

Mixed finite element solution of a semi-conductor problem by Dissection sparse direct solver

Atsushi Suzuki¹

¹Cybermedia Center, Osaka University
`atsushi.suzuki@cas.cmc.osaka-u.ac.jp`

December 15, 2017

Mixed finite element formulation

Find $(u, p) \in V \times Q$

$$a(u, v) + b(v, p) = (f, v) \quad \forall v \in V,$$

$$b(u, q) = (g, q) \quad \forall q \in Q.$$

Stokes equations

$$-\nabla \cdot 2D(u) + \nabla p = f, \quad [D(u)]_{ij} = (\partial_j u_i + \partial_i u_j), \quad 1 \leq i, j < d$$

$$\nabla \cdot u = 0,$$

$$u = 0 \quad \text{on } \Gamma_D.$$

$$V := \{v \in H^1(\Omega)^d; v = 0 \text{ on } \Gamma_D\}, \quad Q := L^2(\Omega).$$

$$a(u, v) = 2 \int_{\Omega} D(u) : D(v), \quad b(v, q) = - \int_{\Omega} \nabla \cdot v q.$$

Poisson equation

$$u = -\nabla p,$$

$$\nabla \cdot u = g,$$

$$u = 0 \quad \text{on } \partial\Omega.$$

$$V := H(\text{div}; \Omega), \quad Q := L^2(\Omega).$$

$$a(u, v) = 2 \int_{\Omega} u \cdot v, \quad b(v, q) = - \int_{\Omega} \nabla \cdot v q.$$

matrix form of mixed finite element method : 1/2

$$\vec{u} \in \mathbb{R}^{N_u}, \vec{p} \in \mathbb{R}^{N_p}$$

$$K \begin{bmatrix} \vec{u} \\ \vec{p} \end{bmatrix} = \begin{bmatrix} A & B^T \\ B & -\epsilon I \end{bmatrix} \begin{bmatrix} \vec{u} \\ \vec{p} \end{bmatrix} = \begin{bmatrix} \vec{f} \\ \vec{g} \end{bmatrix}$$

- ▶ A : coercive $(A\vec{x}, \vec{x}) > 0 \forall \vec{x} \neq \vec{0}$
- ▶ B^T : satisfies discrete inf-sup condition, i.e. $\ker B^T = \{\vec{0}\}$
- ▶ $\epsilon > 0$

Schur complement matrix $S = \epsilon I + BA^{-1}B^T$

$$(S\vec{p}, \vec{p}) = \epsilon(\vec{p}, \vec{p}) + (BA^{-1}B^T\vec{p}, \vec{p}) \geq \epsilon(\vec{p}, \vec{p}) > 0$$

- ▶ LDL^T -factorization is possible for any ordering
- ▶ we need to set **appropriate regularization** $\epsilon > 0$

$\sqrt{\varepsilon}$ -perturbation

a regularization technique

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & \begin{matrix} 0 & \alpha \\ \beta & 0 \end{matrix} \end{bmatrix} \rightarrow \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & \begin{matrix} \sqrt{\varepsilon} & \alpha \\ \beta & 0 \end{matrix} \end{bmatrix}$$

- ▶ iterative refinement to improve accuracy of a solution
- ▶ user **can/have to** specify perturbation parameter for unsymmetric matrix (default = 10^{-13} for Pardiso)

matrix form of mixed finite element method : 2/2

$$\vec{u} \in \mathbb{R}^{N_u}, \vec{p} \in \mathbb{R}^{N_p}$$

$$K \begin{bmatrix} \vec{u} \\ \vec{p} \end{bmatrix} = \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \vec{u} \\ \vec{p} \end{bmatrix} = \begin{bmatrix} \vec{f} \\ \vec{g} \end{bmatrix}$$

- ▶ A : coercive $(A\vec{x}, \vec{x}) > 0 \forall \vec{x} \neq 0$
- ▶ B^T : satisfies discrete inf-sup condition, i.e. $\ker B^T = \{\vec{0}\}$

