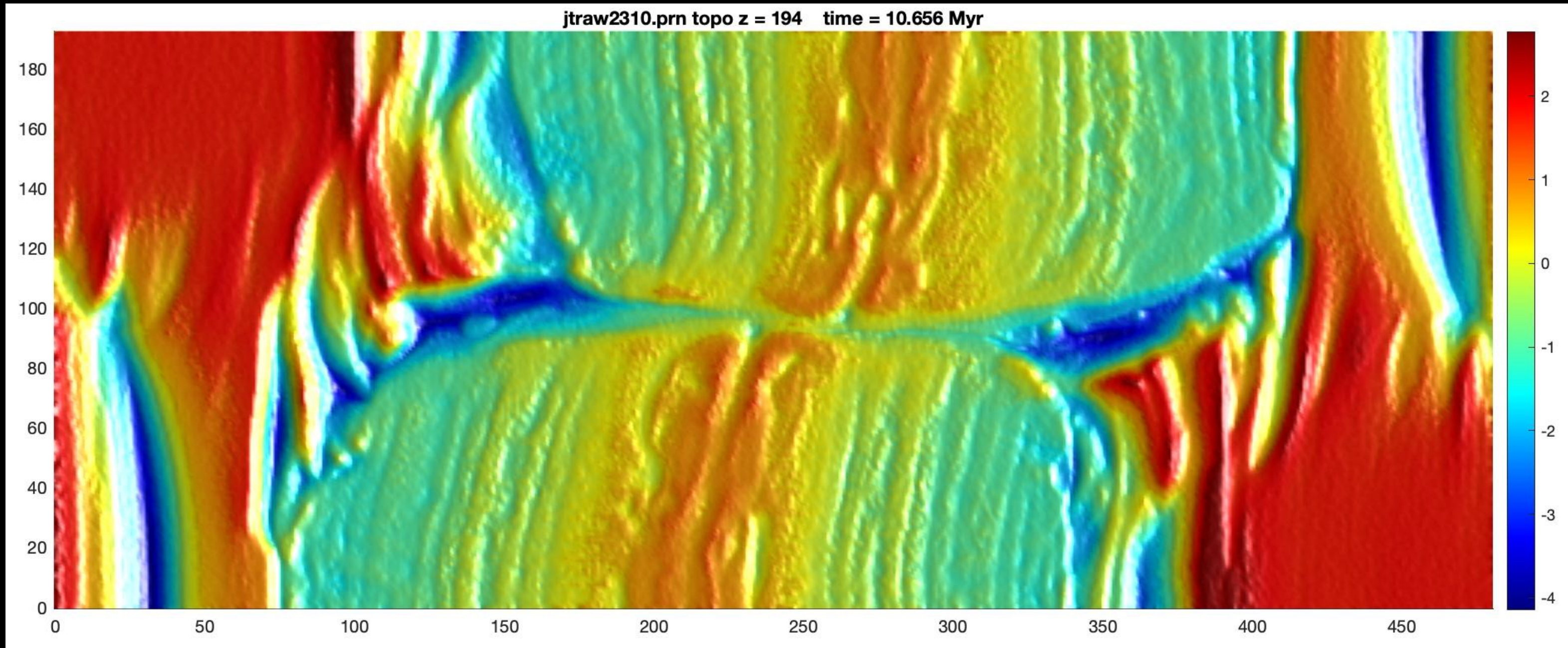
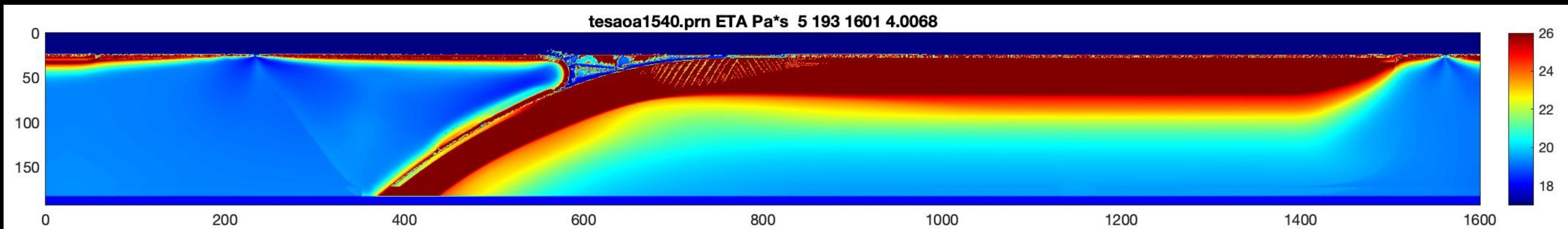
New I3ELVIS: Robust visco-elasto-plastic geodynamic modelling code based on staggered finite differences and marker in cell





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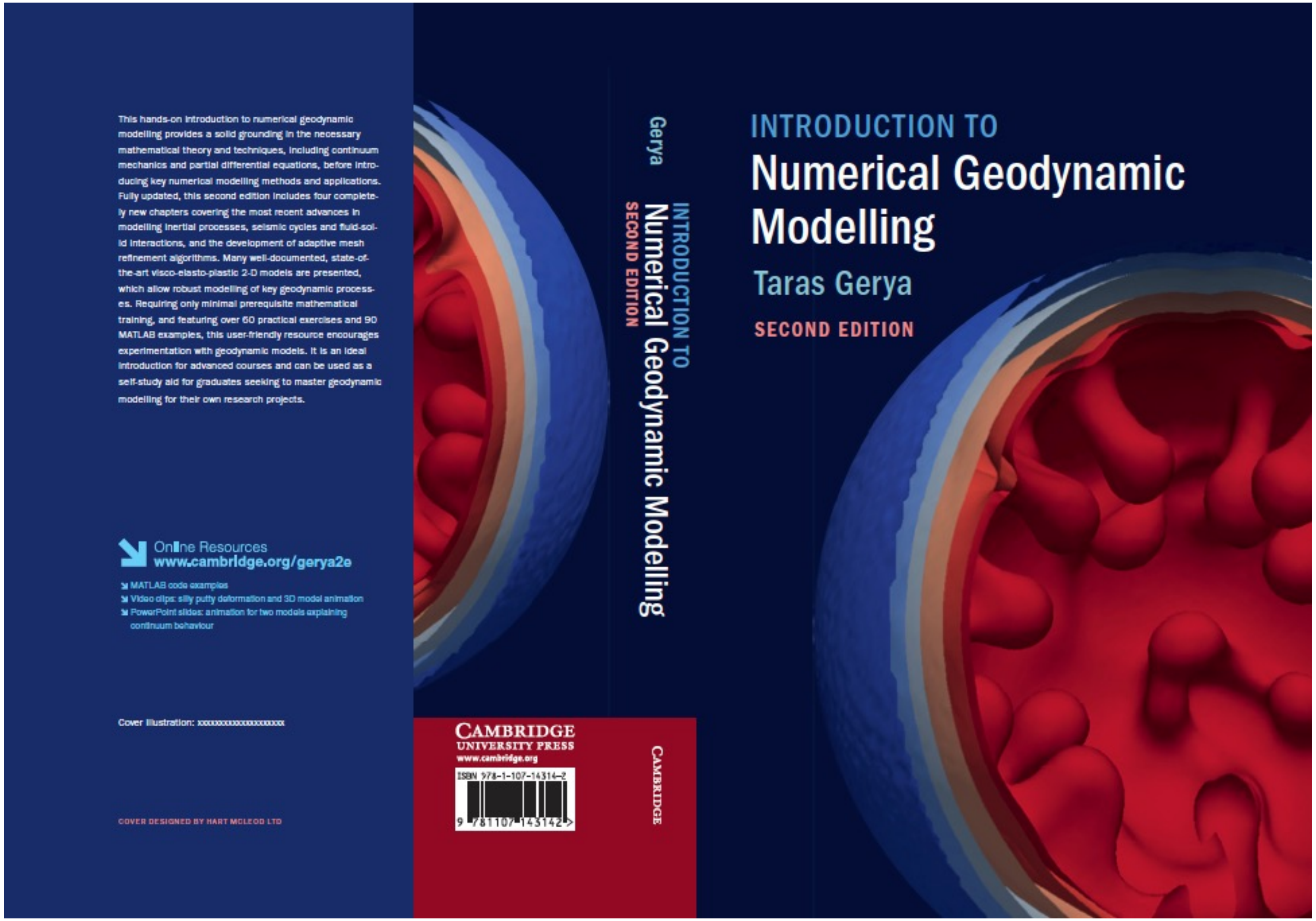
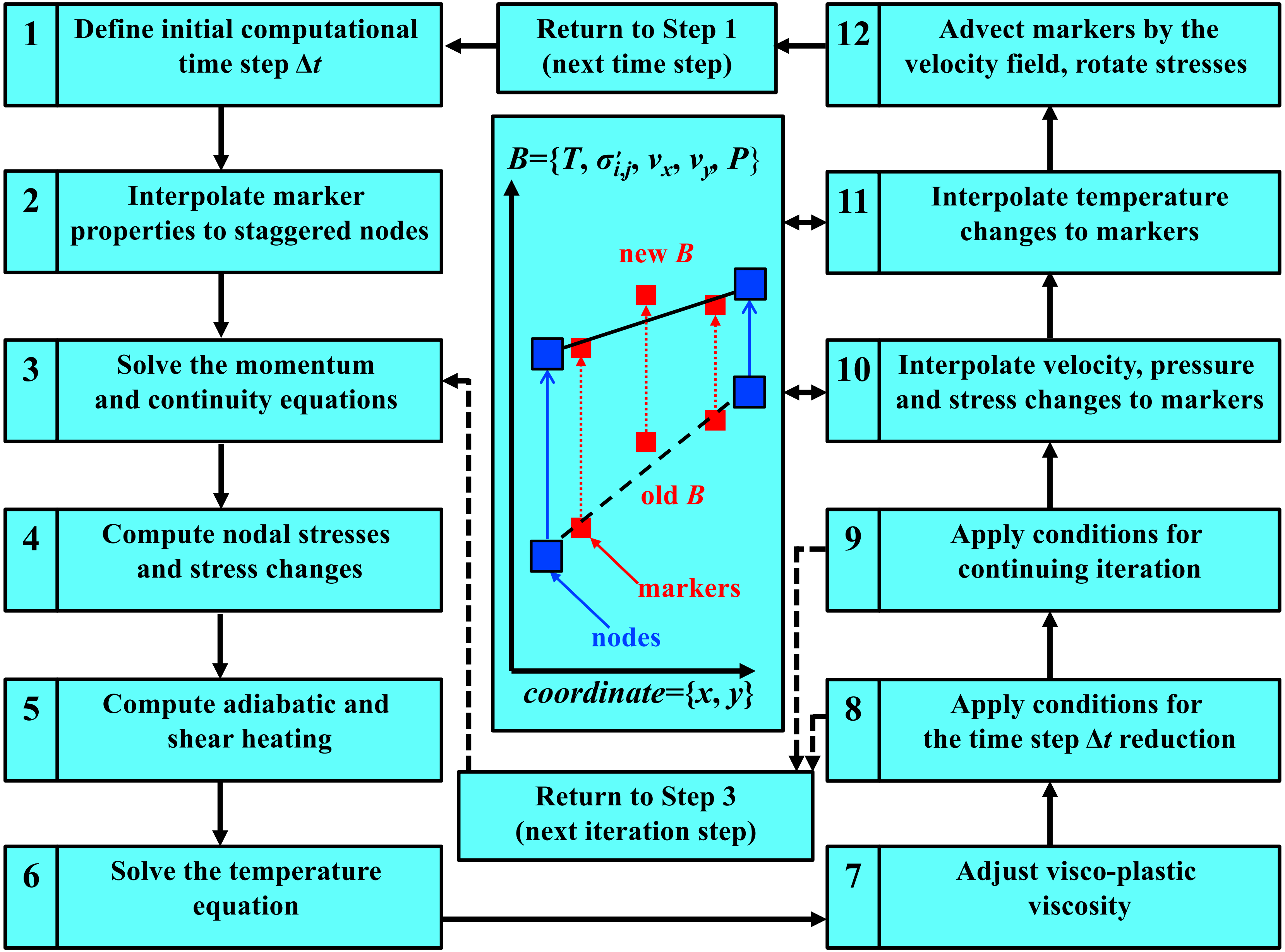
Institute of Geophysics, ETH Zurich

