Continuous upscaling

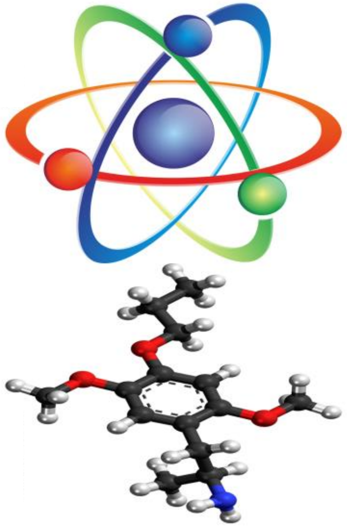
Alexander A. Shapiro

Publications:
Physics of fluids 36 (2024), 027118
Chemical Engineering Science 248 (2022), 117247
Chemical Engineering Science 234 (2021), 116454

Prepared for the online PoreLab Seminar
May 15, 2024

Multiple scales in physics

Atoms and molecules



Macro-world

Earth

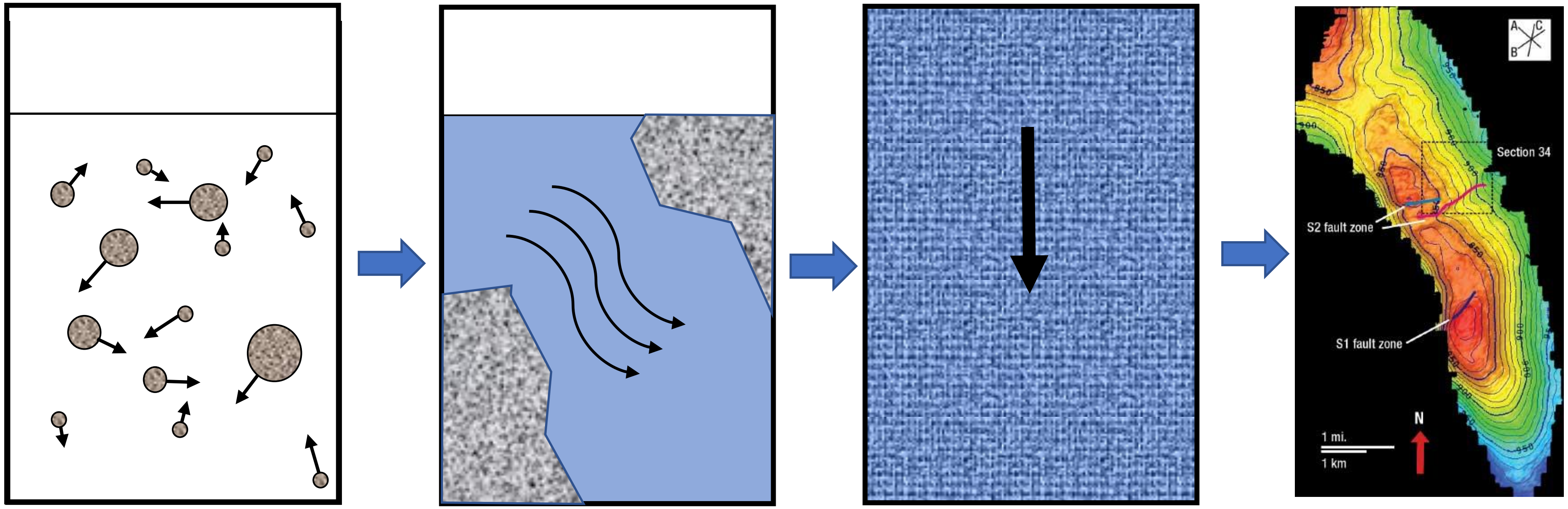
Universe

<u>Physics</u>: What is the difference and the interaction between the different “worlds”?

<u>Mathematics</u>: How the asymptotic transitions between the different scales are organized?

Multiple scales in porous media

Molecular scale | **Hydrodynamic (pore) scale** | **Continuous (Darcy) scale** | **Reservoir scale**



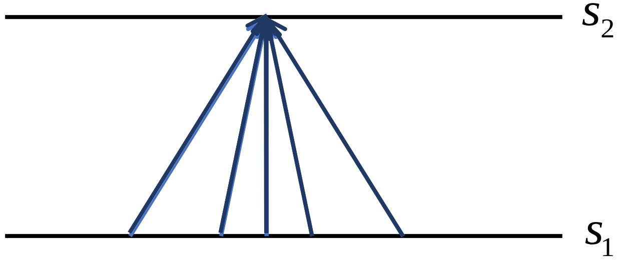
Molecular dynamics | Hydrodynamics (Navier-Stokes) | Hydrodynamics in porous media (Darcy) | Geological heterogeneity

How to transfer:

- From the molecular properties to the flow equations
- From the laboratory experiments to the reservoir level
- From the fine-grid to the coarse-grid reservoir description
- .....

Gray, Miller: Introduction to thermodynamics constrained averaging, 2014

Traditional ways of upscaling:



Simple averaging

$$\langle m\rangle(x) = \frac{1}{V}\int_{V-x} m(y)dy$$

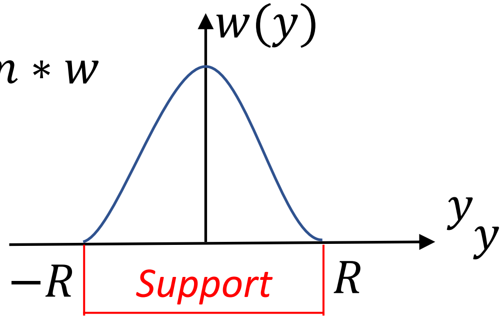
R.E-V – representative elementary volume

Weight averaging

$$\langle m\rangle(x) = \int m(x-y)w(y)dy = m * w$$

Here $w(y)$ is the weight function:

$$\int w(y)dy = 1$$



Mention non-uniqueness

<u>Other methods are system-specific</u>

(statistical mechanics, homogenization in periodic media, multiphase flows in porous media,…)

Weight averaging as averaging over "random step"

$$\langle m \rangle(x) = \int m(x-y)w(y)dy = m * w$$

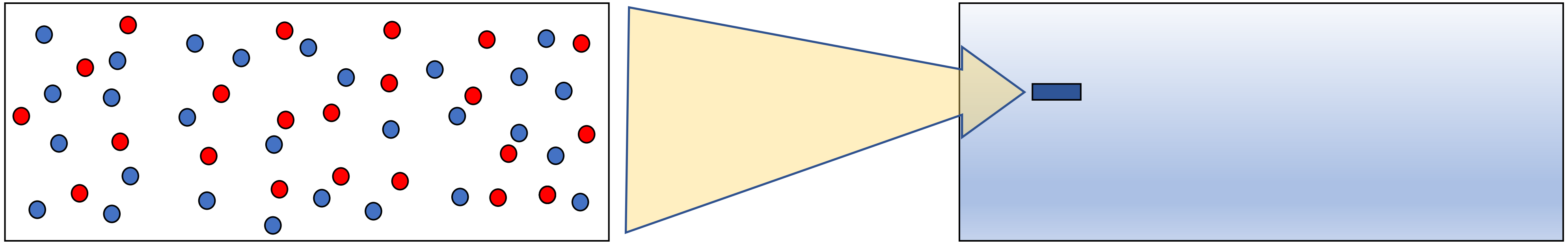
Consider a random variable ("step") $\boldsymbol{Y}$ with the distribution $w(y)$. The last equality may be interpreted as

$$\boxed{\langle m \rangle(x) = \langle m(x-\boldsymbol{Y}) \rangle,}$$

where averaging on the rhs is over all $\boldsymbol{Y}$.

That is, *weighted averaging may be interpreted as an average value of a density in a given point, coming there by a random step.*

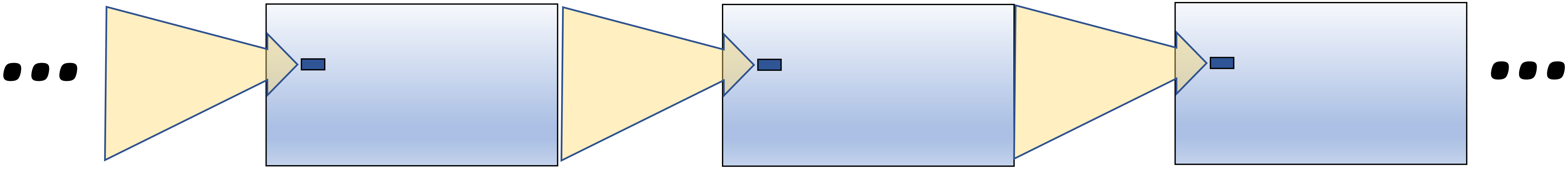
Asymptotics – R.E.V. (representative elementary volume)



