Scharfetter Gummel Schemes for Non-Boltzmann Statistics

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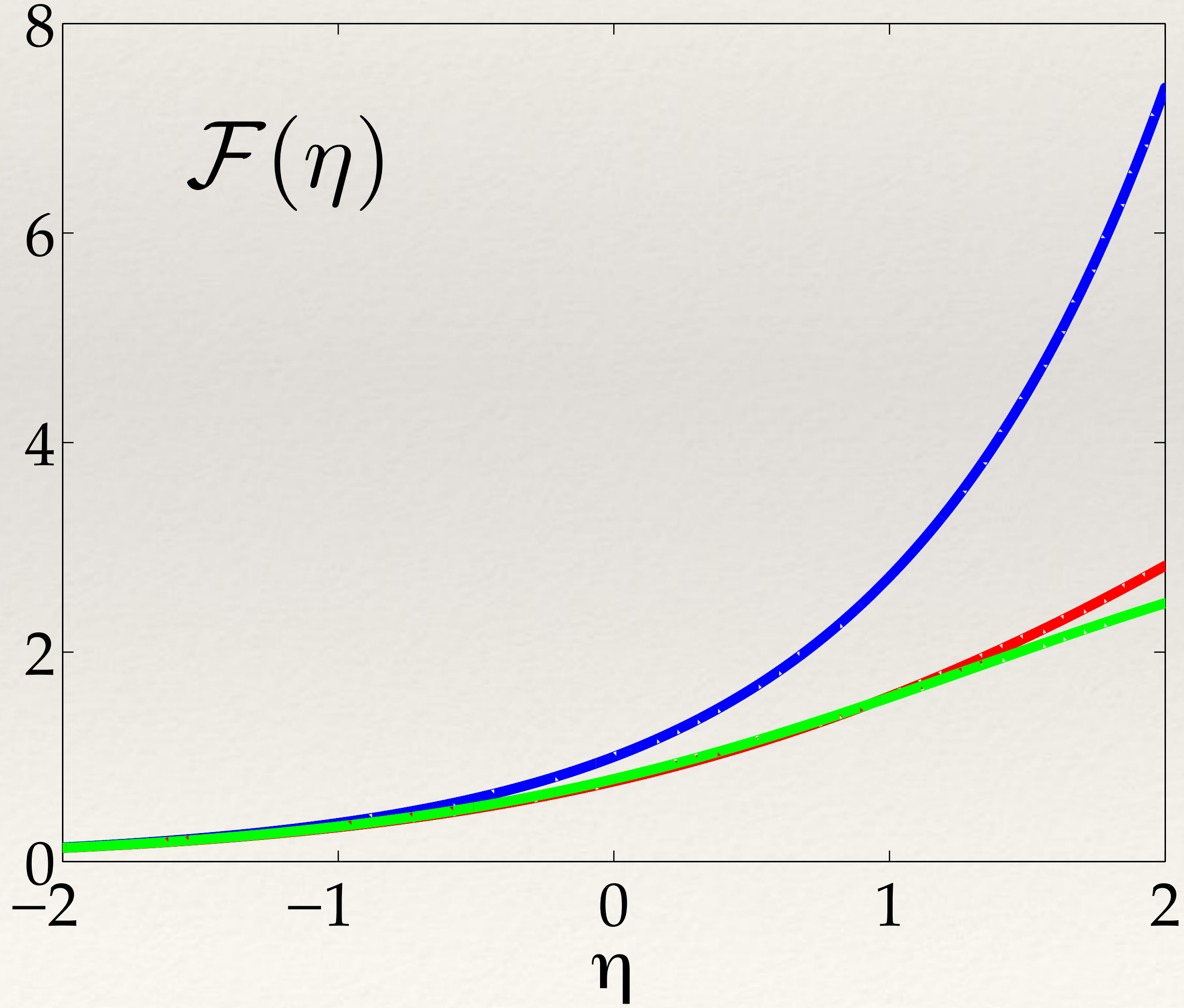
Leibniz Association

Numerical methods for interesting physics

Boltzmann ●	Blakemore ●	Fermi-Dirac ●
e^{η}	$\frac{1}{e^{-\eta}+\gamma}$	$\frac{1}{\Gamma(\alpha+1)} \int_0^\infty \frac{E^\alpha}{1+e^{(E-\eta)}}\,\mathrm{d}E$



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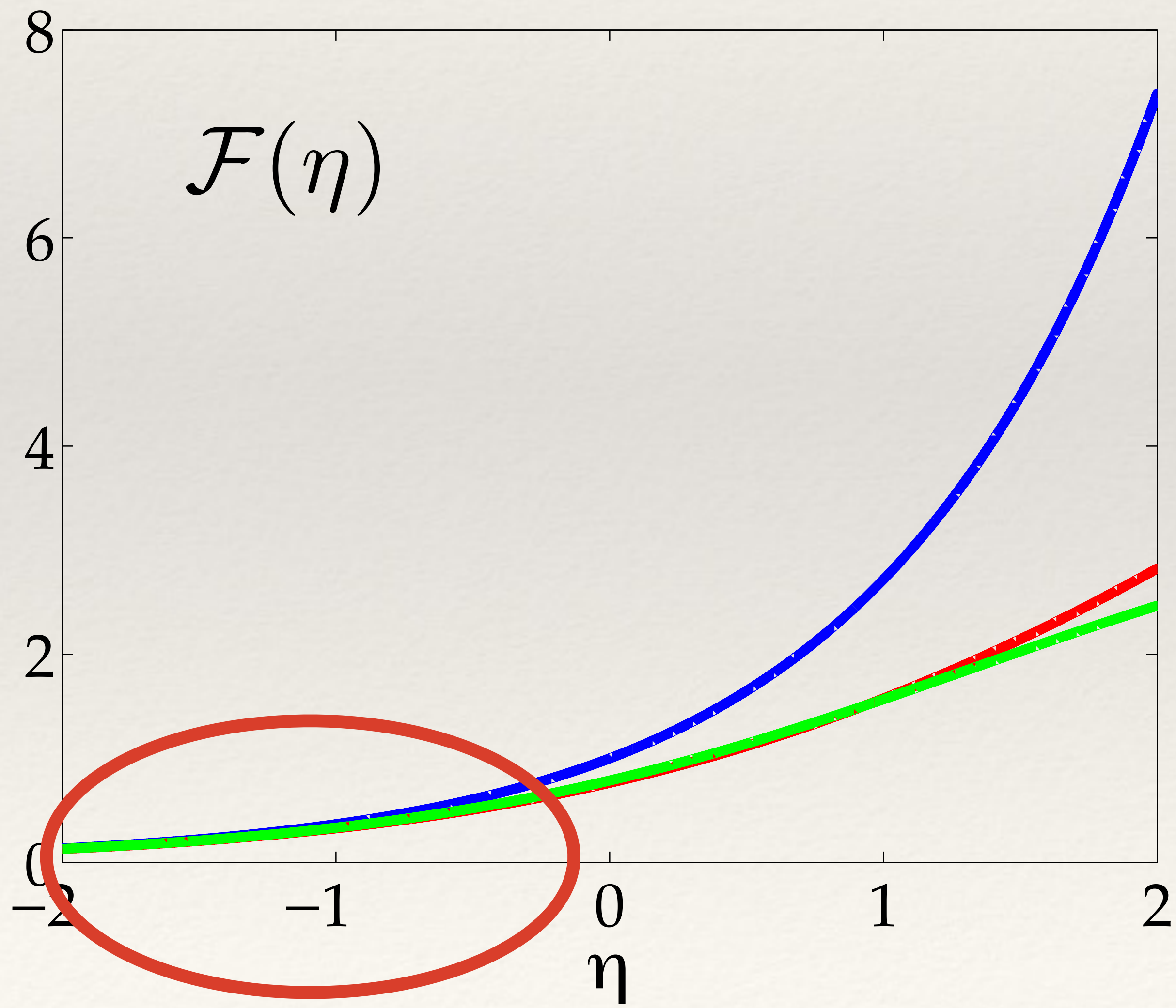
Physics and numerics "easy"



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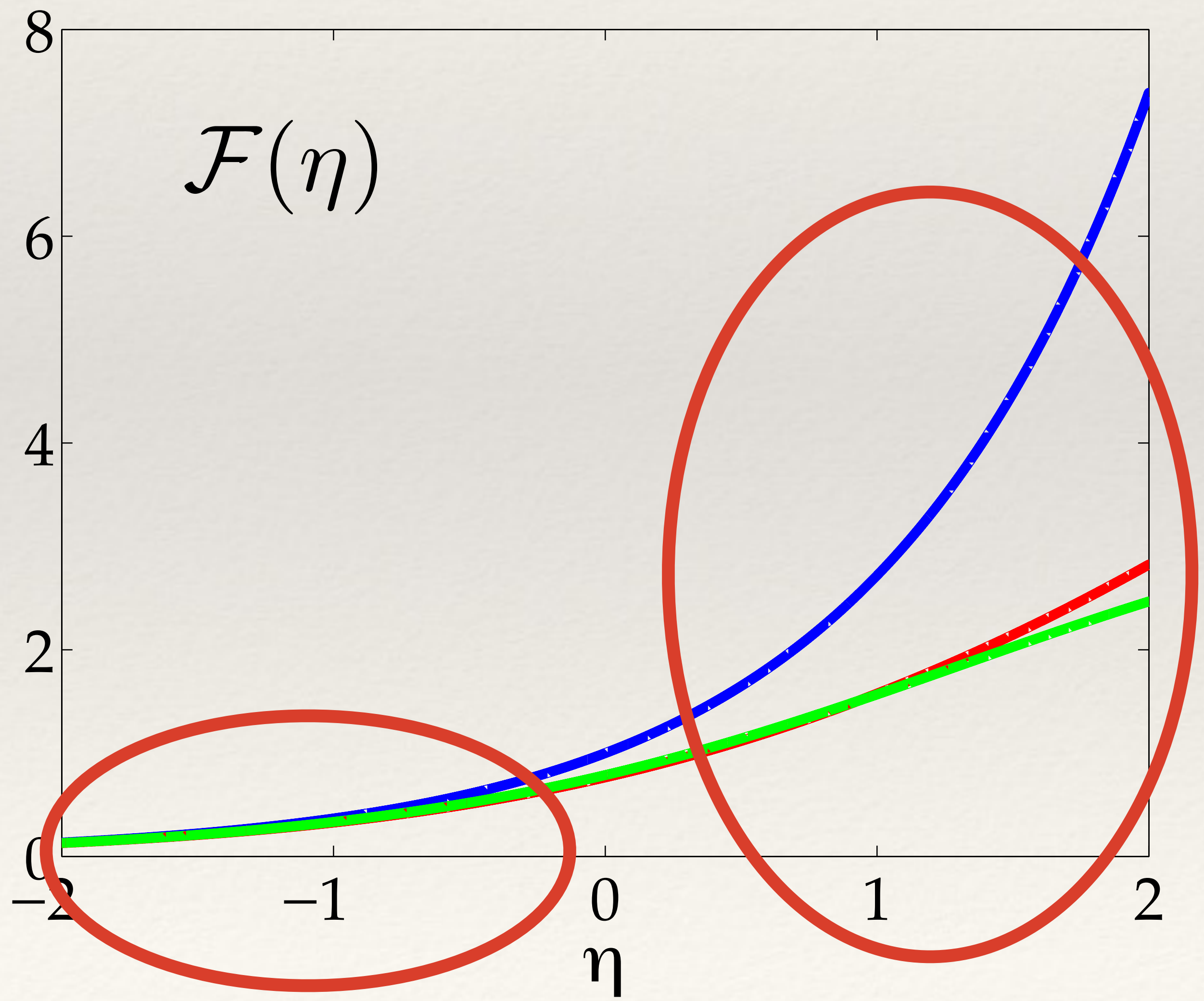

