Statistical algorithm for estimating the derivatives of the solution to the elliptic BVP

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$$\Delta u(r) = \kappa^2 u(r) - c(r)u(r) - \big(v(r), \nabla u(r)\big) - g(r), \;\; r \in \Omega \subset \mathbb{R}^3, \qquad (1)$$
$$u(y) = \psi(y), \;\; y \in \partial\Omega = \Gamma.$$

$$u(r') = ?, \;\; \frac{\partial u}{\partial x_i}(r') = ?, \;\; \frac{\partial^2 u}{\partial x_i \partial x_j}(r') = ?.$$

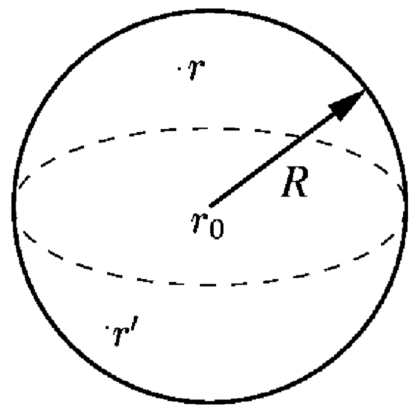
- boundary Γ is simply-connected and piecewise smooth,
- function $v(\cdot)$ satisfies the Hölder condition in $\mathbb{R}^3$,
- function $g(\cdot)$ satisfies the Hölder condition in $\overline{\Omega}$,
- function $\psi(\cdot)$ is continuous on Γ.

Estimation of the first derivatives

We can apply the mean value theorem for the ball $B(r_0, R)$:

$$\Delta_\kappa u(r) \equiv \Delta u(r) - \kappa^2 u(r) = -c(r)u(r) - \big(v(r), \nabla u(r)\big) - g(r).$$

For $r' \in B(r_0, R)$ we have



$$u_1(r') = -\int\limits_{S(r_0,R)} \frac{\partial \mathcal{G}^\kappa_{r_0}}{\partial \mathrm{n}_r}(r, r')u_1(r)\mathrm{d}S_r + \int\limits_{B(r_0,R)} \mathcal{G}^\kappa_{r_0}(r, r')g(r)\mathrm{d}r$$
$$+ \int\limits_{B(r_0,R)} \mathcal{G}^\kappa_{r_0}(r, r') \left[|v(r)|\frac{\partial u_1}{\partial \omega}(r) + c(r)u_1(r)\right] \mathrm{d}r,$$

here $S = \partial B$, $\mathcal{G}^\kappa_{r_0}$ is non-central Green's function and $v = |v|\omega$.

The non-central Green's function for the operator Δ_κ in the ball $B(r_0, R)$:

$$\mathcal{G}^{\kappa}_{r_0}(r, r') = \frac{1}{4\pi}\left[\frac{\sinh\{\kappa(R - |r - r'|)\}}{\sinh\{\kappa R\}\,|r - r'|}\right] - \mathcal{G}(r, r'), \tag{2}$$

here function $\mathcal{G}(r, r')$ is the solution for the following BVP:

$$\begin{cases} \Delta_\kappa \mathcal{G}(r, r') = 0, & \text{for } |r - r_0| < R; \\ \mathcal{G}(r, r') = \frac{1}{4\pi}\left[\frac{\sinh\{\kappa(R - |r - r'|)\}}{\sinh\{\kappa R\}\,|r - r'|}\right], & \text{for } |r - r_0| = R. \end{cases} \tag{3}$$

We can solve (3) using spherical coordinates:

$$\mathcal{G}(r, r') = \sum_{n=0}^{\infty} \varrho_n(r') P_n(\xi) \frac{\nu_n(\kappa|r - r_0|)}{\nu_n(\kappa R)},$$

here $\xi = \cos\theta$ is a cosine of the angle between $(r - r_0)$ and $(r' - r_0)$, $P_n(\cos\theta)$ are Legendre polynomials, and coefficients $\varrho_n(r)$ are the following:

$$\varrho_n(r') = \frac{2n+1}{2} \int_{-1}^{1} \frac{1}{4\pi} \left[\frac{\sinh\left\{\kappa(R - \sqrt{R^2 + |r' - r_0|^2 - 2R|r' - r_0|\xi})\right\}}{\sinh\{\kappa R\}\sqrt{R^2 + |r' - r_0|^2 - 2R|r' - r_0|\xi}} \right] P_n(\xi)\mathrm{d}\xi.$$

