magma matters

Numerical modelling of igneous processes

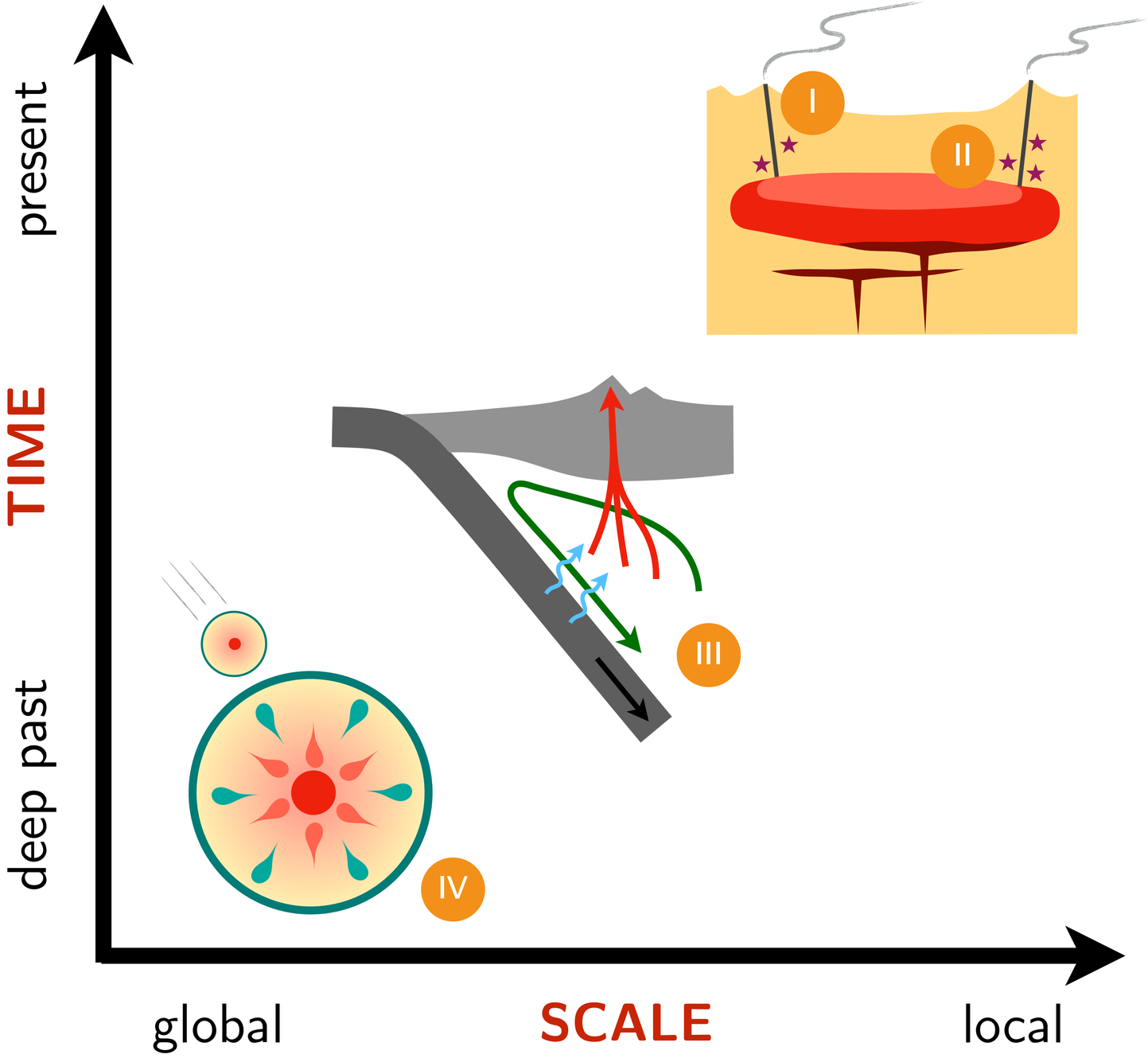
GD Division Outstanding ECS Award Lecture 2020

Tobias Keller | @magmamatters

29 March 2021 | EGU General Assembly

University of Glasgow

research themes



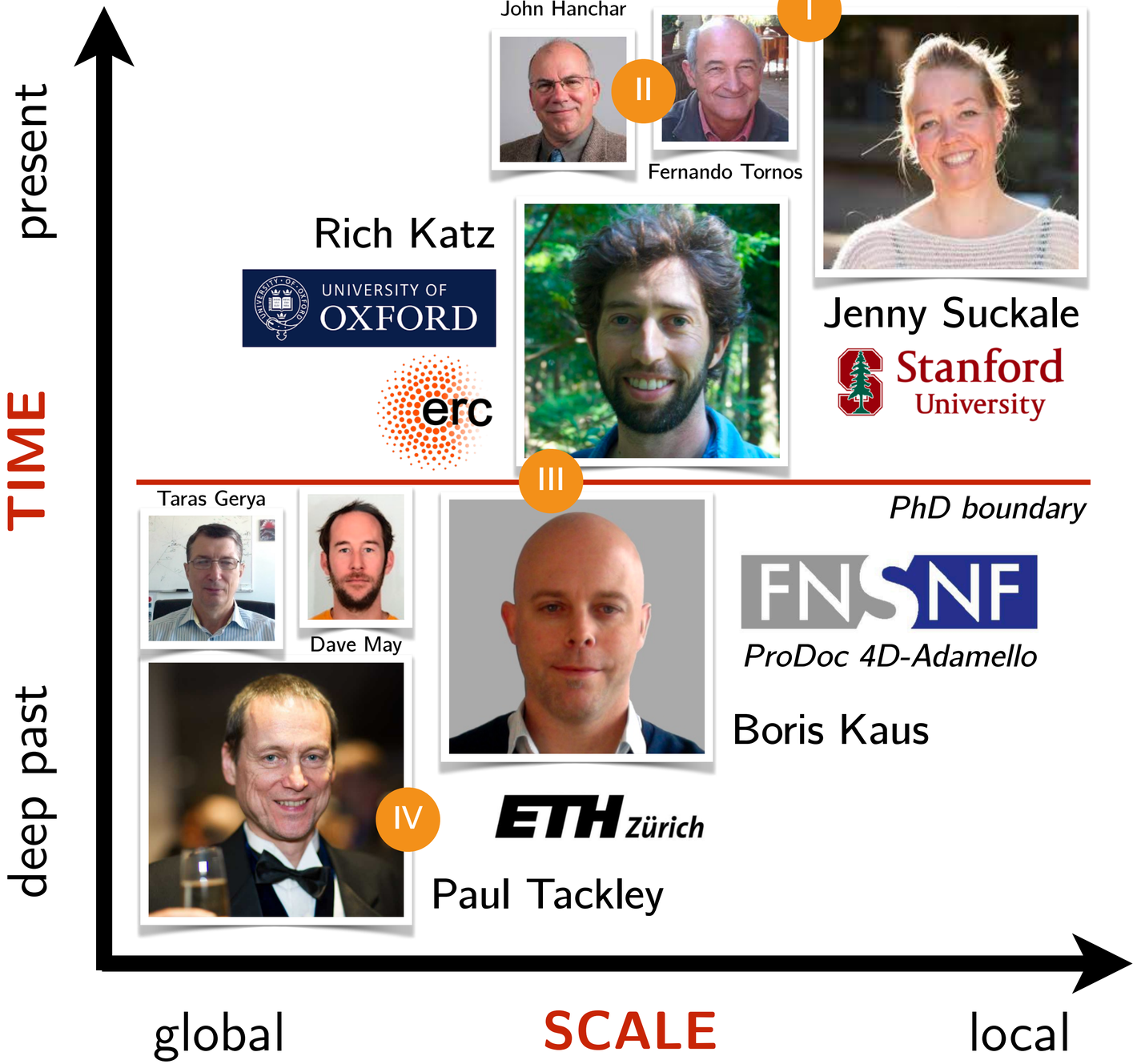
I *volcanic activity*

II *mineral resources*

III *magmatism & tectonics*

IV *planetary differentiation & evolution*

research themes



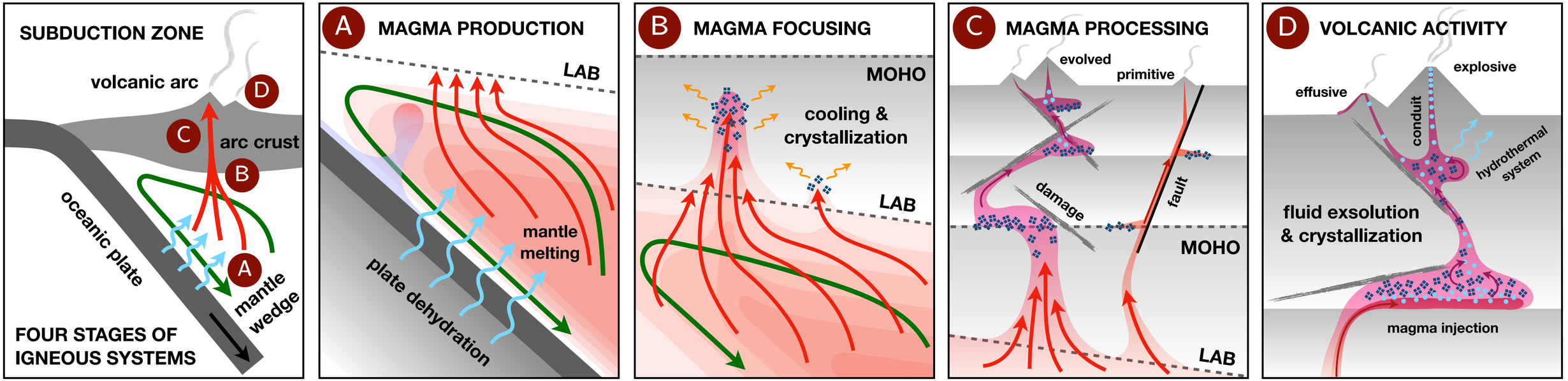
I *volcanic activity*

II *mineral resources*

III *magmatism & tectonics*

IV *planetary differentiation & evolution*

IGNEOUS PROCESSES



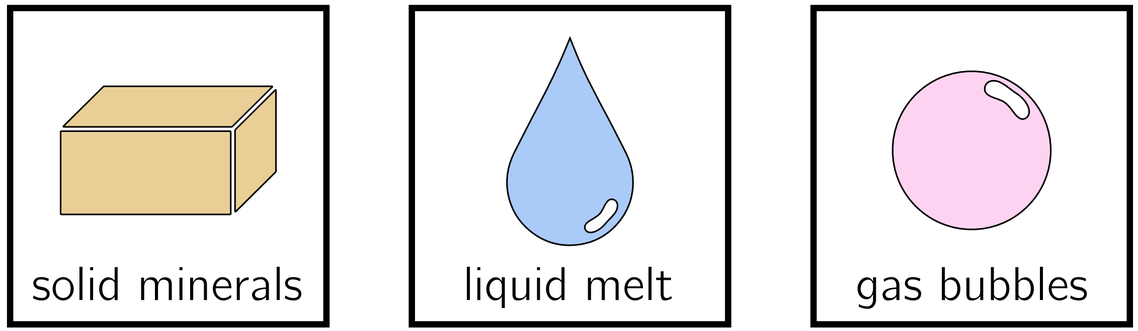
Keller & Suckale, *GJI*, (2019)

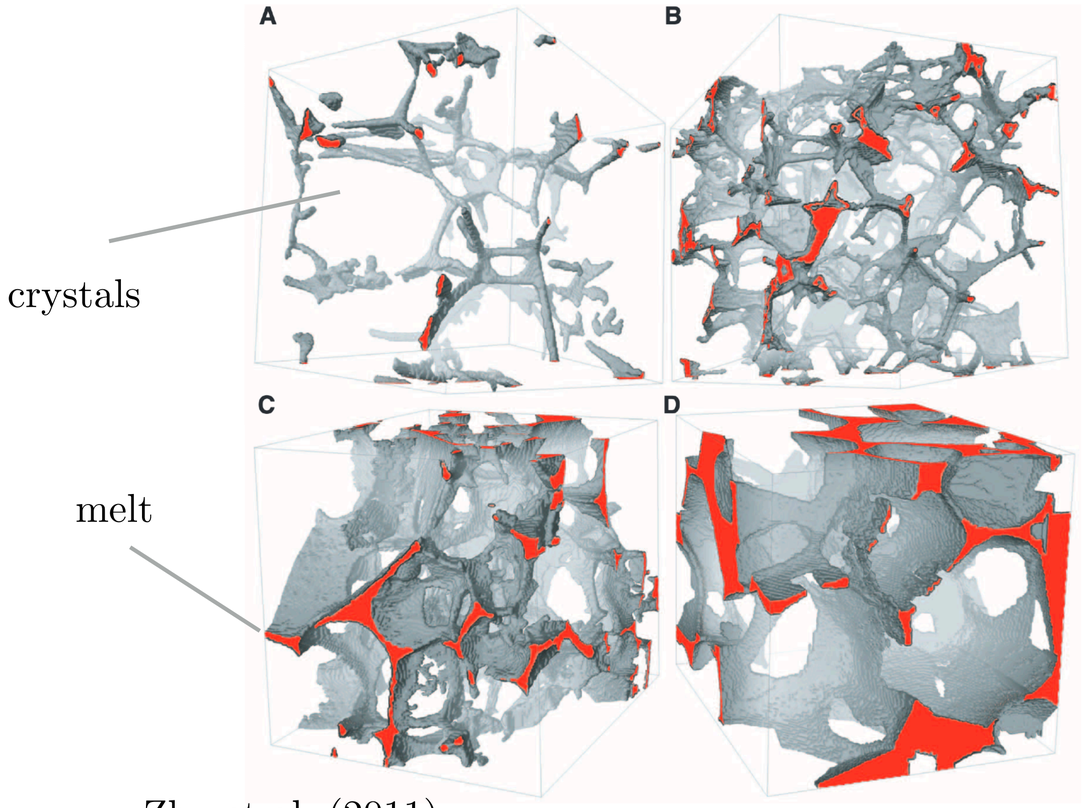
multi-phase aggregates of solids, liquids, and gas phases

reactive mass transfer, element partitioning between phases

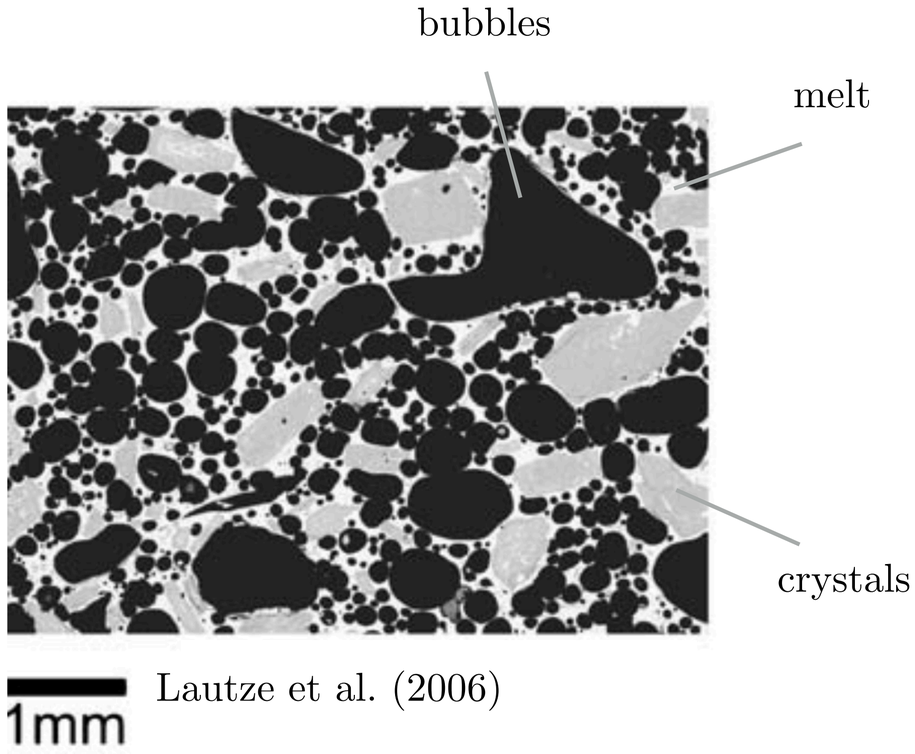
transport contrasting phase mobility, segregation, compaction

MULTI-PHASE MAGMA





Zhu et al. (2011)



Lautze et al. (2006)