Part I

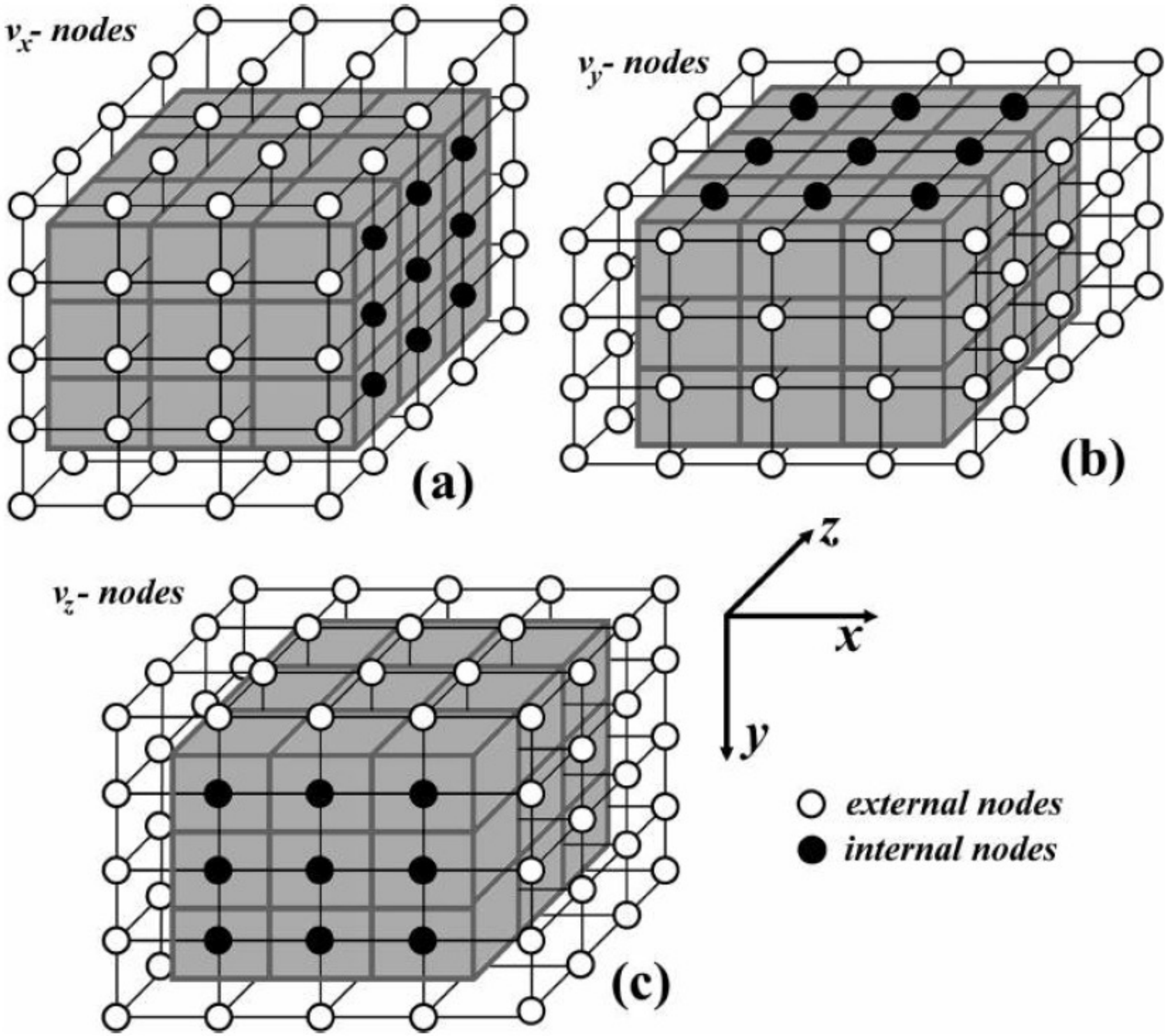
New I3ELVIS development based on own textbook...



New compressible visco-elasto-plastic I3ELVIS: What has been developed (in both C and MatLab)



1. Staggered grid with external velocity, pressure, temperature and stress nodes (temperature is in pressure nodes, not in basic nodes).



2. Fully coupled thermomechanical multigrid solver with global iterations
(non-linear feedbacks from shear and adiabatic heating and thermal expansion)

$$\mathrm{div}(\vec{v}) + \beta\frac{DP}{Dt} = \Gamma_{plastic} + \alpha\frac{DT}{Dt}, \qquad (14.3)$$

$$\alpha = -\frac{\partial \ln(\rho)}{\partial T}, \qquad (14.4)$$

$$\beta = \frac{\partial \ln(\rho)}{\partial P}, \qquad (14.5)$$

$$\rho C_P\frac{DT}{Dt} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + H_r + H_a + H_s, \qquad (14.6)$$

$$H_s = 2\sigma'_{xx}\dot{\varepsilon}'_{xx(visco\_plastic)} + 2\sigma'_{xy}\dot{\varepsilon}'_{xy(visco\_plastic)}, \qquad (14.7)$$

$$H_a = \alpha T\frac{DP}{Dt}. \qquad (14.8)$$

Dilatant plastic deformation

$$\Gamma_{plastic} = 2\sin(\psi)\dot{\varepsilon}_{\mathrm{II}(plastic)}$$

Regularised Kelvin plasticity model

Duretz et al. (2018)

$$\sigma_{yield} = \sigma_c + \gamma_{int}P + \eta_{reg}\,\dot{\varepsilon}_{\mathrm{II}(plastic)}$$

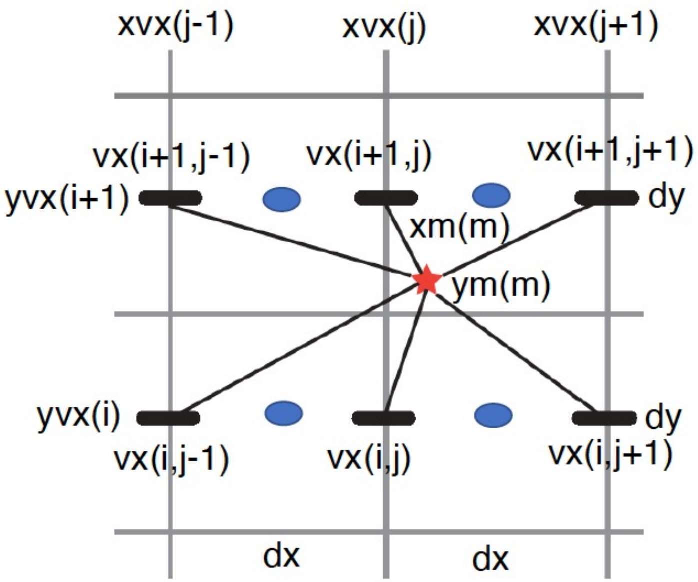
3. Continuity-based marker advection (***ultimate MQS advection scheme***).

The scheme guarantee bi-linear interpolation of dvx/dx and dvy/dy from pressure nodes where they are defined by solving (in)compressible continuity equation

Modified Quadratic Spline

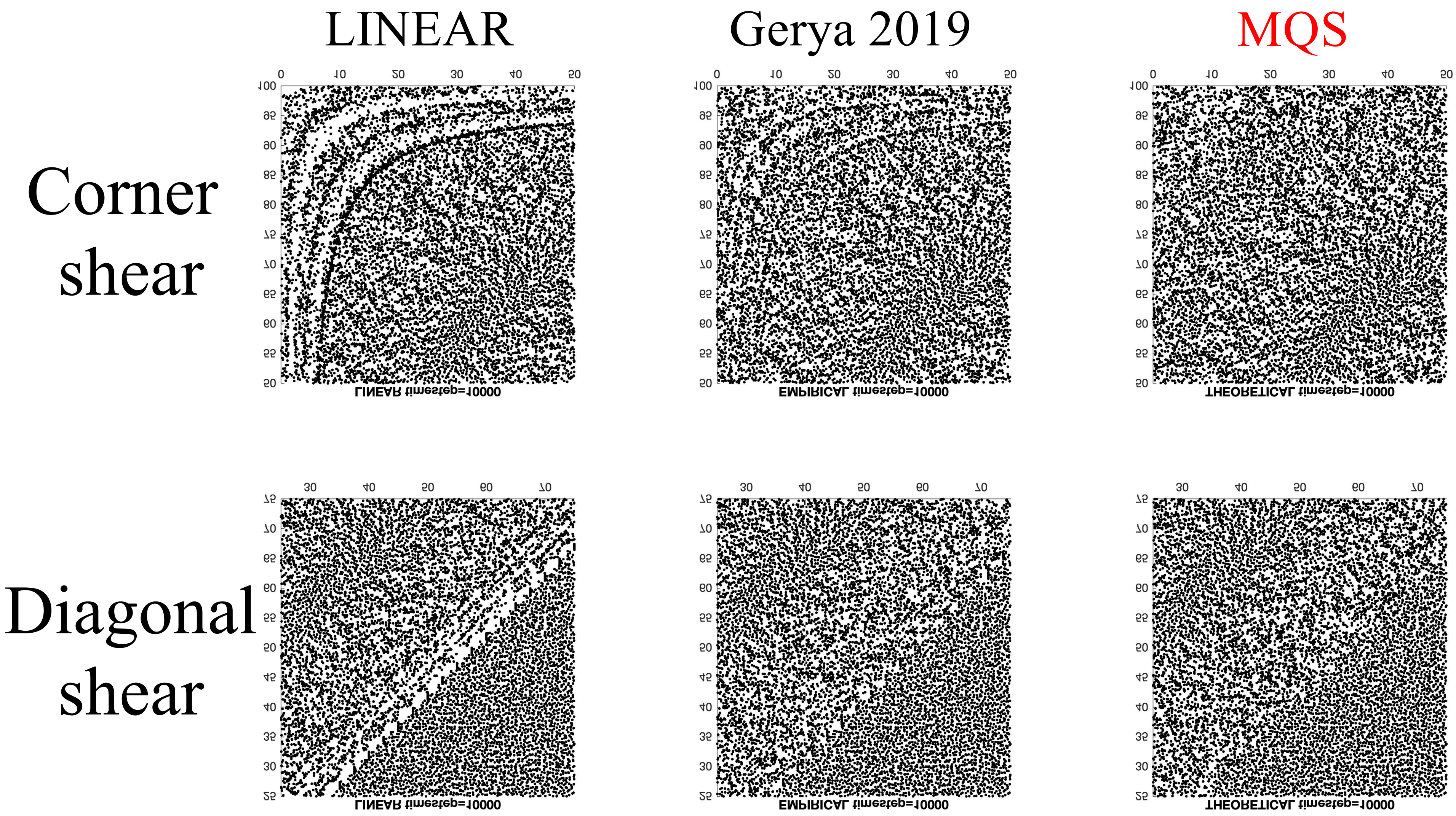
reproduces average velocity in pressure nodes but not in original velocity nodes

Example of vx interpolation for the regular staggered grid

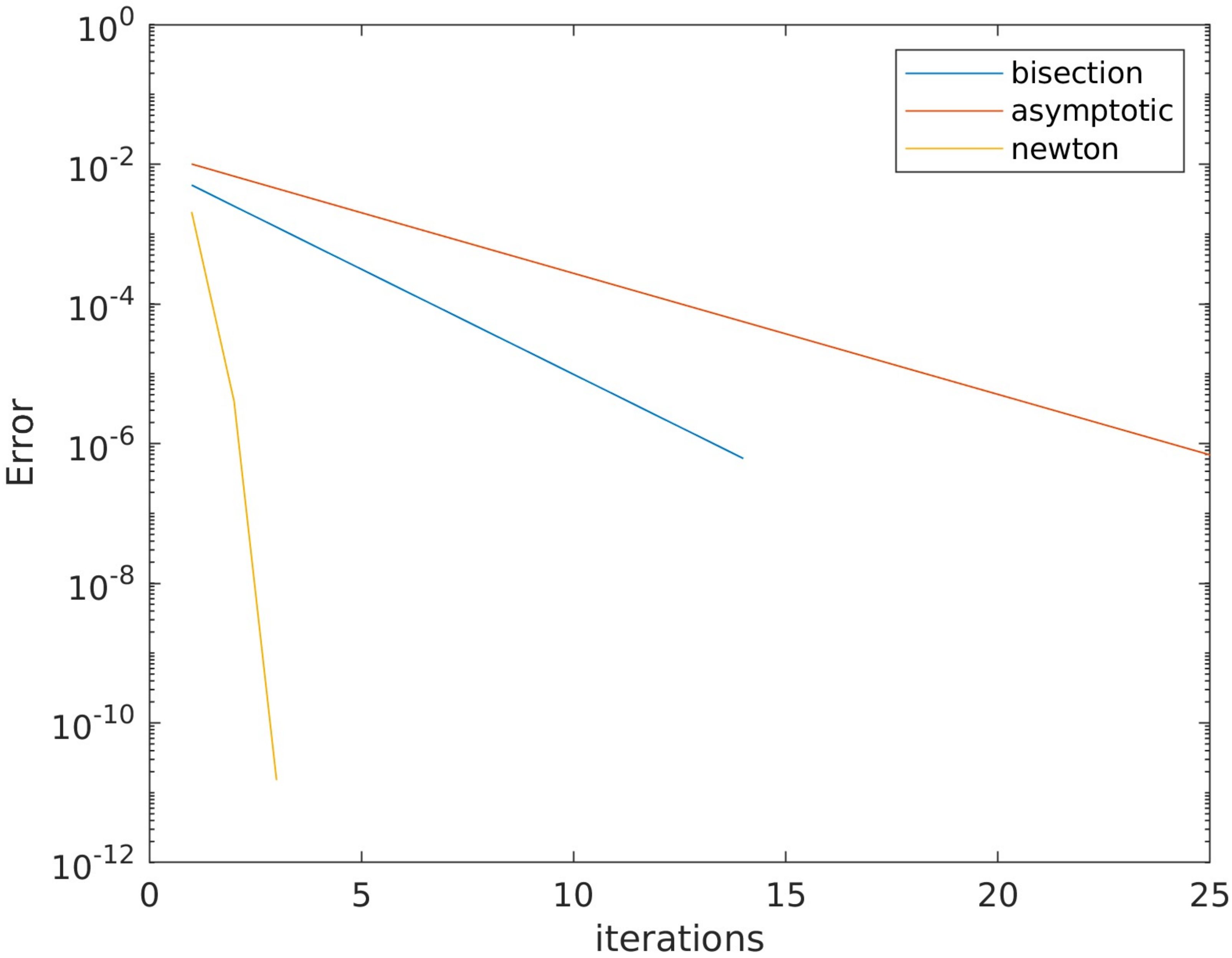



```
% Compute distances
dxmj=xm(m)-xvx(j);
dymi=ym(m)-yvx(i);
% Compute vx velocity with bi-linear scheme for the bottom and top
vxm13=vx(i,j)*(1-dxmj/dx)+vx(i,j+1)*dxmj/dx;
vxm24=vx(i+1,j)*(1-dxmj/dx)+vx(i+1,j+1)*dxmj/dx;
% Compute second order vx correction for the bottom and top
vxm13=vxm13+1/2*((dxmj/dx-0.5)^2)*(vx(i,j-1)-2*vx(i,j)+vx(i,j+1));
vxm24=vxm24+1/2*((dxmj/dx-0.5)^2)*(vx(i+1,j-1)-2*vx(i+1,j)+vx(i+1,j+1));
% Compute vx of the marker with bi-linear scheme in vertical direction
vxm=(1-dymi/dy)*vxm13+(dymi/dy)*vxm24;
```

3. Continuity-based marker advection (***ultimate MQS advection scheme***).



4. Newton iteration for dislocation creep to compute effective viscosity for markers



Luca Blum, 2018 (BSc Thesis)

5. Accurate 3D elastic stress rotation for markers

The 3D algorithm can then be summarized as follows (Popov et al., 2014a, personal communication).

