Formulation of the thermohaline flow problem in FEFLOW

$$S\frac{\partial\varphi}{\partial t}+\mathrm{div}(\mathbf{q})=0$$

$$\mathbf{q}=-\mathbf{K}\left(\mathbf{grad}(\varphi)+\frac{\rho_f-\rho_{0f}}{\rho_{0f}}\mathbf{u}\right)$$

$$\mathbf{K}=\frac{\mathbf{k}\rho_{0f}g}{\mu_f(C,T)}$$

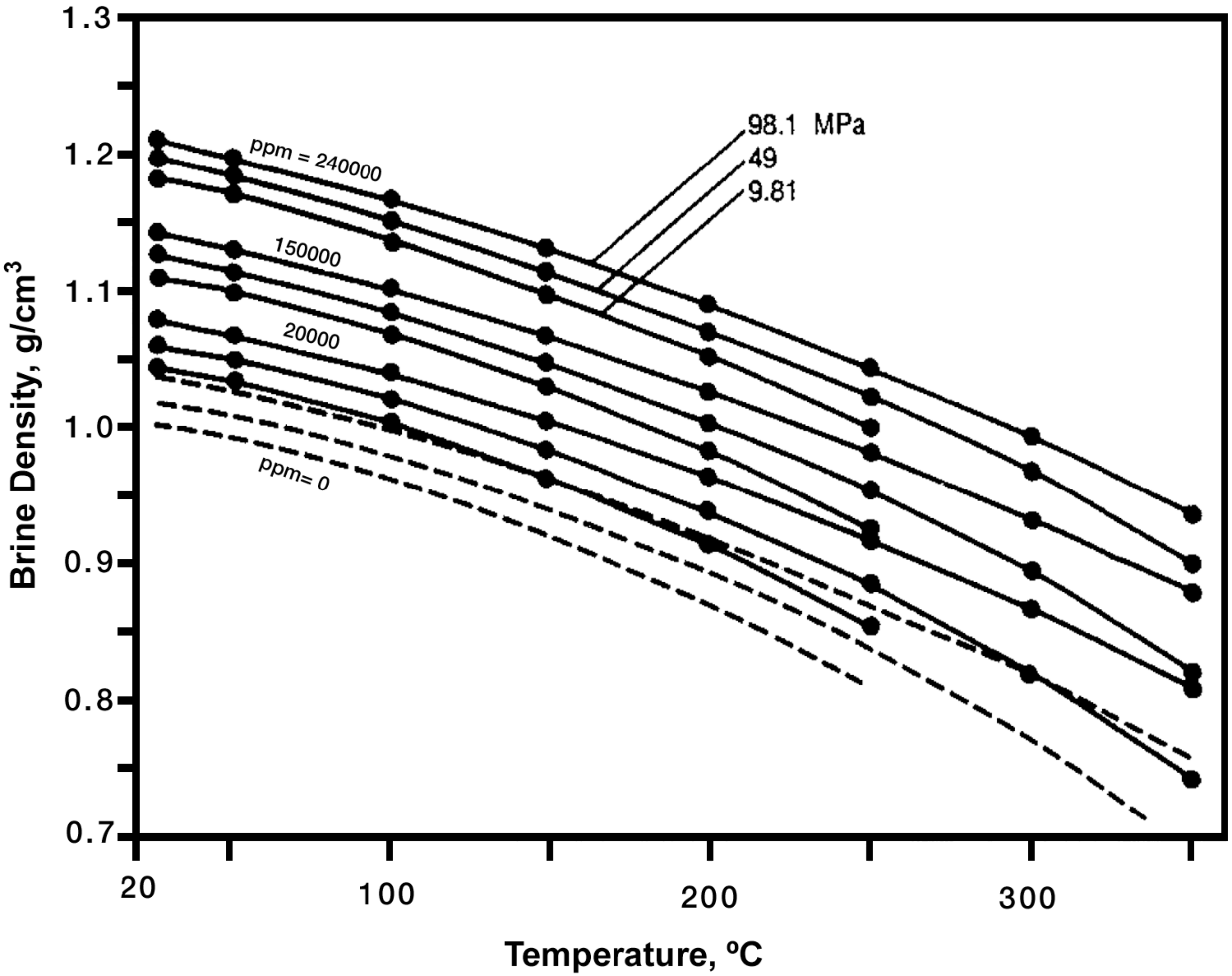
$$\rho_f=\rho_f(\varphi,T,C)$$

$$\phi\frac{\partial C}{\partial t}+\mathrm{div}\left(\mathbf{q}C\right)-\mathrm{div}\left(\mathbf{Dgrad}(C)\right)=0$$

$$\frac{\partial}{\partial t}\left(\left(\phi\rho_f c_f+(1-\phi)\rho_s c_s\right)T\right)+\mathrm{div}(\rho_f c_f T\mathbf{q})-\mathrm{div}\left(\mathbf{\Lambda grad}(T)\right)=0$$

Equations Of State in FEFLOW: brine density

$$\rho_f = \rho_{f0}\left(1+\bar{\gamma}(p_f - p_{f0}) - \bar{\beta}(T_f - T_{f0}) + \bar{\alpha}(C_\alpha - C_{\alpha 0})\right)$$