Physics and numerics "complex"

Outline

- semiconductor equations (arb. distribution function) and their discretisation
- discuss three numerical flux approximations
- assess quality by looking at a benchmark

Semiconductor Equations (van Roosbroeck)

For the electrostatic potential, electron and hole densities

$$
\begin{aligned}
-\nabla \cdot (\varepsilon \nabla \psi) &= q(C + p - n) \\
n_t - \frac{1}{q}\nabla \cdot \mathbf{j}_n &= -R(n,p) \\
p_t + \frac{1}{q}\nabla \cdot \mathbf{j}_p &= -R(n,p)
\end{aligned}
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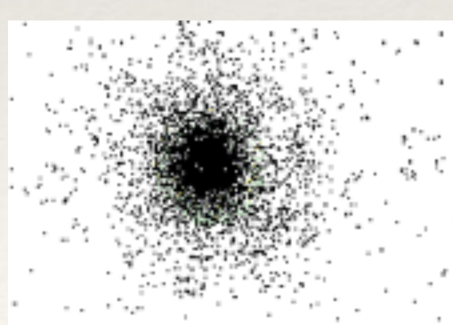
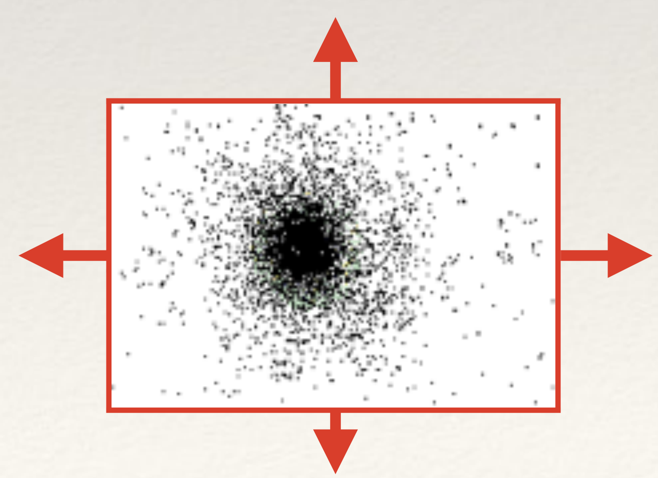


change in mass

=



flow through boundary

Relationships

Currents

Chemical potentials

Diffusion and mobility

Relationships

Currents

$$\mathbf{j}_n = -q\mu_n n \nabla \psi + qD_n \nabla n \quad \text{and} \quad \mathbf{j}_p = -q\mu_p p \nabla \psi - qD_p \nabla p$$

Chemical potentials

Diffusion and mobility

Relationships

Currents

$$\mathbf{j}_n = \underbrace{-q\mu_n n \nabla\psi}_{\text{advection}} + \underbrace{qD_n \nabla n}_{\text{diffusion}} \quad \text{and} \quad \mathbf{j}_p = \underbrace{-q\mu_p p \nabla\psi}_{\text{advection}} - \underbrace{qD_p \nabla p}_{\text{diffusion}}$$

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Chemical potentials

$$n = N_c \mathcal{F}\left(\frac{q(\psi - \varphi_n) + E_{ref} - E_c}{k_B T}\right) \quad \text{and} \quad p = N_v \mathcal{F}\left(-\frac{q(\psi - \varphi_p) + E_{ref} - E_v}{k_B T}\right)$$

Diffusion and mobility

Relationships

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$$n = N_c \mathcal{F}(\eta_n) \quad \text{and} \quad p = N_v \mathcal{F}(\eta_p)$$

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Diffusion and mobility

$$\frac{D_n}{\mu_n U_T} = \frac{n}{N_c} (\mathcal{F}^{-1})' \left(\frac{n}{N_c} \right) \quad \text{and} \quad \frac{D_p}{\mu_p U_T} = \frac{p}{N_v} (\mathcal{F}^{-1})' \left(\frac{p}{N_v} \right)$$

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Chemical potentials

$$n = N_c \mathcal{F}(\eta_n) \quad \text{and} \quad p = N_v \mathcal{F}(\eta_p)$$

Diffusion and mobility

$$\frac{D_n}{\mu_n U_T} = g\left(\frac{n}{N_c}\right) \quad \text{and} \quad \frac{D_p}{\mu_p U_T} = g\left(\frac{p}{N_v}\right)$$

Relationships

Currents

$$\mathbf{j}_n = -q\mu_n \left\{ n\nabla\psi - U_T g\left(\frac{n}{N_c}\right)\nabla n \right\} \quad \text{and} \quad \mathbf{j}_p = -q\mu_p \left\{ p\nabla\psi + U_T g\left(\frac{p}{N_v}\right)\nabla p \right\}$$

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drift and diffusion

quasi Fermi potential

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densities ↔ chemical potentials

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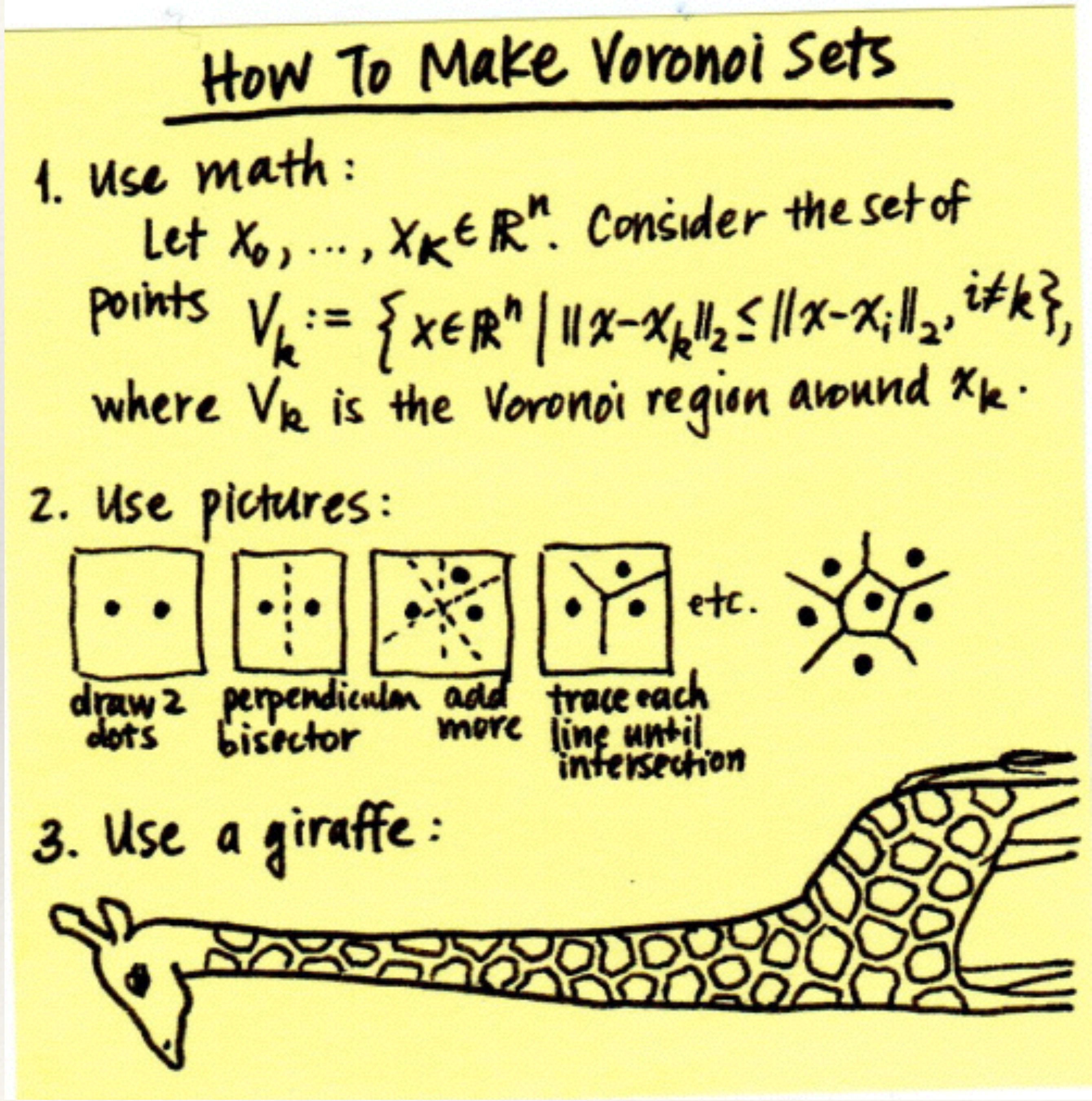
nonlinear

