0)}}{1 + e^{\beta(x - x_0)}}\,, \quad x \in \mathbb{R}$$



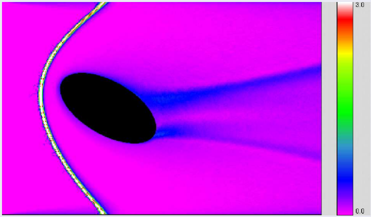


Motivation

Criterion of local equilibrium



$Kn = 0.08$



$Kn = 0.02$

with

$$Crit = \frac{1}{\varrho\, T}\left(\frac{1}{2}\|P - p\, I\|_F^2 + \frac{2}{5\, T}|q|^2 + \frac{1}{120\, T^2}\gamma^2\right)^{1/2}$$

$$f(v) \approx f_M(v)\Big(1 + a + (b, v) + (Cv, v) + (d, v)|v|^2 + e|v|^4\Big)$$

Adaptive Cross Approximation

Approximation of the function $K(x, y)$

$$X = \{x_1, \ldots, x_n\}, \quad Y = \{y_1, \ldots, y_m\}$$

with

$$K(x, y) = \sum_{k=1}^{r} u_k(x) v_k(y) + R_r(x, y), \quad r = r(\varepsilon)$$

Approximation of the matrix $A \in \mathbb{R}^{n \times m}$

$$a_{ij} = K(x_i, y_j)$$

with

$$\tilde{A} = \sum_{k=1}^{r} u_k v_k^\top, \quad u_k \in \mathbb{R}^n, \quad v_k \in \mathbb{R}^m$$

Accuracy, Memory

$$A \approx \tilde{A}, \ \|A - \tilde{A}\|_F \le \varepsilon \|A\|_F, \ Mem(\tilde{A}) : O(n\,m) \to O(n+m)$$

Adaptive Cross Approximation

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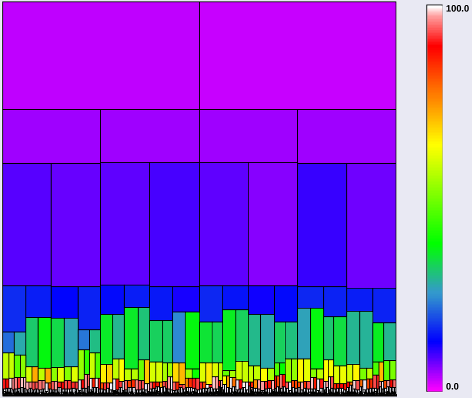
$$A \approx \tilde{A}, \; \|A - \tilde{A}\|_F \leq \varepsilon \|A\|_F, \; Mem(\tilde{A}) : O(n\,m) \to O(n+m)$$

Adaptive Cross Approximation

Approximation of blocks



Adaptive Cross Approximation

Full pivoted ACA

$$R_0 = A\,,\;\; S_0 = 0$$

for $k = 0, 1, 2, \ldots$

$$\begin{aligned} i_{k+1}\,, j_{k+1} &= \arg\max_{i,j} |(R_k)_{i,j}| \\ R_{k+1} &= R_k - \gamma_{k+1} \big(R_k\, e_{j_{k+1}}\big)\big(e^T_{i_{k+1}}\, R_k\big) \\ S_{k+1} &= S_k + \gamma_{k+1} \big(R_k\, e_{j_{k+1}}\big)\big(e^T_{i_{k+1}}\, R_k\big) \end{aligned}$$