Brinedensity as function of pressure and temperature

Equations Of State in FEFLOW: fluid viscosity

$$\mu_f(C,T) = \mu 0(1 + aC + bC^2 + cC^3 + dT(1 - e^{kC})$$

a,b,c,d,k are constants

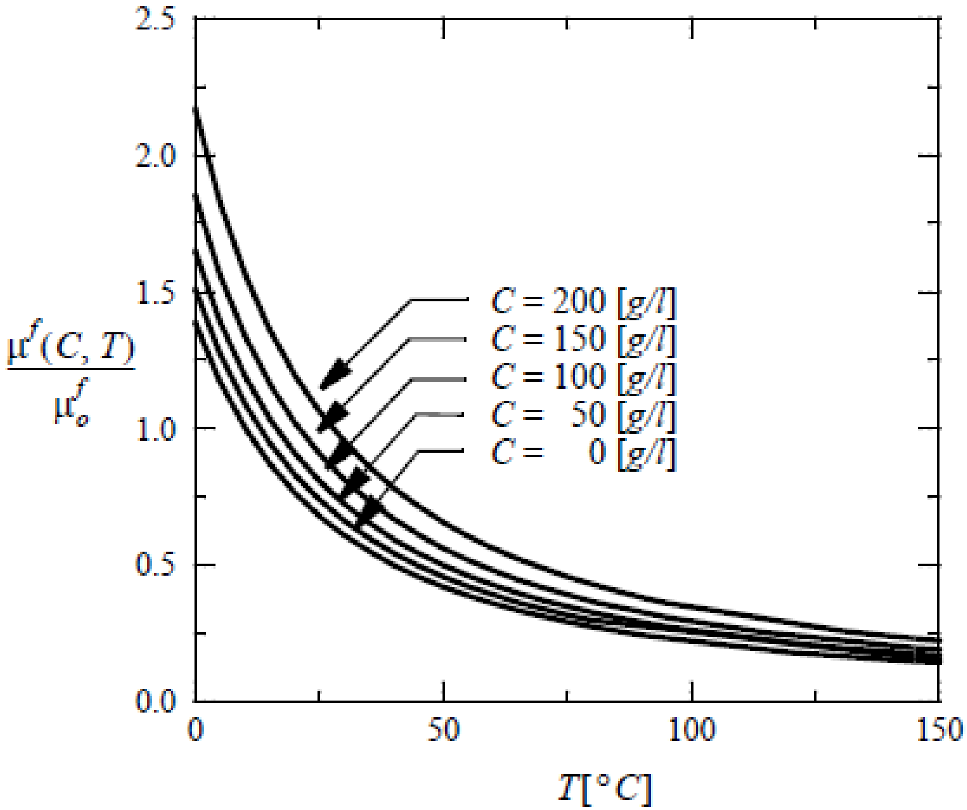
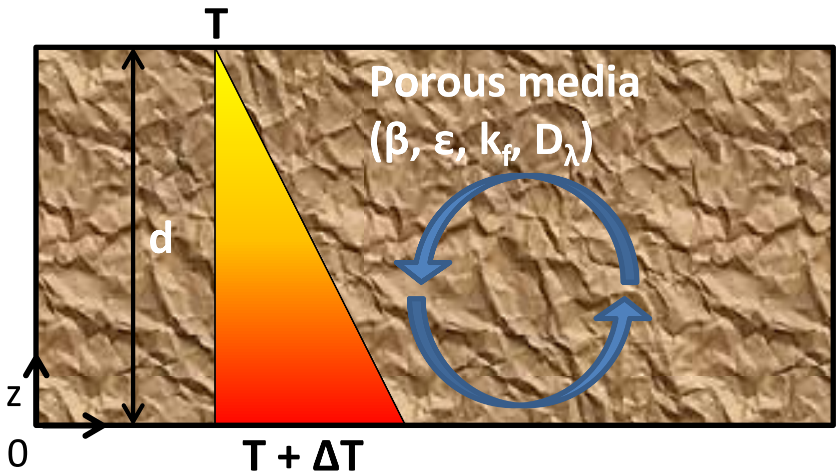
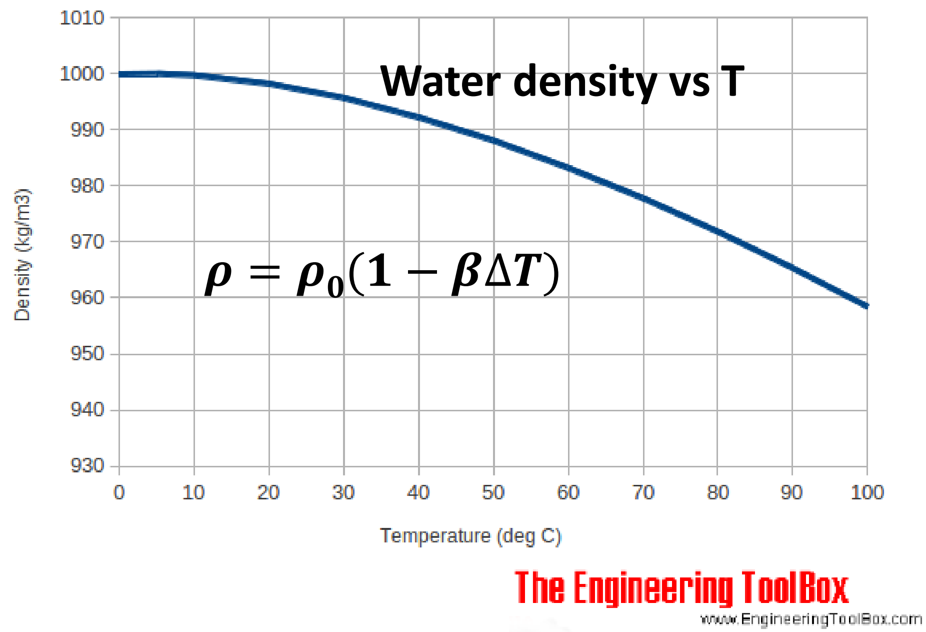


Figure 1.7 Relative viscosity μ^f/μ^f_o as function of temperature $T[°C]$ and concentration $C[g/l]$ with μ^f_o for the reference temperature of $T_o = 10\ °C$ and reference concentration of $C_o = 0$ (freshwater).

Thermal Rayleigh-Number (Ra_T) for an homogeneous porous media heated from below



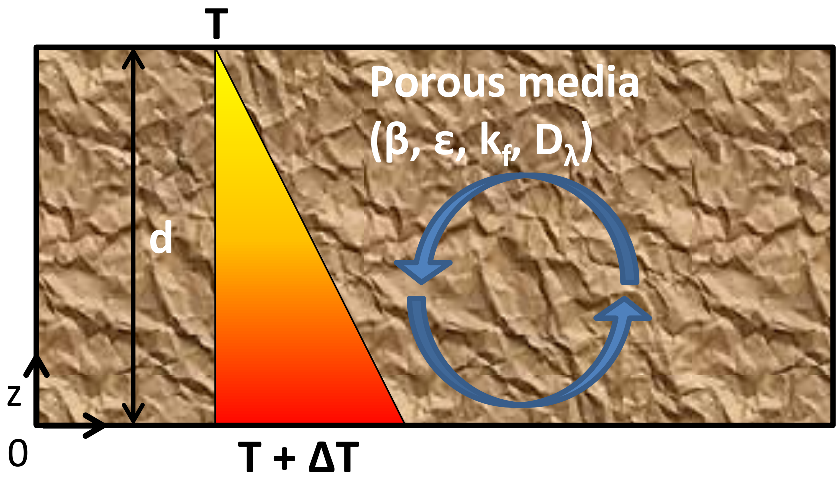


The Rayleigh number(Ra) allows to predict the onset of convection:

$$Ra = \frac{\beta \Delta T k_f d}{D_\lambda}$$

β	Expansion coefficient	[Θ^{-1}]
ΔT	temperature difference	[Θ]
K_f	hydraulic conductivity	[$L*T^{-1}$]
d	height	[L]
D_λ	Thermal diffusivity	[L^2*T^{-1}]