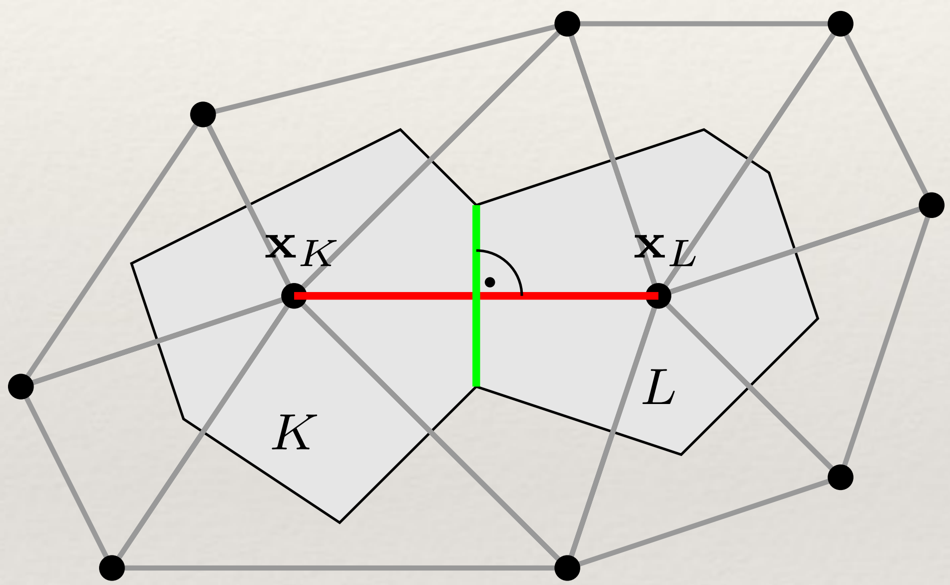
Voronoi Cells



http://postitdoodling.tumblr.com

Voronoi Cells

Flux along 1D edge



Finite Volume Discretisation

$$\nabla \cdot (\varepsilon \nabla \psi) + q(C + p - n) = 0$$

$$\frac{\partial}{\partial t} n - \frac{1}{q} \nabla \cdot \mathbf{j}_n + R(n, p) = 0$$

$$\frac{\partial}{\partial t} p + \frac{1}{q} \nabla \cdot \mathbf{j}_p + R(n, p) = 0$$

Finite Volume Discretisation

$$\int_K \nabla \cdot (\varepsilon \nabla \psi) d\mathbf{x} + q \int_K (C + p - n) d\mathbf{x} = 0$$

$$\frac{\partial}{\partial t} \int_K n d\mathbf{x} - \frac{1}{q} \int_K \nabla \cdot \mathbf{j}_n d\mathbf{x} + \int_K R(n,p) d\mathbf{x} = 0$$

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Finite Volume Discretisation

$$\int_K \nabla \cdot (\varepsilon \nabla \psi) d\mathbf{x} + q|K|(C_K + p_K - n_K) = 0$$

$$\frac{\partial}{\partial t}|K|n_K - \frac{1}{q}\int_K \nabla \cdot \mathbf{j}_n d\mathbf{x} + |K|R(n_K, p_K) = 0$$

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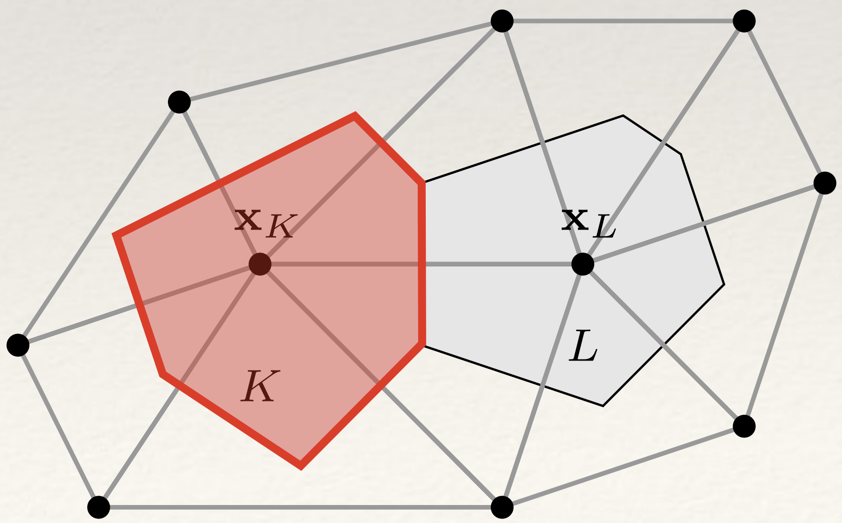

Finite Volume Discretisation

$$\int_{\partial K} \mathbf{n} \cdot (\varepsilon \nabla \psi) dS + q|K|(C_K + p_K - n_K) = 0$$

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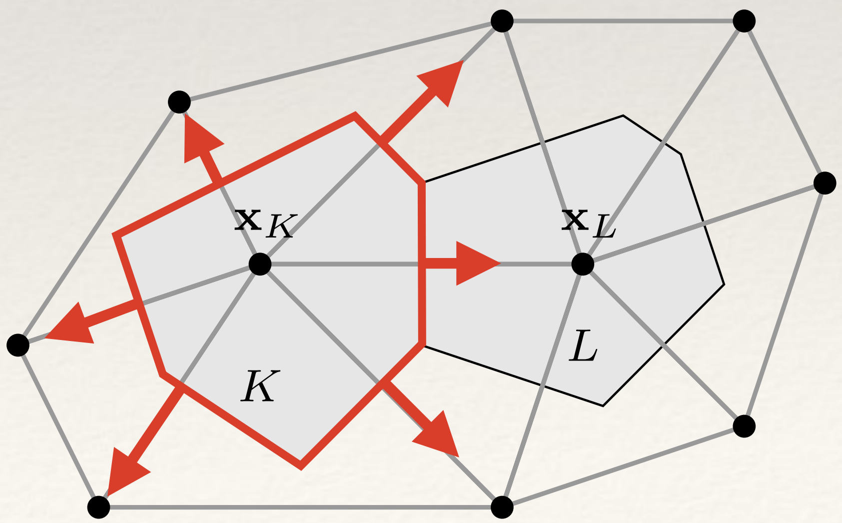

Finite Volume Discretisation

$$\sum_{L \in N(K)} \sigma_{KL} \left(\mathbf{x}_L - \mathbf{x}_K \right) \cdot \left(\varepsilon \nabla \psi \right) + q|K|(C_K + p_K - n_K) = 0$$

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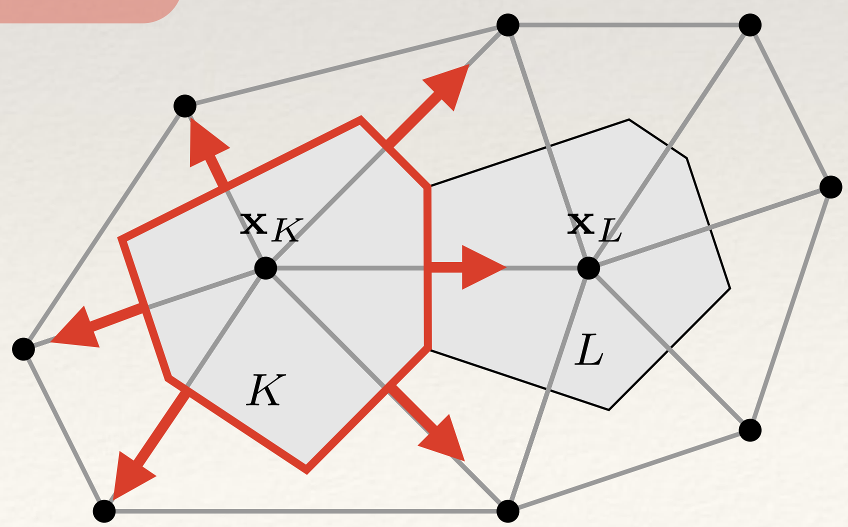

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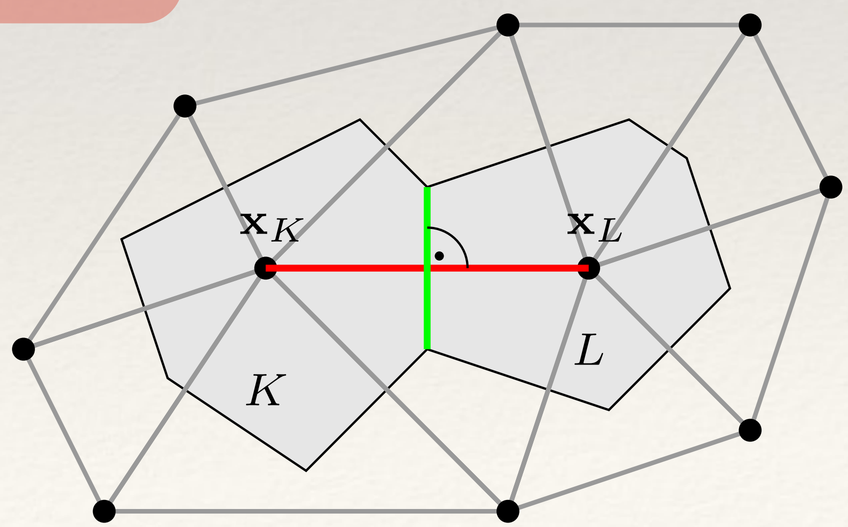

How to choose the fluxes?

Desired properties:

- stable
- preservation of max principle
- approximate boundary layers well
- consistency with thermodynamic equilibrium

Consistency with equilibrium

Zero current leads to

$$\mathbf{0} = \nabla \psi - U_T \nabla \eta_n$$

Consistency with equilibrium

Zero current leads to

$$\mathbf{0} = \nabla\psi - U_T \nabla\eta_n$$

Mimic this numerically via

$$0 = \delta\psi - U_T \delta\eta_n$$

with

$$\delta\psi = \psi_L - \psi_K \qquad \text{and} \qquad \delta\eta = \eta_L - \eta_K$$

Consistency with equilibrium

Zero current leads to

$$\mathbf{0} = \nabla\psi - U_T \nabla \eta_n$$

Mimic this numerically via

Important for coupling!

$$0 = \delta\psi - U_T \delta\eta_n$$

with

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$$\sum_{L\in N(K)} \sigma_{KL}\,(\mathbf{x}_L - \mathbf{x}_K)\cdot(\varepsilon\nabla\psi) + q|K|(C_K + p_K - n_K) = 0$$

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$$\frac{\partial}{\partial t}|K|p_K + \frac{1}{q}\sum_{L\in N(K)} \sigma_{KL}\, j_{p,KL} + |K|R(n_K, p_K) = 0$$

constant!

How to choose the fluxes?

Scharfetter & Gummel (1969) for Boltzmann statistics:

$$\frac{d}{dx} j_{n,KL} = 0 \qquad \text{with} \qquad \begin{aligned} n(\mathbf{x}_K) &= n_K \\ n(\mathbf{x}_L) &= n_L \end{aligned}$$

How to choose the fluxes?