The R.E.V. should be “infinitely large” compared to molecular sizes…

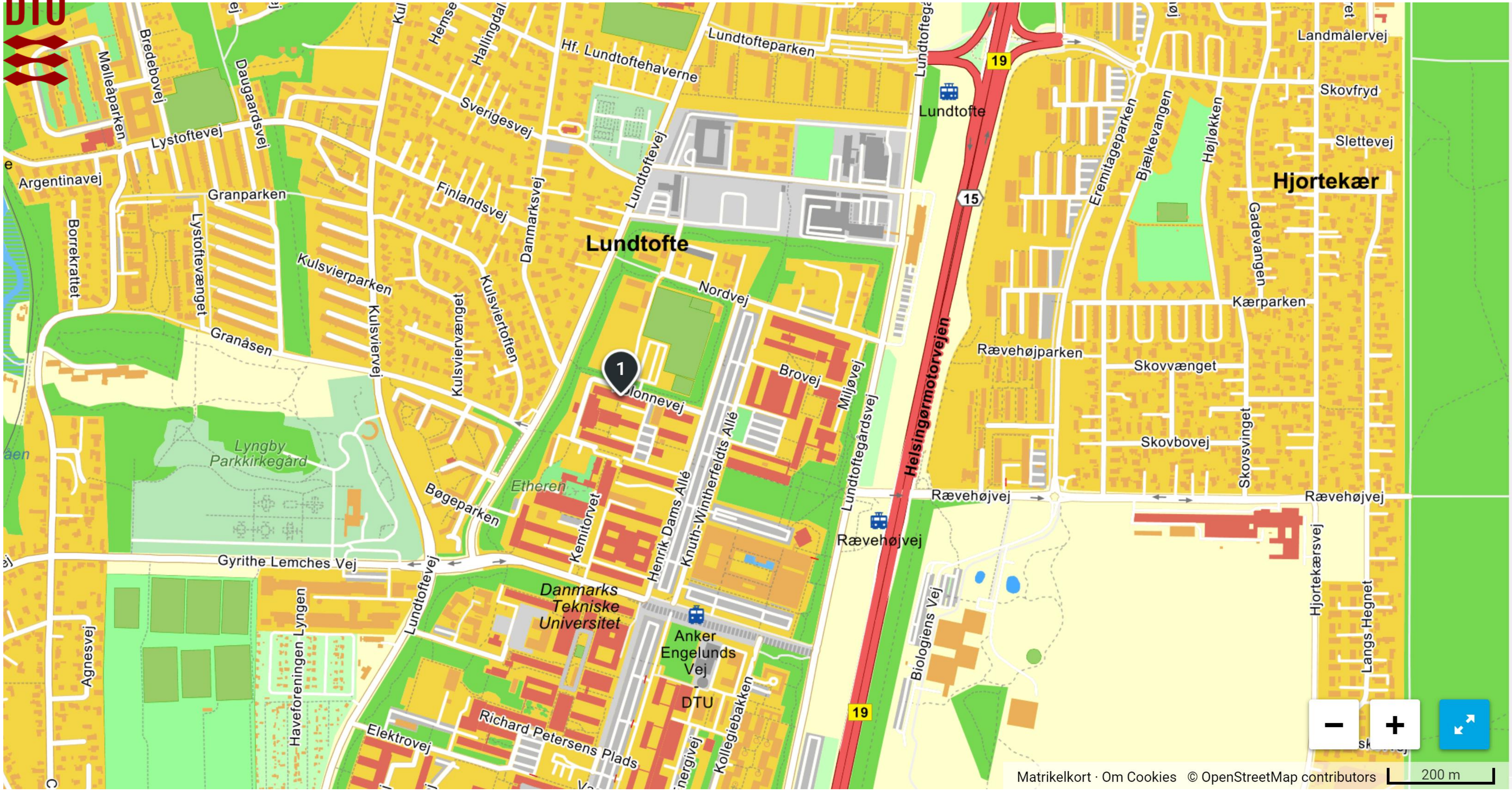
…but “infinitely small” compared to the size of a problem

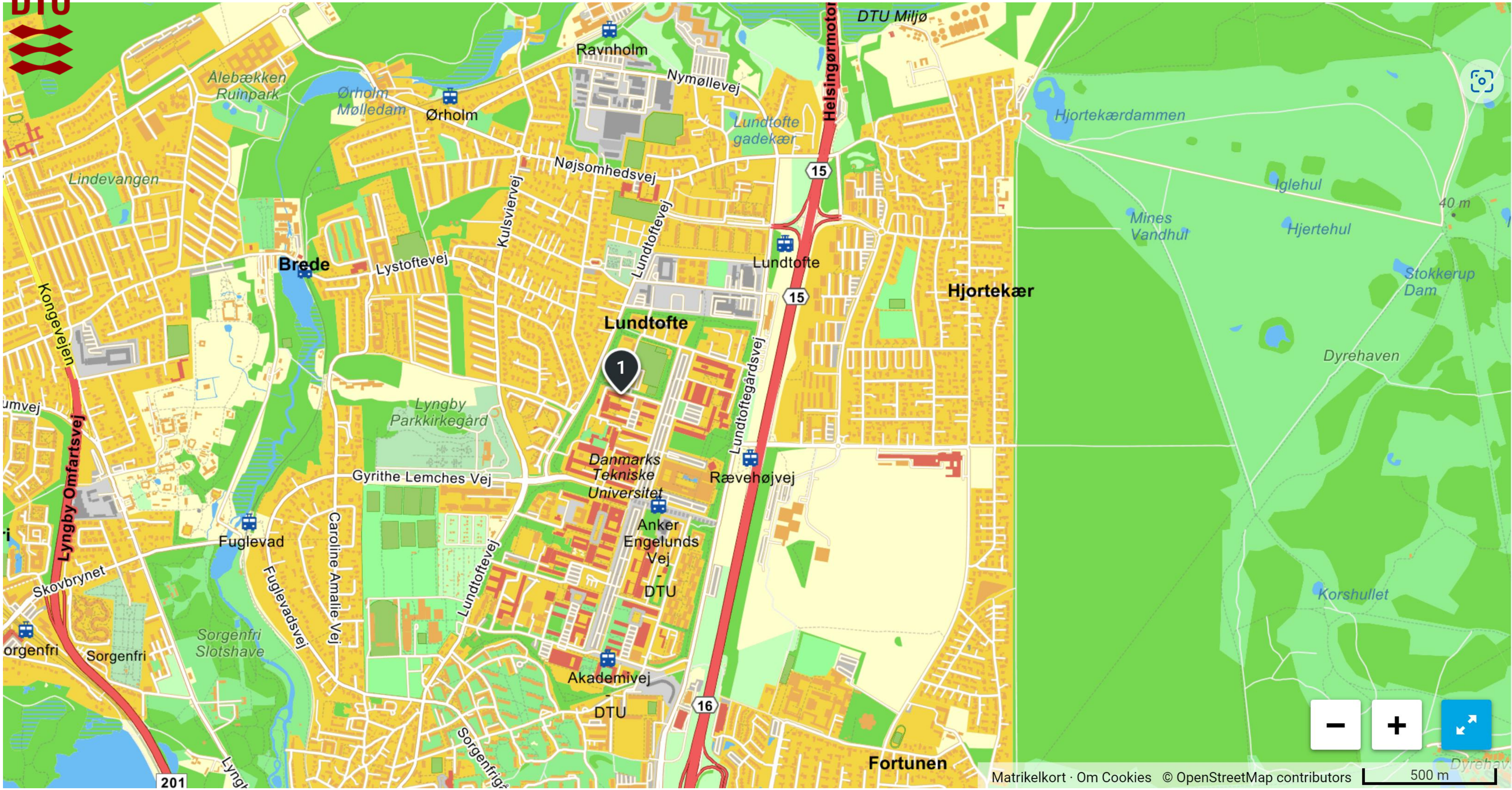
- ***How is this transition made mathematically?***
- ***What happens with multiple asymptotic transitions?***
- ***Is the result unique, or it depends on a procedure?***