Thermal Rayleigh-Number (Ra_T) for an homogeneous porous media heated from below



$$Ra_T = \frac{\beta . \Delta T . k_f . d}{D_\lambda}$$

$$D_\lambda = \frac{\Lambda}{\rho . cl} \quad [L^2 * T^{-1}]$$

$$\Lambda = \lambda_{cond} + \lambda_{disp} [M * L * T^{-3} * \Theta^{-1}]$$

ρ	Fluid density	[M*L-3]
C	heat capacity	$[M*L^2*T^{-2}*\Theta^{-1}]$
C_l	specific heat capacity	$[L^2*T^{-2}*\Theta^{-1}]$
ρ(c/[M])	volumetric heat capacity	$[M*L^{-1}*T^{-2}*\Theta^{-1}]$
k_f	hydraulic conductivity	$[L*T^{-1}]$
β	expansion coefficient	$[\Theta^{-1}]$
ΔT	temperature difference	[Θ]
d	length (height)	[L]
D_λ	Thermal Diffusivity tensor	$[L^2*T^{-1}]$
Λ	hydrodynamic thermodispersion	$[M*L*T^{-3}*\Theta^{-1}]$
λ	thermal conductivity	$[M*L*T^{-3}*\Theta^{-1}]$
ε	Porosity	[1]

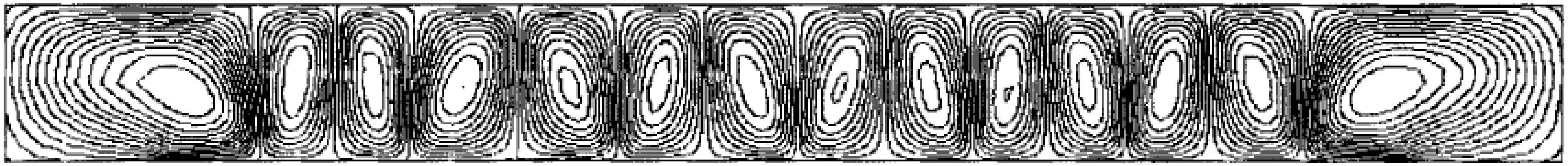
Critical Rayleigh-Numbers

2D homogenous medium / infinite porous medium

$Ra_{critical1} = 4\pi^2 = \mathbf{39,48}$

$Ra_{critical2} = \mathbf{240\text{-}300}$

$Ra < Ra_{critical1}$	→ pure conduction
$Ra_{critical1} < Ra < (240\text{-}300)$	→ stable convergent solution develops and various steady-state flows occur
$Ra > Ra_{critical2}$	→ convection regime is unstable



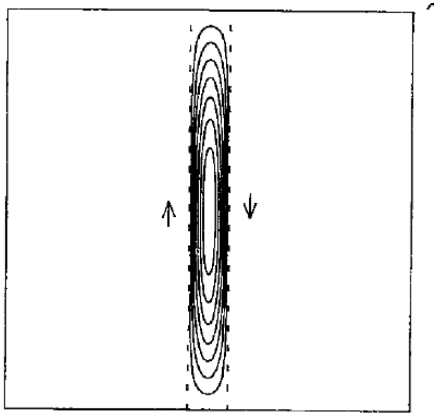
Streamlines for a 2D convective problem (Diersch, 2002)

Critical Rayleigh-Numbers

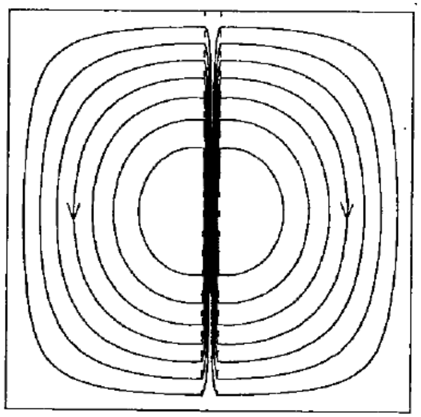
Problem: nature is heterogeneous

→ **$Ra_{critical}$ = 4π² is not indicative of the onset of convection for heterogeneous media**

In a fault surrounded by an impervious rock,
the onset of convection occurs for much higher Rayleigh!



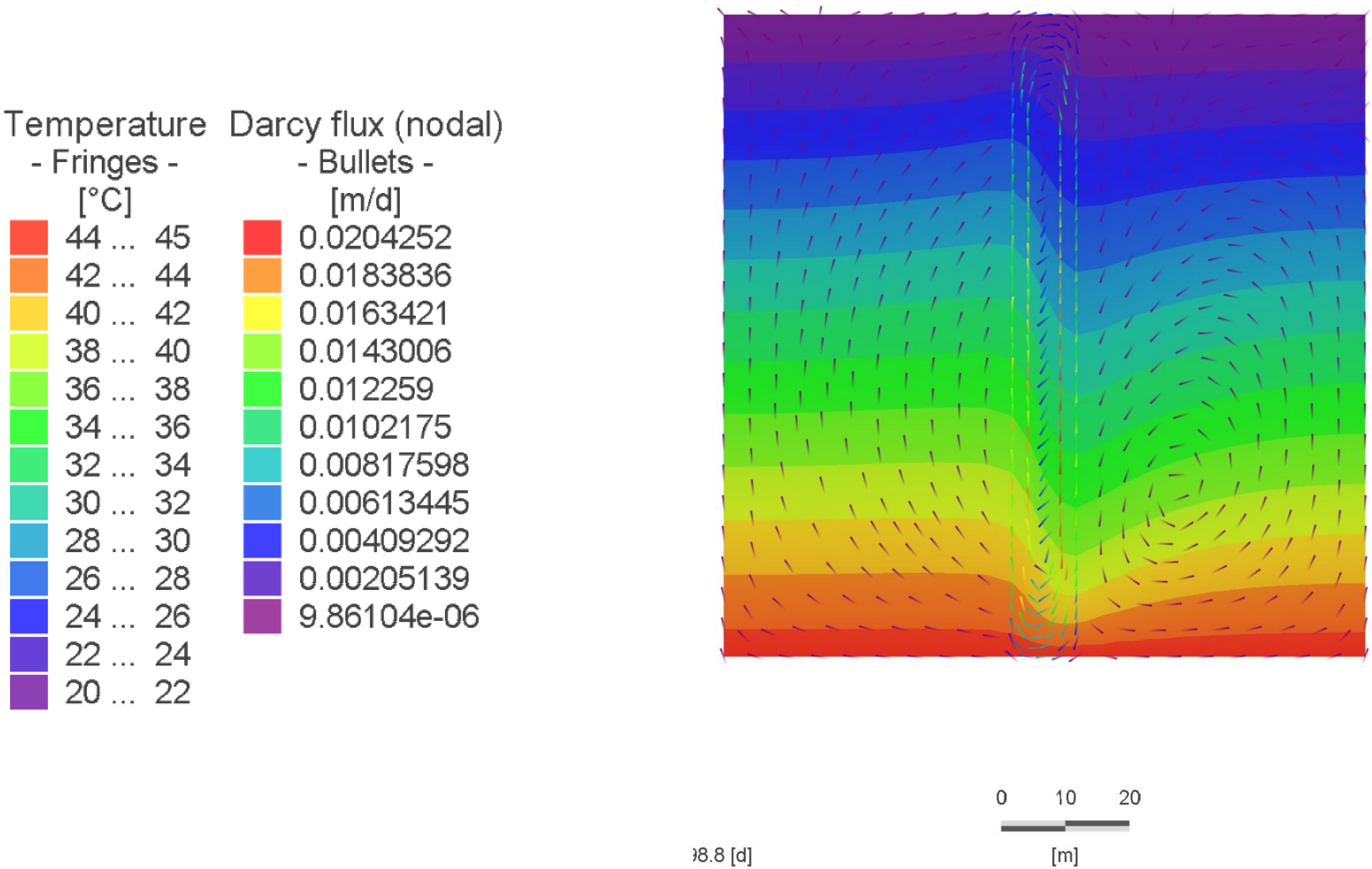
Ra_{fault} = **1054**
$Ra_{surrounding}$ = 10



