Grain Boundary Diffusion due to Stress and Electromigration

Jon Wilkening

Courant Institute of Mathematical Sciences
wilken@cims.nyu.edu

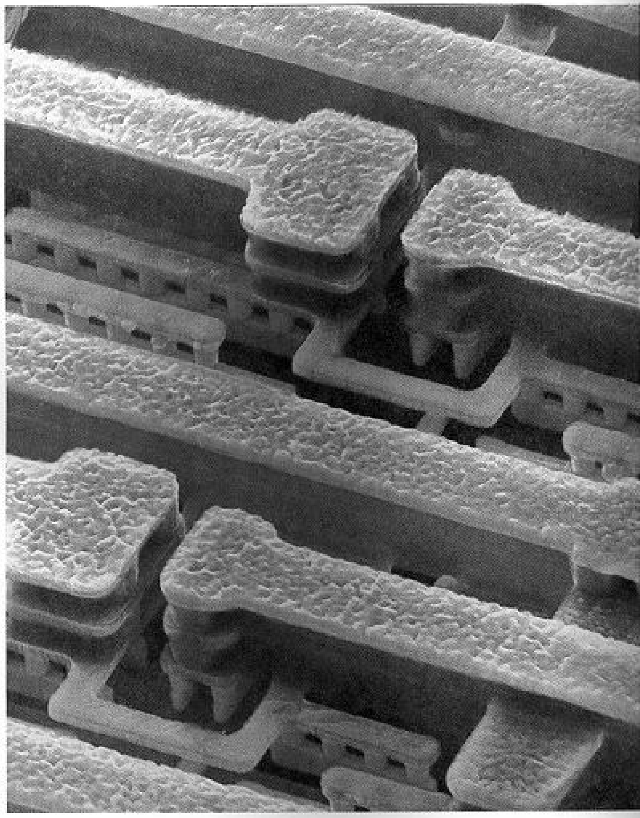
November 15, 2003

Acknowledgements

Prof. James Sethian,
UCB, LBNL

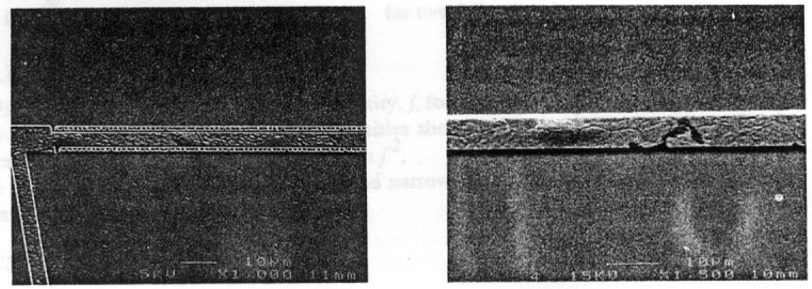
Dr. Len Borucki,
Motorola

Department of Energy
CSGF Fellowship



Multi-level copper metallization of a complementary metal oxide semiconductor (CMOS) chip. This scanning electron micrograph (scale: 1 cm = 3.5 microns) of a CMOS integrated circuit shows six levels of copper metallization that are used to carry electrical signals on the chip. The inter-metal dielectric insulators have been chemically etched away here to reveal the copper interconnects. (Photograph courtesy of IBM.)

Solid State Electronic Devices
Streetman/Banerjee



(a) (b)

Figure 4. EM damage in Type A lines. An extrusion forms first (a), and a fatal erosion void develops afterwards upstream of the extrusion (b).

Characterization of two Electromigration Failure Modes in Submicron VLSI, by Atakov, Clement, Miner

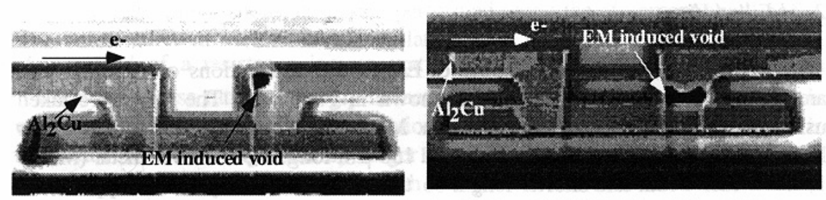


FIGURE 15(a) **FIGURE 15(b)**
Cross-sectional SEM micrographs of Al depletion at the Al filled via. (a) Al depletion starting at the line edge. (b) Al depletion starts at the interface between CVD Al and the glue layer at the bottom of the via.

Comparison of Via Electromigration for Cu, CVD-Al, and CVD-W
Kawasaki, et. al.

Electromigration causes failure in circuits at high current density.

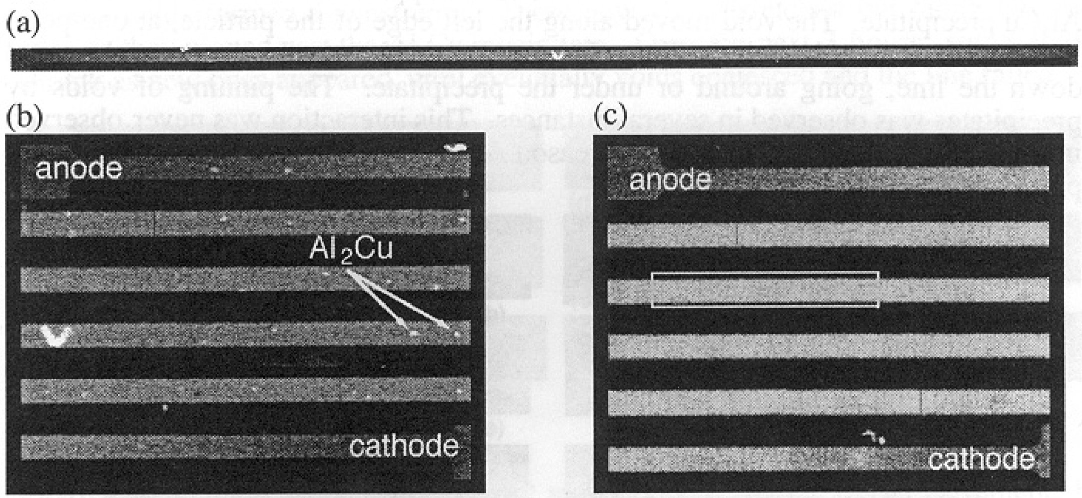


FIGURE 2. (a) A 300µm Al-0.5%Cu line. The line is at 240°C but without test current. (b) The same Al-Cu line displayed at a higher magnification. The image is divided into six segments and stacked from top to bottom. (c) A 300µm Al-0.1%Sc line shown as six segments. The boxed segment designates a region where void nucleation, motion, and line failure were observed.

Comparison of Electromigration Behavior in Passivated Aluminum Interconnects
Lee, Doan, Bravman, Flinn, Marieb, Ogawa

0.6μm $\times$ 3μm $\times$ 300μm
240°C, 20mA$/\mu$m^2
TEM allows for testing with passivation in tact.

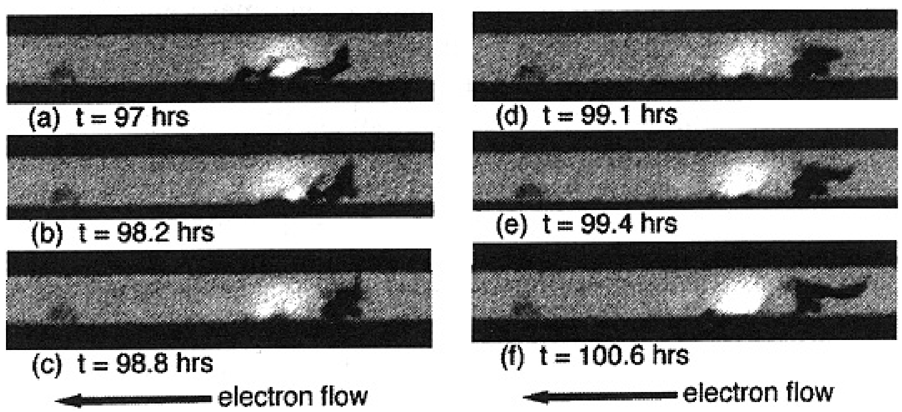


FIGURE 5. An Al-0.5%Cu line segment showing a void which appears to breach the line.

Surface diffusion can lead to a significant change in geometry.

Stress generation by electromigration

I. A. Blech and Conyers Herring

Bell Laboratories, Murray Hill, New Jersey 07974
(Received 16 April 1976)

Stresses in aluminum thin films on TiN were studied *in situ* by transmission x-ray topography. Stress gradients were seen to build up in thin aluminum films during passage of electrical currents. The stresses are more compressive in the anode regions. These stress gradients seem to be a concomitant of the backflow responsible for the reported threshold in electromigration, and can probably be correlated quantitatively with it.

PACS numbers: 68.60.+q, 66.30.Fq, 82.45.+z

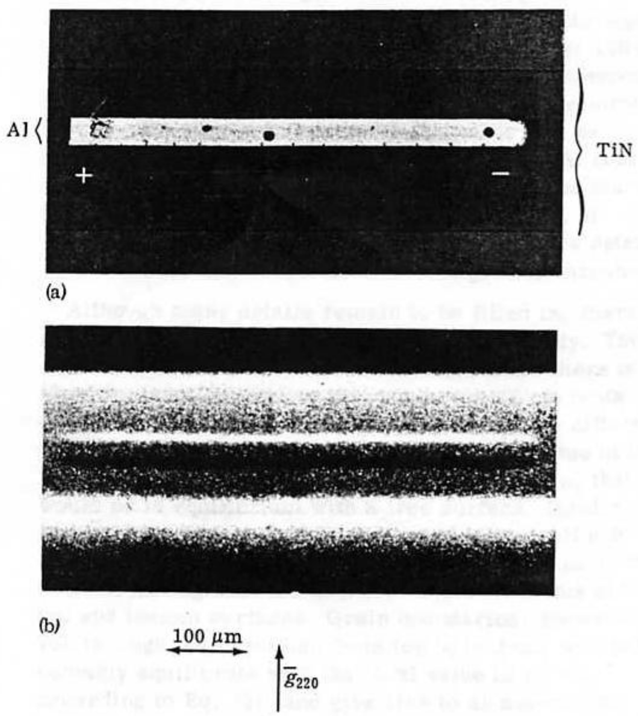


FIG. 1. (a) Photomicrograph of Al test stripe on TiN. (b) X-ray transmission topograph Cu K_α, of the stripe in (a) at 25 °C, showing the Al in tension.