with

$$\gamma_{k+1} = \frac{1}{(R_k)_{i_{k+1}, j_{k+1}}}$$

$A = R_k + S_k$ and $(R_k)_{i_m, j} = (R_k)_{i, j_m} = 0$ for $m = 1, \ldots, k$

Adaptive Cross Approximation

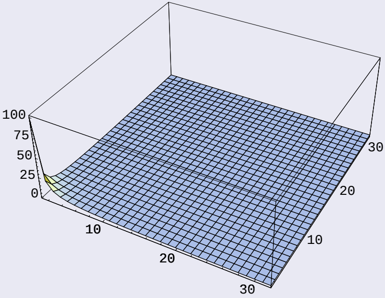
Corner singularity

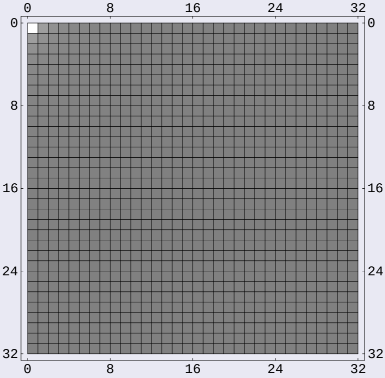
$$K(x,y) = \frac{1}{\alpha + x + y}, \quad \alpha = 10^{-2}$$

Step	Pivot row	Pivot column	Pivot value	Relative error
1	1	1	$1.00 \cdot 10^{+2}$	$3.43 \cdot 10^{-1}$
2	2	2	$7.91 \cdot 10^{+0}$	$1.62 \cdot 10^{-1}$
3	6	6	$1.10 \cdot 10^{+0}$	$3.66 \cdot 10^{-2}$
4	28	28	$2.25 \cdot 10^{-1}$	$2.26 \cdot 10^{-3}$
5	3	3	$6.10 \cdot 10^{-2}$	$8.40 \cdot 10^{-4}$
6	13	13	$9.87 \cdot 10^{-3}$	$2.28 \cdot 10^{-5}$
7	4	4	$3.91 \cdot 10^{-4}$	$8.85 \cdot 10^{-6}$
8	20	20	$1.02 \cdot 10^{-4}$	$2.69 \cdot 10^{-7}$
9	9	9	$6.32 \cdot 10^{-6}$	$3.30 \cdot 10^{-8}$
10	32	32	$1.97 \cdot 10^{-6}$	$1.13 \cdot 10^{-9}$

