Microstructural Modeling of Snow and Firn Processes

Thomas Kaempfer,
Mark Hopkins, Don Perovich

Cold Regions Research and Engineering Laboratory,
Hanover, NH, USA and AF-Consult Switzerland AG

Martin Schneebeli,
Bernd Pinzer

WSL Institute for Snow and Avalanche Research
SLF, Davos, Switzerland

Mathis Plapp

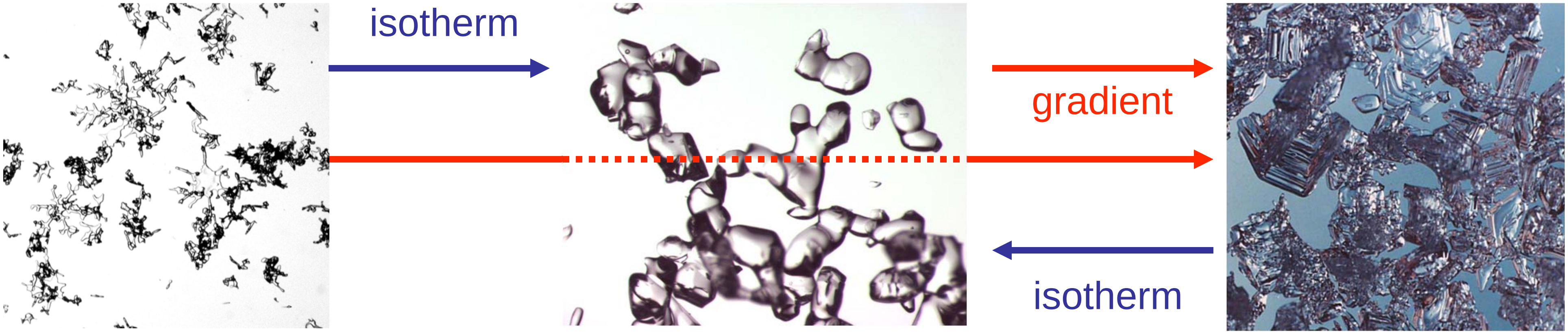
Ecole Polytechnique, Laboratoire PMC,
Palaiseau, France

thomas.kaempfer@a3.epfl.ch

Microstructural Modeling of Snow and Firn Processes

- Snow properties and processes
  - the material snow and metamorphism
  - snow-… interactions
- Natural and Digital snow
  - micro-tomography vs. discrete elements
- Microstructural modeling
  - metamorphism
  - mechanics
  - fluid (and air) flow
  - radiative transfer

Snow: a granular material ?



dendritic

rounded

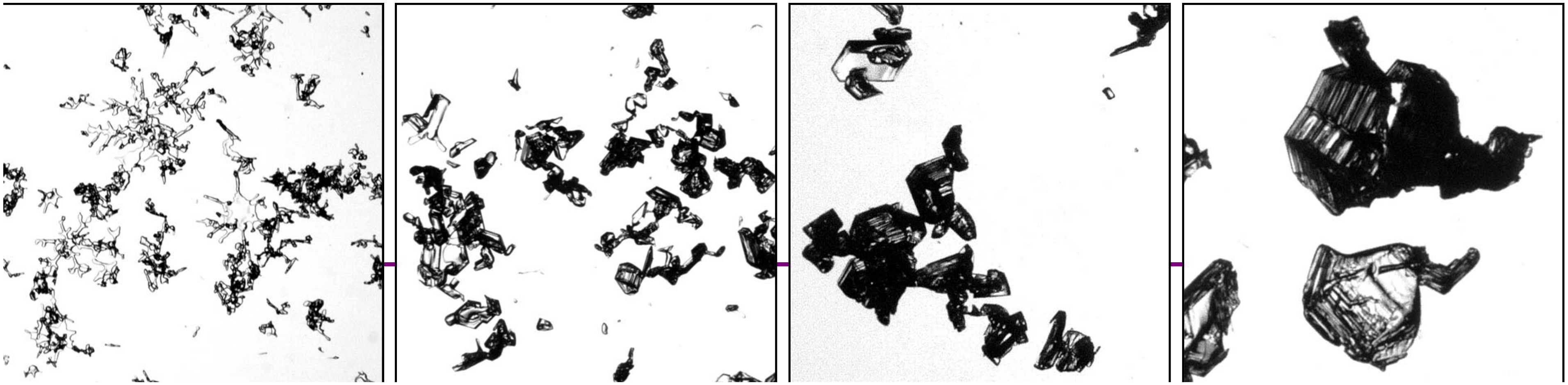
depth hoar

isotherm

gradient

isotherm

Lab exp.: 130 kg m^{-3}, temperature gradient: 120 K m^{-1}



Day 0 (25 Mar 1999)

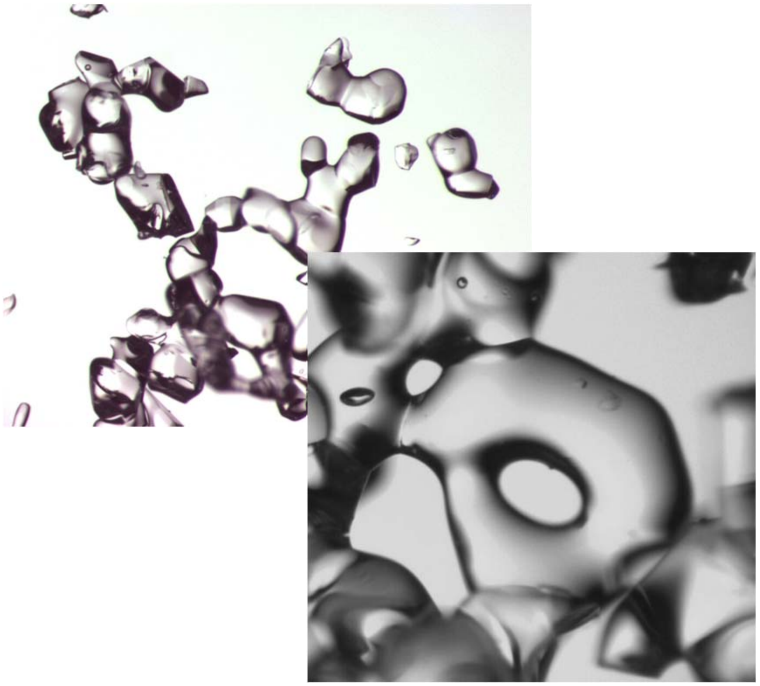
Day 3

Day 7

Day 13

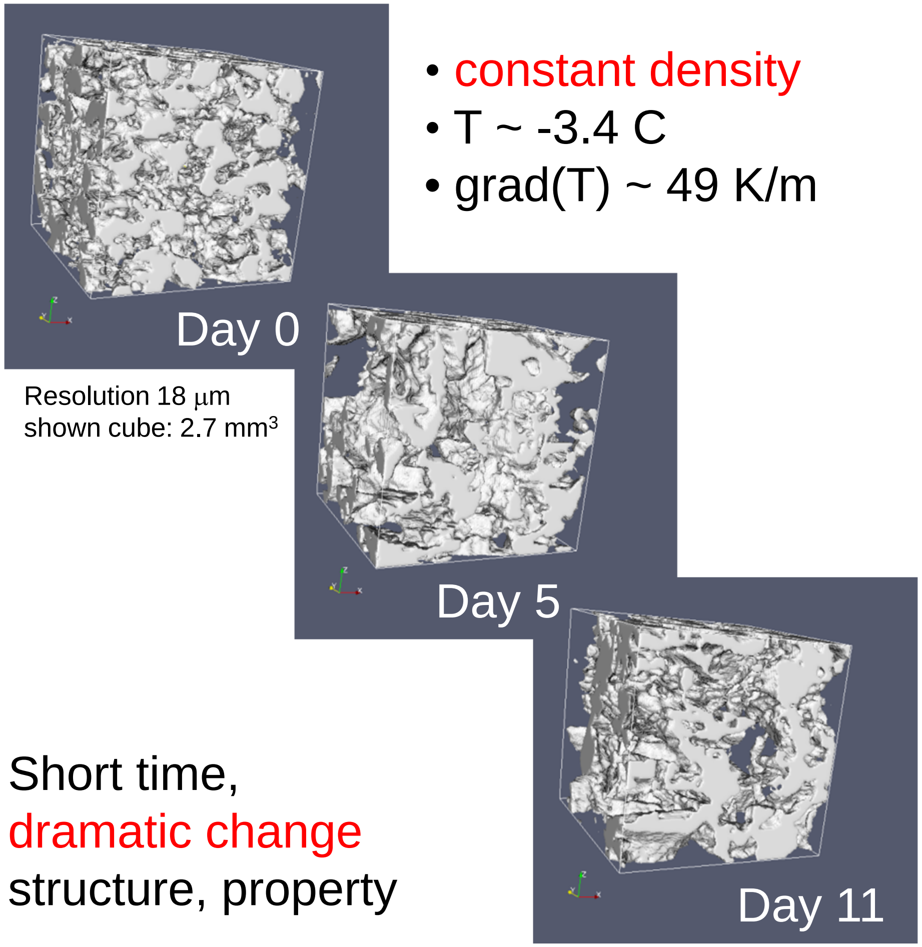
Snow on the ground

(1) Is a sintered,
porous material



Grain type, size, density
+ micro-structure

(2) metamorphoses

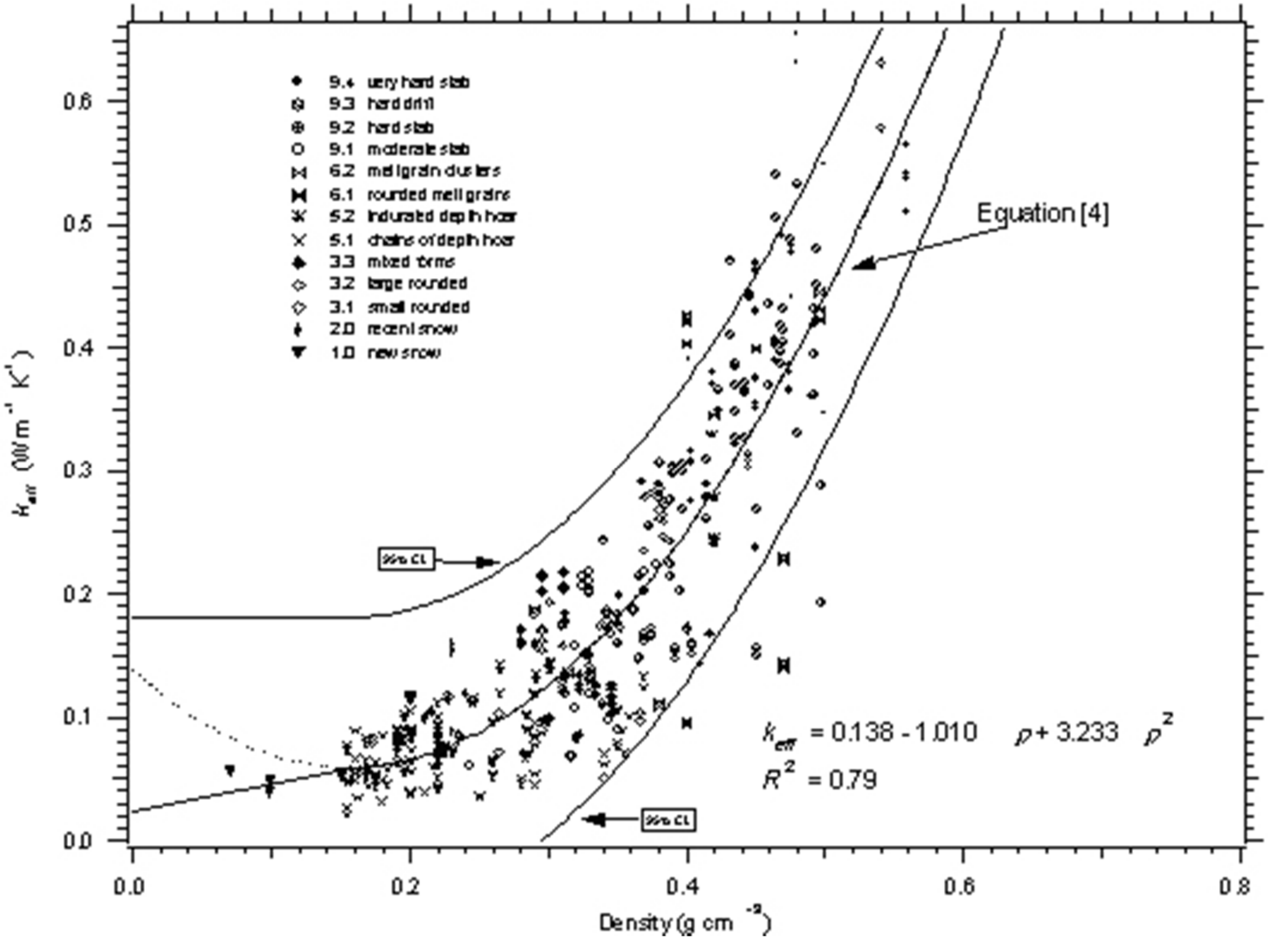


Resolution 18 µm
shown cube: 2.7 mm^3

- constant density
- T ~ -3.4 C
- grad(T) ~ 49 K/m

Short time,
dramatic change
structure, property

Issue 1: Effective heat conductivity

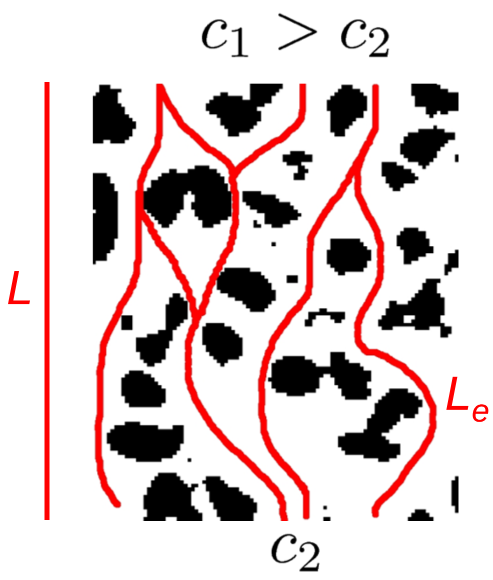


Similar crystal type and density, but highly different EHC

Sturm et al., J.Glaciology, 1997

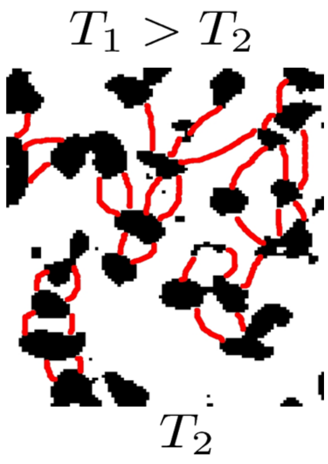
Issue 2: Snow-atmosphere interaction

NO_x



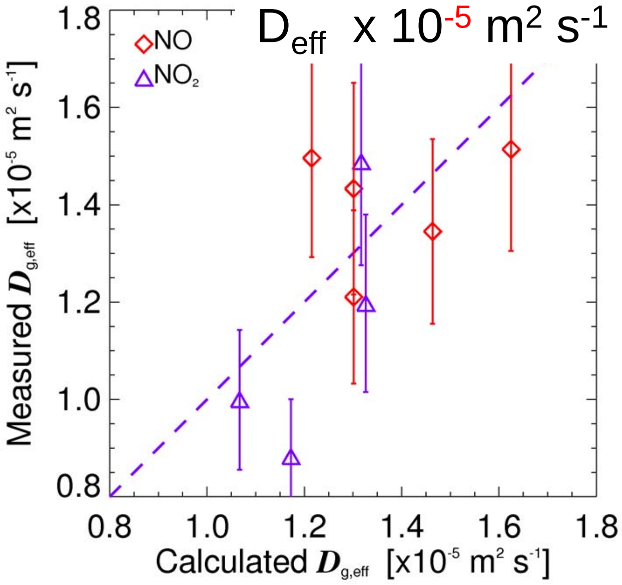
- Diffusive and advective transport
- Reactive surface
- Pore close-off

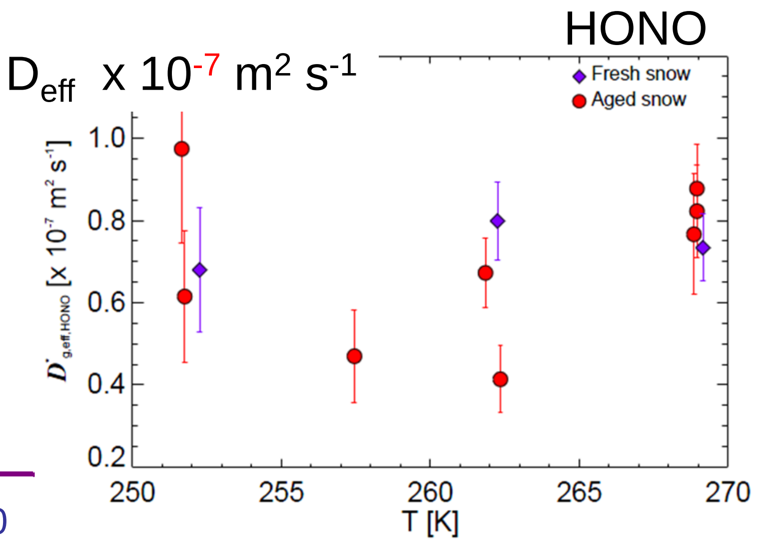
water vapor HONO ?



