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Abstract

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1. Introduction

(H ., 1996). (B r & H , 1983; D , 1974; M r y, 1976; Tw y, 1977). y Å r (1929),

$$\tau(\lambda) = \int_0^{\infty} \pi r^2 Q(r, \lambda, \eta) n(r) \, r + \varrho(\lambda), \tag{1}$$

w r r ; $n(r)$; η

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r ; λ w ; $\varrho(\lambda)$ rr r/ ; Q (r, λ, η) fi y r r M ry. S r (AOT) r r fl y w AOT r r T y ry, w y r y r r r r r , r r. T r $n(r)$, r (B , 2001; P , 1962; S w, 1979; S r & Z , 1996; Tw y, 1963; W , F , F , Y , & G , 2006) r (B & K r , 2006; C , 1970; F rr , B , & P , 1995; Gr , 1971; L & R , 1994; Tw y, 1975; V & K , 2000; W , F , & F , 2007; Y & T , 1969). W r r y r r r r, w y r r (W , 2007). S r CE 318, w w r (W ., 2006, 2007) r y y r r r r y r r . N CE 318 y y r r , w r fi r r r r r $n(r)$ y . E . (1). T r r , r fi y r . T r r fi y, w fir r r y r r r fi r r .

T r r r r w : S 2 r S 3 r r . I S 3.1, w y r r y r . I S 3.2, w r fi : BB y . S 3.3 r r r r r . I S 4, w fir r ; w r - r y r r y r r . I S 5, r r r . F y, r r y, w r r r B r B rw r (BB y) r y r .

T r r, w w : := fi , $\vec{n}$ r n, r r r r , r y, , r y, $(\cdot)$ r , A^{T} r r A . .

2. Forward model and standard regularizing methods

2.1. Mathematical model formulation by moment problem

U r r r r r r y Wr (2000) Wr . (2002) r r . W r r w y y r r y - r y r r . A $n(y)$ r - y r $[a, b]$ $n \geqslant 0$, $g(y)$ $n(y)$ fi

$$\langle g(y) \rangle = \int_a^b g(y) n(y) \, \mathrm{d}y.$$

I w $g(y) = k_i(y)$, $i = 1, 2, \ldots, m$, m w k_i, r r r y fi r w y (W , 2007):

$$\int_a^b k_i(y) n(y) \, \mathrm{d}y = o_i, \quad i = 1, 2, \ldots, m. \tag{2}$$

C r y, w $o_i = o(x_i)$ $k_i(\cdot) = k(x_i, \cdot)$. I (2), $[a, b]$ r r w r r w r r r ; o_i r i rr r- r r ; x_i r r r w ; k_i w (r r r y, r) r r fi , r r r y .

Pr y, r r , , y y . H , r (2) w r o_i r , $n(y)$

d_i

. I w , $n(r)$ (, rr r, r r r r). T r r y fi . T r r y r r w y y (y) r r y r . U , w r r r r

$$M(n) := \frac{1}{2}\|Kn - d\|^2 \quad \text{. .} \quad -H(n) \leqslant \Delta_1, \quad \|Ln\|^2 \leqslant \Delta_2, \quad 0 \leqslant n < \infty, \tag{10}$$

w r L r r $n(r)$, . . ., L r r. I r r, r r S $W^{1,2}$ $n(r)$, w y r r (W ., 2006 r). T fir r E . (10) r rr r y r ; r E . (10) r rr r . T r r , E . (10) r r r y y rr r r (W , 2007; W & Y , 2005; Y , 1993). W r r.

S r (10) w r r :

$$\begin{aligned}\Psi(n) &:= \frac{1}{2}\|Kn - d\|^2 + v\|Ln\|^2 + \mu(-H(n)) \\ &= \frac{1}{2}\|Kn - d\|^2 + v\|Ln\|^2 + \mu\int n(r) \quad n(r) \quad r\end{aligned} \tag{11}$$

w $S = \{n : n$ r r $0 \leqslant n < \infty\}$, w r v μ r w r . r r r w r r .

N r y, (11) r r fi

$$\tilde{\Psi}(\vec{n}) := \frac{1}{2}\|\mathscr{K}\vec{n} - \vec{d}\|^{2\|}$$

3.2. A gradient method for solving a regularized solution

S r y , $\tilde{\Psi}$ r y , , r r (13). I , r $\tilde{\Psi}$,

$$g(\vec{n}) = \mathscr{K}^{\mathrm{T}}(\mathscr{K}\vec{n} - \vec{d}) + v\mathscr{L}^{\mathrm{T}}(\mathscr{L}\vec{n}) + \mu \quad (1 + \quad (w_{\vec{n}} \cdot \vec{n})),$$

w r $(1 + \quad (w_{\vec{n}} \cdot \vec{n})) := [1 + \quad (w_{n_1} \cdot n_1), 1 + \quad (w_{n_2} \cdot n_2), \ldots, 1 + \quad (w_{n_p} \cdot n_p)]^{\mathrm{T}}$, p r r r r.