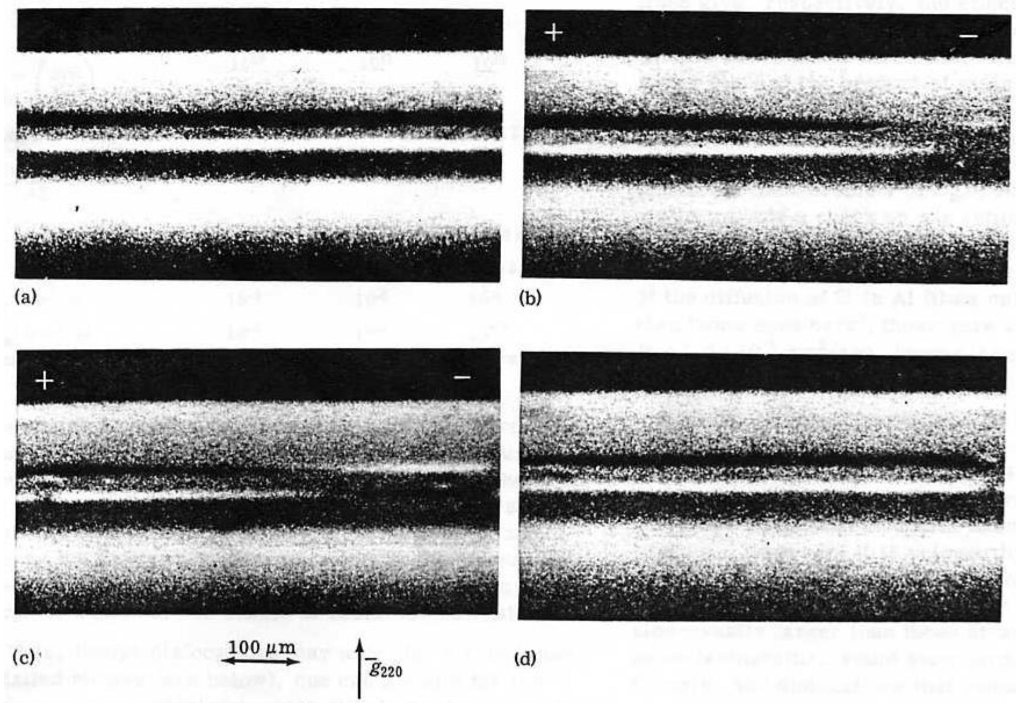
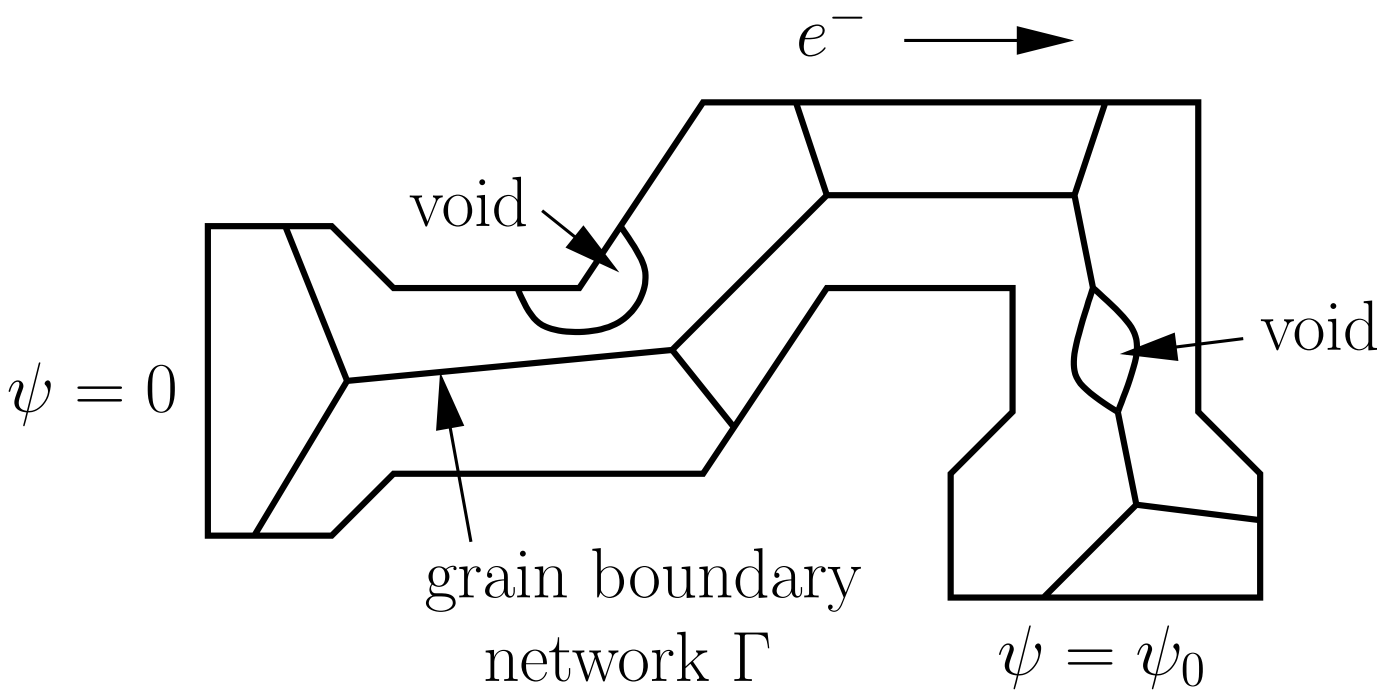


FIG. 2. Transmission x-ray topographs of an Al stripe on TiN at 330 °C. (a) No current. (b) $j=2.7\times10^4$ A 2.7×10^4 A/cm^2, 96—116 h. (d) No current (after current passage).

The Setup



Chemical potentials, continuity equations

bulk: $\mu = \mu_1 - f\Omega\,\mathrm{tr}(\sigma) - kT\log(c_v\Omega)$

grain boundary: $\mu = \mu_0 - \Omega\sigma_{nn}$

free surface: $\mu = \mu_0 - \gamma\Omega(\kappa_1 + \kappa_2)$

μ_1 energy of vacancy formation

μ_0 cohesive energy per atom

γ surface tension ~ 0.1 erg$/$cm

Einstein-Nernst: $\mathbf{J} = -\frac{c_v D}{kT}\nabla\mu$

include electromigration: $\nabla\mu \longrightarrow \nabla\mu + Z^* e\nabla\psi$ $\quad (Z^* = -5)$

bulk: $\mathbf{J} = \frac{c_v D}{kT}\left(f\Omega\nabla\,\mathrm{tr}(\sigma) + \frac{kT}{c_v}\nabla c_v - Z^* e\nabla\psi\right)$

grain boundary: $\mathbf{J}_b = \frac{\nu_b D_b}{kT}\left(\Omega\nabla_s\sigma_{nn} - Z^* e\nabla_s\psi\right)$

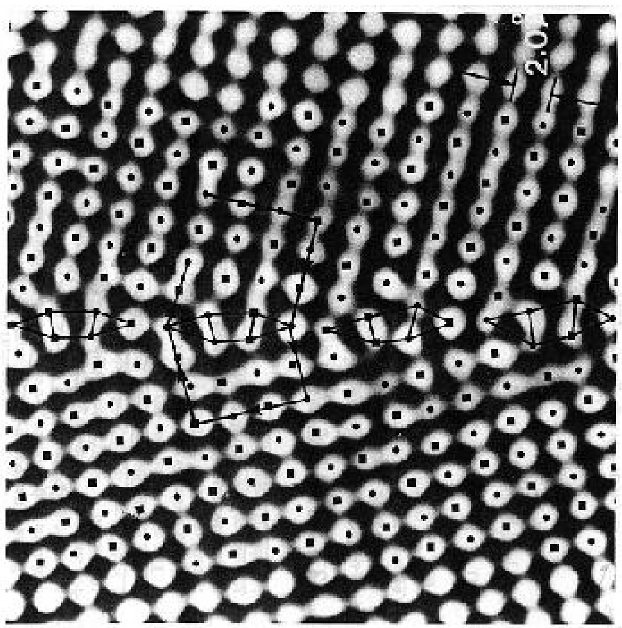
free surface: $\mathbf{J}_s = \frac{\nu_s D_s}{kT}\left(\gamma\Omega\nabla_s(\kappa_1 + \kappa_2) - Z^* e\nabla_s\psi\right)$

$$-\frac{\partial c_v}{\partial t} + \nabla\cdot\mathbf{J} = 0$$

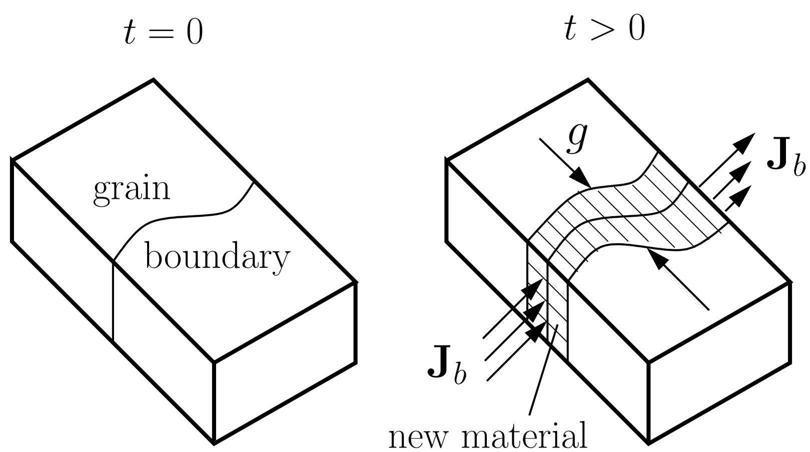
$$g_t + \Omega\nabla_s\cdot\mathbf{J}_b = 0$$

$$v_n + \Omega\nabla_s\cdot\mathbf{J}_s = \Omega\mathbf{J}\cdot\mathbf{n}$$

grain growth rate



Electronic Thin Film Science for Electrical Engineers and material scientists
Tu, Mayer, Feldman



$$g_t + \partial_s J = 0$$

$$J = \partial_s(\eta + \psi), \quad \eta = \sigma_{nn}$$

$$\frac{\partial g}{\partial t} = -\frac{\partial^2}{\partial s^2}(\eta + \psi)$$

Synopsis

- no voids. ψ solved once and for all.
- linearized version of the model.
  - stress/displ. evolve on fixed polygons
  - grain growth with no sliding

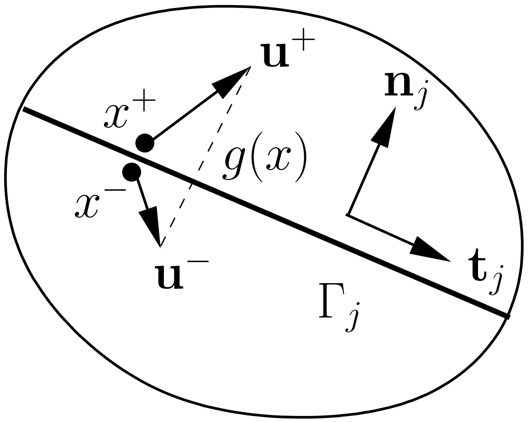
$$\mathbf{u}(x^+) - \mathbf{u}(x^-) = g(x)\mathbf{n} \quad (x \in \Gamma)$$

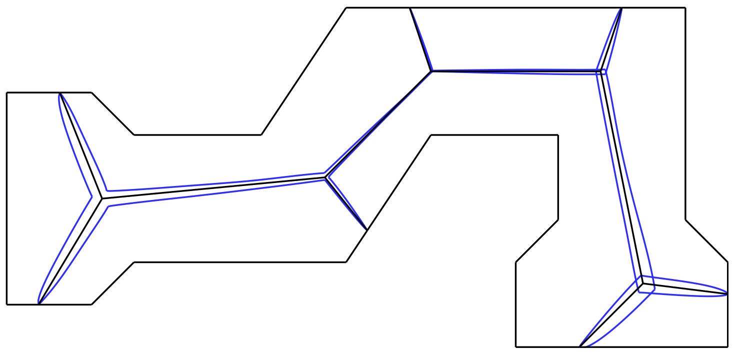
  - forces balance along grain boundaries