Schur complement matrix $S = BA^{-1}B^T$

$$(S\vec{p}, \vec{p}) = (BA^{-1}B^T\vec{p}, \vec{p}) = (A^{-1}B^T\vec{p}, B^T\vec{p})$$

$$\ker B^T = \{\vec{0}\} \bigwedge \vec{p} \neq \vec{0} \Rightarrow (A^{-1}B^T\vec{p}, B^T\vec{p}) > 0.$$

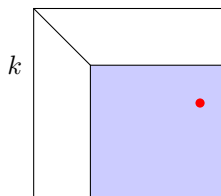
- ▶ LDL^T -factorization of K with “block” ordering as $[\vec{u}, \vec{p}]$
- ▶ not clear with node-wise $[u_1, u_2, p]$ ordering

\Rightarrow postponing factorization + 2×2 pivoting

pivoting strategy

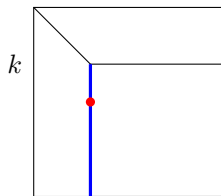
full pivoting : $A = \Pi_L^T L U \Pi_R$

find $\max_{k < i, j \leq n} |A(i, j)|$



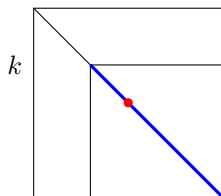
partial pivoting : $A = \Pi L U$

find $\max_{k < i \leq n} |A(i, k)|$



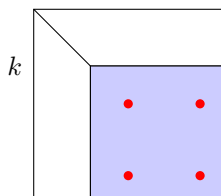
symmetric pivoting : $A = \Pi^T L D U \Pi$

find $\max_{k < i \leq n} |A(k, k)|$



2×2 pivoting : $A = \Pi^T L \tilde{D} U \Pi$

find $\max_{k < i, j \leq n} \det \begin{vmatrix} A(i, i) & A(i, j) \\ A(j, i) & A(j, j) \end{vmatrix}$



sym. pivoting is mathematically not always possible

understanding pivoting strategy by solution in subspaces

$A = \Pi^T L D U \Pi$: symmetric pivoting

D : diagonal, L : lower triangle, $L(i, i) = 1$, U : upper tri., $U(i, i) = 1$.


- ▶ index set $\{i_1, i_2, \dots, i_m\}$
- ▶ $V_m = \text{span}[\vec{e}_{i_1}, \vec{e}_{i_2}, \dots, \vec{e}_{i_m}] \subset \mathbb{R}^N$
- ▶ $P_m : \mathbb{R}^N \rightarrow V_m$ orthogonal projection.

find $\vec{u} \in V_m$ ($A\vec{u} - \vec{f}, \vec{v}) = 0 \quad \forall \vec{v} \in V_m$.

$\exists \Pi : A = \Pi^T L D U \Pi$

$\Rightarrow \exists \{i_1, i_2, \dots, i_N\}$ s.t. $P_m A P_m^T$: invertible on $V_m \quad 1 \leq \forall m \leq N$.

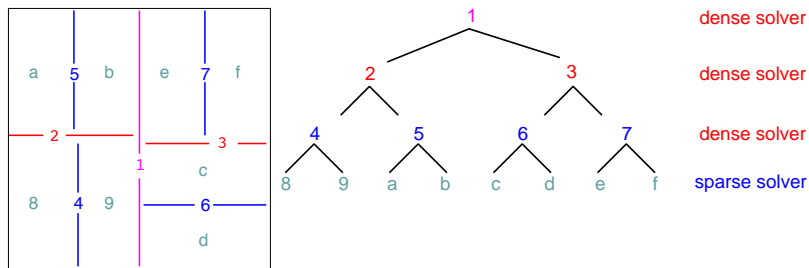
2×2 pivoting: $V_{m-1}, V_m, V_{m+1}, V_{m+2}, V_{m+3}$, by skipping V_{m+1} .