P r r

$$\vec{n}_{k+1} = \vec{n}_k + \omega_k s_k, \tag{15}$$

w r $s_k = -g_k$, $g_k = g(\vec{n}_k)$, ω_k w y r , ω_k^* fi $\omega_k^* =$ r $_\omega \tilde{\Psi}(\vec{n}_k + \omega_k s_k)$. H w r, w r r r r (Y , 1993). I w r r ω_k $(0, \|\mathscr{K}\|^{-2})$ r , w r w w L w r r

$$\vec{n}_{k+1} = \vec{n}_k + \omega s_k. \tag{16}$$

H w r, r r w r r r r (E ., 2000; W ., 2007).

W r r . T w fir r y B r B rw r , r r , BB (B r & B rw , 1988). T r r r y $\alpha_k^{\mathrm{BB1}} = s_{k-1}^{\mathrm{T}} s_{k-1} / s_{k-1}^{\mathrm{T}} y_{k-1}$ r $\alpha_k^{\mathrm{BB2}} = s_{k-1}^{\mathrm{T}} y_{k-1} / y_{k-1}^{\mathrm{T}} y_{k-1}$, w r $y_k = g_{k+1} - g_k$, $s_k = \vec{n}_{k+1} - \vec{n}_k$ (A A r).

T y r r r r r . B r r r r r r r r (F r, 2001). S r r $\tilde{\Psi}(\vec{n})$ ry r r r , $M(\vec{n})$, w BB . By r y, r $\vec{n}_k$ $(k = 1, 2, \ldots)$. T r r , r , r r . I ry fir y r $\vec{n}_k$ r r r y r r r r r r E . (13). T r r , r r $\vec{n}_k$, w r rr w $w_{\vec{n}}$ 1, ., r y r $\vec{n}_k$ r r r y r r fi $\vec{n}_k$ r r .

T r r , $\tilde{\Psi}$ w , y l. D fi , , $\tilde{\Psi}$, $\tilde{\Psi}$ w . T fi r r , $\tilde{\Psi}_r$,

$$\tilde{\Psi}_r - \tilde{\Psi}(\vec{n}_k + \beta s_k) \geqslant -\beta\gamma_1 s_k^T g_k. \tag{20}$$

I r , r r , $\tilde{\Psi}_r$ r . T r r r r $L_r > 0$, $\tilde{\Psi}_r$ r , r r , , $\tilde{\Psi}(\vec{n})$ L_r r . T r r , r , r , fi r , $\tilde{\Psi}$, r .

I r r , r r . r r . T r fir r , w , W r r . y BB . A , w , w- (W & M , 2007) r - r (r D & F r, 2003; M r & T r , 1991) r r :

$$\|\tilde{g}_k\|_2 \leqslant \varepsilon \|g_1\|_2, \tag{21}$$

w r ε r r $\tilde{g}_k$ fi

$$(\tilde{g}_k)_i = \begin{cases} (g_k)_i & (\vec{n}_k)_i > 0, \\ \{(g_k)_i, 0\} & (\vec{n}_k)_i = 0. \end{cases}$$

N w, w r r w :

Algorithm 3.1 (*BB method for maximum entropy regularization*).

Step 1: I : G $\vec{n}_0$, r $\varepsilon > 0$ $k := 1$.
Step 2: C w r : I (21) fi , ; O rw , $s_k = -g_k$.
Step 3: I $k = 1$, , α_k y W r r . y (17) (18). O rw , α_k y α_k^{BB1} r α_k^{BB2}.
Step 4: U , rr r y $\vec{n}_{k+1} = \vec{n}_k + \alpha_k s_k$.
Step 5: F r r , $\tilde{\Psi}_r$ y A r 3.2 w r E . (20) fi . I y , , w r r $s_{k+1} = -g_{k+1}$ S 7; O rw , S 6.
Step 6: N r : L A r 3.2 , r , w r r :

$$\vec{n}_{k+1} = \vec{n}_k + \beta s_k, \quad s_{k+1} = -g_{k+1}.$$

Step 7: L : $k := k + 1$ S 2.