$\nu_n(x) = \sqrt{\dfrac{\pi}{2x}} I_{n+\frac{1}{2}}(x)$, here $I_{n+\frac{1}{2}}(x)$ are modified Bessel functions

The series expansion

$$\nu_n(x) = x^n \sum_{k=0}^{\infty} \frac{x^{2k}}{(2k)!} \prod_{j=0}^{n} \frac{1}{2j+1+2k},$$

The asymptotics

$$\frac{\nu_n(\kappa|r-r_0|)}{\nu_n(\kappa R)} \to \frac{|r-r_0|^n}{R^n}, \qquad \text{when } \kappa \to 0.$$

First functions

$$\nu_0(x) = \frac{\sinh(x)}{x},$$
$$\nu_1(x) = \left(\frac{\cosh(x)}{x} - \frac{\sinh(x)}{x^2}\right),$$
$$\nu_2(x) = \frac{\sinh(x)}{x} - \frac{3}{x^2}\left(\cosh(x) - \frac{\sinh(x)}{x}\right).$$

Further we use central functions (i.e. $r_0 = r'$) for internal BVP:

$$
\begin{aligned}
u_1(r') &= -\int\limits_{S(r',R)} \overbrace{\frac{\partial \mathcal{G}^{\kappa}_{r'}}{\partial \mathrm{n}_r}(r,r')}^{\text{(B)}} u_1(r)\mathrm{d}S_r + \int\limits_{B(r',R)} \mathcal{G}^{\kappa}_{r'}(r,r') g(r)\mathrm{d}r \\
&+ \int\limits_{B(r',R)} \underbrace{\mathcal{G}^{\kappa}_{r'}(r,r')}_{\text{(A)}} \left[|v(r)| \frac{\partial u_1}{\partial \omega}(r) + c(r) u_1(r) \right] \mathrm{d}r,
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial u_1}{\partial \omega}(r') &= -\int\limits_{S(r',R)} \overbrace{\frac{\partial}{\partial \omega}\left(\frac{\partial \mathcal{G}^{\kappa}_{r'}}{\partial \mathrm{n}_r}\right)(r,r')}^{\text{(D)}} u_1(r)\mathrm{d}S_r + \int\limits_{B(r',R)} \frac{\partial \mathcal{G}^{\kappa}_{r'}}{\partial \omega}(r,r') g(r)\mathrm{d}r \\
&+ \int\limits_{B(r',R)} \underbrace{\frac{\partial \mathcal{G}^{\kappa}_{r'}}{\partial \omega}(r,r')}_{\text{(C)}} \left[|v(r)| \frac{\partial u_1}{\partial \omega}(r) + c(r) u_1(r) \right] \mathrm{d}r.
\end{aligned}
$$

$$
U(w) \equiv U(r,j) = \begin{cases} u_1(r), & j = 0; \\ \dfrac{R(r)}{3}\dfrac{\partial u_1}{\partial \omega}(r), & j = 1. \end{cases} \Rightarrow \boxed{\quad U = KU + G. \quad}
$$

Let us denote $\rho = |r - r'|$; $\tilde{\nu}(\rho) = \kappa\rho\cosh\{\kappa(R-\rho)\} + \sinh\{\kappa(R-\rho)\}$;

$$a_\omega(r, r') = (\mathrm{n}(r'), \omega) = \left(\frac{r' - r}{|r' - r|}, \omega\right).$$

Central ($r \to r_0$) Green's function in the ball $B(r', R)$:

$$\mathcal{G}^{\kappa}_{r'}(r, r') = \frac{\sinh\{\kappa(R-\rho)\}}{4\pi\rho\sinh\{\kappa R\}} = F_0(r, r') \cdot \frac{C_{01}(\kappa R)R^2}{6}. \tag{A}$$