J. R. Bunch, L. Kaufman. Some stable methods for calculating inertia and solving symmetric linear systems, *Math. Comput*, 31 (1977) 163–179.

R. Bank, T.-F. Chan. An analysis of the composite step biconjugate gradient method. *Numer. Math*, 66 (1993) 295–320.

nested dissection by graph decomposition



A. George. Numerical experiments using dissection methods to solve n by n grid problems. *SIAM J. Num. Anal.* 14 (1977), 161–179.

software package:

METIS : **V. Kumar, G. Karypis**, A fast and high quality multilevel scheme for partitioning irregular graphs. *SIAM J. Sci. Comput.* 20 (1998) 359–392.

SCOTCH : **F. Pellegrini J. Roman J, P. Amestoy**, Hybridizing nested dissection and halo approximate minimum degree for efficient sparse matrix ordering. *Concurrency: Pract. Exper.* 12 (2000) 69–84.

recursive generation of Schur complement

$$\begin{bmatrix} A_{11} & A_{21} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & 0 \\ A_{21} & S_{22} \end{bmatrix} \begin{bmatrix} I_1 & A_{11}^{-1}A_{12} \\ 0 & I_2 \end{bmatrix}$$

$S_{22} = A_{22} - A_{21}A_{11}^{-1}A_{12} = A_{22} - (A_{21}U_{11}^{-1})D_{11}^{-1}L_{11}^{-1}A_{12}$: recursively computed

88 99 aa bb cc dd ee ff	84 94 a5 b5 c6 d6 e7 f7	82 92 91 a2 b1 b2 b1 c1 d3 d1 e3 e1 f3
48 49 5a 5b 6c 6d 7e 7f	44 55 66 77	42 52 61 73
28 29 2a 2b 3d 3e 3f 19 1b 1c 1d 1e	24 25 37 16	22 21 33 31 12 13 11

Schur complement
by sparse solver

44 55 66 77	42 41 52 51 63 61 73 71
24 25 36 37 14 15 16 17	22 21 33 31 12 13 11

Schur complement
by dense solver

Schur complement
by dense solver

11

dense factorization

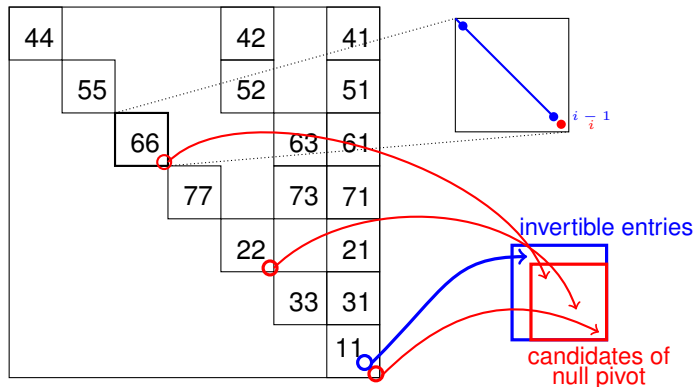
22 33	21 31
12 13 11	

sparse part : completely in parallel
dense part : better use of **BLAS 3**; dgemm, dtrsm

symmetric pivoting with postponing for block strategy

- ▶ nested-dissection decomposition may produce singular sub-matrix for indefinite matrix

τ : given threshold for postponing, 10^{-2} for MUMPS, Dissection
 $|A(i, i)|/|A(i-1, i-1)| < \tau \Rightarrow \{A(k, j)\}_{i \leq k, j}$ are postponed



Schur complement matrix from postponed pivots is computed
kernel detection algorithm : QR -factorization by MUMPS

Parallel performance of Dissection solver : 1/2

matrices are given from TOSHIBA memory by a joint project:
n=569, 139, nnz=8, 338, 291, cond= $1.90090141 \cdot 10^5$

sovler	relative error	error
dissection	$7.5867639 \cdot 10^{-6}$	$4.5545655 \cdot 10^{-13}$
pardiso	$6.4318791 \cdot 10^{-2}$	$1.8114969 \cdot 10^{-7}$