S 5 A r 3.1 , r r r s_{k+1} r y (20). I y, w $\tilde{\Psi}_r = \infty$. T $\tilde{\Psi}_r$ w $\tilde{\Psi}(\vec{n}_k) \geqslant \tilde{\Psi}(\vec{n}_1)$ r y r . I fi r , , fi r $k_{fi} \leqslant L_r$, , $\tilde{\Psi}_r$ r , . O rw , r L_r, , $\tilde{\Psi}_r$ $\tilde{\Psi}$ r , . ., $\tilde{\Psi}_r := \tilde{\Psi}$, $\tilde{\Psi} := \tilde{\Psi}(\vec{n}_k)$. T r , A r 3.2.

Algorithm 3.2 (*Nonmonotone line search*).

Step 1: G r r r $L_r > 0$, $\tilde{\Psi}$, $\tilde{\Psi}$ $\tilde{\Psi}_r = \infty$.
Step 2: A r :

- I $\tilde{\Psi}(\vec{n}_k) < \tilde{\Psi}$, $\tilde{\Psi} := \tilde{\Psi}(\vec{n}_k)$, $\tilde{\Psi} := \tilde{\Psi}(\vec{n}_k)$, $l := 0$.
- O rw , $\tilde{\Psi} :=$ $\{\tilde{\Psi}, \tilde{\Psi}(\vec{n}_k)\}$, $l := l + 1$. I $l = L$, $\tilde{\Psi}_r := \tilde{\Psi}$, $\tilde{\Psi} := \tilde{\Psi}(\vec{n}_k)$, $l := 0$.
- U $\tilde{\Psi}_r$, (20) fi .

3.3. Aerosol particle size distribution function retrieval

T r r r r r , , $n(r)$, w r , (6) r AOT r w . W r r w r r [0.1, 10] μm. N r r r ($N \leqslant 20$) r r r rr r, r r w r y r r r , $N = 200$.

T r r r w y K , Byr , H r , R (1978), .., w r r r w $h(r)$ $f(r)$: $n(r) = h(r)f(r)$, w r $h(r)$ r y ry r, w $f(r)$ r wy ry . T $h(r)$ J r (J , 1955), $h(r) = r^{-(v^*+1)}$, w v^* 3.0. I w y w

$$\tau_{\ r}(\lambda) = \int_a^b [k(r, \lambda, \eta)h(r)] f(r) \ r, \tag{22}$$

w r $k(r, \lambda, \eta) = \pi r^2 Q \ (r, \lambda, \eta)$ w $k(r, \lambda, \eta)h(r)$ w r w rr w r r Ξ:

$$(\Xi f)(\lambda) = \tau_{\ r}(\lambda). \tag{23}$$

F r y , r Ξ y r $\mathscr{K}$. N w, w r r r r r

$$\frac{1}{2}\|\mathscr{K}\vec{f} - \overrightarrow{\tau_{\ r}}\|^2 + v\|\mathscr{L}\vec{f}\|^2 + \mu\sum_i f_i \ (w_{f_i} \cdot f_i), \tag{24}$$

w r $w_{\vec{f}} := [w_{f_1}, w_{f_2}, \ldots]^{\mathrm{T}}$ w $\vec{f}$ y r r r r y r r r r

$$e^{\mathrm{T}}\vec{f} \quad .. \ \mathscr{K}\vec{f} = \overrightarrow{\tau_{\ r}}, \ \vec{f} \geqslant 0 \tag{25}$$

w $\{\vec{f} : \mathscr{K}\vec{f} = \overrightarrow{\tau_{\ r}}, \ \vec{f} \geqslant 0\}$, w r e r w 1. T r y r , $w_{\vec{f}}$ fi r r S 3.2 w r r $\vec{f}$.

N r y, r r r r v μ r . I ry, v μ r r r . A r - r r r $\mathscr{K}$. T r r w y r r : *a priori* w y *a posteriori* w y. S rr r r δ w y , w w y *a posteriori* W . (2006). Pr y, r *a priori* r r r r, v μ w (0, 1). F r r r , w r r v *a priori* μ r r:

$$\mu_k = \mu_0 \cdot \xi^{k-1}, \quad 0 < \xi < 1, \tag{26}$$

w r $\mu_0 \in (0, 1)$ w r y r , r , $\mu_0 = 0.5$, k k r . I r r r r ry, μ_k r r k r fi y.

4. Numerical experiments

4.1. Theoretical simulation

T r y y r r , w y r . T w . F r , ( ) r y r r E . (3) r r r r $n_{\ r}(r)$ (r) r r r η. T , r r r r , r r r r w .