CHALLENGE OF SCALES

sub-μm

to 10s cm

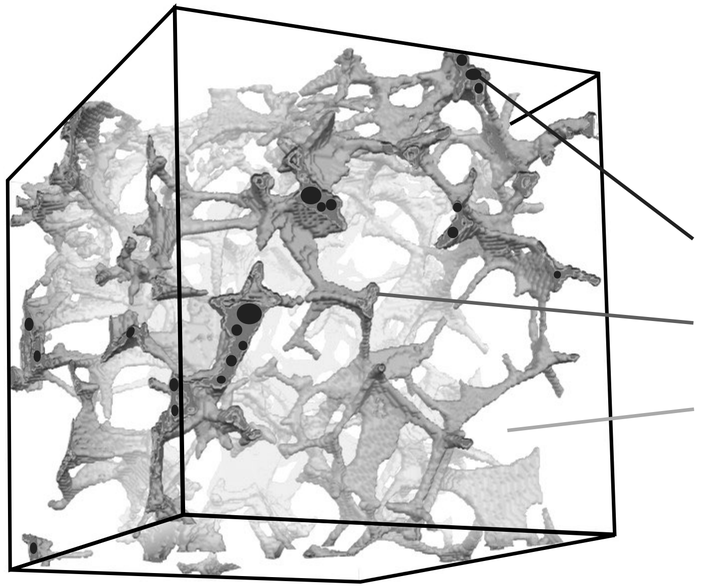
LOCAL

SCALE

SYSTEM

10s m

to 100s km



direct observations

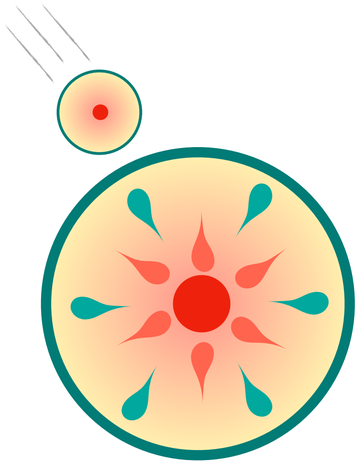
at local scale

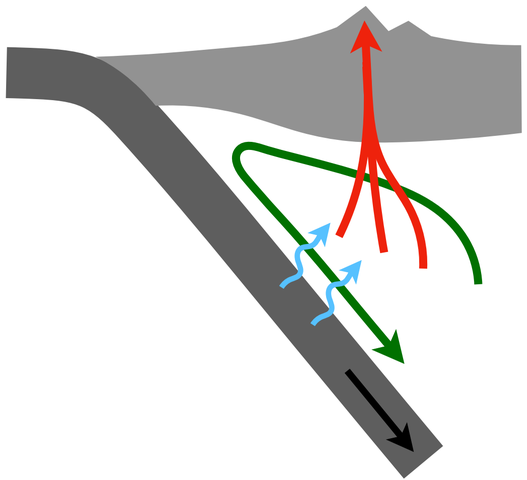
localisation of flow &

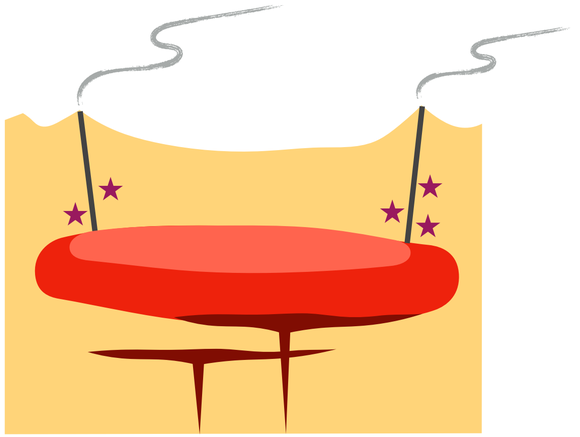
deformation at meso-scale

phenomena of interest at

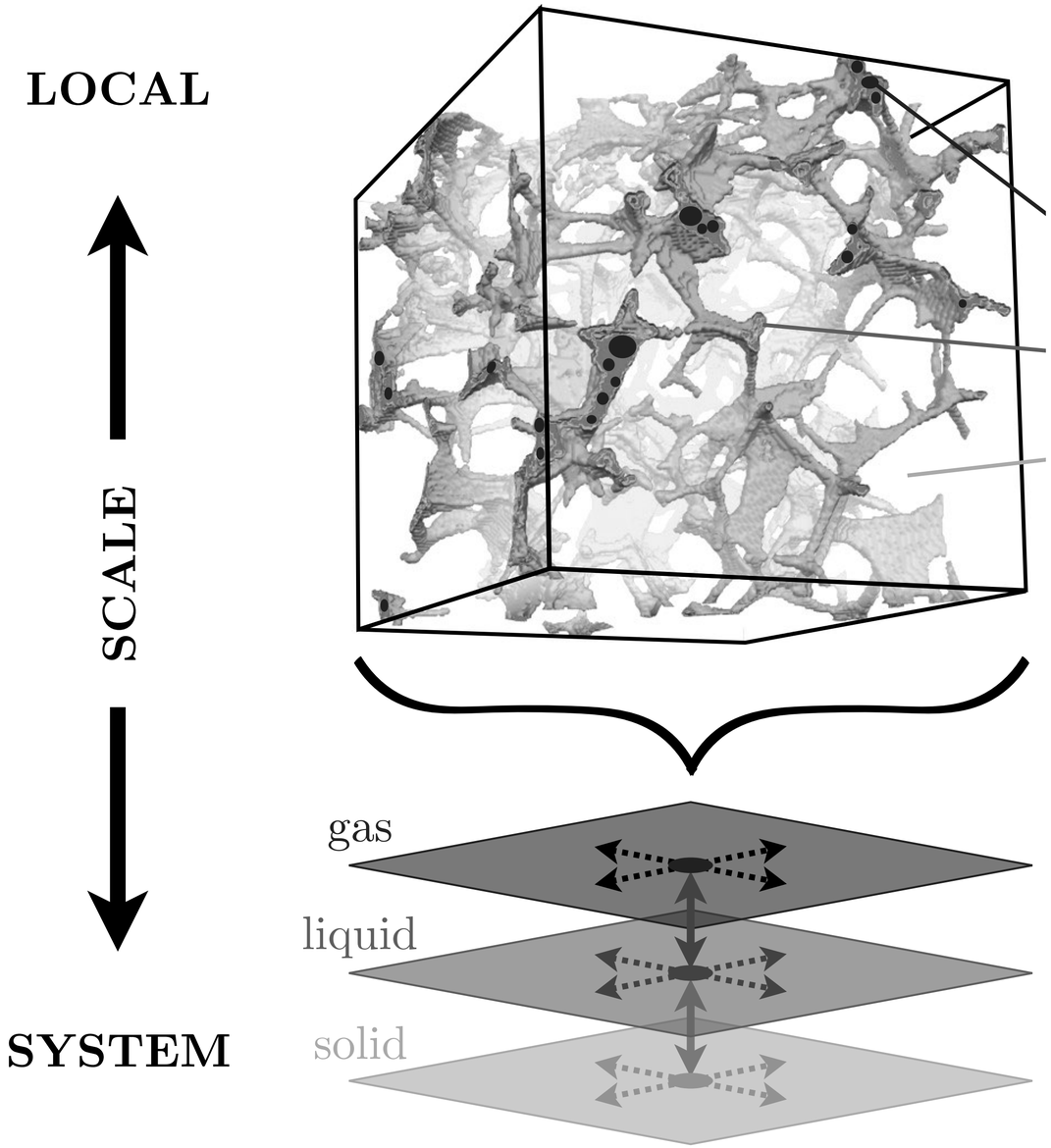
system scale







CHALLENGE OF SCALES



local properties

density, viscosity, surface energy, etc.

local topology

grain/bubble size, wetting angle, etc.

UPSCALING

averaged properties

phase fractions, mixture density, etc.

effective media coefficients

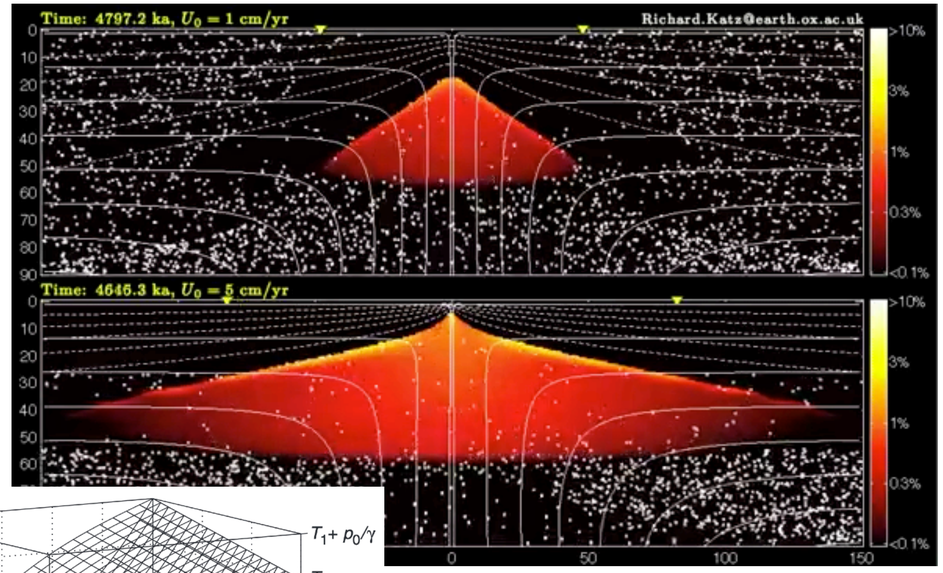
mixture viscosity, permeability, etc.

=> continuum mixture models

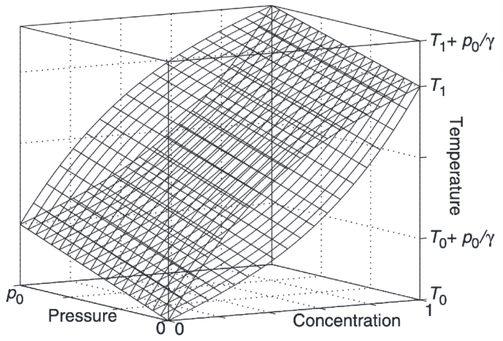
MODELLING CHALLENGES

modelling 10 years ago

- diffuse porous flow
- viscous matrix deformation
- one-dimensional chemistry



video source



Katz, *J Pet* (2008)

challenge of scales

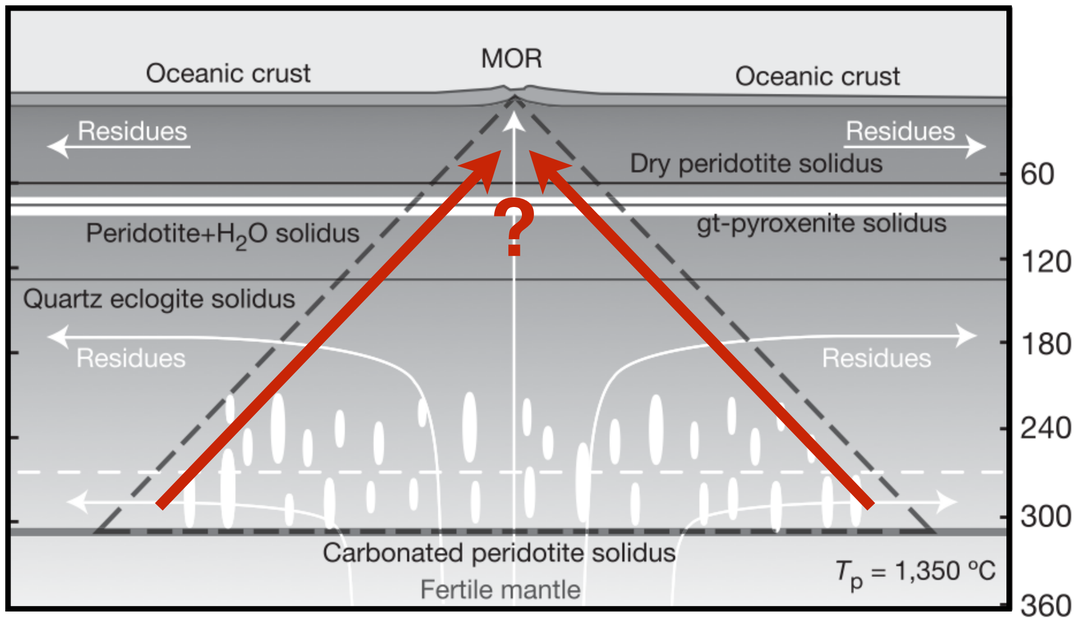
i multi-component reactions

ii flow to fracture transition

iii solid- to liquid-dominated flows

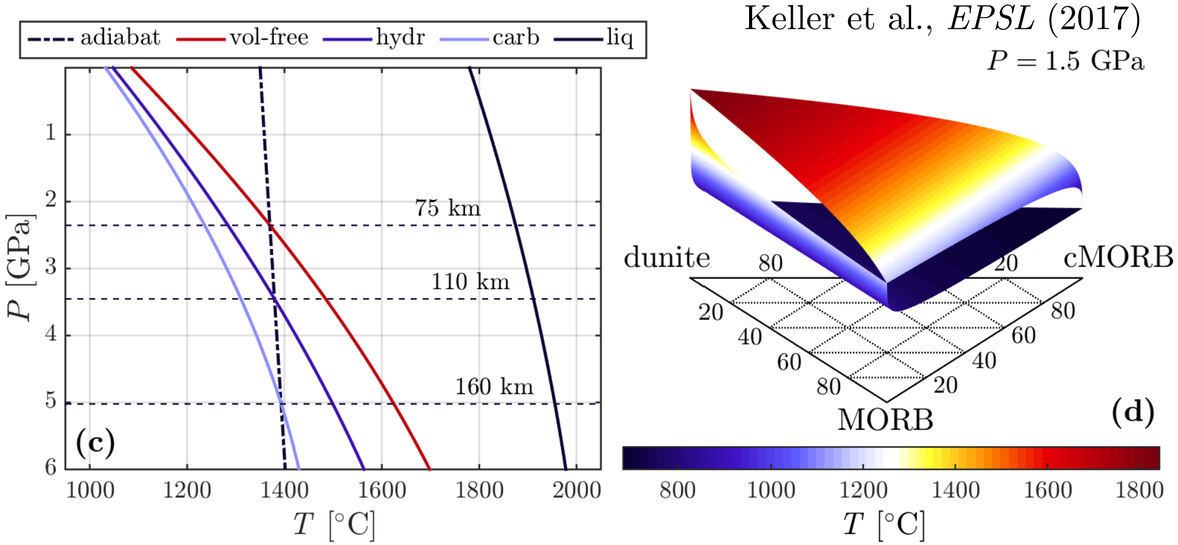
iv single- to multi-phase flows

VOLATILES BENEATH MOR



Dasgupta et al. (2006)

Keller et al., *EPSL* (2017)



challenge

- multiple chemical components in reactions (e.g., major oxides + volatiles)
- equilibrium (melt fraction, phase compositions) required at each grid / time step
- direct use of thermodynamic solvers in reaction transport model not (yet) practical

way forward

Keller & Katz, *J Pet* (2016)

- select few pseudo-components (unite + basalt + hydr./carb. basalt) for *petrological hypothesis*
- simplified linear solution thermodynamics
- flexibly calibrated multi-component phase loops
- linear kinetic reaction rates (or enforce eq.)

VOLATILES BENEATH MOR

Stokes flow
of matrix

Darcy flow
of melt

four-component
reaction model

forced
plate spreading

i *reactive transport*

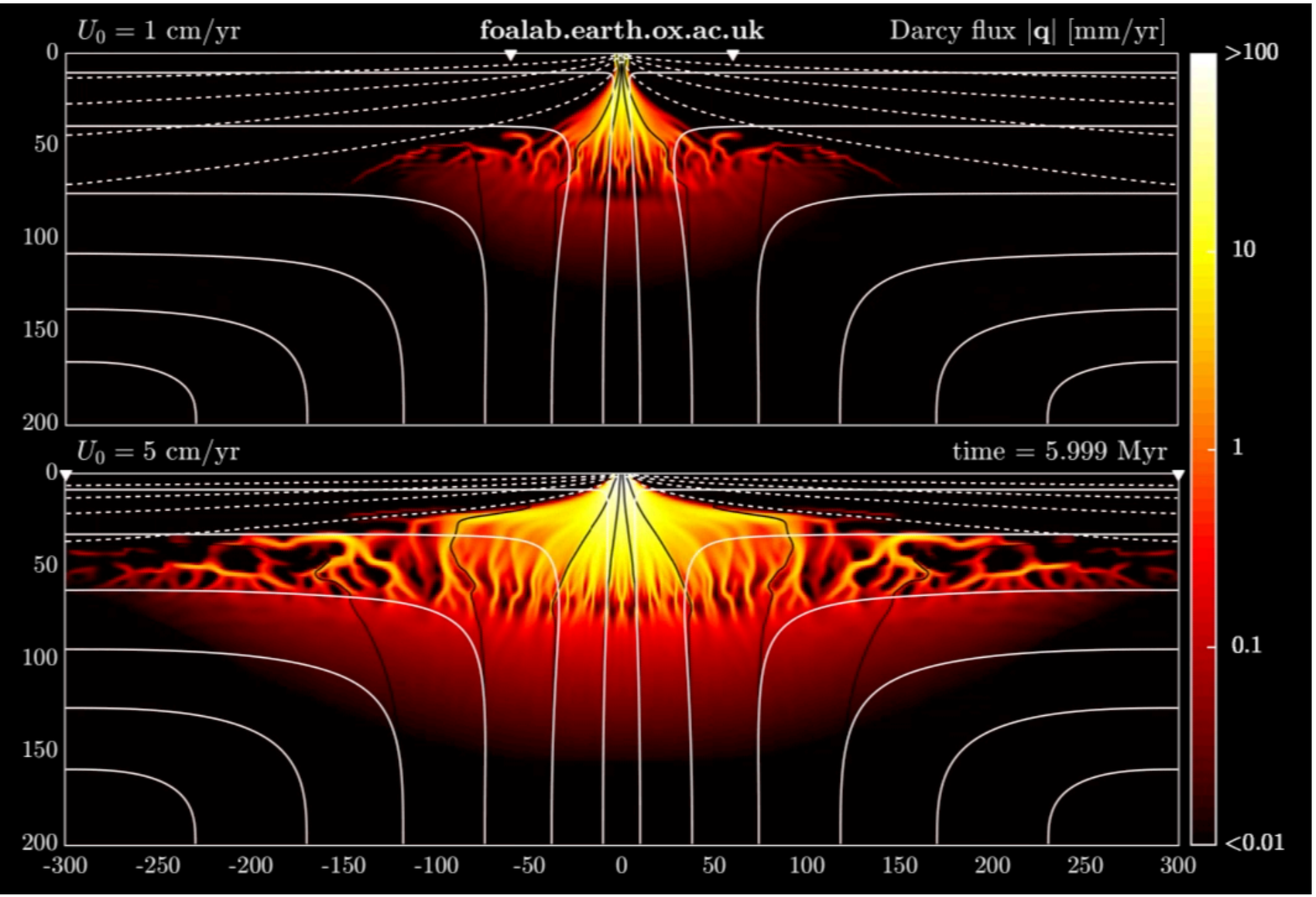
III *magma/tectonics*

IV *planet evolution*

A *melt production*

B *melt focusing*

VOLATILES BENEATH MOR

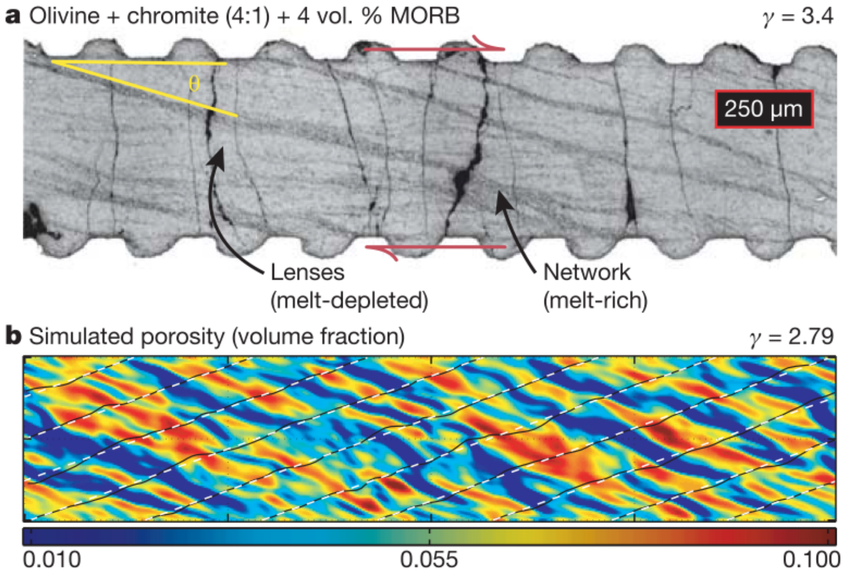


- solid-dominated system, porous flow
- liquid segregates from deforming solid matrix
- segregation speed exceeds matrix flow
- phase-pressure diff. cause de/compaction
- reactive feedback causes channeling

