数值代数中 Gummel 迭代方法的补充与 MSP 方法公式推导

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考虑引入量子修正效应的半导体器件方程:

$$\begin{cases} f_1: & \varepsilon\Delta\psi + q(p - n + N_D^+ - N_A^-) + \rho_s = 0, \\ f_2: & \frac{1}{q}\nabla\cdot J_n - (U - G) = 0, \\ f_3: & -\frac{1}{q}\nabla\cdot J_p - (U - G) = 0, \\ f_4: & b_n(\Delta \ln n + \frac{1}{2}\varepsilon(\ln n)^2) - \Lambda_n = 0 \\ f_5: & b_p(\Delta \ln p + \frac{1}{2}\varepsilon(\ln p)^2) - \Lambda_p = 0. \end{cases} \tag{1.1}$$

现在已知第 k 次迭代时自变量 $(\psi, \phi_n, \phi_p, \Lambda_n, \Lambda_p)$ 的值 $(\psi_k, \phi_{n,k}, \phi_{p,k}, \Lambda_{n,k}, \Lambda_{p,k})$，要迭代求出第 $k+1$ 次迭代时自变量 $(\psi, \phi_n, \phi_p, \Lambda_n, \Lambda_p)$ 的值 $(\psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1}, \Lambda_{n,k+1}, \Lambda_{p,k+1})$ 使以下方程组的残差接近于 0。

$$f_i(\psi_{k+1}, \phi_{n,k+1}, \phi_{p,k+1}, \Lambda_{n,k+1}, \Lambda_{p,k+1}) = 0, i = 1, 2, 3, 4, 5.$$

广义 Gummel 线性化

假设准费米势 ϕ_n, ϕ_p，量子修正 Λ_n, Λ_p 是静电势 ψ 的函数：

$$n = n(\psi, \phi_n, \Lambda_n) \tag{1.2}$$

$$dn = \frac{\partial n}{\partial \psi} d\psi + \frac{\partial n}{\partial \phi_n} d\phi_n + \frac{\partial n}{\partial \Lambda_n} d\Lambda_n = \frac{\partial n}{\partial \psi} d\psi + \frac{\partial n}{\partial \phi_n}\frac{d\phi_n}{d\psi} d\psi + \frac{\partial n}{\partial \Lambda_n}\frac{d\Lambda_n}{d\psi} d\psi \tag{1.3}$$

$$= \frac{\partial n}{\partial \psi} d\psi + \frac{\partial n}{\partial \phi_n}\alpha_n^k d\psi + \frac{\partial n}{\partial \Lambda_n}\beta_n^k d\psi = \left(\frac{\partial n}{\partial \psi} + \frac{\partial n}{\partial \phi_n}\alpha_n^k + \frac{\partial n}{\partial \Lambda_n}\beta_n^k\right) d\psi \tag{1.4}$$

原 Possion 方程：$-\frac{\varepsilon \Delta \psi^{k+1}}{q} - p^{k+1} + n^{k+1} - N_D^+ + N_A^- + \frac{\rho_s}{q} = 0.$

普通 Gummel 迭代：令 p^{k+1}, n^{k+1} 分别在 p^k, n^k 处对 ψ 一阶 Taylor 展开：

$$-\frac{\varepsilon \Delta \psi^{k+1}}{q} - \left(p^k + \frac{\partial p}{\partial \psi}\left(\psi^{k+1} - \psi^k\right)\right) + \left(n^k + \frac{\partial n}{\partial \psi}\left(\psi^{k+1} - \psi^k\right)\right) - N_D^+ + N_A^- + \frac{\rho_s}{q} = 0. \tag{1.5}$$

令 p^{k+1}, n^{k+1} 分别在 p^k, n^k 处对 $\psi, \phi_n, \phi_p, \Lambda_n, \Lambda_p$ 一阶 Taylor 展开：

$$n^{k+1} = n^k\left(\psi^k, \phi_n^k, \Lambda_n^k\right) + \frac{\partial n}{\partial \psi}\left(\psi^{k+1} - \psi^k\right) + \frac{\partial n}{\partial \phi_n}\left(\phi_n^{k+1} - \phi_n^k\right) + \frac{\partial n}{\partial \Lambda_n}\left(\Lambda_n^{k+1} - \Lambda_n^k\right)$$