I r , r r - $\vec{\sigma}$ E . (2) r y, r r r $\vec{d}$. N r y, r $\vec{d}$ r . H r , r y, w , y G r , . ., w

$$\vec{d} = \vec{\sigma} + \delta \cdot r \quad (\quad (\vec{\sigma})),$$

w r δ (0, 1), r (($\vec{\sigma}$)) G r w $\vec{\sigma}$.
T r r r r y r - r rr r (r)

$$r = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\frac{(\tau \quad (\lambda_i) - \tau \quad (\lambda_i))^2}{(\tau \quad (\lambda_i))^2}},$$

w r r r r r r r . I w , τ r r r r , τ r r r .
I r , r $n_{\mathrm{r}}(r)$ y (W ., 2007)

$$n_{\mathrm{r}}(r) = 10.5r^{-3.5} \quad (-10^{-12}r^{-2}).$$

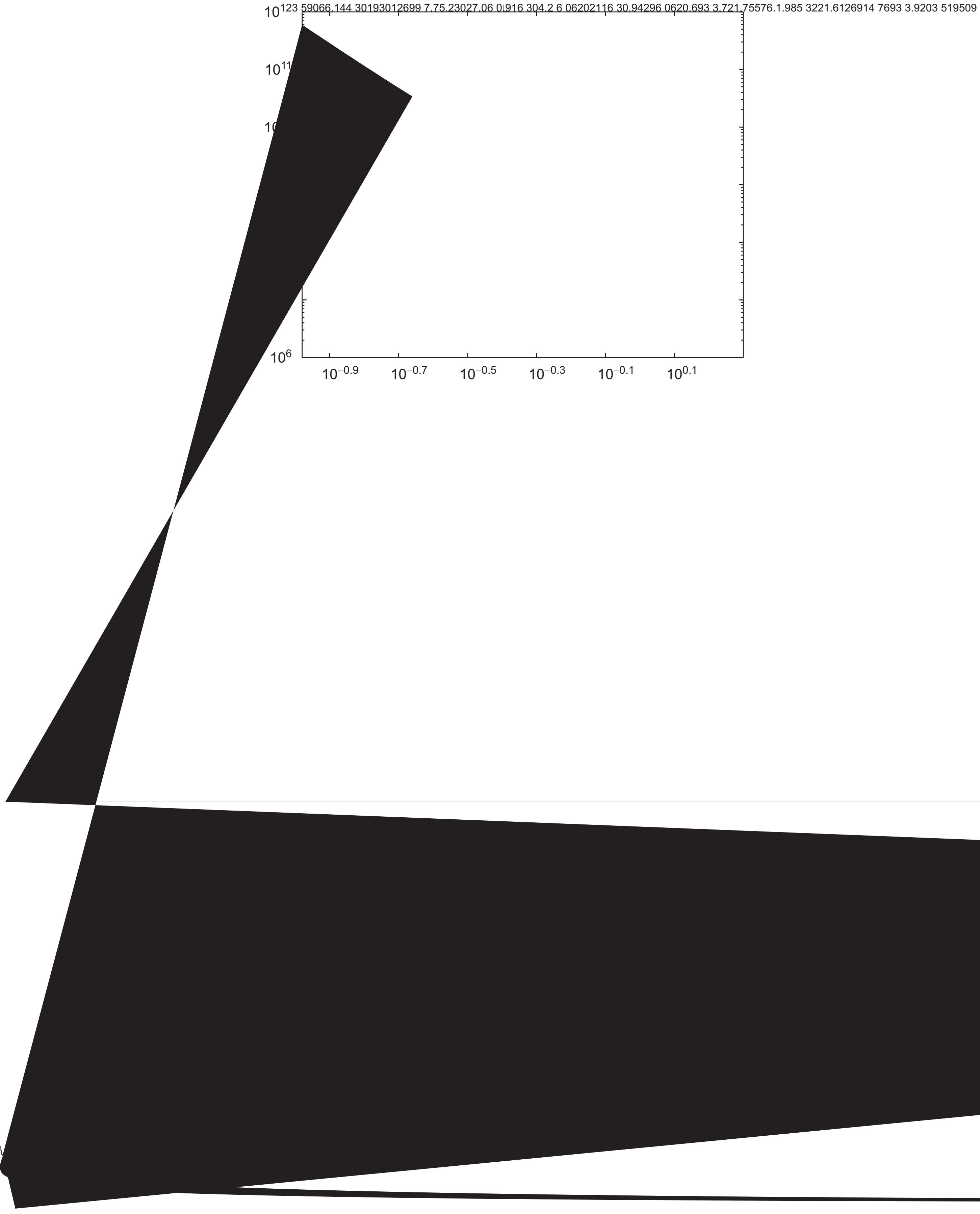
T r r r r [0.1, 2] μ.
N w w fi A r 3.1 3.2 r r r : $\lambda_1 = 1.0 \times 10^{-4}$, $\lambda_2 = 0.9$, $\varepsilon = 1.0 \times 10^{-6}$, r r r r $v = 0.001$, $\mu_0 = 0.55$, r r r y $\xi = \frac{1}{10}$, μ_k r y y r r (26), $L_{\mathrm{r}} = 7$, $\tilde{\Psi}_{\mathrm{r}} = 1.0 \times 10^{10}$, w $w_{\vec{n}}$ r E . (14) (W ., 2007 r r r), $\vec{n}_0 = w_{\vec{n}}$, r r $N = 200$.
F r r r (24), r r $\mathscr{L}$ r r r r