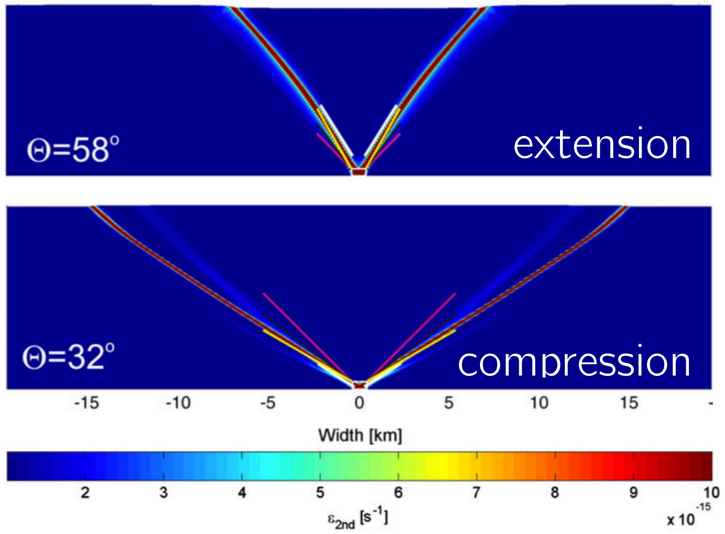
video source

Keller et al., *EPSL*, (2017)

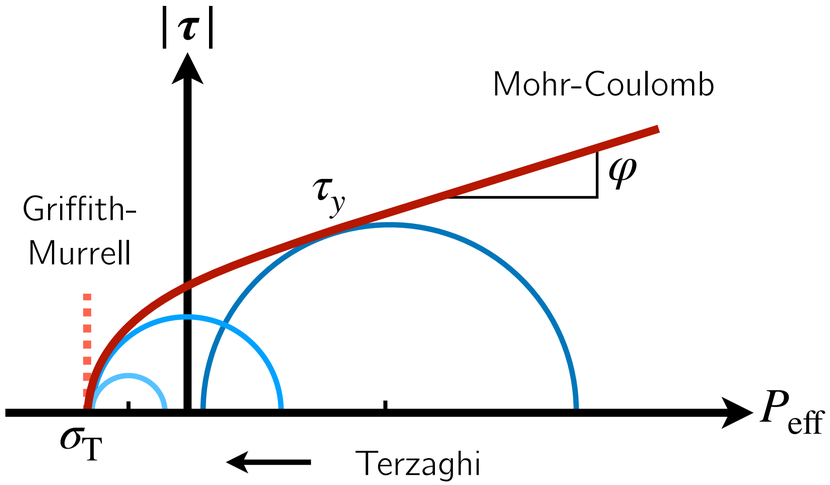
FLOW TO FRACTURE



Katz et al. (2006)



Kaus (2010)



challenge

- diffuse porous flow fails to explain localised and fracture-bound flow & deformation
- viscous matrix deformation not appropriate for ductile to brittle crustal host rocks

way forward Keller, May & Kaus, *GJI* (2013)

- generalise effective-viscosity approach from single- to two-phase visco-elasto-plastic flow
- cohesive-frictional Mohr-Coulomb + tensile Griffith-Murrell failure criterion

FLOW TO FRACTURE

Stokes flow
of matrix

Darcy flow
of melt

visco-elasto-plastic
shear & compaction

forced extensional /
compressional tectonics

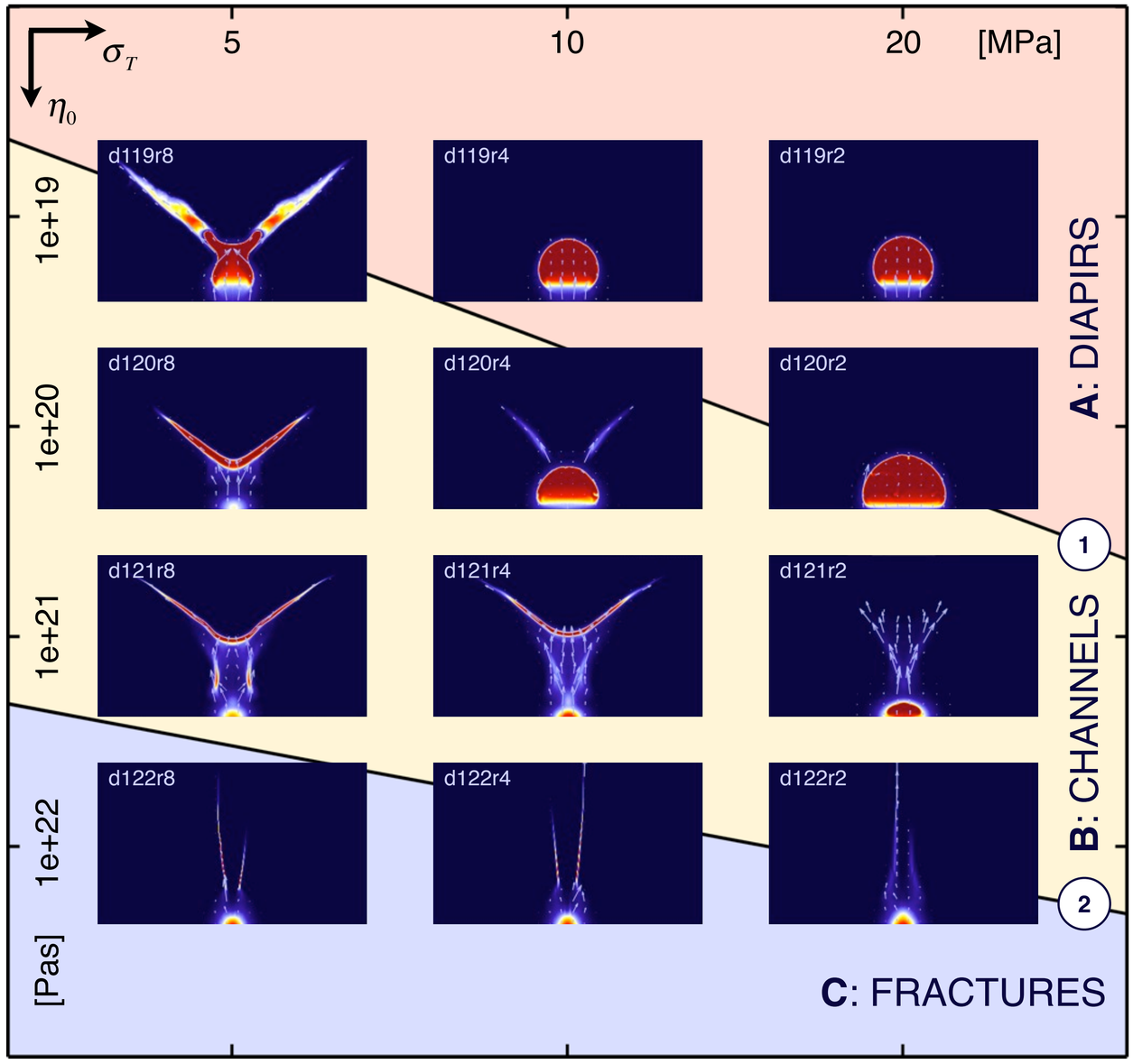
ii *flow to fracture*

III *magma/tectonics*

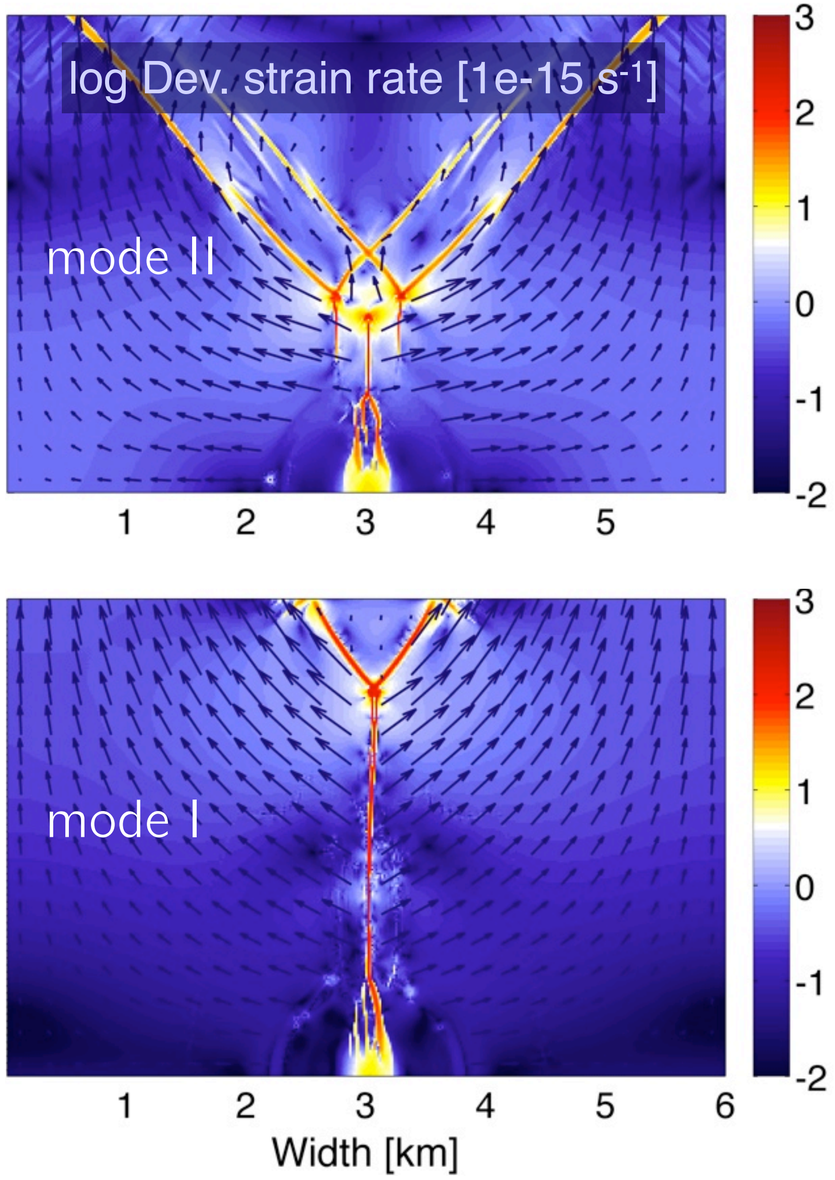
A *magma focusing*

B *magma processing*

FLOW TO FRACTURE

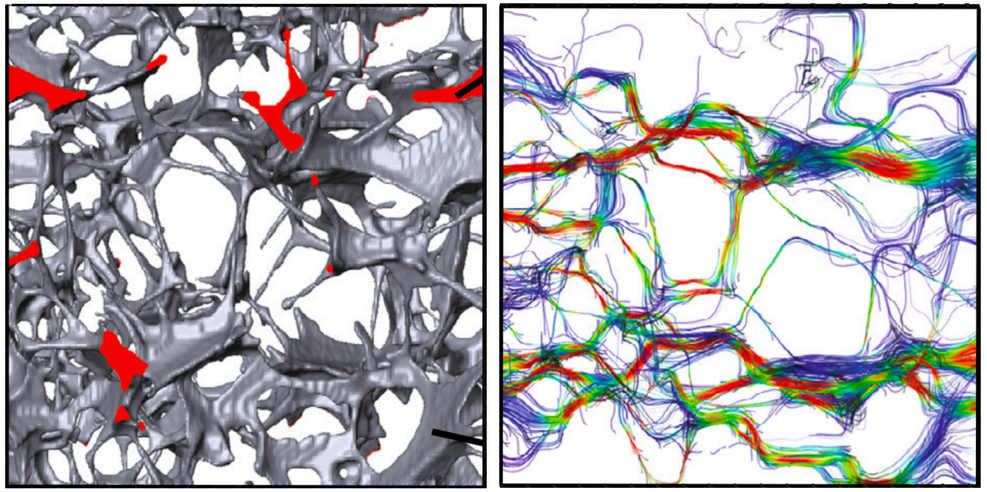


Keller, May & Kaus, *GJI* (2013)



SOLID TO LIQUID REGIMES

POROUS FLOWS

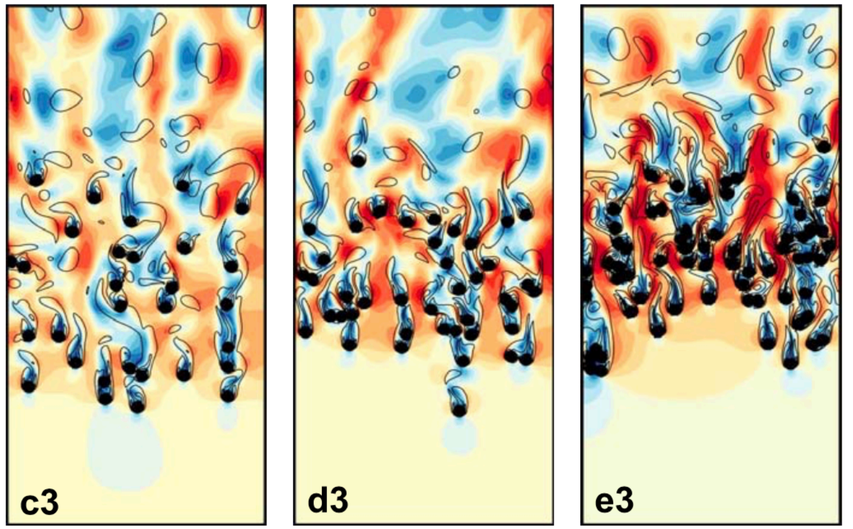


Miller et al. (2014)

liquid percolates
through deforming solid

?

SUSPENSION FLOWS



Suckale et al. (2012)

particles settle / bubbles rise
through convecting liquid

challenge

- crustal magmatic to volcanic systems transition from solid- to liquid-dominated aggregates
- separate models for porous, suspension flow
- separate research communities address limits

way forward Keller & Suckale, *GJI* (2019)

- general model where end-member regimes emerge as special cases in solid-/liquid-rich limits
- conceptualise as carrier vs segregating phase
- close gap in effective media closures