Central normal derivative (i. e. $r \to r_0$ and $|r' - r| = R$):

$$\left.\frac{\partial \mathcal{G}^{\kappa}_{r'}}{\partial \mathrm{n}_r}(r, r')\right|_{|r'-r|=R} = -\frac{1}{4\pi R^2}\frac{1}{\nu_0(\kappa R)} = -F_S(r, r') \cdot C_{00}(\kappa R). \tag{B}$$

$$\frac{\partial \mathcal{G}^{\kappa}_{r'}}{\partial \omega}(r, r') = \frac{a_\omega}{4\pi\sinh\{\kappa R\}}\left[\frac{\tilde{\nu}(\rho)}{\rho^2} - \frac{\kappa}{R}\frac{\nu_1(\kappa\rho)}{\nu_1(\kappa R)}\right] = F_1(r, r') \cdot \frac{3RC_{11}(\kappa R)a_\omega}{4}. \tag{C}$$

$$\frac{\partial}{\partial \omega}\left(\frac{\partial \mathcal{G}^{\kappa}_{r'}}{\partial \mathrm{n}_r}\right)(r, r')\Big|_{|r'-r|=R} = -\frac{a_\omega}{4\pi R^2}\frac{\kappa}{\nu_1(\kappa R)} = -F_S(r, r') \cdot \frac{3C_{10}(\kappa R)a_\omega}{R}. \tag{D}$$

$$C_{00}(x) = \frac{1}{\nu_0(x)}, \qquad C_{01}(x) = \frac{6}{x^2} \cdot \frac{\nu_0(x) - 1}{\nu_0(x)},$$
$$C_{10}(x) = \frac{x}{3\nu_1(x)}, \qquad C_{11}(x) = \frac{4}{3}\left[\mathrm{t}_0(x) - \frac{\mathrm{t}_0(x) - 1}{x\nu_1(x)}\right],$$

$$\nu_0(x) = \frac{\sinh(x)}{x}, \;\; \nu_1(x) = \frac{1}{x}\left(\cosh(x) - \frac{\sinh(x)}{x}\right), \;\; \mathrm{t}_0(x) = \frac{\tanh(x/2)}{x/2},$$

Let $p_0^c + p_1^c = 1$ and $c_0 \equiv \text{const} < \frac{6}{R_{\text{max}}}$, then $p(r) = 1 - \frac{c_0 R^2(r)}{6} \in (0,1)$.

We can use "Random Walk by Spheres and Balls" Algorithm to solve the equation

$$\underbrace{U = KU + G}_{\text{randomization}}$$
$$\Downarrow$$

$$U(r,j) = p(r)\Bigg(\int\limits_{S(r)} F_S(r,r')U(r',0)\underbrace{Q_{j0}(r')}_{\text{weights}}\mathrm{d}S_{r'} + G(r,j)/p(r)\Bigg)$$
$$+ (1-p(r)) \int\limits_{B(r)} F_j(r,r')[p_1^c U(r',1)\underbrace{Q_{j1}^c(r,r')}_{\text{weights}} + p_0^c U(r',0)\underbrace{Q_{j0}^c(r,r')}_{\text{weights}}]\mathrm{d}r'.$$

The estimator $\xi^{(0)}=\zeta(r_0,0)$ for the function $u(r_0)$, and the estimator $\xi_\omega^{(0)}=\zeta(r_0,1)$ for the function $\dfrac{R(r_0)}{3}\dfrac{\partial u}{\partial\omega}(r_0)$ have the following recurrent forms:

$$\xi^{(0)} = \begin{cases} Q_{00}\xi^{(1)} + \dfrac{G}{p}, & \mathbb{P} = p; \\ Q^c_{01}\xi^{(1)}_\omega, & \mathbb{P} = (1-p)p^c_1; \\ Q^c_{00}\xi^{(1)}, & \mathbb{P} = (1-p)p^c_0; \end{cases} \qquad \xi^{(0)}_\omega = \begin{cases} Q_{10}\xi^{(1)} + \dfrac{G_\omega}{p}, & \mathbb{P} = p; \\ Q^c_{11}\xi^{(1)}_\omega, & \mathbb{P} = (1-p)p^c_1; \\ Q^c_{10}\xi^{(1)}, & \mathbb{P} = (1-p)p^c_0. \end{cases}$$

Here $\xi^{(1)}$ and $\xi^{(1)}_\omega$ are estimators for $u(r_1)$ and $\dfrac{R(r_1)}{3}\dfrac{\partial u}{\partial\omega}(r_1)$, respectively.