(1) Compute the vorticity vector magnitude:

$$\omega_{mag} = \sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}\ . \tag{12.38}$$

(2) Compute the unit rotation vector $\vec{n}$, which also has three components:

$$n_x = \frac{\omega_x}{\omega_{mag}},\ n_y = \frac{\omega_y}{\omega_{mag}},\ n_z = \frac{\omega_z}{\omega_{mag}}. \tag{12.39}$$

(3) Integrate the incremental rotation angle:

$$\theta = \omega_{mag}\Delta t. \tag{12.40}$$

(4) Evaluate the rotation matrix using the Euler–Rodrigues formula:

$$R_{mat} = \cos(\theta)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \sin(\theta)\begin{pmatrix} 0 & -n_z & n_y \\ n_z & 0 & -n_x \\ -n_y & n_x & 0 \end{pmatrix} + \left(1 - \cos(\theta)\right)\begin{pmatrix} n_x n_x & n_x n_y & n_x n_z \\ n_y n_x & n_y n_y & n_y n_z \\ n_z n_x & n_z n_y & n_z n_z \end{pmatrix}. \tag{12.41}$$

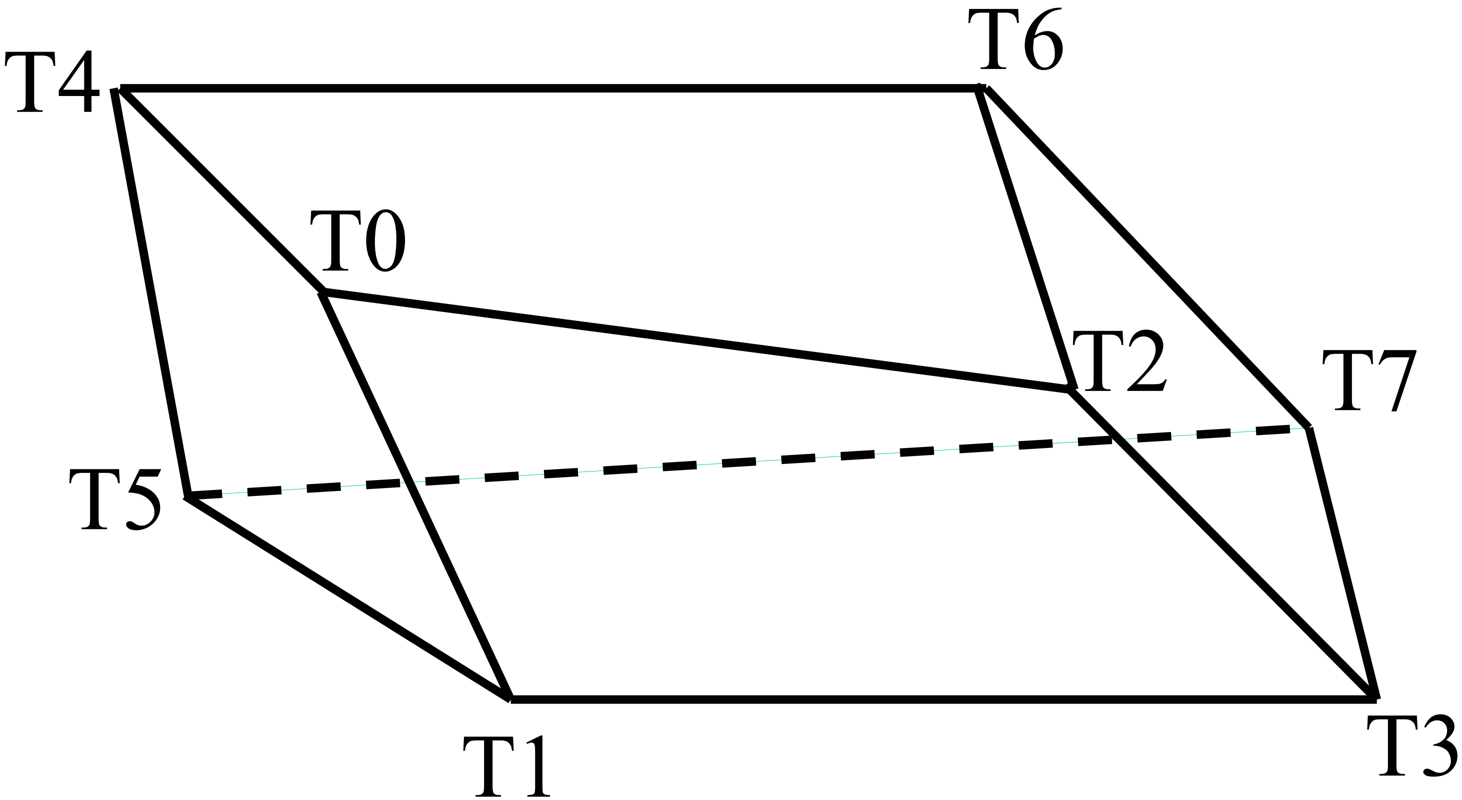
(5) Compute the rotated stress matrix by multiplying R_{mat}, σ' and $R_{mat}{}^T$ matrices:

$$\sigma'_{rotated} = R_{mat} \times \sigma' \times R_{mat}{}^T, \tag{12.42}$$

where $R_{mat}{}^T$ is the *transpose* of the matrix R_{mat} ($R_{mat}{}^T$ is obtained by reflecting the elements of the matrix R_{mat} along its main diagonal).

Anton Popov (personal communication)

6. Arbitrary shapes for thermal and material rectangles

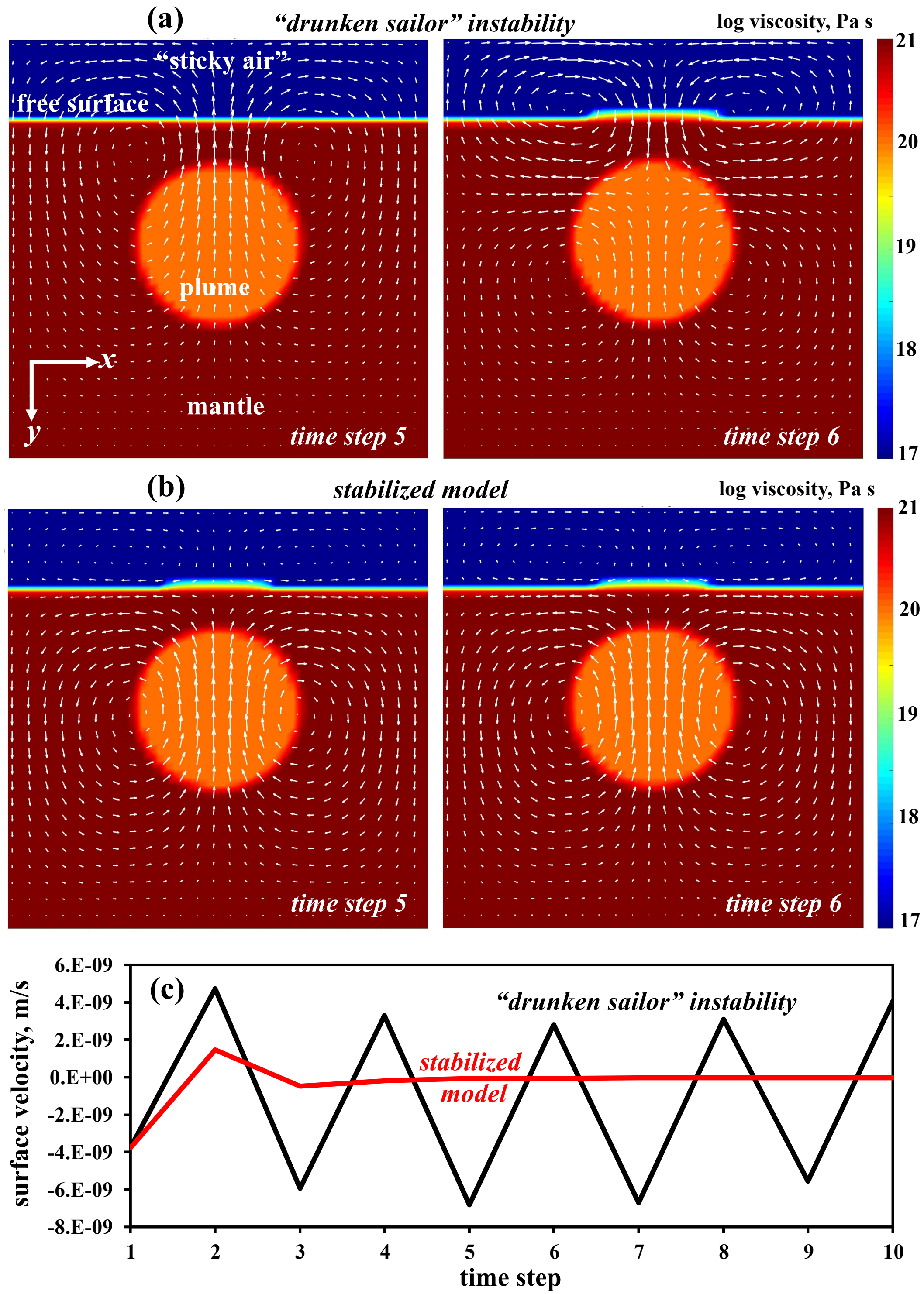


7. Free surface stabilization

$$\rho_{\Delta t} = \rho + \frac{\partial \rho}{\partial t}\Delta t = \rho - v_x \frac{\partial \rho}{\partial x}\Delta t - v_y \frac{\partial \rho}{\partial y}\Delta t,$$

$$\frac{\partial \sigma'_{yy}}{\partial y} + \frac{\partial \sigma'_{yx}}{\partial x} - \frac{\partial P}{\partial y} + \rho_{\Delta t} g_y = 0$$

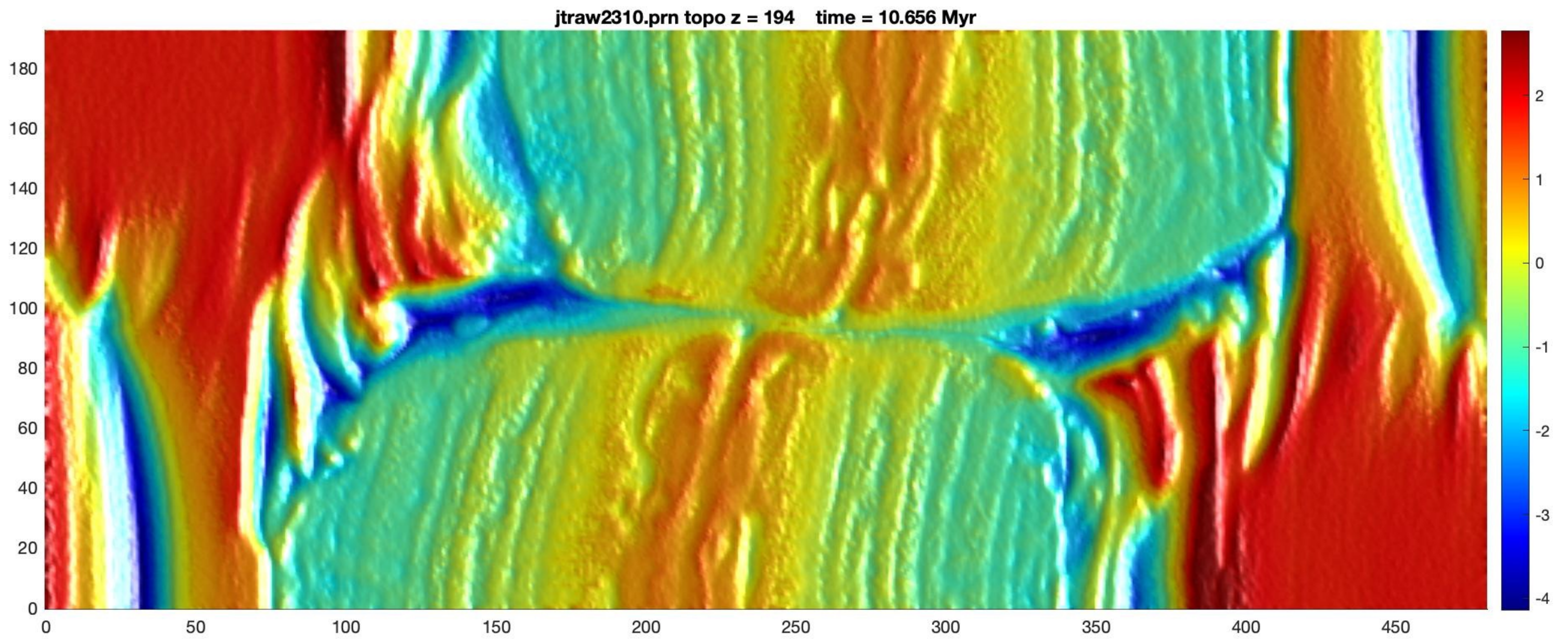
$$\frac{\partial \sigma'_{yy}}{\partial y} + \frac{\partial \sigma'_{yx}}{\partial x} - \frac{\partial P}{\partial y} - g_y \Delta t \left(v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} \right) = -\rho g_y$$