LAVA LAKE DYNAMICS

Stokes flow
of magma

hindered settling/rising
of crystals/bubbles

T-dependent xtallinity
controls rheology

forced lava supply
from conduit

iii *solid to liquid*

I *volcano dynamics*

D *shallow exsolution*

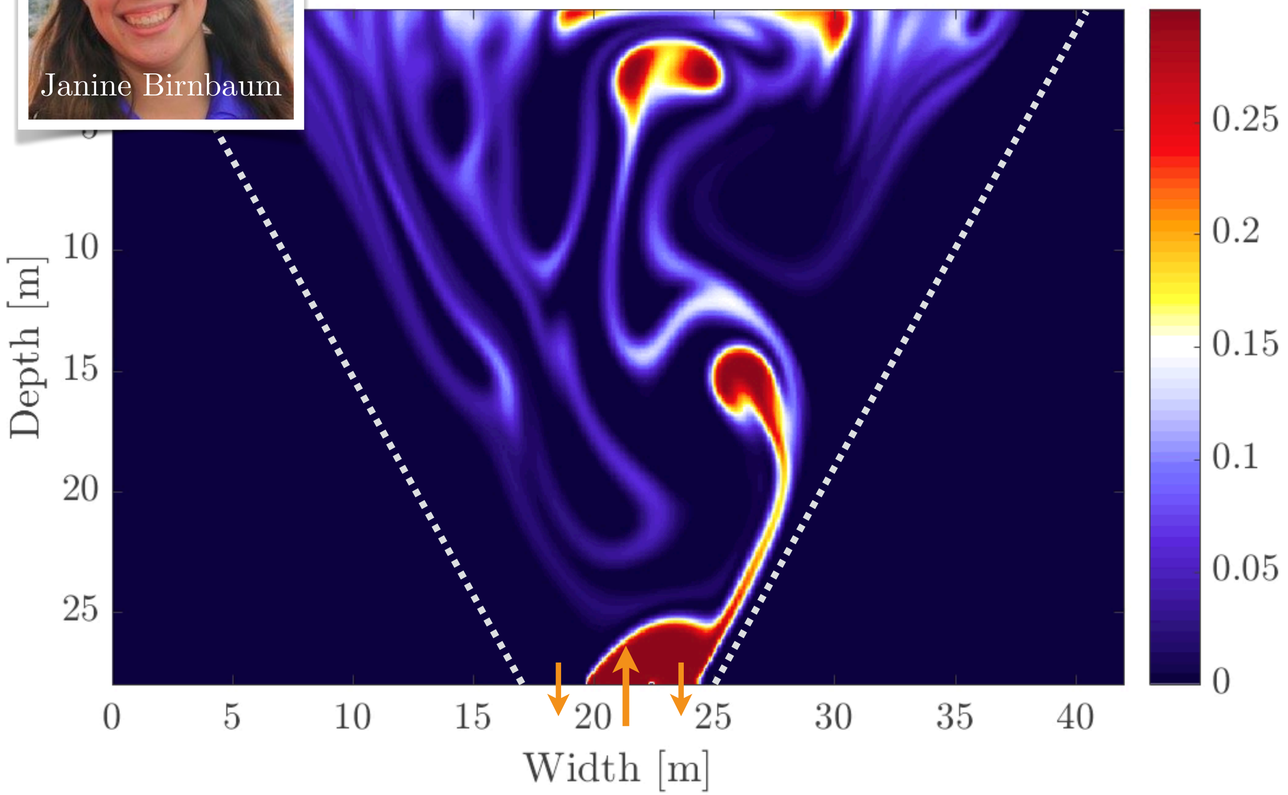
LAVA LAKE DYNAMICS

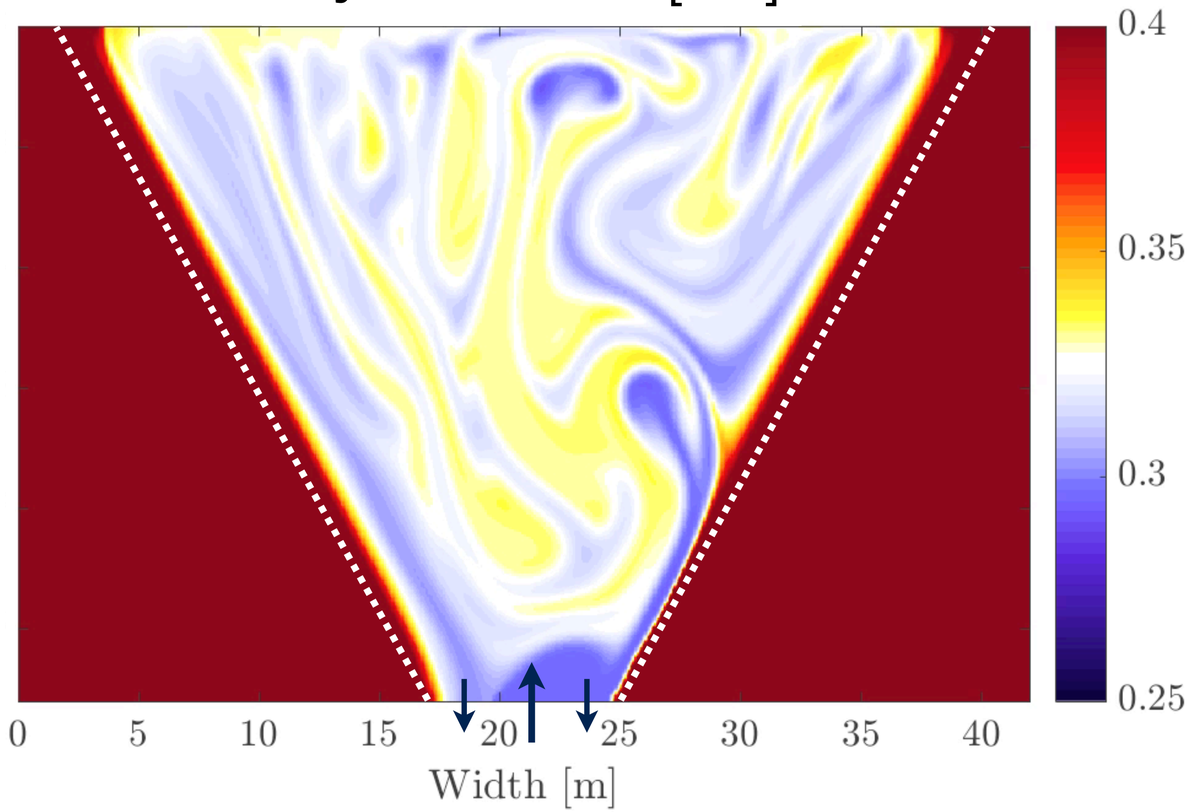


bubble fract. [vol]

Birnbaum et al., *EPSL*, (2020)

crystal fract. [vol]

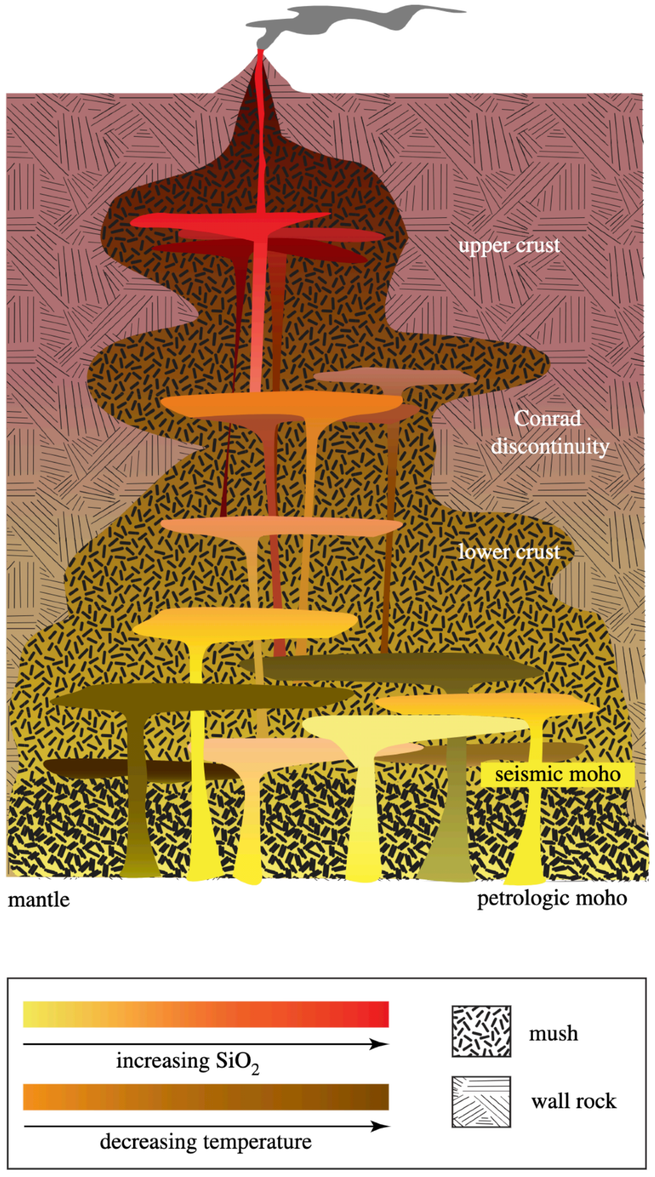


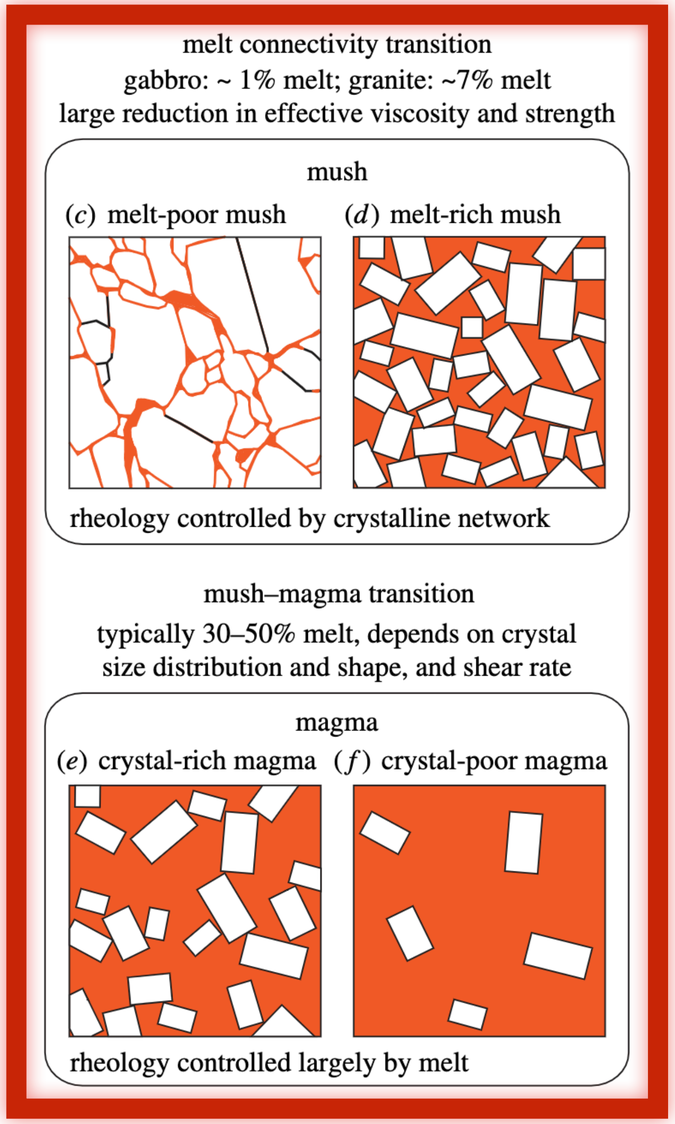


- solid- to liquid-dominated
- bubbles/crystals segregate from convecting carrier liquid

- convective speed exceeds particle settling/rising
- phase-pressure diff. negligible

MUSH DYNAMICS?





Sparks et al. (2019)

crustal mush bodies

- may dominate trans-crustal processing
- may produce ephemeral melt lenses
- solid- to liquid-supported rheology
- porous or suspension flow model?
  both? neither?

MODEL FRAMEWORK

Geophysical Journal International

Geophys. J. Int. (2019) **219,** 185–222
Advance Access publication 2019 June 25
GJI General Geophysical Methods

doi: 10.1093/gji/ggz287

A continuum model of multi-phase reactive transport in igneous systems

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Accepted 2019 June 23. Received 2019 June 14; in original form 2018 August 28

SUMMARY

Multiphase reactive transport processes are ubiquitous in igneous systems. A challenging aspect of modelling igneous phenomena is that they range from solid-dominated porous to liquid-dominated suspension flows and therefore entail a wide spectrum of rheological conditions, flow speeds and length scales. Most previous models have been restricted to the two-phase limits of porous melt transport in deforming, partially molten rock and crystal settling in convecting magma bodies. The goal of this paper is to develop a framework that can capture igneous system from source to surface at all phase proportions including not only rock and melt but also an exsolved volatile phase. Here, we derive an *n*-phase reactive transport model building on the concepts of Mixture Theory, along with principles of Rational Thermodynamics and procedures of Non-equilibrium Thermodynamics. Our model operates at the macroscopic system scale and requires constitutive relations for fluxes within and transfers between phases, which are the processes that together give rise to reactive transport phenomena. We introduce a phase- and process-wise symmetrical formulation for fluxes and transfers of entropy, mass, momentum and volume, and propose phenomenological coefficient closures that determine how fluxes and transfers respond to mechanical and thermodynamic forces. Finally, we demonstrate that the known limits of two-phase porous and suspension flow emerge as special cases of our general model and discuss some ramifications for modelling pertinent two- and three-phase flow problems in igneous systems.

Key words: Dynamics of lithosphere and mantle; Mechanics, theory, and modelling; Magma genesis and partial melting; Physics and chemistry of magma bodies.

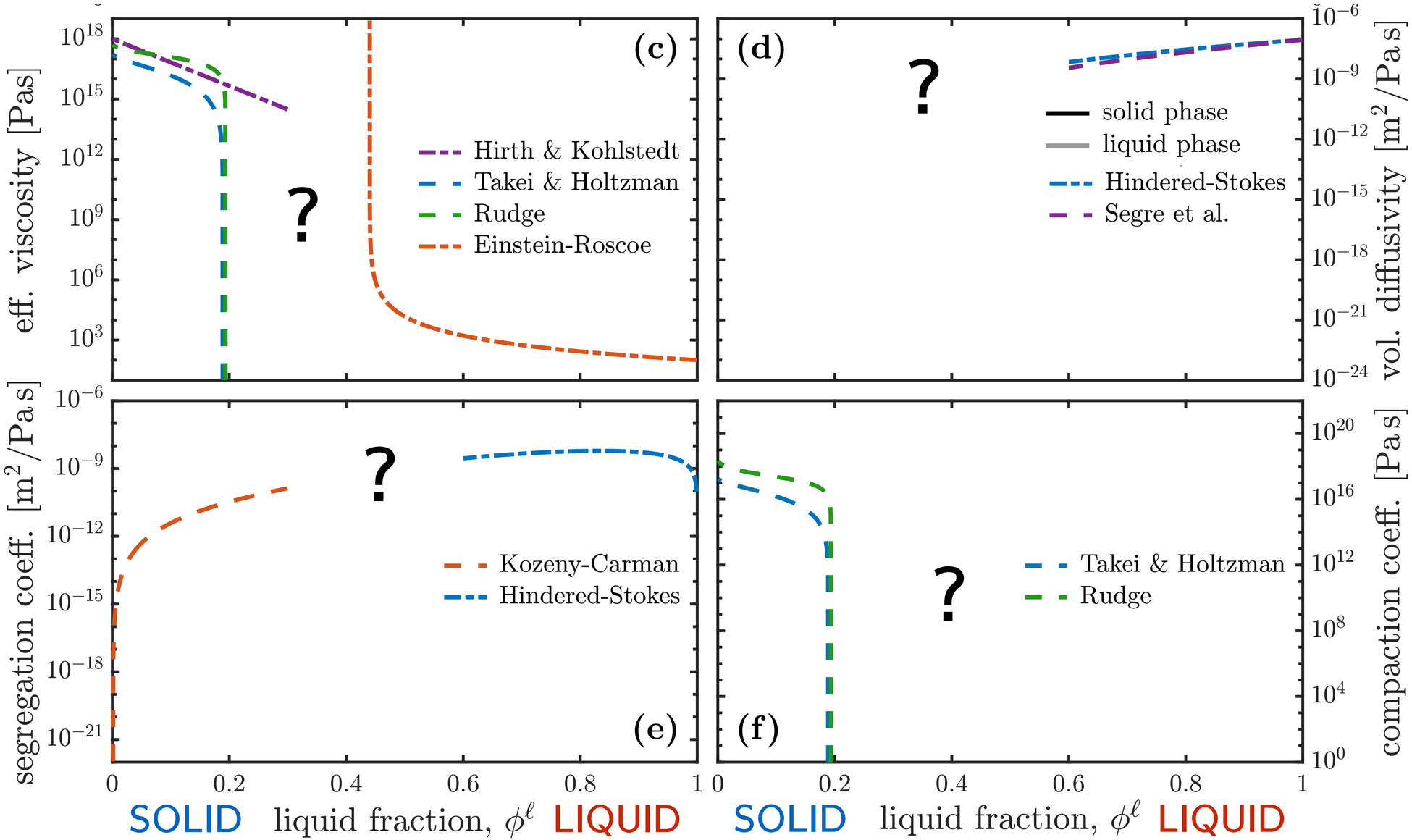
- from source to surface
- porous to suspension flows
- two-, three-, *n*-phase flows
- phase-, process-wise symmetric

"A problem clearly stated is a problem half solved"