Adaptive Cross Approximation

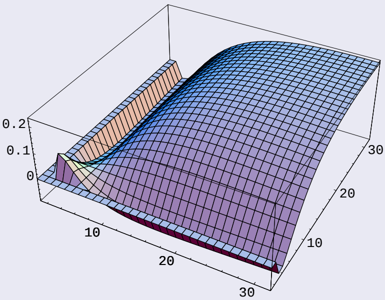
Initial situation

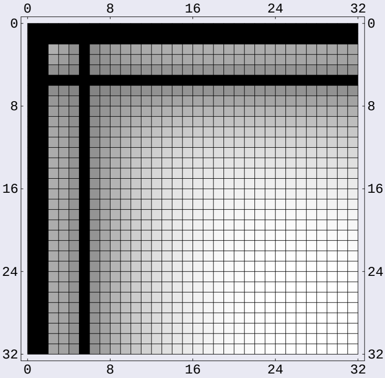




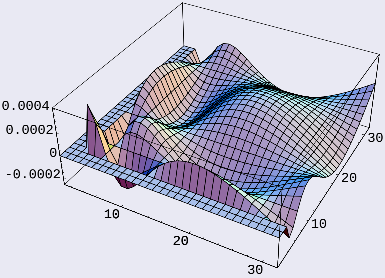
Adaptive Cross Approximation

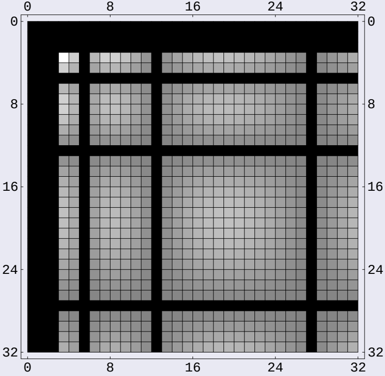
After 3 Iterations





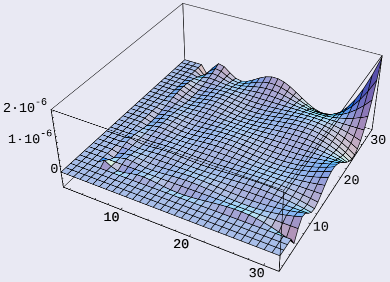
After 6 Iterations

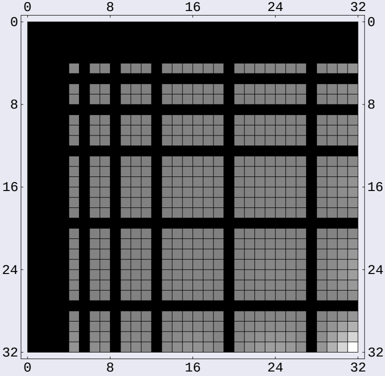




Adaptive Cross Approximation

After 9 Iterations





Main ideas

Extension of the ACA

$$S_0(x,y,z) = 0\,, \quad R_0(x,y,z) = K(x,y,z)$$

$$C_m(x,y,z) = \frac{R_{m-1}(x_{i_m},y_{j_m},z_{k_m})R_{m-1}(x_{i_m},y,z)R_{m-1}(x,y_{j_m},z)R_{m-1}(x,y,z_{k_m})}{R_{m-1}(x_{i_m},y_{j_m},z)R_{m-1}(x_{i_m},y,z_{k_m})R_{m-1}(x,y_{j_m},z_{k_m})}$$

$$S_m(x,y,z) = S_{m-1}(x,y,z) + C_m(x,y,z)\,,$$

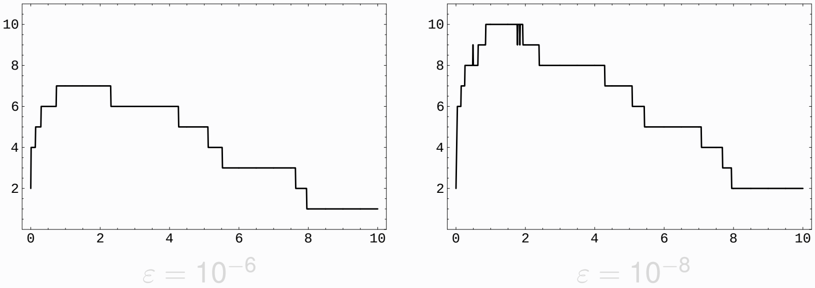
$$R_m(x,y,z) = R_{m-1}(x,y,z) - C_m(x,y,z)$$

Numerical experiments

Initial condition

$$f_0(v) = \frac{1}{2(2\pi)^{3/2}} \left(e^{-\frac{|v-(2,2,0)^\top|^2}{2}} + e^{-\frac{|v+(-2,0,0)^\top|^2}{2}} \right)$$

Relaxation of the numerical rank



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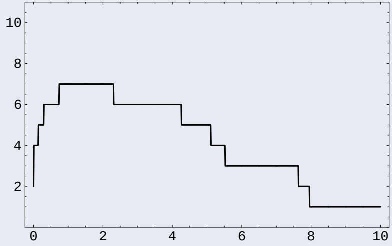
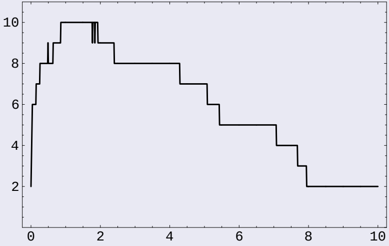


$\varepsilon = 10^{-6}$



$\varepsilon = 10^{-8}$

Numerical experiments

Computational times

n	$\varepsilon = 0$		$\varepsilon = 10^{-6}$		$\varepsilon = 10^{-8}$	
16	$0.2s$	$8.0s$	$0.4s$	$19.0s$	$0.5s$	$22.0s$
32	$11.0s$	$12.0m$	$0.8s$	$70.0s$	$1.0s$	$81.0s$
64	$7.0m$	$15.0h$	$3.3s$	$7.0m$	$3.4s$	$7.0m$
128	$6.0h$	$--$	$49.0s$	$3.6h$	$49.0s$	$3.6h$

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