将 $dn = \left(\frac{\partial n}{\partial \psi} + \frac{\partial n}{\partial \phi_n}\alpha_n^k + \frac{\partial n}{\partial \Lambda_n}\beta_n^k\right) d\psi$ 代入：

$$n^{k+1} = n^k\left(\psi^k, \phi_n^k, \Lambda_n^k\right) + \left(\frac{\partial n}{\partial \psi} + \frac{\partial n}{\partial \phi_n}\alpha_n^k + \frac{\partial n}{\partial \Lambda_n}\beta_n^k\right) d\psi,$$

$$-\frac{\varepsilon \Delta \psi^{k+1}}{q} + n^k - p^k + \left(\frac{\partial n}{\partial \psi} - \frac{\partial p}{\partial \psi}\right)\left(\psi^{k+1} - \psi^k\right) + C +$$

$$\left(\alpha_n^k \frac{\partial n}{\partial \phi_n} - \alpha_p^k \frac{\partial p}{\partial \phi_p} + \beta_n^k \frac{\partial n}{\partial \Lambda_n} - \beta_p^k \frac{\partial p}{\partial \Lambda_p}\right)\left(\psi^{k+1} - \psi^k\right) = 0$$

更新策略:

$$\phi_n^{k+1} = \phi_n^k + \alpha_n^k(\psi^{k+1} - \psi^k), \quad \phi_p^{k+1} = \phi_p^k + \alpha_p^k(\psi^{k+1} - \psi^k),$$
$$\Lambda_n^{k+1} = \Lambda_n^k + \beta_n^k(\psi^{k+1} - \psi^k), \quad \Lambda_p^{k+1} = \Lambda_p^k + \beta_p^k(\psi^{k+1} - \psi^k).$$
$$n_{k+1} = n(\psi^{k+1}, \phi_n^{k+1}, \Lambda_n^{k+1}), \quad p_{k+1} = p(\psi^{k+1}, \phi_p^{k+1}, \Lambda_p^{k+1}),$$
$$R_{k+1} = R(\psi^{k+1}, \phi_n^{k+1}, \phi_p^{k+1}, \Lambda_n^{k+1}, \Lambda_p^{k+1}).$$

$\alpha_p^{k+1}, \alpha_n^{k+1}, \beta_n^{k+1}, \beta_p^{k+1}$ 的更新策略:

$$dn = \left(\frac{\partial n}{\partial \psi} + \frac{\partial n}{\partial \phi_n}\alpha_n^k + \frac{\partial n}{\partial \Lambda_n}\beta_n^k\right) d\psi \Rightarrow \alpha_n^k = \frac{dn/d\psi - \partial n/\partial \psi - \partial n/\partial \Lambda_n \cdot \beta_n^k}{\partial n/\partial \phi_n}$$
$$\beta_n^k = \frac{dn/d\psi - \partial n/\partial \psi - \partial n/\partial \phi_n \cdot \alpha_n^k}{\partial n/\partial \Lambda_n}$$

1. 对于 ψ 问题：求解 ψ^{k+1} 使得

$$-\frac{\varepsilon\Delta\psi^{k+1}}{q}+n^k-p^k+\left(\frac{\partial n}{\partial\psi}-\frac{\partial p}{\partial\psi}\right)(\psi^{k+1}-\psi^k)+C+$$
$$\left(\alpha_n^k\frac{\partial n}{\partial\phi_n}-\alpha_p^k\frac{\partial p}{\partial\phi_p}+\beta_n^k\frac{\partial n}{\partial\Lambda_n}-\beta_p^k\frac{\partial p}{\partial\Lambda_p}\right)(\psi^{k+1}-\psi^k)=0.$$

2. 对于 ϕ,Λ 问题，更新准费米势以及量子修正：

$$\phi_n^{k+1}=\phi_n^k+\alpha_n^k(\psi^{k+1}-\psi^k),\quad \phi_p^{k+1}=\phi_p^k+\alpha_p^k(\psi^{k+1}-\psi^k),$$
$$\Lambda_n^{k+1}=\Lambda_n^k+\beta_n^k(\psi^{k+1}-\psi^k),\quad \Lambda_p^{k+1}=\Lambda_p^k+\beta_p^k(\psi^{k+1}-\psi^k).$$