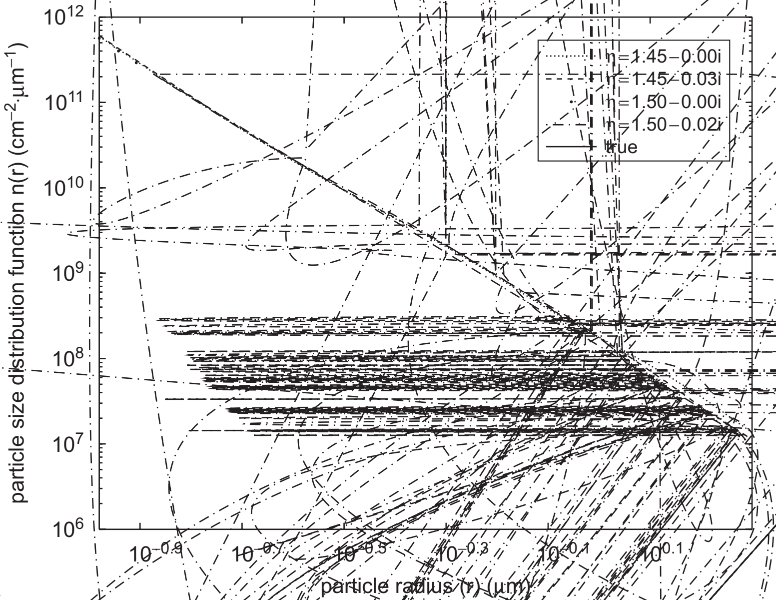
$$\mathscr{L} = \begin{bmatrix} 1+\frac{1}{s_{\mathrm{r}}^2} & -\frac{1}{s_{\mathrm{r}}^2} & 0 & \cdots & 0 \\ -\frac{1}{s_{\mathrm{r}}^2} & 1+\frac{2}{s_{\mathrm{r}}^2} & -\frac{1}{s_{\mathrm{r}}^2} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & -\frac{1}{s_{\mathrm{r}}^2} & 1+\frac{2}{s_{\mathrm{r}}^2} & -\frac{1}{s_{\mathrm{r}}^2} \\ 0 & \cdots & 0 & -\frac{1}{s_{\mathrm{r}}^2} & 1+\frac{1}{s_{\mathrm{r}}^2} \end{bmatrix}.$$

I w , $s_{\mathrm{r}} = (2-0.1)/(N-1)$ r [a, b]. T r $\mathscr{L}$ w r $\vec{f}$, w r r r r r r r - (W ., 2006).
T r w r r r P (R) r w CPU 1.0 GH . I fir , r r η 1.45 − 0.00 1.50 − 0.00 . T w r , η ry r . T r r η 1.45 − 0.03 1.50 − 0.02 , r y.
N r r r F . 1, 3 5 w $\delta = 0.005, 0.01$ 0.05 r r r r , r y. T r fi r r r F . 2, 4 6, r y. T r r r w T 1. I r , r μ_k r r r r ry r , w fi r r ry (T & Ar , 1977; X ., 2003). T w fi y, w r r r CPU , w T 2.
T w y BB r , w r r r rr r $\mathrm{Err}_{\mathrm{r}}$:

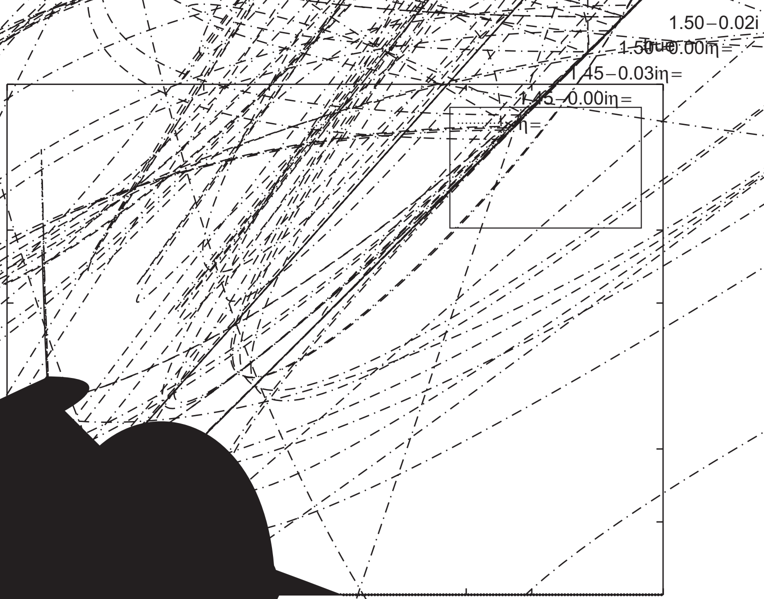
$$\mathrm{Err}_{\mathrm{r}}^{k} = \frac{\|\mathscr{K}\vec{n}_k - \vec{\sigma}\|}{\|\vec{\sigma}\|}.$$

T r r rr r BB r $\eta = 1.50 - 0.02$ $\delta = 0.05$ ry r w F . 7. I r y r F . 7 r rr r r y y BB .


10^12
10^11
10^6
10^−0.9
10^−0.7
10^−0.5
10^−0.3
10^−0.1
10^0.1

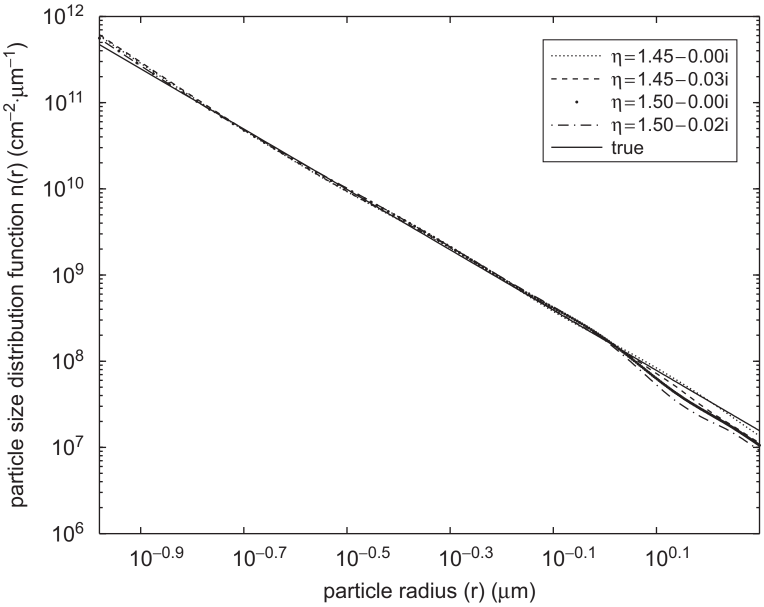


F . 3. L r r r , w r r = 0.01 r r r



F . 4. L r r δ = 0.01 r r r

w r [redacted] 6, p_2 [redacted] $\sigma_2^2 = 0.036$ r r r f (r) w
[redacted] 1.45 − 0.00 , 1.45 − 0.03 , 1.50 − 0.00
1.5 [redacted] y. B f r r . N r , r r



F . 5. L r r r w r r rr r $\delta = 0.05$ r r r .

T 1
T r - r rr r r r

N	$\eta = 1.45 - 0.00$	$\eta = 1.45 - 0.03$	$\eta = 1.50 - 0.00$	$\eta = 1.50 - 0.02$
$\delta = 0.005$	1.4501×10^{-4}	8.7595×10^{-5}	9.8996×10^{-5}	1.0632×10^{-4}
$\delta = 0.01$	1.5067×10^{-4}	9.2079×10^{-5}	6.8340×10^{-5}	1.0414×10^{-4}
$\delta = 0.05$	3.1027×10^{-4}	2.5333×10^{-4}	1.8165×10^{-4}	2.1722×10^{-4}