– Fortune Cookie

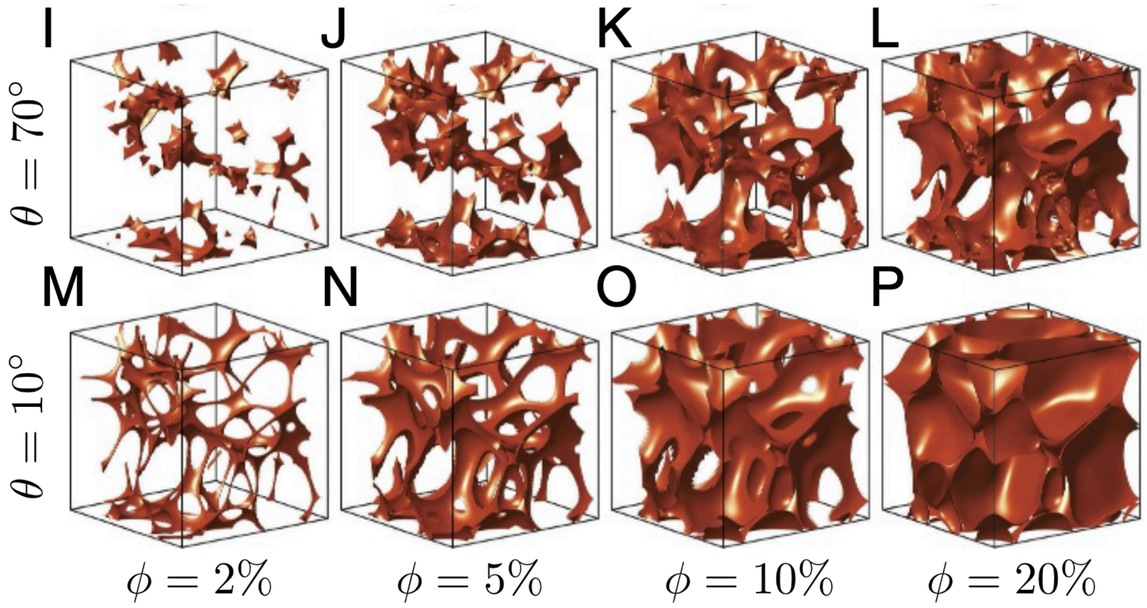
EFFECTIVE MEDIA COEFFS

experimental & theoretical closures for porous & suspension flows

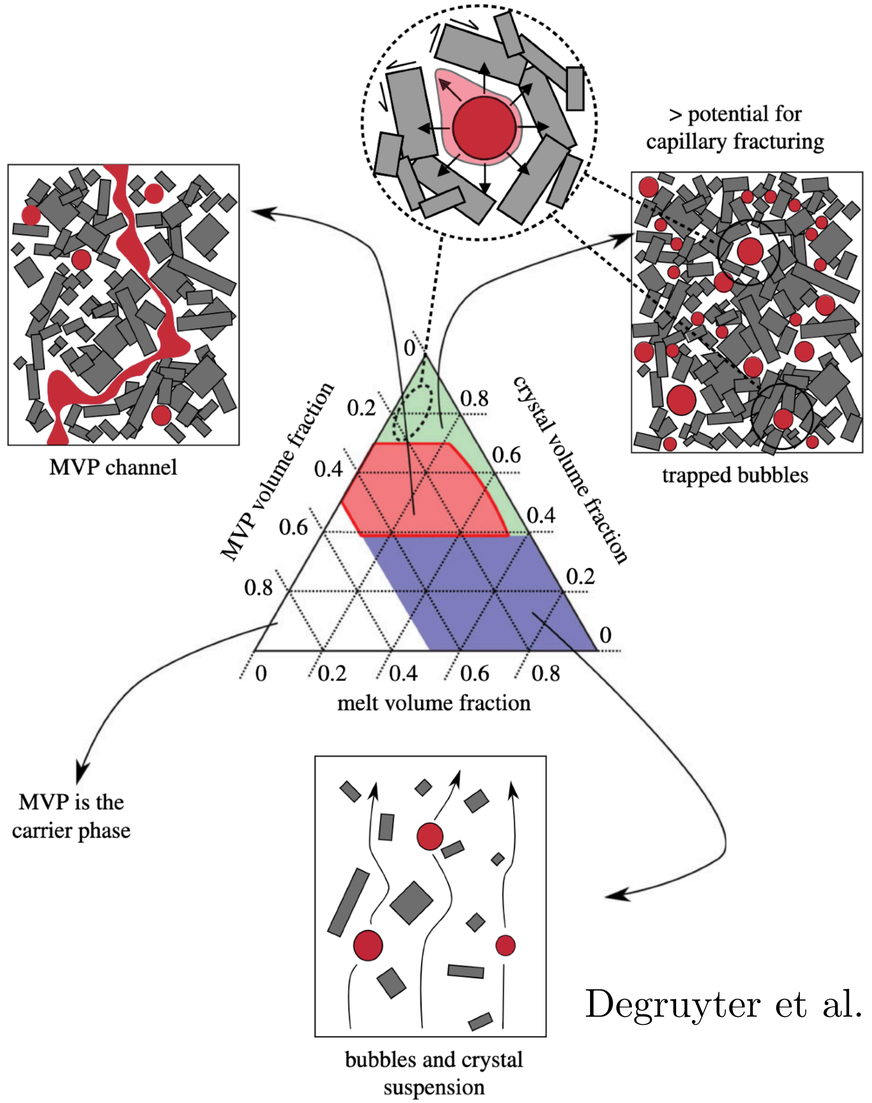


PHASE CONNECTIVITY

local-scale phase topology permits system-scale transport



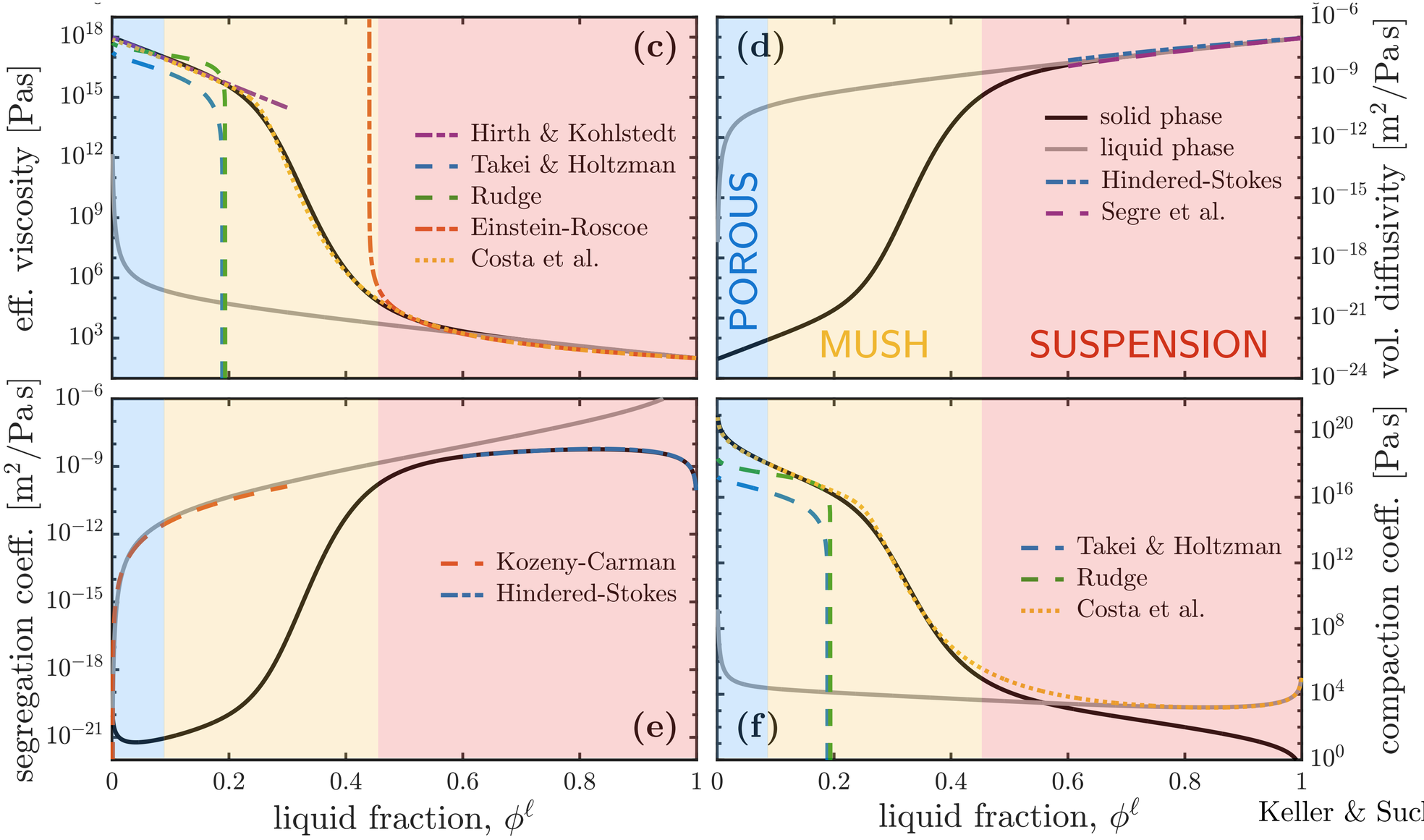
Ghanbarzadeh et al. (2017)



Degruyter et al. (2019)

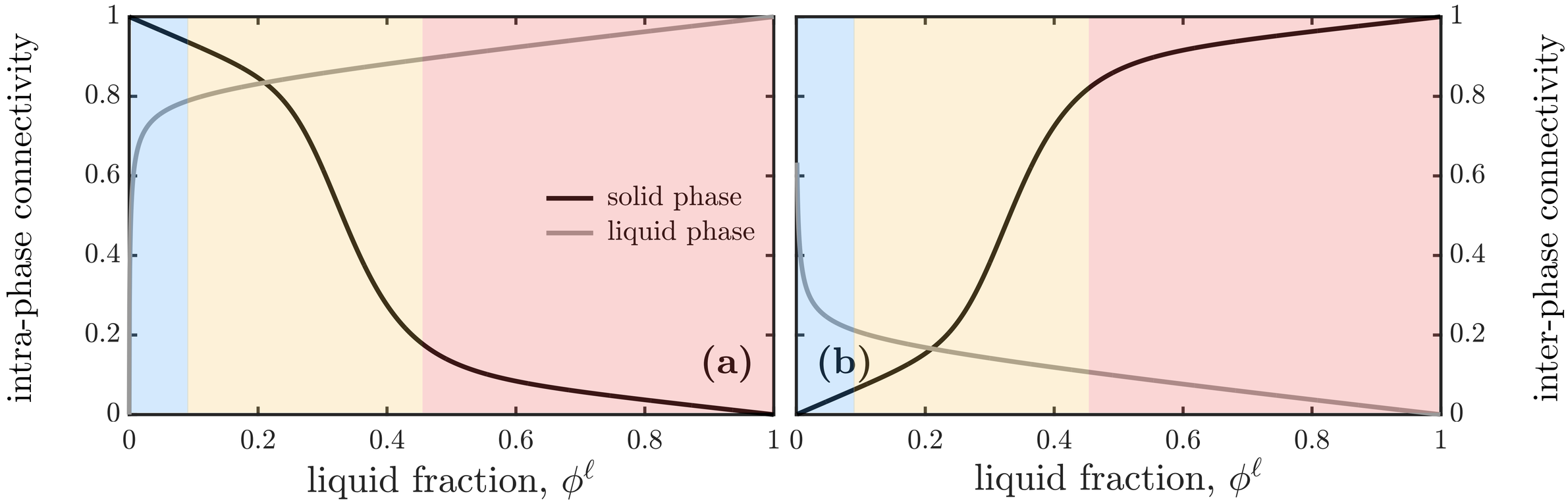
COEFFICIENT CALIBRATION

two-phase calibration: olivine (10^{18} Pas) **+ basalt** (10^{2} Pas), d = 1 mm



COEFFICIENT CALIBRATION

two-phase calibration: olivine (10^{18} Pas) **+ basalt** (10^{2} Pas), $d = 1$ mm

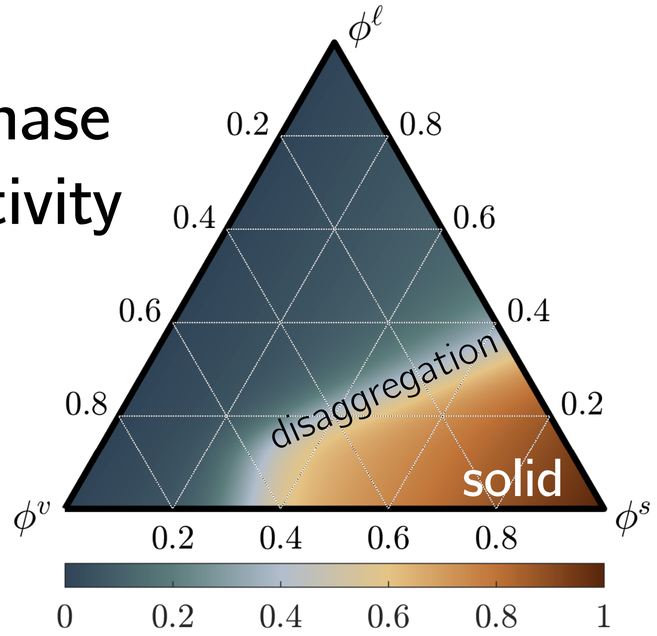


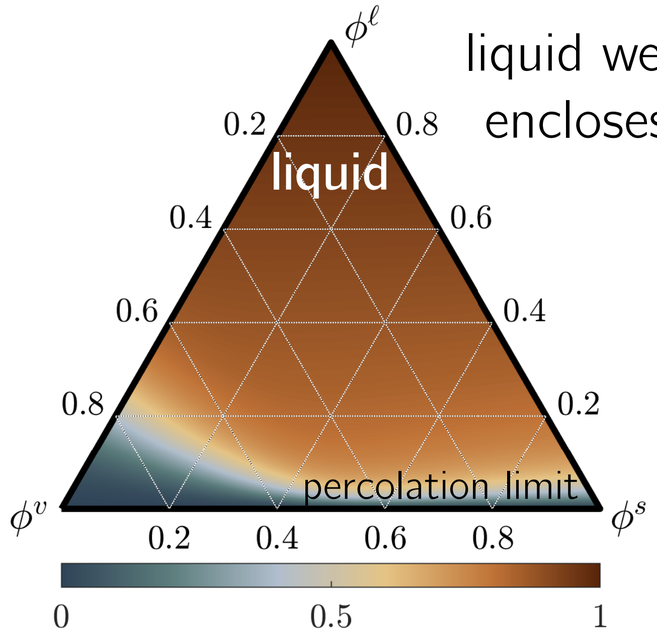
measured **pure-phase diffusivities** & calibrated **connectivity weights**