3. 更新载流子浓度以及 R:

$$n_{k+1}=n(\psi^{k+1},\phi_n^{k+1},\Lambda_n^{k+1}),\quad p_{k+1}=p(\psi^{k+1},\phi_p^{k+1},\Lambda_p^{k+1}),$$
$$R_{k+1}=R(\psi^{k+1},\phi_n^{k+1},\phi_p^{k+1},\Lambda_n^{k+1},\Lambda_p^{k+1}).$$

4. **for** $i \in \mathcal{I}$
   4.1 设 $\nabla \cdot \mathbf{J}_n - qR = 0, \nabla \cdot \mathbf{J}_p + qR = 0$ 的离散格式，分别记为 f_n^J 以及 f_p^J，及量子修正方程的离散格式，分别记为 f_n^Q 以及 f_p^Q。
   4.2 更新节点 i 处的 n,p:

$$n_i^* = f_n^J(N(i), n^{k+1}, R^{k+1}),\ \ p_i^* = f_p^J(N(i), p^{k+1}, R^{k+1}),$$
$$\Lambda_{n,i}^* = f_n^Q(N(i), n^{k+1}),\ \ \Lambda_{p,i}^* = f_p^Q(N(i), p^{k+1}).$$

5. 更新离散节点的 $\alpha_n, \alpha_p, \beta_n, \beta_p$:

$$\beta_n^{k+1} = \frac{\Lambda_n^* - \Lambda_n^k}{\psi^{k+1} - \psi^k} \simeq \frac{d\Lambda_n}{d\psi}, \alpha_n^{k+1} = \frac{\frac{n^* - n^k}{\psi^{k+1} - \psi^k} - \partial n/\partial\psi - \partial n/\partial\Lambda_n \cdot \beta_n^{k+1}}{\partial n/\partial\phi_n}$$
$$\beta_p^{k+1} = \frac{\Lambda_p^* - \Lambda_p^k}{\psi^{k+1} - \psi^k} \simeq \frac{d\Lambda_p}{d\psi}, \alpha_p^{k+1} = \frac{\frac{p^* - p^k}{\psi^{k+1} - \psi^k} - \partial p/\partial\psi - \partial p/\partial\Lambda_p \cdot \beta_n^{k+1}}{\partial p/\partial\phi_p}$$

$$\begin{cases} -\frac{\varepsilon}{q}\Delta\psi + n - p + C = 0 \\ \nabla\cdot\mathbf{J}_n - qR = 0, \mathbf{J}_n = -q\mu_n n\nabla\phi_n \\ \nabla\cdot\mathbf{J}_p + qR = 0, \mathbf{J}_p = -q\mu_p p\nabla\phi_p \end{cases} \Rightarrow \begin{cases} f_1 : -\frac{\varepsilon}{q}\Delta\psi + n - p + C = 0, \\ f_2 : \nabla\cdot[-q\mu_n n\nabla\phi_n] - qR = 0, \\ f_3 : \nabla\cdot[-q\mu_p p\nabla\phi_p] + qR = 0. \end{cases} \tag{2.1}$$

（1）考虑对 $\phi_p^{k+1}, d\phi_p$ 的求解：

- **近似牛顿**： $\nabla\cdot[\mu_p p(\nabla d\phi_p + \nabla\phi_p)] = R + \frac{\partial R}{\partial\phi_p} d\phi_p$.
- **MSP-Gummel**： $\nabla\cdot[\mu_p p\nabla\phi_p^{k+1}] = -qR$. **Gummel 迭代的核心思想**： f_3: 求解 $\phi_{p,k+1}$
  - 固定 $\psi_{k+1} = \psi_k; \phi_{n,k+1} = \phi_{n,k}$；迭代方程： $f_3(\psi_{k+1} = \psi_k, \phi_{n,k+1} = \phi_{n,k}, \phi_{p,k+1})$。