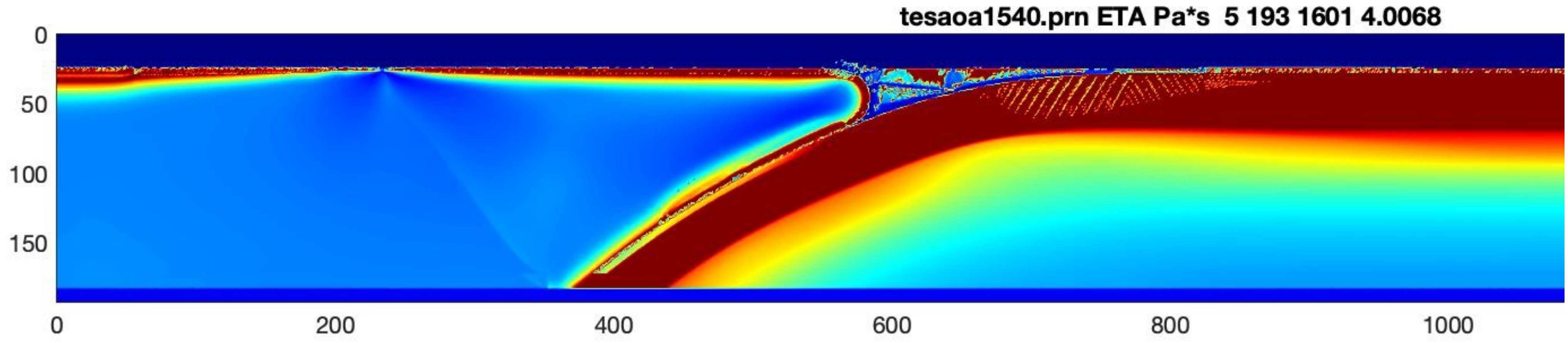
Part II

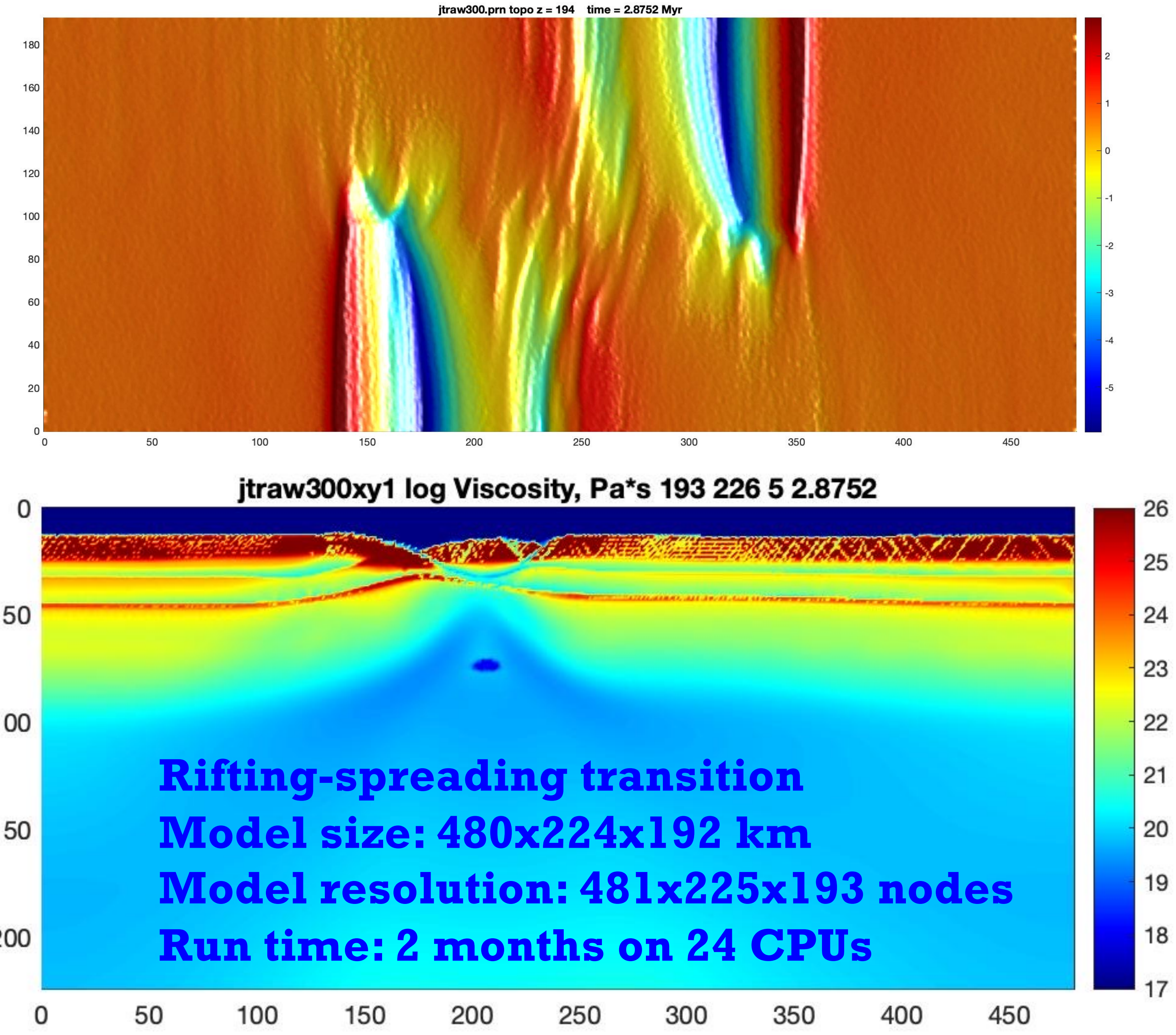
New I3ELVIS model examples:

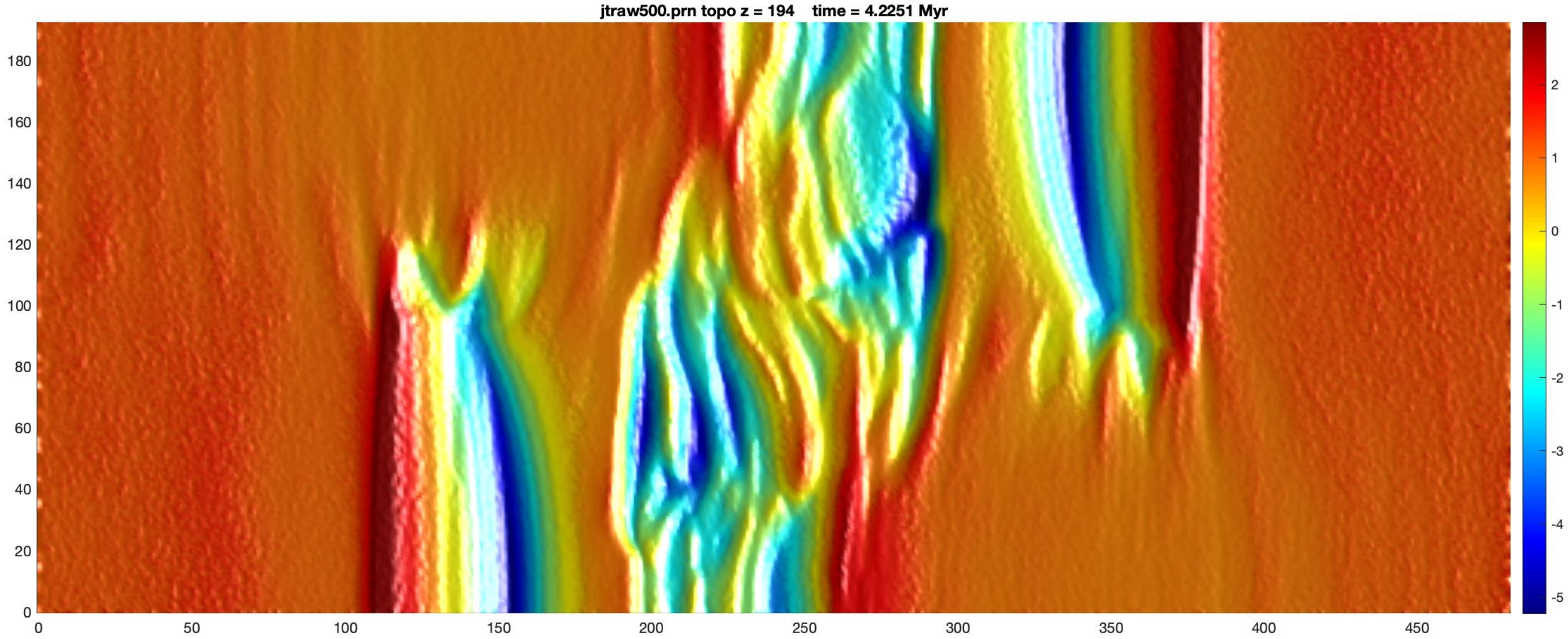
Rifting-spreading transition



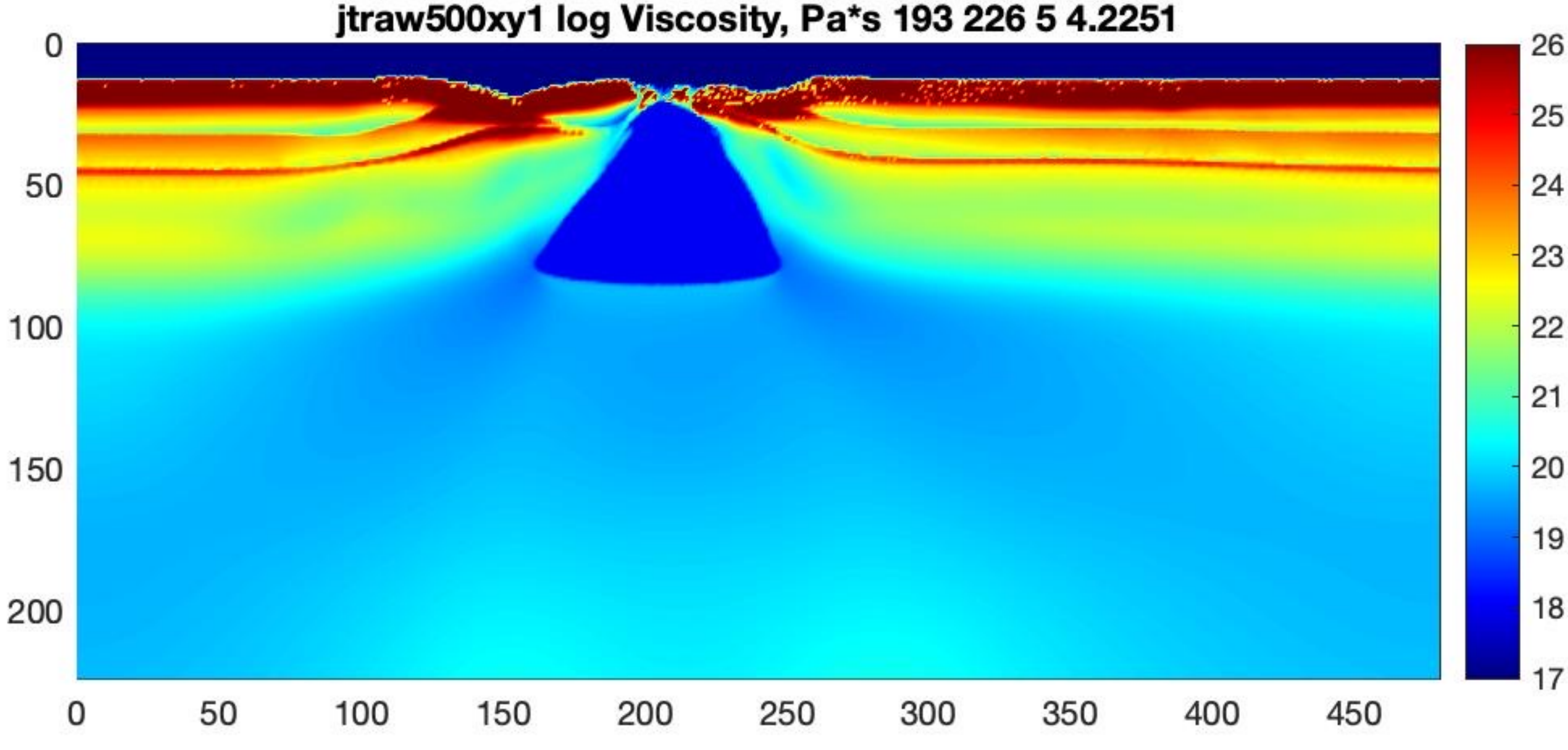
Subduction with grain damage



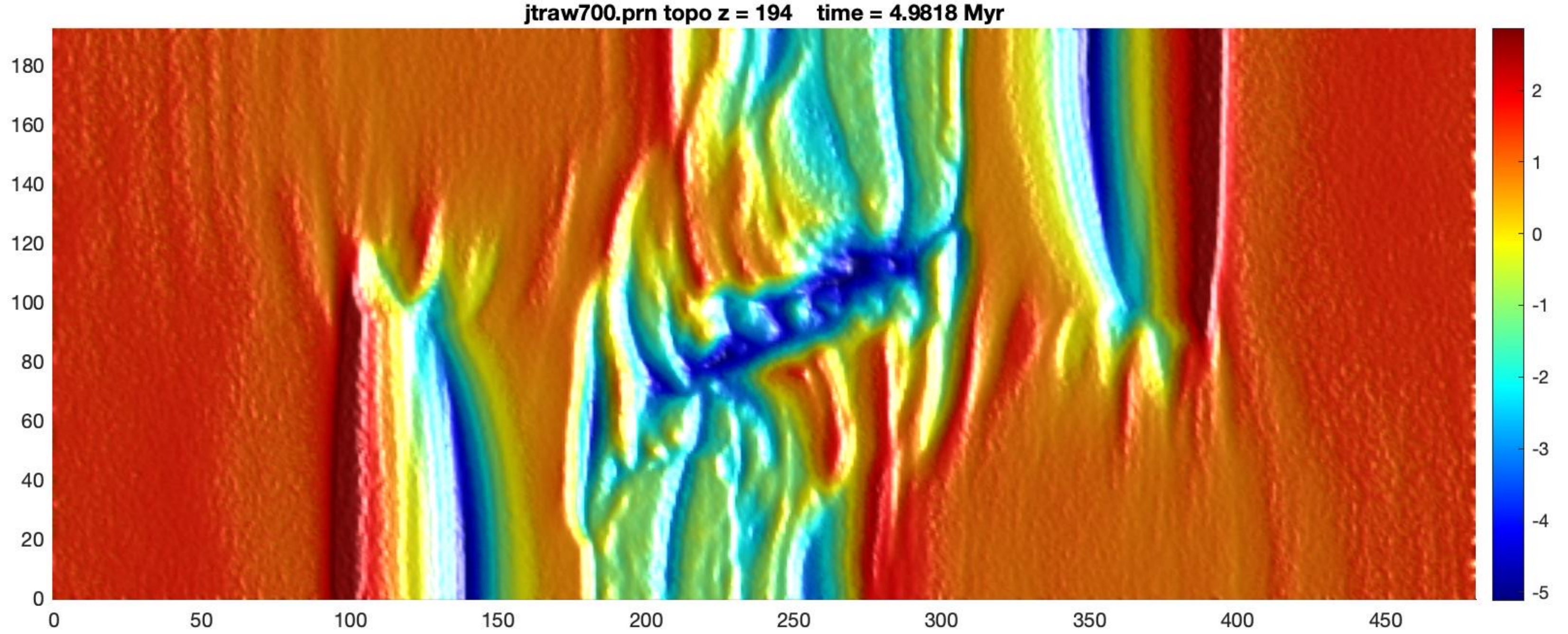

jtraw300.prn topo z = 194 time = 2.8752 Myr
jtraw300xy1 log Viscosity, Pa*s 193 226 5 2.8752
Rifting-spreading transition
Model size: 480x224x192 km
Model resolution: 481x225x193 nodes
Run time: 2 months on 24 CPUs

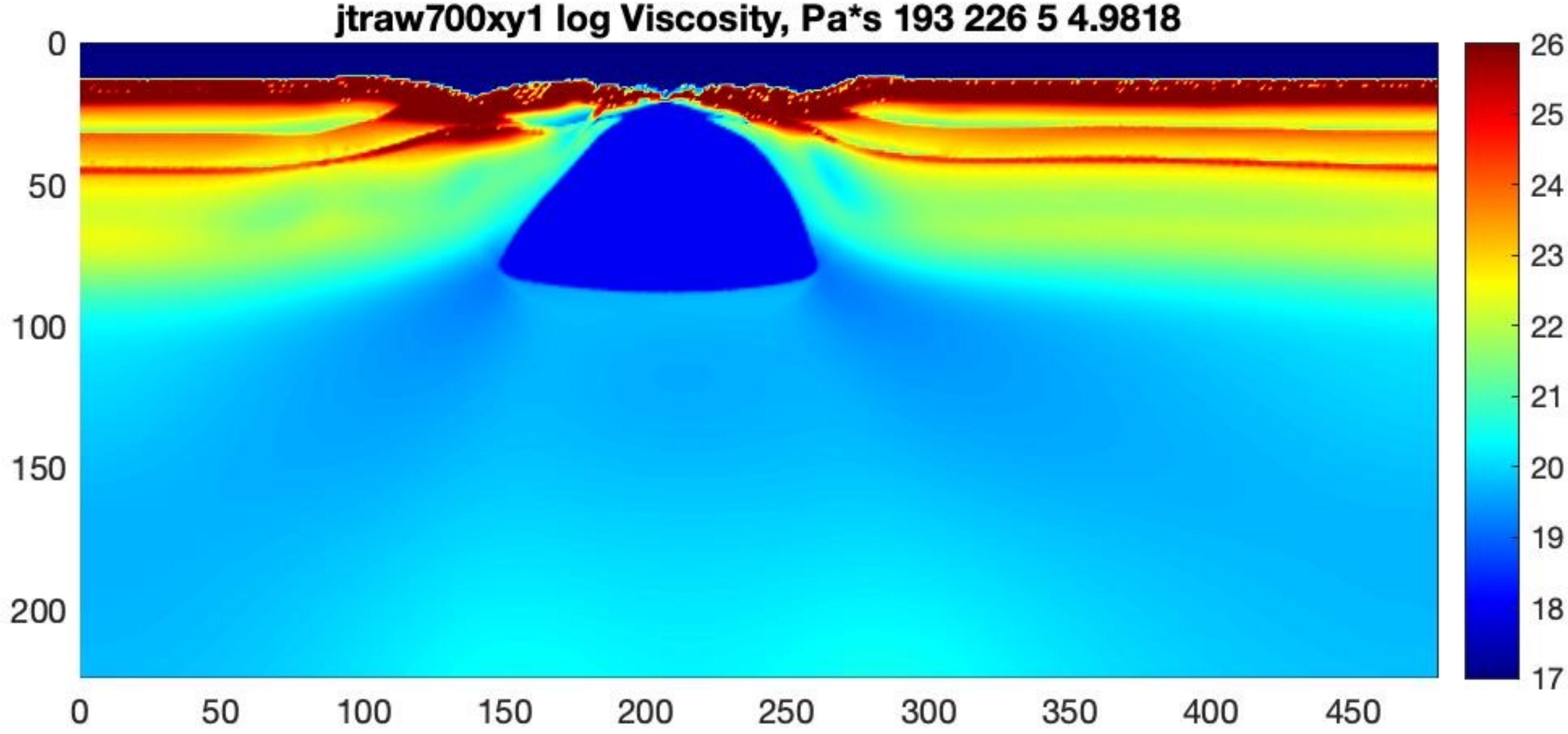


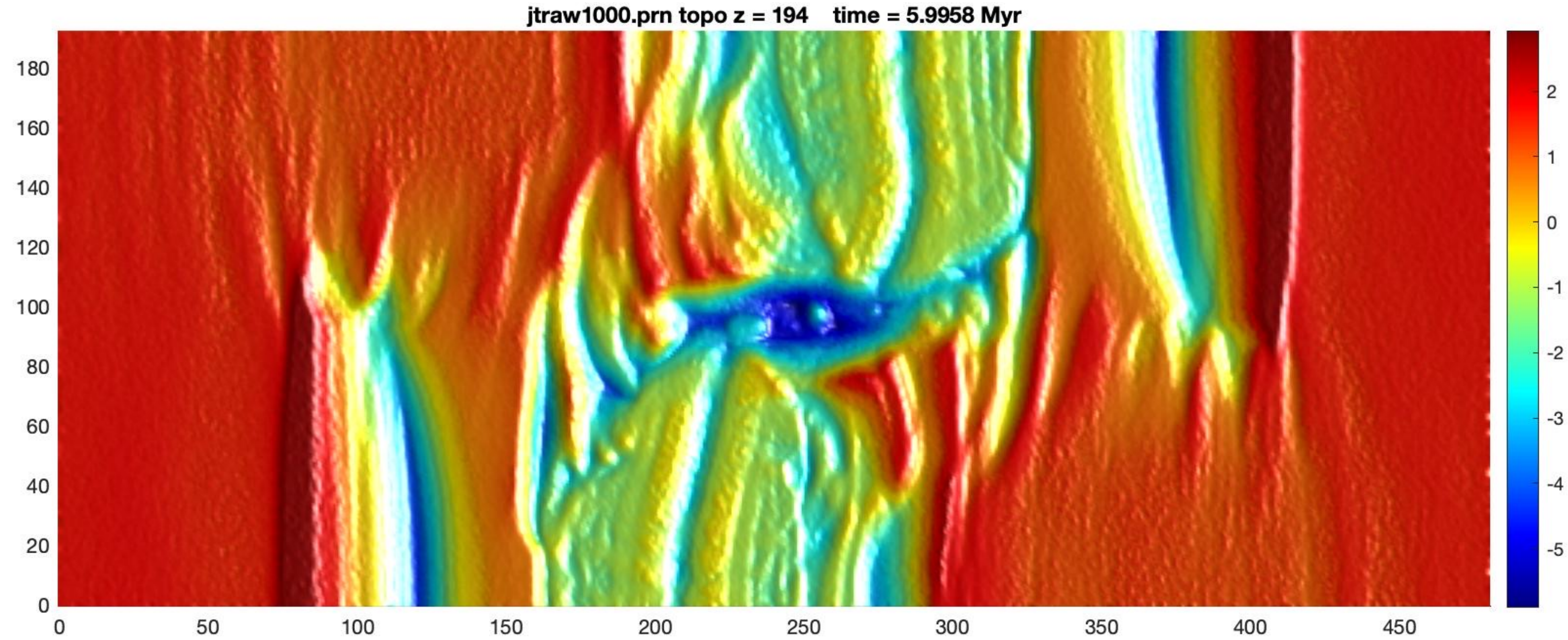
jtraw500.prn topo z = 194   time = 4.2251 Myr
180
160
140
120
100
80
60
40
20
0
0
50
100
150
200
250
300
350
400
450
2
1
0
-1
-2
-3
-4
-5



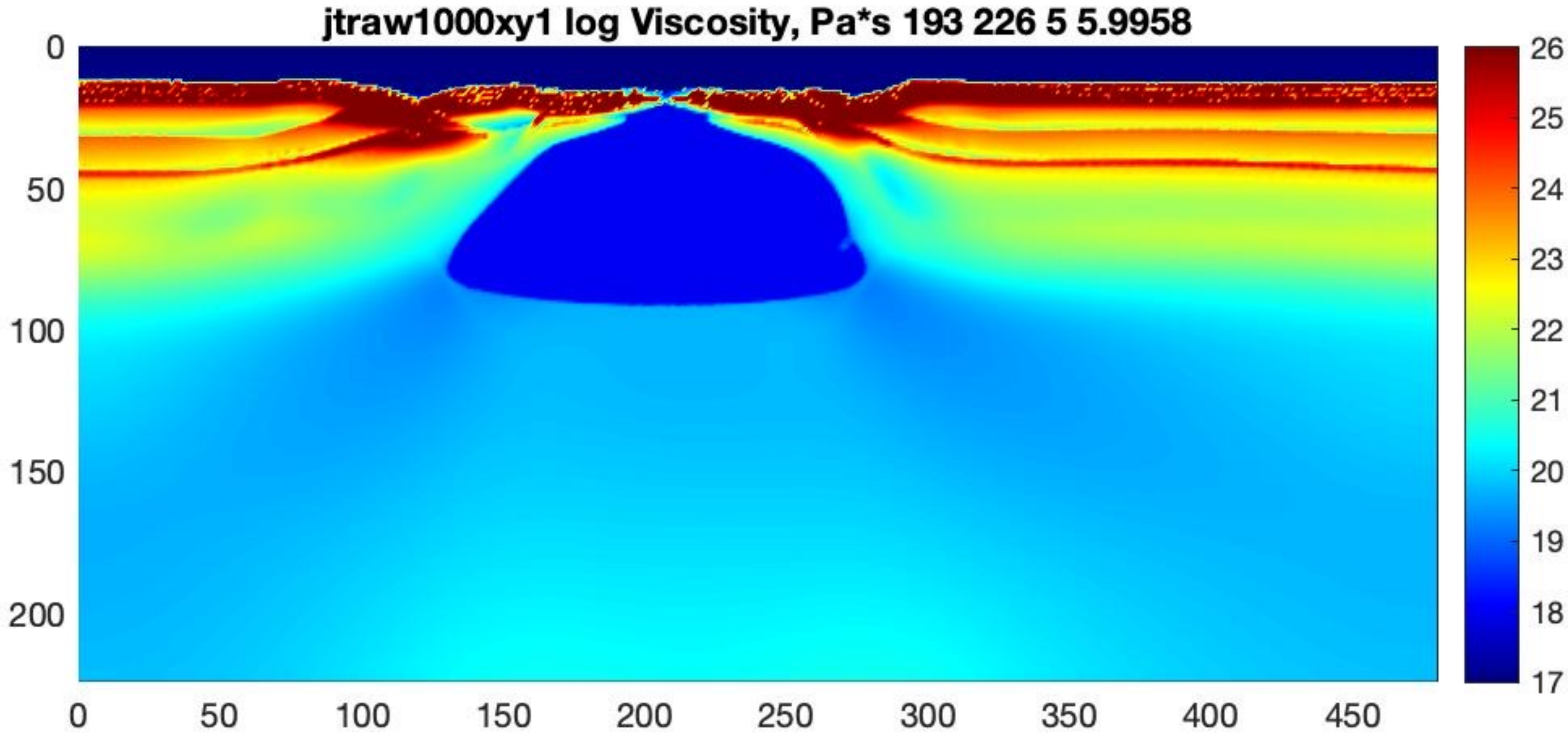
jtraw500xy1 log Viscosity, Pa*s 193 226 5 4.2251
0
50
100
150
200
0
50
100
150
200
250
300
350
400
450
26
25
24
23
22
21
20
19
18
17


jtraw700.prn topo z = 194   time = 4.9818 Myr
0 20 40 60 80 100 120 140 160 180
0 50 100 150 200 250 300 350 400 450
2 1 0 -1 -2 -3 -4 -5