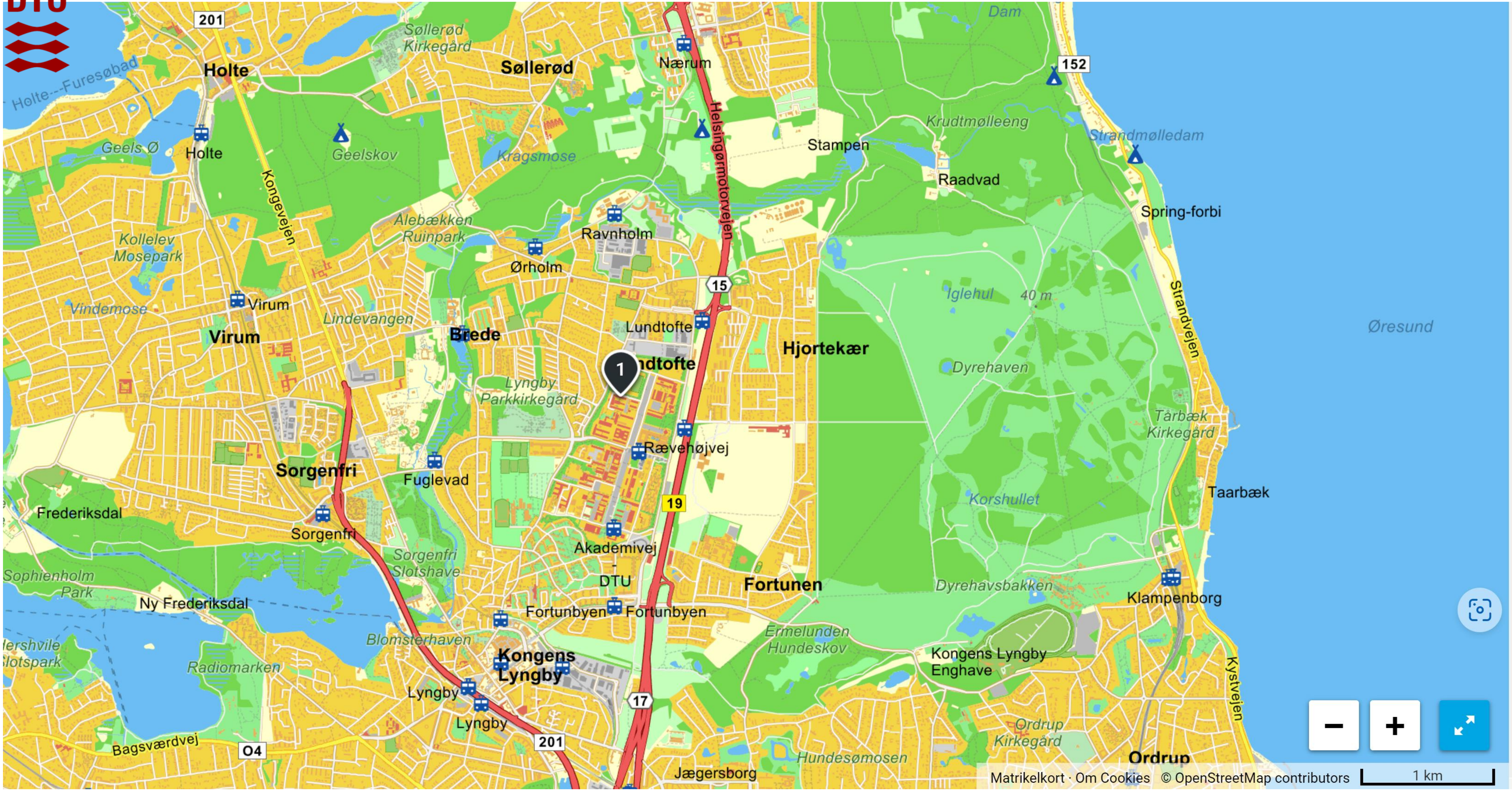
Continuous upscaling

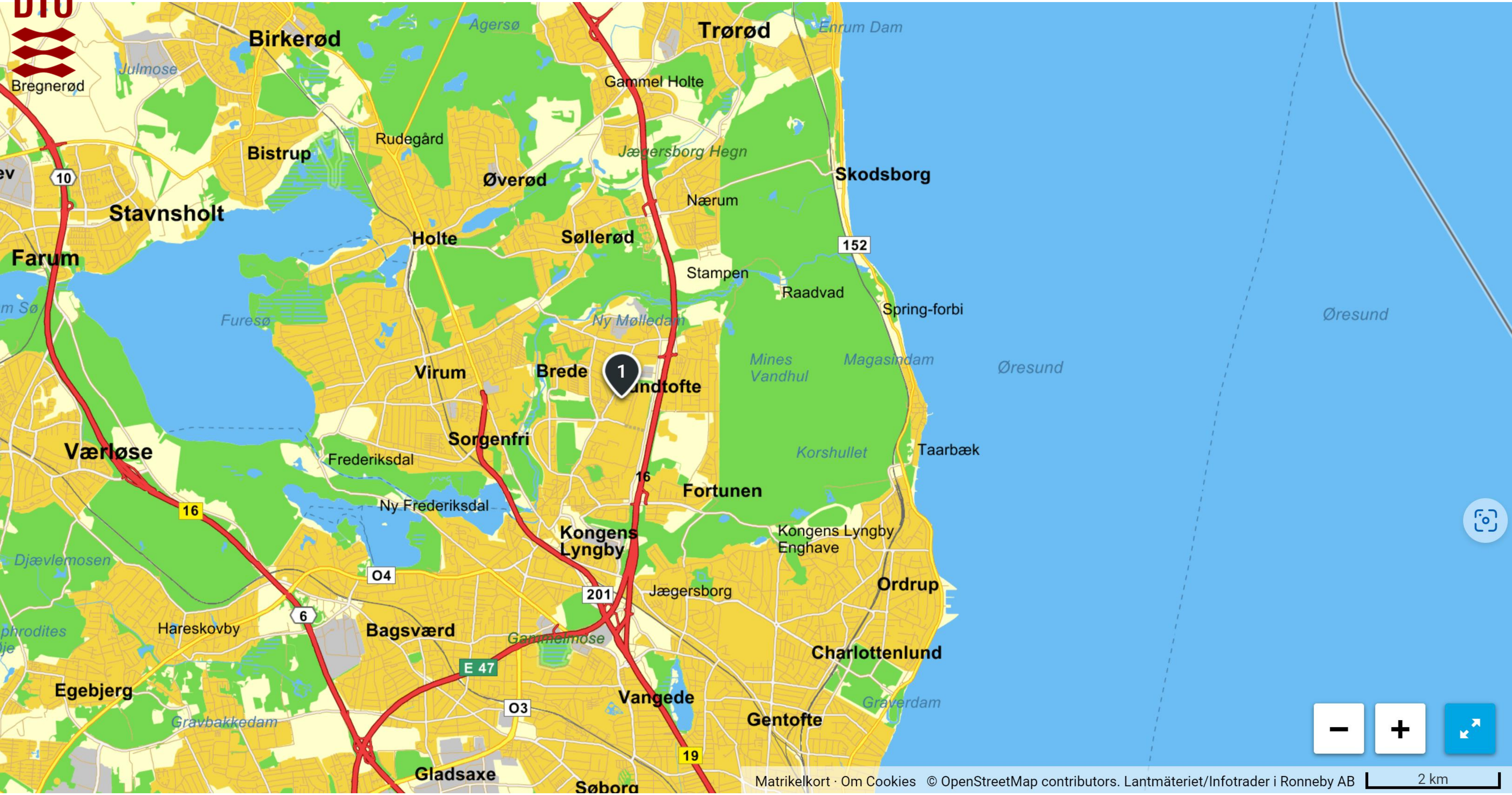
DTU


Lundtofte
Hjortekær
Danmarks
Tekniske
Universitet
Lyngby
Parkkirkegård
Etheren
Anker
Engelunds
Vej
DTU
Rævehøjvej
Helsingørmotorvejen
Lundtofteparken
Hf. Lundtoftehaverne
Sverigesvej
Finlandsvej
Danmarksvej
Lundtoftevej
Nordvej
Brovej
Miljøvej
Lundtoftegårdsvej
Knuth-Winterfeldts Allé
Henrik Dams Allé
Kemitorvet
Anker Engelunds Vej
Bøgeparken
Gyrithe Lemches Vej
Kulsvierparken
Kulsviertoften
Kulsviervænget
Kulsvierivej
Granåsen
Granparken
Lystoftevej
Lystoftevænget
Argentinavej
Borrekrattet
Bredebovej
Mølleåparken
Daugaardsvej
Hallingdal
Hemse
Haveforeningen Lyngen
Agnesvej
Elektrovej
Richard Petersens Plads
Kollegiebakken
Biologiens Vej
Hjortekærsvej
Langs Hegnet
Skovsvinget
Skovbovej
Skovvænget
Rævehøjparken
Kærparken
Gadevangen
Højløkken
Bjælkevangen
Eremitageparken
Slettevej
Skovfryd
Landmålervej
19
15
1
Matrikelkort · Om Cookies
© OpenStreetMap contributors
200 m

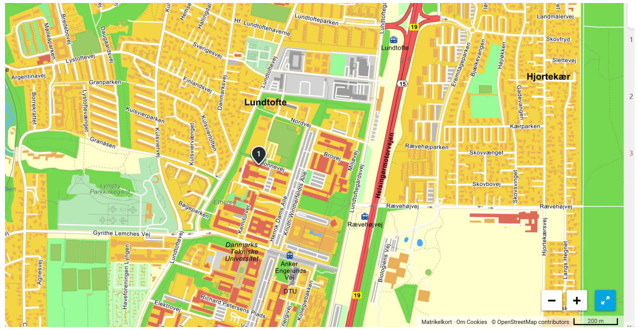

DTU Miljø
Ravnholm
Nymøllevej
Helsingørmotor
Ålebækken Ruinpark
Ørholm Mølledam
Ørholm
Lundtofte gadekær
Hjortekærdammen
Nøjsomhedsvej
15
Lindevangen
Kulsviervej
Lundtoftevej
Iglehul
40 m
Mines Vandhul
Hjertehul
Brede
Lystoftevej
Lundtofte
Stokkerup Dam
Kongevejen
Hjortekær
Lundtofte
Dyrehaven
1
Lundtoftegårdsvej
umvej
Lyngby Parkkirkegård
Lyngby Omfartsvej
Danmarks Tekniske Universitet
Gyrithe Lemches Vej
Rævehøjvej
Anker Engelunds Vej - DTU
Fuglevad
Caroline Amalie Vej
Fuglevadsvej
Skovbrynet
Korshullet
Sorgenfri Slotshave
orgenfri
Sorgenfri
Akademivej - DTU
16
Fortunen
201
Matrikelkort · Om Cookies © OpenStreetMap contributors
500 m