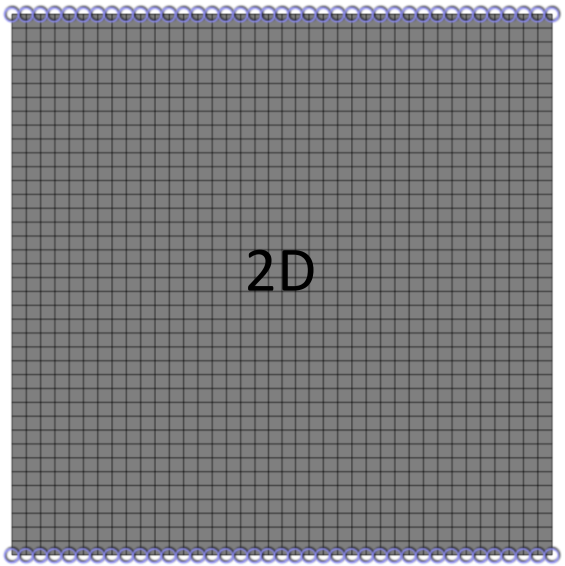
Ra_{fault} = **2625**
$Ra_{surrounding}$ = 26

Streamline patterns (McKibbin,1986)

McKibbin example nicely reproduced



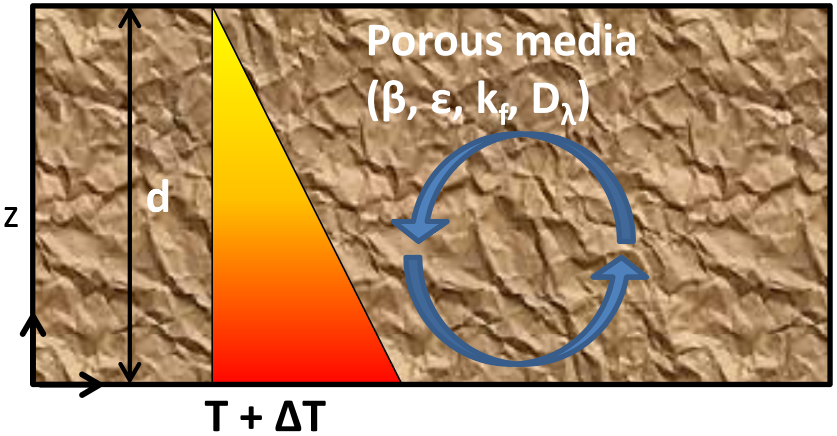
FEFLOW Exercise



When will convection occur?

Change **β or ΔT or kf**

Compare with Ra theory



- **1st-kind (Dirichlet) heat transport BC**
  → *fixed temperature at the top and the bottom*

- **1st-kind (Dirichlet) flow BC**
  → *fixed Hydraulic-Head in the upper left and right corner as a reference value*

- (the surrounding bounds are set as No-Flow-BC by default)

Additional slides

Critical Rayleigh-Number (Zhao et al. 2008)

Fault and surrounding rock

$$Ra^{3D}_{Tcritical} = \frac{\left[\left(\frac{H_3}{H_1}\right)^2 + \left(\frac{H_3}{H_2}\right)^2 + 1\right]^2 \pi^2}{\left(\frac{H_3}{H_1}\right)^2 + \left(\frac{H_3}{H_2}\right)^2}.$$

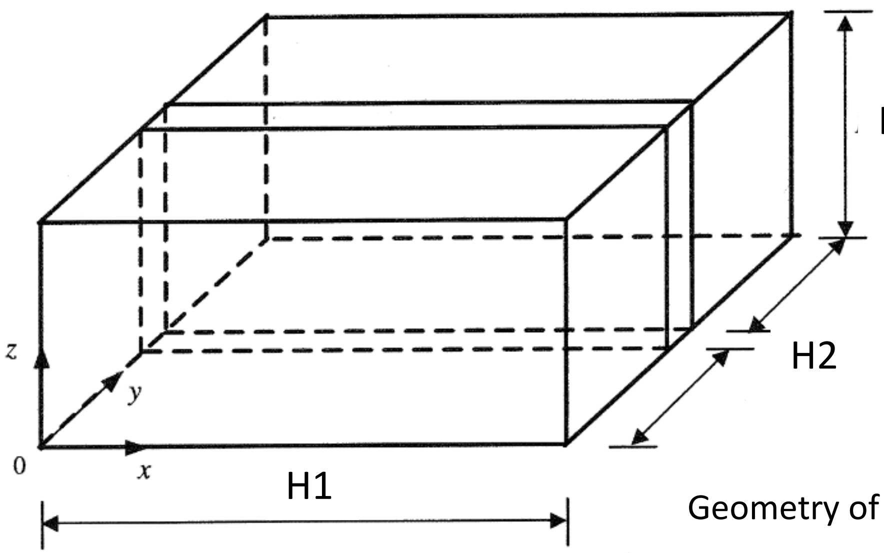
H3/H1 << 1 — *$H3_{(height)}$ << $H1_{(length)}$*

$$Ra^{2D}_{Tcritical} = \frac{\left[\left(1 + \left(\frac{H_3}{H_2}\right)^2\right]^2 \pi^2}{\left(\frac{H_3}{H_2}\right)^2}.$$