produce set of phase-, process-wise symmetrical coefficient closures

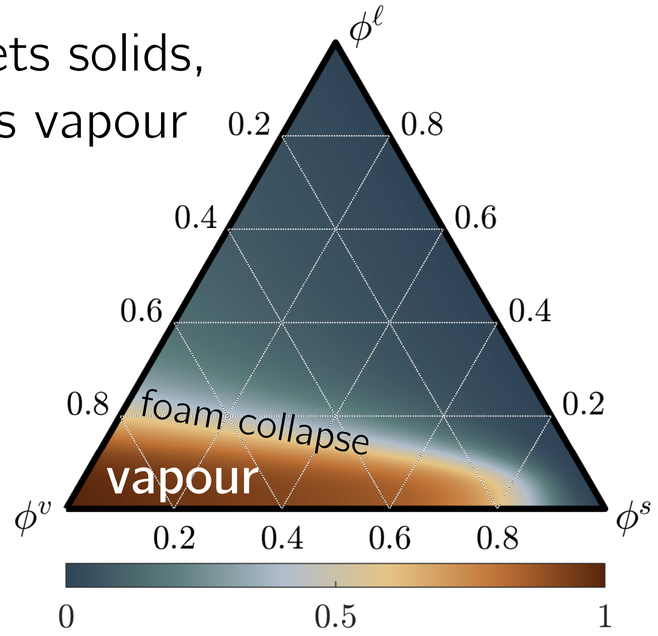
THREE-PHASE CALIBRATION

intra-phase connectivity

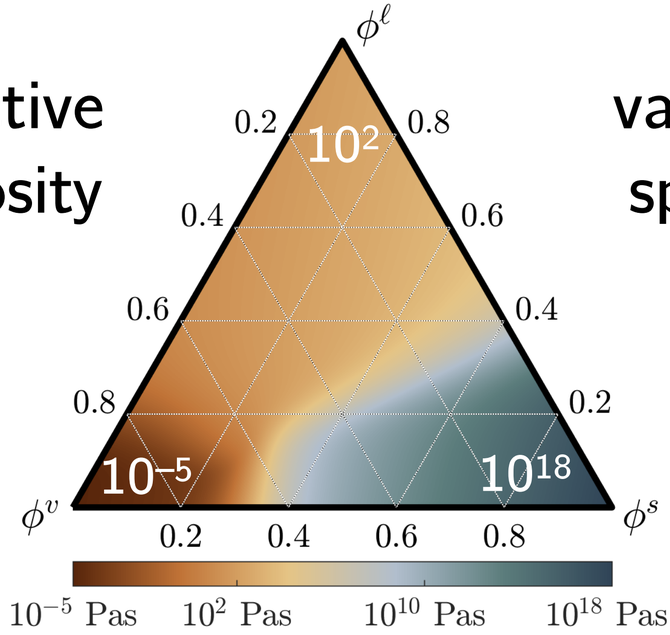




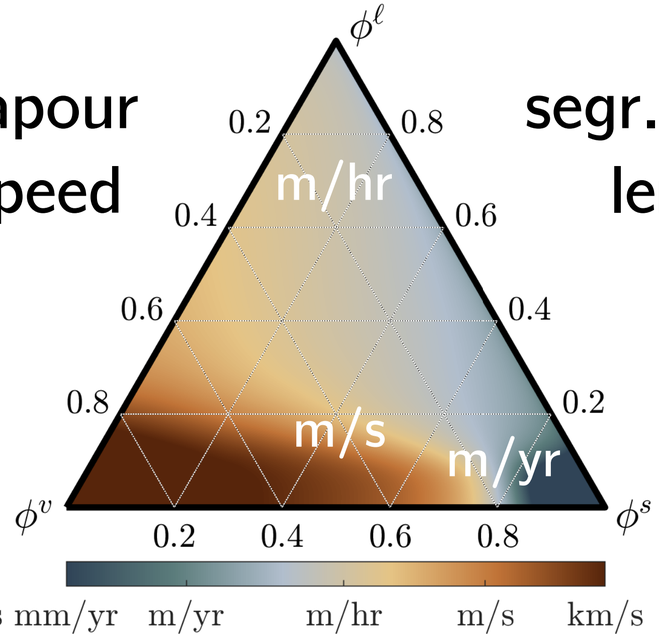
liquid wets solids, encloses vapour



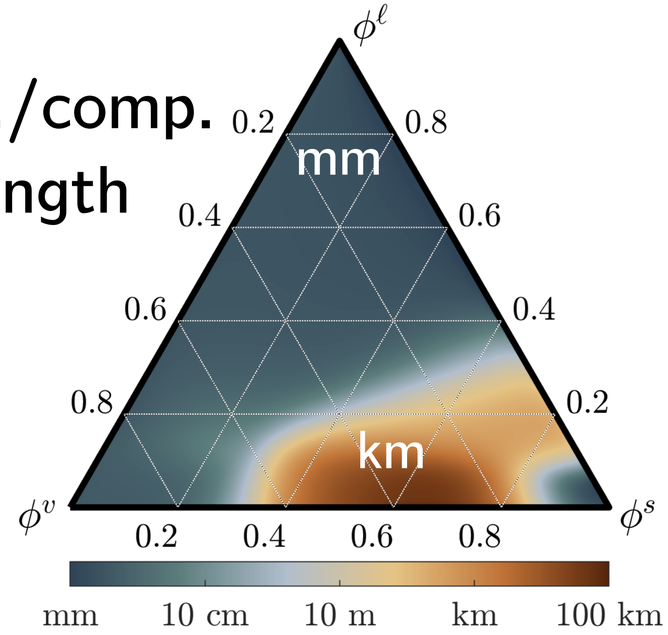
effective viscosity



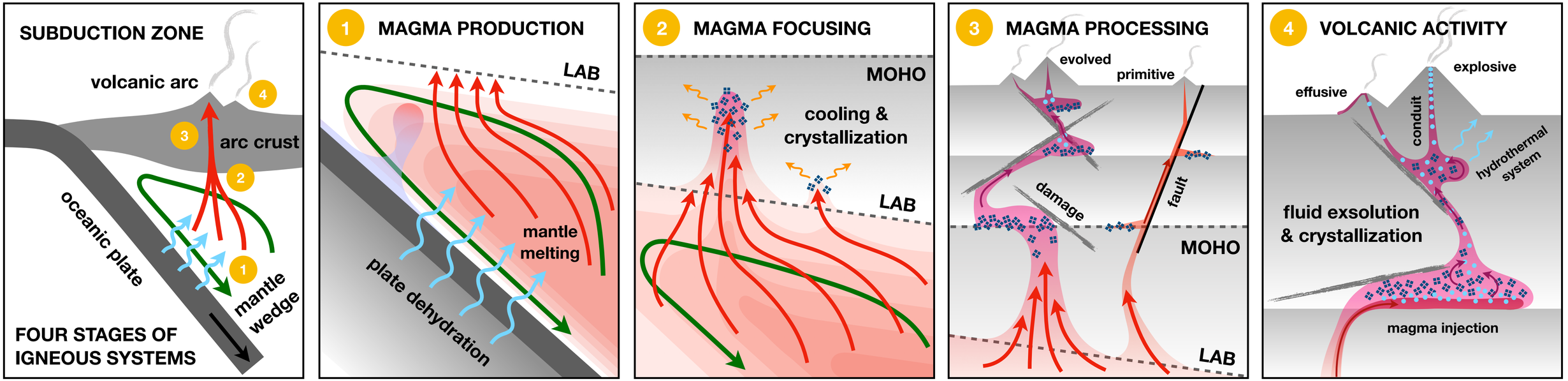
vapour speed



segr./comp. length



CHALLENGES REMAIN



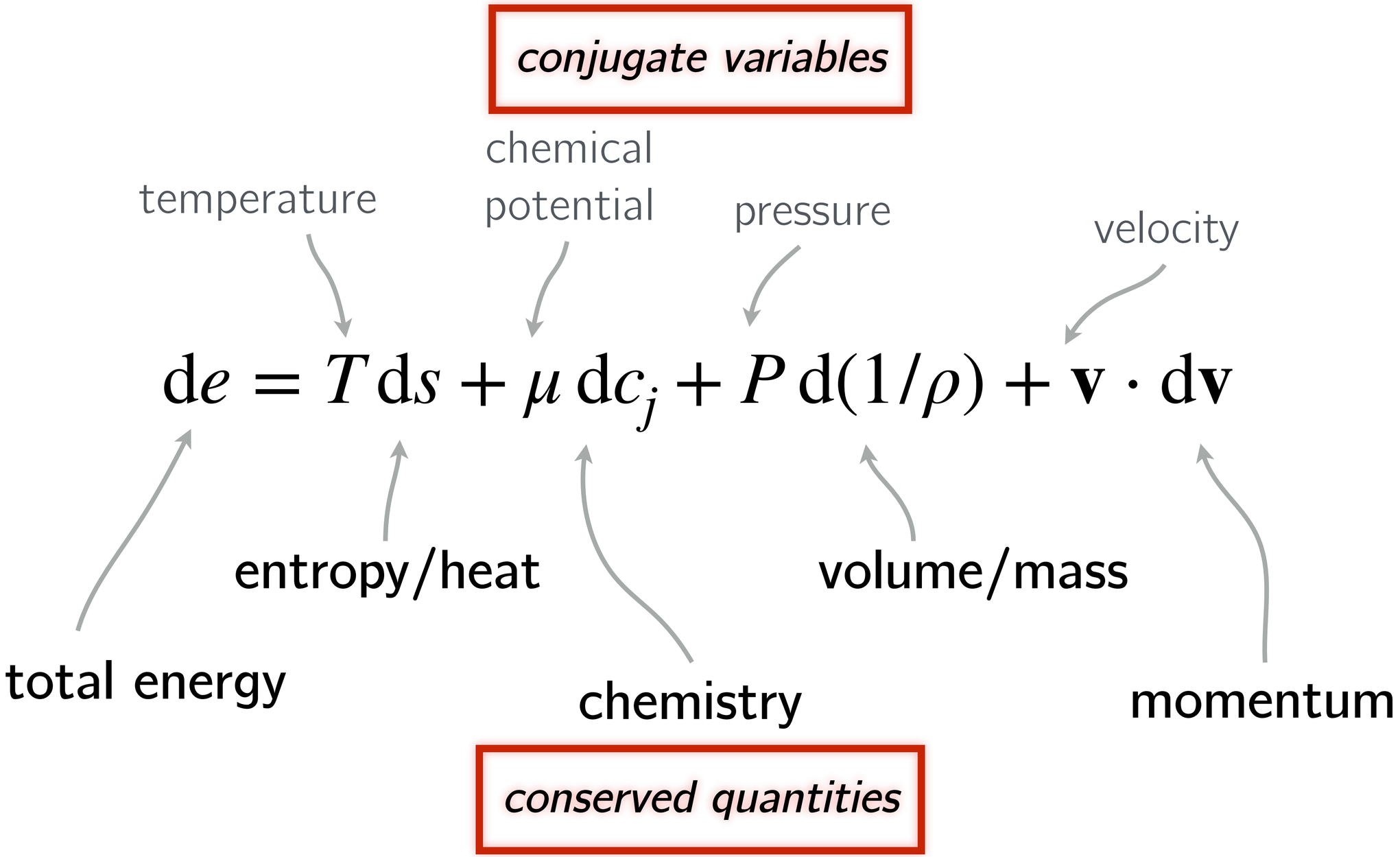
i **reactions** couple fluid mechanic & thermodynamic solvers

ii **failure** couple multi-phase flow with dike/sill emplacement

iii **mush** strong contrasts in properties, time & length scales

iv **three-phase** calibrate coefficients with phase connectivity

SYSTEM ENERGY



CONSERVATION LAWS

phase i, volume fraction

phase density

mass-specific quantity

n material phases (i)
phase-wise symmetrical
process-wise symmetrical

$$\frac{\partial \phi^i \rho^i a^i}{\partial t} + \nabla \cdot (\mathbf{q}^i_\phi \rho^i a^i) + \nabla \cdot \mathbf{q}^i_a + \Gamma^i_a = Q^i_a$$

rate of change
quantity/m^3/s

advection flux

diffusion flux

transfer

source

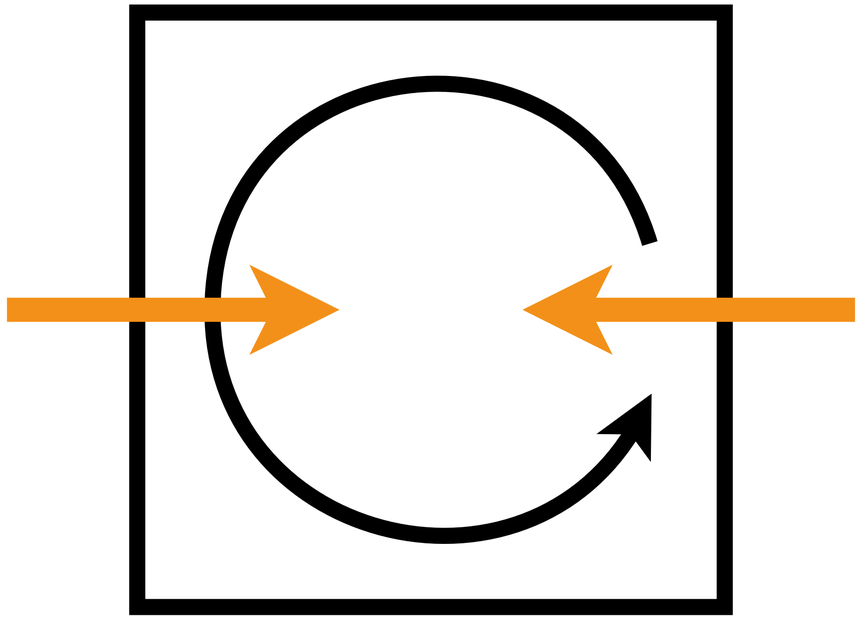
write equations for heat/entropy, chemistry, mass/volume, momentum, in each phase

CONSTITUTIVE RELATIONS

SOURCES

external input of heat (e.g., radiogenic heating), momentum (e.g., gravity)

provides “fuel” to disequilibrate system, drive reaction-transport dynamics

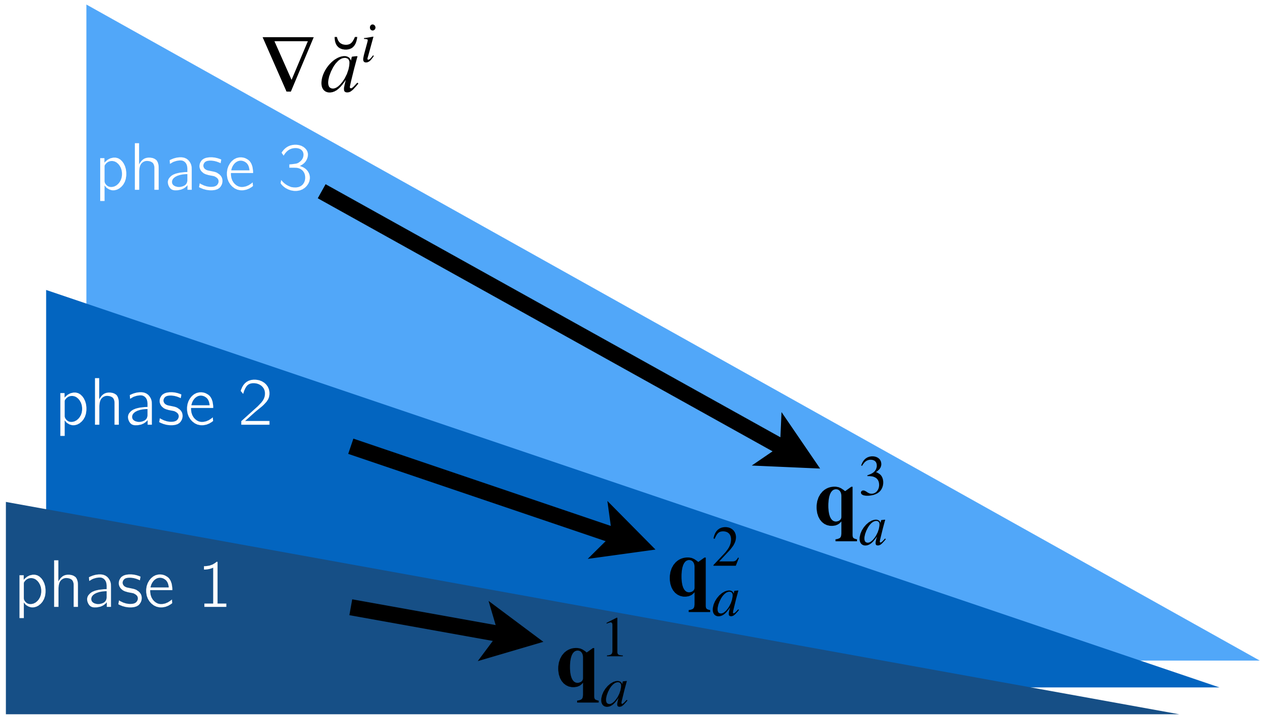


CONSTITUTIVE RELATIONS

FLUXES

intra-phase transport of **heat, chemistry, momentum, volume**

down gradients in temperature, chemical potentials, velocity, pressure



$$\mathbf{q}_a^i = -K_a^i \nabla \breve{a}^i$$

intra-phase flux

flux coefficient

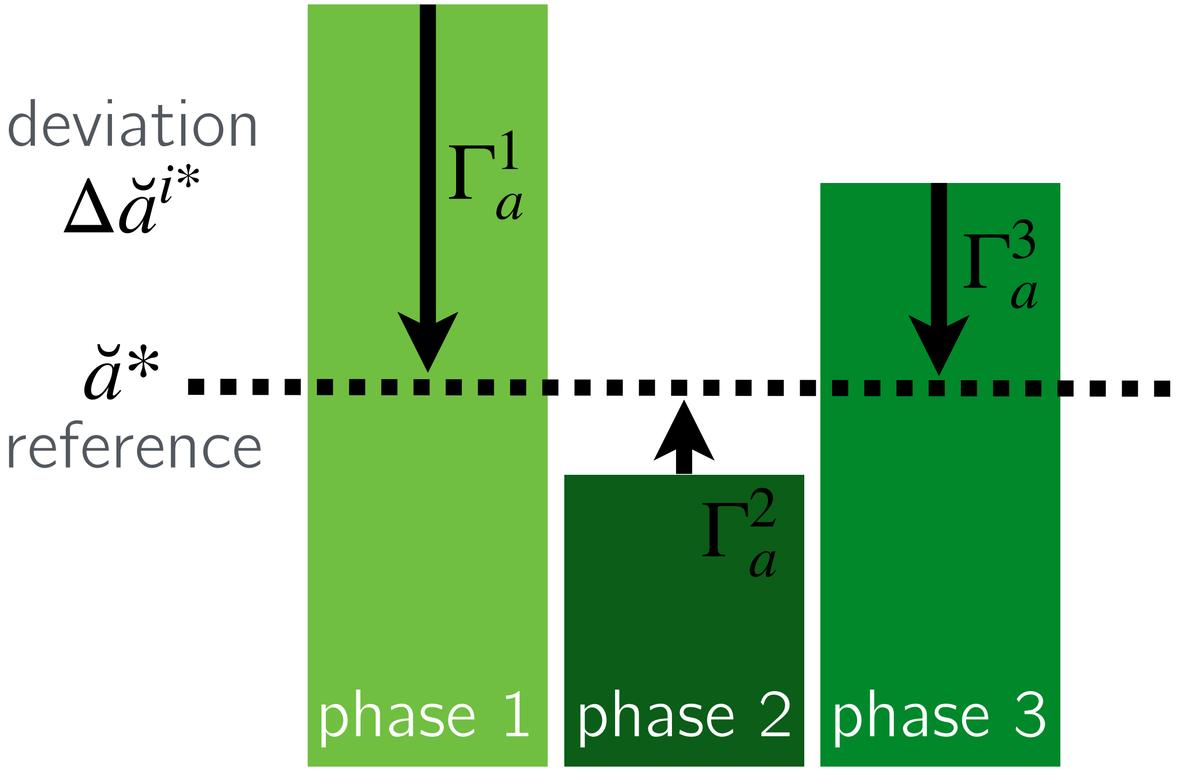
phase gradient

CONSTITUTIVE RELATIONS

TRANSFERS

inter-phase exchange of **heat, chemistry, momentum, volume**

down deviations in temperature, chemical potentials, velocity, pressure



$$\Gamma_a^i = -C_a^i \Delta\breve{a}^{i*}$$

inter-phase transfer

transfer coefficient

phase deviation

$$\Delta\breve{a}^{i*} = \breve{a}^i - \breve{a}*$$

COEFFICIENT CLOSURES

n material phases (i)
phase-wise symmetrical
process-wise symmetrical

$$\frac{\partial \phi^i \rho^i a^i}{\partial t} + \nabla \cdot (\phi^i \mathbf{v}^i \rho^i a^i) - \nabla \cdot K_a^i \nabla \breve{a}^i - C_a^i \Delta \breve{a}^{i*} = Q_a^i$$

flux coefficients

transfer coefficients

write equations for heat/entropy, chemistry, mass/volume, momentum, in each phase

COEFFICIENT CLOSURES

assume transport limited by diffusion at local scale,
modulated by pure-phase diffusivity, phase connectivity

FLUX COEFFS

pure-phase
diffusion parameter

$$K_a^i = \phi^i k_a^i \theta_a^i$$

permission function,
encodes phase connectivity

TRANSFER COEFFS

$$C_a^i = (1 - \phi^i)\phi^i k_a^i \theta_a^i / d^{i^2}$$

phase constituent size

maintain phase-wise, process-wise symmetry
keep effective media aspects formally separate

REFERENCE STATES

phase sum by relative weights of transfer coefficients,
reference state tends to most abundant, fastest equilibrating phase

reference state is weighted sum of phase states

$$a^* = \sum_i \omega_a^i a^i$$

reference weights

phase transfer coefficient

$$\omega_a^i = \frac{C_a^i}{\sum_k C_a^k}$$

sum over all phases

CLOSED GOVERNING EQUATIONS



phase i, volume fraction

phase density

mass-specific quantity

constitutive relations & coefficient closures found
next step: model calibration

$$\frac{\partial \phi^i \rho^i a^i}{\partial t} + \nabla \cdot (\mathbf{q}^i_\phi \rho^i a^i) + \nabla \cdot \mathbf{q}^i_a + \Gamma^i_a = Q^i_a$$

rate of change
quantity/m^3/s

advection flux

diffusion flux

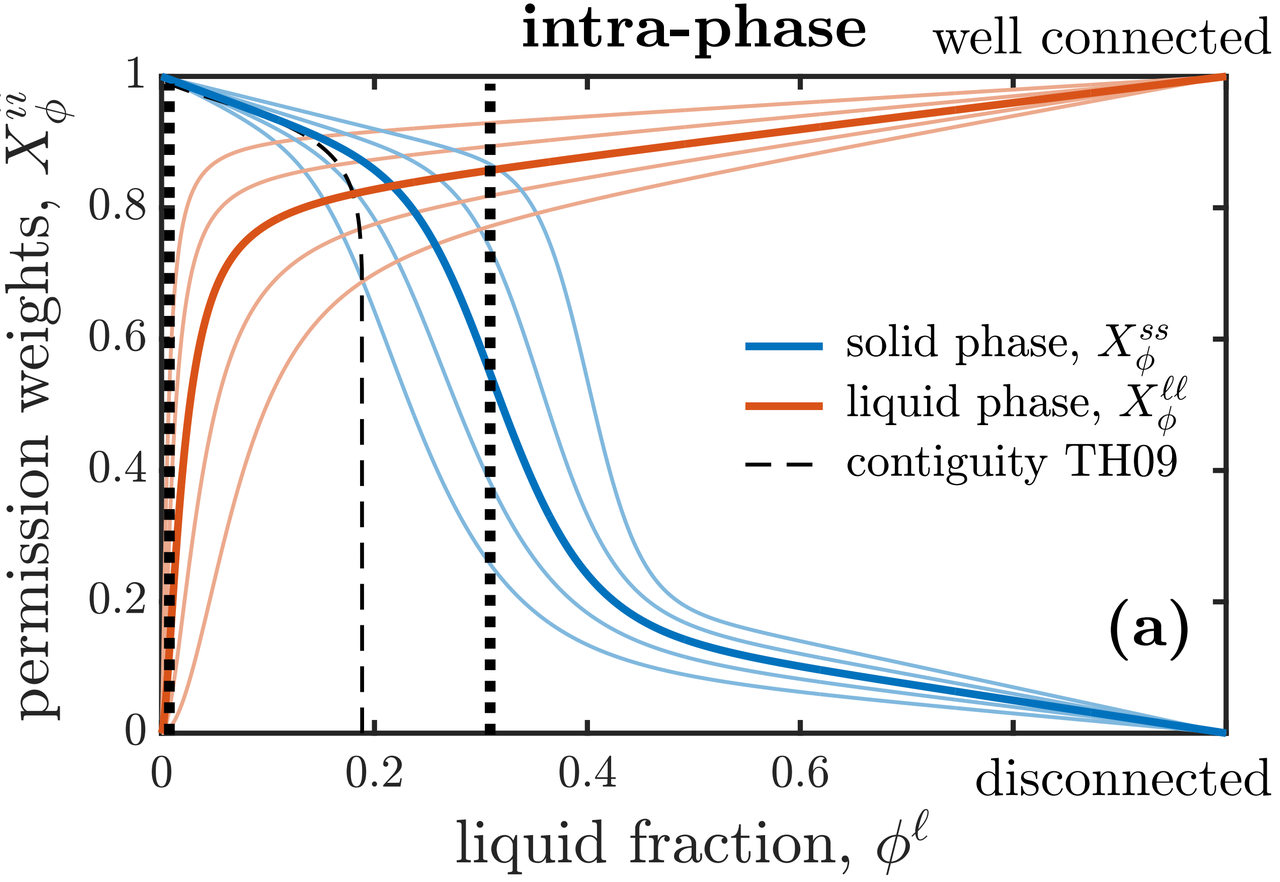
transfer

source

write equations for heat/entropy, chemistry, mass/volume, momentum, in each phase