  得到 $\phi_{p,k+1} = \phi_1$。

（2）考虑对 $\psi_1, d\psi_1$ 的求解：

- **近似牛顿**： $-\frac{\varepsilon}{q}(\Delta d\psi_1 + \Delta\psi) + n - p + C - \frac{\partial p}{\partial\psi} d\psi_1 - \frac{\partial p}{\partial\phi_p} = 0$
- **MSP-Gummel**： $-\frac{\varepsilon}{q}\Delta\psi^{k+1} + n - p + C = 0.$

(3) 考虑对 $d\phi_n, \phi_n^{k+1}$ 的求解:

- **近似牛顿**:

$$\nabla \cdot [\mu_n n(\nabla d\phi_n + \nabla \phi_n)] = -R - \frac{\partial R}{\partial \phi_n} d\phi_n - \frac{\partial R}{\partial \phi_p} d\phi_p - \mu_n \nabla \cdot [\frac{\partial n}{\partial \psi} \nabla \phi_n d\psi_1].$$

- **MSP-Gummel**: $\nabla \cdot [\mu_n n(\psi^{k+1}, \phi_n^{k+1}) \nabla \phi_n] = -R$, 而 $\psi_{k+1} = g(\phi_{n,k+1}) :=$ $\psi_1 - (\frac{\partial f_0}{\partial \phi_n}\left(\psi_{k+\frac{1}{2}}, \phi_{n,k}, \phi_{p,k+1}\right))/(\frac{\partial f_0}{\partial \psi}\left(\psi_{k+\frac{1}{2}}, \phi_{n,k}, \phi_{p,k+1}\right)) \cdot (\phi_{n,k+1} - \phi_{n,k})$.

(4) 考虑对 $d\psi, \psi^{k+1}$ 的求解:

- **近似牛顿**: $-\frac{\varepsilon}{q}(\Delta d\psi + \Delta \psi) + n - p + C = \frac{\partial p}{\partial \phi_p} d\phi_p - \frac{\partial n}{\partial \phi_n} d\phi_n - \frac{\partial n}{\partial \psi} d\psi + \frac{\partial p}{\partial \psi} d\psi.$
- **MSP-Gummel**: $-\frac{\varepsilon}{q}\Delta \psi^{k+1} + n - p + C = 0.$

1 广义 Gummel 线性化

2 MSP-Gummel 与近似牛顿迭代法的比较

3 Modified Singular Perturbation 算法理解
- Singular Perturbation Schema
- Modified Singular Perturbation Schema

4 Application of Matrix Transformation Methods in Block Newton Method

观察以 ψ, u, v 为自变量的 Non-linear 方程组：

$$
\begin{aligned}
f_1 &: -\Delta\psi + e^{\psi}u - e^{-\psi}v - C(x) = 0, \\
f_2 &: \nabla\cdot\left[\mu_n e^{\psi}\nabla u\right] - R(\nabla\psi, u, v) = 0, \\
f_3 &: \nabla\cdot\left[\mu_p e^{-\psi}\nabla v\right] - R(\nabla\psi, u, v) = 0.
\end{aligned} \tag{3.1}
$$

- ***The first step:*** $\frac{\partial f_3}{\partial v}(\psi_k, u_k, v_k)dv = -f_3(\psi_k, u_k, v_k), \quad v_{k+1} := v_k + dv.$
- ***The Second step:***

$$
\frac{\partial f_1}{\partial\psi}\left(\psi_k, u_k, v_{k+1}\right)\widetilde{d\psi} + \frac{\partial f_1}{\partial u}\left(\psi_k, u_k, v_{k+1}\right)du = -f_1\left(\psi_k, u_k, v_{k+1}\right).
$$

$$
\frac{\partial f_1}{\partial u} = e^{\psi}du, \quad \frac{\partial f_1}{\partial\psi} = -\Delta\widetilde{d\psi} + e^{\psi}ud\psi + e^{-\psi}v\widetilde{d\psi}
$$

- ▶ 对第二步补充推导：忽略 Laplace 项，则可以得到

$$-\Delta \widetilde{d\psi} + e^{\psi} u \widetilde{d\psi} + e^{-\psi} v \widetilde{d\psi} + e^{\psi} du = -f_1 \Rightarrow \widetilde{d\psi} = \frac{-f_1 - e^{\psi} du}{e^{\psi} u + e^{-\psi} v}.$$