$$\tau = \frac{L_e}{L}$$

$$D_{\mathrm{eff}} = D_{\mathrm{air}} \frac{\Phi}{\tau^2}$$





Pinzer et al., JGR 2010

In order to improve

- snow assessment
- forecasting of snow properties
- ice core analyses
- …

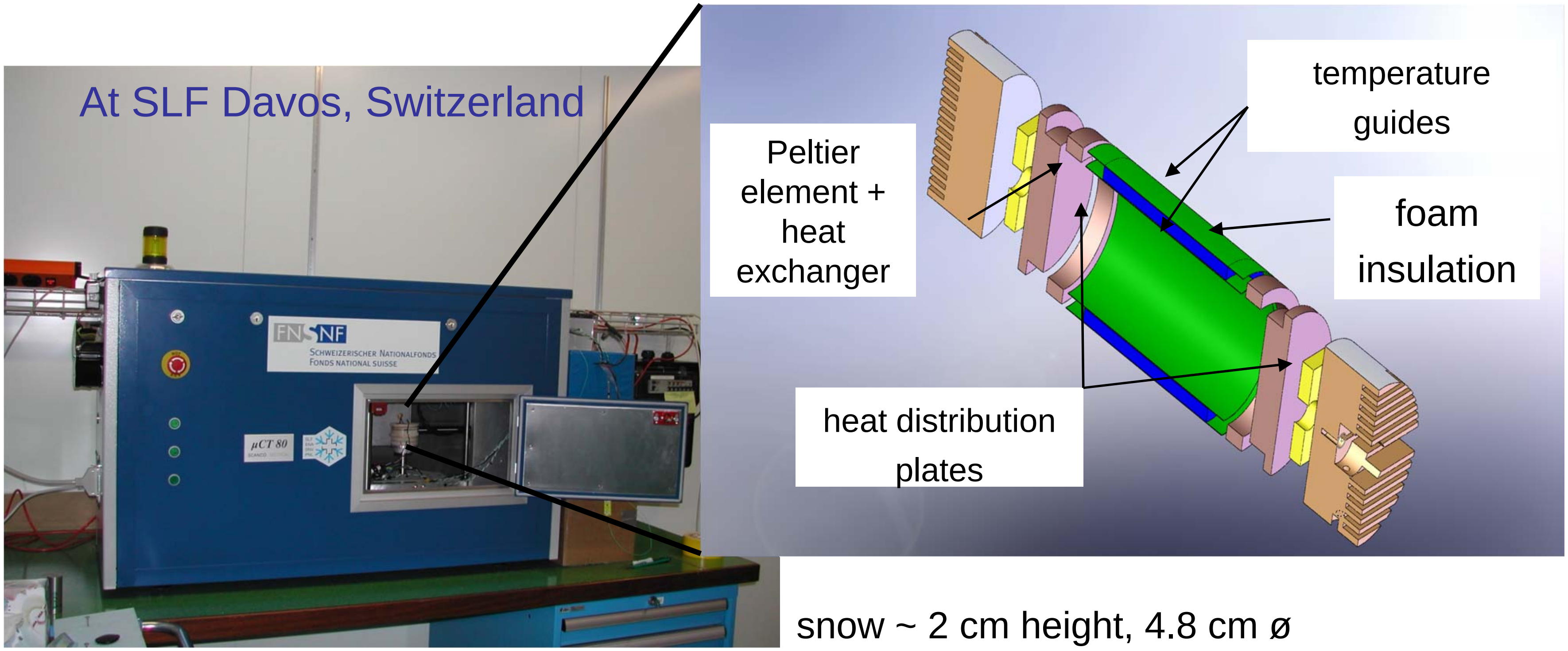
It is necessary to understand

- the relation between
  micro-structure and macro-properties
- the physics of snow metamorphsim

A solution is

- combined physics based modeling and experiments

Metamorphism experiments inside µ-CT

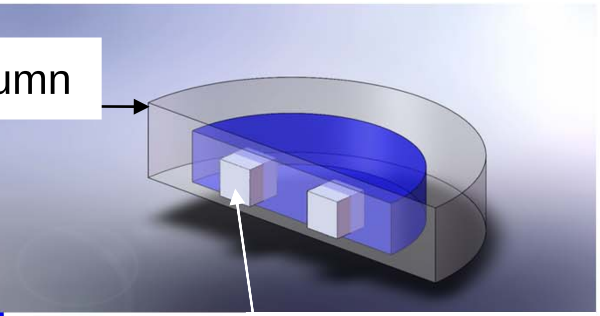


snow ~ 2 cm height, 4.8 cm ø

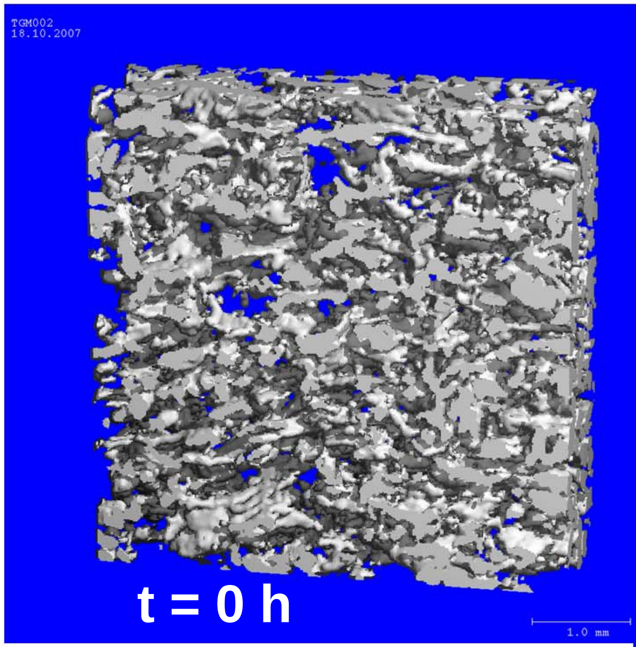
- controlled T and grad(T)
- undisturbed snow structure observation
  high resolution: 10-40 µm, every 2-8h
- simultaneous heat flux measurements

Pinzer & Schneebeli, Meas. Sci. Technol. 2009

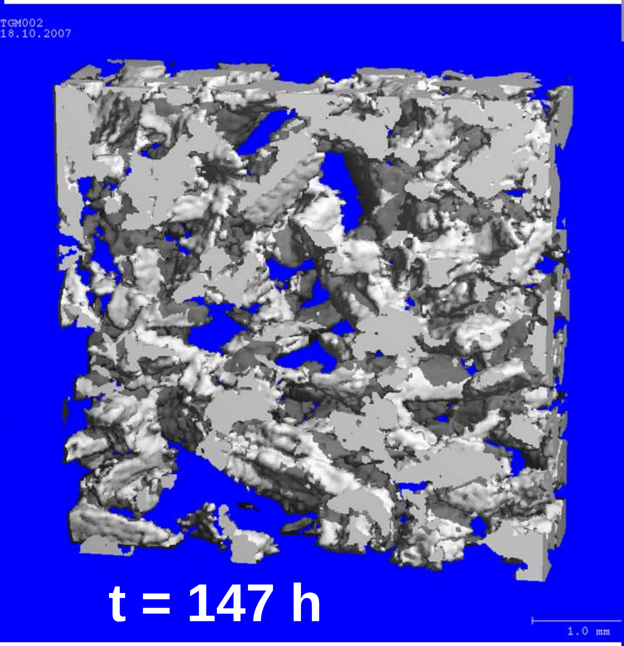
Structural changes (unidirectional TG)


snow column

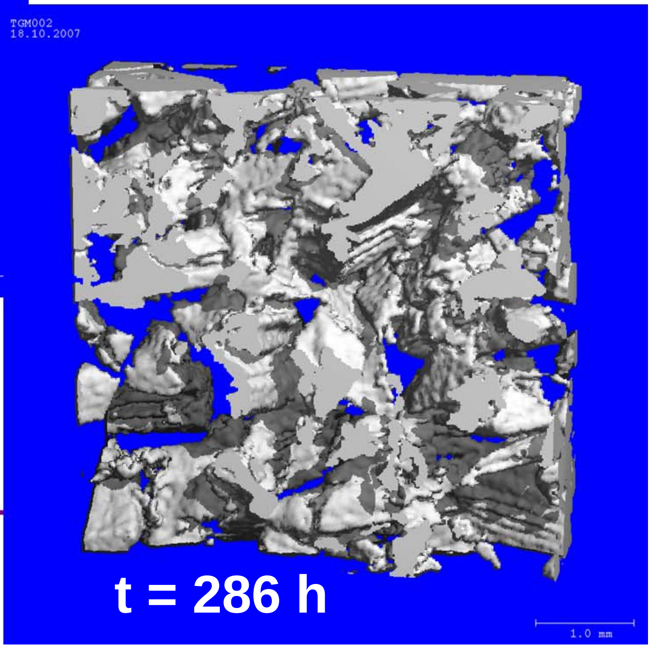
investigated CT subvolume



t = 0 h



t = 147 h



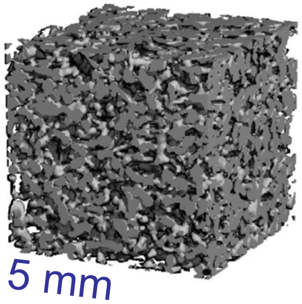
t = 286 h

depth hoar formation

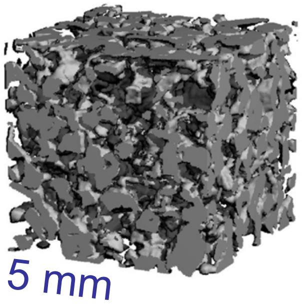
Schneebeli & Sokratov, Hydrol. Proc., 2004

Sublimation-deposition (unidirectional TG)

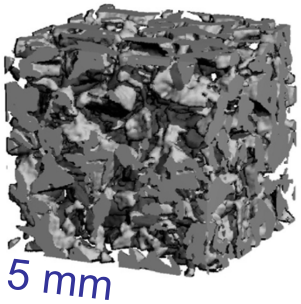
day 0



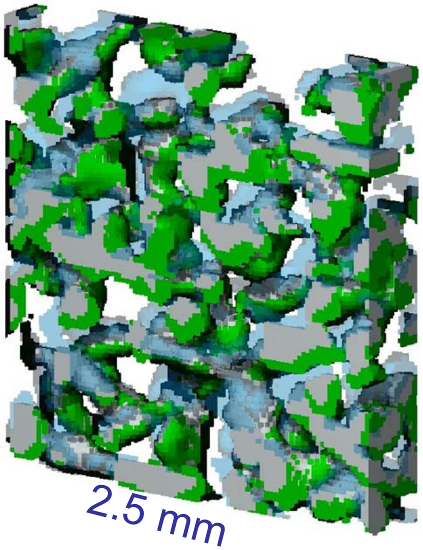
day 8



day 16



day 1 – day 0

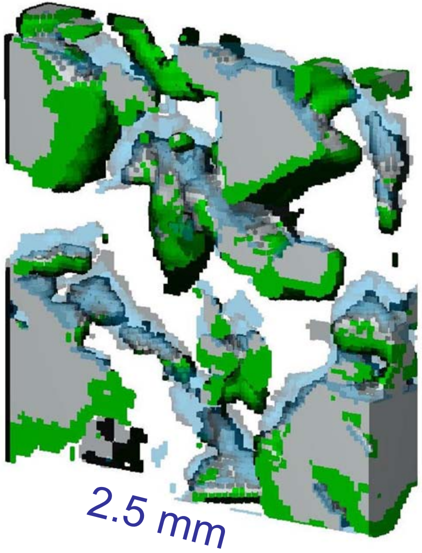


🟦 lost

⬜ constant

🟩 gained

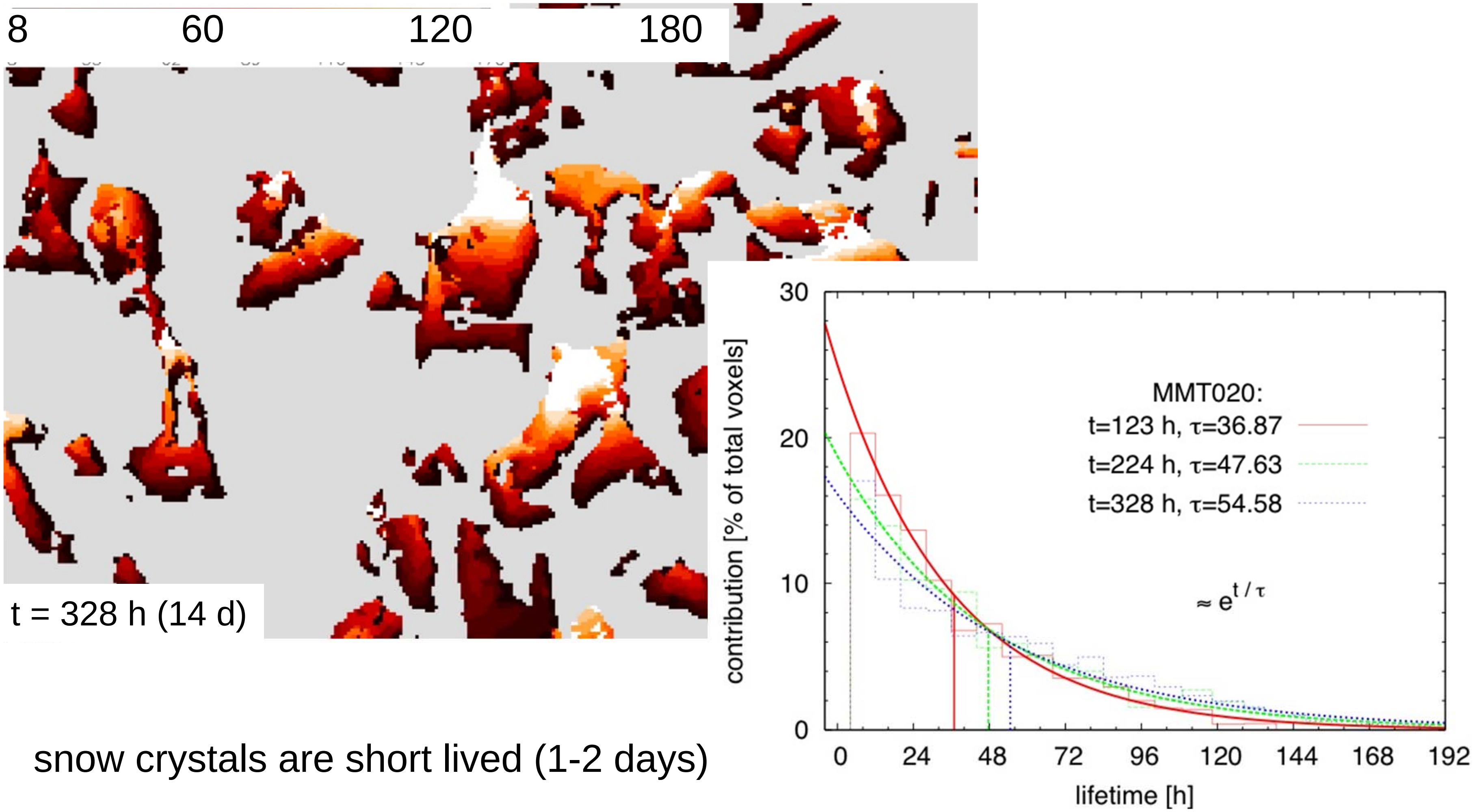
day 16 – day 15



Evolution of snow structure (unidirectional TG)

- coarsening
- high mass flux
- rate of mass loss
  and gain
  >>
  growth rate
- grain ≠ grain

Crystal lifetime in hours (unidirectional TG)

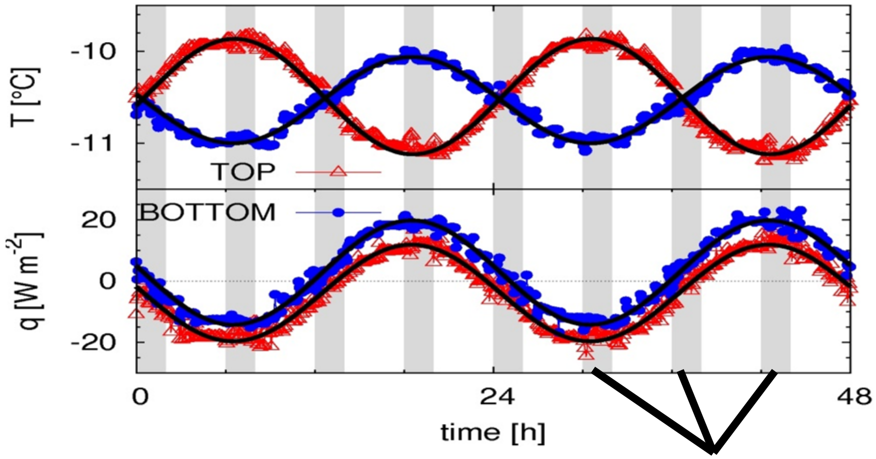


snow crystals are short lived (1-2 days)