$$\sigma(x^+)\mathbf{n} = \sigma(x^-)\mathbf{n} \quad (x \in \Gamma)$$

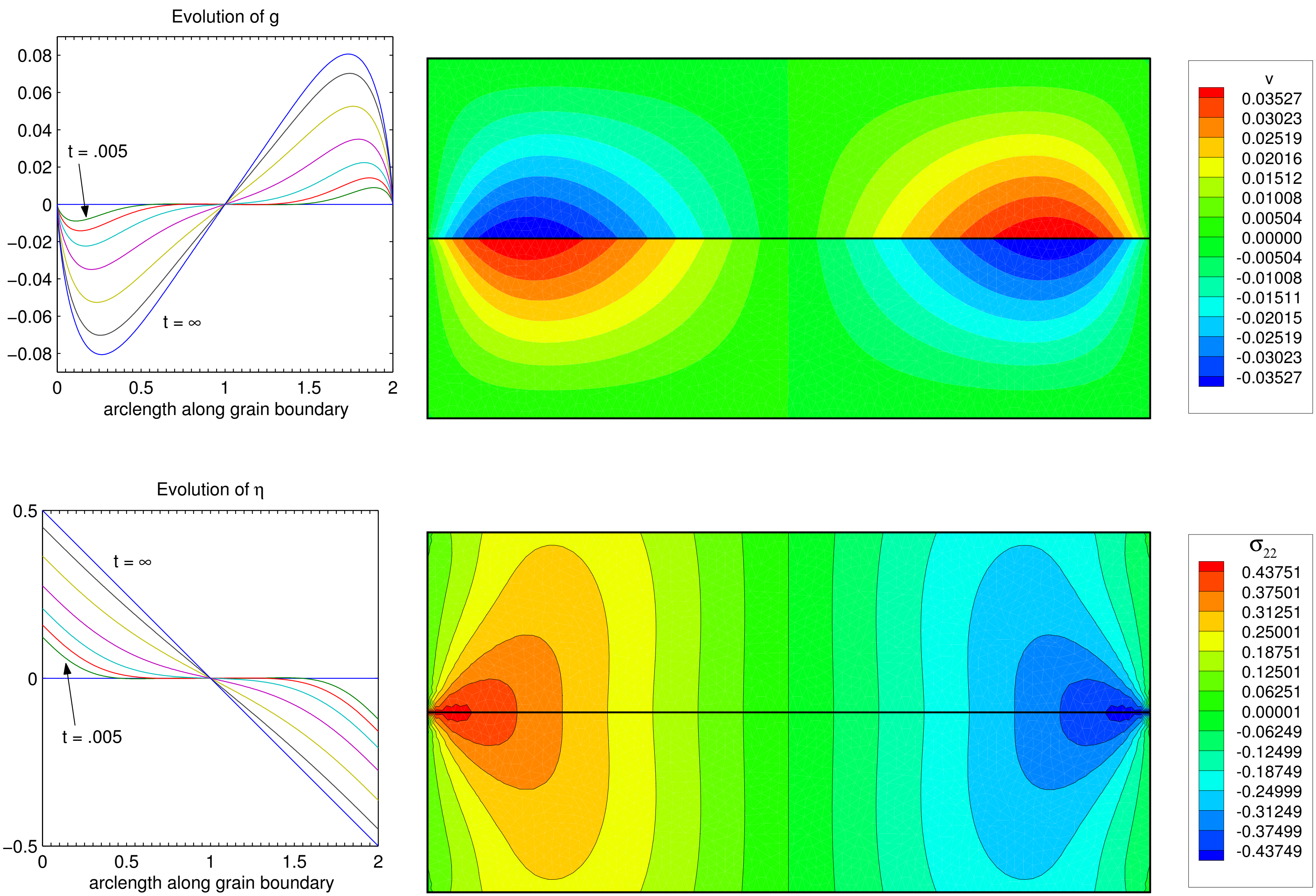
  - normal stress given by

$$\eta(x) := \mathbf{n} \cdot \sigma(x)\mathbf{n} \quad (x \in \Gamma)$$



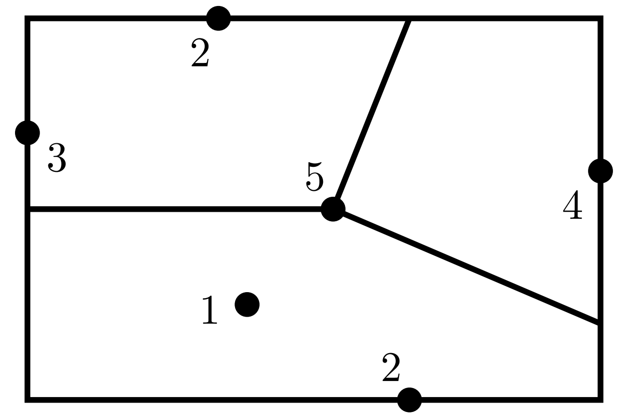


plot of $x - C\mathbf{u}(x^{\pm}),\ x \in \Gamma$


Evolution of g
t = .005
t = ∞
arclength along grain boundary
v
0.03527
0.03023
0.02519
0.02016
0.01512
0.01008
0.00504
0.00000
-0.00504
-0.01008
-0.01511
-0.02015
-0.02519
-0.03023
-0.03527
Evolution of η
t = ∞
t = .005
arclength along grain boundary
σ22
0.43751
0.37501
0.31251
0.25001
0.18751
0.12501
0.06251
0.00001
-0.06249
-0.12499
-0.18749
-0.24999
-0.31249
-0.37499
-0.43749

Electric Potential

1. $\nabla^2\psi = 0$
2. $\partial_n\psi = 0$
3. $\psi = 0$
4. $\psi = \psi_0$
5. Grain boundaries are invisible to ψ



Elasticity and Grain Growth

1a. $\mu\Delta\mathbf{u} + (\lambda+\mu)\nabla(\nabla\cdot\mathbf{u}) = 0$

2a. $\mathbf{u} = 0$

3a. $\mathbf{u}(x^+) - \mathbf{u}(x^-) = g(x)\mathbf{n}$

3b. $\sigma(x^+) = \sigma(x^-)$

3c. $\mathbf{n}\cdot\sigma(x)\mathbf{n} = \eta(x)$

3d. $\partial_t g = -\partial_s^2(\eta+\psi)$ $\quad \begin{cases} J = \partial_s(\eta+\psi) \\ g_t + J_s = 0 \end{cases}$

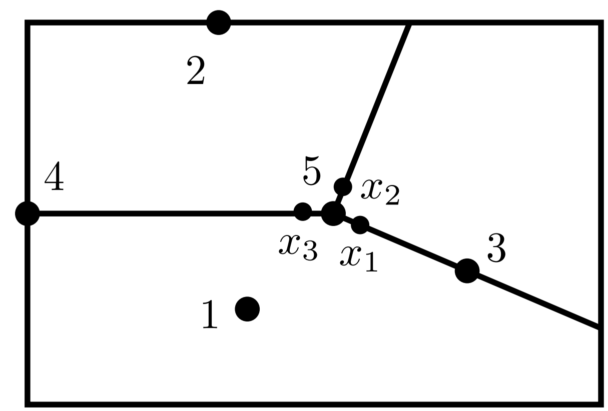
4a. $g = 0$

4b. $\partial_s(\eta+\psi) = 0$

5a. $g(x_1)\mathbf{n}_1 + g(x_2)\mathbf{n}_2 + g(x_3)\mathbf{n}_3 = 0$

5b. $\eta(x_1) = \eta(x_2) = \eta(x_3)$

5c. $\partial_{s_1}(\eta+\psi) + \partial_{s_2}(\eta+\psi) + \partial_{s_3}(\eta+\psi) = 0$



Initial Condition: $g \equiv 0$

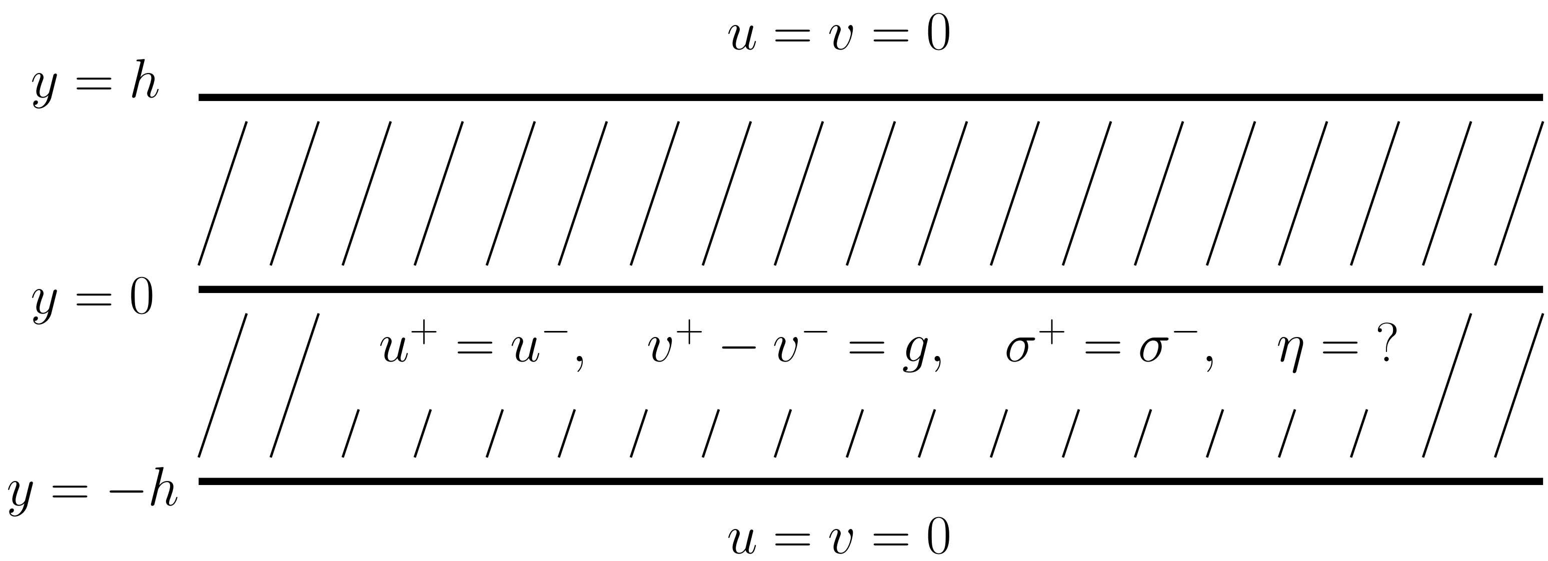
comments

- Equations are very stiff: two derivatives of stress!
- Equations and boundary conditions are non-local.
- Boundary conditions overspecified? (displacement and flux)

$$u_t = u_{xx} \quad \text{yes} \qquad u_t = -u_{xxxx} \quad \text{no} \qquad g_t = -\eta_{xx} \quad ??$$

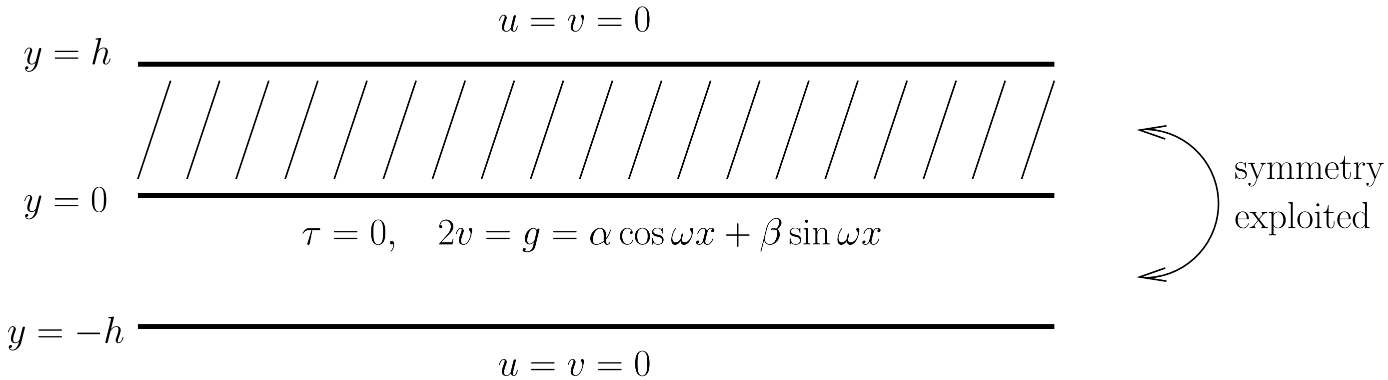
- What role will singularities play?
  - Does it make sense to impose b.c.'s on η, $\partial_s \eta$ at a junction?
- Can we make use of the fact that we have linearized the model?

infinite interconnect line



- start simple
- no singularities or junctions
- gain insight about nature of the diffusion process