再继续求解 f_2 方程：

$$\frac{\partial f_2}{\partial \psi}(\psi_k, u_k, v_{k+1}) \widetilde{d\psi} + \frac{\partial f_2}{\partial u}(\psi_k, u_k, v_{k+1}) du = -f_2(\psi_k, u_k, v_{k+1}),$$
$$u_{k+1} = u_k + du.$$

- ***The Third step:***

$$-\Delta \psi + e^{\psi} u_{k+1} - e^{-\psi} v_{k+1} - C(x) = 0.$$

在具有单载流子的半导体器件方程求解器中，电子电流连续性方程与 Possion 方程：

$$
\begin{cases}
F_\psi : \nabla \cdot (\varepsilon \nabla \psi) = n - p + N_A - N_D, \\
F_{\Phi_n} : \nabla \cdot J_n = 0, J_n = -q\mu_n n \nabla \phi_n \\
n = e^{\psi - \phi_n}, \quad p = e^{\phi_p - \psi}, \\
\Phi_n = e^{-\phi_n}, \quad \Phi_p = e^{-\phi_p}.
\end{cases}
\tag{3.2}
$$

使用块对角矩阵公式：

$$
Ax = -F \equiv \begin{bmatrix} A_{\psi\psi} & D_{\psi\Phi_n} \\ A_{\Phi_n\psi} & A_{\Phi_n\Phi_n} \end{bmatrix} \begin{pmatrix} \delta\psi \\ \delta\Phi_n \end{pmatrix} = -\begin{pmatrix} F_\psi \\ F_{\Phi_n} \end{pmatrix}. \tag{3.3}
$$

其中 $\Phi_n = e^{-\phi_n}$，$\Phi_p = e^{-\phi_p}$ 为 Slotboom Variables。

Advantages of Using the Slotboom Variables:

- The current continuity equation becomes linear and that its matrix becomes definite and symmetric.
- Symmetric matrices take less time to solve than asymmetric ones.
- For low-bias applications where Gummel iteration converges rapidly, using the Slotboom Variables offers higher computational efficiency.

Disadvantages of Using the Slotboom Variables:

- The disadvantage of using the Slotboom variables is that these variables overflow at large voltage bias. Using IEEE standard double precision capabilities, the maximum number which can be represented is about 10^{300}. However, even this huge number can only accommodate a bias of about 18 V at room temperature. At low temperatures, the maximum voltage is further reduced, to less than 5 V at 77 K.

对上述块对角矩阵进行拆分:

$$A_{\psi\psi}\delta\psi = \frac{\partial F_\psi(\psi,\Phi_n)}{\partial\psi}\delta\psi = \nabla\cdot(\varepsilon\nabla d\psi) - nd\psi - pd\psi,$$

$$D_{\psi\Phi_n}\delta\Phi_n = \frac{\partial F_\psi(\psi,\Phi_n)}{\partial\Phi_n}\delta\Phi_n = -e^{\psi}d\Phi_n,$$

$$A_{\Phi_n\psi}\delta\psi = \frac{\partial F_{\Phi_n}(\psi,\Phi_n)}{\partial\psi}\delta\psi = \nabla\cdot(J_n d\psi),$$

$$A_{\Phi_n\Phi_n}\delta\Phi_n = \frac{\partial F_{\Phi_n}(\psi,\Phi_n)}{\partial\Phi_n}\delta\Phi_n =$$

$$\nabla\cdot\left[-q\mu_n e^{\psi}\nabla(-\ln\Phi_n)\, d\Phi_n\right] + \nabla\cdot\left[-q\mu_n e^{\psi}\Phi_n\nabla(-d\Phi_n/\Phi_n)\right]$$

在线性化的电子电流连续性方程中:

$$A_{\Phi_n\psi}\delta\psi + A_{\Phi_n\Phi_n}\delta\Phi_n = -F_{\Phi_n}.$$

传统 Gummel 迭代忽略了 $A_{\Phi_n\psi}\delta\psi$ 项，在 SP 方法中则用 $\widetilde{\delta\psi}$ 作为 $\delta\psi$ 的估计:

$$A_{\Phi_n\psi}\widetilde{\delta\psi} + A_{\Phi_n\Phi_n}\delta\Phi_n = -F_{\Phi_n}. \tag{3.4}$$