$$p^c_1 = \frac{3|v(r_1)|}{R(r_1)p_{cv}}, \;\; p^c_0 = \frac{|c(r_1)|}{p_{cv}}, \quad \text{here } p_{cv} = \frac{3|v(r_1)|}{R(r_1)} + |c(r_1)|;$$

$$Q_{10}(r_1,r_0) = \frac{a_\omega C_{10}}{p(r_0)}, \;\; Q^c_{10}(r_1,r_0) = \frac{3a_\omega c(r_1)C_{11}}{2p^c_0 c_0}, \;\; Q^c_{11}(r_1,r_0) = \frac{9a_\omega|v(r_1)|C_{11}}{2p^c_1 c_0 R(r_1)},$$

$$Q_{00}(r_1,r_0) = \frac{C_{00}}{p(r_0)}, \;\; Q^c_{00}(r_1,r_0) = \frac{c(r_1)C_{01}}{p^c_0 c_0}, \;\; Q^c_{01}(r_1,r_0) = \frac{3|v(r_1)|C_{01}}{p^c_1 c_0 R(r_1)}.$$

Theorem 1 *Let the first derivatives of $u(r)$ to be bounded in Ω, $-c^*$ is the first eigen value of Laplacian in Ω and for any $r \in \Omega$:*

$$|Q_{ij}^c| \leq 1, \quad c_0 < \frac{6}{\pi^2} c^* \simeq 0.6079 c^*,$$

then there exists the unique solution of the integral equation $U = KU + G$ and

$$U(r,0) = u(r), \quad U(r,1) = \frac{R(r)}{3} \frac{\partial u}{\partial \omega}(r),$$

where $u(r)$ is the solution of initial differential problem. Moreover

$$|u(r) - \mathbf{E}\zeta_\varepsilon(r,0)| \leq C_u \varepsilon, \quad \left| \frac{R(r)}{3} \frac{\partial u}{\partial \omega} - \mathbf{E}\zeta_\varepsilon(r,1) \right| \leq C_d \varepsilon, \;\; \varepsilon > 0, \;\; r \in \Omega.$$

Theorem 2 *Let $y = \kappa/\sqrt{c^*}$ and*

$$\frac{c_0}{c^*} < \min_{x \in [0,\pi]} \left[\frac{6}{x^2} \left(1 - \frac{yx}{\sinh(yx)} \sqrt{\frac{\sin(x)}{x}} \right) \right],$$

then $\mathbf{V}\zeta_\varepsilon < C_V < +\infty \;\; \forall \varepsilon > 0$.

Estimation of the second derivatives $(\kappa = 0)$

Green's function

$$\mathcal{G}^0_{r_0} = g_1 + g_2 = \frac{1}{4\pi|r - r'|} + \frac{-R}{4\pi|r - r_0|}\frac{1}{\left|\frac{R^2}{|r-r_0|^2}(r - r_0) - (r' - r_0)\right|}.$$

Let us denote

$$\mathcal{F}(u, r) \equiv c(r)u(r) + \big(v(r), \nabla u(r)\big) + g(r), \;\; a_i = \cos(r - r', e_i), \;\; c_{ij} = \frac{(3a_i a_j - \delta_{ij})}{2},$$

here δ_{ij} is the Kronecker delta. Note that $|a_i| \leq 1$ and $|c_{ij}| \leq 1$.

$$\frac{\partial^2 u}{\partial x'_j x'_i}(r') = -\int\limits_{S(r_0,R)} \frac{\partial^2}{\partial x'_j x'_i}\left(\frac{\partial \mathcal{G}^0_{r_0}}{\partial \mathrm{n}_r}\right)(r, r')u(r)\mathrm{d}S_r + \int\limits_{B(r_0,R)} \frac{\partial^2 g_2}{\partial x'_j x'_i}(r, r')\mathcal{F}(u, r)\mathrm{d}r$$
$$+ \int\limits_{B(r_0,R)} \frac{\partial g_1}{\partial x'_j}(r, r')\frac{\partial \mathcal{F}(u, r)}{\partial x_i}\mathrm{d}r - \int\limits_{S(r_0,R)} \frac{\partial g_1}{\partial x'_j}(r, r')\mathcal{F}(u, r)\cos(\mathrm{n}_r, e_i)\mathrm{d}r.$$

