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近似牛顿迭代法的数值离散格式

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(a) $-\lambda^2\Delta\psi + e^{\psi}u - e^{-\psi}v - C(x) = 0,$
(b) $-\operatorname{div} J_n + R = 0,$
(c) $J_n = \mu_n e^{\psi}\nabla u,$
(d) $\operatorname{div} J_p + R = 0,$
(e) $J_p = -\mu_p e^{-\psi}\nabla v$

本周工作：

- 设计了数值离散格式；
- 写了一部分牛顿迭代法的 C++ 代码。

引入 Scharfetter-Gummel 数值离散格式：

$$J_{n_{i+\frac{1}{2}}} = \frac{1}{h_i}\left[B\left(\psi_{i+1}-\psi_i\right)n_{i+1} - B\left(\psi_i-\psi_{i+1}\right)n_i\right], \tag{1.1}$$

$$J_{n_{i-\frac{1}{2}}} = \frac{1}{h_i}\left[B\left(\psi_i-\psi_{i-1}\right)n_i - B\left(\psi_{i-1}-\psi_i\right)n_{i-1}\right]. \tag{1.2}$$

其中 $B(x) = \frac{x}{e^x-1}$ 是 Bernoulli 函数。

- 由牛顿迭代法的原理：

$$-F(x) = dF(x) = \nabla F(x)dx. \tag{1.3}$$

$$dJ_{n_{i+\frac{1}{2}}} - dJ_{n_{i-\frac{1}{2}}} = -\left[J_{n_{i+\frac{1}{2}}} - J_{n_{i-\frac{1}{2}}}\right],$$

$$\begin{aligned} dJ_{n_{i+\frac{1}{2}}} &= \frac{1}{h_i}\left[B\left(\psi_{i+1}-\psi_i\right) dn_{i+1} - B\left(\psi_i-\psi_{i+1}\right) dn_i\right] \\ &+ \left[G\left(\psi_i-\psi_{i+1}\right)\left(d\psi_i - d\psi_{i+1}\right) + d\psi_i\right] J_{n_{i+\frac{1}{2}}} \end{aligned}$$

$$\begin{aligned} dJ_{n_{i-\frac{1}{2}}} &= \frac{1}{h_i} B\left(\psi_i-\psi_{i-1}\right) dn_i - B\left(\psi_{i-1}-\psi_i\right) dn_{i-1}\Big] \\ &+ \left[\left[G\left(\psi_{i-1}-\psi_i\right)\left(d\psi_{i-1} - d\psi_i\right) + d\psi_{i-1}\right] J_{n_{i-\frac{1}{2}}},\right. \end{aligned}$$

$$\begin{aligned} &\frac{1}{h_i}\left[B\left(\psi_{i+1}-\psi_i\right) dn_{i+1} - \left[B\left(\psi_i-\psi_{i+1}\right) dn_i + B\left(\psi_i-\psi_{i-1}\right)\right] dn_i + B\left(\psi_{i-1}-\psi_i\right) dn_{i-1}\right] \\ &+ \left[G\left(\psi_i-\psi_{i+1}\right)\left(d\psi_i - d\psi_{i+1}\right) + d\psi_i\right] J_{n_{i+\frac{1}{2}}} \\ &- \left[\left[G\left(\psi_{i-1}-\psi_i\right)\left(d\psi_{i-1} - d\psi_i\right) + d\psi_{i-1}\right] J_{n_{i-\frac{1}{2}}} = -\left[J_{n_{i+\frac{1}{2}}} - J_{n_{i-\frac{1}{2}}}\right]\right. \end{aligned}$$

电子电流连续性方程

$$
\begin{bmatrix}
B(\psi_1-\psi_2) & -\begin{pmatrix} B(\psi_2-\psi_3)+ \\ B(\psi_2-\psi_1) \end{pmatrix} & B(\psi_3-\psi_2) & & & \\
 & & & & & \\
 & & & B(\psi_{N-1}-\psi_N) & -\begin{pmatrix} B(\psi_N-\psi_{N+1}) \\ +B(\psi_N-\psi_{N-1}) \end{pmatrix} & B(\psi_{N+1}-\psi_N)
\end{bmatrix}
\begin{bmatrix} dn_1 \\ dn_2 \\ \vdots \\ \\ dn_N \end{bmatrix}
=
\begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ \\ F_N \end{bmatrix}
\tag{1.4}
$$

$$
\begin{aligned}
F_i = -\left[J_{n_{i+\frac{1}{2}}} - J_{n_{i-\frac{1}{2}}}\right] + \left[\left[G\left(\psi_{i-1}-\psi_i\right)\left(d\psi_{i-1}-d\psi_i\right) + d\psi_{i-1}\right] J_{n_{i-\frac{1}{2}}}\right. \\
\left. - \left[G\left(\psi_i-\psi_{i+1}\right)\left(d\psi_i-d\psi_{i+1}\right) + d\psi_i\right] J_{n_{i+\frac{1}{2}}}\right.
\end{aligned}
$$