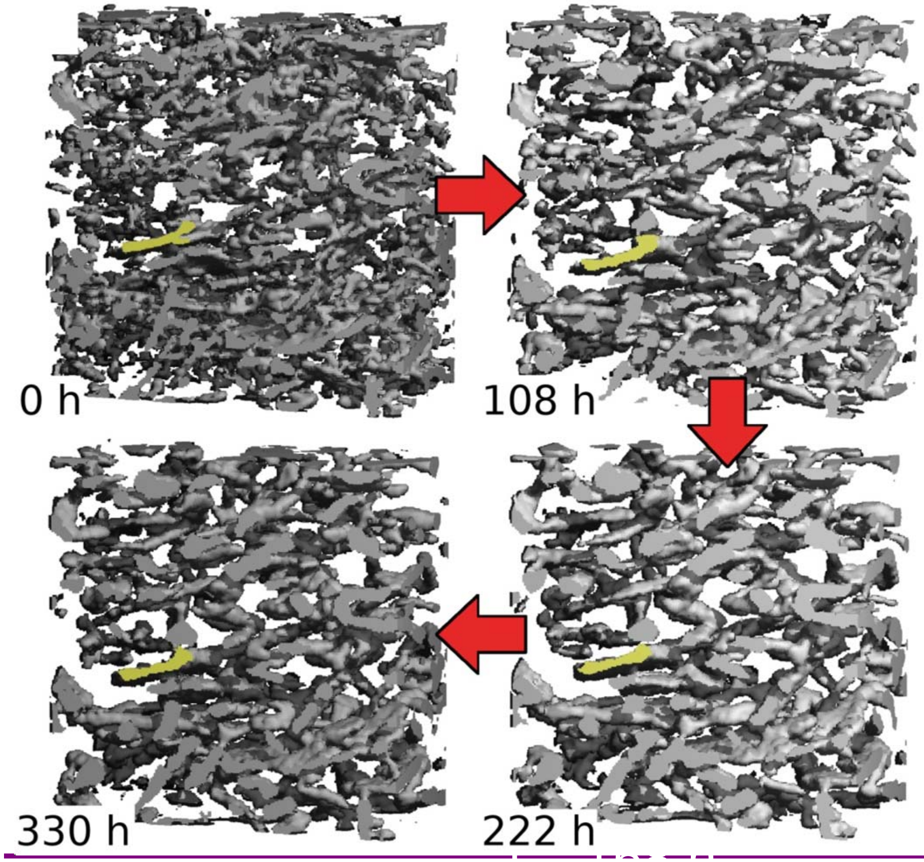
Pinzer (et al.), Thesis ETH 2009

Experiments under sinusoidal TG

- Alternating TG similar to snow surface in nature
- max(grad(T)) ~ 100 K/m



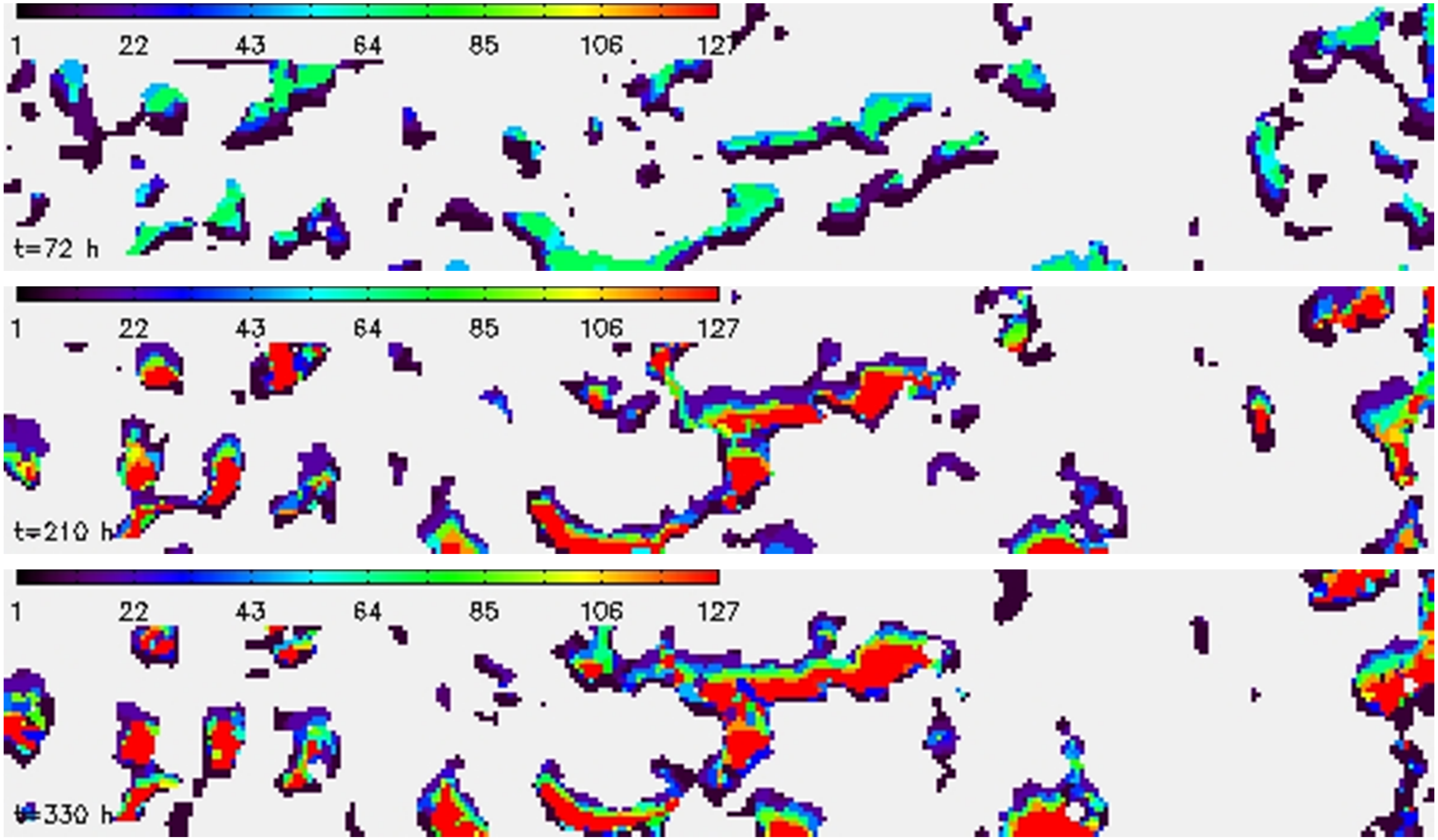
CT scans



- The “critical gradient” for faceting was exceeded during 86% of the time
- No sign of faceting was observed
- Slow 3D-structure evolution

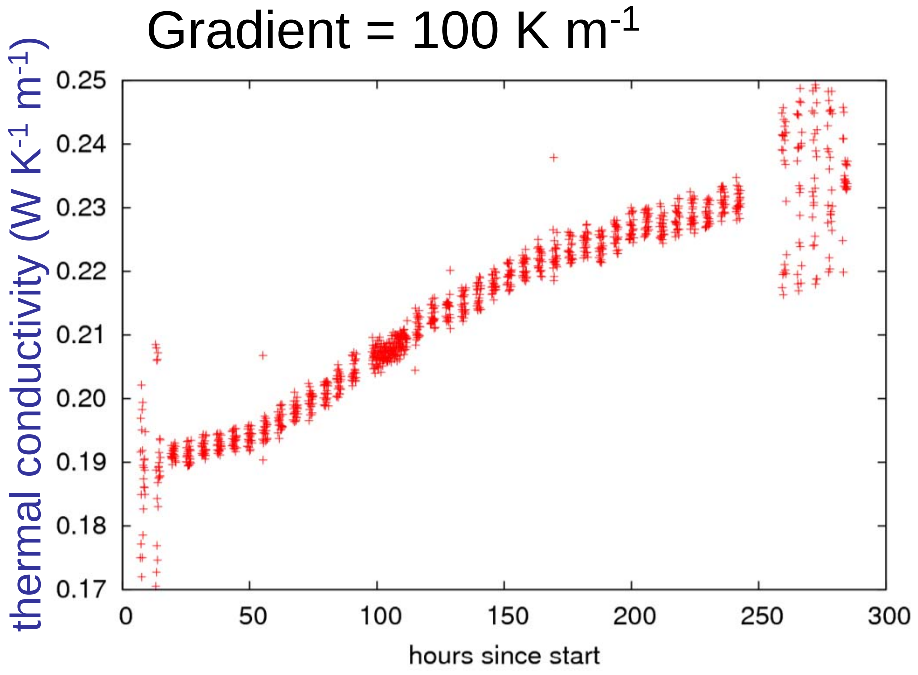
Pinzer & Schneebeli, GRL 2009

Life-time (sinusoidal TG)

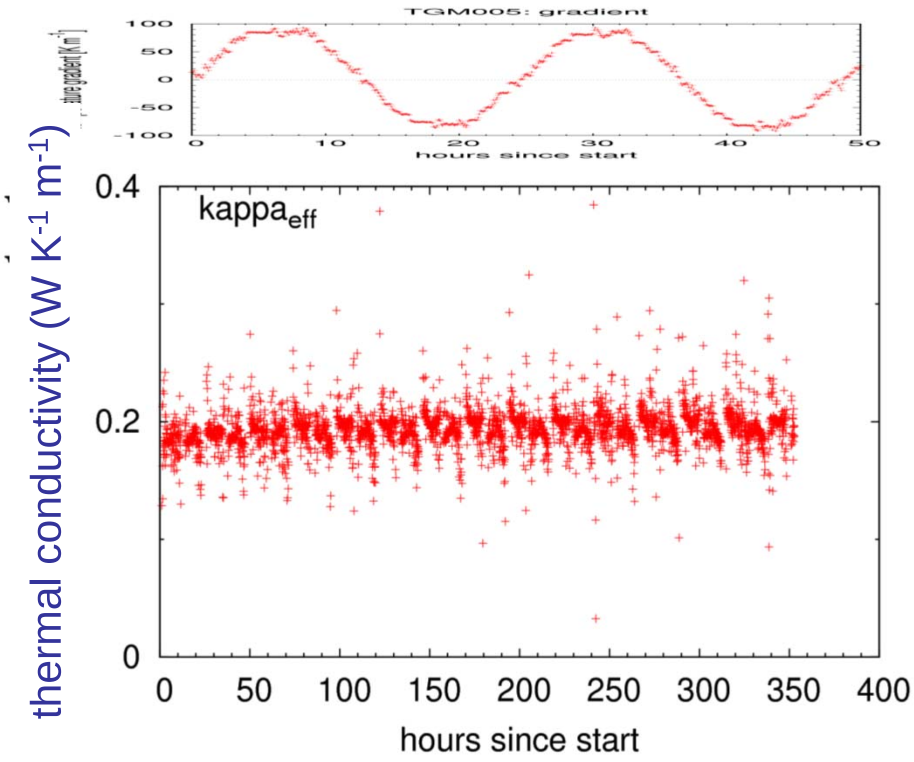


Pinzer & Schneebeli, GRL 2009

Heat conductivity
Unidirectional vs. sinusoidal TG



=> effective heat conductivity calculated from temperature and flux measurements increases



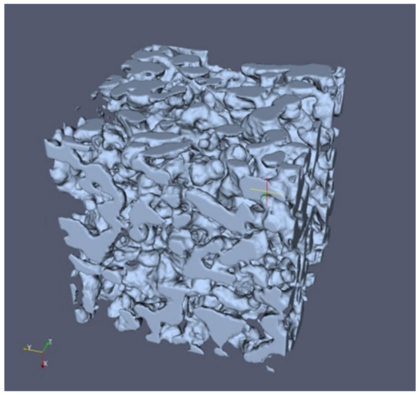
=> heat conductivity does not change!

topology conserved?

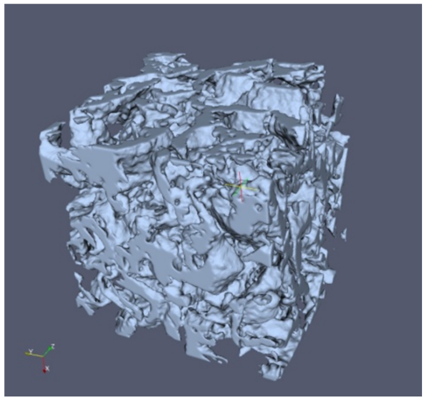
Pinzer (et al.), Thesis ETH 2009

A “virtual” snow lab

Natural snow



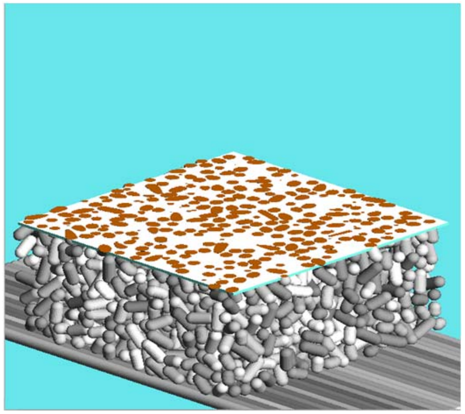
metamorphism



1.

Numerical modeling

Model snow

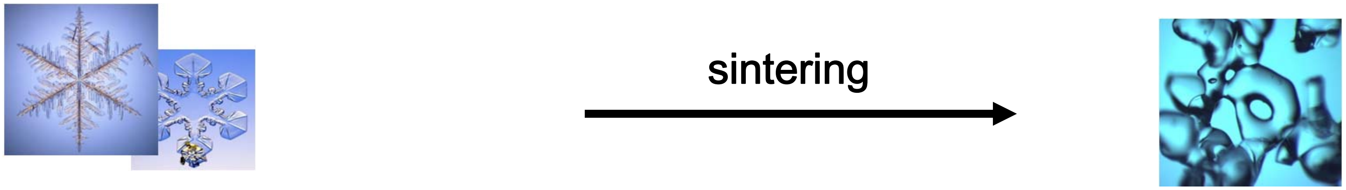


Controlled, variable
structural properties

2.

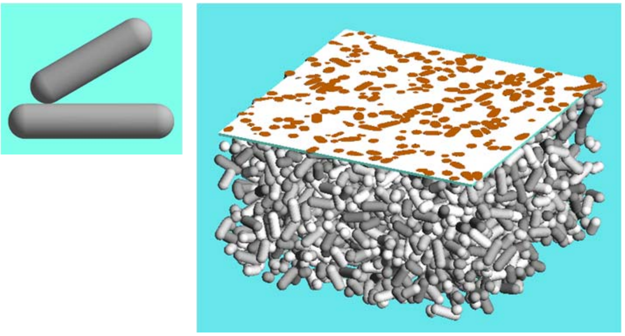
Study processes,
Predict properties:
- air flow
- optics

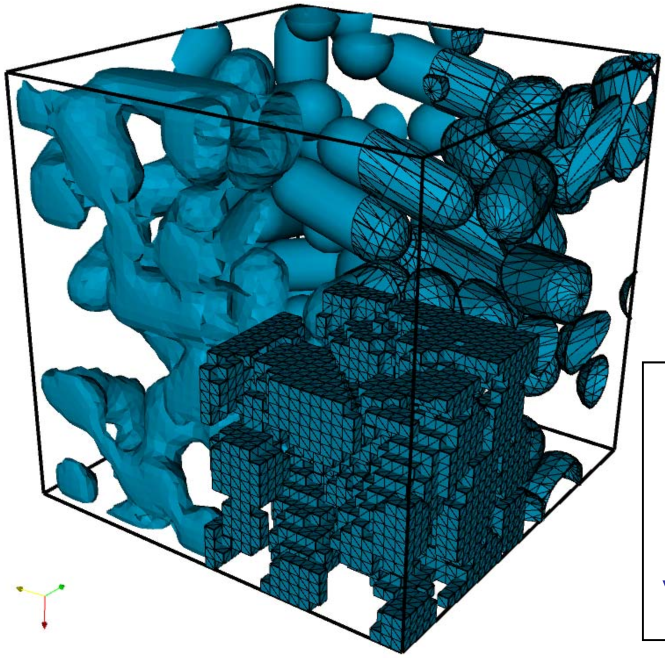
Snow: a granular and porous medium

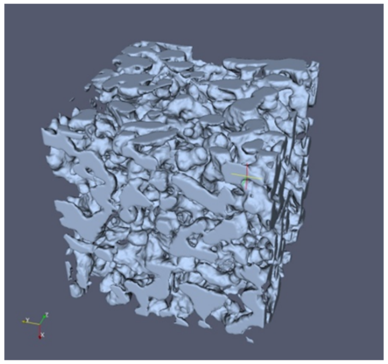


When inter-granular processes dominate:
Discrete Element (DEM)

For matrix and pore-space structures and interactions:
2-phase continuum, FE, FDM



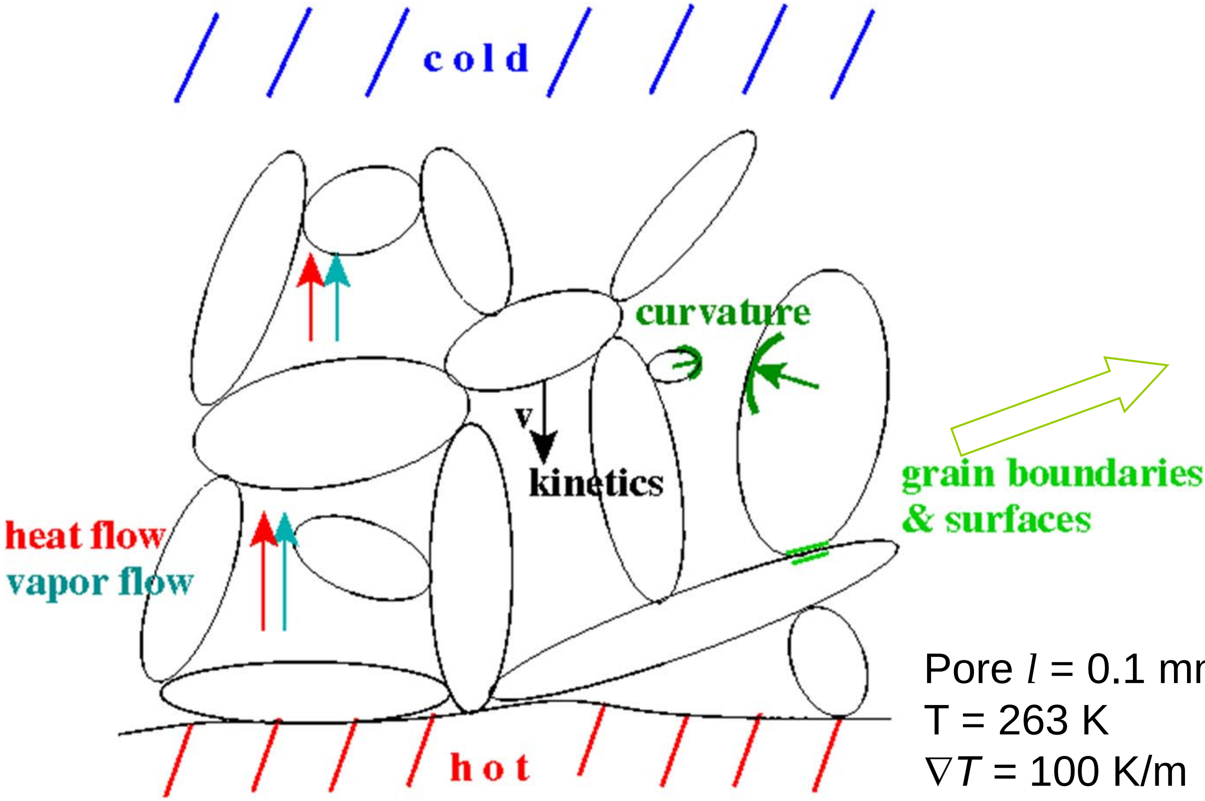


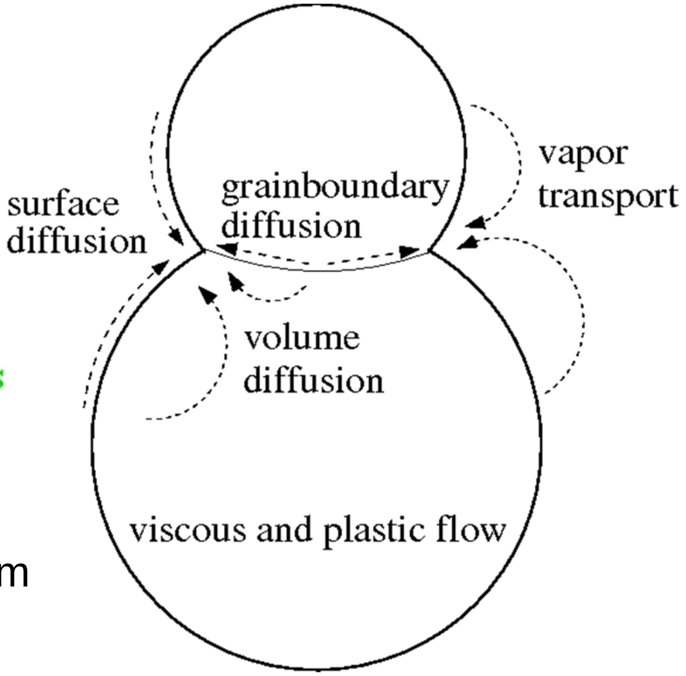


Matrix-Particle interaction
DEM + triangulated Microstructure

Monte-Carlo ice particles, Lattice Boltzmann
Voxel-Microstructure

Snow metamorphism: processes





Pore *l* = 0.1 mm
T = 263 K
∇T = 100 K/m

$$P_{sat}^{bottom} / P_{sat}^{top} \approx 1 + 9 \cdot 10^{-4}$$

κ = 0.1 mm

$$P_{sat}^{\kappa} / P_{sat}^{flat} \approx 1 + 6 \cdot 10^{-6}$$

Grain boundary, surface, volume diffusion; viscous flow;
(re)sublimation+vapor transport; … what dominates?