# cores	i7-6770HQ@2.60GHz		E5-2695v4@2.10GHz	
	elapsed	CPU	elapsed	CPU
1	17.019	17.018	27.028	27.030
2	9.217	18.300	13.564	26.980
3	6.281	18.490	9.251	27.390
4	5.224	20.461	7.085	27.780
8			3.744	28.530
12			2.686	29.340
16			2.185	30.620

Parallel performance of Dissection solver : 2/2

$n=1,867,029$ $nnz=29,311,205$, $cond=8.93145673 \cdot 10^5$

sovler	relative error	error
dissection	$1.2970417 \cdot 10^{-5}$	$3.3747264 \cdot 10^{-12}$
pardiso	$7.0464281 \cdot 10^{-1}$	$1.6031101 \cdot 10^{-5}$

E5-2695v4@2.10GHz x2

# cores	double precision		quadruple precision	
	elapsed	CPU	elapsed	CPU
1	197.58	197.89	23,988.0	23,988.0
2	102.73	200.02	12,225.0	24,007.0
4	55.22	204.66	6,195.5	24,022.0
8	30.17	208.47	3,154.5	24,016.0
16	18.08	222.63	1,567.3	24,036.0
24	14.95	250.26	1,088.9	24,059.0
32	13.47	289.29	824.5	24,083.0
36	13.38	311.15	754.1	24,124.0

quadruple arithmetic \Leftarrow double-double `qd` library 2.3.17
+ Dissection C++ template

Drift-Diffusion system at stationary state : 1/2

- ▶ φ : electrostatic potential
- ▶ n : electron concentration
- ▶ p : hole concentration

$$\operatorname{div}(\varepsilon E) = q(p - n + C(x))$$

$$E = -\nabla\varphi$$

$$-\operatorname{div}J_n = 0$$

$$J_n = -q(\mu_n n \nabla\varphi - \mu_n D_n \nabla n)$$

$$\operatorname{div}J_p = 0$$

$$J_p = -q(\mu_p p \nabla\varphi + \mu_p D_p \nabla p)$$

following Maxwell-Boltzmann statistics : $p = n_i \exp\left(\frac{\varphi_p - \varphi}{V_{th}}\right)$

- ▶ q : positive electron charge
- ▶ ε : dielectric constant of the materials
- ▶ φ_p : quasi-Fermi level
- ▶ n_i : intrinsic concentration of the semiconductor
- ▶ $V_{th} = K_B T / q$: thermal voltage
- ▶ K_B : Boltzmann constant
- ▶ T : lattice temperature

Drift-Diffusion system at stationary state : 2/2

dimensionless system (by **unit scaling**)

$$-\operatorname{div}(\lambda^2 \nabla \varphi) = p - n + C(x)$$

$$-\operatorname{div} J_n = 0$$

$$\operatorname{div} J_p = 0$$

$$J_n = \nabla n - n \nabla \varphi$$

$$J_p = -(\nabla p + p \nabla \varphi)$$

with boundary conditions

$$\varphi = f \text{ on } \Gamma_D \quad \frac{\partial \varphi}{\partial \nu} = 0 \text{ on } \Gamma_N$$

$$n = g \text{ on } \Gamma_D \quad J_n \cdot \nu = 0 \text{ on } \Gamma_N \leftarrow \frac{\partial n}{\partial \nu} = 0$$

$$p = h \text{ on } \Gamma_D \quad J_p \cdot \nu = 0 \text{ on } \Gamma_N \leftarrow \frac{\partial p}{\partial \nu} = 0$$