忽略 Possion 方程中的 Laplace 项:

$$\frac{\partial F_\psi}{\partial\psi}\widetilde{\delta\psi} + \frac{\partial F_\psi}{\partial\Phi_n}\delta\Phi_n = -F_\psi \Rightarrow (n_j + p_j)\,\widetilde{\delta\psi}_j + n_j\frac{\delta\Phi_{n,j}}{\Phi_{n,j}} = -F_{\psi,j}$$

$$\widetilde{\delta\psi}_j = -\frac{n_j}{n_j + p_j}\frac{\delta\Phi_{n,j}}{\Phi_{n,j}} - \frac{F_{\psi,j}}{n_j + p_j}. \tag{3.5}$$

将 (3.5) 代入 (3.4) 中即可。

- The success of the Singular Perturbation Schema depends on how closely $\widetilde{\delta\psi}$ approximates $\delta\psi$.
- 将 $A_{\psi\psi}\delta\psi$ 替换为 $D^{SP}_{\psi\psi}\widetilde{\delta\psi}$:

$$D^{SP}_{\psi\psi}\widetilde{\delta\psi} + D_{\psi\Phi_n}\delta\Phi_n = -F_\psi, \tag{3.6}$$

$$A_{\psi\psi}\delta\psi + D_{\psi\Phi_n}\delta\Phi_n = -F_\psi. \tag{3.7}$$

$$D^{SP}_{\psi\psi,j} = n_j + p_j.$$

- Argument for the SP Schema: since the mobile carrier terms almost always **dominate the diagonal** of $A_{\psi\psi}$, which makes $A_{\psi\psi}$ approximately a diagonal matrix, one can use $D^{SP}_{\psi\psi}$ to approximate $A_{\psi\psi}$.

Modified Singular Perturbation Schema:

$$(n_j + p_j)\,\widetilde{\delta\psi}_j + n_j \frac{\delta\Phi_{n,j}}{\Phi_{n,j}} = -F_{\psi,j} \Rightarrow \widetilde{\delta\psi}_j = -\frac{n_j}{n_j + p_j}\frac{\delta\Phi_{n,j}}{\Phi_{n,j}} - \frac{F_{\psi,j}}{n_j + p_j}. \tag{3.8}$$

$$\left(n_j + p_j + V_j^{-1}\sum_k \frac{\varepsilon_{jk}A_{jk}}{d_{jk}}\right)\widetilde{\delta\psi}_j + n_j \frac{\delta\Phi_{n,j}}{\Phi_{n,j}} = -F_{\psi,j}. \tag{3.9}$$

- 原始 SP 方案在模拟 MOSFET 器件时性能不稳定。
- 原始 SP 在 $n \gg p$ 时，$\widetilde{\delta\psi}$ 仅随 Φ_n 的相对变化（F_ψ, F_{Φ_n} 之间有密切的耦合，$n = e^\psi \Phi_n$ 保持不变为一个较为严格的约束）。
- 原始 SP 适用于 n 型电荷中性区域，不适用于空间电荷区域（受到了杂志电荷而非移动载流子的影响）。

在 (3.8) 的基础上，加入对 Slotboom Variable Φ_p 变量的偏微分项：

$$\left(n_j + p_j + V_j^{-1}\sum_k \frac{\varepsilon_{jk}A_{jk}}{d_{jk}}\right)\widetilde{\delta\psi}_j + n_j\frac{\delta\Phi_{n,j}}{\Phi_{n,j}} = -F_{\psi,j},$$

$$A_{\psi\psi}\widetilde{\delta\psi} + A_{\psi\Phi_n}\delta\Phi_n + A_{\psi\Phi_p}\delta\Phi_p = -F_\psi.$$

双载流子器件的 MSP 求解步骤：

1. $f_3(f_{\Phi_p})$：求解 $\Phi_{p,k+1}$
   - 固定 $\psi_{k+1} = \psi_k; \Phi_{n,k+1} = \Phi_{n,k}$；迭代方程：$f_3(\psi_{k+1} = \psi_k, \Phi_{n,k+1} = \Phi_{n,k}, \Phi_{p,k+1})$。