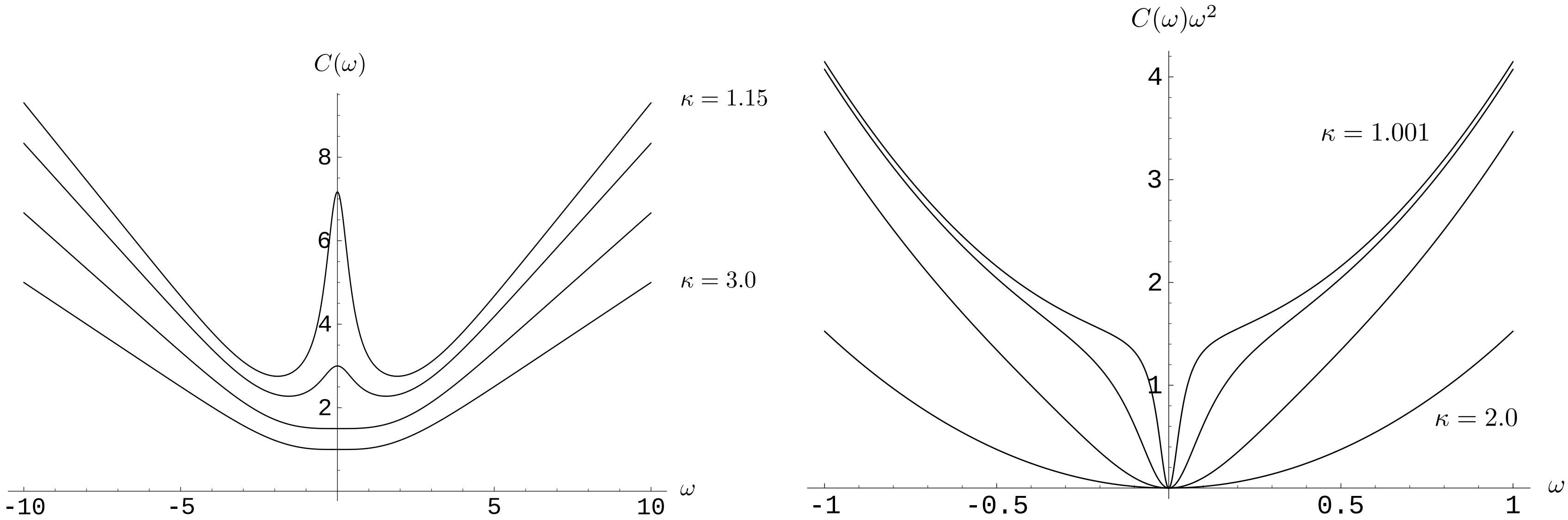
Fourier transform



$$\eta(x) = \sigma_{22}(x,0) = -C(\omega)g(x)$$

$$C(\omega) = \frac{\omega[1+\kappa^2+4h^2\omega^2+2\kappa\cosh 2h\omega]}{(1+\kappa)[\kappa\sinh 2h\omega - 2h\omega]}$$

$$g_t = -\eta_{xx} \quad \Rightarrow \quad g(x,t) = \int_{-\infty}^{\infty} e^{i\omega x} e^{-C(\omega)\omega^2 t}\hat{g}_0(\omega)\,d\omega$$

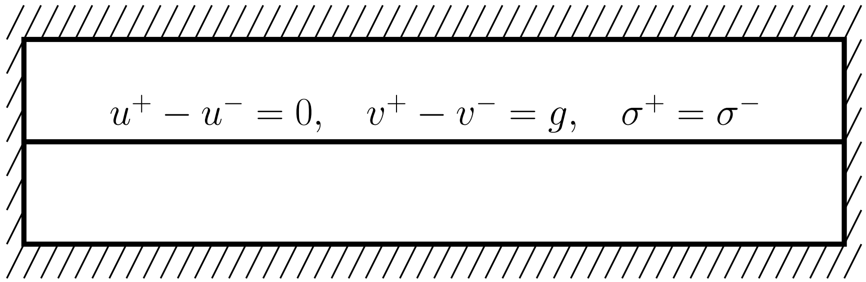


$$C(\omega) = \frac{1}{h}\left\{\frac{\kappa+1}{2(\kappa-1)} - \frac{(\kappa-2)(\kappa-3)}{3(\kappa-1)^2}(h\omega)^2 + \dots\right\}, \qquad (|h\omega| \ll 1)$$

$$C(\omega) = \frac{2\omega}{1+\kappa}, \qquad (|h\omega| \gg 1)$$

Dissipation Rate	Equation
$b\omega^2$	$u_t = \quad bu_{xx} \qquad (b > 0)$
$C(\omega)\omega^2$	$g_t = -\eta_{xx}$
$b\omega^4$	$u_t = -bu_{xxxx} \quad (b > 0)$

finite geometry



$$g \quad \underset{B}{\overset{S}{\rightleftarrows}} \quad \eta \quad \underset{G}{\overset{L}{\rightleftarrows}} \quad -\partial_s^2 \eta$$

$$g(0) = g(1) = 0 \qquad \frac{\partial}{\partial s}\Big|_{0,1}(\eta + \psi) = 0$$

$$g_t = L(Sg + \psi) \qquad S \quad \text{Dirichlet to Neumann map}$$

$$\eta_t = SL(\eta + \psi) \qquad L \quad -\frac{\partial^2}{\partial s^2}$$

The operator $B : L^2(\Gamma) \to L^2(\Gamma)$

(gb normal stress problem) $$\begin{cases} \mu\Delta\mathbf{u} + (\lambda+\mu)\nabla(\nabla\cdot\mathbf{u}) = 0, & (x \in \Omega_k), \\ \mathbf{u}(x) = \mathbf{0}, & (x \in \Gamma_0), \\ [\mathbf{u}(x^+) - \mathbf{u}(x^-)]\cdot\mathbf{t}_j = 0, & (x \in \Gamma_j), \\ [\sigma(x^+) - \sigma(x^-)]\mathbf{n}_j = \mathbf{0}, & (x \in \Gamma_j), \\ \mathbf{n}_j\cdot\sigma(x)\mathbf{n}_j = \eta(x), & (x \in \Gamma_j). \end{cases}$$

$$(B\eta)(x) = [\mathbf{u}(x^+) - \mathbf{u}(x^-)]\cdot\mathbf{n}_j, \quad (x \in \Gamma_j).$$

- $E = -\frac{1}{2}\int_\Gamma \eta g = -\frac{1}{2}\int_\Gamma \eta B\eta$
- B is self-adjoint and negative
- B is compact
  - a sort of Neumann to Dirichlet map
  - trace operators are involved

The operator G

Poisson problem on network: $\begin{cases} -\frac{\partial^2}{\partial s^2}\eta = f & \text{on each segment} \\ \eta \text{ continuous} & \text{at each junction} \\ \mathcal{F}_i\eta = 0 & \text{at each junction} \end{cases}$

$$A = L + \sum_1^d (\cdot, e_j)e_j, \qquad P = I - \sum_1^d (\cdot, e_j)e_j, \qquad L = AP = PA$$

$$G = A^{-1}P = PA^{-1} \quad \text{(self-adjoint, positive, compact)}$$

$$A^{-1/2} : L^2(\Gamma) \to H^1(\Gamma) \text{ is an isomorphism}$$

$$\begin{matrix} f = \sum a_n\varphi_n \\ L\varphi_n = \mu_n^2\varphi_n \end{matrix} \quad \Rightarrow \quad \|f\|^2 = \sum_{n=0}^{\infty} |a_n|^2, \qquad \|f'\|^2 = \sum_{n=0}^{\infty} |a_n\mu_n|^2$$

semigroup theory

$$\dot{\eta} = SL\eta, \quad \eta(0) = \eta_0 \qquad \Rightarrow \qquad \eta(t) = E_t\eta_0$$

$E_{t+s} = E_t E_s$

$E_0 = id_{H^1(\Gamma)}$

$t \mapsto E_t x$ continuous on $[0, \infty)$ for each fixed x

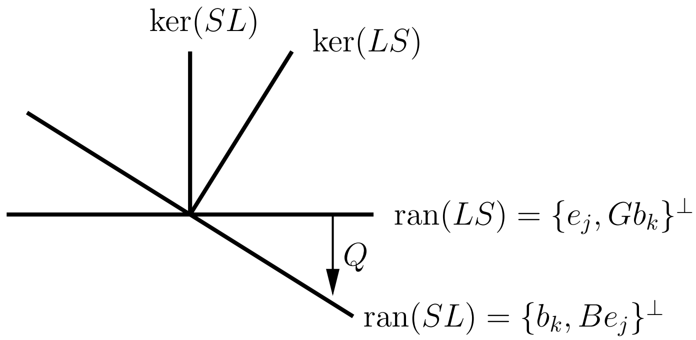
$$\Rightarrow \frac{d}{dt}E_t x = SLE_t x = E_t SLx, \quad (x \in \mathcal{D}(SL),\ 0 \leq t < \infty)$$

Electromigration: a passive driving force

$$\eta_t = SL(\eta + \psi) \qquad \Rightarrow \qquad \eta(t) = E_t(\eta_0 + \psi) - \psi.$$

Suffices to solve $\eta_t = SL\eta$ to get E_t.

a pseudo-inverse



$K = QGBQ$ (compact)

$$SL\phi = \lambda\phi \;\Leftrightarrow\; K\phi = \lambda^{-1}\phi \quad (\lambda \neq 0)$$

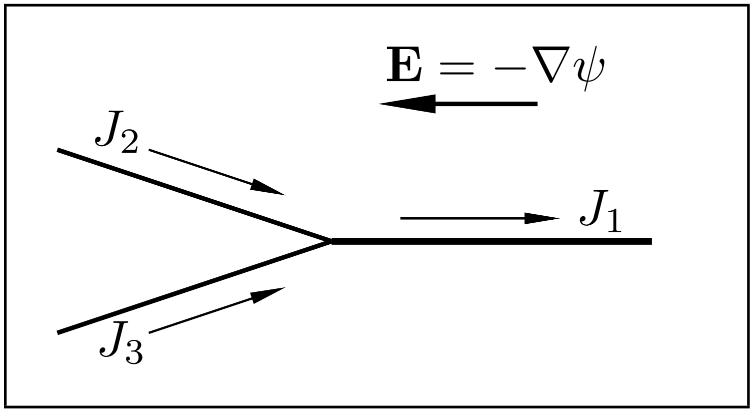
$$SL\phi = 0 \;\Leftrightarrow\; K\phi = 0$$

$$\eta_0 = \sum_{k=1}^{\infty} a_k\phi_k, \qquad E_t\eta_0 = \sum_{k=1}^{\infty} a_k e^{\lambda_k t}\phi_k, \qquad a_k = (\eta_0, \phi_k^*)_{L^2(\Gamma)}$$

Analyze $L^{\frac{1}{2}}SL^{\frac{1}{2}}$ in parallel:

- the ϕ_k are a Riesz basis for $H^1(\Gamma)$
- the semigroup E_t is analytic $\left(\limsup_{t\to 0} t\|E_t'\| = \alpha < \infty\right)$

boundary conditions



(possible flux imbalance at $t = 0$)