Scharfetter & Gummel (1969) for Boltzmann statistics:

$$\frac{d}{dx} j_n = \frac{d}{dx} q\mu \left\{ U_T \frac{d}{dx} n - n \frac{d}{dx} \psi \right\} = 0 \quad \text{with} \quad \begin{array}{l} n(\mathbf{x}_K) = n_K \\ n(\mathbf{x}_L) = n_L \end{array}$$

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leads to exact solution

$$j = q\mu U_T \left[B\Big(\frac{\delta\psi_{KL}}{U_T}\Big) n_L - B\Big(-\frac{\delta\psi_{KL}}{U_T}\Big) n_K \right],$$

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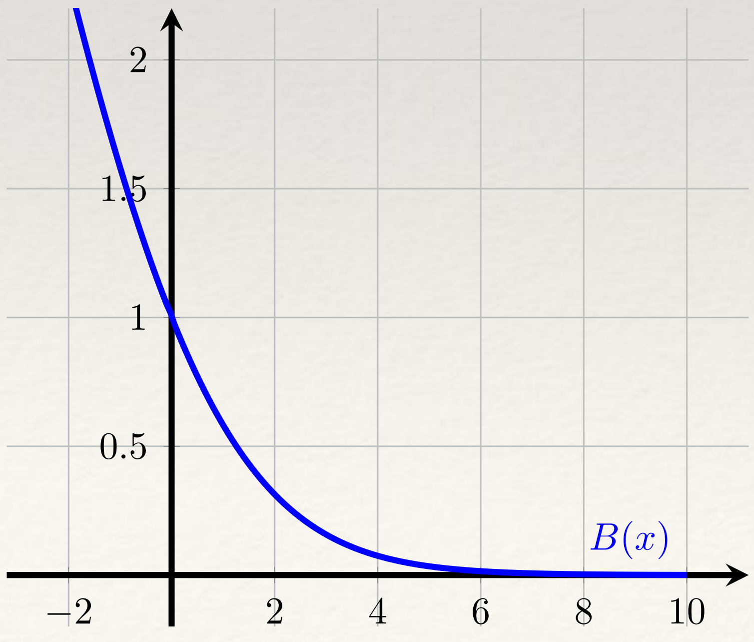

$$B(x) := \frac{x}{e^x - 1}$$

Bernoulli function

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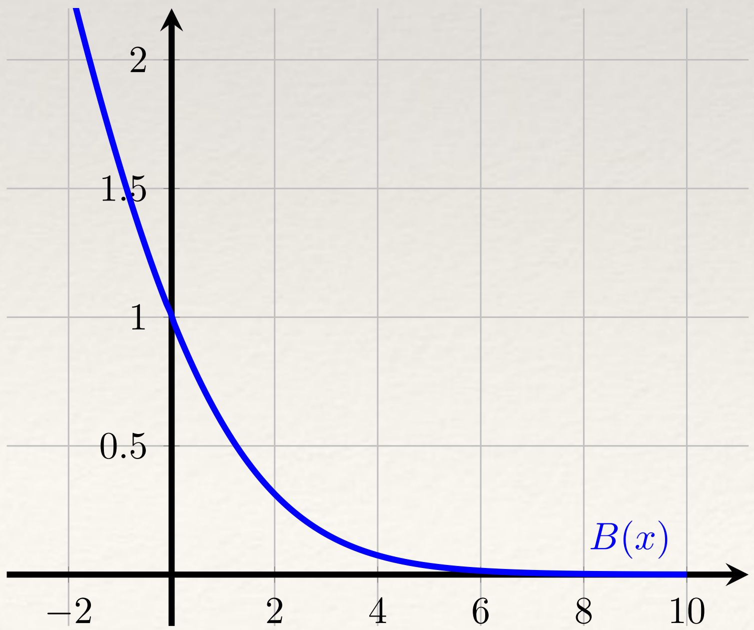

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Bernoulli function

Exact solution for Boltzmann statistics! What about other $\mathcal{F}$?

How to choose the fluxes?

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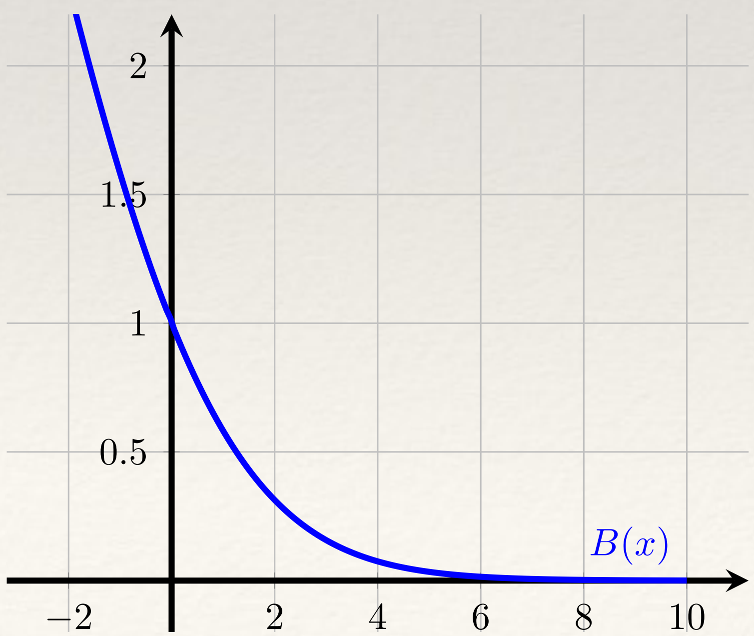

$$B(x) := \frac{x}{e^x - 1}$$

Bernoulli function

Exact solution for Boltzmann statistics! What about other $\mathcal{F}$?

Three flux approx. for Blakemore!

General Scharfetter-Gummel

Koprucki / Gärtner (2013):

$$\frac{d}{dx} j_n = \frac{d}{dx} q\mu \left\{ U_T g\left(\frac{n}{N_c}\right) \frac{d}{dx} n - n \frac{d}{dx} \psi \right\} = 0 \quad \text{with} \quad \begin{aligned} n(\mathbf{x}_K) &= n_K \\ n(\mathbf{x}_L) &= n_L \end{aligned}$$

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Exact solution for Blakemore

$$j = j_0\left\{g\left(\tfrac{n_L}{N_C}\right)B\left(\tfrac{\delta\psi_{KL}}{U_T}+\gamma\tfrac{j}{j_0}\right)\tfrac{n_L}{N_C} - g\left(\tfrac{n_K}{N_C}\right)B\left(-\tfrac{\delta\psi_{KL}}{U_T}-\gamma\tfrac{j}{j_0}\right)\tfrac{n_K}{N_C}\right\}$$

with

$$g(x) = x(\mathcal{F}^{-1})'(x) = \tfrac{1}{1-\gamma x} \qquad \text{and} \qquad j_0 = q\mu N_C U_T$$

General Scharfetter-Gummel

Koprucki / Gärtner (2013):

$$\frac{d}{dx} j_n = \frac{d}{dx} q\mu \left\{ U_T g\left(\frac{n}{N_c}\right) \frac{d}{dx} n - n \frac{d}{dx}\psi \right\} = 0 \quad \text{with} \quad \begin{array}{l} n(\mathbf{x}_K) = n_K \\ n(\mathbf{x}_L) = n_L \end{array}$$

Exact solution for Blakemore

fixed point equation
exact (up to machine precision)

$$j = j_0 \left\{ g\left(\frac{n_L}{N_C}\right) B\left(\frac{\delta\psi_{KL}}{U_T} + \gamma \frac{j}{j_0}\right) \frac{n_L}{N_C} - g\left(\frac{n_K}{N_C}\right) B\left(-\frac{\delta\psi_{KL}}{U_T} - \gamma \frac{j}{j_0}\right) \frac{n_K}{N_C} \right\}$$

with

$$g(x) = x(\mathcal{F}^{-1})'(x) = \frac{1}{1-\gamma x} \qquad \text{and} \qquad j_0 = q\mu N_C U_T$$

Diffusion averaging

Bessemoulin-Chatard (2012) and Koprucki et al. (2014):

$$\frac{d}{dx} j_n = \frac{d}{dx} q\mu \left\{ U_T g\left(\frac{n}{N_c}\right) \frac{d}{dx} n - n \frac{d}{dx} \psi \right\} = 0 \quad \text{with} \quad \begin{matrix} n(\mathbf{x}_K) = n_K \\ n(\mathbf{x}_L) = n_L \end{matrix}$$

Diffusion averaging

Bessemoulin-Chatard (2012) and Koprucki et al. (2014):

$$j = q\mu U_T \bar{g}_{KL} \left[B\left(-\frac{\delta\psi_{KL}}{U_T \bar{g}_{KL}} \right) n_K - B\left(\frac{\delta\psi_{KL}}{U_T \bar{g}_{KL}} \right) n_L \right]$$

Diffusion averaging

Bessemoulin-Chatard (2012) and Koprucki et al. (2014):

$$j = q\mu U_T \bar{g}_{KL} \left[B\left(-\frac{\delta\psi_{KL}}{U_T \bar{g}_{KL}} \right) n_K - B\left(\frac{\delta\psi_{KL}}{U_T \bar{g}_{KL}} \right) n_L \right]$$

where

$$\bar{g}_{KL} = \frac{\mathcal{F}^{-1}\left(\frac{n_L}{N_c}\right) - \mathcal{F}^{-1}\left(\frac{n_K}{N_c}\right)}{\log(n_L/N_c) - \log(n_K/N_c)}$$

only consistent average!

approximates

$$g(x) = x(\mathcal{F}^{-1})'(x) = \frac{(\mathcal{F}^{-1})'(x)}{\log'(x)}$$

Inverse Activity Coefficients

Fuhrmann (2015):

$$\frac{d}{dx} j_n = \frac{d}{dx}\left(-q\mu N_c \beta(\eta) e^{\eta} \frac{d}{dx}\varphi_n\right) = 0 \quad \text{with} \quad \begin{aligned} \eta(\mathbf{x}_K) &= \eta_K \\ \eta(\mathbf{x}_L) &= \eta_L \end{aligned}$$

with $\beta(\eta) = \dfrac{\mathcal{F}(\eta)}{e^{\eta}}$ leads to

Inverse Activity Coefficients

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with $\beta(\eta) = \dfrac{\mathcal{F}(\eta)}{e^{\eta}}$ leads to

$$j = -q\mu U_T N_c \beta_{KL} \left\{ e^{\eta_L} B\left(\frac{\delta\psi_{KL}}{U_T}\right) - e^{\eta_k} B\left(-\frac{\delta\psi_{KL}}{U_T}\right)\right\}$$

Inverse Activity Coefficients

Fuhrmann (2015):

$$\frac{d}{dx} j_n = \frac{d}{dx}\left(-q\mu N_c \beta(\eta) e^{\eta} \frac{d}{dx}\varphi_n\right) = 0 \quad \text{with} \quad \begin{array}{c} \eta(\mathbf{x}_K) = \eta_K \\ \eta(\mathbf{x}_L) = \eta_L \end{array}$$

with $\beta(\eta) = \dfrac{\mathcal{F}(\eta)}{e^{\eta}}$ leads to

consistent for any average!