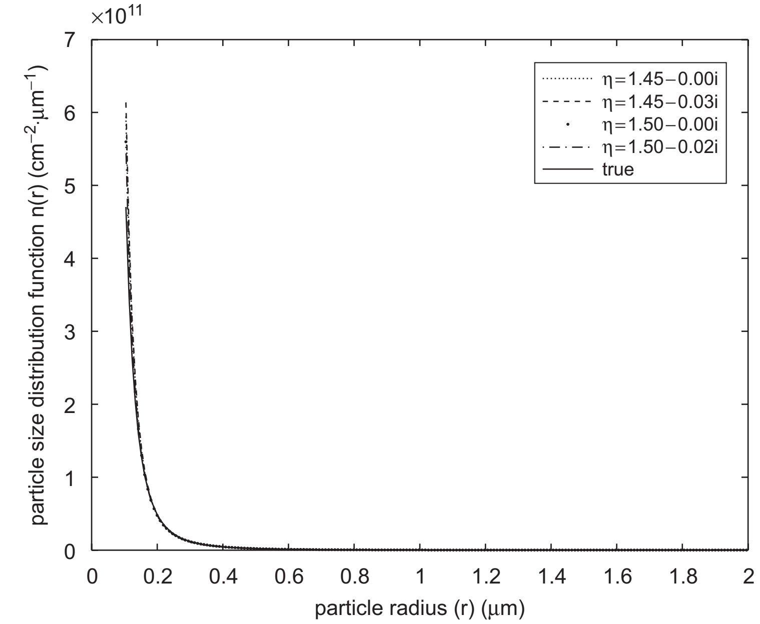
T 2
T r (CPU ( )) r r

N	$\eta = 1.45 - 0.00$	$\eta = 1.45 - 0.03$	$\eta = 1.50 - 0.00$	$\eta = 1.50 - 0.02$
$\delta = 0.005$	1995 (2.8130)	1492 (2.1400)	1130 (1.6090)	1133 (1.4060)
$\delta = 0.01$	1311 (1.8900)	1575 (2.5940)	781 (1.0630)	1102 (1.6880)
$\delta = 0.05$	1348 (1.9210)	2000 (2.8590)	1329 (1.5470)	894 (1.2810)

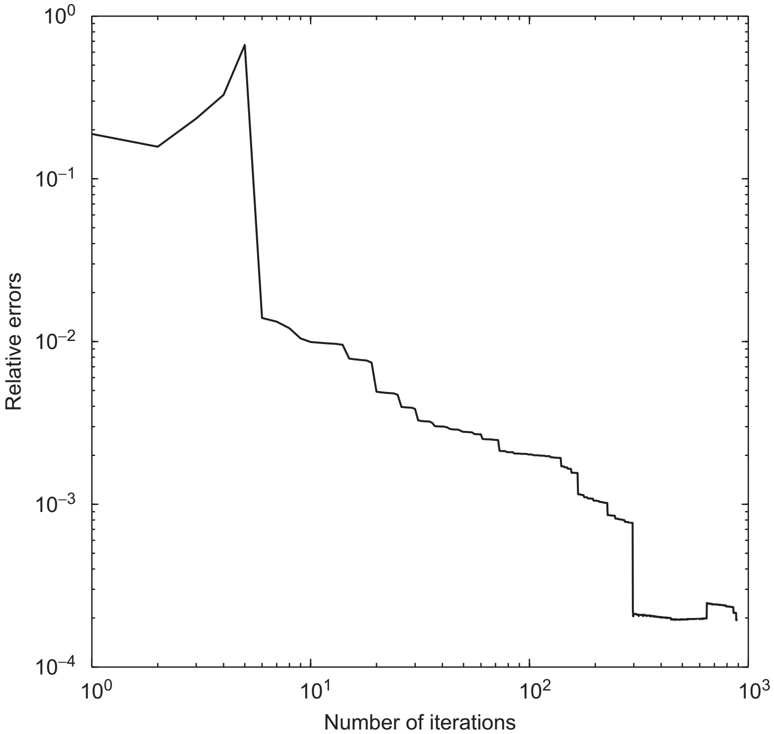
F . 8, 9 10 w $\delta = 0.005, 0.01$ 0.05 r r r r , r y. T r w w y ry G y r w r r .
I r r r r r y r r r . T r r , r rr r r r r .

4.2. Discussions on numerical results

I , w r r y - r CE 318 (r r , r r fi , r r W ., 2006) y r



F. . 6. L r , r r. r , w. , r. r. rr r $\delta = 0.05$ r r r .



F. . 7. N y r rr r .

r. . W r r. , *in situ* r. , . CE 318 r O r 17 O r 31 y r 2005. T r r r y Y. T A. r. , r E S CERN (C E y R r N w r).