Slotboom variables, η, ξ : $n = \eta e^\varphi, \quad p = \xi e^{-\varphi}$

$$\nabla n = \nabla \eta e^\varphi + \eta e^\varphi \nabla \varphi = \nabla \eta e^\varphi + n \nabla \varphi$$

$$J_n = \nabla n - n \nabla \varphi = e^\varphi \nabla \eta$$

$$e^{-\varphi} J_n = \nabla \eta \quad e^\varphi J_p = -\nabla \xi$$

Finite volume discretization with Scharfetter-Gummel method

approximation of $e^\varphi J_p = -\nabla \xi$ in an interval $[x_i, x_{i+1}]$, $h = x_{i+1} - x_i$

$$\int_{x_i}^{x_{i+1}} e^\varphi dx J_{p\ i+1/2} = -h \nabla \xi_{i+1/2} \simeq -(\xi_{i+1} - \xi_i)$$

- ▶ φ : assumed to be linear in the interval $[x_i, x_{i+1}]$.

$$\int_{x_i}^{x_{i+1}} e^\varphi dx = \frac{1}{\frac{d\varphi}{dx}} \left[e^{\varphi(x)} \right]_{x_i}^{x_{i+1}} = \frac{h}{\varphi_{i+1} - \varphi_i} (e^{\varphi_{i+1}} - e^{\varphi_i})$$

$$\begin{aligned} J_{p\ i+1/2} &\simeq -(\xi_{i+1} - \xi_i) \frac{\varphi_{i+1} - \varphi_i}{h} \frac{1}{e^{\varphi_{i+1}} - e^{\varphi_i}} \\ &= -\frac{\varphi_{i+1} - \varphi_i}{h} \left(\frac{e^{-\varphi_{i+1}} \xi_{i+1}}{1 - e^{\varphi_i - \varphi_{i+1}}} - \frac{e^{-\varphi_i} \xi_i}{e^{\varphi_{i+1} - \varphi_i} - 1} \right) \\ &= -\frac{\varphi_{i+1} - \varphi_i}{h} \left(\frac{p_{i+1}}{1 - e^{\varphi_i - \varphi_{i+1}}} - \frac{p_i}{e^{\varphi_{i+1} - \varphi_i} - 1} \right) \\ &= -\frac{1}{h} (B(\varphi_i - \varphi_{i+1}) p_{i+1} - B(\varphi_{i+1} - \varphi_i) p_i) \end{aligned}$$

- ▶ $B(x) = x/(e^x - 1)$: Bernoulli function

mixed variational formulation : 1 / 2

Slotboom variable $\xi : p = \xi e^{-\varphi}$

$$\begin{aligned}\operatorname{div}(J_p) &= 0 && \text{in } \Omega, \\ e^\varphi J_p &= -\nabla \xi && \text{in } \Omega.\end{aligned}$$

function space :

$$\begin{aligned}H(\operatorname{div}) &= \{v \in L^2(\Omega)^2; \operatorname{div} v \in L^2(\Omega)\}, \\ \Sigma &= \{v \in H(\operatorname{div}); v \cdot \nu = 0 \text{ on } \Gamma_N\}\end{aligned}$$

integration by parts leads to

$$\begin{aligned}\int_{\Omega} e^\varphi J_p \cdot v &= - \int_{\Omega} \nabla \xi \cdot v = \int_{\Omega} \xi \nabla \cdot v - \int_{\partial\Omega} \xi v \cdot \nu \\ \int_{\Omega} e^\varphi J_p \cdot v - \int_{\Omega} \xi \nabla \cdot v &= - \int_{\Gamma_D} h e^\varphi v \cdot \nu - \int_{\Gamma_N} \xi v \cdot \nu \quad \forall v \in \Sigma \\ \int_{\Omega} \nabla \cdot J_p q &= 0 \quad \forall q \in L^2(\Omega)\end{aligned}$$