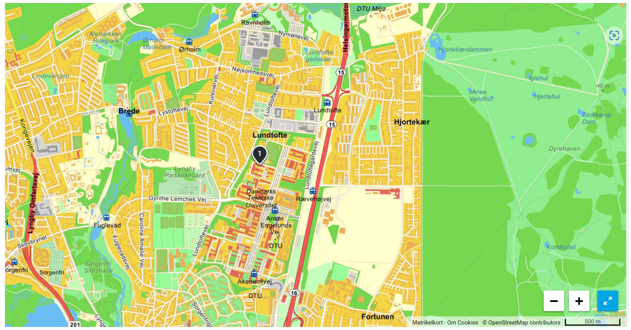
DTU

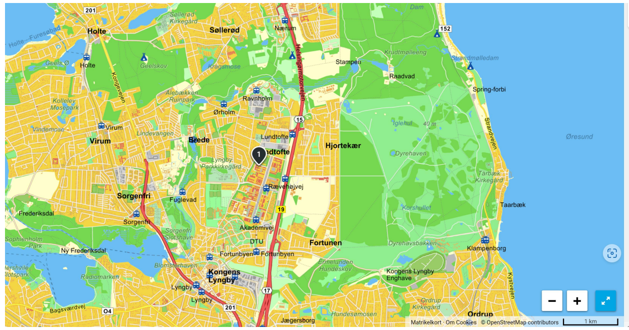

201
Holte
Søllerød Kirkegård
Søllerød
Nærum
Dam
152
Holte--Furesøbad
Geels Ø
Holte
Geelskov
Kragsmose
Kongevejen
Helsingørmotorvejen
Krudtmølleeng
Strandmølledam
Stampen
Raadvad
Spring-forbi
Alebækken Ruinpark
Ravnholm
Kollelev Mosepark
Ørholm
15
Virum
Vindemose
Lindevangen
Lundtofte
Brede
Virum
Hjortekær
Iglehul
40 m
Strandvejen
Øresund
1
ndtofte
Lyngby Parkkirkegård
Dyrehaven
Tårbæk Kirkegård
Rævehøjvej
Sorgenfri
Fuglevad
Taarbæk
Frederiksdal
19
Korshullet
Sorgenfri
Akademivej
Sorgenfri Slotshave
DTU
Fortunen
Dyrehavsbakken
Sophienholm Park
Ny Frederiksdal
Fortunbyen
Fortunbyen
Klampenborg
Blomsterhaven
Ermelunden Hundeskov
lershvile Slotspark
Kongens Lyngby
Radiomarken
Kongens Lyngby Enghave
Lyngby
17
Kystvejen
Lyngby
Ordrup Kirkegård
Bagsværdvej
O4
201
Hundesømosen
Ordrup
Jægersborg
Matrikelkort · Om Cookies © OpenStreetMap contributors
1 km

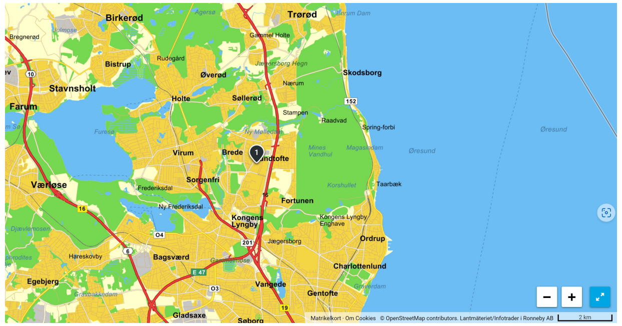

Birkerød
Agersø
Trørød
Enrum Dam
Bregnerød
Julmose
Gammel Holte
Rudegård
Bistrup
Øverød
Jægersborg Hegn
Skodsborg
Nærum
10
Stavnsholt
Holte
Søllerød
152
Farum
Stampen
Raadvad
Spring-forbi
Øresund
Furesø
Ny Mølledam
Mines Vandhul
Magasindam
Øresund
Virum
Brede
1
Sorgenfri
Frederiksdal
Korshullet
Taarbæk
Værløse
16
Fortunen
16
Ny Frederiksdal
Kongens Lyngby
Kongens Lyngby Enghave
Djævlemosen
O4
201
Jægersborg
Ordrup
6
Hareskovby
Bagsværd
Gammelmose
Charlottenlund
E 47
Egebjerg
Vangede
O3
Gravbakkedam
Graverdam
Gentofte
19
Gladsaxe
Søborg
Matrikelkort · Om Cookies
© OpenStreetMap contributors. Lantmäteriet/Infotrader i Ronneby AB
2 km

Continuous **axis of scales**









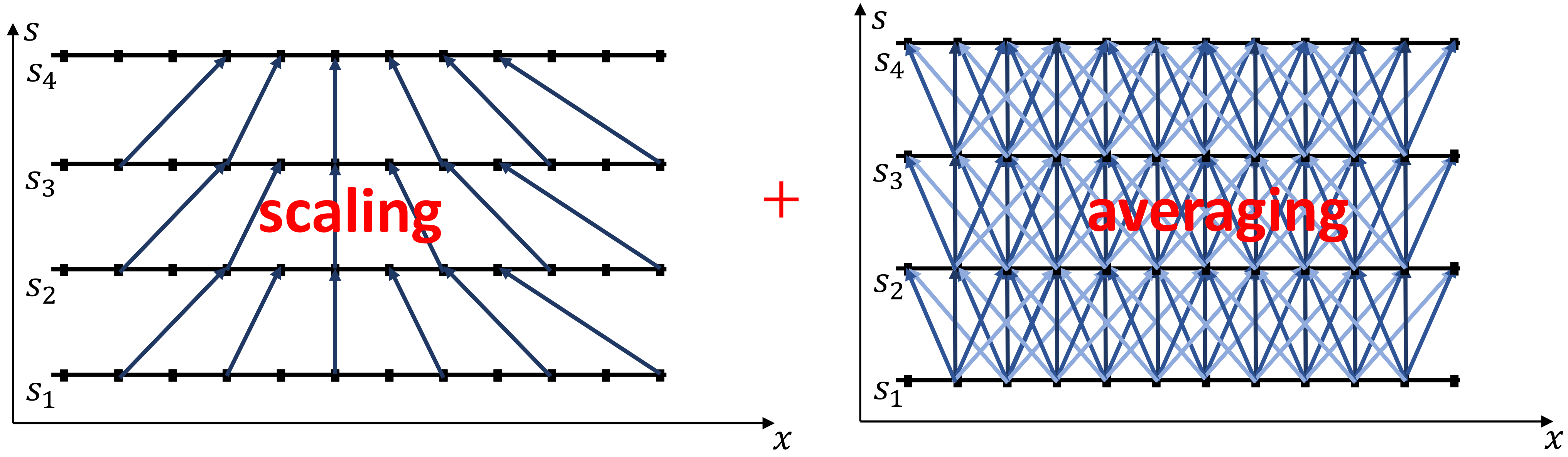
$\alpha_1 = 1{:}\,200$ $\alpha_2 = 1{:}\,500$ $\alpha_3 = 1{:}\,1000$ $\alpha_4 = 1{:}\,2000$

s

The scale parameter: $s = -\ln \alpha$

s increases from a fine to a coarse scale

Upscaling = Scaling + Averaging ("smoothing")



<u>Scaling</u>: Simple change of the scale without loss of the detail

<u>Averaging</u>: Smoothing, loss of the resolution

Transition to the “next scale”

Averaging:

$$\langle m\rangle(x) = \langle m(x - \boldsymbol{Y})\rangle$$

Scaling:

$$m_\alpha(x) = \frac{1}{\alpha} m\left(\frac{x}{\alpha}\right)$$

Scaling after averaging:

$$\langle m\rangle_\alpha(x) = \frac{1}{\alpha}\left\langle m\left(\frac{1}{\alpha}(x - \boldsymbol{Y})\right)\right\rangle$$

Averaging after scaling:

$$\langle m\rangle_\alpha(x) = \frac{1}{\alpha}\left\langle m\left(\frac{1}{\alpha}x - \boldsymbol{Y}\right)\right\rangle$$

- *The two expressions are not equivalent*

Transition to the "next scale": Asymptotic expansion

$$\frac{1}{\alpha} = e^s \approx 1 + s; \quad m(x - \boldsymbol{Y}) \approx m(x) - \boldsymbol{Y}\frac{\partial m}{\partial x} + \frac{1}{2}\boldsymbol{Y}^2\frac{\partial^2 m}{\partial x^2}; \quad \langle \boldsymbol{Y} \rangle = 0:$$