$$j = -q\mu U_T N_c \beta_{KL} \left\{ e^{\eta_L} B\left(\frac{\delta\psi_{KL}}{U_T}\right) - e^{\eta_k} B\left(-\frac{\delta\psi_{KL}}{U_T}\right)\right\}$$

where

$$\beta_{KL} = \frac{\beta(\eta_K) + \beta(\eta_L)}{2} \in [\beta(\eta_K), \beta(\eta_L)]$$

Compare three schemes

- General Scharfetter-Gummel

$$j_{\mathrm{GENSG}} = j_0 \left\{ e^{\eta_L} B\left(\delta\psi_{KL} + \gamma \frac{j}{j_0}\right) - e^{\eta_K} B\left(-\delta\psi_{KL} - \gamma \frac{j}{j_0}\right) \right\}$$

- Diffusion enhanced Scharfetter-Gummel

$$j_{\mathrm{DESG}} = j_0 g_{KL} \left\{ \mathcal{F}(\eta_L) B\left(\frac{\delta\psi_{KL}}{g_{KL}}\right) - \mathcal{F}(\eta_K) B\left(-\frac{\delta\psi_{KL}}{g_{KL}}\right) \right\}$$

- Inverse activity based scheme

$$j_{\mathrm{IACT}} = j_0 \beta_{KL} \left\{ e^{\eta_L} B\left(\delta\psi_{KL}\right) - e^{\eta_K} B\left(-\delta\psi_{KL}\right) \right\}$$

How to design a benchmark?

Leave equilibrium!

$$\delta\varphi_{KL} = -\delta\eta_{KL} + \delta\psi_{KL} \qquad \nabla\varphi = -\nabla\eta + \nabla\psi$$

How to design a benchmark?

Leave equilibrium!

$$\delta\varphi_{KL} = -\delta\eta_{KL} + \delta\psi_{KL}$$

$$\nabla\varphi = -\nabla\eta + \nabla\psi$$

$$\frac{h_{KL}}{L}\delta\psi$$ (linear potential)

coarse grid

large bias

How to design a benchmark?

Leave equilibrium!

$$\delta\varphi_{KL} = -\delta\eta_{KL} + \delta\psi_{KL}$$

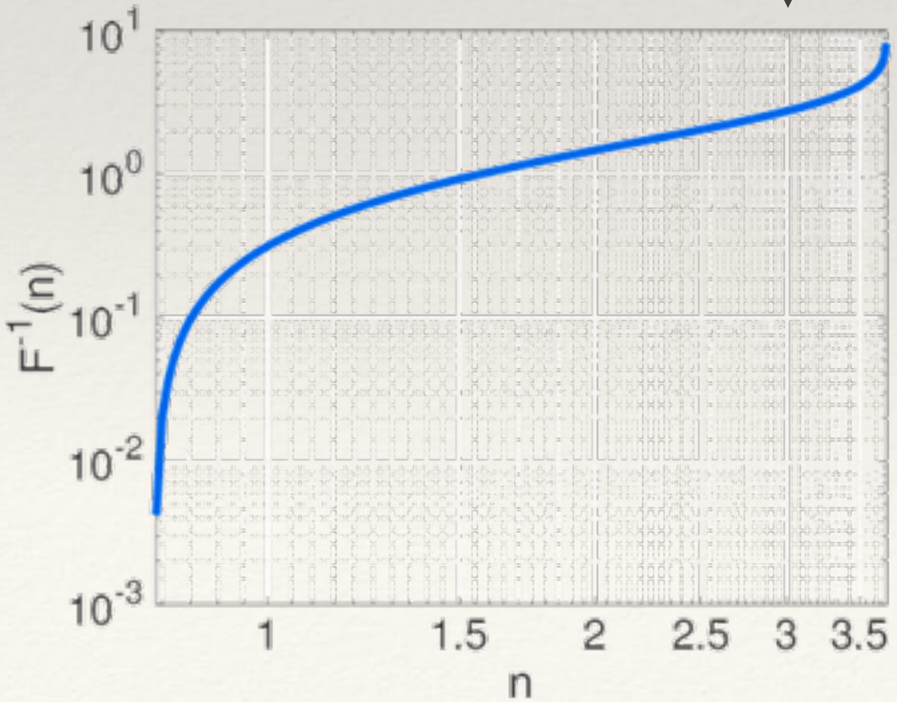
$$\nabla\varphi = -\nabla\eta + \nabla\psi$$

large contrast
with opposite sign

$$\frac{h_{KL}}{L}\delta\psi$$ (linear potential)