F . 108 I

10

particle radius (r)

By r r , r r r r $n(r)$ r F . 11 r r . I r fi r r r r r y. I y, r r r r r r 1.0 μm. O r . . 1.0 μm, y y. T r r r r w r W . (2007). T r r , r r r r r , w r r r Y . T y y r r . T r r [5.0, 10.0] μm, w r y r y rr , r y r r . T r r w r r .

5. Concluding remarks

I r, w r r r r r r r r . W fir r y r r , r r y r r . F r , w r r BB y .

W fir r r y y r r . O rr w r η . T , w r r r r y r CE 318. T r r r r w r w r w r r r r r r .

T r r r r r: w r y N w y . A y, H (13) y

$$H(\vec{n}) = \mathscr{K}^{\mathrm{T}}\mathscr{K} + \nu\mathscr{L}^{\mathrm{T}}\mathscr{L} + \mu \left(\frac{1}{n_1}, \frac{1}{n_2}, \ldots, \frac{1}{n_p}\right).$$

T r r , fi N w -N w . H w r, H $\vec{n}$. I y w r w $\vec{n}$ r r . T r r r r y .

F y, w w r r - r , r r y r r rr r r r (W ., 2007).

Acknowledgments

I ry r r w r ry r. T r r w r y N S F r Gr N . 10501051 S fi R r F H R r M ry. I r y r y C N 973 r r Gr N . 2007CB714400.

Appendix A. BB method

T B r B rw (BB) r r , w w fir r y B r B rw (1988) r r r r r r

$$q(x) := \tfrac{1}{2}(Ax, x) - (b, x), \tag{A.1}$$

w r $q : \mathbb{R}^m \longrightarrow \mathbb{R}$, A y r fi r . L x_k k r g_k r q x_k. A r r (A.1) r

$$x_{k+1} = x_k - \alpha_k g_k, \tag{A.2}$$

w r α_k . T y B r B rw . rr r .

L -N w E . (A.1)

$$y_k = As_k, \tag{A.3}$$

w r $y_k = g_{k+1} - g_k$, $s_k = x_{k+1} - x_k$. R A y r $\alpha^{-1} I\ (\alpha > 0)$

$\|y_{k-1} - \alpha^{-1} I s_{k-1}\|^2$

y

$$\alpha_k^{\mathrm{BB1}} = \frac{s_{k-1}^{\mathrm{T}} s_{k-1}}{s_{k-1}^{\mathrm{T}} y_{k-1}}. \tag{A.4}$$

S r y, w αI r r A, w α_k r

$\|\alpha I y_{k-1} - s_{k-1}\|^2$

$$\alpha_k^{\mathrm{BB2}} = \frac{s_{k-1}^{\mathrm{T}} y_{k-1}}{y_{k-1}^{\mathrm{T}} y_{k-1}}. \tag{A.5}$$

N $s_{k-1} = -\alpha_{k-1} g_{k-1}$ $y_{k-1} = A s_{k-1}$, w r E . (A.4) (A.5):

$$\alpha_k^{\mathrm{BB1'}} = \frac{g_{k-1}^{\mathrm{T}} g_{k-1}}{g_{k-1}^{\mathrm{T}} A g_{k-1}} \tag{A.6}$$

α g

Step 3: C (B.2) fi r : I (B.2) fi , , , β_k; O rw , $a_{k+1} := \alpha_k$, $b_{k+1} := b_k$. I $b_{k+1} < +\infty$, S 4, O rw , $\alpha_{k+1} := t\alpha_k$, $k := k+1$, S 2.
Step 4: C w r y r , ., $\alpha_{k+1} := (a_{k+1} + b_{k+1})/2$ $k := k+1$, S 2.

I r r , S 1, w $\lambda_1 = 1.0 \times 10^{-4}$ $\lambda_2 = 0.9$.
BB subroutine: T r fi r $\overrightarrow{n}_{k+1}$ y . $\overrightarrow{n}_{k+1} = \overrightarrow{n}_k + s_k$. N r r r w y α_k^{BB}, w y y α_k^{BB1} y E . (A.4), r w y y α_k^{BB2} y E . (A.5). O α_k^{BB1} α_k^{BB2}, . ., $\alpha_k^{BB} = \alpha_k^{BB1}$ $\alpha_k^{BB} = \alpha_k^{BB2}$. I y , α_k^{BB1} y α_k^{BB2}, y E . (A.7), α_k^{BB2} r r - r .
F r *nonmonotone subroutine*, w r y y A r 3.2.

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