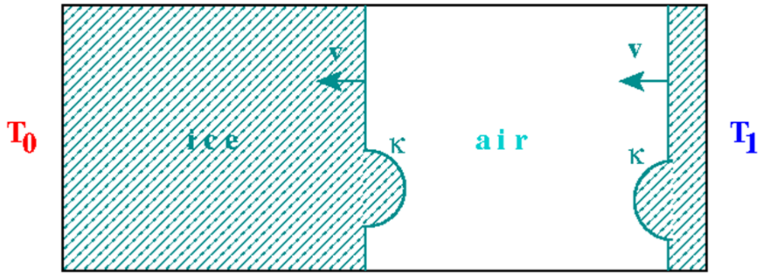
κ = 0.01 mm

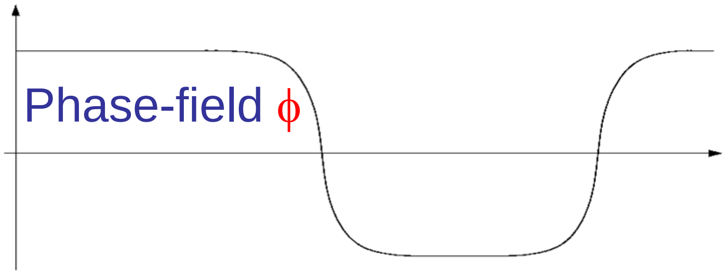
$$P_{sat}^{\kappa} / P_{sat}^{flat} \approx 1 + 6 \cdot 10^{-5}$$

TGM Phase-field model: idea

Hypothesis: Dominating driving forces are
water vapor gradients in the pore space

ice: heat diffusion Air: heat diffusion (T)
\+ water vapor diffusion (chemical potential u)

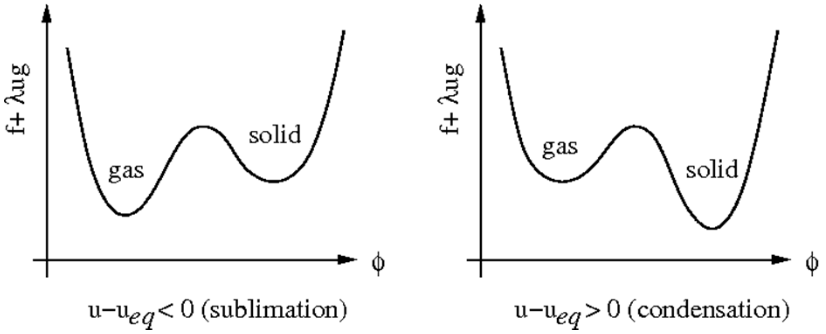




Free energy functional:

$$F = \int_V W^2 (\nabla\phi)^2 / 2 + f(\phi) + \lambda(u - u_{eq}) g(\phi)$$

surface volume tilting



TGM Phase-field model: equations

Phase field

$$\tau \frac{\partial \phi}{\partial t} = W^2 \nabla^2 \phi + \phi - \phi^3 + \lambda \frac{\rho_v^{eq}(T_0)}{\rho_i}(u - u_{eq}(T))(1-\phi^2)^2, \qquad \left(\tau \partial_t \phi(x,t) = -\frac{\delta F}{\delta \phi(x,t)} \right)$$

Energy

$$\rho c_p(\phi) \frac{\partial T}{\partial t} = \nabla(\kappa(\phi)\nabla T) \boxed{+ \frac{L_{sv}\rho_i}{2}\frac{\partial \phi}{\partial t},}$$

Latent heat

Mass

$$\frac{\partial u}{\partial t} = \nabla(D(\phi)\nabla u) \boxed{- \frac{\rho_i}{\rho_v^{eq}(T_0)} \frac{1}{2} \frac{\partial \phi}{\partial t},}$$

Sublimation, condensation

Parameters:

Phase-field:

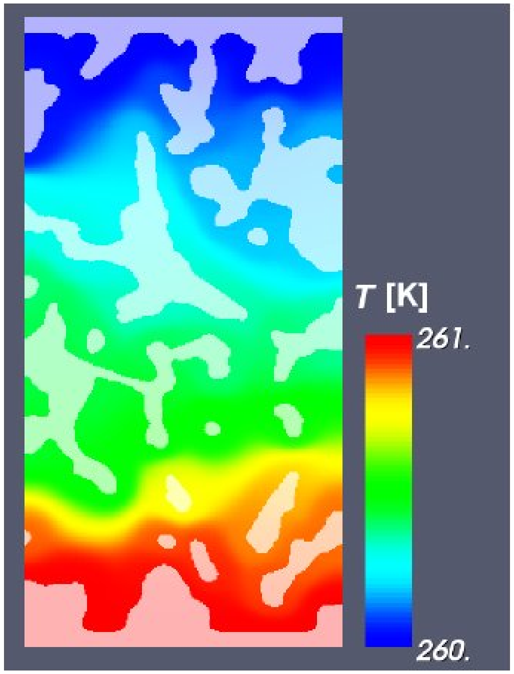
$\lambda, \quad \tau, \quad W$

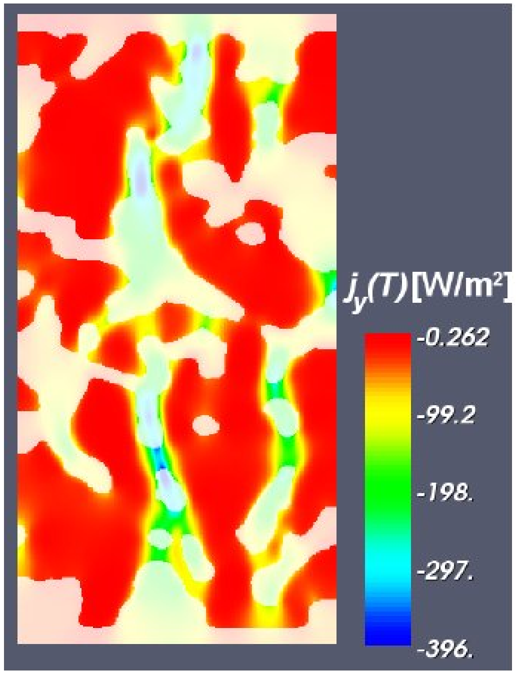
Physical:

$\beta, \quad d_0$

Kaempfer & Plapp, Phys. Rev. E 2009

Modeling grad(T) metamorphism



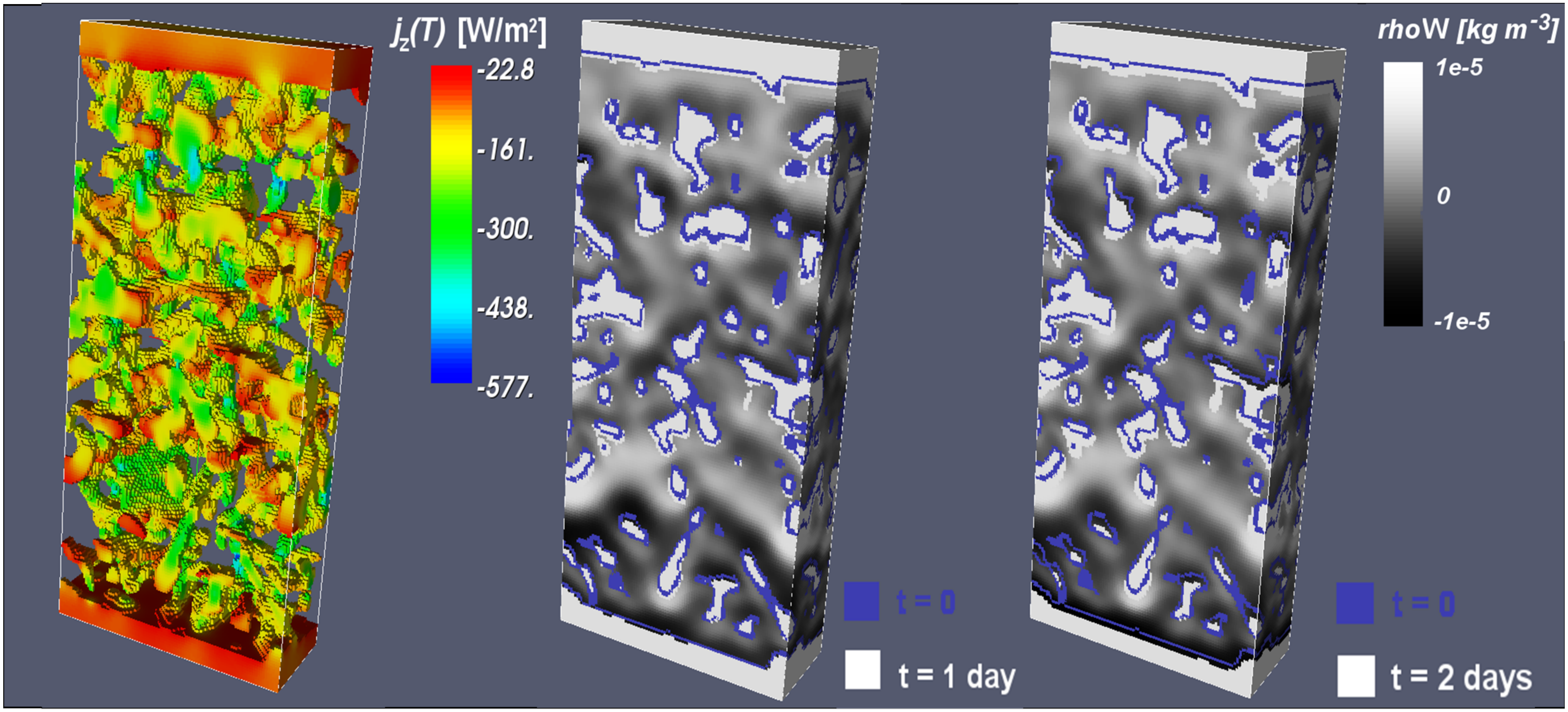


- heat and mass diffusion with phase-change using phase-field technique: no grain boundaries, induced vapor transport dominant

- heat diffusion field disturbed (with respect to linear one)
- heat flow follows ice matrix ⇒ high gradients across pores (heat and water vapor)
- Phase-field model: Topological changes are handled implicitly

Kaempfer & Plapp, Phys. Rev. E 2009

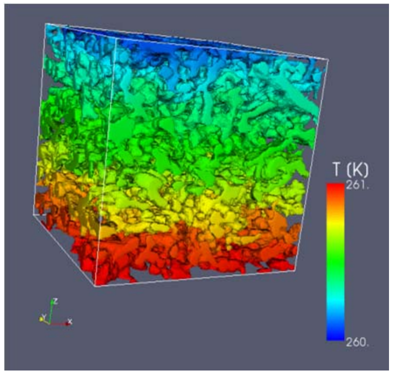
Results - 3D snow



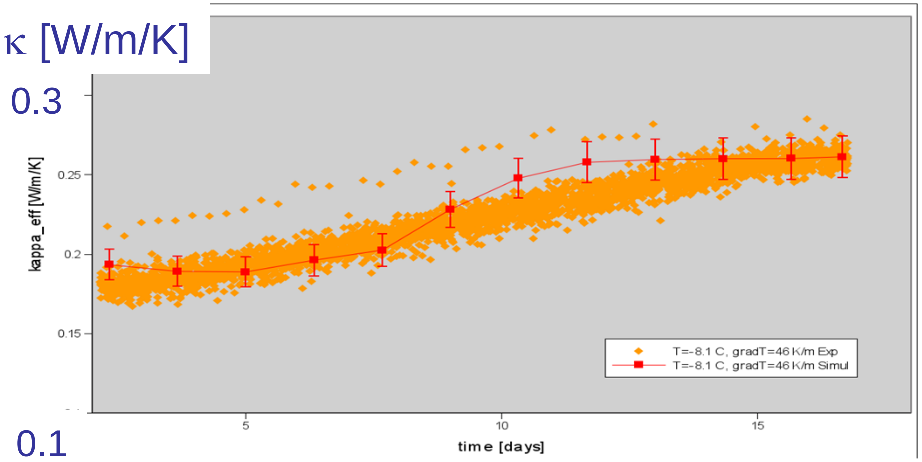
Snow density 270 kg/m^3, grad(T)=190 K/m
Domain size: 100x40x210 voxels (1.8x0.7x3.8 mm)

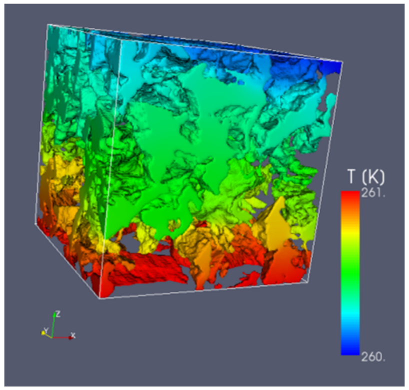
Kaempfer & Plapp, Phys. Rev. E 2009

Simulation of heat (and mass) flow through snow

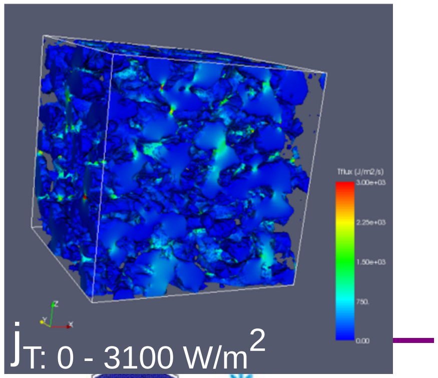


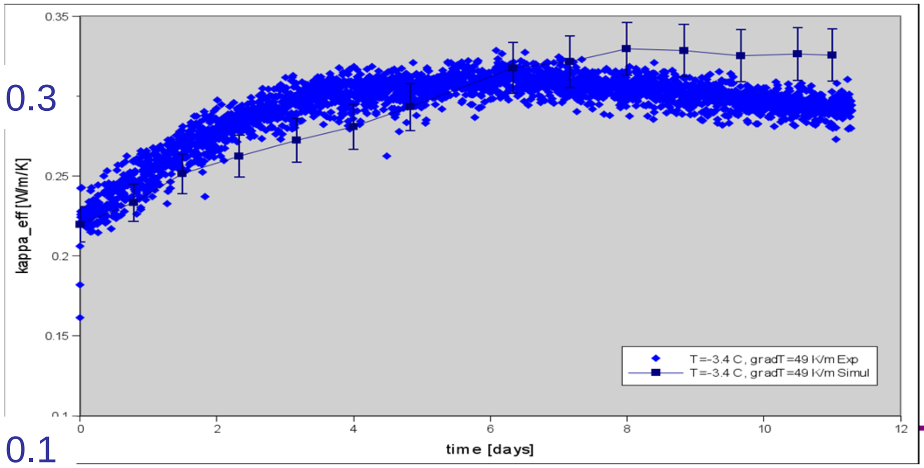
T ~ -8.1 C, grad(T) ~ 46 K/m

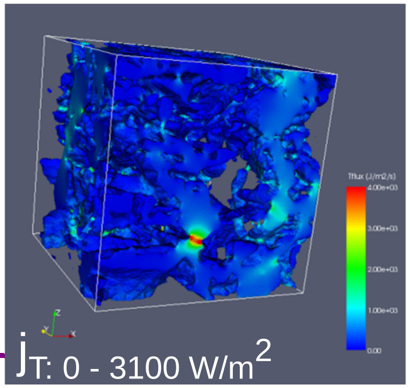




T ~ -3.4 C, grad(T) ~ 49 K/m





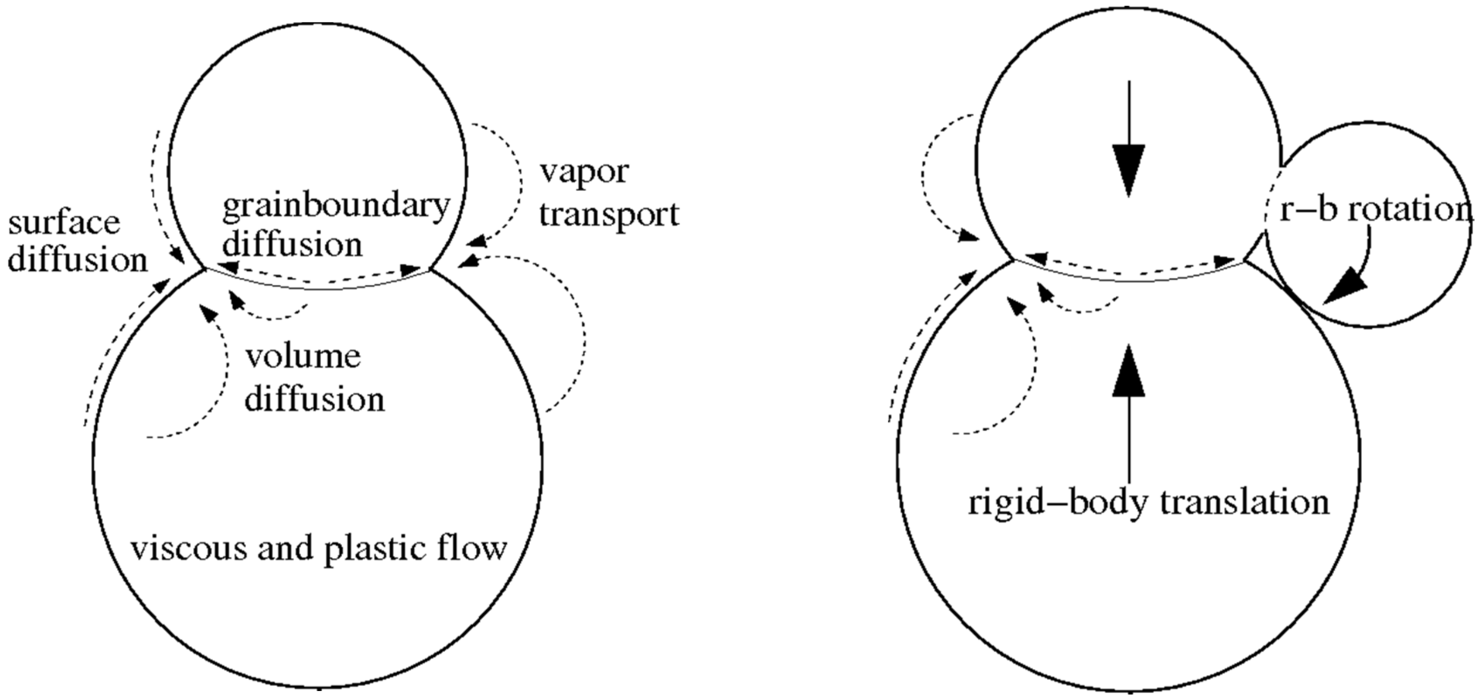


Kaempfer et al., GRL 2005

Isothermal (low gradient) metamorphism

We must consider:

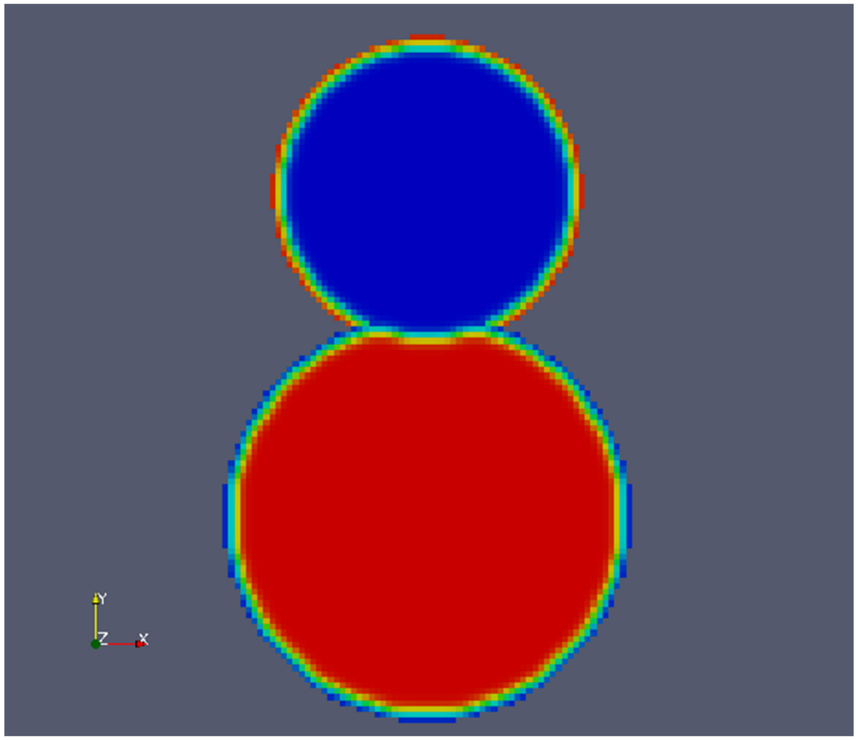
many transport processes and rigid body motion