   得到 $\Phi_{p,k+1}$。
2. $f_1(f_\psi)$：求解 $\psi_{k+1} = \psi_k + \widetilde{\delta\psi}$

$$\partial f_1/\partial\psi \cdot \widetilde{\delta\psi} + \partial f_1/\partial\Phi_n \cdot \delta\Phi_n + \partial f_1/\partial\Phi_p \cdot \delta\Phi_p = -f_1.$$

3. $f_2(f_{\Phi_n})$： **求解** $\Phi_{n,k+1}$
   - **固定** $\psi_{k+1} = \psi_k + \widetilde{\delta\psi}; \Phi_{p,k+1} = \Phi_{p,k+1}$； **迭代方程**：

$$f_2(\psi_{k+1} = \psi_k + \widetilde{\delta\psi}, \Phi_{p,k+1} = \Phi_{p,k+1}, \Phi_{n,k+1}) = 0.$$

4. $f_1(f_\psi)$： **求解** ψ_{k+1}
   - **固定** $\Phi_{n,k+1} = \Phi_{n,k+1}; \Phi_{p,k+1} = \Phi_{p,k+1}$； **迭代方程**：

$$f_1(\psi_{k+1}, \Phi_{n,k+1} = \Phi_{n,k+1}; \Phi_{p,k+1} = \Phi_{p,k+1}).$$

With a block matrix transformation, the system of equations for a new update is as follows :

$$Ax = -F \equiv \begin{bmatrix} A_{\psi\psi} & D_{\psi\Phi_n} \\ A_{\Phi_n\psi} & A_{\Phi_n\Phi_n} \end{bmatrix} \begin{pmatrix} \delta\psi \\ \delta\Phi_n \end{pmatrix} = -\begin{pmatrix} F_\psi \\ F_{\Phi_n} \end{pmatrix}. \tag{4.1}$$

$A_{\psi\psi}, A_{\Phi_n\Phi_n}$ are the main matrices of Poisson and current continuity equation respectively while $D_{\psi\Phi_n}$ and $A_{\Phi_n\psi}$ are the corresponding coupling matrices.

- **MSP 方法的应用**:

$$T_{MSP}Ax = -T_{MSP}F, \quad T_{MSP} = \begin{bmatrix} I & 0 \\ -A_{\Phi_n\psi}D_{\psi\psi}^{-1} & I \end{bmatrix}.$$

- **Altenate-Block-Factorization (ABF) 的应用**

$$AT_{ABF}T_{ABF}^{-1}x = -F, \quad T_{ABF} = \begin{bmatrix} I & -D_{\psi\psi}^{-1}D_{\psi\Phi_n} \\ -D_{\Phi_n\Phi_n}^{-1}D_{\Phi_n\psi} & I \end{bmatrix}.$$

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- MSP & Block Newton Method
- Altenate-Block-Factorization (ABF) 算法公式推导
- Altenate-Block-Factorization (ABF) 算法在 Semiconductor Equation 的应用

算法核心公式：$(AD^{-1})(Dx) = b.$

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & A_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mm} \end{bmatrix}, A_{ij} \in \mathbb{R}^{\nu\times\nu}$$

$$\tilde{A} = PAP^T = \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} & \cdots & \tilde{A}_{1\nu} \\ \tilde{A}_{21} & \tilde{A}_{22} & \cdots & \tilde{A}_{2\nu} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{A}_{\nu 1} & \tilde{A}_{\nu 2} & \cdots & \tilde{A}_{\nu\nu} \end{bmatrix}, \tilde{A}_{ij} = \begin{bmatrix} (A_{11})_{ij} & (A_{12})_{ij} & \cdots & (A_{1m})_{ij} \\ (A_{21})_{ij} & (A_{22})_{ij} & \cdots & (A_{2m})_{ij} \\ \vdots & \vdots & \ddots & \vdots \\ (A_{m1})_{ij} & (A_{m2})_{ij} & \cdots & (A_{mm})_{ij} \end{bmatrix} \in \mathbb{R}^{m\times m}$$