We use the following functions in the integral representations of $u(r')$, $\frac{\partial u}{\partial x'_i}(r')$, $\frac{\partial^2 u}{\partial x'_j x'_i}(r')$:

$$\mathcal{G}^0_{r'}(r, r') = \frac{1}{4\pi}\left[\frac{1}{|r - r'|} - \frac{1}{R}\right] = \frac{R^2}{6} \cdot F_0(r, r'),$$

$$\frac{\partial \mathcal{G}^0_{r'}}{\partial x'_i}(r, r') = \frac{a_i}{4\pi}\left[\frac{1}{|r - r'|^2} - \frac{|r - r'|}{R^3}\right] = a_i\frac{3R}{4} \cdot F_1(r, r'),$$

$$\frac{\partial^2 g_2}{\partial x'_j x'_i}(r, r') = -\frac{2}{5}c_{ij} \cdot F_2(r, r'),$$

$$\frac{\partial g_1}{\partial x'_j}(r, r') = a_j \cdot F_S(r, r') = a_j R \cdot F_3(r, r'),$$

$$-\frac{\partial \mathcal{G}^0_{r'}}{\partial \mathrm{n}_r}(r, r') = \frac{1}{4\pi R^2} = F_S(r, r'),$$

$$-\frac{\partial}{\partial x'_i}\left(\frac{\partial \mathcal{G}^0_{r'}}{\partial \mathrm{n}_r}\right)(r, r') = \frac{a_i}{4\pi R^2}\frac{3}{R} = a_i\frac{3}{R} \cdot F_S(r, r'),$$

$$-\frac{\partial^2}{\partial x'_j x'_i}\left(\frac{\partial \mathcal{G}^0_{r_0}}{\partial \mathrm{n}_r}\right)(r, r') = c_{ij}\frac{10}{R^2} \cdot F_S(r, r').$$

The estimator $\xi_{ji}^{(0)}$ for the function $\dfrac{R^2(r_0)}{10}\dfrac{\partial^2 u}{\partial x_j \partial x_i}(r_0)$:

$$\xi_{ji}^{(0)} = \begin{cases} \dfrac{c_{ij}}{p}\xi^{(1)} + \dfrac{G_{ji}}{p}, & \mathbb{P} = p; \\ -a_i a_j \left[q_0 \xi^{(1)} + \sum_{k=1}^{3} q_k \xi_k^{(1)} \right], & \mathbb{P} = p_{_S} = 3(1-p)/15; \\ -c_{ij} \left[q_0 \xi^{(1)} + \sum_{k=1}^{3} q_k \xi_k^{(1)} \right], & \mathbb{P} = p_{_{F_2}} = 4(1-p)/25; \\ a_j \dfrac{15R}{4} \left[q_{0i}\xi^{(1)} + q_{00}\xi_i^{(1)} + \sum_{k=1}^{3} q_{ki}\xi_k^{(1)} + \sum_{k=1}^{3} q_{k0}\xi_{ik}^{(1)} \right], & \mathbb{P} = p_{_{F_3}} = 6(1-p)/25. \end{cases}$$

$$\xi^{(0)} = \begin{cases} \dfrac{1}{p}\xi^{(1)} + \dfrac{G}{p}, & \mathbb{P} = p; \\ Q_{0j}^c \xi_j^{(1)}, & \mathbb{P} = (1-p)p_j^c; \\ Q_{00}^c \xi^{(1)}, & \mathbb{P} = (1-p)p_0^c; \end{cases} \qquad \xi_i^{(0)} = \begin{cases} \dfrac{a_i}{p}\xi^{(1)} + \dfrac{G_i}{p}, & \mathbb{P} = p; \\ Q_{ij}^c \xi_j^{(1)}, & \mathbb{P} = (1-p)p_j^c; \\ Q_{i0}^c \xi^{(1)}, & \mathbb{P} = (1-p)p_0^c. \end{cases}$$

$$q_0 = \frac{c(r_1)}{c_0}; \;\; q_j = \frac{3v_j(r_1)}{R(r_1)c_0}; \;\; q_{0i} = \frac{c'_{x_i}(r_1)}{c_0};$$

$$q_{00} = \frac{3c(r_1)}{R(r_1)c_0}; \;\; q_{ji} = \frac{3v'_{x_i}(r_1)}{R(r_1)c_0}; \;\; q_{j0} = \frac{10v_j(r_1)}{R^2(r_1)c_0}.$$

We introduce probabilities p_k, p_{kj} and weights Q_k, Q_{kj} such as

$$q_k = Q_k p_k, \;\; q_{kj} = Q_{kj} p_{kj},$$

$$\sum_{k=0}^{3} p_k = 1, \;\; \sum_{k=0}^{3} (p_{ki} + p_{k0}) = 1.$$

Theorem 3 *Let the second derivatives of $u(r)$ to be bounded in Ω and*

$$|Q_k| \le 1, \;\; |Q_{kj}| \le 1.$$

Under the hypothesis of theorem 1, $\xi_{ji}^{(0)}$ is ε-biased estimator for $\frac{R^2(r_0)}{10} \frac{\partial^2 u}{\partial x_j \partial x_i}(r_0)$. Moreover, under the hypothesis of theorem 2, the variance of $\xi_{ji}^{(0)}$ is bounded $\forall \varepsilon > 0$.