mixed variational formulation : 2 / 2

mixed-type weak formulation

$$\begin{aligned} \text{find } (J_p, \xi) &\in \Sigma \times L^2(\Omega) \\ \int_{\Omega} e^{\varphi} J_p \cdot v - \int_{\Omega} \xi \nabla \cdot v &= - \int_{\Gamma_D} h e^{\varphi} v \cdot \nu & \forall v \in \Sigma \\ - \int_{\Omega} \nabla \cdot J_p q &= 0 & \forall q \in L^2(\Omega) \end{aligned}$$

symmetric indefinite

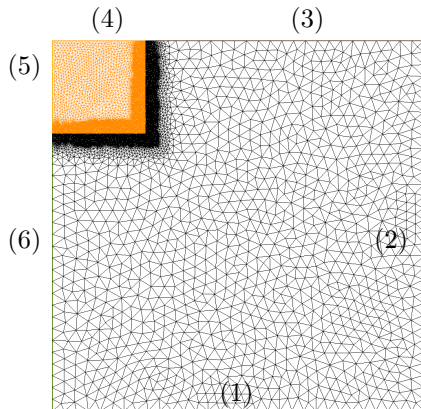
replacing $\xi = e^{\varphi} p$ again,

$$\begin{aligned} \text{find } (J_p, p) &\in \Sigma \times L^2(\Omega) \\ \int_{\Omega} e^{\varphi} J_p \cdot v - \int_{\Omega} e^{\varphi} p \nabla \cdot v &= - \int_{\Gamma_D} h e^{\varphi} v \cdot \nu & \forall v \in \Sigma \\ - \int_{\Omega} \nabla \cdot J_p q &= 0 & \forall q \in L^2(\Omega) \end{aligned}$$

unsymmetric indefinite

hybridization of mixed formulation + mass lumping \Rightarrow FVM

boundary conditions for a diode device (thanks to Dr. Sho)



N region : $x < 1/4 \wedge y > 3/4$,

$$C(x, y) = n_d = 10^{17}$$

P region : others

$$C(x, y) = -n_a = -10^{20}$$

$$np = n_i^2, \quad n_i = 1.08 \times 10^{10}$$

charge neutrality

$$p - n + C(x, y) = 0 \text{ on } (1), (4).$$

N region :

$$n = \sqrt{n_i^2 + C^2/4} + C/2 \simeq n_d$$

P region :

$$p = \sqrt{n_i^2 + C^2/4} - C/2 \simeq n_a$$

$$(1) \quad \varphi = -\log\left(\frac{n_a}{n_i}\right) + \frac{1}{V_{th}} \varphi_{\text{appl}} \quad n = \frac{n_i}{n_a} \quad p = \frac{n_a}{n_i}$$

$$(2), (3), (5), (6) \quad \partial_\nu \varphi = 0 \quad \partial_\nu n = 0 \quad \partial_\nu p = 0$$

$$(4) \quad \varphi = \log\left(\frac{n_d}{n_i}\right) \quad n = \frac{n_d}{n_i} \quad p = \frac{n_i}{n_d}$$

nonlinear iteration to obtain the stationary state

a variant of Gummel map

φ^m, n^m, p^m : given $\rightarrow \varphi^{m+1}, n^{m+1}, p^{m+1}$ by a fixed point method

Slotboom variable ξ^m, η^m

$$p^m = \xi^m e^{-\varphi^m} \quad n^m = \eta^m e^{\varphi^m}$$

to find a solution of the nonlinear eq. : $-\text{div}(\lambda^2 \nabla \varphi) = p - n + C(x)$

$$F(\eta^m, \xi^m; \varphi, \psi) = \lambda^2 \int_{\Omega} \nabla \varphi \cdot \nabla \psi - \int_{\Omega} (\xi^m e^{-\varphi} - \eta^m e^{\varphi} + C) \psi = 0$$

differential calculus with $\delta\varphi \in \{H^1(\Omega); \psi = 0 \text{ on } \Gamma_D\}$ leads to