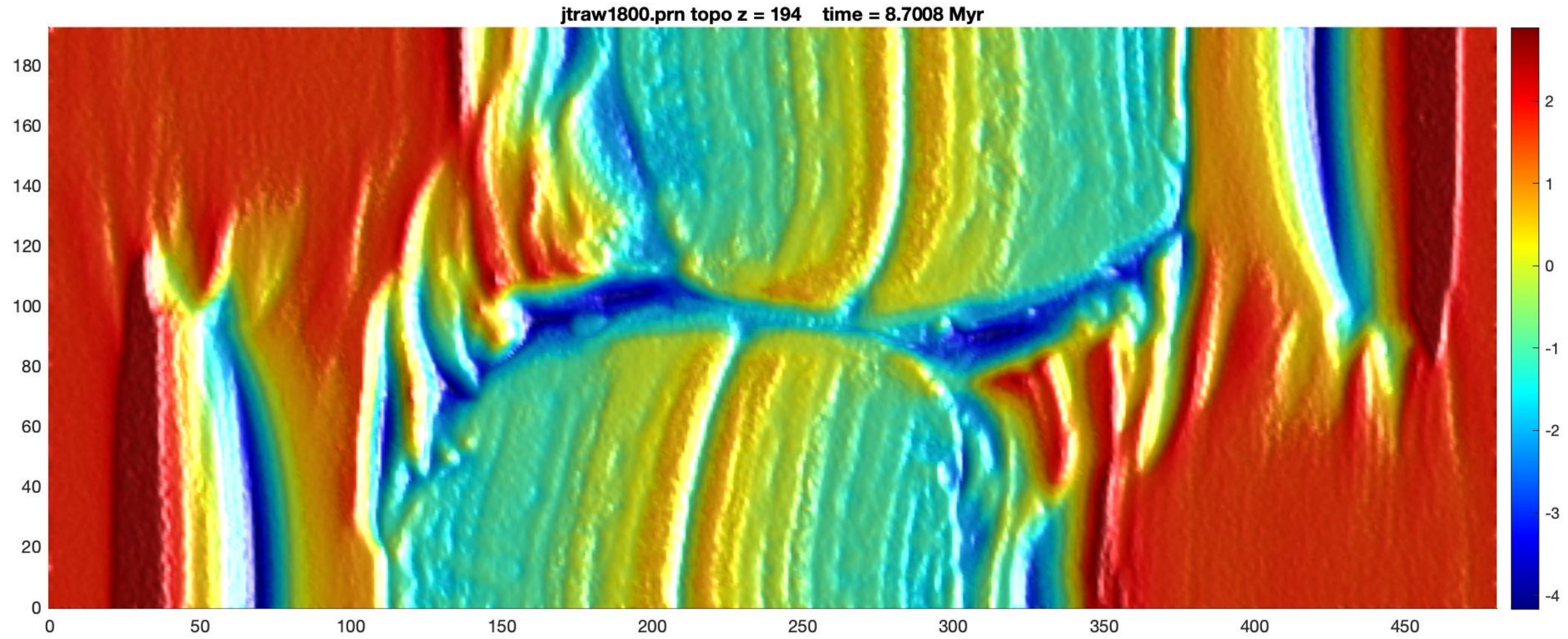

jtraw700xy1 log Viscosity, Pa*s 193 226 5 4.9818
0 50 100 150 200
0 50 100 150 200 250 300 350 400 450
26 25 24 23 22 21 20 19 18 17

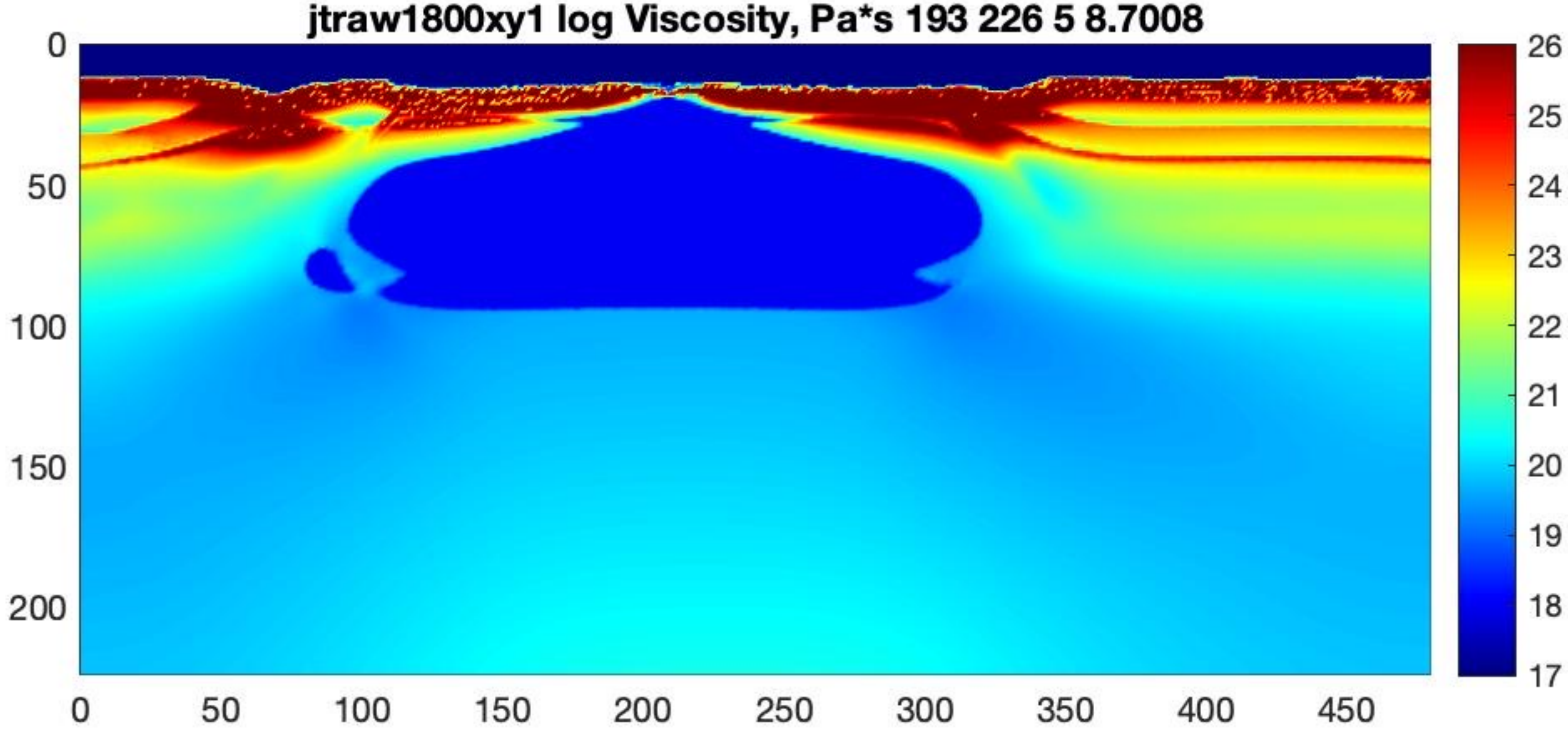


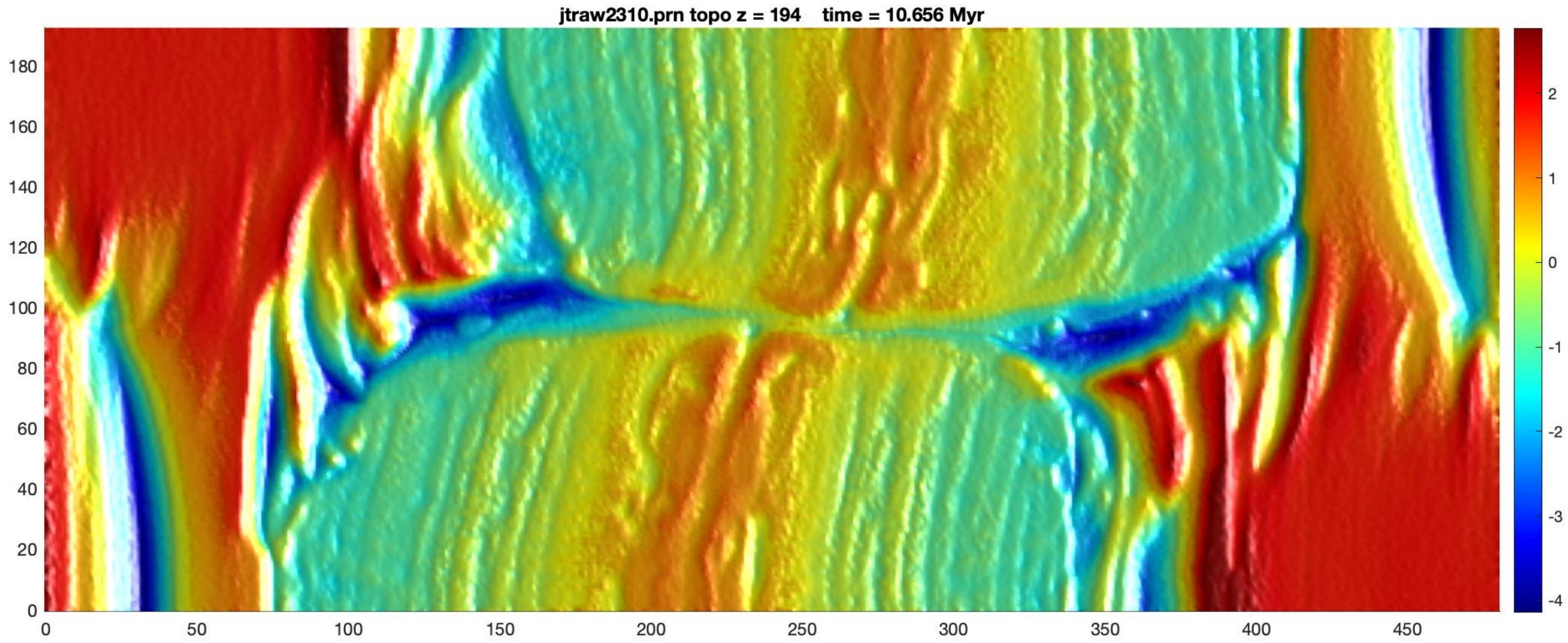
jtraw1000.prn topo z = 194   time = 5.9958 Myr