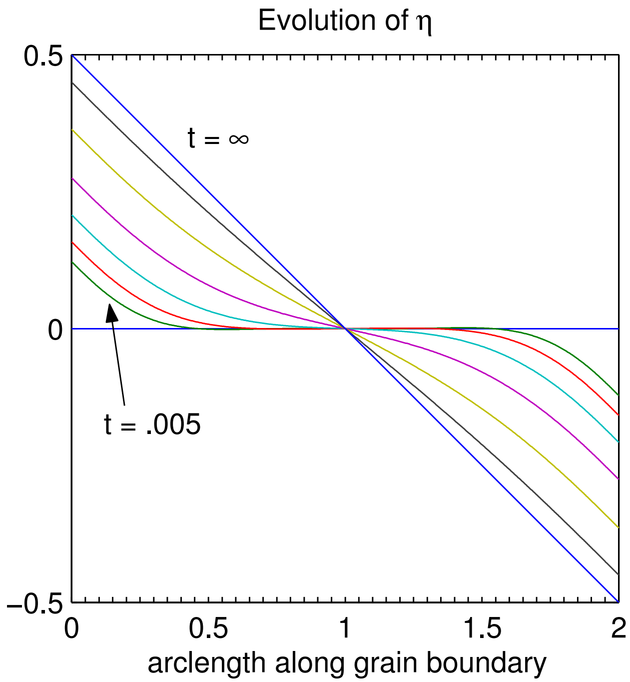
$\psi \in \mathcal{D}(L^{1/2})$ but $\psi \notin \mathcal{D}(L)$

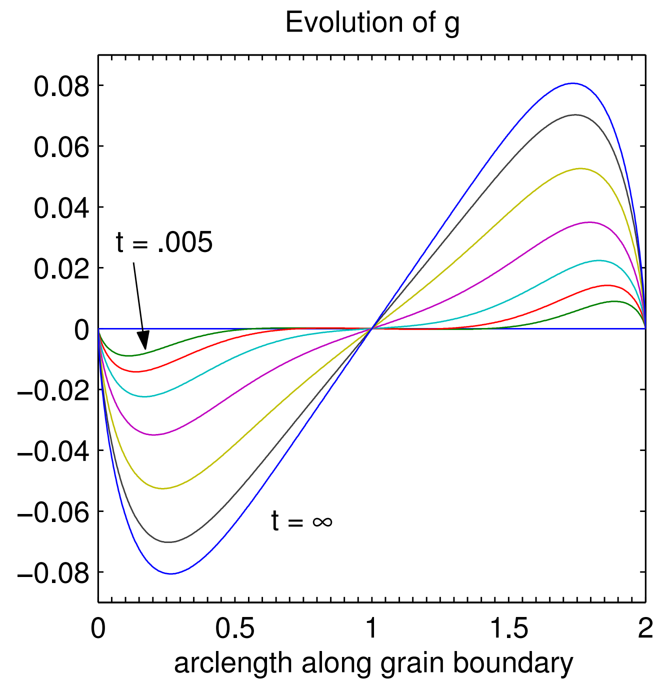
$$\eta_t = SL(\eta + \psi), \quad \eta = E_t(\eta_0 + \psi) - \psi, \quad J = \partial_s(\eta + \psi)$$

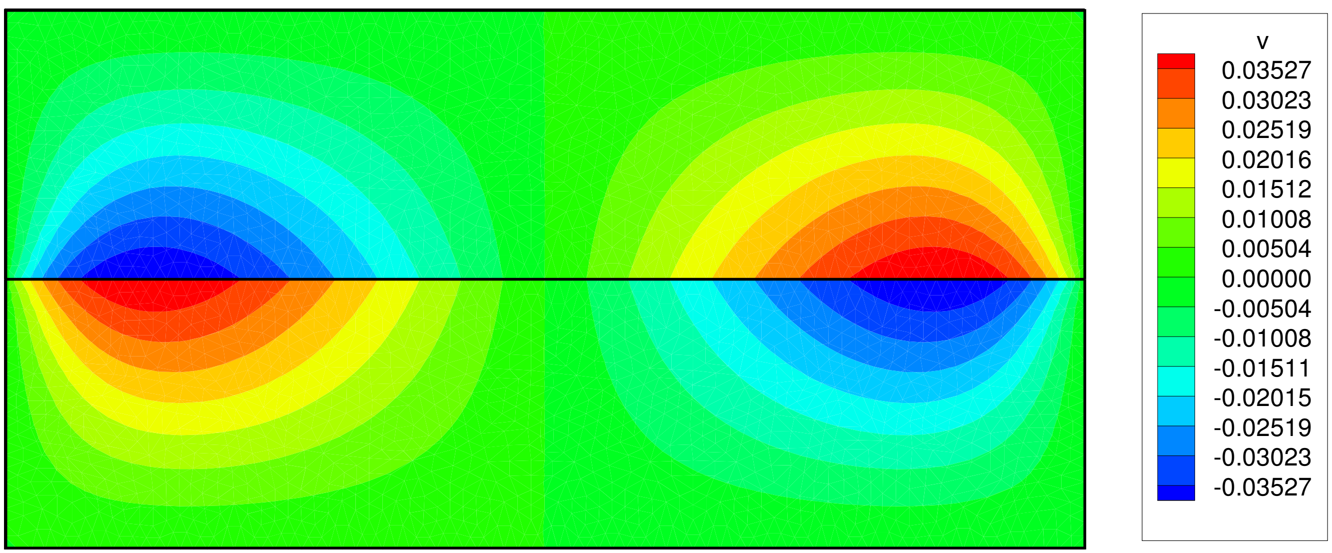
E_t analytic $\quad \Rightarrow \quad \mathrm{range}(E_t) \subset \mathcal{D}(SL) \qquad (t > 0)$

$\eta(t) + \psi \in \mathcal{D}(L) \qquad (t > 0) \quad \longleftarrow \quad \begin{cases} \eta \text{ remains finite (not singular),} \\ \text{flux balances at junctions} \end{cases}$

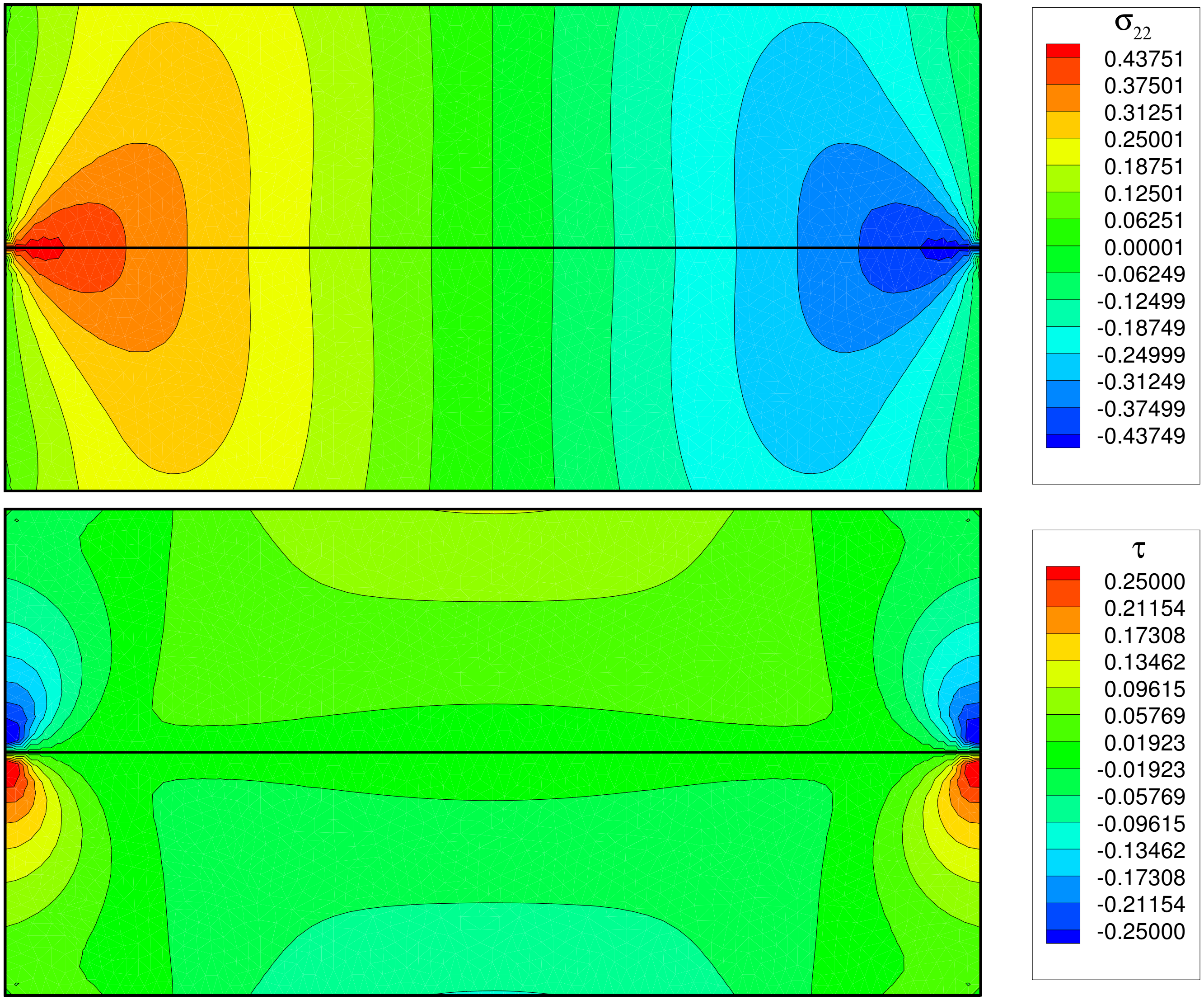
$g_t = L(\eta + \psi) \in \mathrm{range}(L) \quad \Rightarrow \quad \dfrac{\partial}{\partial t} \displaystyle\int_{\Gamma_j} g\, ds = 0$ (mass cons.)


Evolution of η
0.5
0
−0.5
t = ∞
t = .005
0
0.5
1
1.5
2
arclength along grain boundary

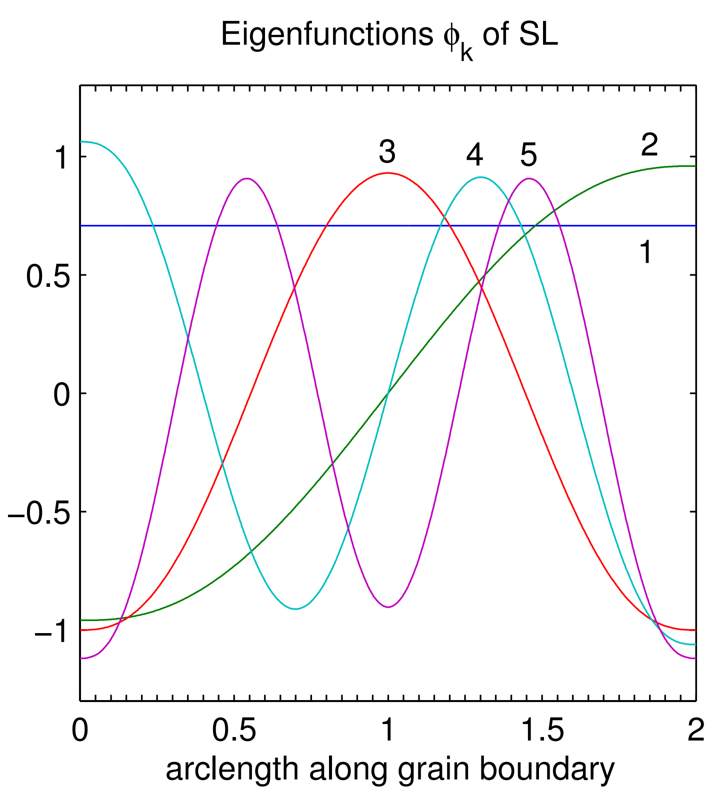

Evolution of g
0.08
0.06
0.04
0.02
0
−0.02
−0.04
−0.06
−0.08
t = .005
t = ∞
0
0.5
1
1.5
2
arclength along grain boundary