$$\begin{aligned} & F(\eta^m, \xi^m; \varphi^m + \delta\varphi, \psi) - F(\eta^m, \xi^m; \varphi^m, \psi) \\ &= \lambda^2 \int_{\Omega} \nabla \delta\varphi \cdot \nabla \psi - \int_{\Omega} \xi^m \left(e^{-\varphi^m - \delta\varphi} - e^{-\varphi^m} \right) \psi - \eta^m \left(e^{\varphi^m + \delta\varphi} - e^{\varphi^m} \right) \psi \\ &= \lambda^2 \int_{\Omega} \nabla \delta\varphi \cdot \nabla \psi + \int_{\Omega} \left(\xi^m e^{-\varphi^m} + \eta^m e^{\varphi^m} \right) \delta\varphi \psi \\ &= \lambda^2 \int_{\Omega} \nabla \delta\varphi \cdot \nabla \psi + \int_{\Omega} (p^m + n^m) \delta\varphi \psi \quad \varphi^{m+1} = \varphi^m + \delta\varphi \end{aligned}$$

FreeFem++ script

Finite element approximation

- ▶ $J_p \in H(\text{div})$: Raviar-Thomas : $RT1(K) = (P1(K))^2 + \vec{x}P1(K)$,
- ▶ $p \in L^2(\Omega)$: piecewise linear : $P1(K)$,
- ▶ $\varphi \in H^1(\Omega)$: piecewise linear : $P1(K)$.

```
load "Element_Mixte"  
load "Dissection"  
defaulttoDissection();  
fespace Vh(Th, RT1);      fespace Ph(Th, P1);  
fespace Xh(Th, P1);  
Vh [up1, up2], [v1, v2]; Ph pp, q;  
Xh phi; // obtained in Gummel map  
problem DDp([up1, up2, pp],[v1, v2, q],  
            solver=sparsesolver, strategy=3,  
            tolpivot=1.0e-2, tgv=1.0e+30) =  
  int2d(Th, qft=qf9pT) (exp(phi) * (up1 * v1 + up2 * v2)  
                        - exp(phi) * pp * (dx(v1) + dy(v2))  
                        + q * (dx(up1) + dy(up2)))  
+int1d(Th, 1) (gp1 * exp(phi) * (v1 * N.x + v2 * N.y))  
+int1d(Th, 4) (gp4 * exp(phi) * (v1 * N.x + v2 * N.y))  
+ on(2, 3, 5, 6, up1 = 0, up2 = 0);
```

matrix representation and preconditioning

linear system for hole concentration by RT1/P1

$$\begin{bmatrix} A(\vec{\varphi}) & B_1(\vec{\varphi})^T \\ -B_2 & 0 \end{bmatrix} \begin{bmatrix} \vec{u} \\ \vec{p} \end{bmatrix} = \begin{bmatrix} \vec{f}(\vec{\varphi}) \\ \vec{0} \end{bmatrix}$$

matrices and vectors weighted with exponential of electrostatic potential

$$\vec{v}^T A(\vec{\varphi}) \vec{u} = \int_{\Omega} e^{\varphi} u \cdot v$$

$$\vec{v}^T B_1(\vec{\varphi}) \vec{p} = - \int_{\Omega} e^{\varphi} p \nabla \cdot v$$

$$\vec{v}^T \vec{f}(\vec{\varphi}) = - \int_{\Gamma_D} h e^{\varphi} v \cdot \nu$$