<u>Scaling after averaging</u>:

$$\langle m \rangle_\alpha(x) = e^s \langle m(e^s(x - \boldsymbol{Y})) \rangle$$

$$\approx (1+s)\langle m(((1+s)x - (1+s)\boldsymbol{Y})) \rangle$$

<u>Averaging after scaling</u>:

$$\langle m_\alpha \rangle (x) = e^s \langle m(e^s x - \boldsymbol{Y}) \rangle$$

$$\approx (1+s)\langle m(((1+s)x - \boldsymbol{Y})) \rangle$$

$$\approx \langle m(x + (sx - \boldsymbol{Y})) \rangle + s m(x)$$

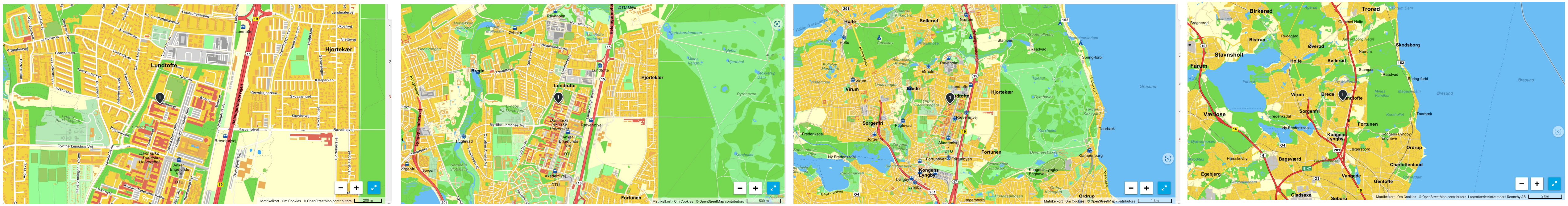
The two expressions become equivalent in the limit of a small step

Expansion and neglect of the higher-order terms: $\langle m \rangle_\alpha(x) \approx \langle m_\alpha \rangle(x) = m_s(x)$

$$\frac{m_s(x) - m(x)}{s} = m(x) + x\frac{\partial m}{\partial x} + \frac{\langle \boldsymbol{Y}^2 \rangle}{2s}\frac{\partial^2 m}{\partial x^2}$$

$$\frac{\partial m_s}{\partial s} = \frac{\partial}{\partial x}(x m_s) + d_0 \frac{\partial^2 m_s}{\partial x^2}, \qquad d_0 = \frac{\langle \boldsymbol{Y}^2 \rangle}{2s}$$

Theory of upscaling: Uniqueness



$\alpha = 1:200$ $\alpha = 1:500$ $\alpha = 1:1000$ $\alpha = 1:2000$

s

Rule 1. If a transition between scales *i* and *j* is performed, the "path" does not matter:

$$W_{13} = W_{12} W_{23}$$

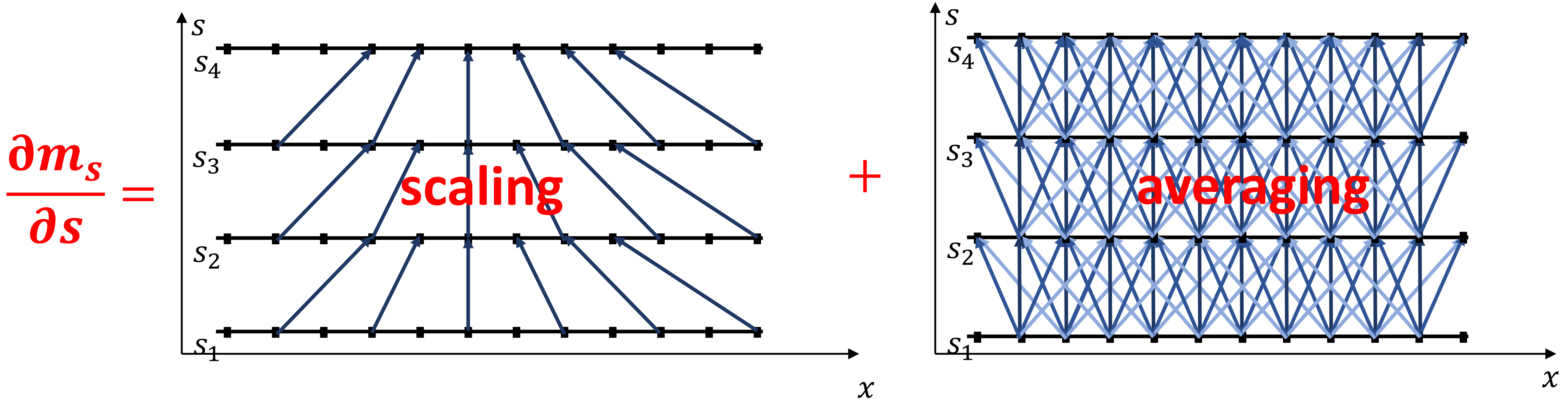
Rule 2. The transition should be *<u>continuous</u>*: If scales 1 and 2 approach each other then W_{12} should tend to unity (identity) transformation.

<u>These rules are sufficient to build the mathematics of upscaling and derive the upscaling equation</u>
(similar to the theory of continuous Markov processes)

Upscaling of densities (1D, steady-state flows):

Scale transformation → $\frac{\partial m_s}{\partial s} = \frac{\partial}{\partial x}\left(x - b_0(s)\right)m_s + d_0 \frac{\partial^2 m_s}{\partial x^2}$ **(*)**

Scaling — Displacement of x=0 — Smoothing (averaging)



In the limit of infinitely small steps, scaling and averaging are interchangeable.

What needs to be upscaled? The flow equations:

Mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = q_m$$

Concentration:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\boldsymbol{v} + J_D) = q_C$$

Momentum:

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} + P\boldsymbol{I} + \Pi) = \boldsymbol{F}$$

Energy:

$$\frac{\partial}{\partial t}\left(E + \frac{\rho v^2}{2}\right) + \nabla \cdot \left(\left(E + \frac{\rho v^2}{2} + P\right)\boldsymbol{v} + \boldsymbol{q}\right) = \boldsymbol{Q}$$

What needs to be upscaled? The flow equations:

Mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = q_m$$

Concentration:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\boldsymbol{v} + J_D) = q_C$$

Momentum:

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} + P\boldsymbol{I} + \Pi) = \boldsymbol{F}$$

Energy:

$$\frac{\partial}{\partial t}\left(E + \frac{\rho v^2}{2}\right) + \nabla \cdot \left(\left(E + \frac{\rho v^2}{2} + P\right)\boldsymbol{v} + \boldsymbol{q}\right) = Q$$

Densities

What needs to be upscaled? The flow equations:

Mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = q_m$$

Concentration:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\boldsymbol{v} + J_D) = q_C$$

Momentum:

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} + P\boldsymbol{I} + \Pi) = \boldsymbol{F}$$

Energy:

$$\frac{\partial}{\partial t}\left(E + \frac{\rho v^2}{2}\right) + \nabla \cdot \left(\left(E + \frac{\rho v^2}{2} + P\right)\boldsymbol{v} + \boldsymbol{q}\right) = Q$$

Densities

Fluxes

What needs to be upscaled? The flow equations:

Mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = q_m$$

Concentration:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\boldsymbol{v} + J_D) = q_C$$

Momentum:

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} + P\boldsymbol{I} + \Pi) = \boldsymbol{F}$$

Energy:

$$\frac{\partial}{\partial t}\left(E + \frac{\rho v^2}{2}\right) + \nabla \cdot \left(\left(E + \frac{\rho v^2}{2} + P\right)\boldsymbol{v} + \boldsymbol{q}\right) = Q$$

Densities

Fluxes

Sources

What needs to be upscaled? The flow equations:

Mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = q_m$$

Concentration:

$$\frac{\partial C}{\partial t} + \nabla \cdot (C\boldsymbol{v} + J_D) = q_C$$

Momentum:

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} + P\boldsymbol{I} + \Pi) = \boldsymbol{F}$$

Energy:

$$\frac{\partial}{\partial t}\left(E + \frac{\rho v^2}{2}\right) + \nabla \cdot \left(\left(E + \frac{\rho v^2}{2} + P\right)\boldsymbol{v} + \boldsymbol{q}\right) = Q$$

Densities

Fluxes

Sources

General form:

$$\frac{\partial m}{\partial t} + \nabla \cdot \boldsymbol{J} = n$$

What needs to be upscaled

A transport (balance) equation: $\frac{\partial m}{\partial t} + \nabla \cdot j = q$

Densities:
Mass density ρ, concentration c, momentum $j = \rho v$, energy e…

Fluxes:
Mass flux $j = \rho v$, momentum flux $J = \rho v v + \Pi$, energy flux $j_e = \rho v h$…

Production:
Density per unit time

- Different physical values should be upscaled according to the different rules
- The overall form of the equation should be preserved under upscaling

Example: Diffusion equation

$$\frac{\partial C}{\partial t} + \nabla \cdot J_D = q_C, \qquad J_D = -D\nabla C$$

1. C is upscaled like density: $$\frac{\partial C_s}{\partial s} = \frac{\partial}{\partial x}(xC_s) + d_0 \frac{\partial^2 C_s}{\partial x^2}$$