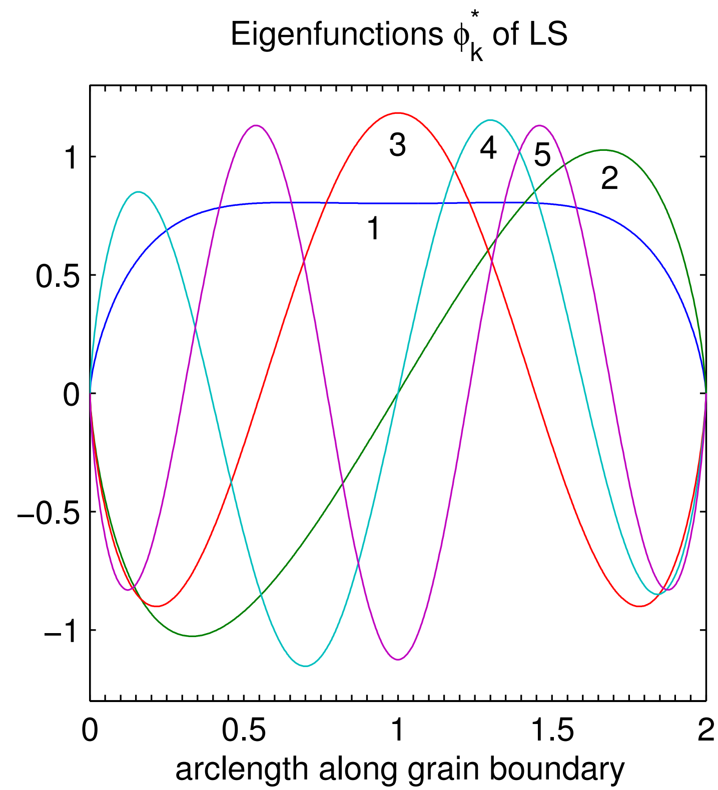

v
0.03527
0.03023
0.02519
0.02016
0.01512
0.01008
0.00504
0.00000
-0.00504
-0.01008
-0.01511
-0.02015
-0.02519
-0.03023
-0.03527

steady state



eigenfunctions





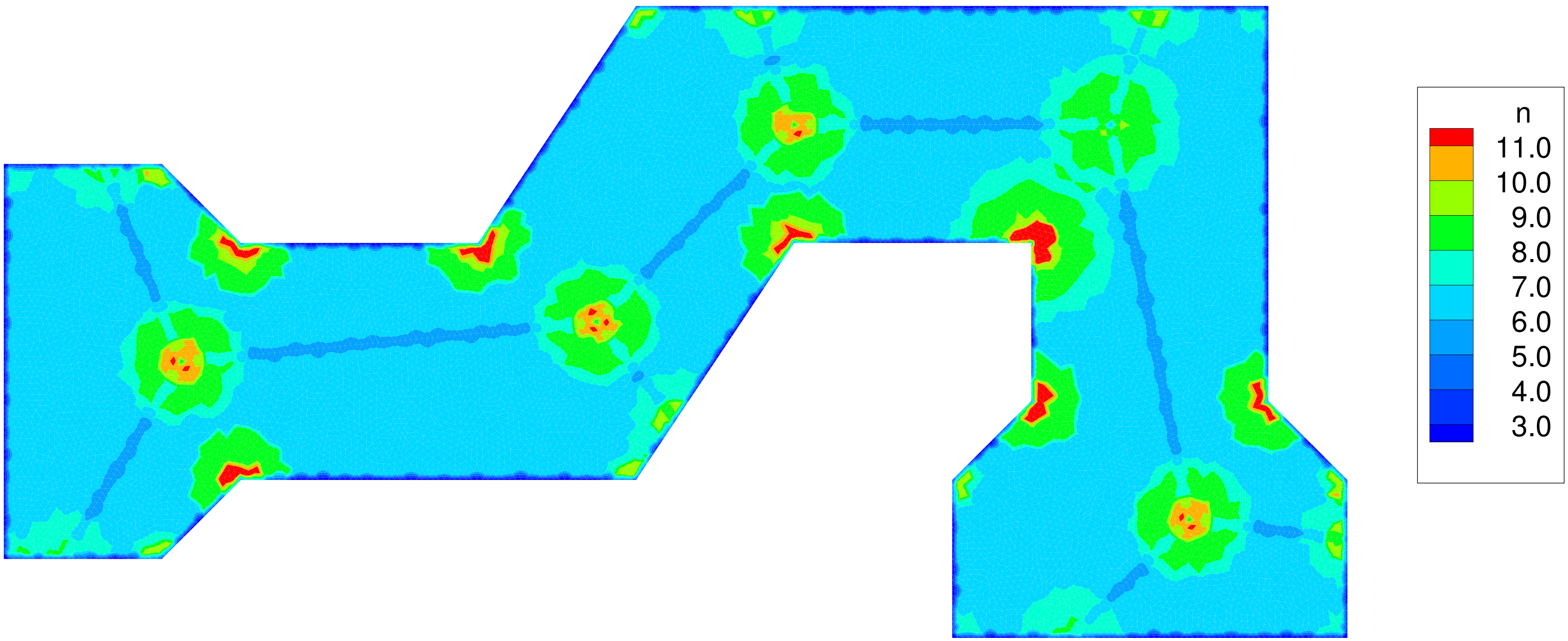
Note that ϕ_k, ϕ_k^* satisfy the boundary conditions for η, g respectively

$$\eta_0 = \sum_{k=1}^{\infty} a_k \phi_k, \qquad E_t \eta_0 = \sum_{k=1}^{\infty} a_k e^{\lambda_k t} \phi_k, \qquad a_k = (\eta_0, \phi_k^*)_{L^2(\Gamma)}$$

numerical method

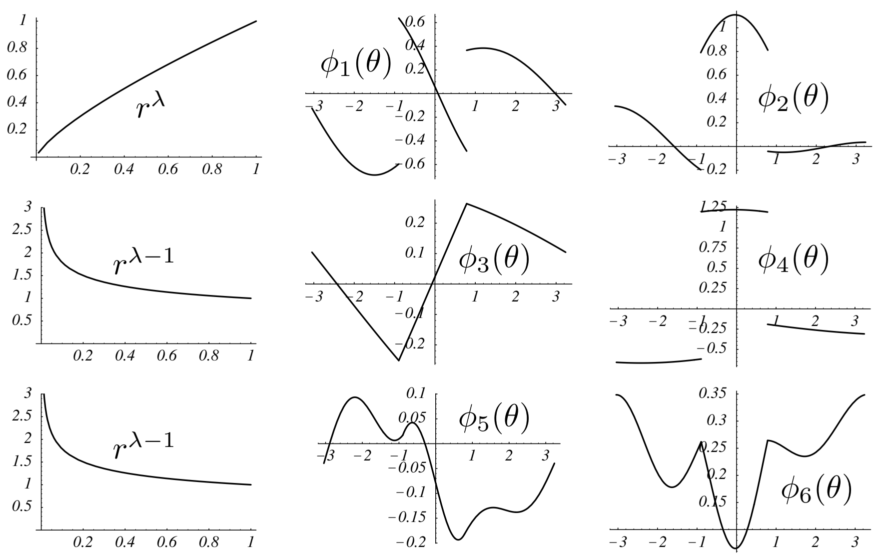
- $K = QGBQ = \mathrm{pinv}(SL)$ is compact
  - well approximated by finite rank operators
- compute B numerically using X-Fosls
  - resolve singularities
  - use compatible stress and displacement spaces
- use 1D Galerkin finite elements to compute G
- compute eigenvalues and eigenfunctions of K
- use them to represent the evolution

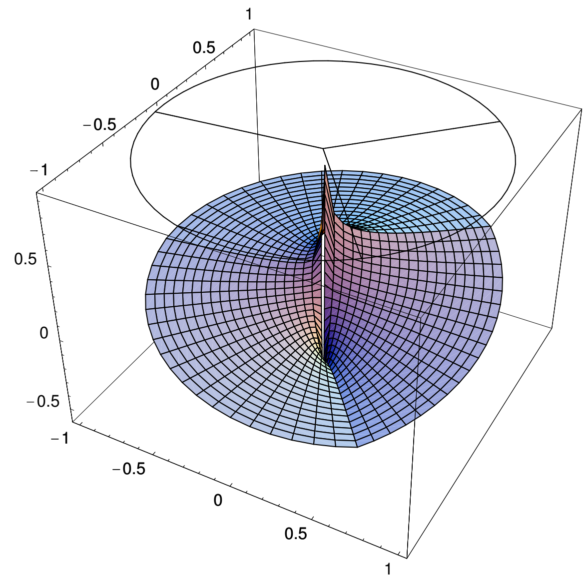
101 singular functions added to FE space



Example

Left: a power solution ($\lambda = .7474$). Right: 3d plot of $\alpha = w_3(r, \theta)$