H3/H2 >> 1 — *$H3_{(height)}$ >> $H2_{(width))}$*

H1/H2 >> 1 — *$H1_{(length)}$ >> $H2_{(width)}$*

if H1 tends to infinity: **$Ra_{critical}$2D = $Ra_{critical}$3D**



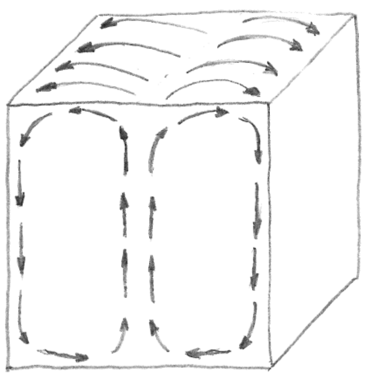
Geometry of the problem (Zhao et al. 2006)

Results - 3D homogenous cube

Same geometry - different Rayleigh-Numbers

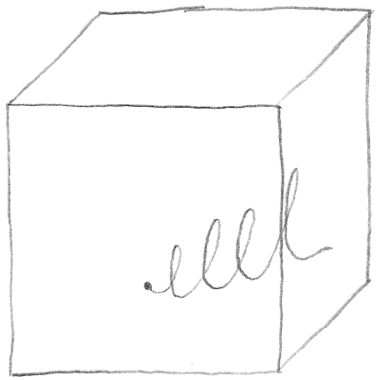
$Ra_{critical} = 4\pi^2 = \mathbf{39{,}5}$