PHASE CONNECTIVITY

local-scale phase topology permits system-scale transport



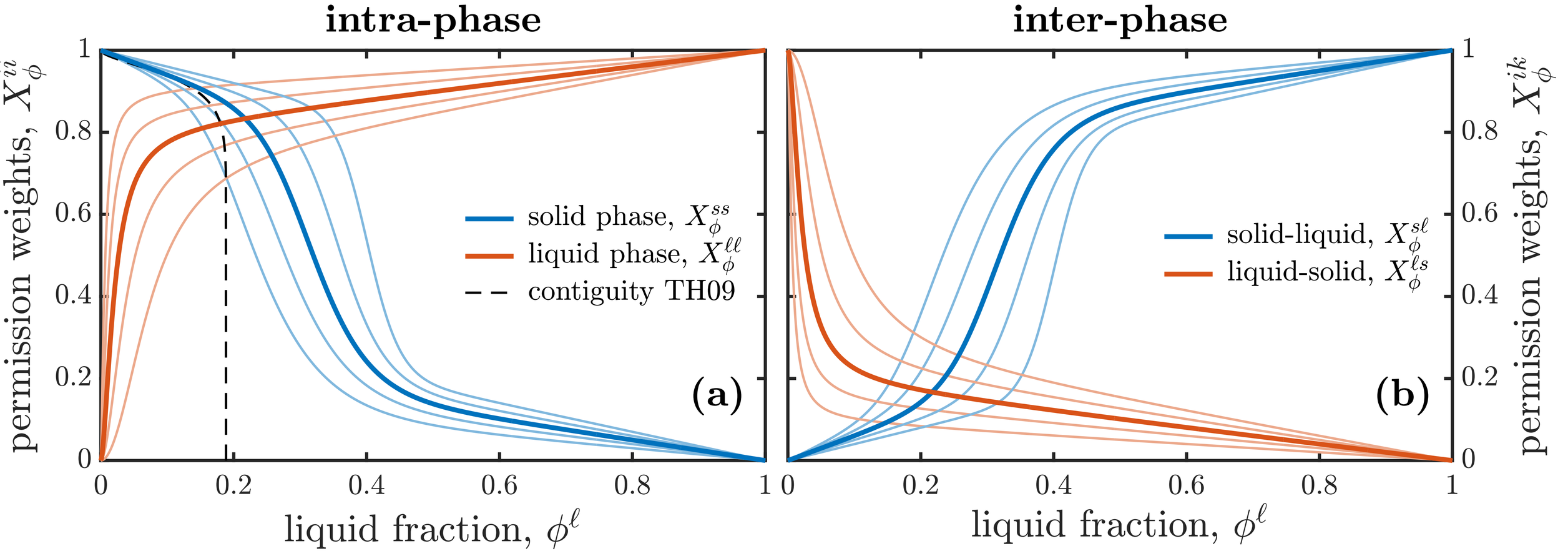
percolation threshold

disaggregation threshold

- phenomenological framework for **effective media coefficients**
- example two-phase system
- calibrate to appropriate exponential softening/hardening, solid disagregation threshold, liquid percolation threshold, smoothness of transition

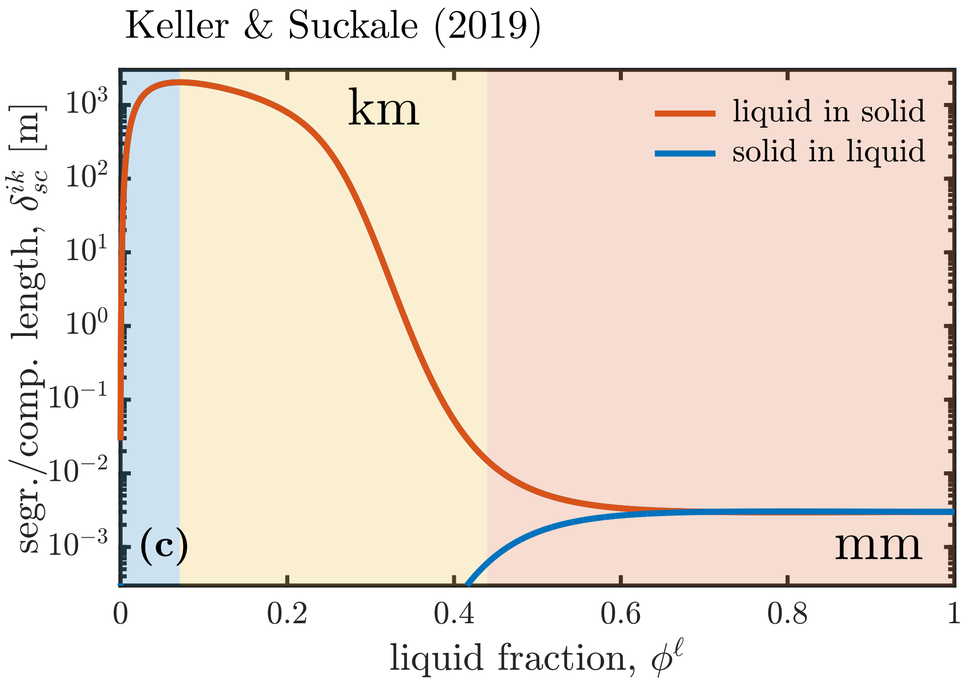
PHASE CONNECTIVITY

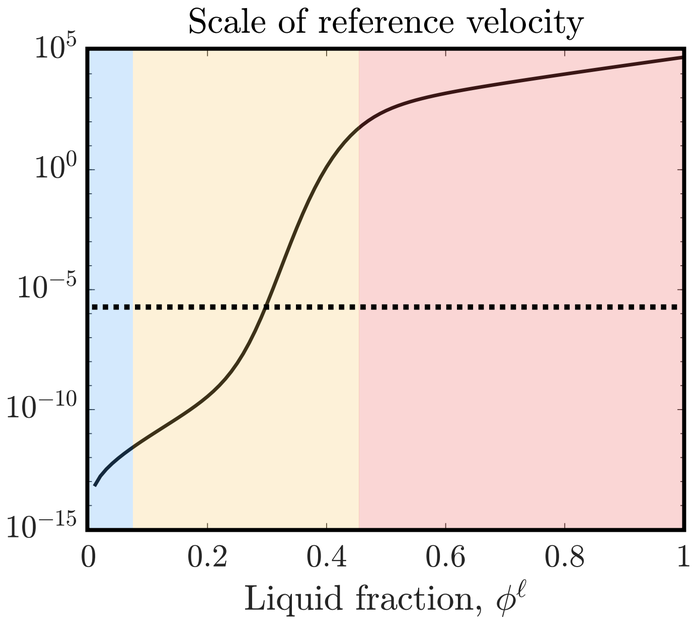
local-scale phase topology permits system-scale transport

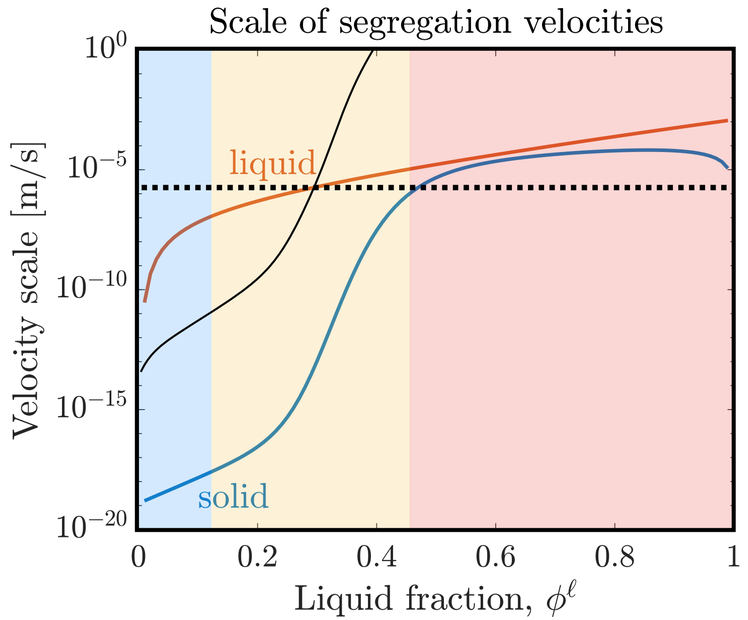


Keller & Suckale (2019)

TWO-PHASE FLOW REGIMES







Wong & Keller (in prep.)

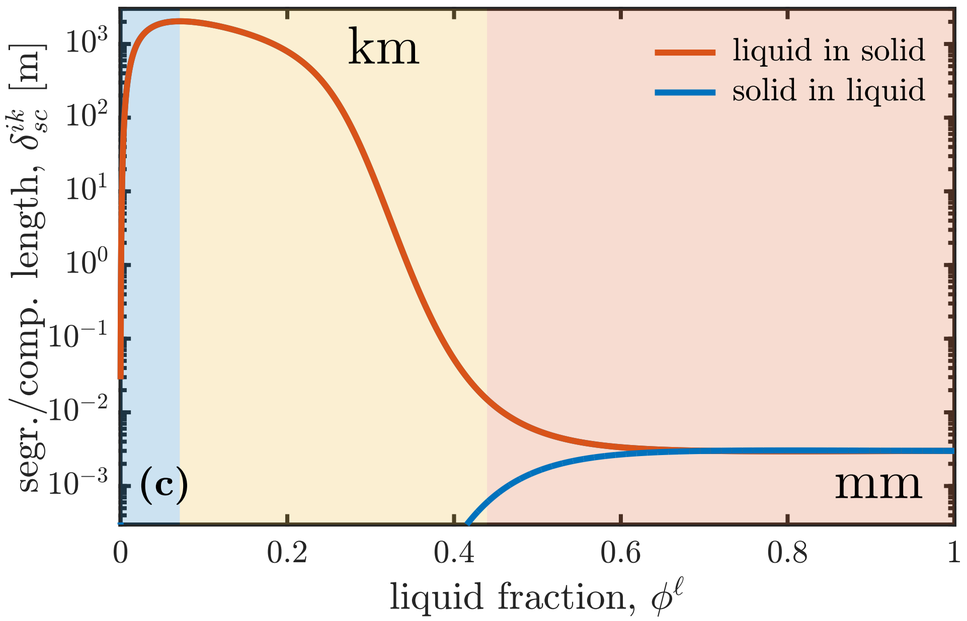
segregation-compaction length

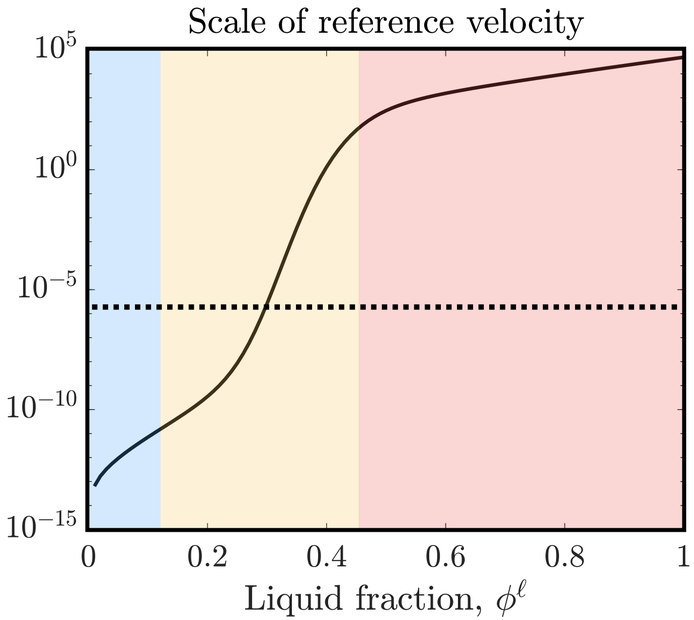
inherent length scale of phase segregation in compacting matrix

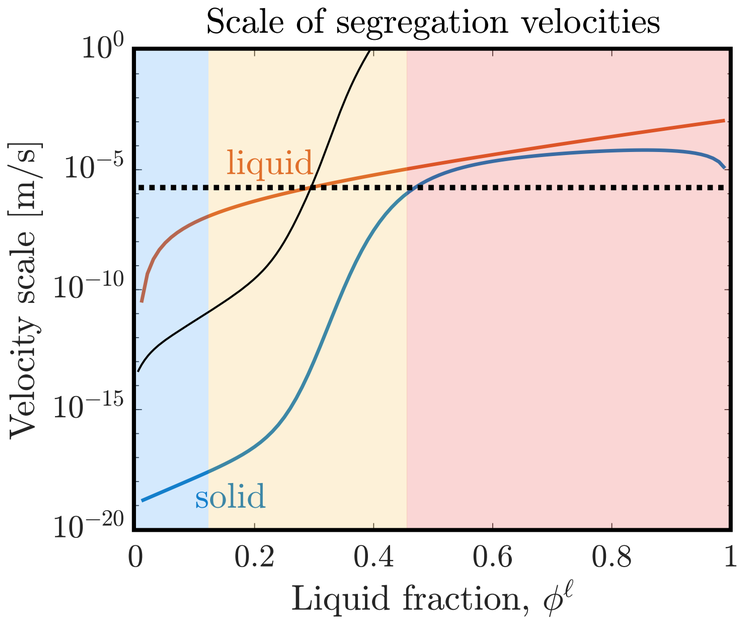
convection, segregation speeds

inherent speed scales of collective and phase segregation flow

TWO-PHASE FLOW REGIMES







Wong & Keller (in prep.)