coarse grid

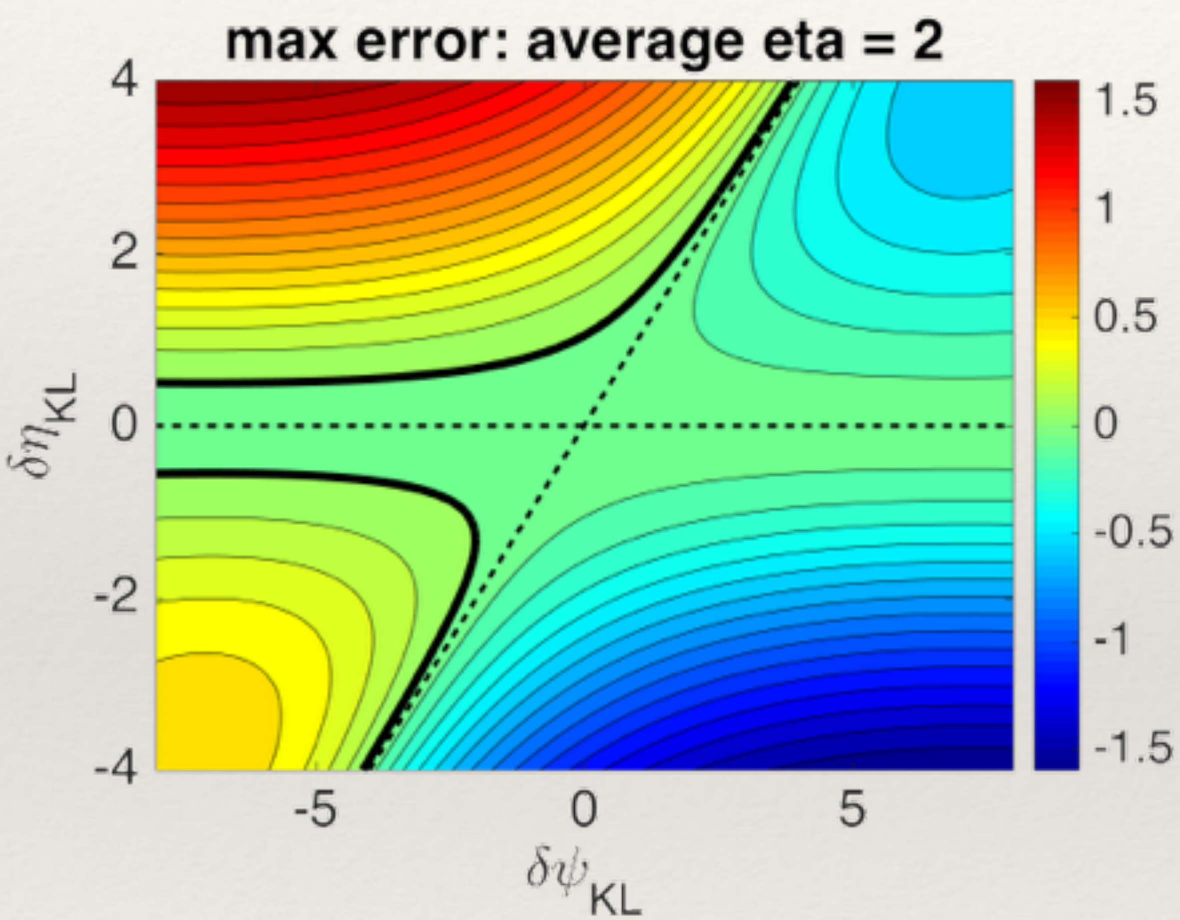
large bias



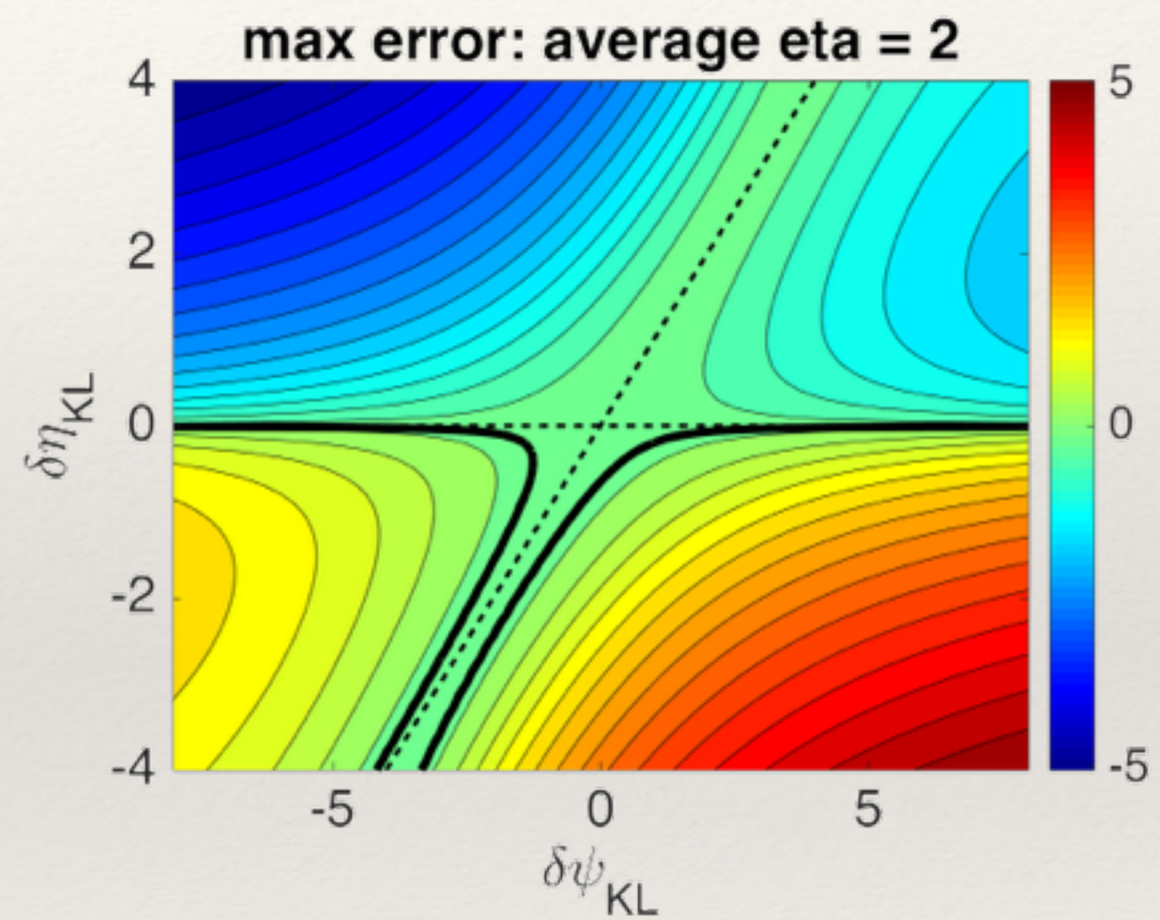
$\eta = \mathcal{F}^{-1}(n)$

large density contrast

Errors between schemes



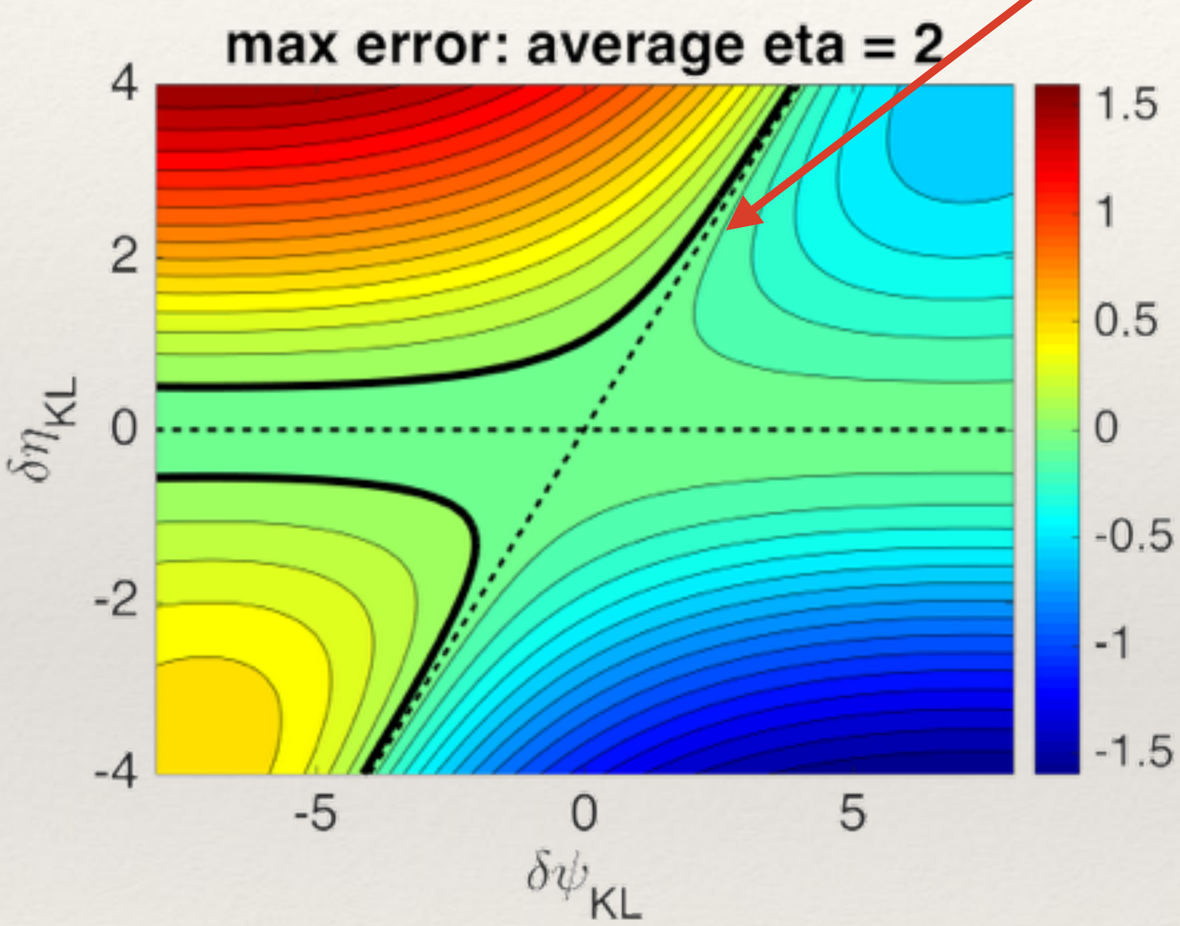
diffusion enhanced vs general SG

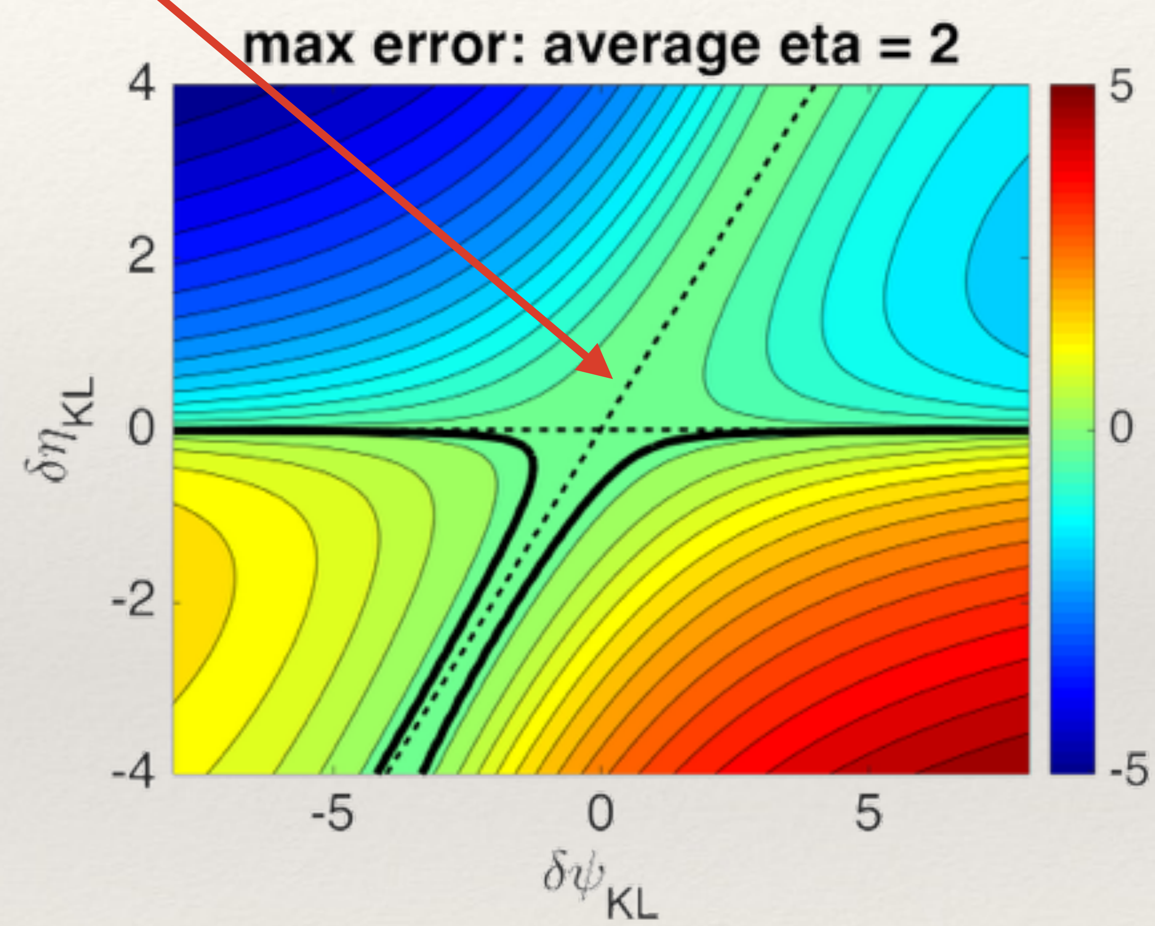


inverse act. vs general SG

Errors between schemes

$\delta\psi_{KL} = \delta\eta_{KL}$



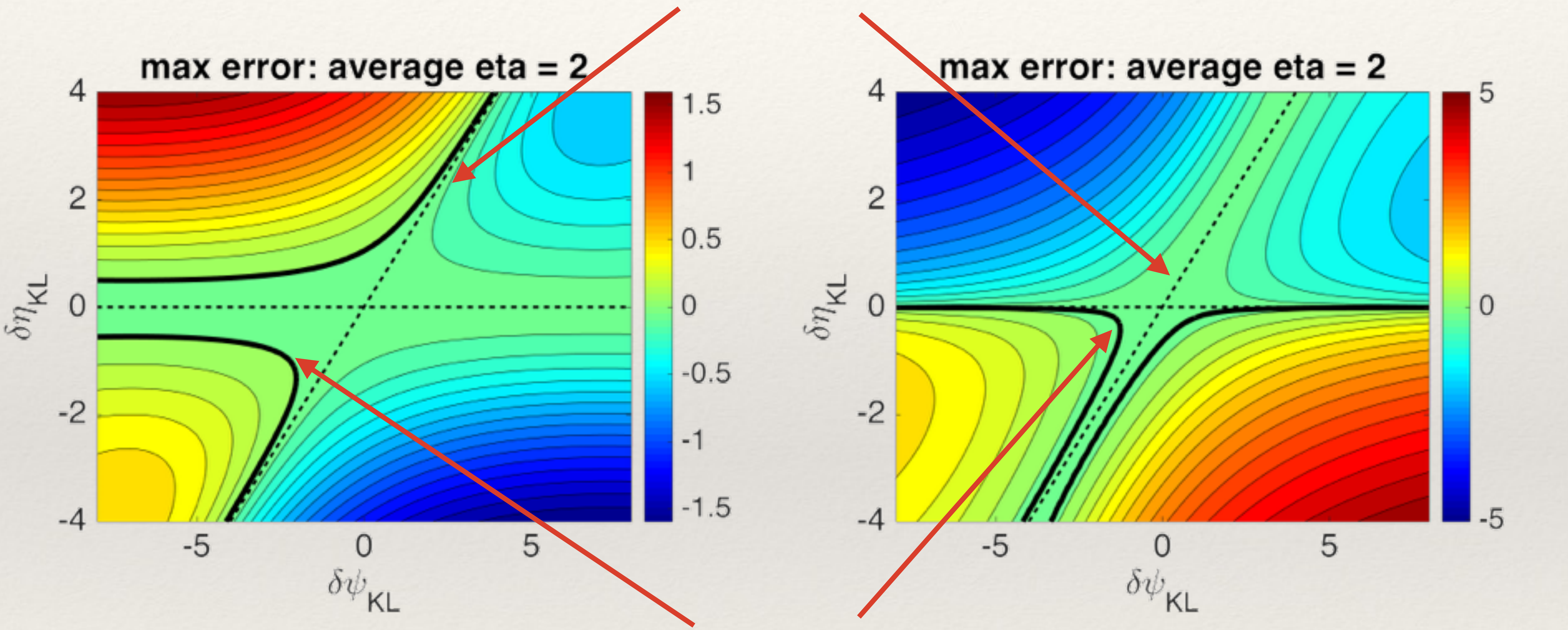


diffusion enhanced vs general SG

inverse act. vs general SG

Errors between schemes

$$\delta\psi_{KL} = \delta\eta_{KL}$$

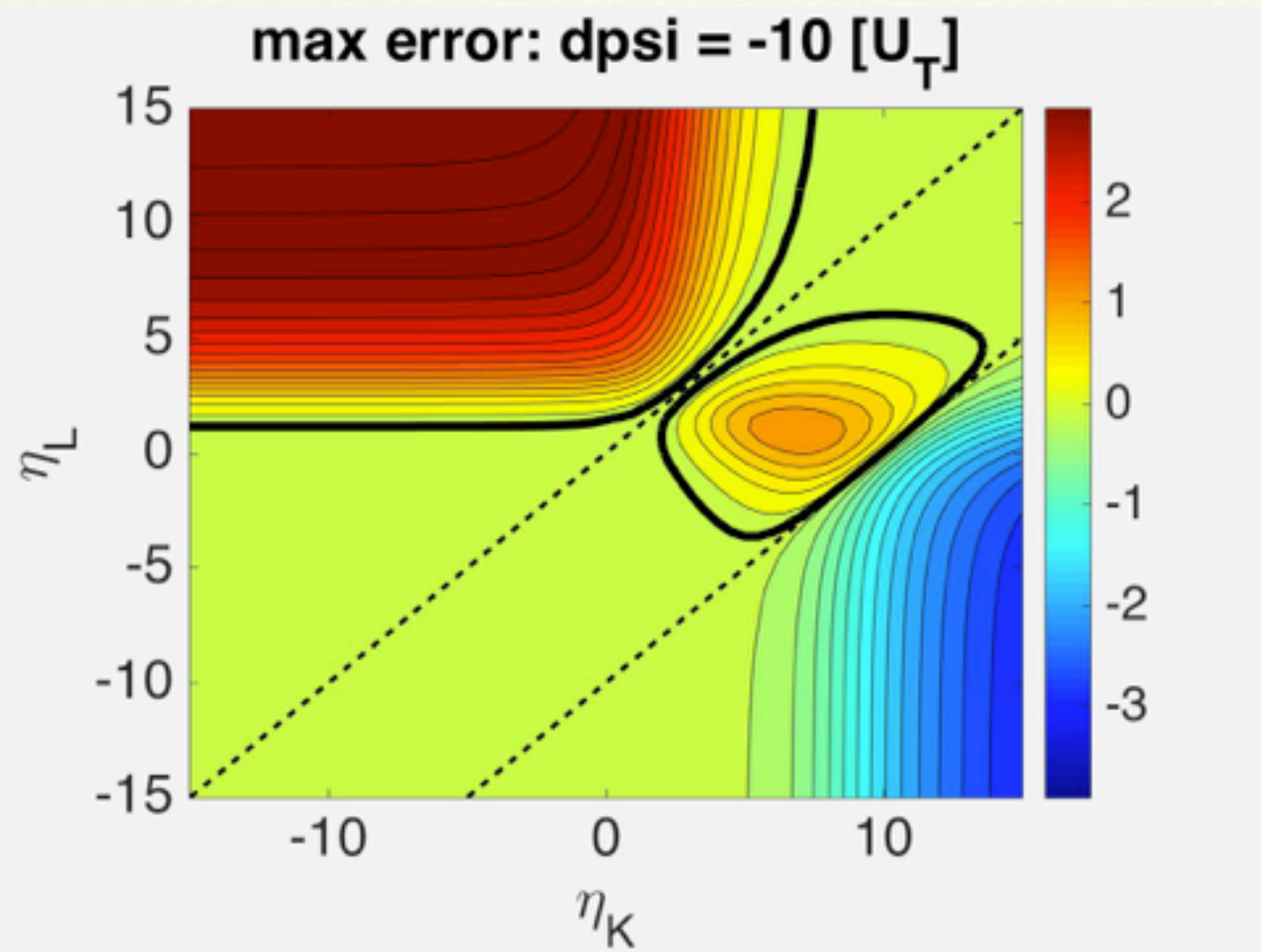


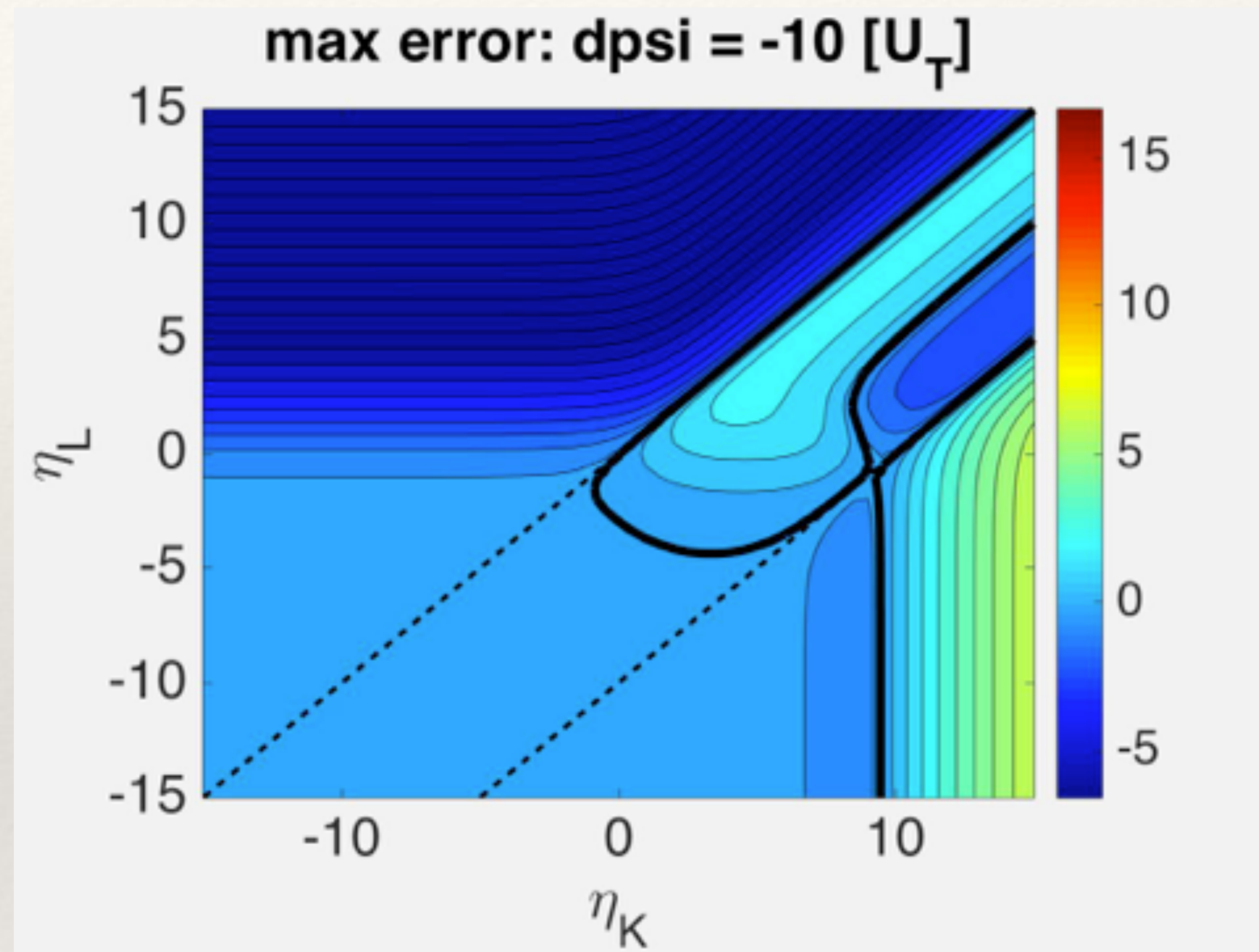
same contour line

diffusion enhanced vs general SG