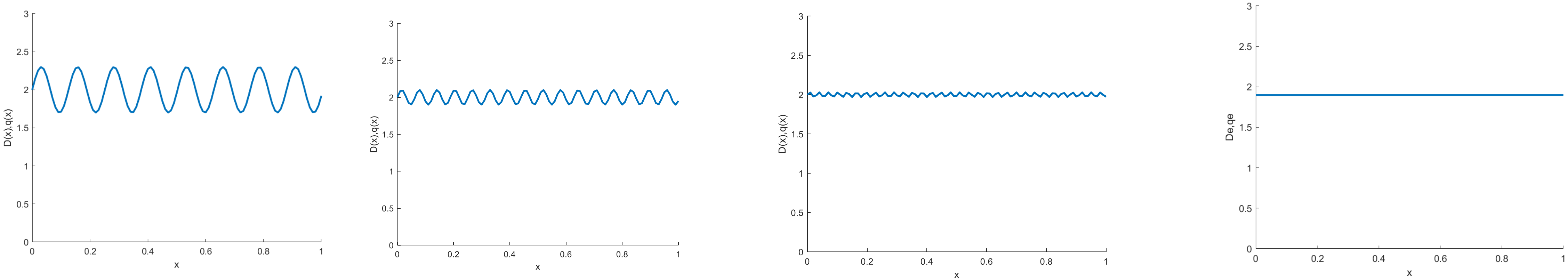
2. J_D is upscaled like density: $$\frac{\partial J_{D,s}}{\partial s} = \frac{\partial}{\partial x}(xJ_{D,s}) + d_0 \frac{\partial^2 J_{D,s}}{\partial x^2}$$ *//Theorem about upscaling fluxes*

3. $q_c, \nabla C$ are upscaled like the derivatives of the density *//The rules for upscaling derivatives*

4. The rule for upscaling the diffusion coefficient D is derived from upscaling the products ($D\nabla C$). *//The rules for upscaling the products*

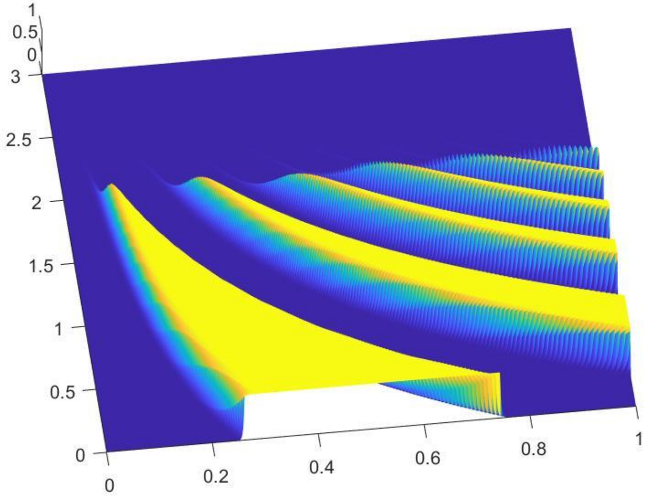
These rules may be different

Continuous upscaling of diffusion coefficient



s

3D plot:



Convective diffusion equation (1D, steady state)

Original

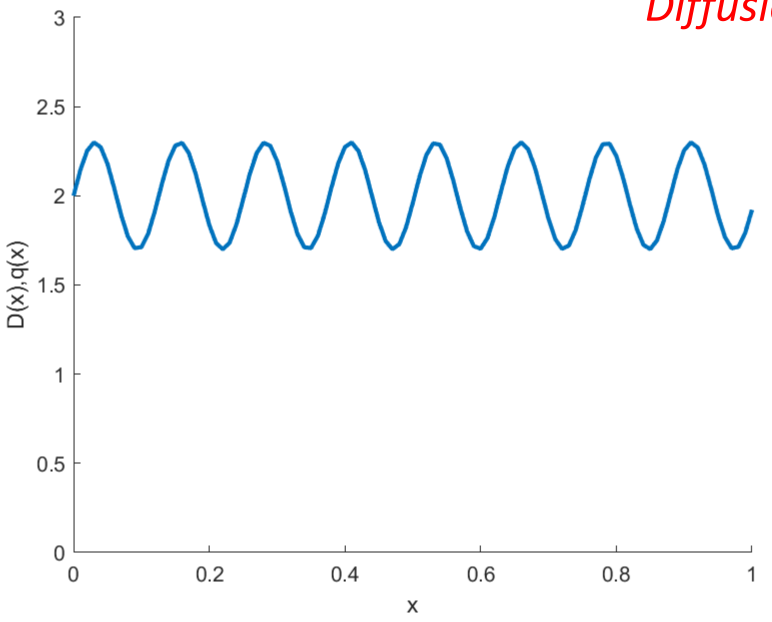
$$\frac{d}{dx}\left(D(x)\frac{dc(x)}{dx}\right) - v\frac{d}{dx}\big(c(x)\big) = q(x)$$

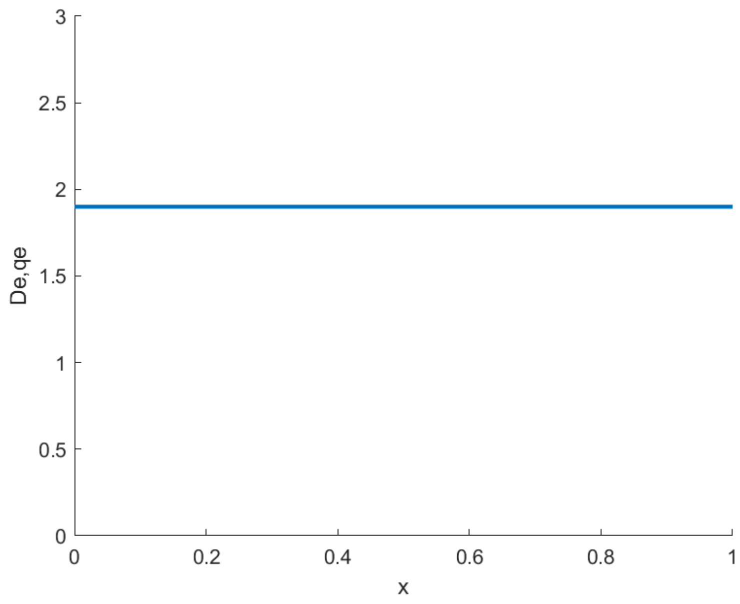
Averaged (upscaled)

$$\frac{d}{dx}\left(D_{av}\frac{dc_{av}(x)}{dx}\right) - v_{av}\frac{d}{dx}\big(c_{av}(x)\big) = q_{av}$$

Diffusion coefficient

Source term





A procedure for transition from periodic to average diffusion coefficients is to be developed

Case 1: “Just” diffusion equation

$$\frac{d}{dx}\left(D(x)\frac{dc(x)}{dx}\right) = 0$$

<u>Evolution of the diffusion coefficient</u>:

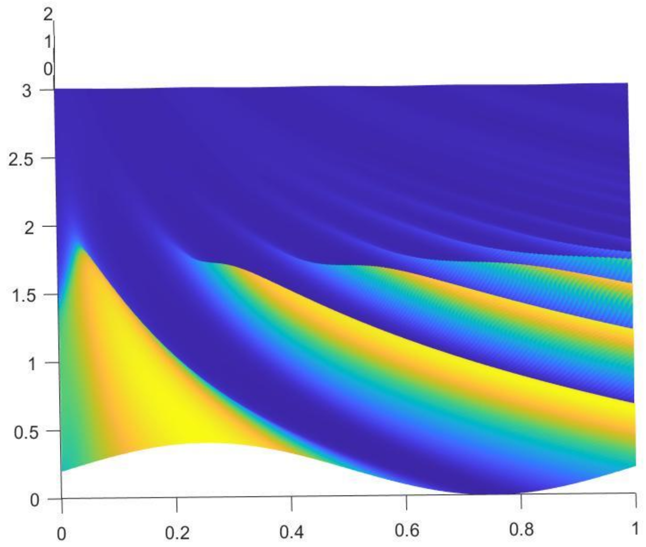
$$\frac{\partial}{\partial s}\left(\frac{1}{D_s(x)}\right) = \frac{\partial}{\partial x}\left(x - b_0(s)\right)\frac{1}{D_s(x)} + d_0(s)\frac{\partial^2}{\partial x^2}\left(\frac{1}{D_s(x)}\right)$$

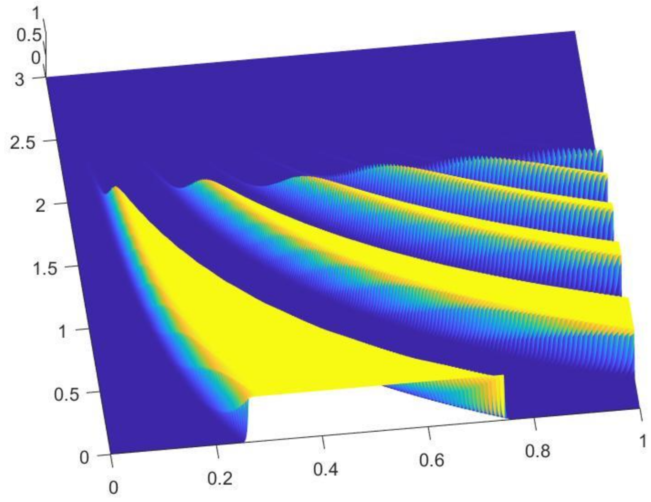
- the inverse diffusion coefficient is upscaled like a density