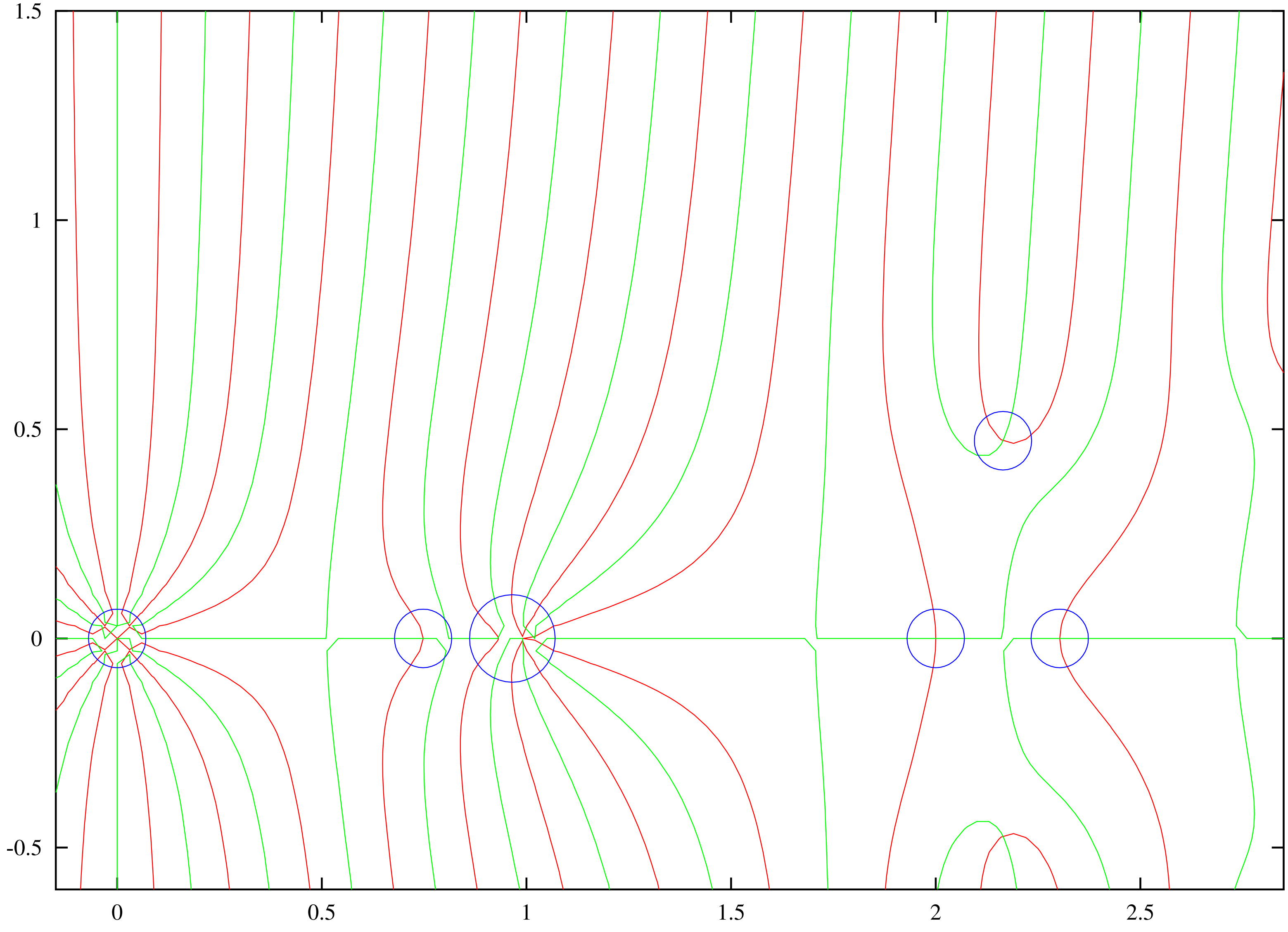




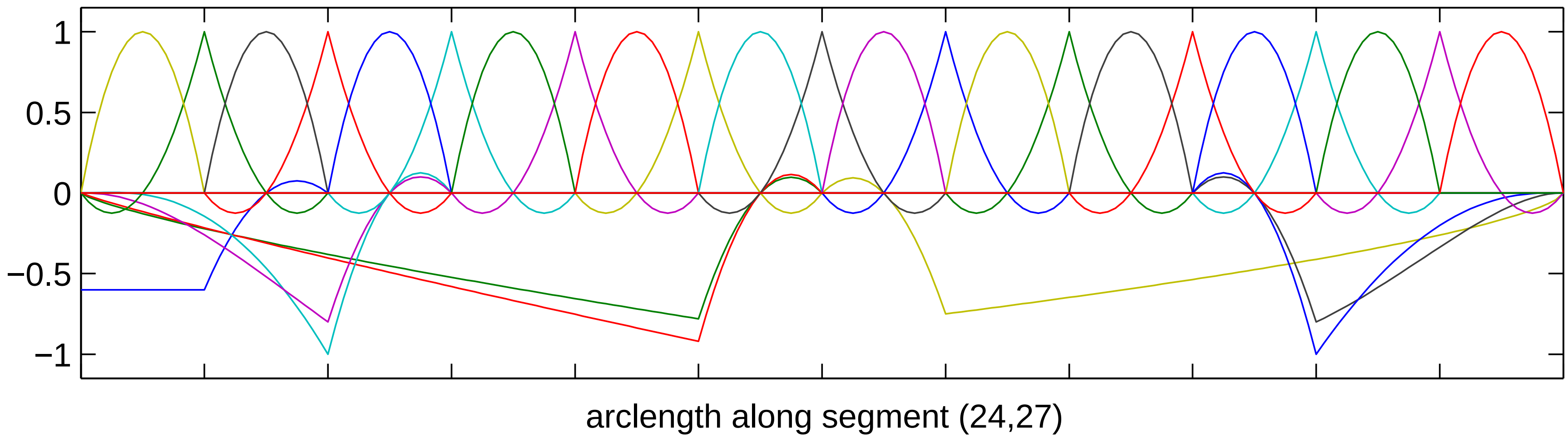
$$w = (u, v, \alpha, \beta, \gamma, \tau)^T$$

$$w_j(r, \theta) = r^{\lambda + t_j} \phi_j(\theta)$$

GB triple junction



singular basis functions affect g but not η

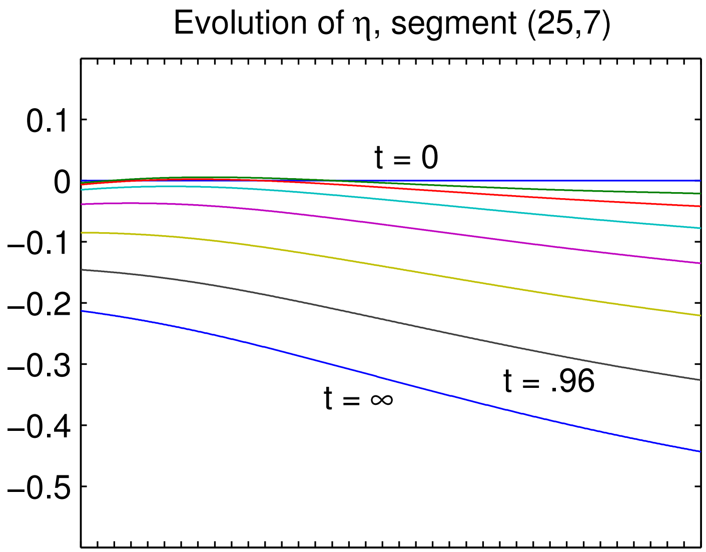


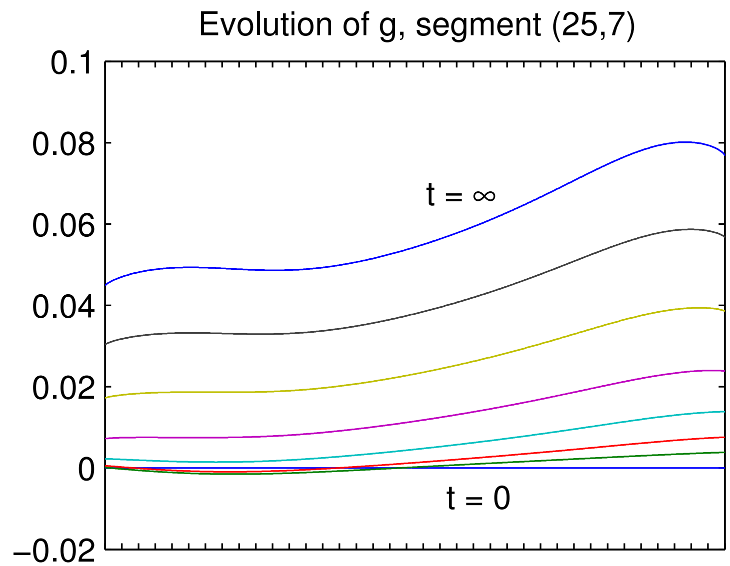
computing G on Γ is *almost* like solving 1D Poisson problem with FE:

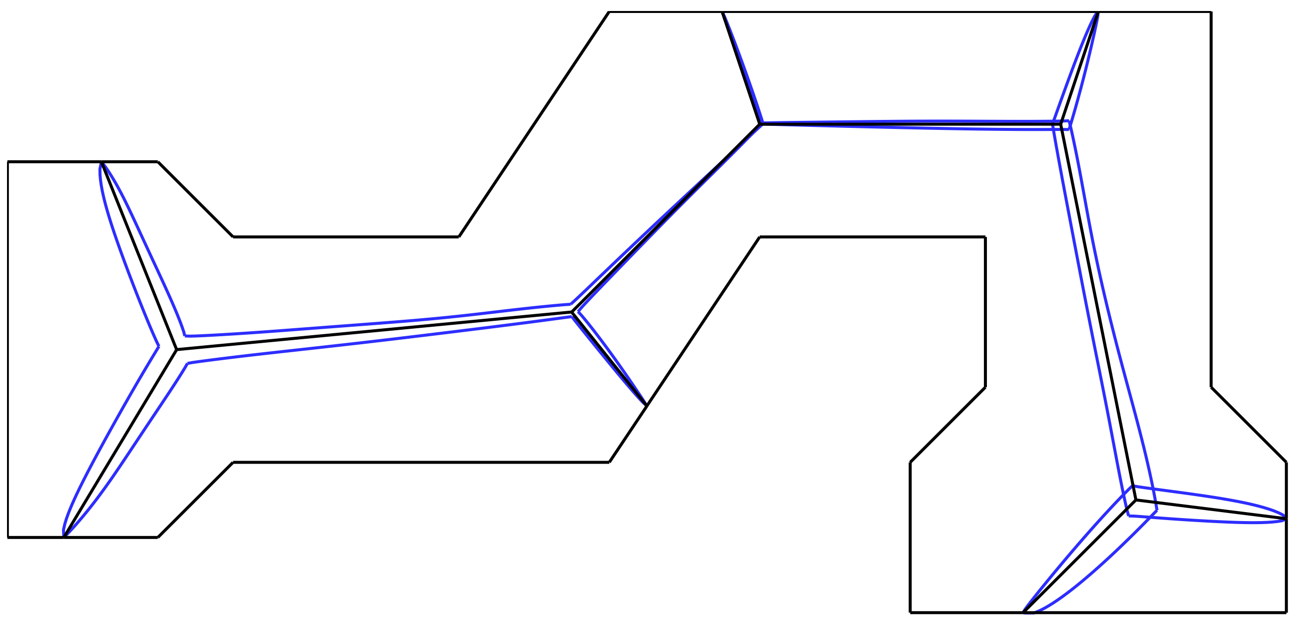
$\{e_i\}_{i=1}^{n}$ basis for grain growth, $\quad g = g_i e_i$

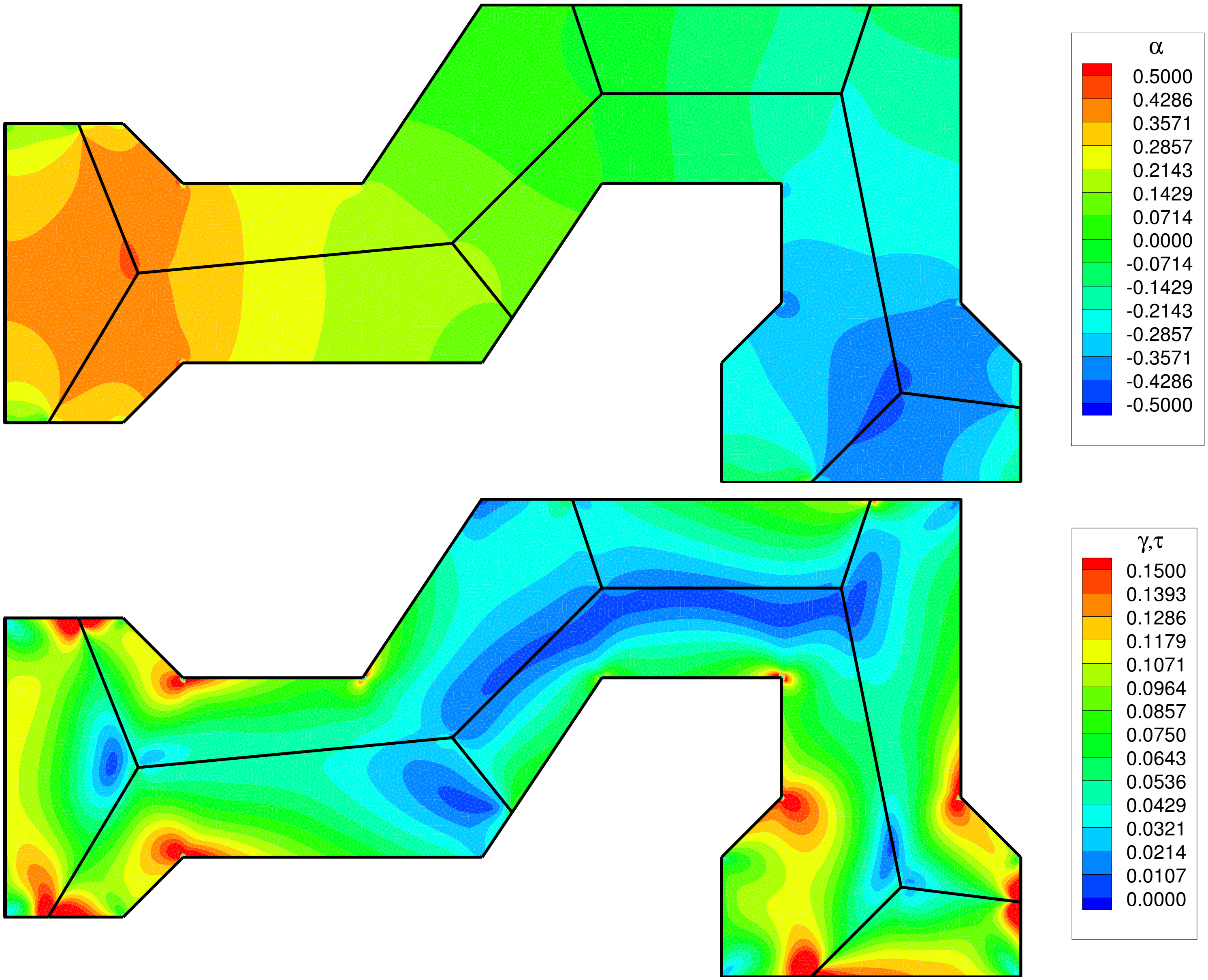
$\{\varepsilon_i\}_{i=1}^{m}$ basis for normal stress, $\quad \eta = \eta_i \varepsilon_i$