Polynomial summand

$$\Delta u(r) - \kappa^2 u(r) + u^n(r) = 0, \;\; u\Big|_\Gamma = \psi, \;\; n \geq 2,$$

$$\xi^{(0)} = \begin{cases} \xi^{(1)} \dfrac{C_{00}(\kappa R)}{p}, & \mathbb{P} = p; \\ \left[\displaystyle\prod_{k=1}^{n} \xi^{(1,k)}\right] \dfrac{C_{01}(\kappa R)}{c_0}, & \mathbb{P} = 1 - p, \end{cases} \qquad \xi_i^{(0)} = \begin{cases} a_i \xi^{(1)} \dfrac{C_{10}(\kappa R)}{p}, & \mathbb{P} = p; \\ a_i \left[\displaystyle\prod_{k=1}^{n} \xi^{(1,k)}\right] \dfrac{9C_{11}(\kappa R)}{2Rc_0}, & \mathbb{P} = 1 - \end{cases}$$

here $R = R(r_0)$, $p = 1 - c_0 R^2/6$.

Theorem 4 *If* $c^{(0)} \geq 1$ *and* $1 < c_0 < 6c^*/\pi^2$, *then*

$$\mathbb{E}\xi^{(0)} = u(r_0) \;\; \textit{and} \;\; \mathbb{E}\xi_i^{(0)} = \frac{\partial u}{\partial x_i}(r_0).$$

Under the hypothesis of theorem 2 the variances are bounded.

$$c(r) = \sin\left(x - \frac{y}{z+2}\right), \quad v(r) = (R(r)/3, 0, 0), \quad \kappa = 2.12.$$

Table 1 shows the numerical results obtained at the point $r_0 = (-0.25, 0.50, 0.88)$.

These numerical results confirm the predicted error order $\mathcal{O}(\varepsilon + M^{-1/2})$.

Table 1: The total and statistical errors of the estimator ζ_ε for the solution $u(r_0) = -0.26273362$ and the gradient $\mathrm{grad}\,u(r_0) = (1.05093449, -0.26273362, -0.24943491)$. The parameter $c_0 = 4.0$.

M	ε	$\delta_T \pm \frac{\sigma(\zeta)}{\sqrt{M}}$ for $u(r_0)$	$\mathbf{E}N$	M	ε	$\delta_T \pm \frac{\sigma(\zeta)}{\sqrt{M}}$ for $\frac{\partial u}{\partial x}(r_0)$	$\mathbf{E}N$
10^5	10^{-2}	$(4.973 \pm 7.887) \cdot 10^{-4}$	10.38	10^4	10^{-3}	$(2.461 \pm 0.213) \cdot 10^{-2}$	17.80
10^7	10^{-3}	$(2.295 \pm 8.006) \cdot 10^{-5}$	17.84	10^6	10^{-4}	$(2.059 \pm 0.211) \cdot 10^{-3}$	25.23
M	ε	$\delta_T \pm \frac{\sigma(\zeta)}{\sqrt{M}}$ for $\frac{\partial u}{\partial y}(r_0)$	$\mathbf{E}N$	M	ε	$\delta_T \pm \frac{\sigma(\zeta)}{\sqrt{M}}$ for $\frac{\partial u}{\partial z}(r_0)$	$\mathbf{E}N$
10^4	10^{-3}	$(3.048 \pm 0.211) \cdot 10^{-2}$	17.80	10^4	10^{-3}	$(5.770 \pm 0.203) \cdot 10^{-2}$	17.80
10^6	10^{-4}	$(2.970 \pm 0.210) \cdot 10^{-3}$	25.23	10^6	10^{-4}	$(3.020 \pm 0.205) \cdot 10^{-3}$	25.23

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