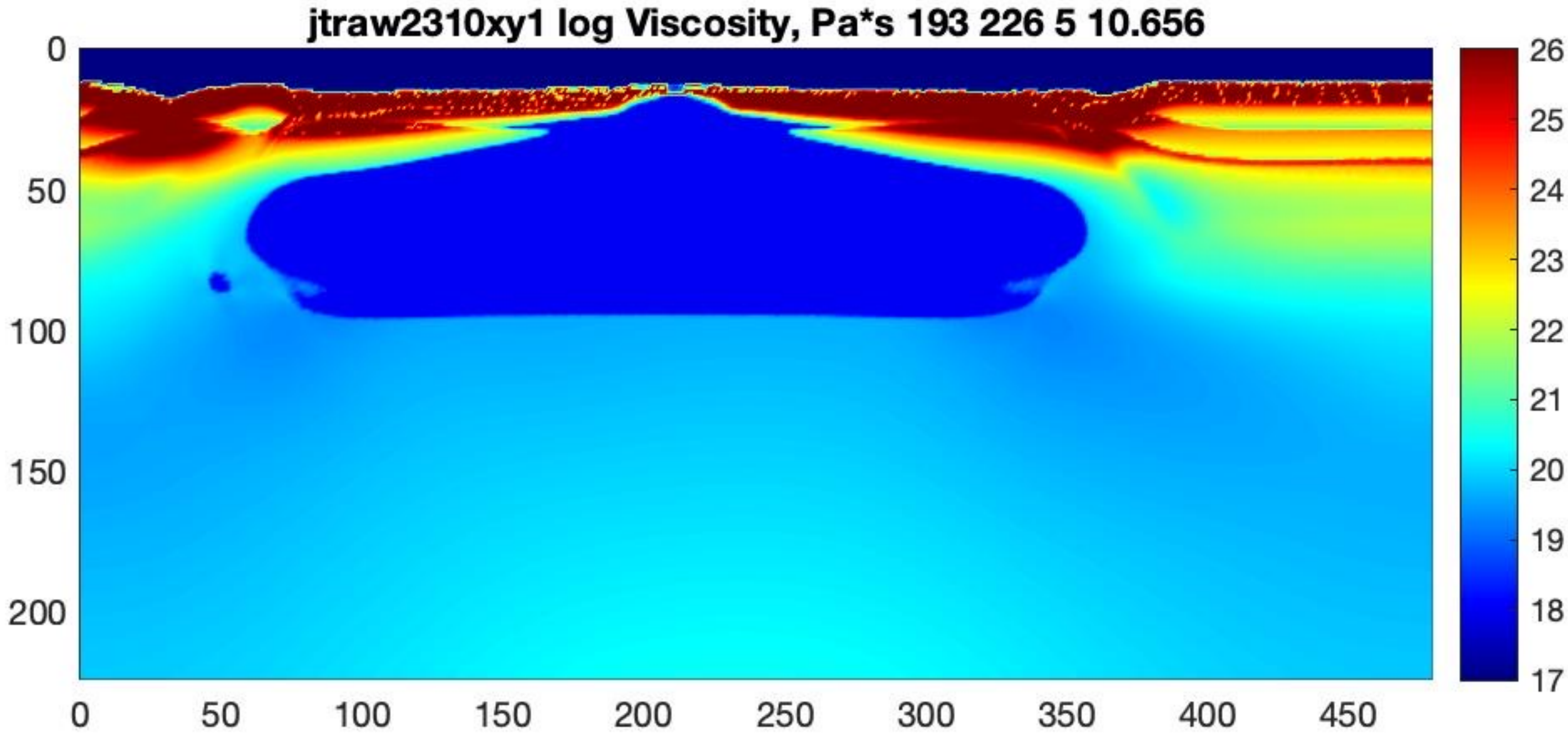


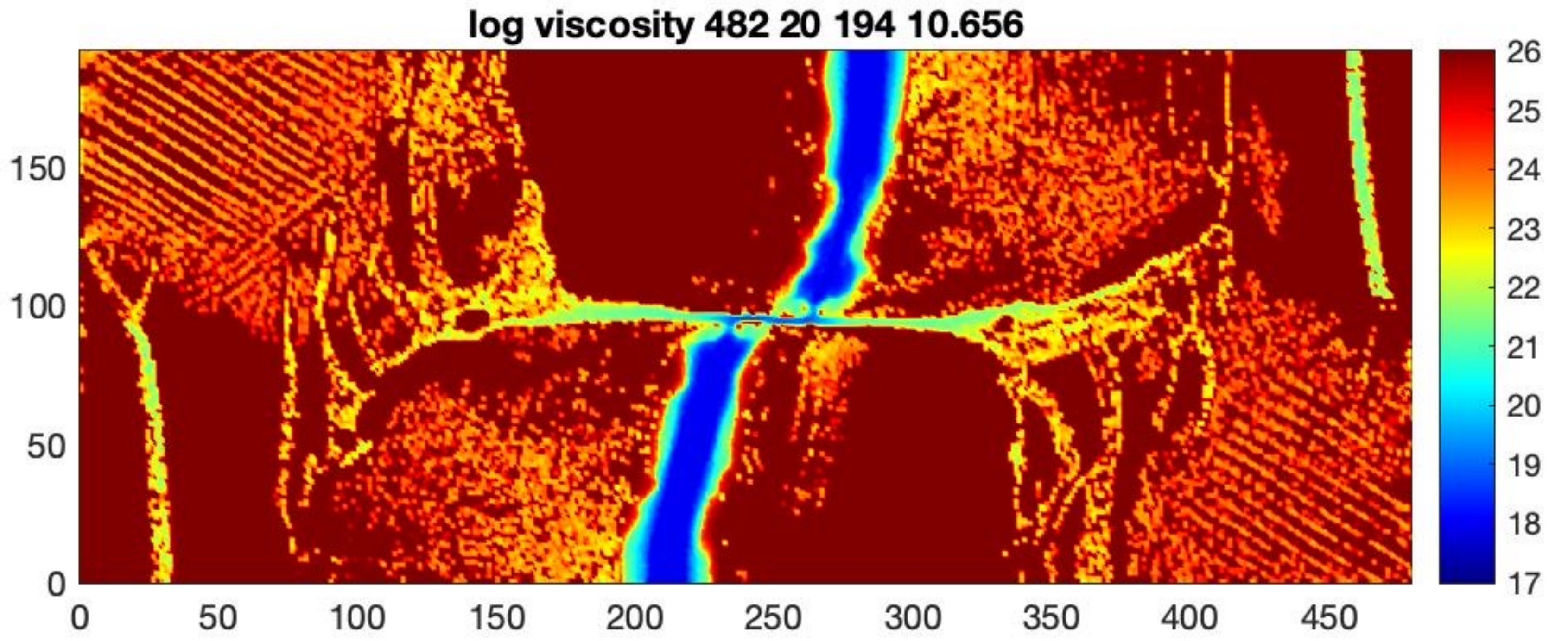
jtraw1000xy1 log Viscosity, Pa*s 193 226 5 5.9958

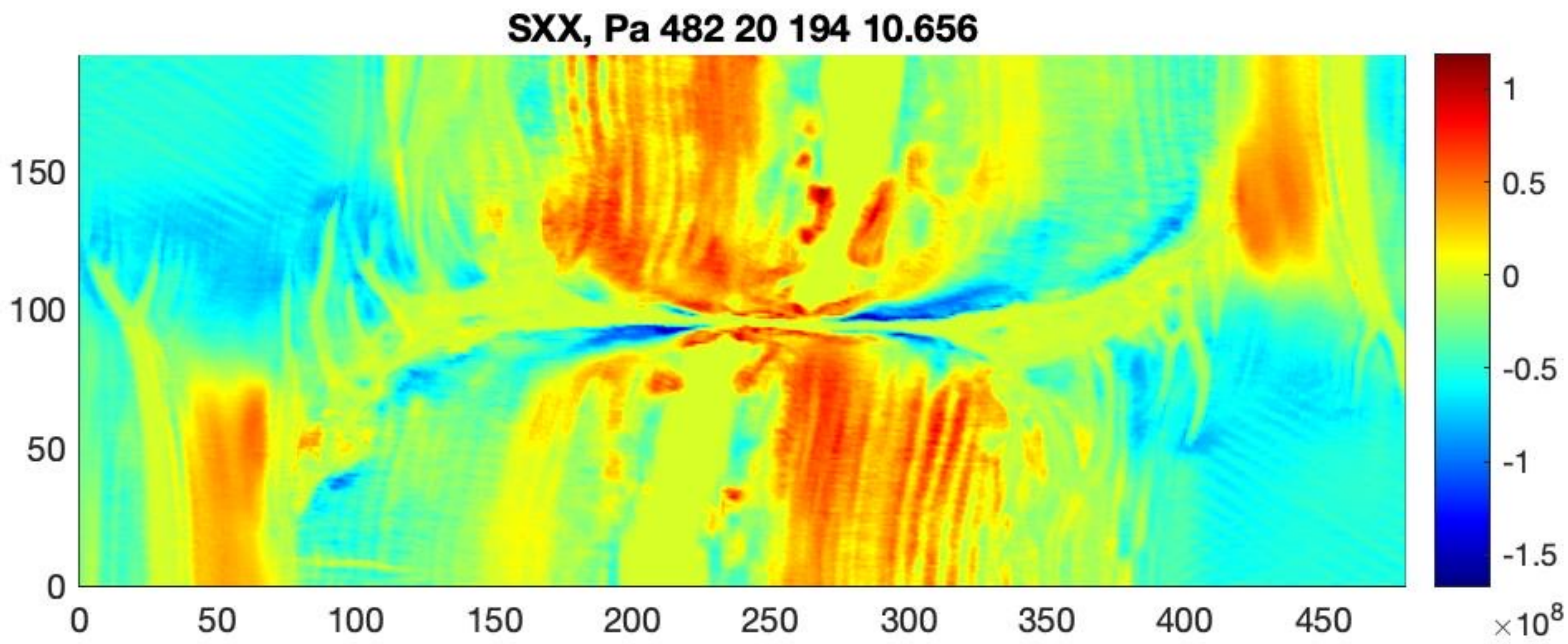

jtraw1800.prn topo z = 194   time = 8.7008 Myr
0
20
40
60
80
100
120
140
160
180
0
50
100
150
200
250
300
350
400
450
2
1
0
-1
-2
-3
-4


jtraw1800xy1 log Viscosity, Pa*s 193 226 5 8.7008
0
50
100
150
200
0
50
100
150
200
250
300
350
400
450
26
25
24
23
22
21
20
19
18
17

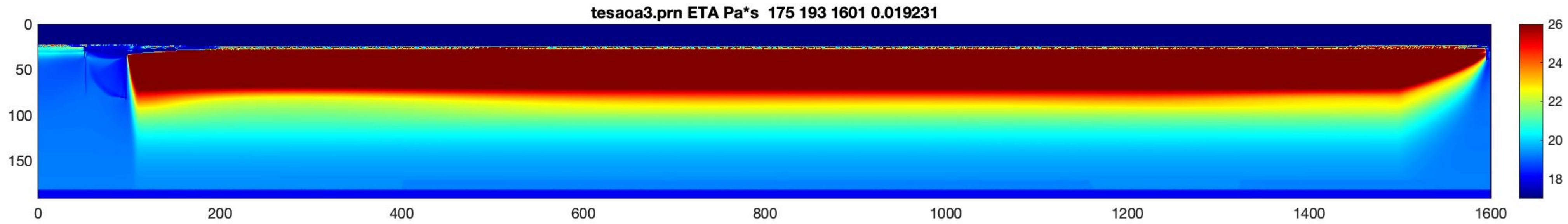

jtraw2310.prn topo z = 194   time = 10.656 Myr
0
20
40
60
80
100
120
140
160
180
0
50
100
150
200
250
300
350
400
450
2
1
0
-1
-2
-3
-4

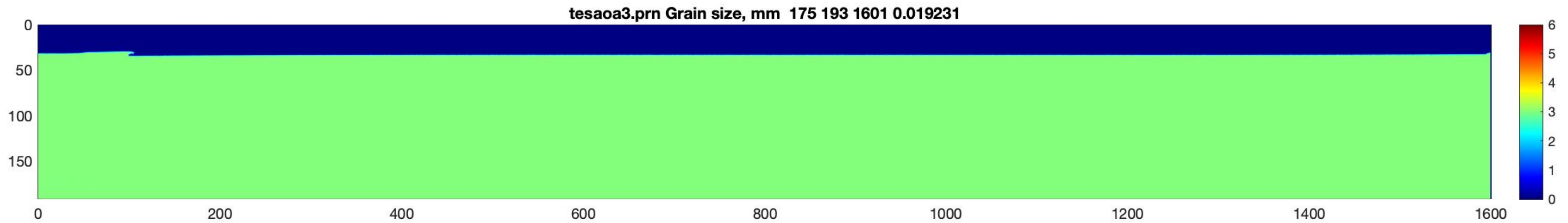

jtraw2310xy1 log Viscosity, Pa*s 193 226 5 10.656
0
50
100
150
200
0
50
100
150
200
250
300
350
400
450
26
25
24
23
22
21
20
19
18
17


log viscosity 482 20 194 10.656
0
50
100
150
200
250
300
350
400
450
26
25
24
23
22
21
20
19
18
17


SXX, Pa 482 20 194 10.656
0
50
100
150
200
250
300
350
400
450
1
0.5
0
-0.5
-1
-1.5
×10^8