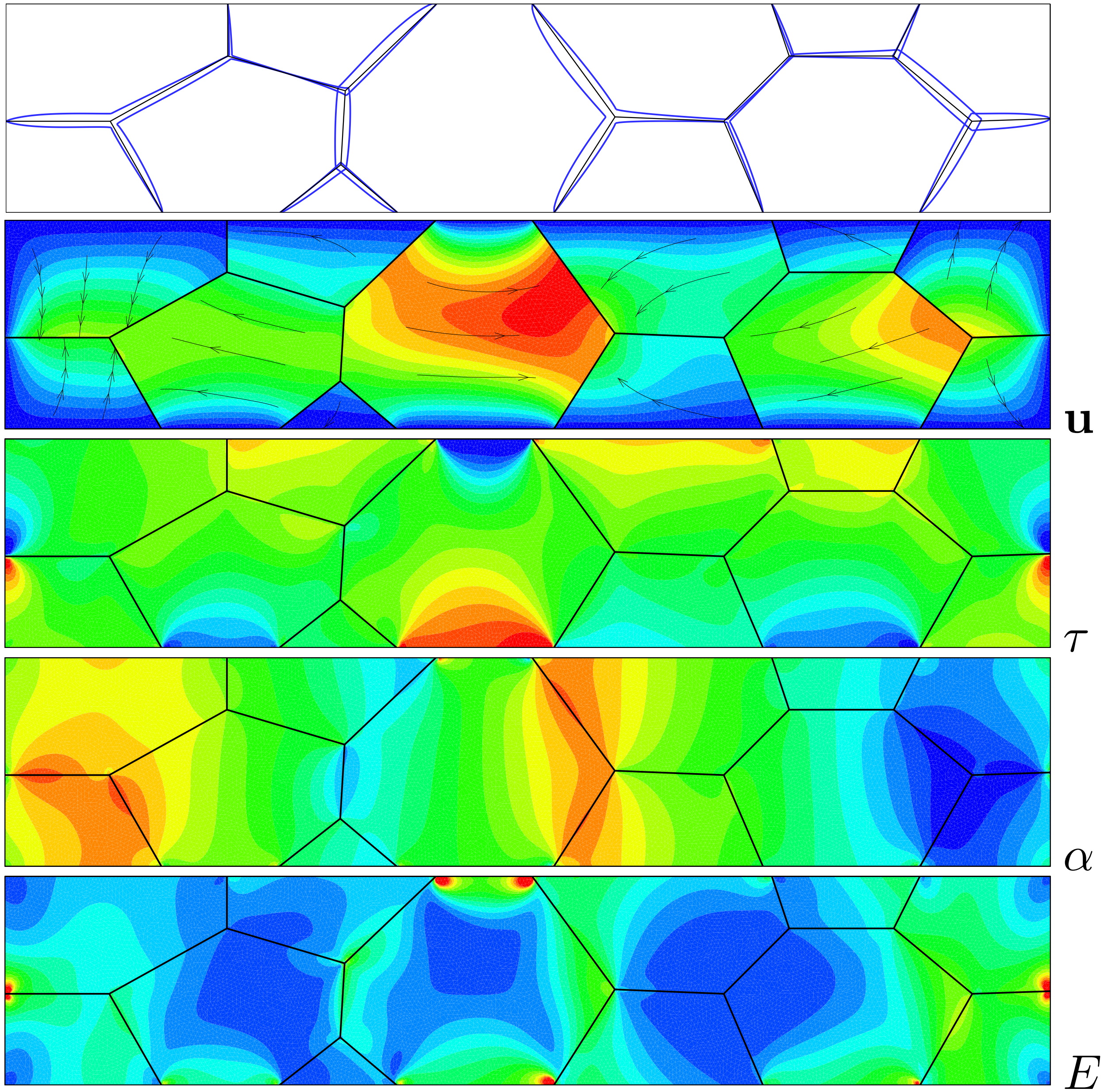
$$-A\eta = \widetilde{M}g, \quad A_{ij} = (\partial_x \varepsilon_i, \partial_x \varepsilon_j)_{L^2}, \quad \widetilde{M}_{ij} = (\varepsilon_i, e_j)_{L^2},$$


Evolution of η, segment (25,7)
0.1
0
−0.1
−0.2
−0.3
−0.4
−0.5
t = 0
t = .96
t = ∞


Evolution of g, segment (25,7)
0.1
0.08
0.06
0.04
0.02
0
−0.02
t = ∞
t = 0




α
0.5000
0.4286
0.3571
0.2857
0.2143
0.1429
0.0714
0.0000
-0.0714
-0.1429
-0.2143
-0.2857
-0.3571
-0.4286
-0.5000
γ,τ
0.1500
0.1393
0.1286
0.1179
0.1071
0.0964
0.0857
0.0750
0.0643
0.0536
0.0429
0.0321
0.0214
0.0107
0.0000


u
τ
α
E

evolution of g from η

$$\eta_t = SL(\eta + \psi), \qquad g_t = L(Sg + \psi), \qquad \eta(t) = E_t(\eta_0 + \psi) - \psi$$

- nondegenerate case: $g(t) = B\eta(t)$
- degenerate case:
  - orthogonal projection $R = SB = BS$

    $$\dim \ker R = \text{ “order of degeneracy”}$$

  - related projection R_1 (along $\operatorname{span}\{b_k\}$ onto $\{Gb_k\}^\perp$)

    $$g(t) = R_1 B\eta(t) + (I - R_1)g_0 + [(I - R_1)L\psi]t$$

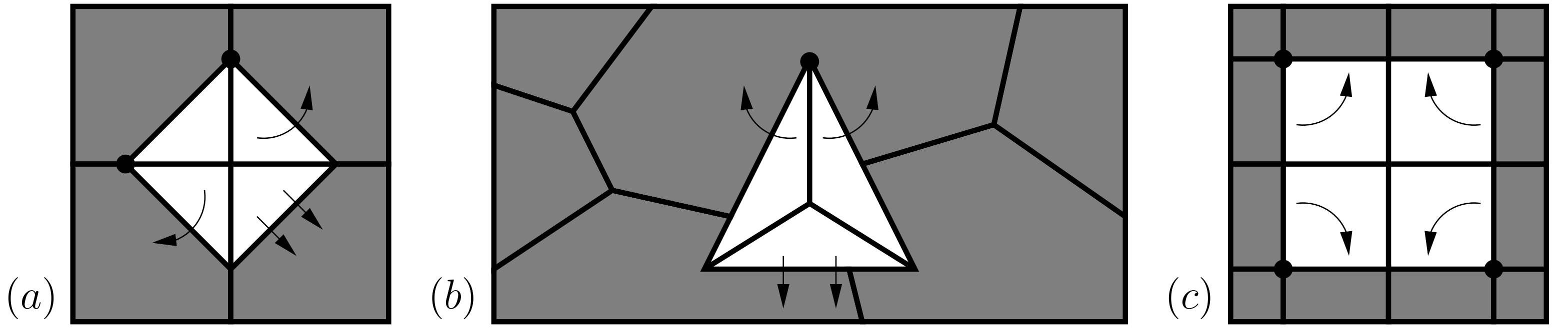
  - η reaches steady state, g has unsuppressed growth modes (plate tectonics)

degenerate grain boundary networks

existence/uniqueness: $\mathbf{u} \equiv 0$ must be the only displacement in H consisting of infinitesimal rigid body motions on each grain

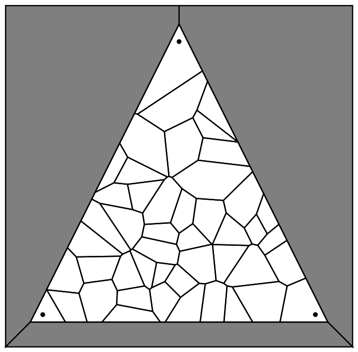
$$H = \{\mathbf{u} \in H^1(\Omega)^2 : \gamma_0\mathbf{u} = 0, \gamma_t\mathbf{u} = 0\}$$

i.r.b.m. : $\varepsilon(\mathbf{u}) = 0 \quad \begin{cases} u_1(x,y) = a - cy \\ u_2(x,y) = b + cx \end{cases}$



- pathologies lead to degeneracy
  - non-convex grains
  - too many quadruple (or higher order) junctions

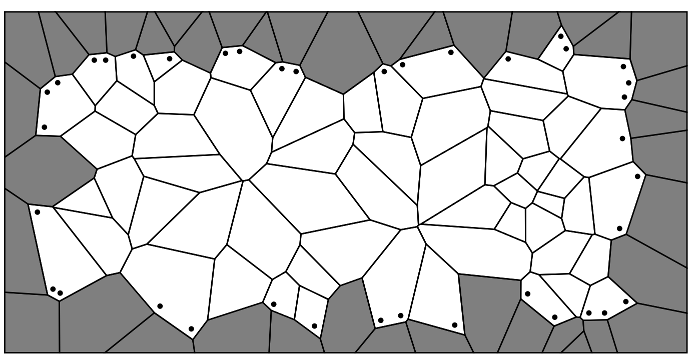
typical grain boundary networks are non-degenerate



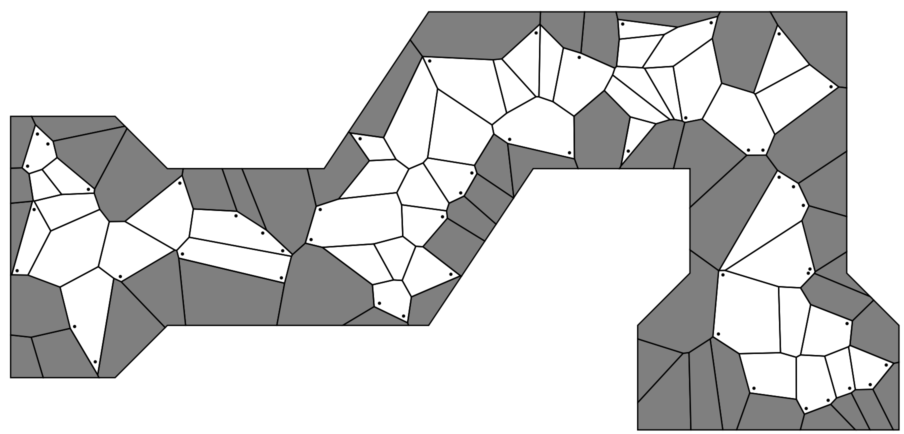
(a)

condition number of matrix (rigid body motions ↔ b.c.'s)

geometry	regions	trials	max	min	mean	std dev
(a)	200	10000	172.6	31.7	37.8	3.2
(a)	100	10000	48.4	21.6	26.2	2.1
(a)	50	10000	35.0	14.4	18.2	1.6
(b)	200	10000	31.8	13.0	16.8	1.3
(b)	100	10000	31.5	8.2	11.1	1.1
(c)	200	10000	26.8	7.4	9.9	1.1
(c)	100	10000	21.4	4.5	6.9	1.1



(b)



(c)

summary

1. Found an exact solution for the infinite interconnect line.

2. Recast problem on a finite geometry as an ODE on a Hilbert space.

3. Developed a machinery for computing the eigenfunctions of the generator of the semigroup.

4. Explored problem numerically, proved well-posedness rigorously.

   - stress components directly involved in transport process remain well-behaved.
   - “hidden” stress components grow very large, develop singularities.
     - may be responsible for voiding and stress induced damage.
     - omitted from most stress generation models in the literature.

5. Developed X-Fosls, a method of adjoining stable representations of singularities near corners and junctions to LSFE basis.

6. To do: void meets grain boundary?