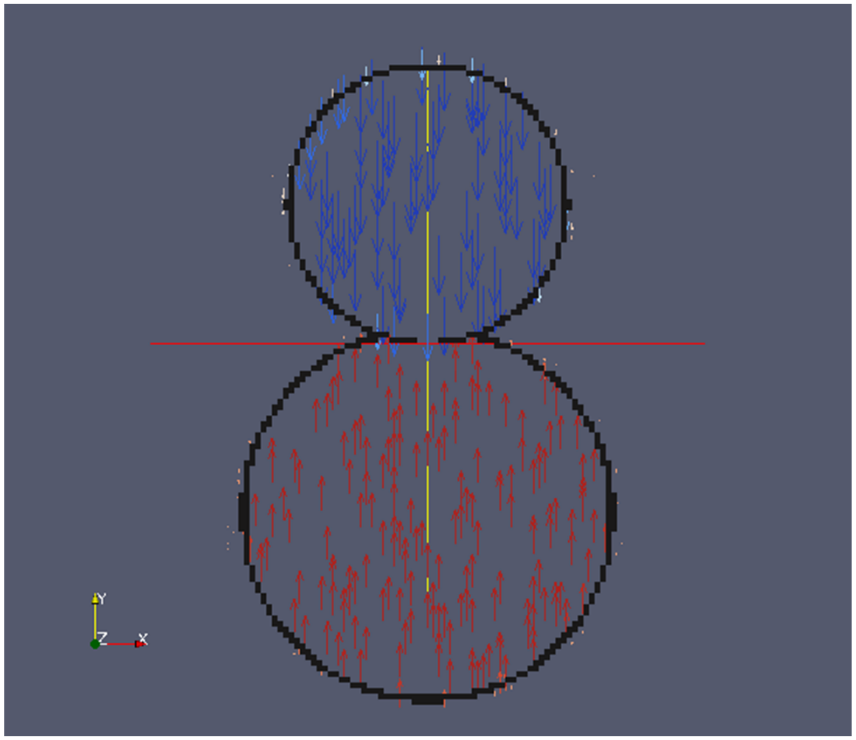
We must distinguish grains ==> more than one phase field

Isothermal modling: 2D first results

Grain phase fields:



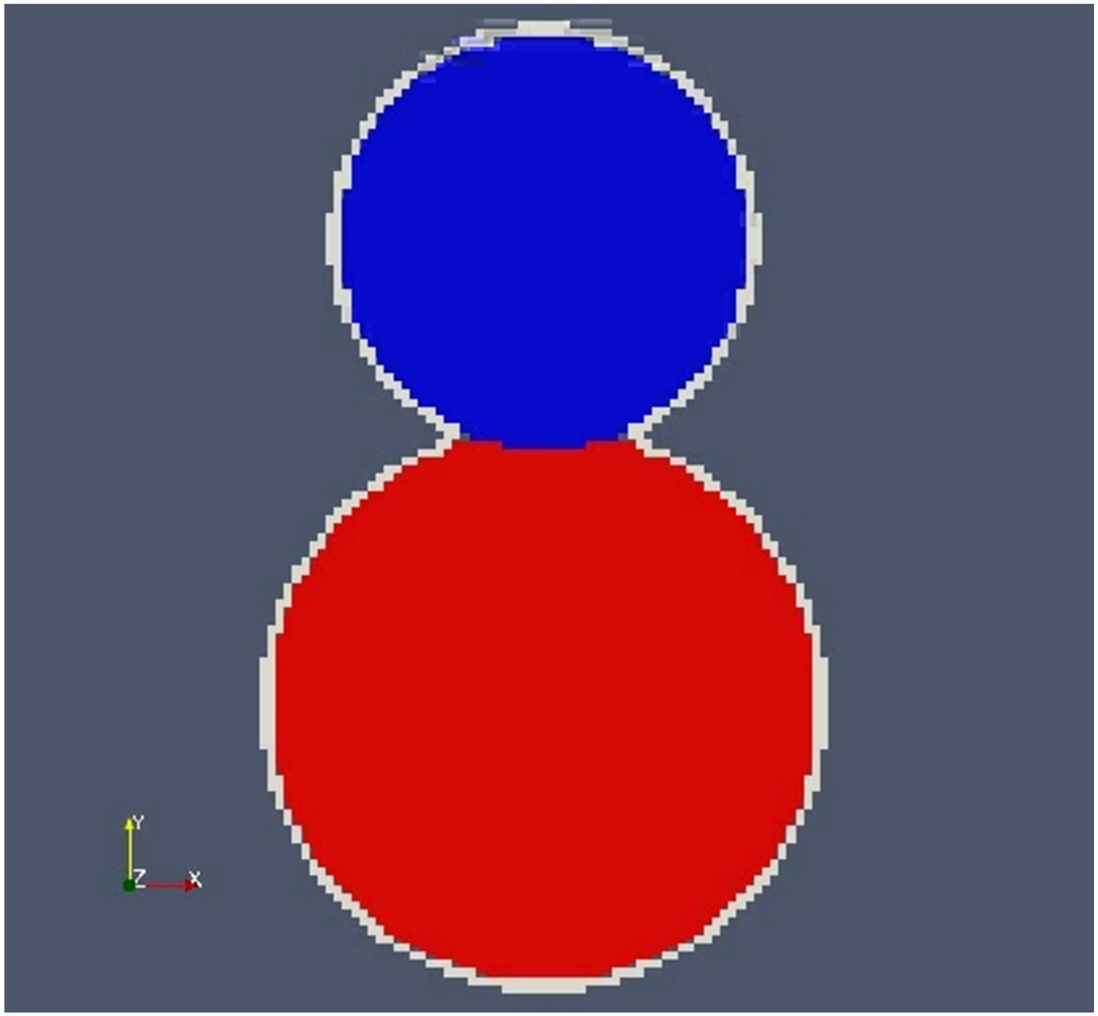
Rigid body advection field:



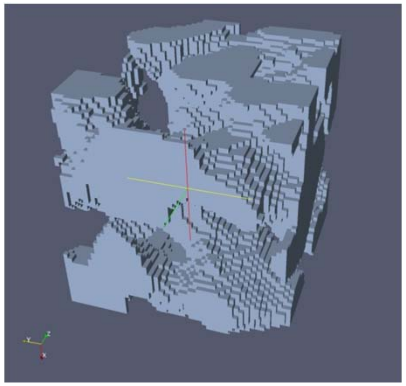
Two grains, different size, sinter together

$D_{\mathrm{surf}} : D_{\mathrm{gb}} : D_{\mathrm{vol}} : D_{\mathrm{vap}} \sim 1000 : 100 : 10 : 1$

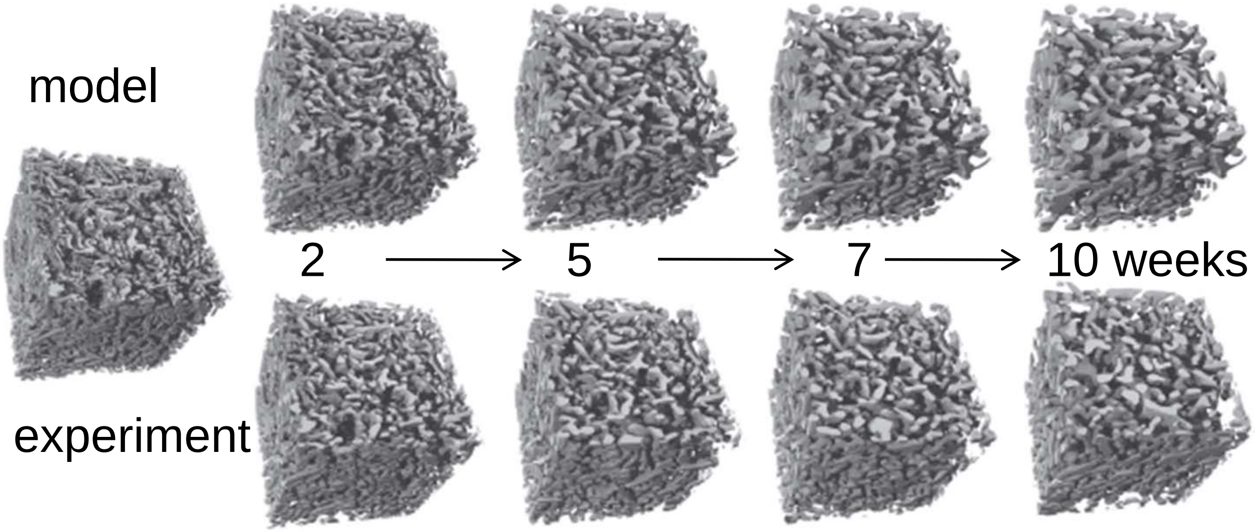
Isothermal modeling: 2D first results



Monte-Carlo (cellular automaton) algorithm for isothermal aging of snow



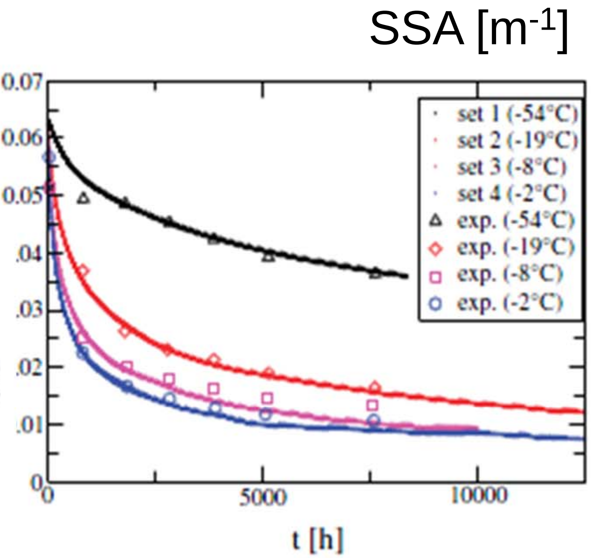
- (Re)sublimation: probabilistic rules
- Diffusion: random walk
- Parameters: experimental fit



model

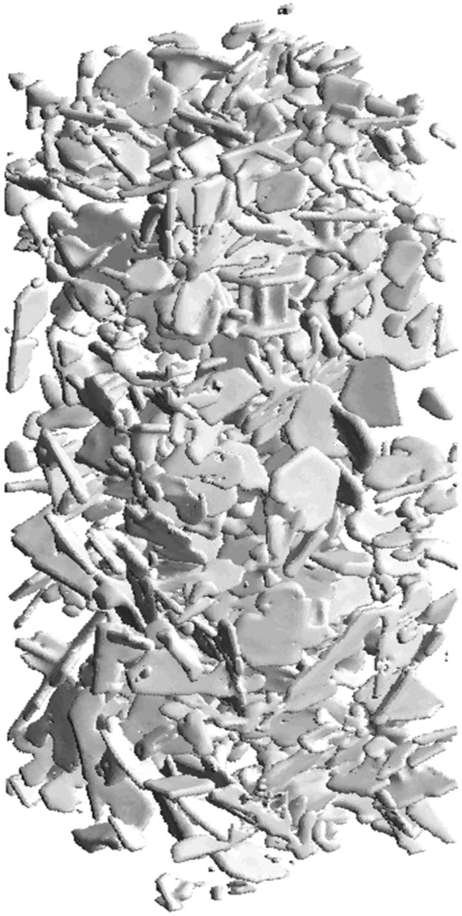
2 → 5 → 7 → 10 weeks

experiment



Vetter et al., EPL 2010

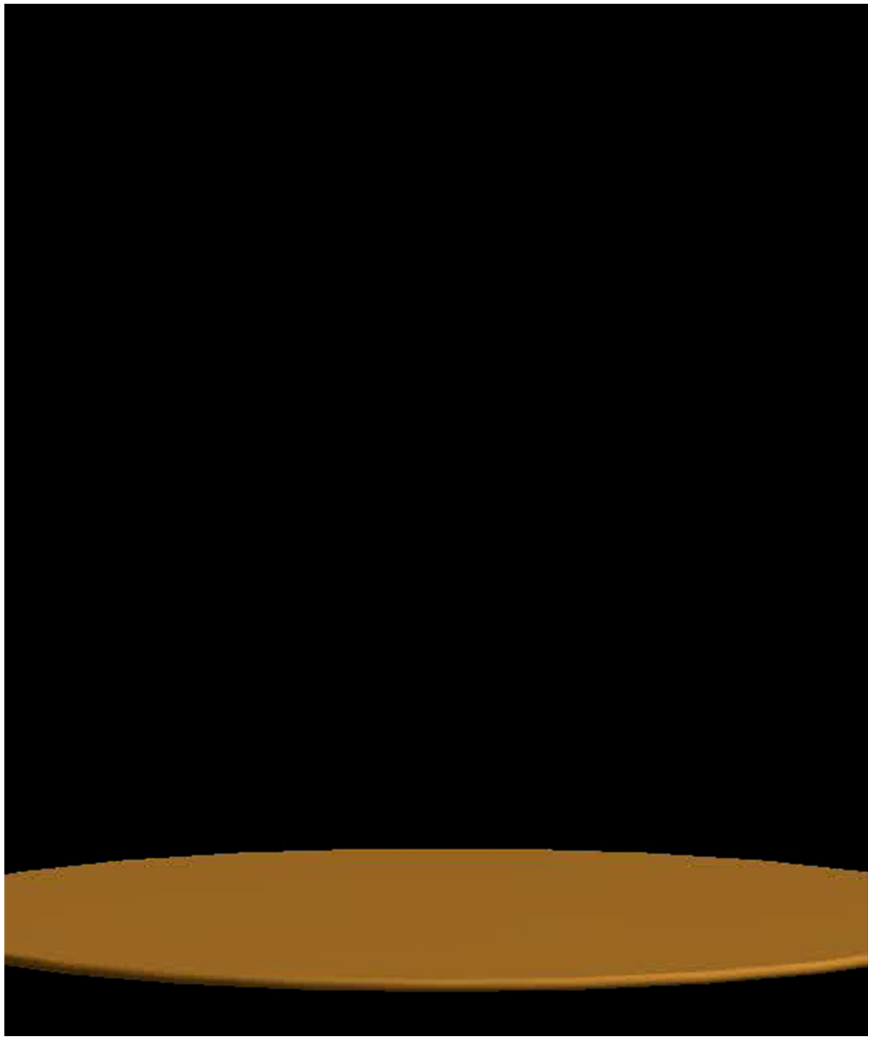
Curvature-driven modeling of settling



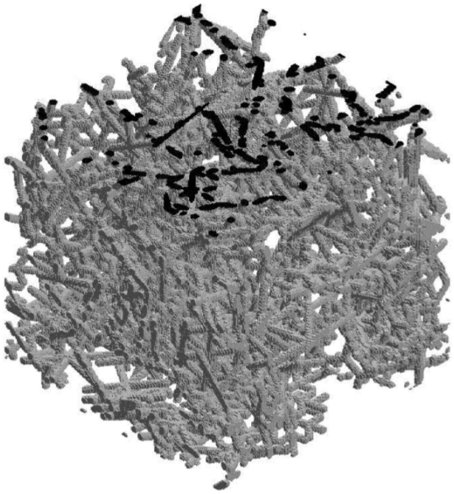
- Curvature effects
  ➔ diffusion and vapor exchange
- sublimation
  ➔ bond breaking
- gravity
  ➔ settling

A. Duffour et al., MOCA 2009

Snowfall: Discrete Element Modeling



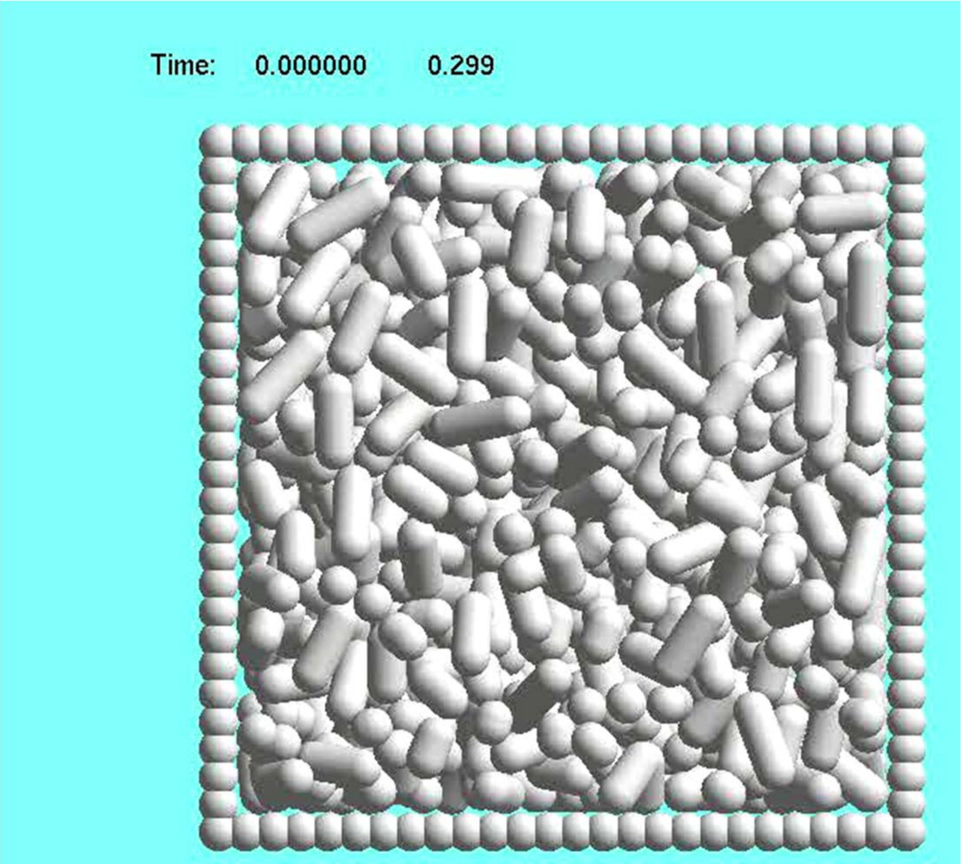
- 3D Discrete Elements (individual ice particles)
- Position and orientation
- Dynamics: contact and body forces on particles (F=ma at each contact)