引入 Scharfetter-Gummel 数值离散格式：

$$J_{p,i+\frac{1}{2}} = -\frac{1}{h_i}\left[B\left(\psi_{i+1}-\psi_i\right)p_i - B\left(\psi_i-\psi_{i+1}\right)p_{i+1}\right],$$

$$J_{p,i-\frac{1}{2}} = -\frac{1}{h_i}\left[B\left(\psi_i-\psi_{i-1}\right)p_{i-1} - B\left(\psi_{i-1}-\psi_i\right)p_i\right].$$

$$\begin{aligned} dJ_{p_{i+\frac{1}{2}}} &= \frac{1}{h_i}\left[B\left(\psi_i-\psi_{i+1}\right)dp_{i+1} - B\left(\psi_{i+1}-\psi_i\right)dp_i\right] \\ &\quad + \left[G\left(\psi_{i+1}-\psi_i\right)\left(d\psi_{i+1}-d\psi_i\right) - d\psi_i\right] J_{p_{i+\frac{1}{2}}} \end{aligned}$$

$$\begin{aligned} dJ_{p_{i-\frac{1}{2}}} &= \frac{1}{h_i} B\left(\psi_{i-1}-\psi_i\right)dp_i - B\left(\psi_i-\psi_{i-1}\right)dp_{i-1}\Big] \\ &\quad + [[G\left(\psi_i-\psi_{i-1}\right)\left(d\psi_i-d\psi_{i-1}\right) - d\psi_{i-1}] J_{p_{i-\frac{1}{2}}} \end{aligned}$$

得到基础的方程:

$$dJ_{p_{i+\frac{1}{2}}} - dJ_{p_{i-\frac{1}{2}}} = -\left[J_{p_{i+\frac{1}{2}}} - J_{p_{i-\frac{1}{2}}}\right] \Rightarrow$$

$$\frac{1}{h_i}\left[B\left(\psi_i - \psi_{i+1}\right) dp_{i+1} - \left[B\left(\psi_{i+1} - \psi_i\right) + B\left(\psi_{i-1} - \psi_i\right)\right] dp_i + B\left(\psi_i - \psi_{i-1}\right) dp_{i-1}\right]$$

$$+\left[G\left(\psi_{i+1} - \psi_i\right)\left(d\psi_{i+1} - d\psi_i\right) - d\psi_i\right] J_{p_{i+\frac{1}{2}}}$$

$$-\left[\left[G\left(\psi_i - \psi_{i-1}\right)\left(d\psi_i - d\psi_{i-1}\right) - d\psi_{i-1}\right] J_{p_{i-\frac{1}{2}}} = -\left[J_{p_{i+\frac{1}{2}}} - J_{p_{i-\frac{1}{2}}}\right].$$

$$
\begin{bmatrix}
B\left(\psi_2-\psi_1\right) & -\begin{pmatrix} B\left(\psi_3-\psi_2\right) \\ +B\left(\psi_1-\psi_2\right) \end{pmatrix} & B\left(\psi_2-\psi_3\right) & & \\
 & \ddots & \ddots & \ddots & \\
 & & B\left(\psi_N-\psi_{N-1}\right) & -\begin{pmatrix} B\left(\psi_{N+1}-\psi_N\right) \\ +B\left(\psi_{N-1}-\psi_N\right) \end{pmatrix} & B\left(\psi_N-\psi_{N+1}\right)
\end{bmatrix}
\begin{bmatrix} dp_1 \\ dp_2 \\ \vdots \\ dp_N \end{bmatrix}
=
\begin{bmatrix} K_1 \\ K_2 \\ \vdots \\ K_N \end{bmatrix}
\tag{2.1}
$$

$$
K_i = -\left[G\left(\psi_{i+1}-\psi_i\right)\left(d\psi_{i+1}-d\psi_i\right)-d\psi_i\right] J_{p_{i+\frac{1}{2}}}
$$

$$
+\left[\left[G\left(\psi_i-\psi_{i-1}\right)\left(d\psi_i-d\psi_{i-1}\right)-d\psi_{i-1}\right] J_{p_{i-\frac{1}{2}}}-\left[J_{p_{i+\frac{1}{2}}}-J_{p_{i-\frac{1}{2}}}\right]\right.
$$

给定 $\psi^k = \left[\psi_0^k, \psi_1^k, \cdots, \psi_N^k, \psi_{N+1}^k\right]$, $n^k = \left[n_0^k, n_1^k, \cdots, n_N^k, n_{N+1}^k\right]$, $p^k = \left[p_0^k, p_1^k, \cdots, p_N^k, p_{N+1}^k\right]$:

- 计算 $b_i^1 (b^1 = \left[b_1^1, b_2^1, \cdots, b_N^1\right])$:

$$b_i^1 = \frac{-2\lambda^2}{h_i + h_{i-1}} \left[\frac{1}{h_i}(\psi_{i+1} - \psi_i) - \frac{1}{h_{i-1}}(\psi_i - \psi_{i-1})\right] + n_i - p_i - C_i. \tag{3.1}$$

- 计算 $d\psi^k = \left[d\psi_1^k, d\psi_2^k, \cdots, d\psi_N^k\right]$:

$$d\psi_i = (n_i + p_i)^{-1} / [-b_i^1 + dp_i - dn_i]. \tag{3.2}$$

- 计算 $dn^k = \left[dn_0^k, dn_1^k, \cdots, dn_N^k, dn_{N+1}^k\right]$:

$$dJ_{n_{i+\frac{1}{2}}} - dJ_{n_{i-\frac{1}{2}}} = -\left[J_{n_{i+\frac{1}{2}}} - J_{n_{i-\frac{1}{2}}}\right]. \tag{3.3}$$

- 计算 $dp^k = \left[dp_0^k, dp_1^k, \cdots, dp_N^k, dp_{N+1}^k\right]$:

$$dJ_{p_{i+\frac{1}{2}}} - dJ_{p_{i-\frac{1}{2}}} = -\left[J_{p_{i+\frac{1}{2}}} - J_{p_{i-\frac{1}{2}}}\right]. \tag{3.4}$$

- 更新变量:

$$\psi^{k+1} = \psi^k + d\psi^k, \quad n^{k+1} = \left(n^k + dn^k\right) e^{d\psi^k}, \quad p^{k+1} = \left(p^k + dp^k\right) e^{-d\psi^k}.$$

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