inverse act. vs general SG

Errors between schemes





diffusion enhanced vs general SG

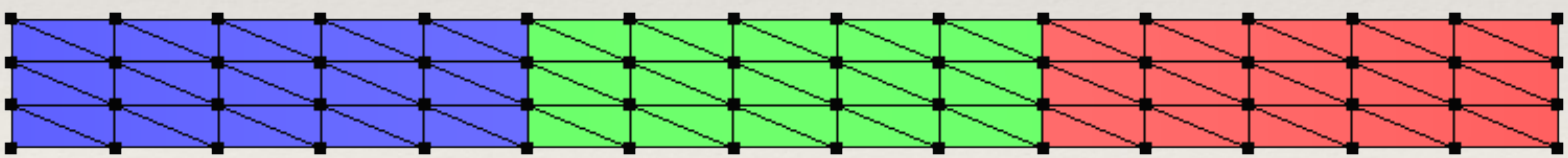
inverse act. vs general SG

pin

$N_I = 0.00/\text{cm}^3$

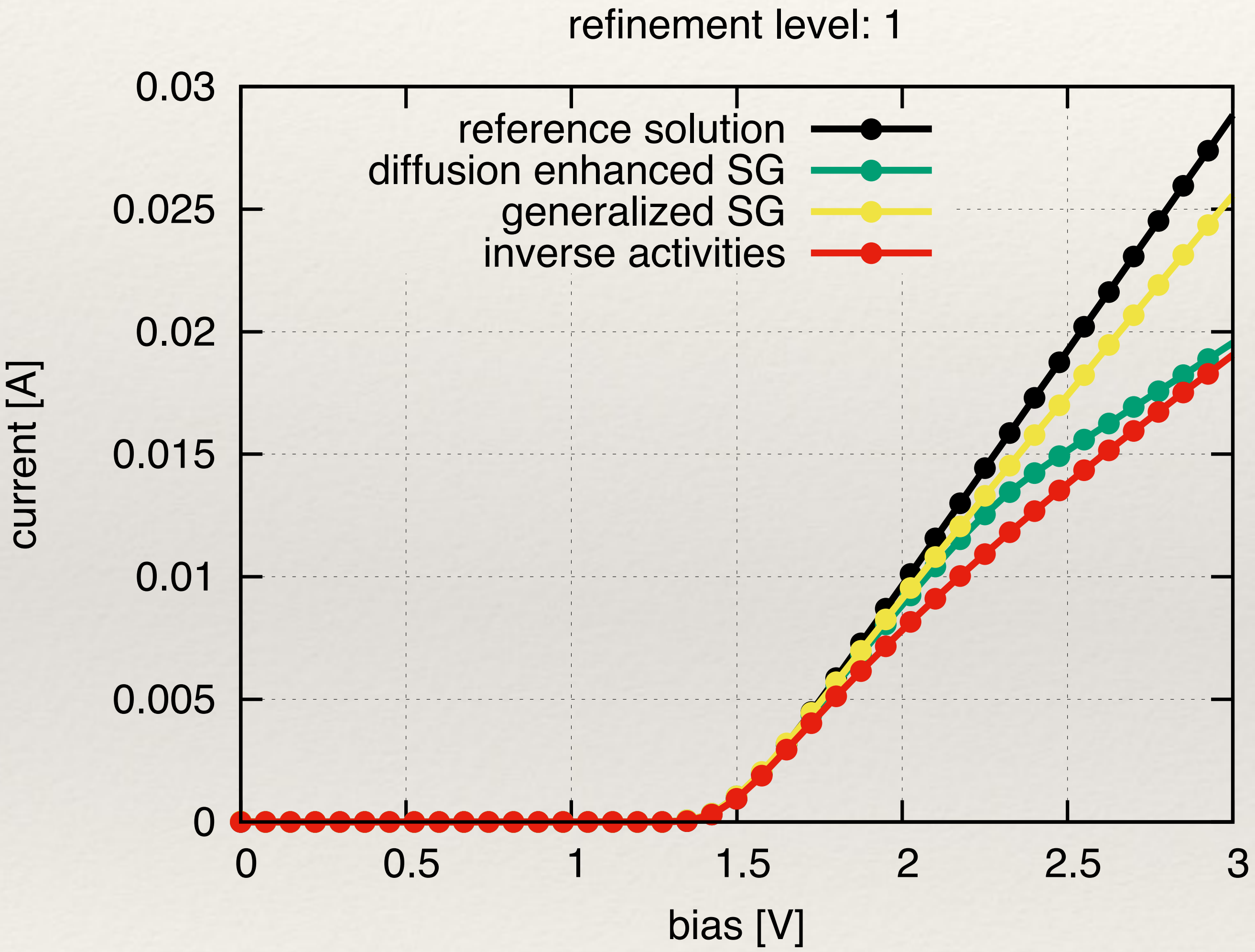
$N_A = 4.35 \times 10^{17}/\text{cm}^3$

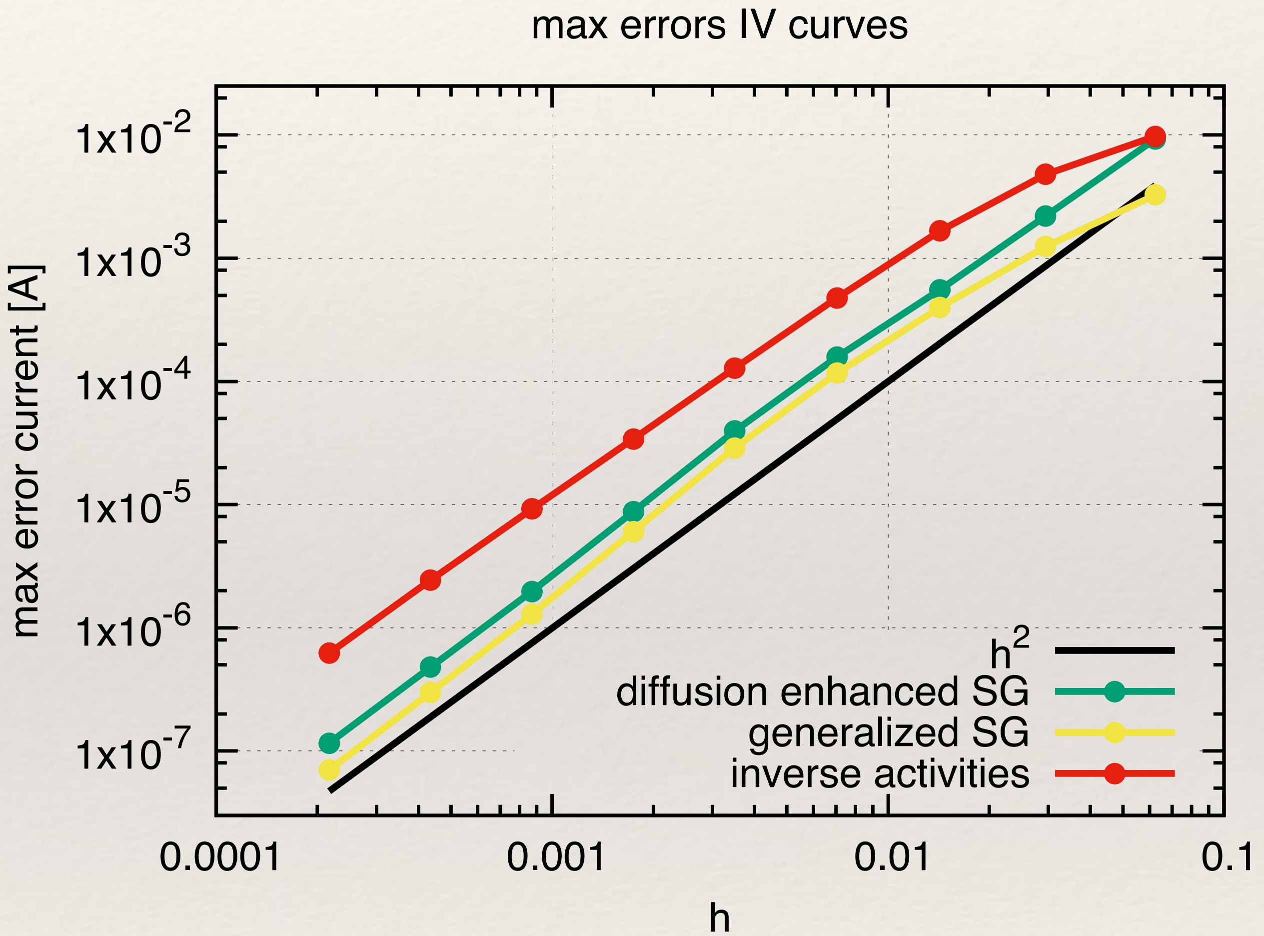
$N_D = 4.20 \times 10^{18}/\text{cm}^3$



How do schemes influence current and electrostatic potential?

IV curves


refinement level: 1
reference solution
diffusion enhanced SG
generalized SG
inverse activities
current [A]
bias [V]
0.03
0.025
0.02
0.015
0.01
0.005
0
0
0.5
1
1.5
2
2.5
3

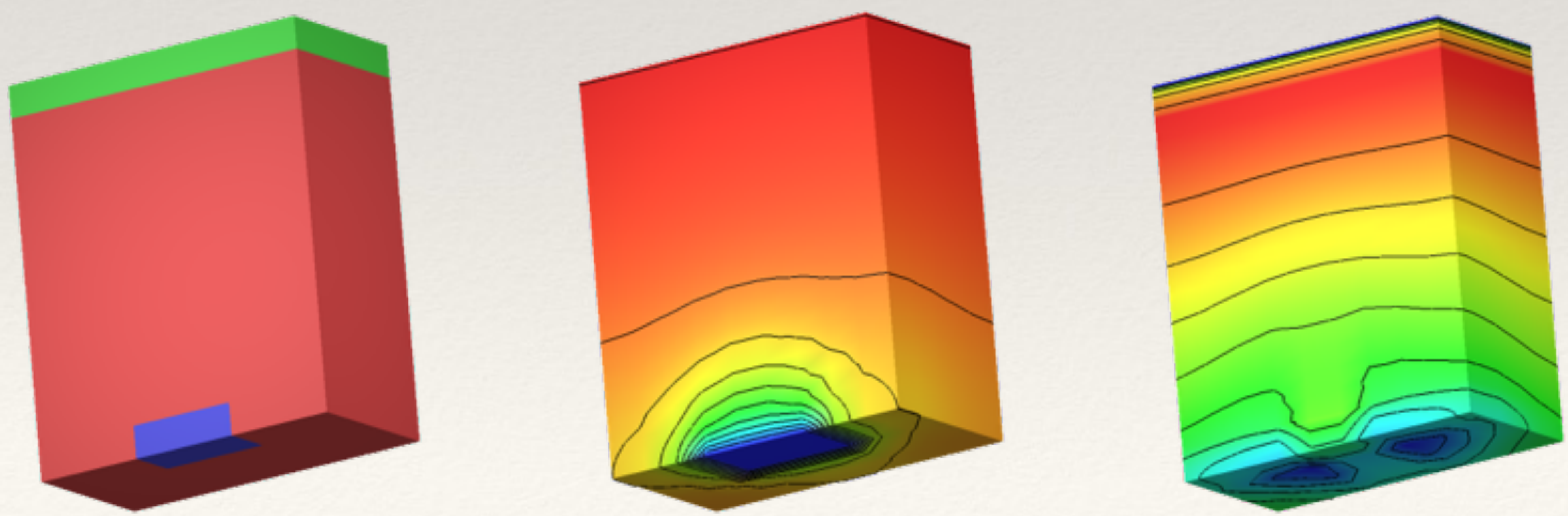

max errors IV curves
max error current [A]
h
h^2
diffusion enhanced SG
generalized SG
inverse activities
$1x10^{-2}$
$1x10^{-3}$
$1x10^{-4}$
$1x10^{-5}$
$1x10^{-6}$
$1x10^{-7}$
0.0001
0.001
0.01
0.1

Results

- three thermodynamically consistent schemes (Blakemore)
- all schemes converge to SG for large negative η
- pin benchmark useful to discriminate accuracy
- exact scheme yields best current approximation; diffusion enhanced scheme good for electrostatic field
- other factors: computation times need to be considered

Outlook

- prototype: ddfermi
- moderately-sized 2D/3D problems
- different variables: heterostructure
- we welcome applications!



Muchas gracias
por su atención!

Thank you for your attention!