<u>Asymptotic behavior</u>:

$$\frac{1}{e^s D_s(e^s x)} \to \left\langle \frac{1}{D_0(x)} \right\rangle$$ - the same as for the direct upscaling

Consequence of scaling





Case 2: Diffusion equation with a source

$$\frac{d}{dx}\left(D(x)\frac{dc(x)}{dx}\right) = q(x), \langle q(x)\rangle = 0$$

Flux

$$J(x) = D(x)\frac{dc(x)}{dx} = J(x_0) + \int_{x_0}^{x} q(x)dx$$

Boundary condition

$$D(x_0)\frac{dc(x_0)}{dx} = J(x_0)$$

Evolution of the diffusion coefficient:

$$\frac{\partial}{\partial s}\left(\frac{J_s(x)}{D_s(x)}\right) = \frac{\partial}{\partial x}(x - b_0(s))\frac{J_s(x)}{D_s(x)} + d_0(s)\frac{\partial^2}{\partial x^2}\left(\frac{J_s(x)}{D_s(x)}\right)$$

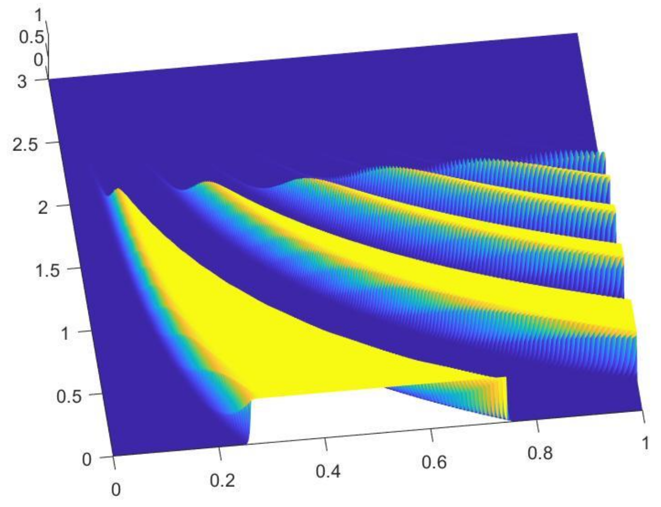
$$\frac{\partial J_s(x)}{\partial s} = \frac{\partial}{\partial x}(x - b_0(s))J_s(x) + d_0(s)\frac{\partial^2 J_s(x)}{\partial x^2}$$

the values of $\frac{J_s(x)}{D_s(x)}$ and $J_s(x)$ are upscaled like densities

Asymptotic behavior:

$$\frac{J_s(e^s x)}{e^{2s}D_s(e^s x)} \to \left\langle\frac{J_0(x)}{D_0(x)}\right\rangle; e^{-s}J_s(e^s x) \to \langle J_0(x)\rangle$$

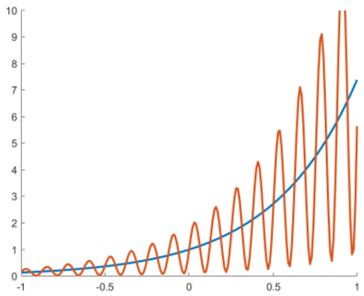
- the same as for the direct upscaling



Either velocity, or the boundary conditions are displaced

Case 3: Diffusion with convection

$$\frac{d}{dx}\left(D(x)\frac{dc(x)}{dx}\right) - v\frac{dc(x)}{dx} = 0$$



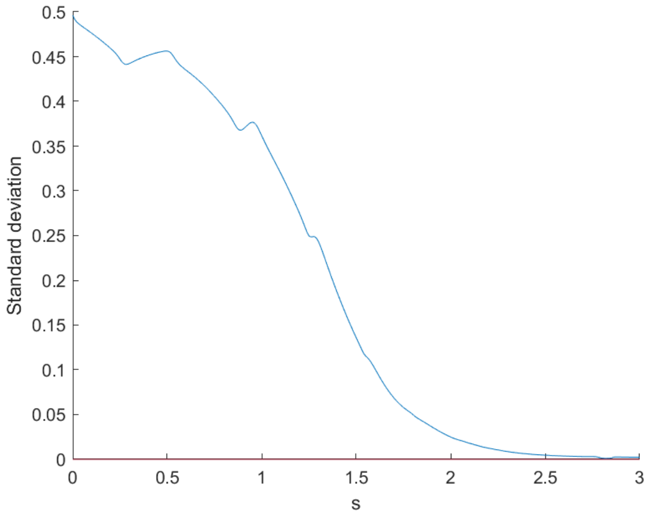
Evolution of the diffusion coefficient:

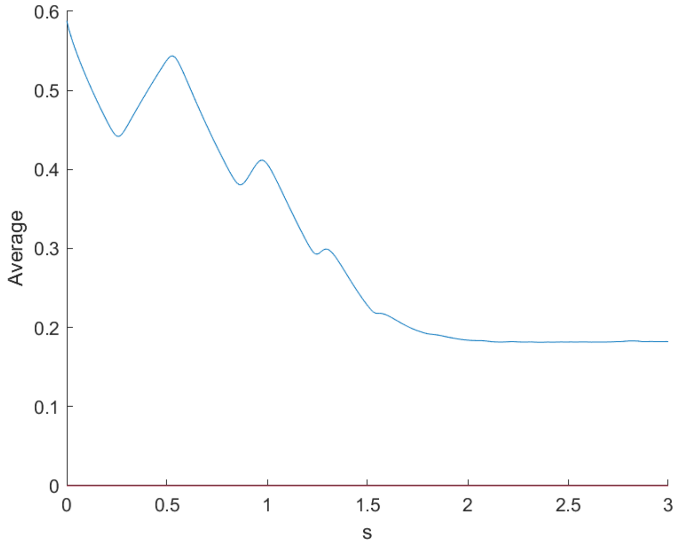
$$\frac{\partial}{\partial s}\left(\frac{1}{D_s(x)}\right) = \frac{\partial}{\partial x}(x - b_0(s))\frac{1}{D_s(x)} + d_0(s)\frac{\partial^2}{\partial x^2}\left(\frac{1}{D_s(x)}\right) + d_0(s)v\frac{\partial}{\partial x}\left(\frac{1}{D_s(x)^2}\right)$$

Asymptotic behavior:

$$\frac{1}{e^s D_s(e^s x)} \to \left\langle \frac{1}{D_0(x)} \right\rangle$$

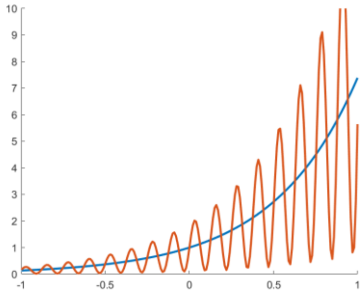
(It seems so, but no proof, only numerical check)





Diffusion equation with convection

$$\frac{d}{dx}\left(D(x)\frac{dc(x)}{dx}\right) - v\frac{dc(x)}{dx} = 0$$



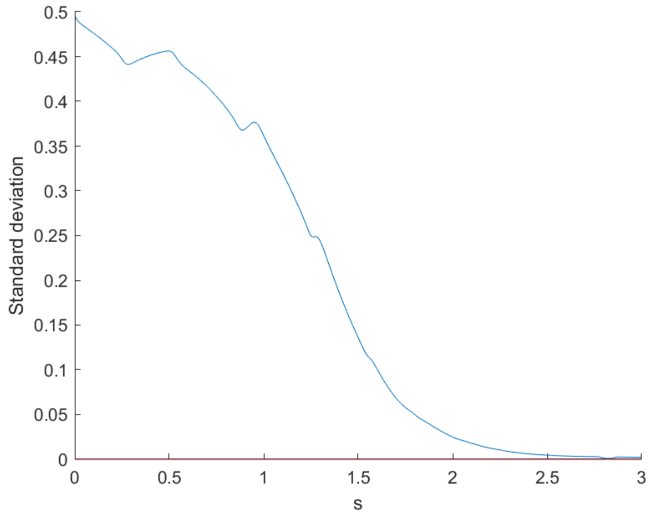
Evolution of the diffusion coefficient:

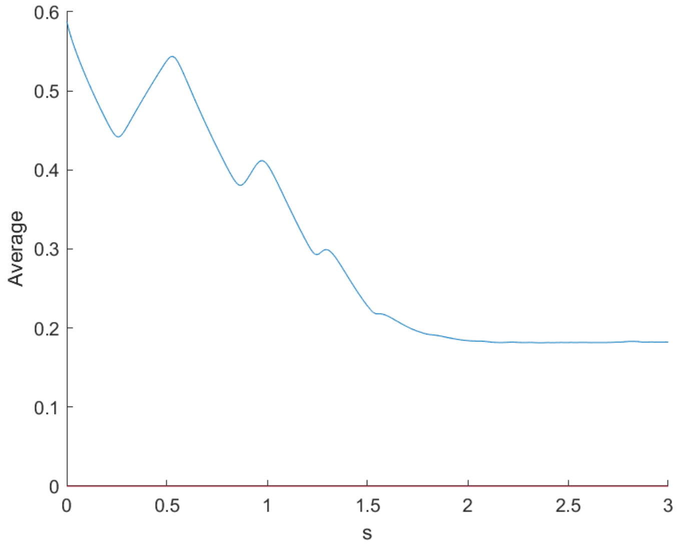
$$\frac{\partial}{\partial s}\left(\frac{1}{D_s(x)}\right) = \frac{\partial}{\partial x}(x - b_0(s))\frac{1}{D_s(x)} + d_0(s)\frac{\partial^2}{\partial x^2}\left(\frac{1}{D_s(x)}\right) + d_0(s)v\frac{\partial}{\partial x}\left(\frac{1}{D_s(x)^2}\right)$$