Fresh DEM snow: ~150 kg m^{-3}

Settlement using DEM

- Collisional interaction
- Frozen bonds support tension, compression, shear, bending, and twisting
- Contact creep acts in tension, compression, shear, bending, and twisting to reduce stress
- Frozen contact failure by brittle rupture
  Sintering using empirical bond-growth law

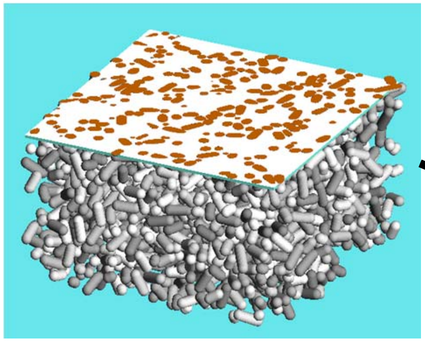


- driven by self-weight and lid mass of 0.125 kg
- Sample is 20x20x20 mm
- Particles diameter 1 mm

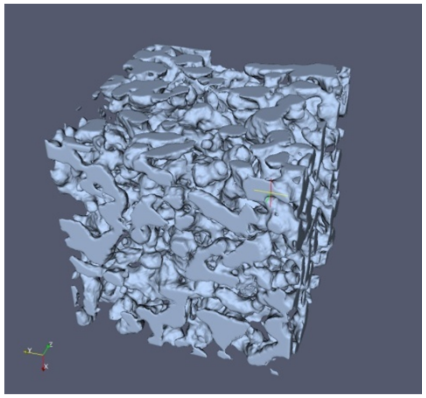
Johnson & Hopkins, J. Glac. 2005

Air flow through digital snow

DEM snow



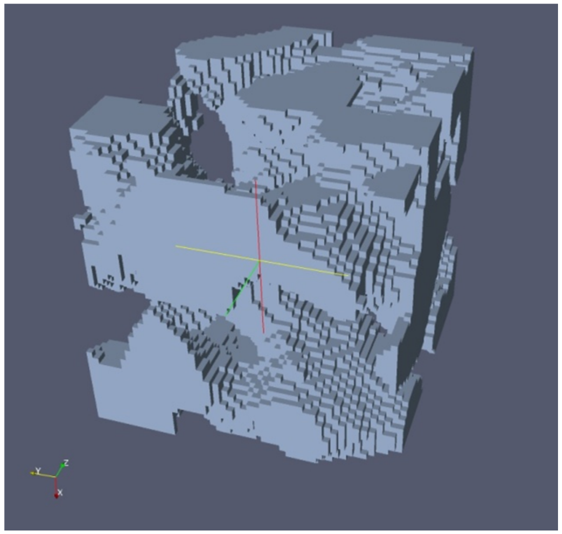
natural snow



Grid overlay

Tomography

- regular grid of pore-space (or ice)
- 2D slice or 3D

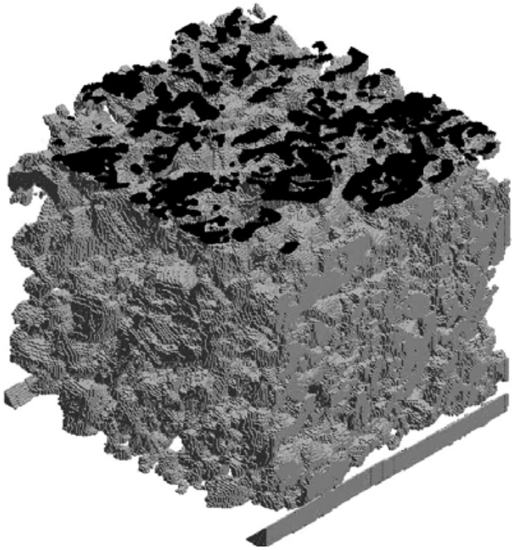


Lattice-Boltzmann (LB)

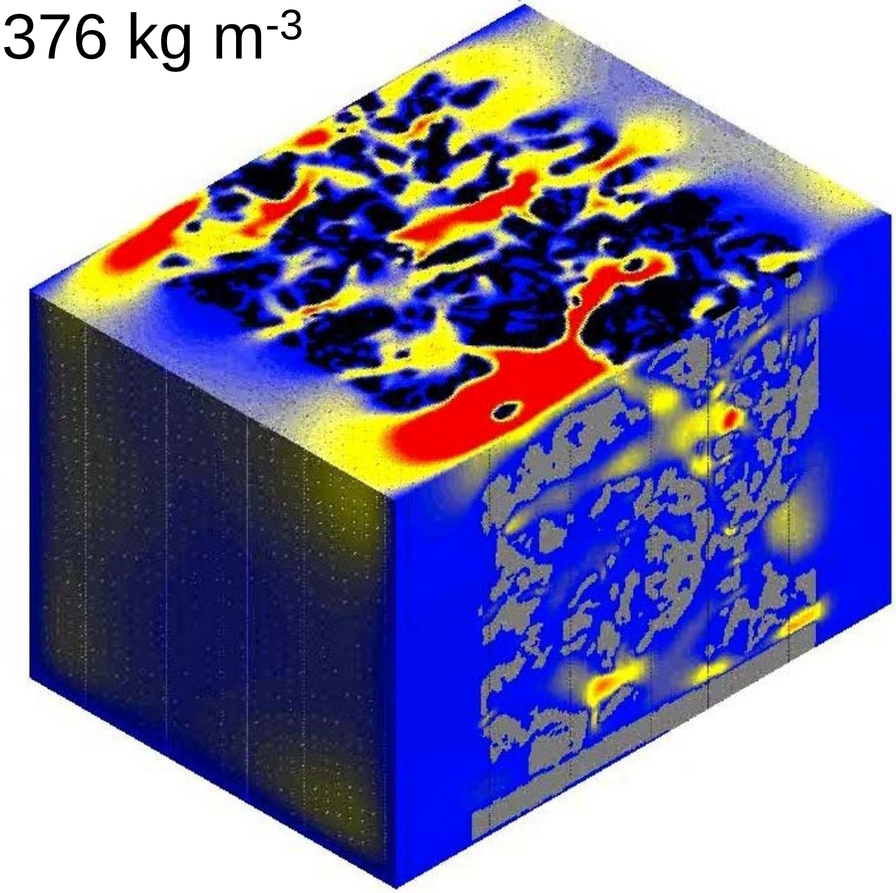
- discrete velocities at nodes
- propagation, collision
- bounce-back at ice-interfaces

Air flow through digital firn

- Antarctic firn tomography
- 2.6 cm side-length, density 376 kg m^{-3}
- 3D simulation



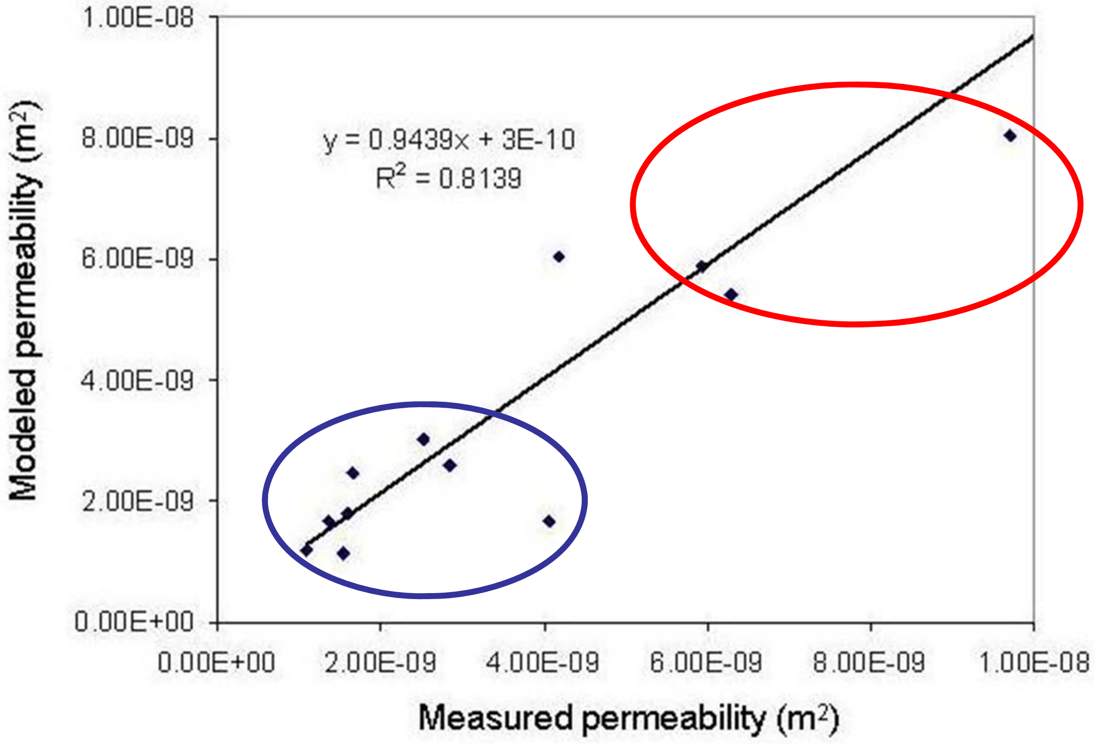
Tomography: A. Wegener Institute



Courville et al., JRG 2010

Permeablity: simulation vs. experiment

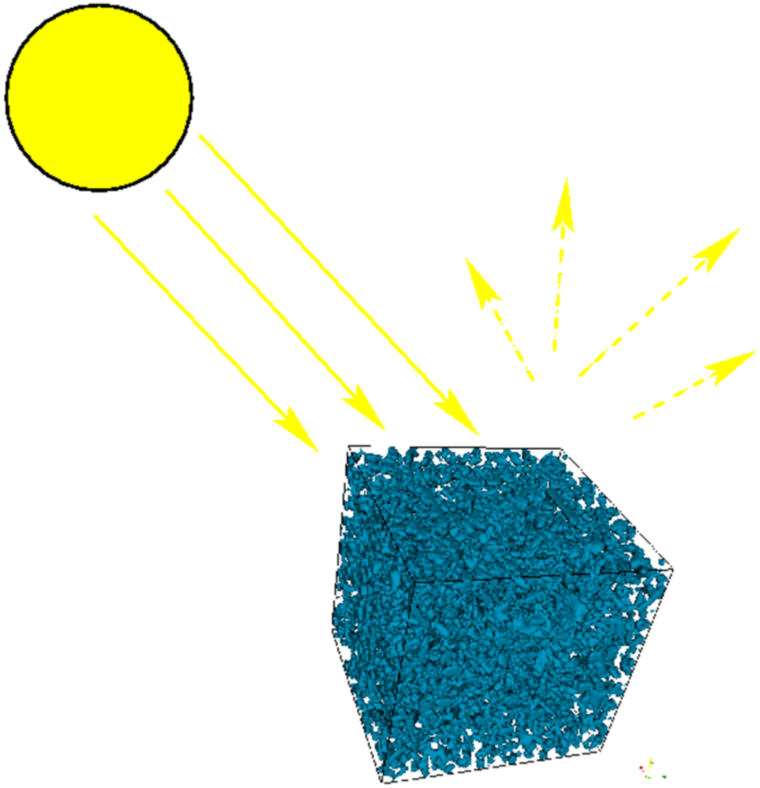
Low accumulation (coarse)



High accumulation (fine)

Courville et al., JGR 2010

Radiative Transfer Modeling

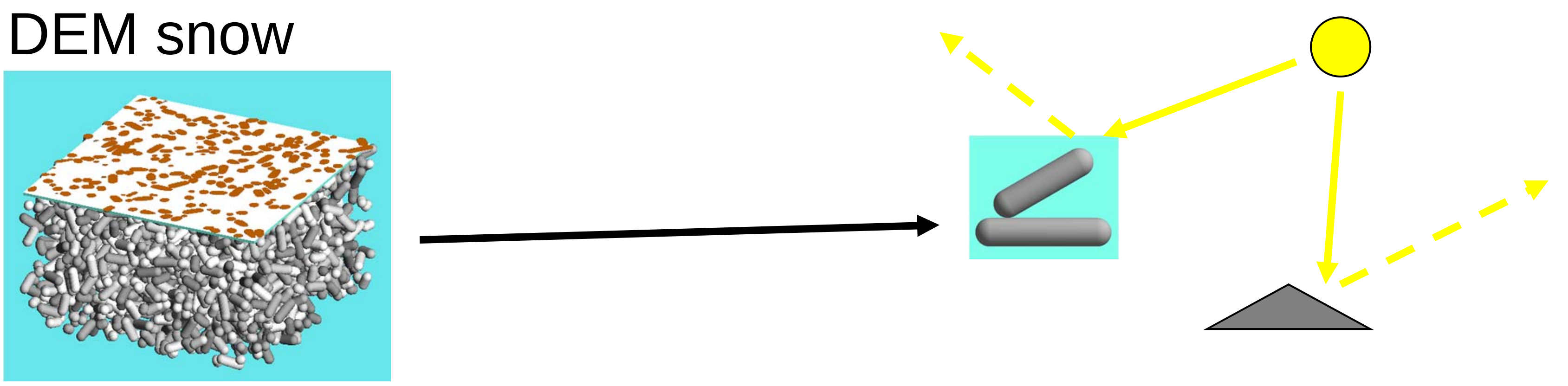


Goal: Study (and predict) albedo, transmittance, reflectivity factors

Hypotheses:
- wave length << structural scale (grain size)
  - ⇒ geometrical optics
- diffraction neglected

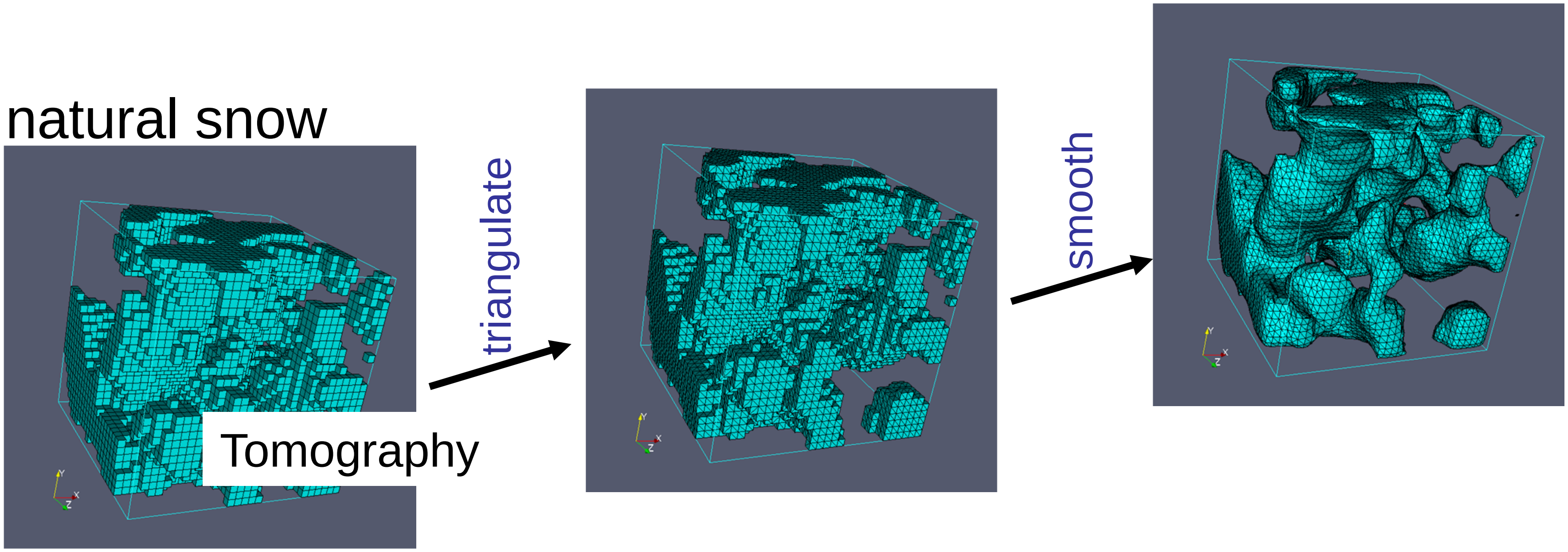
Input:
- Grain based model snow (DEM)
- μ-CT images of natural snow

Optics: snow representation



DEM snow

Photon:
infinitesimal DE



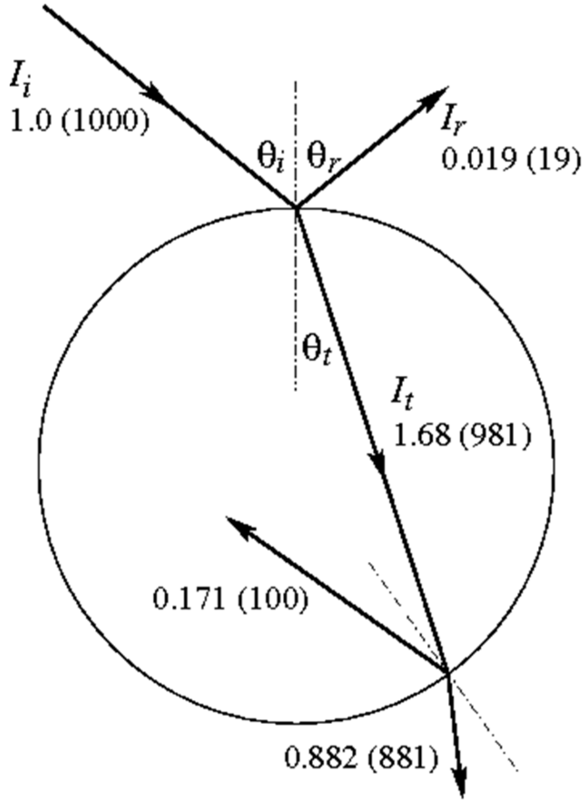
natural snow

triangulate

smooth

Tomography

Geometrical optics approach



At ice-air interface:

- part of energy reflected
- part transmitted, angle: Snell's Law

$$\boxed{n_i} \sin(\theta_i) = \boxed{n_t} \sin(\theta_t)$$

- Radiances are determined by Fresnels equation

$$I_r(\theta_r) = I_o(\theta_i)\frac{1}{2}\left[\frac{\sin^2(\theta_i-\theta_t)}{\sin^2(\theta_i+\theta_t)} + \frac{\tan^2(\theta_i-\theta_t)}{\tan^2(\theta_i+\theta_t)}\right]$$

$$I_t(\theta_t) = (I_o(\theta_i) - I_r(\theta_r))\frac{n_t^{\;2}}{n_i^{\;2}}$$

In the ice: Part of energy absorbed by Bourguer-Lambert equation

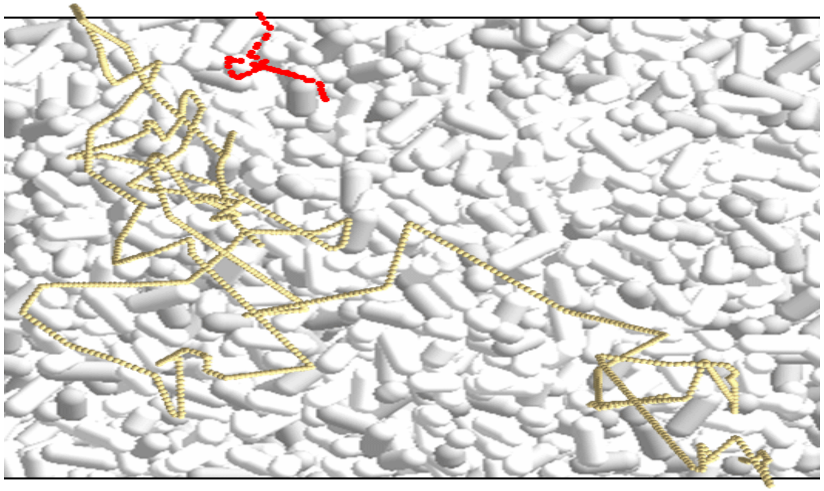
$$I(t+\Delta t) = I(t)\boxed{e^{-kL}}$$

Photon tracking instead of ray tracing

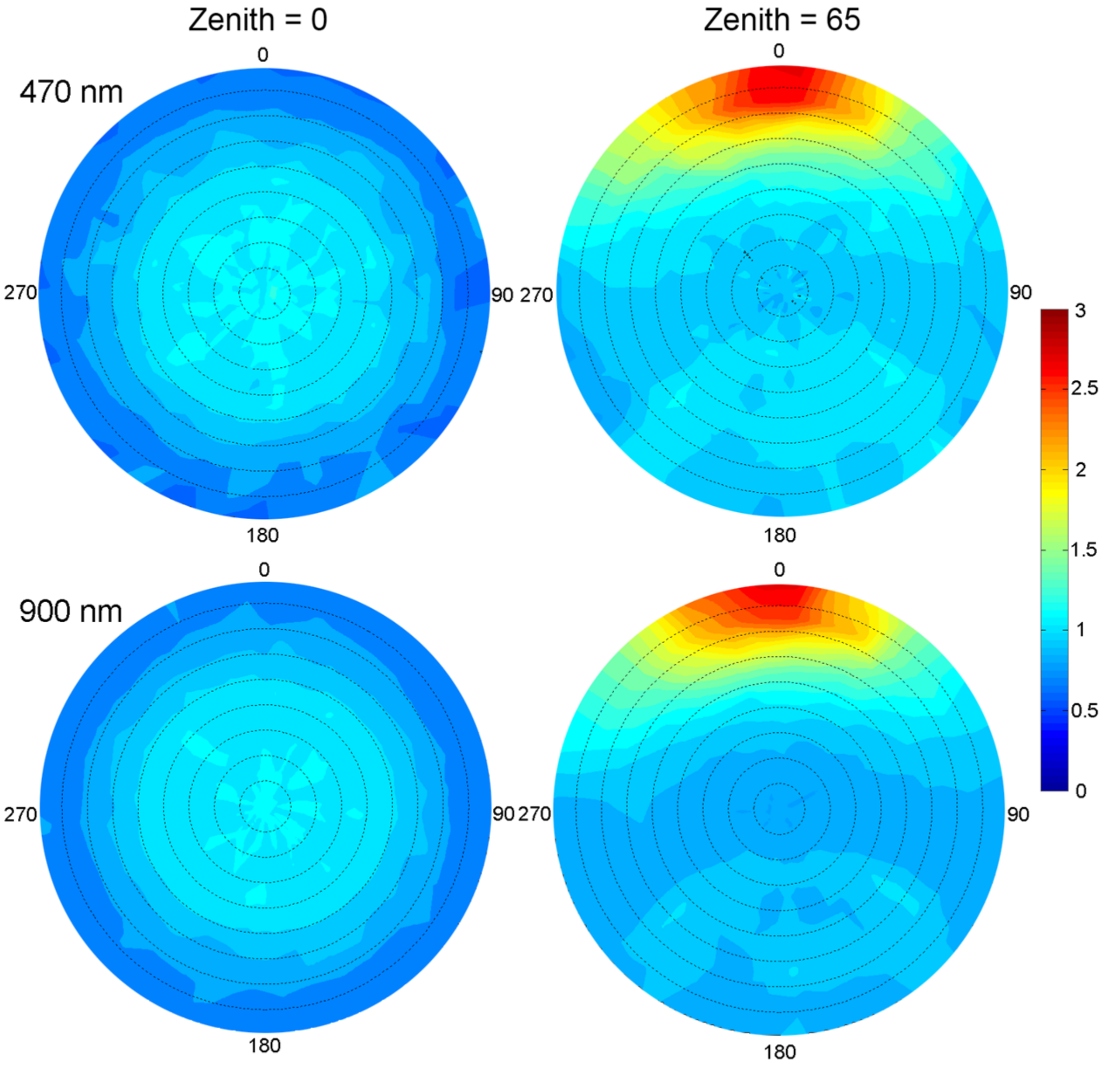
Idea: Each ray of light consists of many photons
(simulation: e.g., 200’000)

Implementation:

- Photons are fired individually
- Optics laws implemented probabilistically
- Discrete element framework tracks photons

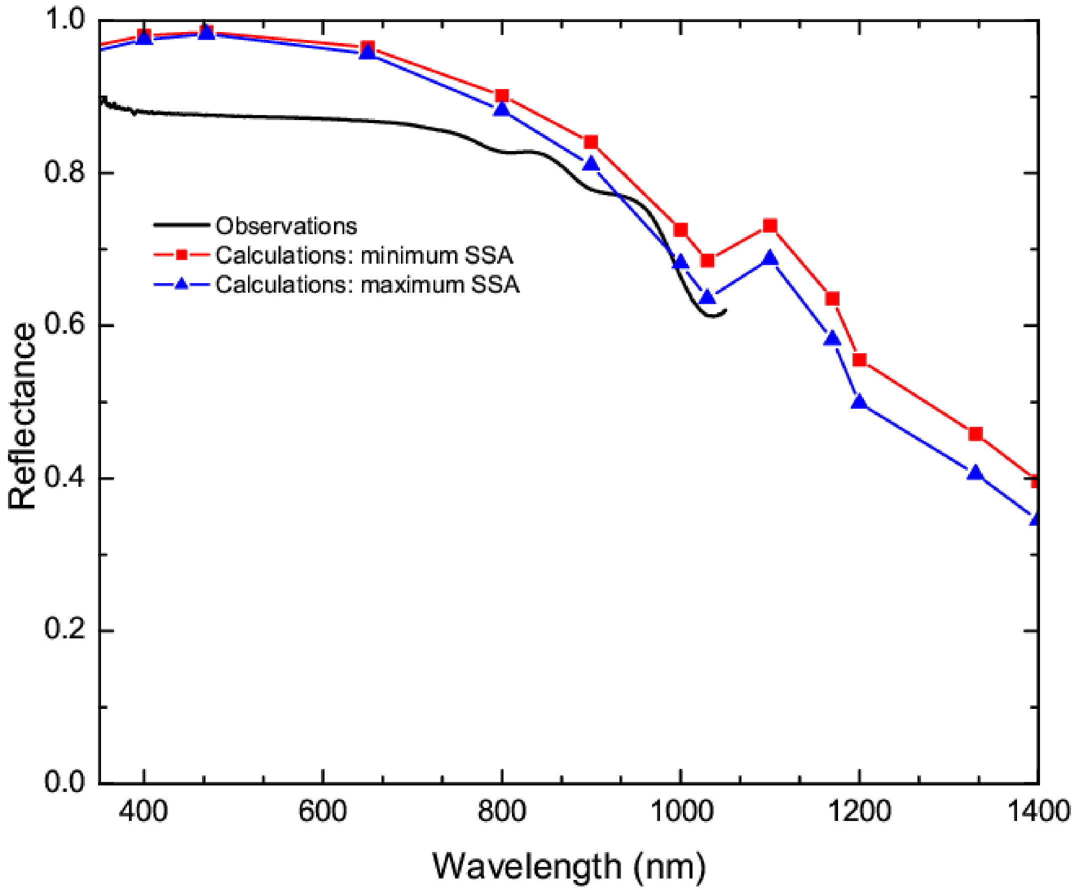


Results: Directional reflectance



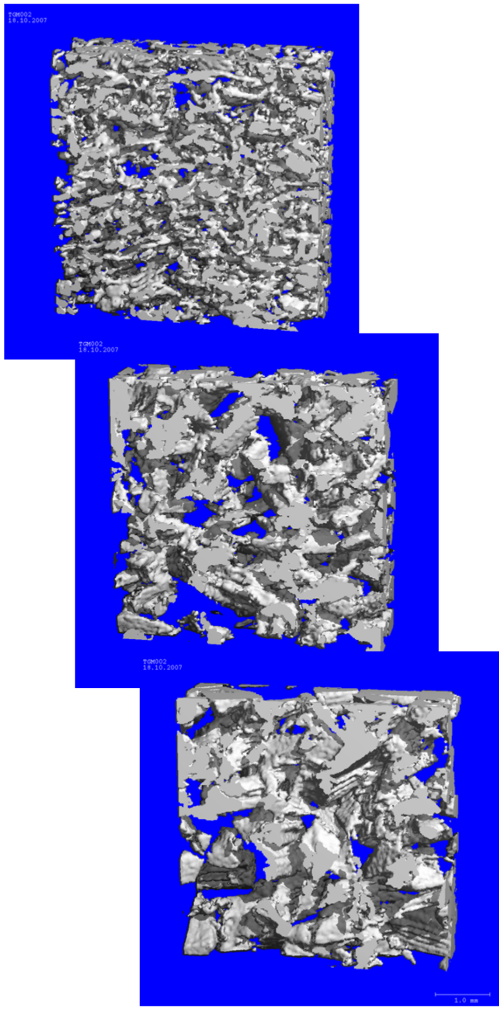
Kaempfer et al., JGR 2007

Results: Comparison with measurement



Kaempfer et al., JGR 2007

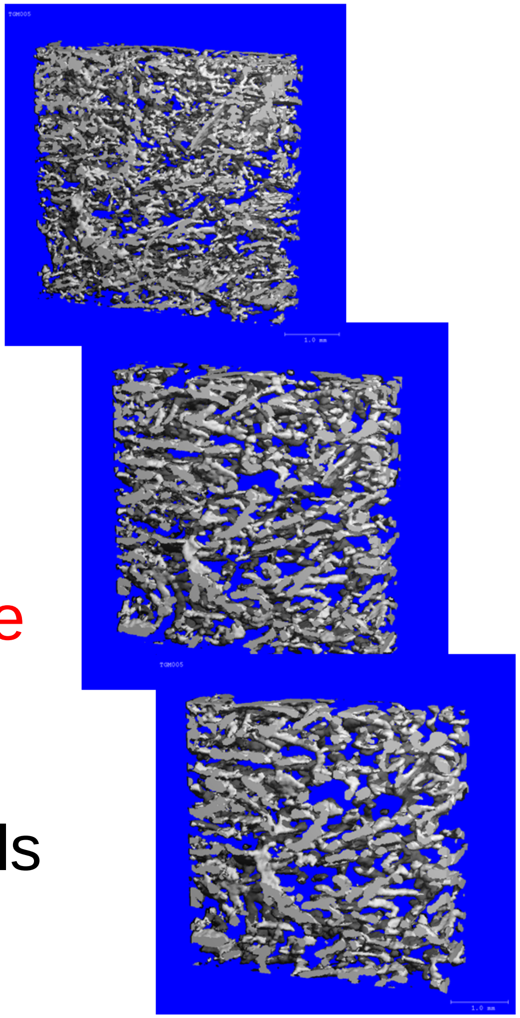
Summary (1)



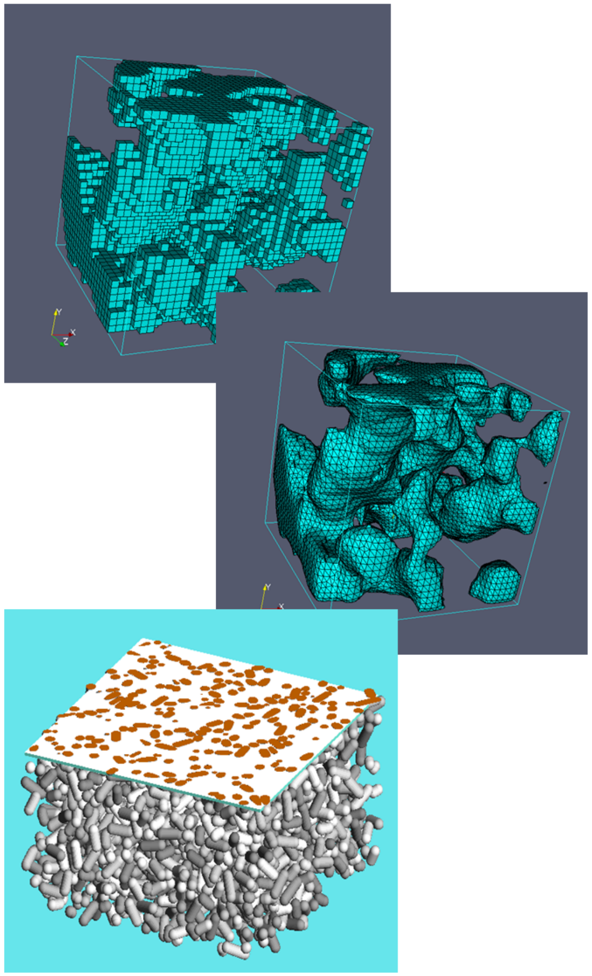
- snow is a very dynamic material
- evolution depends on environment
- interaction with environment depends on (micro)structure

- snow and evolution can be observed on the relevant scales

➔ input to numerical models



Summary (2)

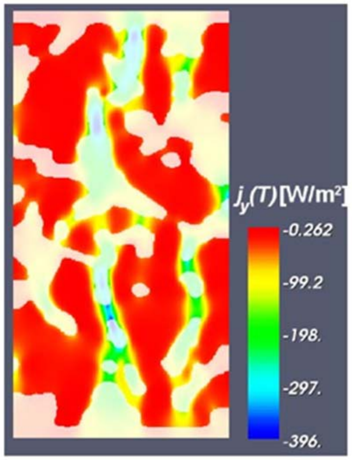


Numerical models for

- + air flow through pore space (LB, FD, FE)
- + radiative transfer (DEM)
- + heat conductivity (FDM, FD, FE)
- + metamorphism (FDM, CA, DEM, FD, FE)
  - + heat and mass transfer
  - + grain boundaries

- – „bits and pieces“
- – coupling
- – chemistry

+ phase-field method



Conclusion

- Combined micro-structural approach: experiments and modeling
- Modeling: Discrete or continuum approach
  - Depending on problem: mechanics, optics, air flow, heat and mass
- Digital snow
  - DEM or tomography (voxels), triangulations
- Detailed studies at the relevant length scale
  - coupling between micro-structure and physical or chemical properties
  - Based on fundamental physics
  - Strength:
    - Complex geometries (natural snow) & Controlled microstructures (DEM)
    - Examine interaction (e.g., flow or scattering) in detail
    - Coupling to modern observation techniques (μ-CT) & virtual snow lab
- Outlook:
  - Impurities, liquid water, …

Acknowledgements

- Collaborators:

  Mathis Plapp
  Ecole Polytechnique

  Mark Hopkins, Don Perovich, Zoe Courville
  CRREL

  Martin Schneebeli, Bernd Pinzer, Henning Löwe
  SLF Davos

- Funding:

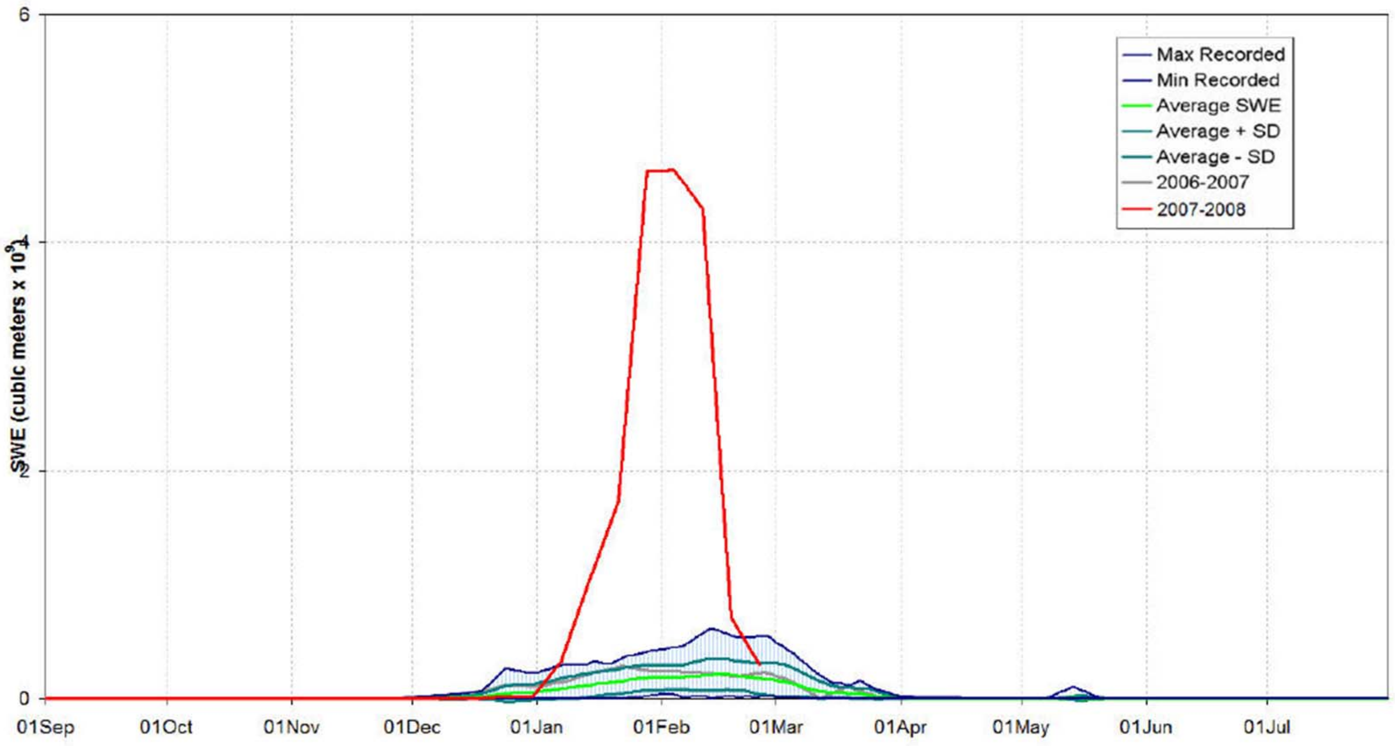
  Army Basic Research Terrain Properties and Processes Program

  Research Participation Program at the USACRREL administered by the Oak Ridge Institute for Science and Education