POROUS

expanding s/c-length

segregation dominates over convection

MUSH

contracting s/c-length

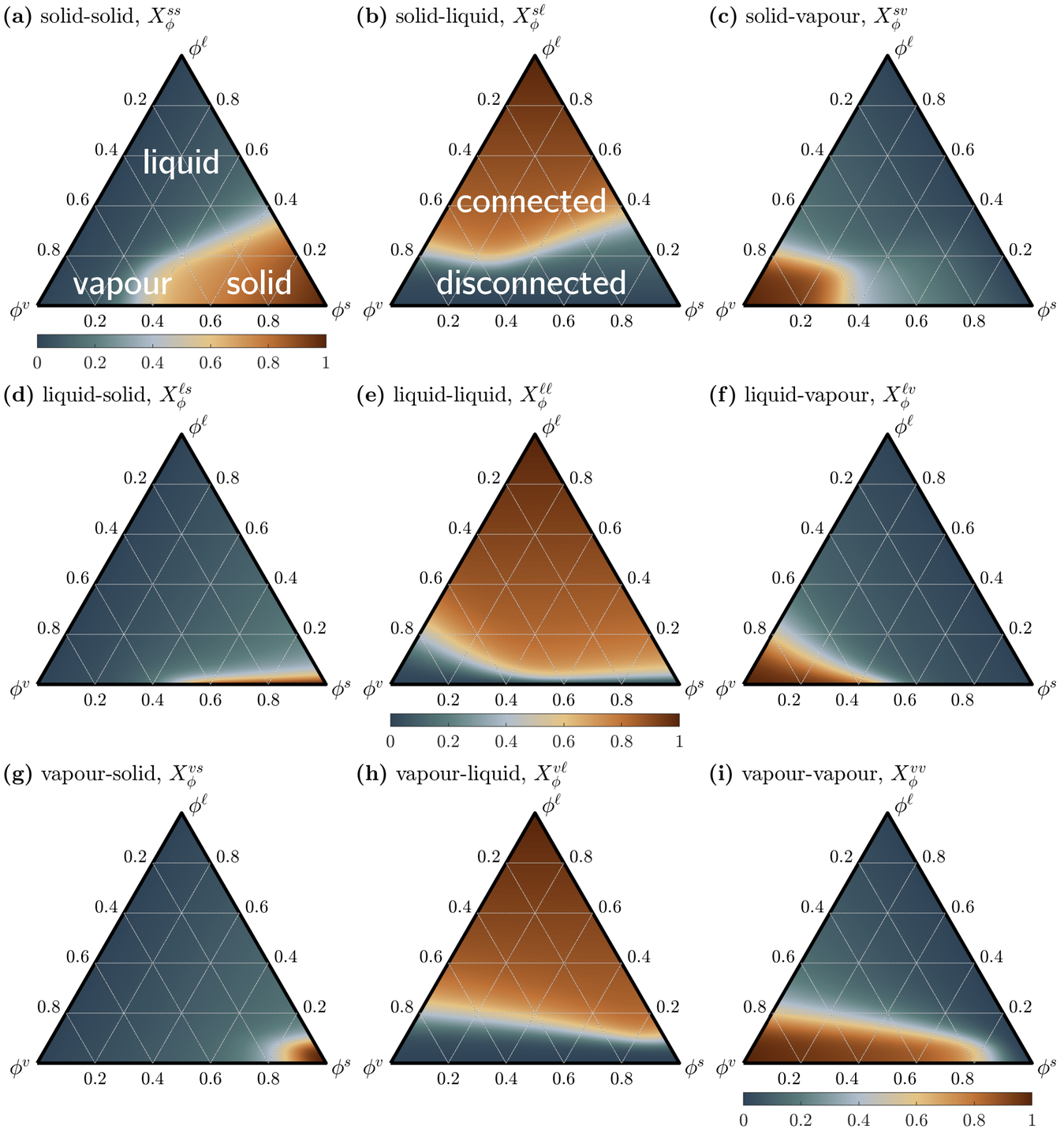
segregation- to convection-dominated

SUSPENSION

s/c-length at grain scale

convection dominates over segregation

3-PHASE CONNECTIVITIES

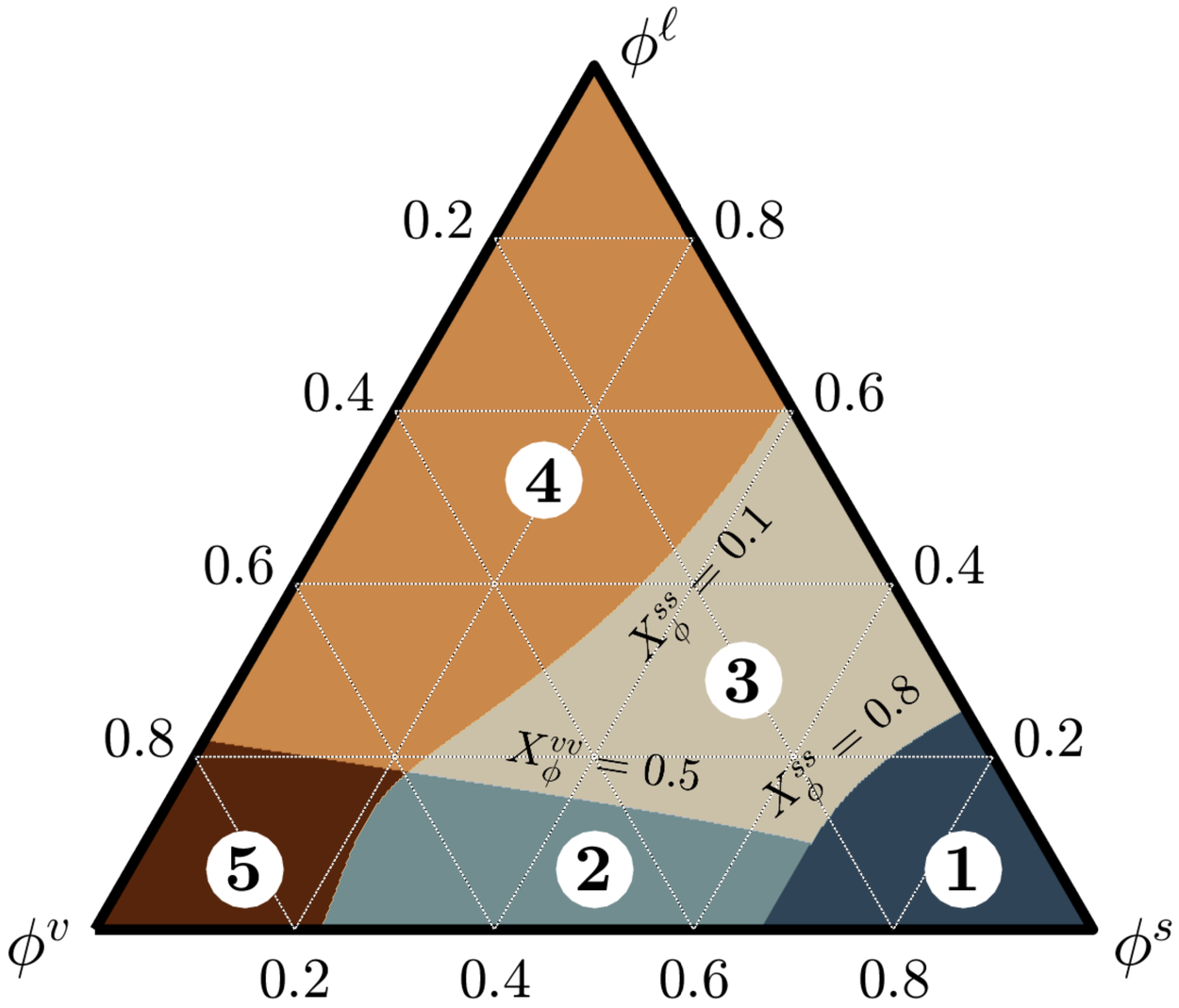


solid

liquid

vapour

THREE-PHASE REGIMES



1. porous flow
2. granular flow
3. mush flow
4. suspension flow
5. ash flow (finite Re)

N-PHASE NUMERICAL MODEL

update fluxes

```
% get momentum flux fields
qvxx  = - Kv .* (diff(u,1,3)./h - 0.*Div_v./3) + f.*p;
qvzz  = - Kv .* (diff(w,1,2)./h - 0.*Div_v./3) + f.*p;
qvxz  = -(Kv(:,im,im)+Kv(:,ip,im)+Kv(:,im,ip)+Kv(:,ip,ip))./4 .* (diff(u(:,ic,:),1,2)./h + diff(w(:,:,ic),1,3)./h)./2;
if strcmp(BC,'closed'); qvxz(:,[1,end],:) = 0; end

% get volume flux fields
qfx = -(Kf(:,:,im)+Kf(:,:,ip))./2 .* (diff(p(:,:,ic),1,3)./h - Gx_pstar) + (f(:,:,im)+f(:,:,ip))./2.*u;
qfz = -(Kf(:,im,:)+Kf(:,ip,:))./2 .* (diff(p(:,ic,:),1,2)./h - Gz_pstar) + (f(:,im,:)+f(:,ip,:))./2.*w;
if strcmp(BC,'closed'); qfz(:,[1,end],:) = 0; end
```

update transfers

```
% get momentum transfer fields
Gvx = (Cv(:,:,im)+Cv(:,:,ip))./2 .* (u-ustar) - (pstar(:,:,im)+pstar(:,:,ip))./2.*diff(f(:,:,ic),1,3)./h;
Gvz = (Cv(:,im,:)+Cv(:,ip,:))./2 .* (w-wstar) - (pstar(:,im,:)+pstar(:,ip,:))./2.*diff(f(:,ic,:),1,2)./h;

%get volume transfer field
Gf  =  Cf                        .* (p-pstar) -  vstar_Gf;
```

update body force

```
% get momentum source fields
Qvx = - (f(:,:,im)+f(:,:,ip))./2.*(rho0-rhomix).*grav(2);
Qvz = - (f(:,im,:)+f(:,ip,:))./2.*(rho0-rhomix).*grav(1);
```

update time step

```
% get physical time step
dt  = min(2*dto,cfl/(max(abs([qfx(:);qfz(:)]))/(h/2) + max(abs(Gf(:)))/1e-2));  % [s]
```

update residuals

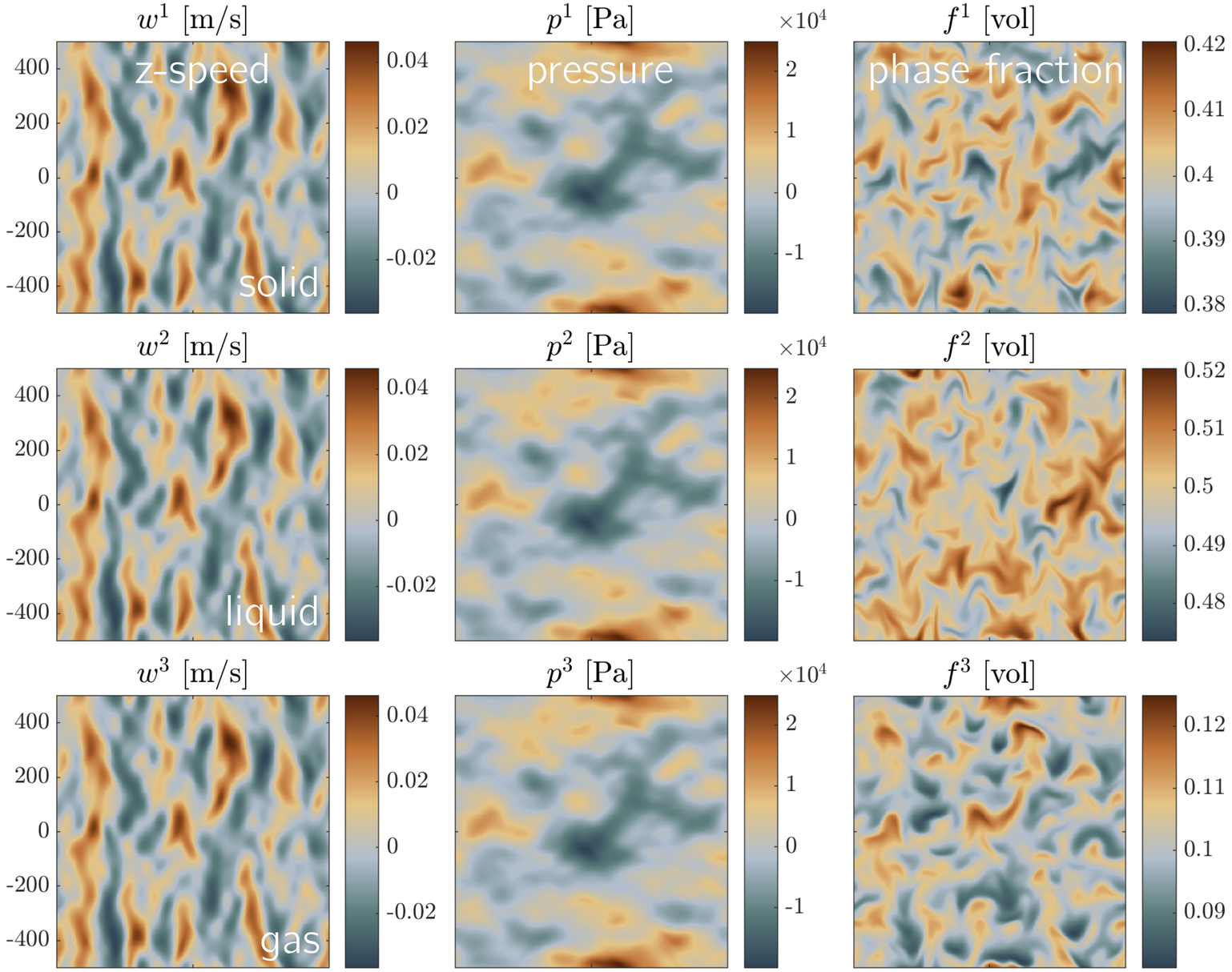
```
% get residual fields
res_u = diff(qvxx(:,:,ic),1,3)./h + diff(qvxz,1,2)./h + Gvx + Qvx;
res_w = diff(qvzz(:,ic,:),1,2)./h + diff(qvxz,1,3)./h + Gvz + Qvz;
res_p = diff(qfx         ,1,3)./h + diff(qfz ,1,2)./h + Gf;
res_f = (f-fo)./dt + (diff(qfx,1,3)./h + diff(qfz,1,2)./h);
if strcmp(BC,'closed'); res_u(:,:,[1,end]) = 0; res_w(:,[1,end],:) = 0; end
```

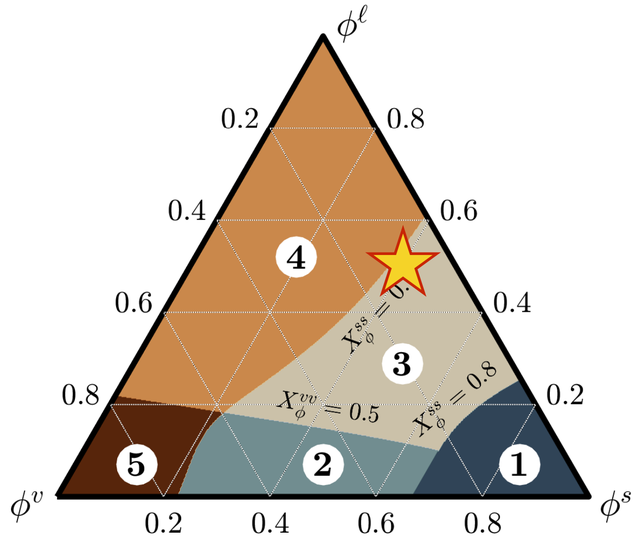
update solution

```
% update solution
u = ui - alpha.*res_u.*dtau_u + beta.*(ui-uii);
w = wi - alpha.*res_w.*dtau_w + beta.*(wi-wii);
p = pi - alpha.*res_p.*dtau_p + beta.*(pi-pii);
f = fi - alpha.*res_f.*dtau_f + beta.*(fi-fii);
```

github.com/kellertobs/pantarhei

0.4 SOLID + 0.5 LIQUID + 0.1 GAS





$\eta^\ell = 10^2$ Pas

$\rho^\ell = 2500$ kg/m^3

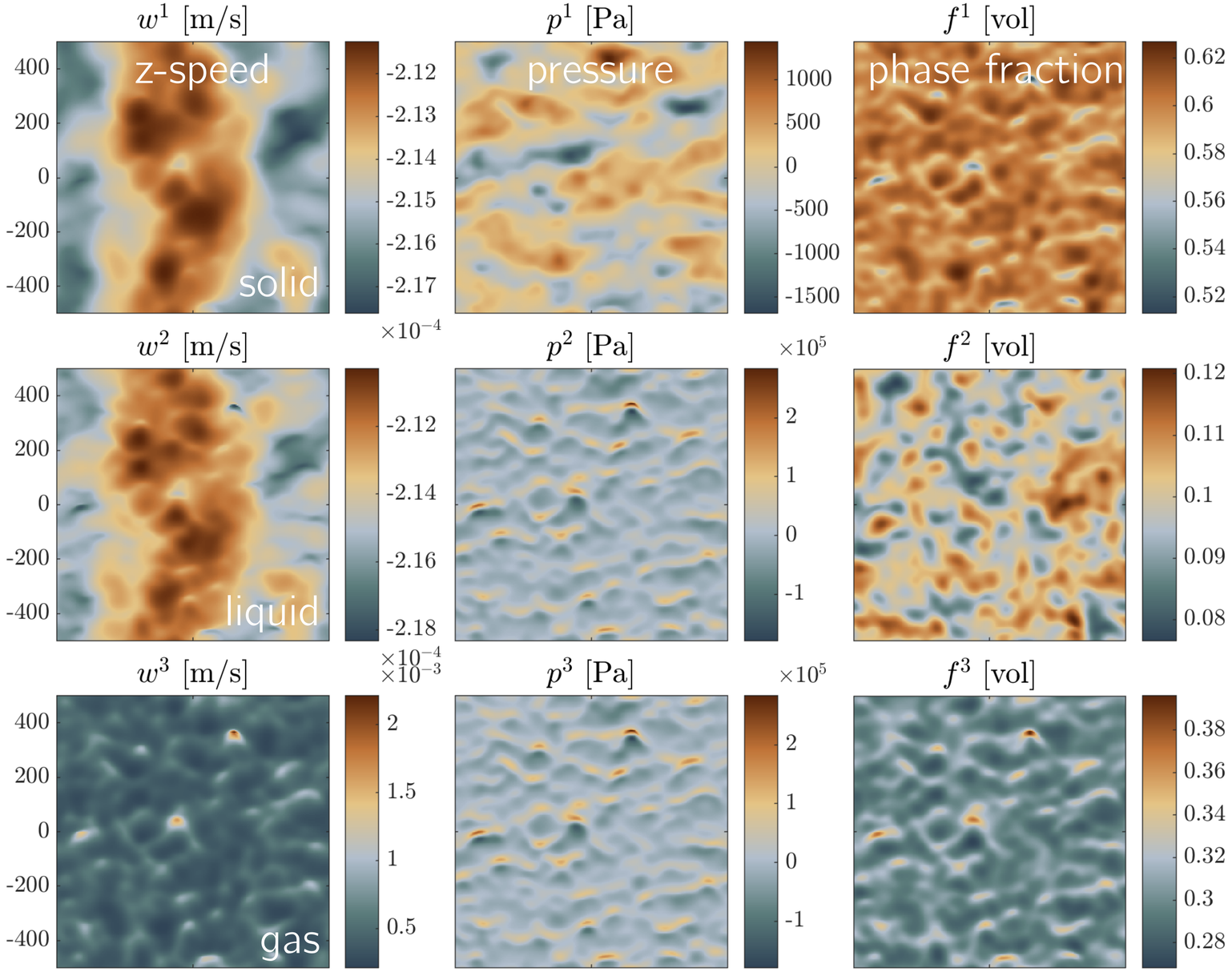
$d^\ell = 1$ mm

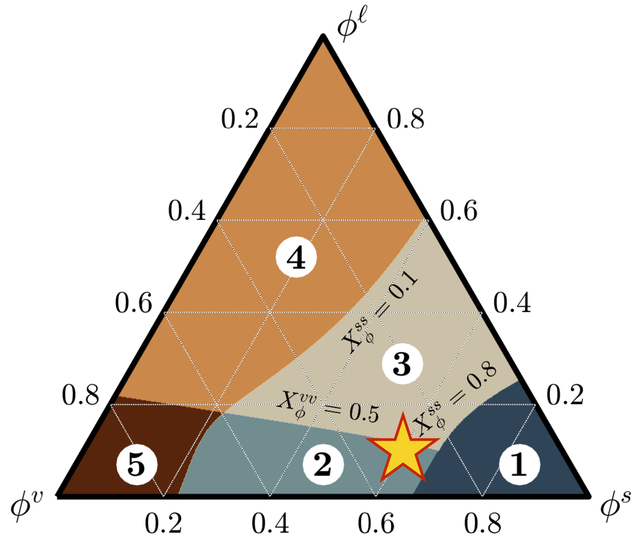
$\eta^g = 10^{-5}$ Pas $\quad \eta^s = 10^{18}$ Pas

$\rho^g = 200$ kg/m^3 $\quad \rho^s = 3000$ kg/m^3

$d^g = 1$ mm $\quad d^s = 1$ mm

0.6 SOLID + 0.1 LIQUID + 0.3 GAS





$$\eta^\ell = 10^2 \text{ Pas}$$
$$\rho^\ell = 2500 \text{ kg/m}^3$$
$$d^\ell = 1 \text{ mm}$$

$$\eta^g = 10^{-5} \text{ Pas} \qquad \eta^s = 10^{18} \text{ Pas}$$
$$\rho^g = 200 \text{ kg/m}^3 \qquad \rho^s = 3000 \text{ kg/m}^3$$
$$d^g = 1 \text{ mm} \qquad d^s = 1 \text{ mm}$$