Asymptotic behavior:

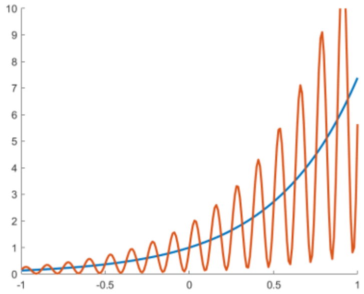
$$\frac{1}{e^s D_s(e^s x)} \to \left\langle\frac{1}{D_0(x)}\right\rangle$$

(It seems so, but no proof, only numerical check)



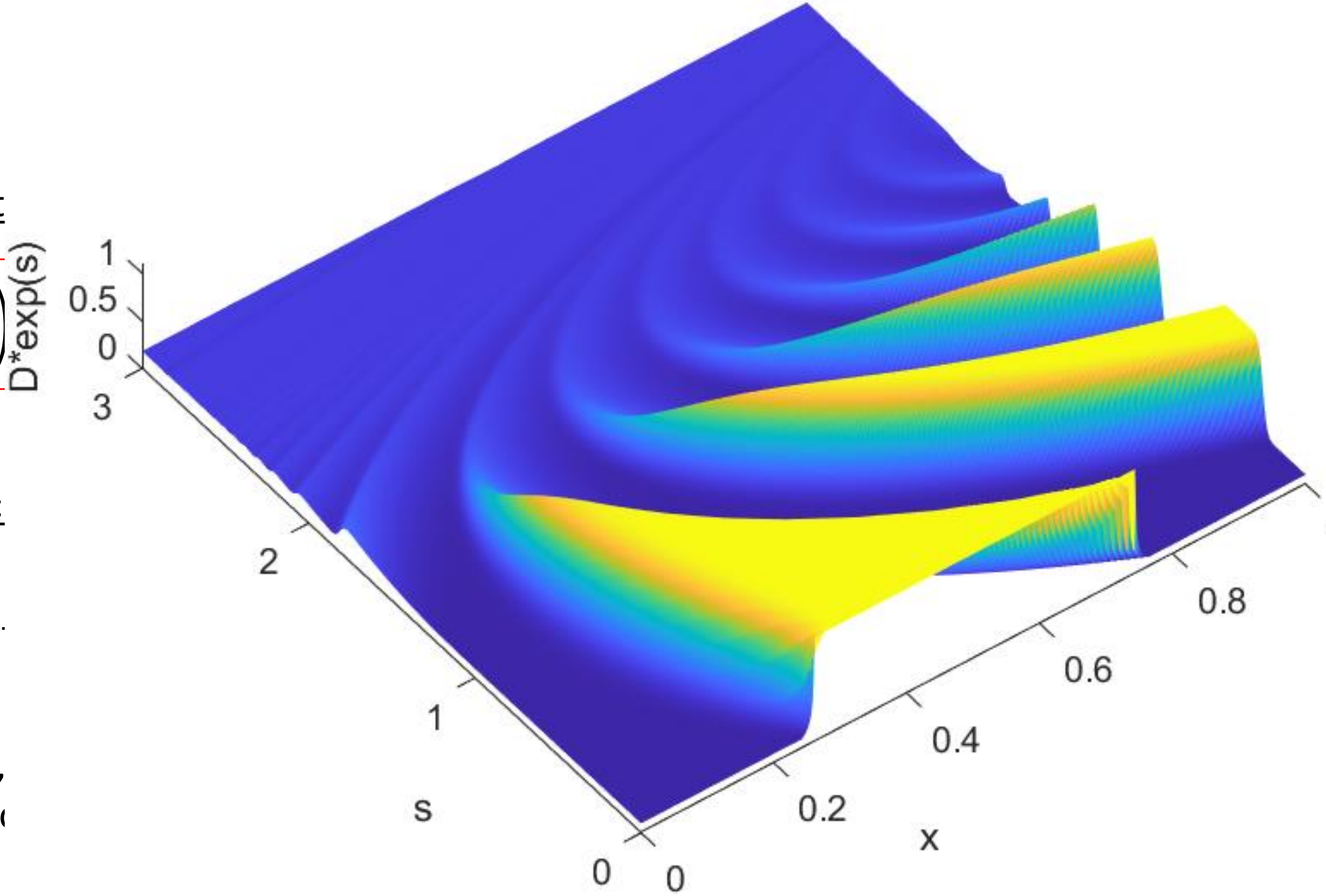


Diffusion equation with convection



Evolution of t

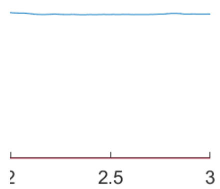
$$\frac{\partial}{\partial s}\left(\frac{1}{D_s(x)}\right)$$



Asymptotic

$$\frac{1}{e^s D_s(e^s x)}$$

(It seems so,
only numeri

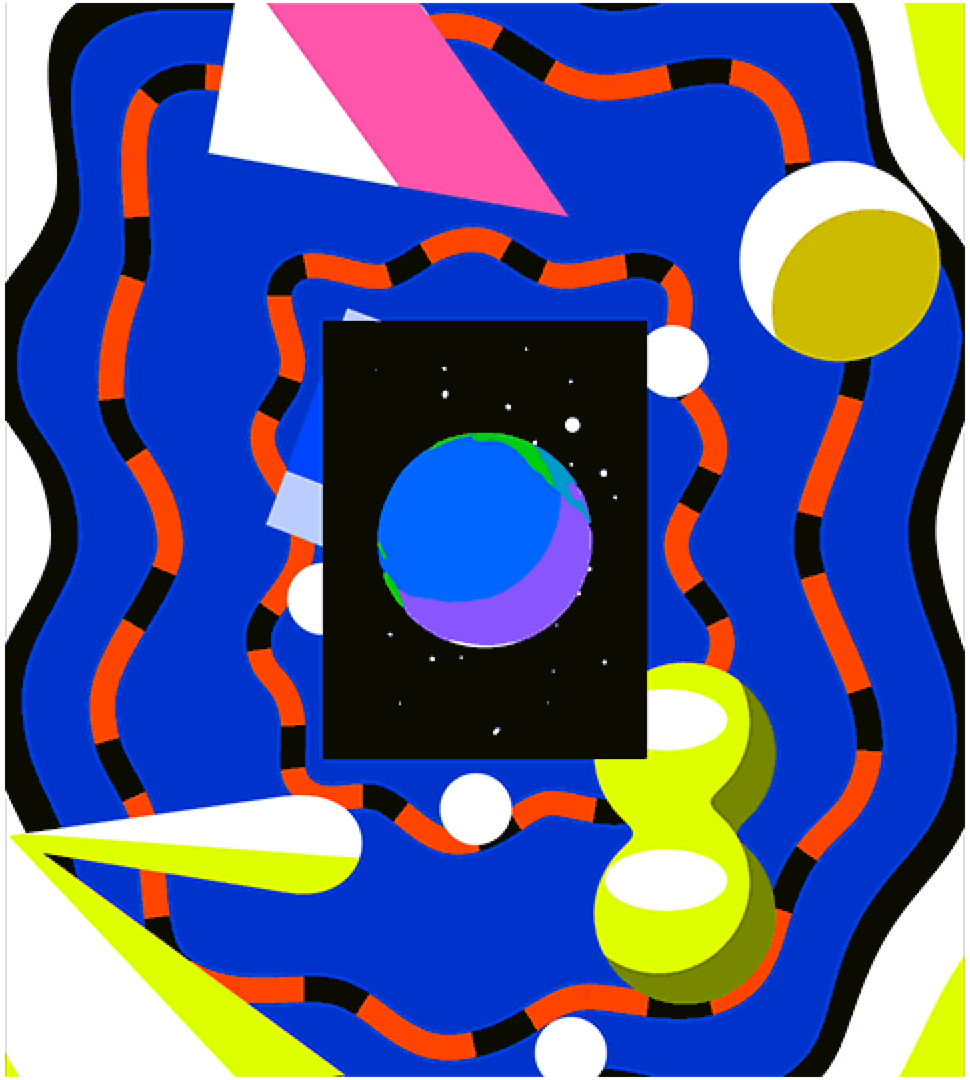


Conclusions

- The theory of continuous upscaling is developed
- The laws for upscaling of densities and fluxes are derived
- The theory is applied to upscaling of the diffusion equation and diffusion coefficients
- Continuous upscaling may be possible and gives asymptotic results even if the direct averaging results in large deviations
- Asymptotic behavior of the continuously upscaled diffusion coefficients is the same as under direct averaging
- In the case of convective diffusion, large differences between fine-scale and core-scale solutions cannot be eliminated

Thank you!

Questions?



”Unity Universe” by Peter Steineck