类似上述构造 post-conditioned matrix $D\,(\tilde{D} = PDP^T)$：

$$\tilde{D}_{ij} = \begin{bmatrix} (D_{11})_{ij} & (D_{12})_{ij} & \cdots & (D_{1m})_{ij} \\ (D_{21})_{ij} & (D_{22})_{ij} & \cdots & (D_{2m})_{ij} \\ \vdots & \vdots & \ddots & \vdots \\ (D_{m1})_{ij} & (D_{m2})_{ij} & \cdots & (D_{mm})_{ij} \end{bmatrix} \overset{D_{ij}=\mathrm{diag}(A_{ij})}{\Longrightarrow}$$

$$\begin{bmatrix} (\mathrm{diag}A_{11})_{ij} & (\mathrm{diag}A_{12})_{ij} & \cdots & (\mathrm{diag}A_{1m})_{ij} \\ (\mathrm{diag}A_{21})_{ij} & (\mathrm{diag}A_{22})_{ij} & \cdots & (\mathrm{diag}A_{2m})_{ij} \\ \vdots & \vdots & \ddots & \vdots \\ (\mathrm{diag}A_{m1})_{ij} & (\mathrm{diag}A_{m2})_{ij} & \cdots & (\mathrm{diag}A_{mm})_{ij} \end{bmatrix}.$$

由此构造出 $(AD^{-1})Dx = b.$

考虑一个由两个 PDE 的系统产生的 2×2 的块系统：

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}, A_{ij} \in \mathbb{R}^{\nu \times \nu}$$

$$\begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix} = \begin{bmatrix} \operatorname{diag}(A_{11}) & \operatorname{diag}(A_{12}) \\ \operatorname{diag}(A_{21}) & \operatorname{diag}(A_{22}) \end{bmatrix} \in \mathbb{R}^{2\nu \times 2\nu}$$

假设 D^{-1} 存在，则构建的 post-conditioned 矩阵为

$$AD^{-1} = A\left(P^T \tilde{D}^{-1} P\right) = \begin{bmatrix} A_{11}D_{22} - A_{12}D_{21} & A_{12}D_{11} - A_{11}D_{12} \\ A_{21}D_{22} - A_{22}D_{21} & A_{22}D_{11} - A_{21}D_{12} \end{bmatrix} \begin{bmatrix} \delta & 0 \\ 0 & \delta \end{bmatrix}.$$

其中 $\delta = (D_{11}D_{22} - D_{21}D_{12})^{-1}$.

考虑问题模型：

$$
Ax = -F \equiv \begin{bmatrix} A_{\psi\psi} & D_{\psi\Phi_n} \\ A_{\Phi_n\psi} & A_{\Phi_n\Phi_n} \end{bmatrix} \begin{pmatrix} \delta\psi \\ \delta\Phi_n \end{pmatrix} = -\begin{pmatrix} F_\psi \\ F_{\Phi_n} \end{pmatrix}.
$$

则 post-condition 矩阵构造如下：

$$
AD^{-1} = A\left(P^T\tilde{D}^{-1}P\right) = \begin{bmatrix} A_{11}D_{22} - A_{12}D_{21} & A_{12}D_{11} - A_{11}D_{12} \\ A_{21}D_{22} - A_{22}D_{21} & A_{22}D_{11} - A_{21}D_{12} \end{bmatrix} \begin{bmatrix} \delta & 0 \\ 0 & \delta \end{bmatrix} \to
$$

$$
AD^{-1} = \begin{bmatrix} \left(A_{\psi\psi}\mathrm{diag}\left(A_{\Phi_n\Phi_n}\right) - \mathrm{diag}\left(A_{\Phi_n\psi}\right)\right)\delta & \left(\mathrm{diag}\left(A_{\psi\psi}\right) - A_{\psi\psi}\right)\delta \\ \left(A_{\Phi_n\psi}\mathrm{diag}\left(A_{\Phi_n\Phi_n}\right) - A_{\Phi_n\Phi_n}\mathrm{diag}\left(A_{\Phi_n\psi}\right)\right)\delta & \left(A_{\Phi_n\Phi_n}\mathrm{diag}A_{\psi\psi} - A_{\Phi_n\psi}\right)\delta \end{bmatrix}.
$$

其中 $\delta = \left(\mathrm{diag}\left(A_{\psi\psi}\right)\mathrm{diag}\left(A_{\Phi_n\Phi_n}\right) - \mathrm{diag}\left(A_{\Phi_n\psi}\right)\right)^{-1}$.

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