  Swiss National Science Foundation

thomas.kaempfer@a3.epfl.ch

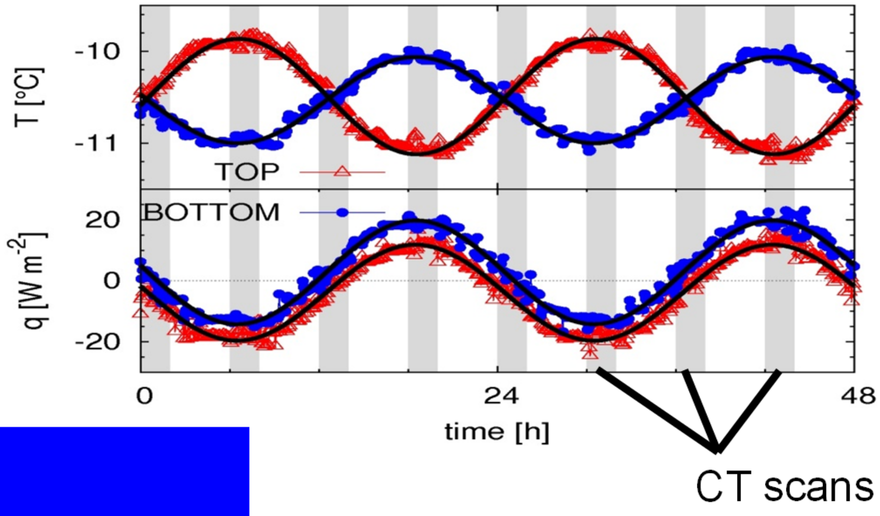
Issue 1: Snow mapping (radiative transfer)

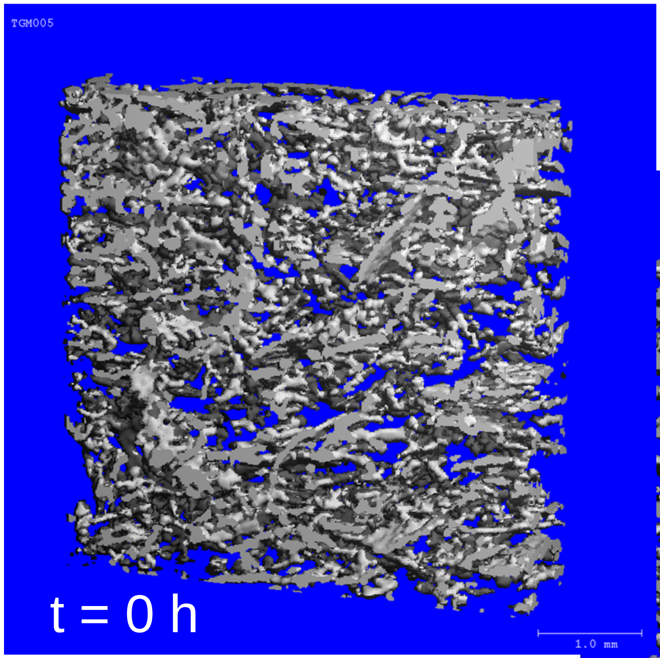


Thin snow and extremely cold temperatures (==> high temperature gradients) led to significant overestimation of snowpack SWE by SSM/I

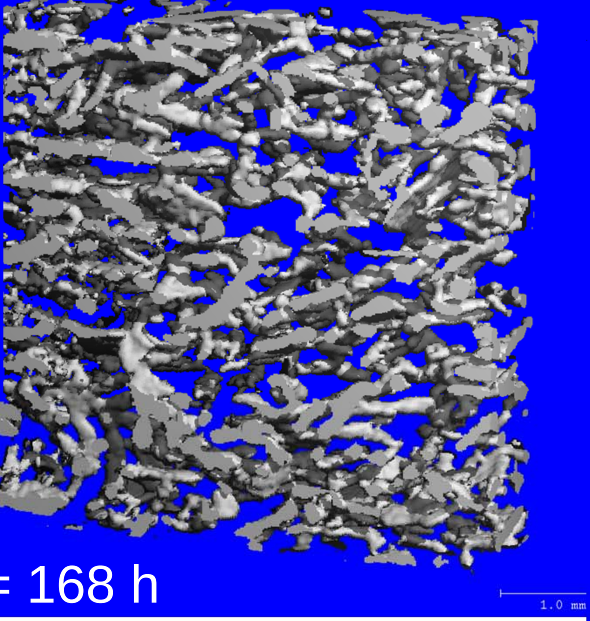
Experiments under sinusoidal TG

- Alternating TG similar to snow surface in nature
- max(grad(T)) ~ 100 K/m

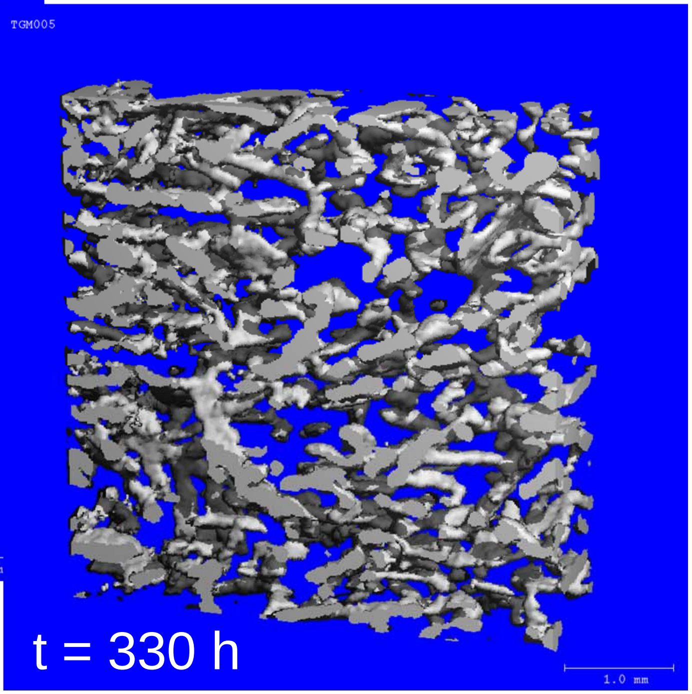




t = 0 h



t = 168 h

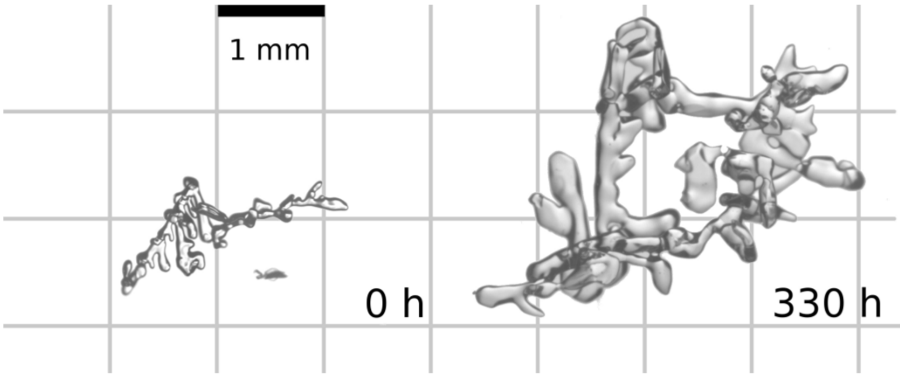


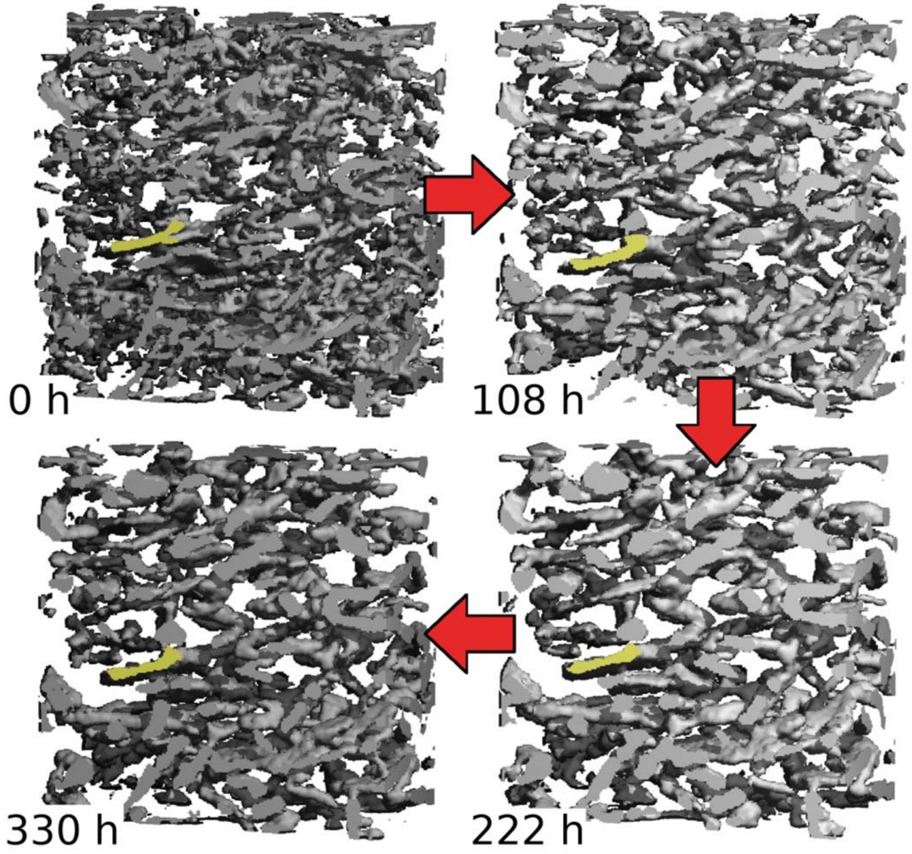
t = 330 h

Pinzer & Schneebeli, GRL 2009

Morphology (sinusoidal TG)

- The “critical gradient” for faceting was exceeded during 86% of the time
- No sign of faceting was observed
- Slow 3D-structure evolution

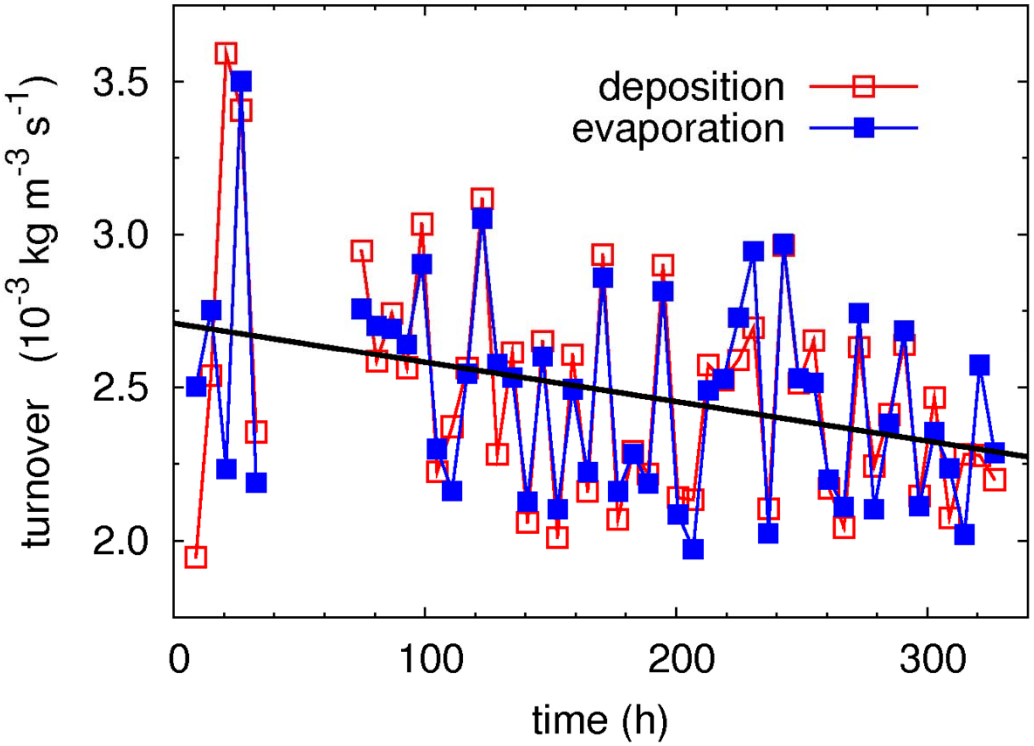




Pinzer & Schneebeli, GRL 2009

Mass turnover rate (sinusoidal TG)

Rate of mass relocation

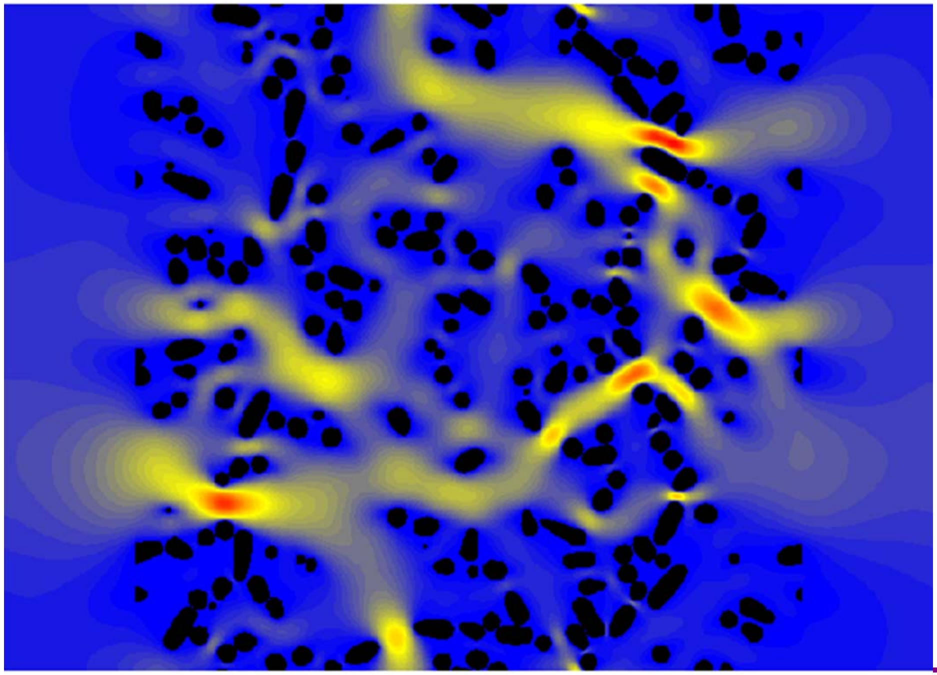


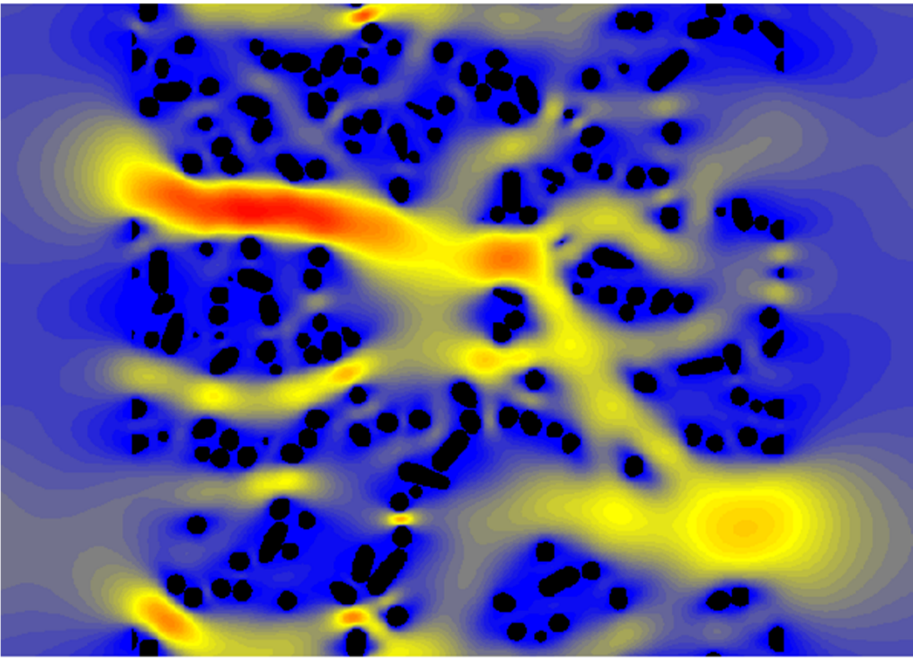
- 2.5 means a recrystallization of 60% of the complete ice mass during 12 h

Pinzer & Schneebeli, GRL 2009

Air flow through digital snow

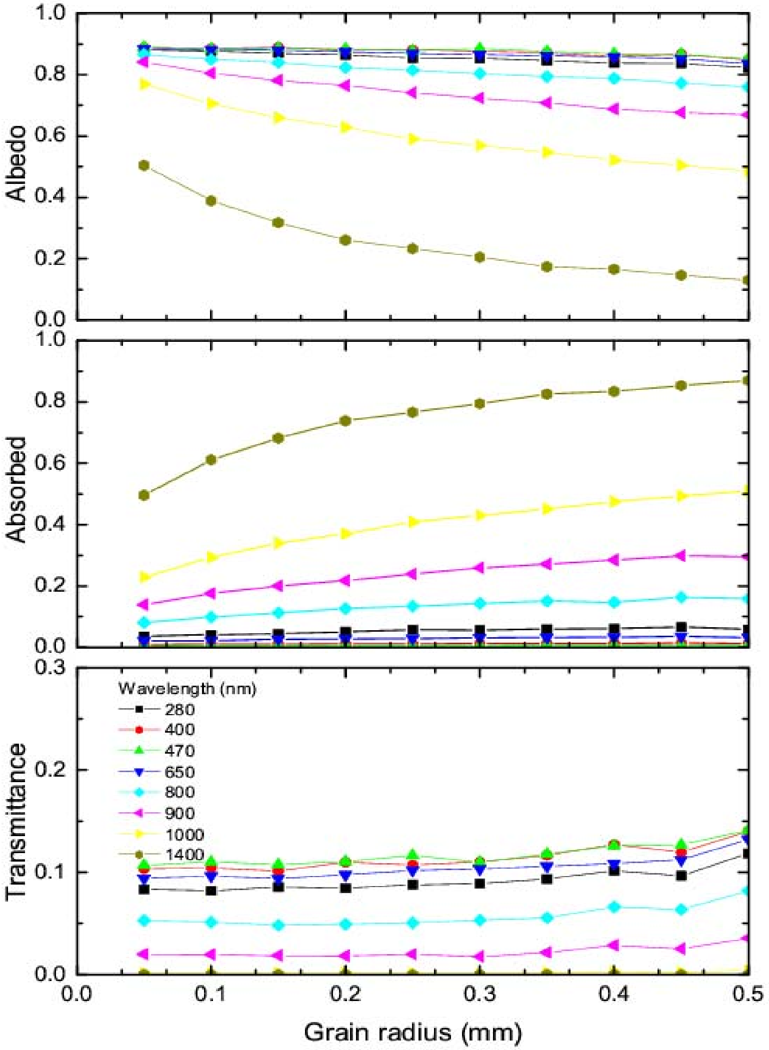
- cylindrical model snow
- porosity 82 and 85%
- 2D slices simulation


exp100.15.25 porosity 82%


exp100.15.55 porosity 86%

Courville et al., JRG 2010

Results: Snow model studies



Kaempfer et al., JGR 2007