Ra_T = **70**



- two stable convection cells
- like in 2D

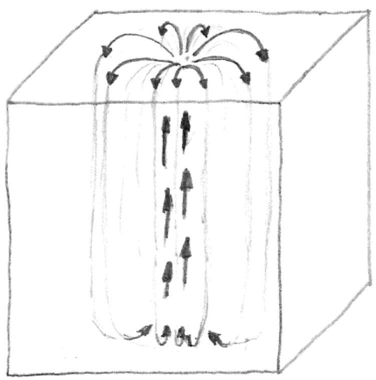
Ra_T = **330**



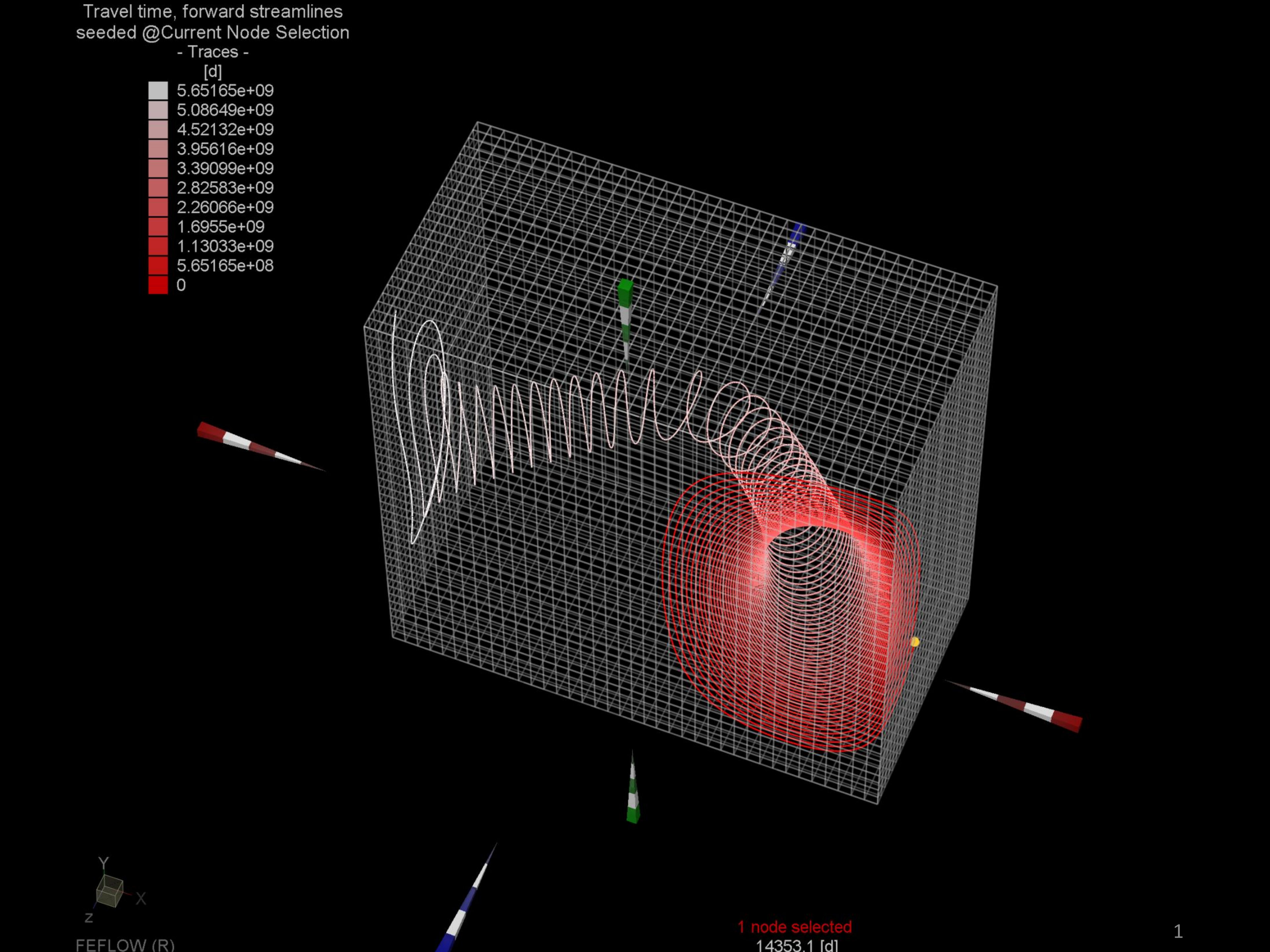
- unstable flow pattern
- no symmetry

→ ≠ 2D

Ra_T = **1200**



- radial symmetric convection cell
- only for a short time stable

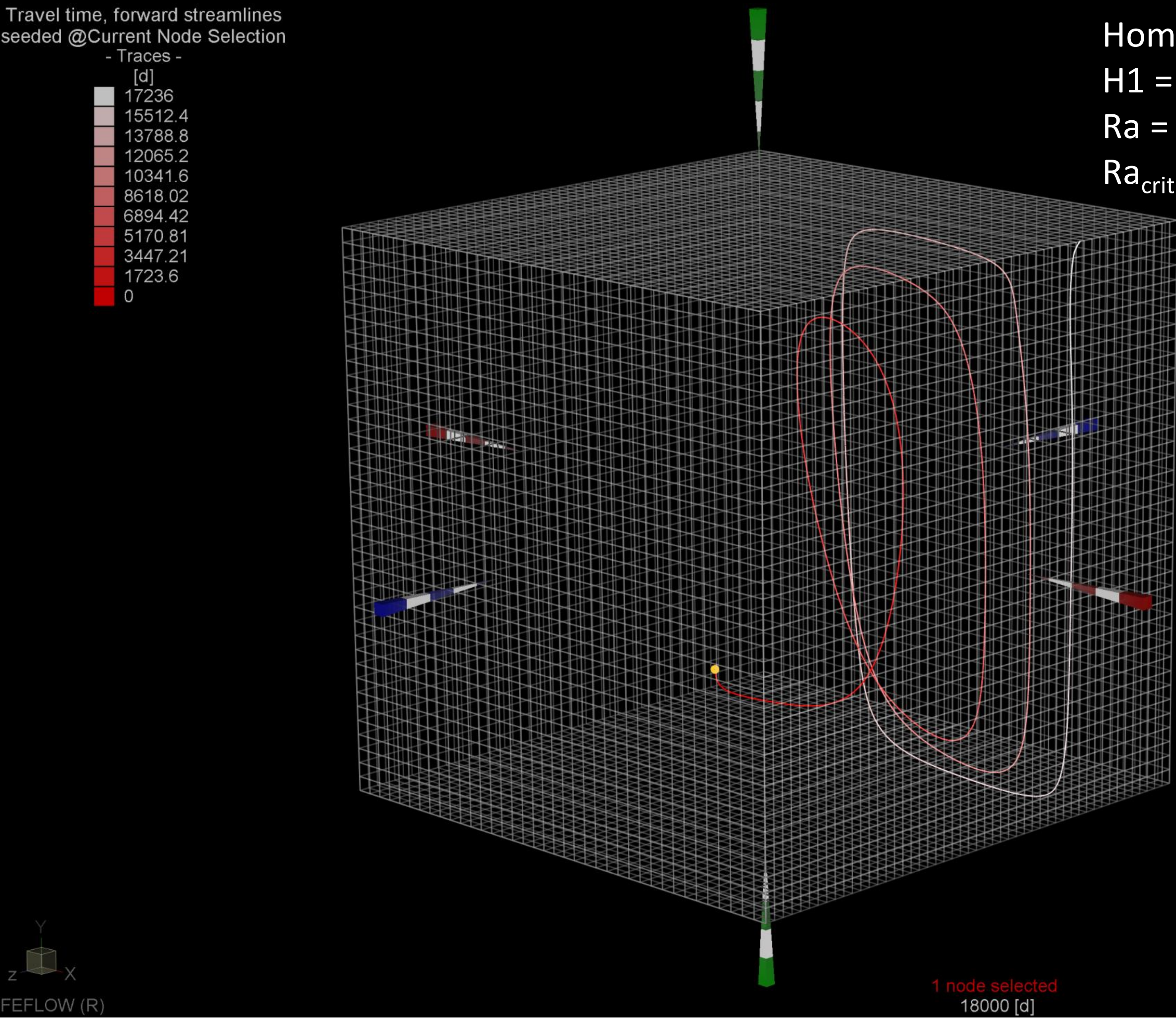

Travel time, forward streamlines
seeded @Current Node Selection
- Traces -
[d]
5.65165e+09
5.08649e+09
4.52132e+09
3.95616e+09
3.39099e+09
2.82583e+09
2.26066e+09
1.6955e+09
1.13033e+09
5.65165e+08
0
Y
X
z
FEFLOW (R)
1 node selected
14353.1 [d]
1