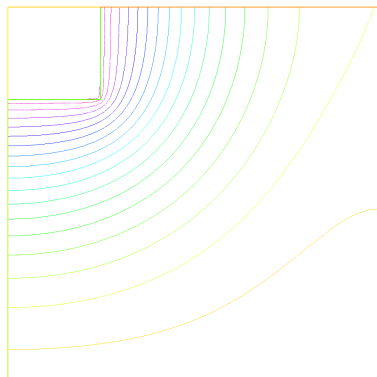
$$\vec{q}^T B_2 \vec{u} = - \int_{\Omega} q \nabla \cdot u$$

preconditioned system by scaling matrix $[W]_{ii} = 1/[A(\vec{\varphi})]_{ii}$

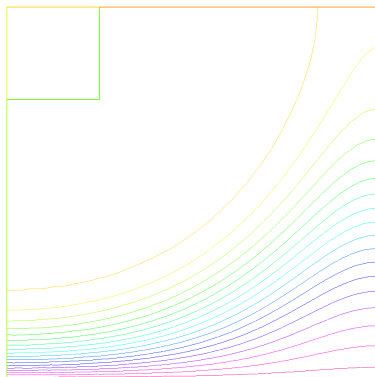
$$\begin{bmatrix} W A(\vec{\varphi}) & W B_1(\vec{\varphi})^T \\ -B_2 & 0 \end{bmatrix} \begin{bmatrix} \vec{u} \\ \vec{p} \end{bmatrix} = \begin{bmatrix} W \vec{f}(\vec{\varphi}) \\ \vec{0} \end{bmatrix}$$

numerical result of a semi-conductor problem

- ▶ compute thermal equilibrium with $p = n_i \exp(-\varphi) V_{th}$ and $n = n_i \exp(\varphi) V_{th}$
- ▶ Newton iteration for the potential equation and fixed point iteration for the whole system : a kind of Gummel map



electrostatic potential

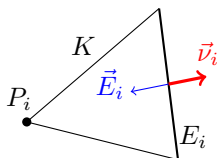


hole concentration

Raviart-Thomas finite element

$$RT0(K) = (P0(K))^2 + \vec{x}P0(K) \subset (P1(K))^2.$$

- ▶ K : triangle element
- ▶ $\{E_i\}$: edges of K
- ▶ $\vec{\nu}_i$: outer normal of K on E_i
- ▶ \vec{E}_i : normal to edge E_i



$$\vec{v} \in RT0(K) \Rightarrow \vec{v}|_{E_i} \cdot \vec{n}_i \in P0(E_i), \quad \text{div} \vec{v} \in P0(K)$$

finite element basis

$$\vec{\Psi}_i(\vec{x}) = \sigma_i \frac{|E_i|}{|K|} (\vec{x} - \vec{P}_i) \quad \sigma_i = \vec{E}_i \cdot \vec{\nu}_i, \quad P_i : \text{node of } K$$

finite element vector value is continuous on the middle point on E_i .
inner finite element approximation of $H(\text{div}; \Omega)$

$$\int_K e^\varphi \vec{\Psi}_i \cdot \vec{\Psi}_j \leftarrow \int_K e^{\varphi_1 \lambda_1 + \varphi_2 \lambda_2 + \varphi_3 \lambda_3} \lambda_k \lambda_l \quad \text{by exact quadrature}$$
$$\int_K e^\varphi \vec{\Psi}_i \cdot \vec{\Psi}_j \simeq \frac{1}{|K|} \int_K e^{\sum_k \varphi_k \lambda_k} \int_K \vec{\Psi}_i \cdot \vec{\Psi}_j \quad : \text{exponential fitting}$$

$\{\lambda_1, \lambda_2, \lambda_3\}$: barycentric coordinates of K

summary

- ▶ Dissection direct solver can factorize indefinite unsymmetric matrix with symmetric pivoting
- ▶ mixed finite element formulation for Dirft-Diffusion equations with standard numerical integration instead of Schafetter-Gummel scheme / exponential fitting
- ▶ possible extension with higher order elements with $RT1(K)/P1(K)/P2(K)$

References

- ▶ F. Brezzi, L. D. Marini, S. Micheletti, P. Pietra, R. Sacco, S. Wang. Discretization of semiconductor device problems (I) F. Brezzi et al., Handbook of Numerical Analysis vol XIII, Elsevier 2005
- ▶ personal communication with Dr. Sho Shohiro @ Osaka Univ.