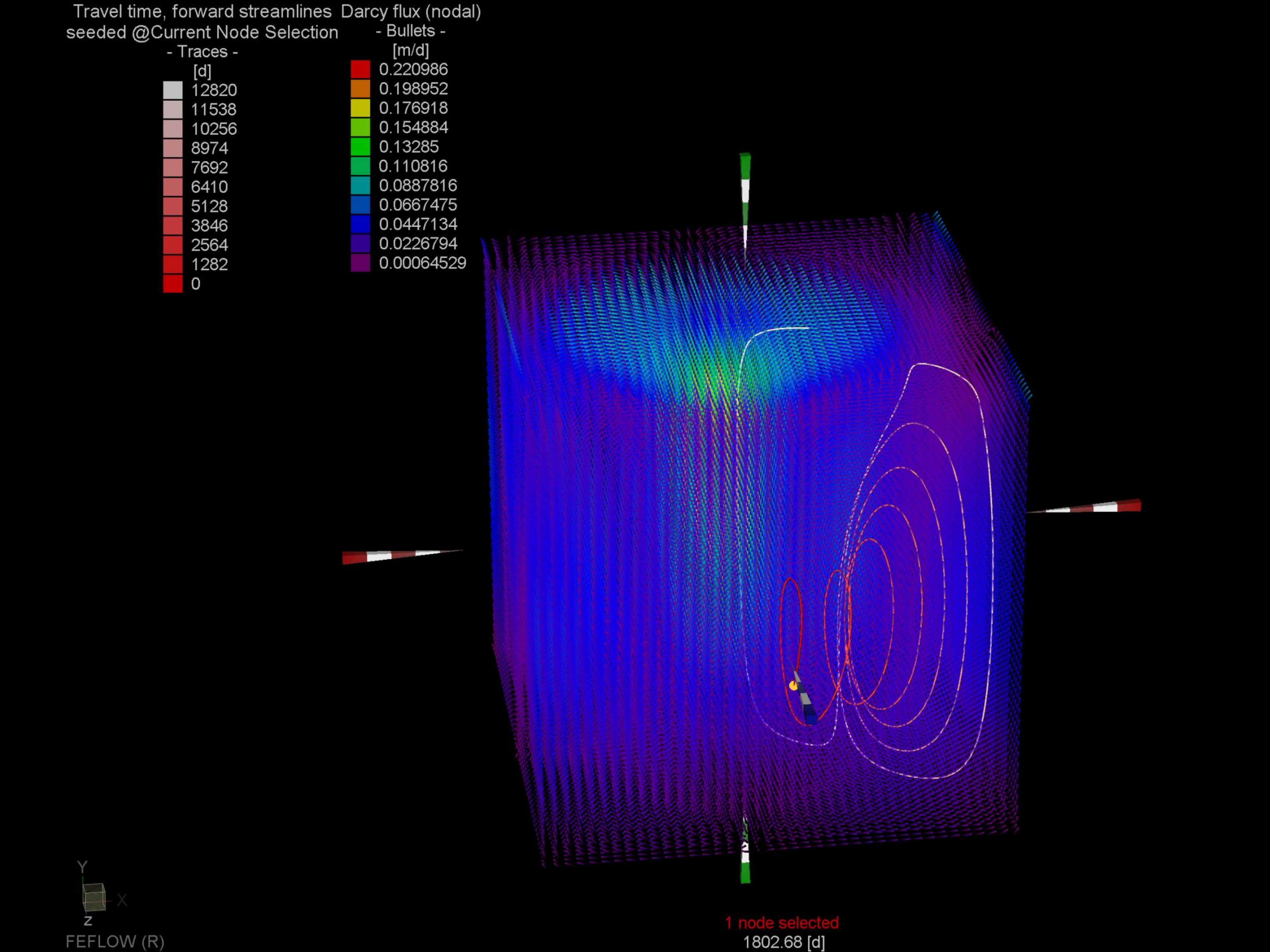
Homogenous cube

H1 = H2 = H3 = 100 m

Ra = 330

$Ra_{critical}3D = 4,5pi^2 = 44,4$




Travel time, forward streamlines
seeded @Current Node Selection
- Traces -
[d]
12820
11538
10256
8974
7692
6410
5128
3846
2564
1282
0
Darcy flux (nodal)
- Bullets -
[m/d]
0.220986
0.198952
0.176918
0.154884
0.13285
0.110816
0.0887816
0.0667475
0.0447134
0.0226794
0.00064529
Y
X
Z
FEFLOW (R)
1 node selected
1802.68 [d]

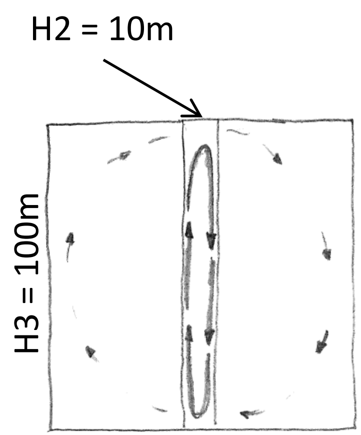
Results - 10 m fault with surrounding rock

Same Rayleigh-Number – different geometry

2D

Ra_T = 1200

$Ra_{critical}2D = 1006$



- different mode of convection compared to the 3D case

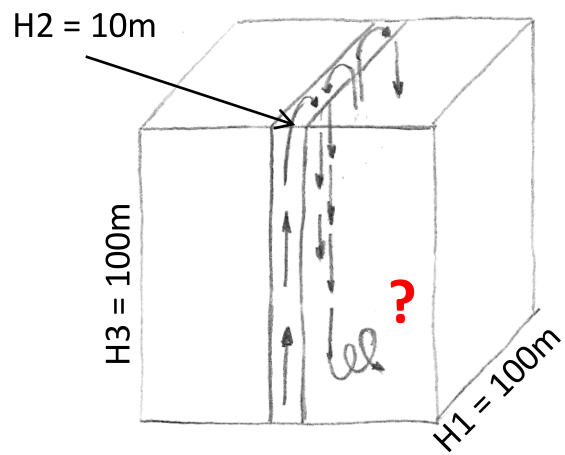
3D

Ra_T = 1200

H1= 100 m

~~$Ra_{critical}2D = 1006$~~

$Ra_{critical}3D = 1016$



$Ra_{critical}3D \neq Ra_{critical}2D$

BUT: 3D and 2D have the same chance to develop, if the height to width ratio is small

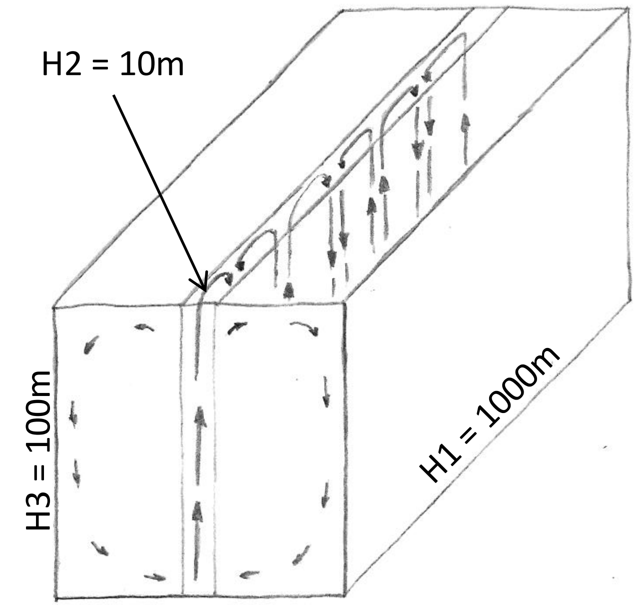
3D

Ra_T = 1200

H1 = 1000m

$Ra_{critical}2D = 1006$

$Ra_{critical}3D = 1006$



$Ra_{critical}3D = Ra_{critical}2D$

→ H1 tends to infinity

Does the system need more time to reach the 3D state?

Is the fault´s height to width ratio to small, so 2D and 3D have the same chance to occur?

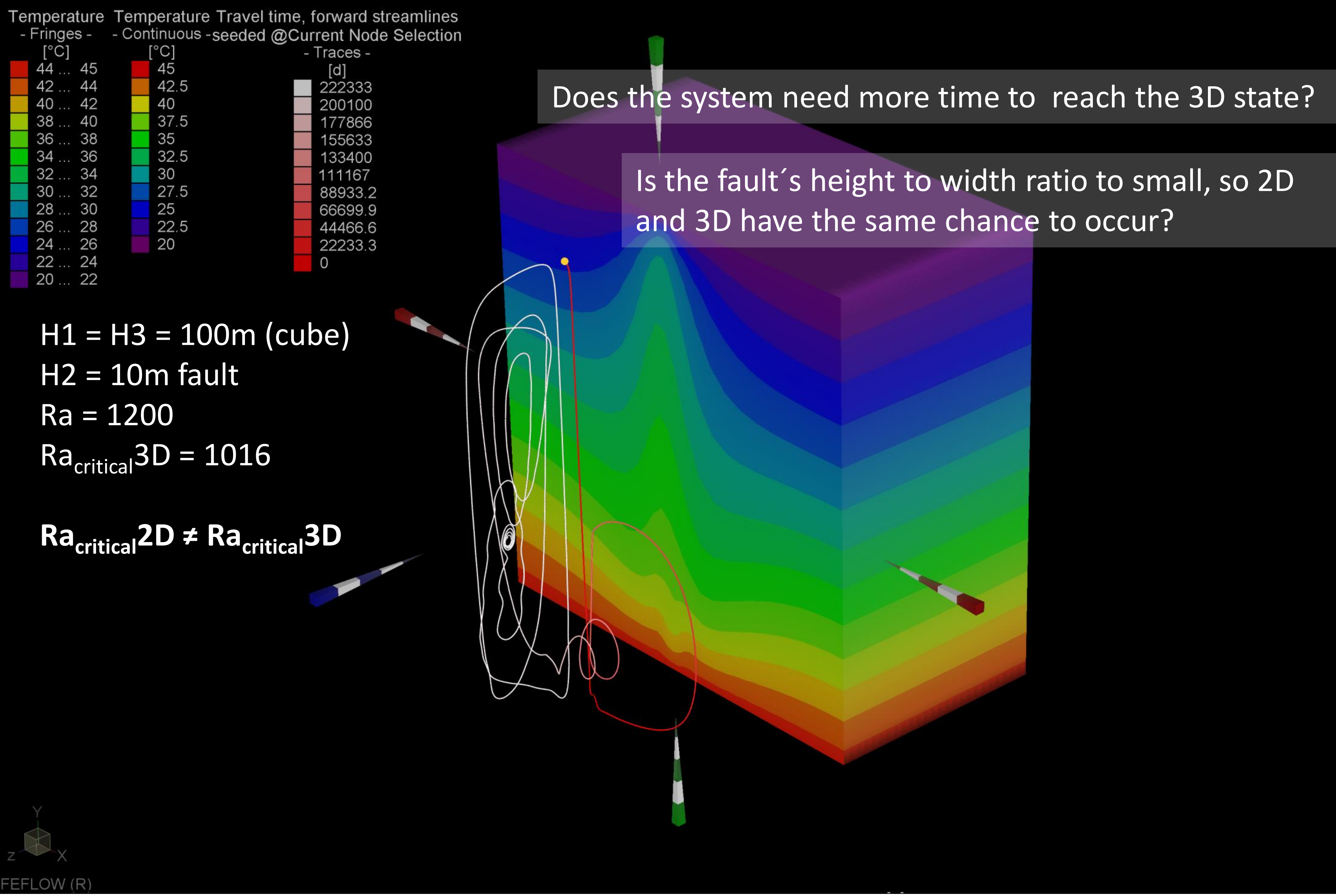
H1 = H3 = 100m (cube)

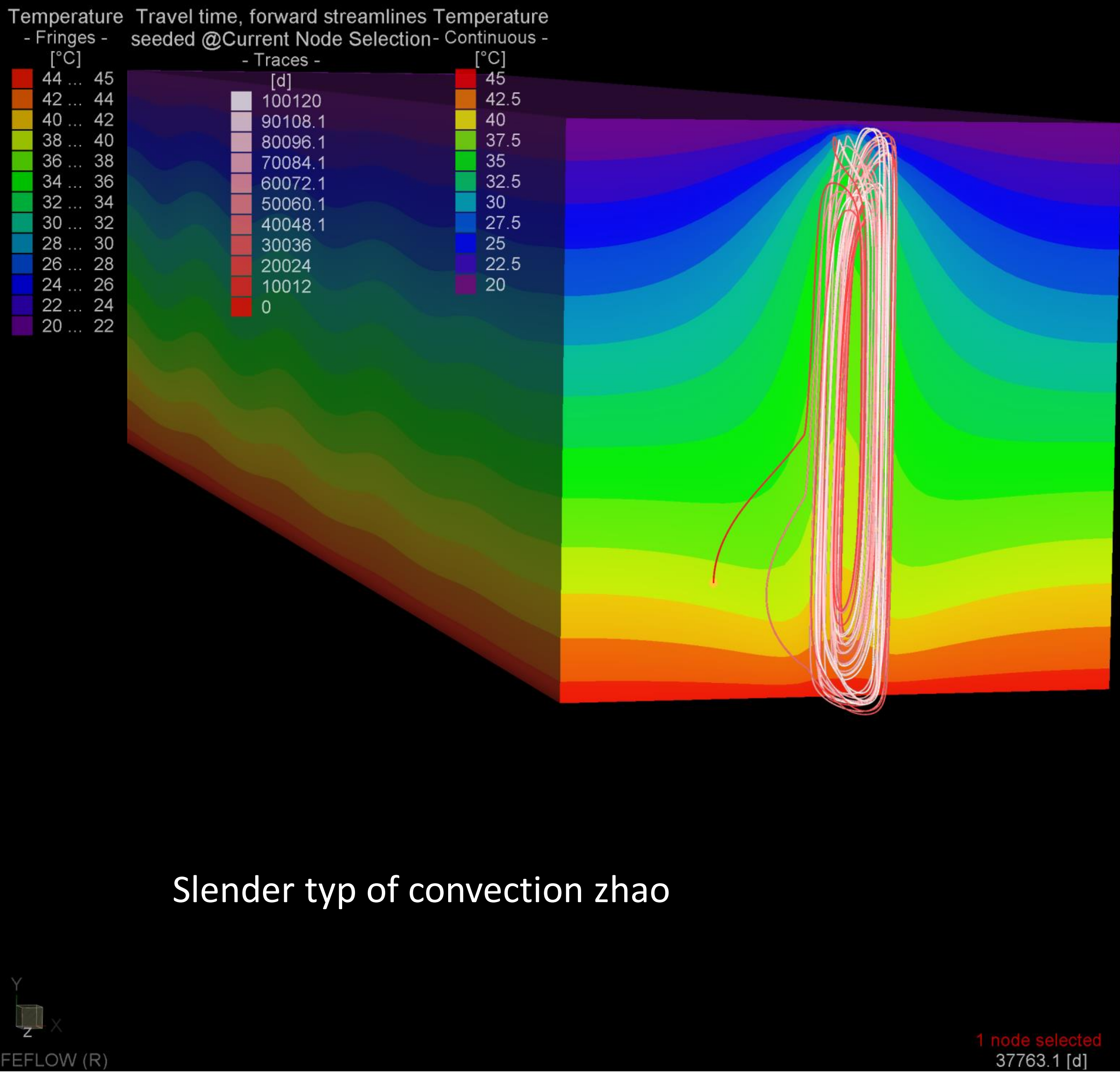
H2 = 10m fault

Ra = 1200

$Ra_{critical}3D = 1016$

$Ra_{critical}2D \neq Ra_{critical}3D$





H1 = 1000 m (length)

H2 = 10 m (fault)

H3 = 100 m (height)

Ra = 1200

$Ra_{critical}3D = 1016$

$Ra_{critical}2D = 1016$

$Ra_{critical}2D = Ra_{critical}3D$

Cause H1 tends to infinity

Slender typ of convection zhao