Subduction with grain damage

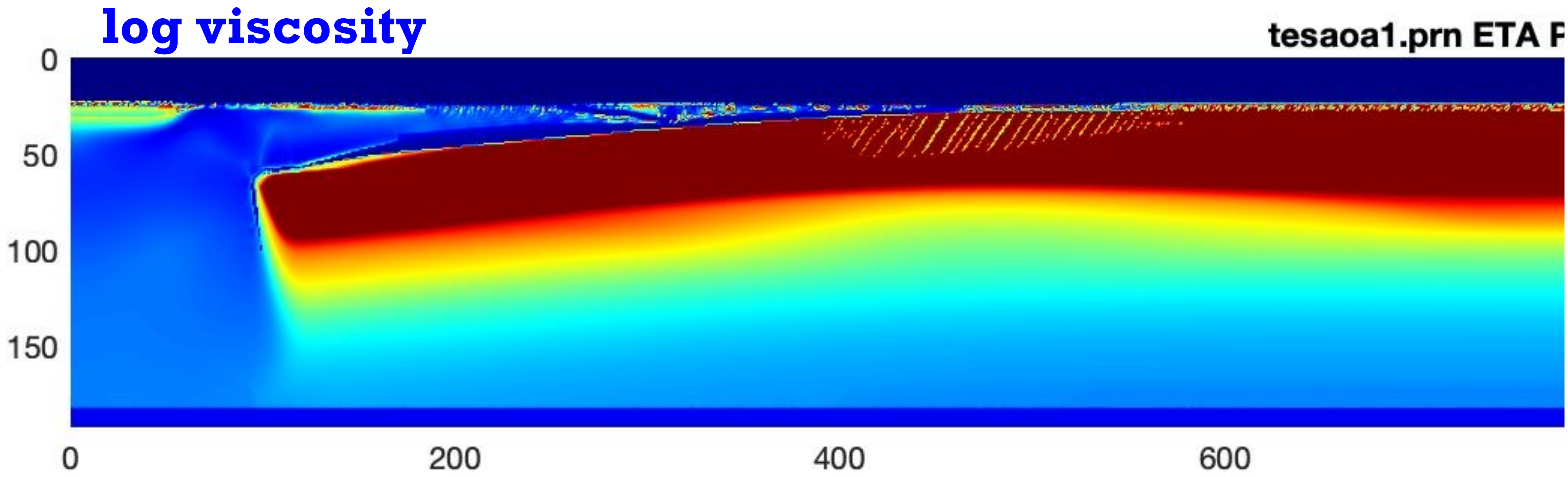


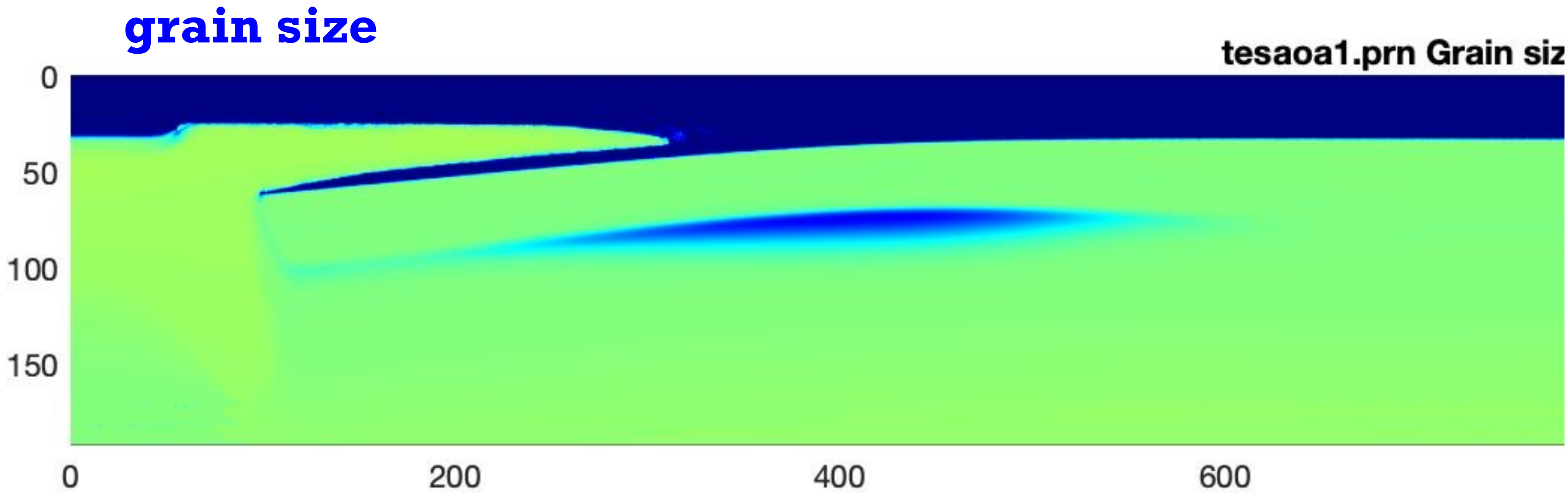


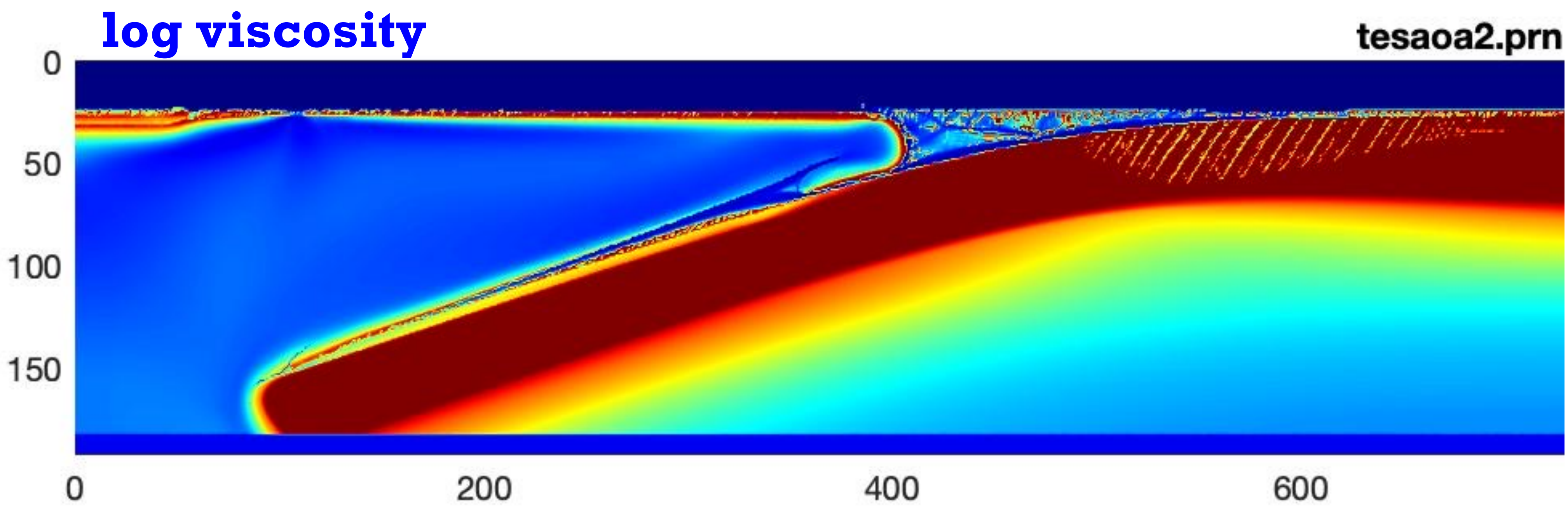
Model size: 1600x192x750 km

Model resolution: 1601x193x145 nodes

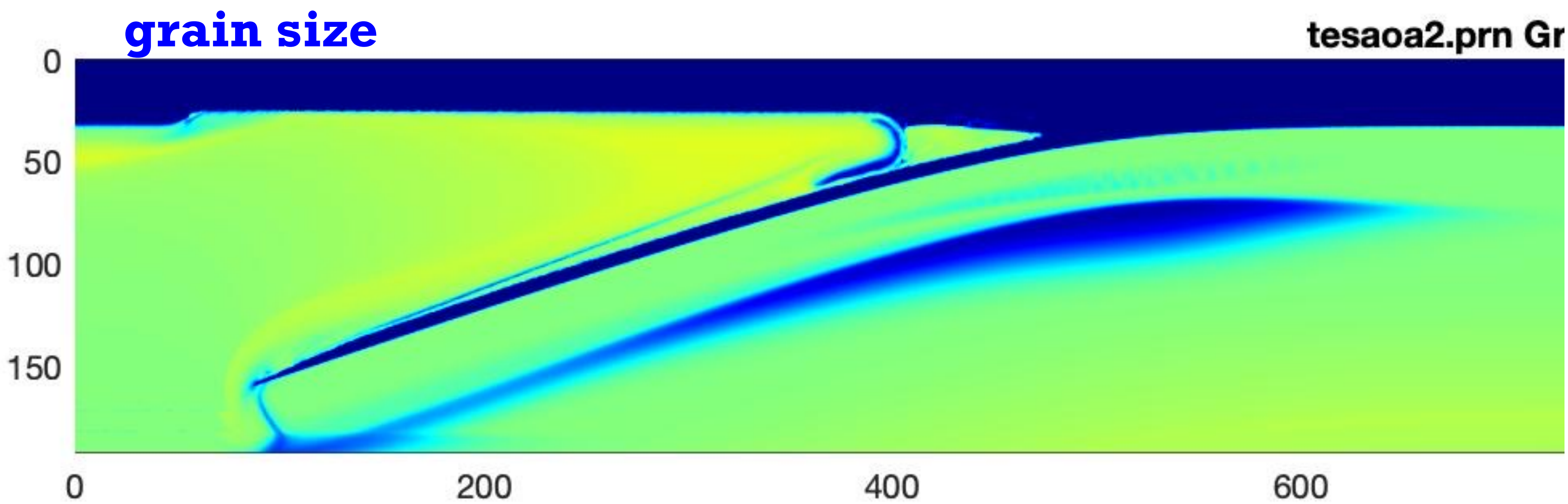
Run time: 2 months on 64 CPUs


log viscosity
tesaoa1.prn ETA P
0
50
100
150
0
200
400
600

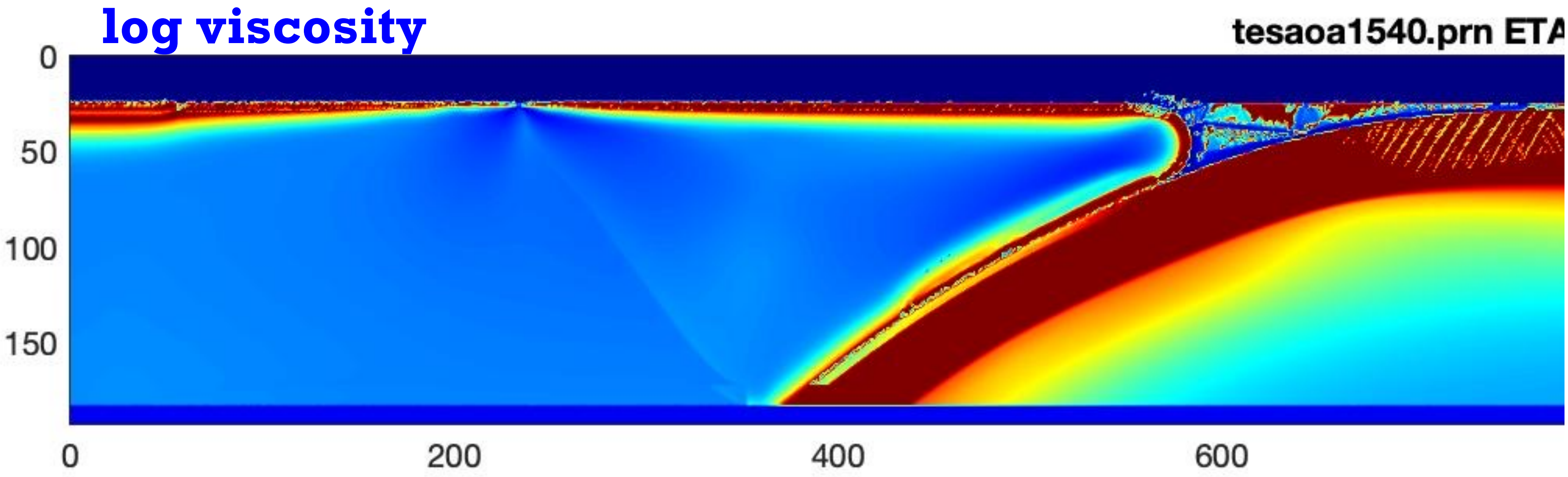

grain size
tesaoa1.prn Grain siz
0
50
100
150
0
200
400
600

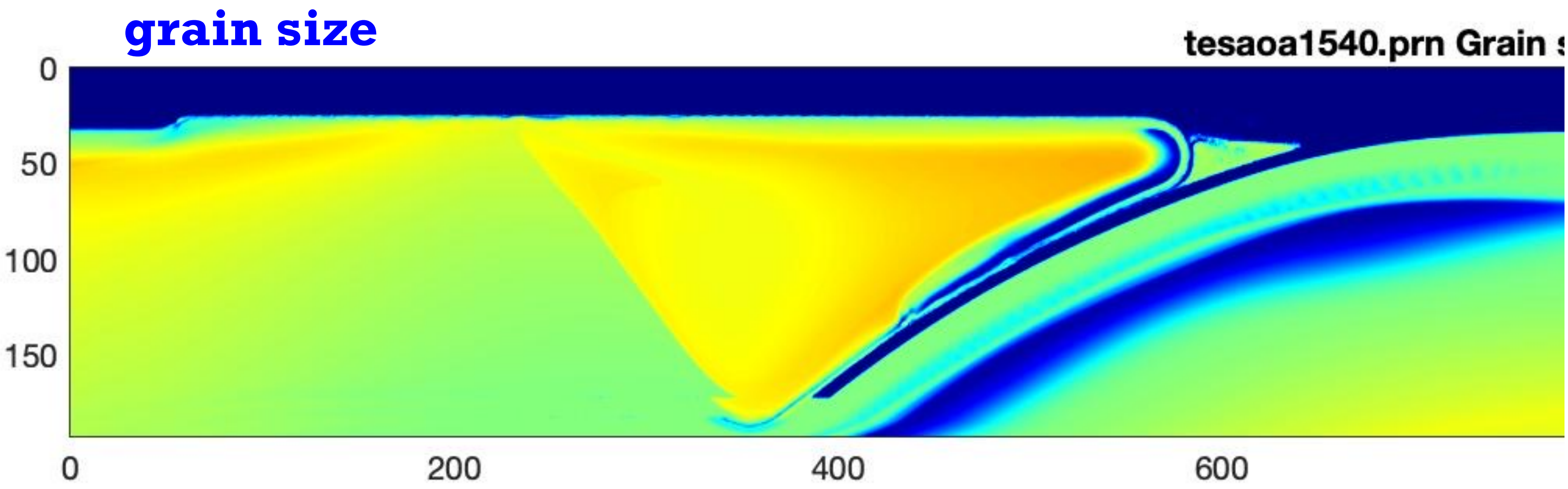


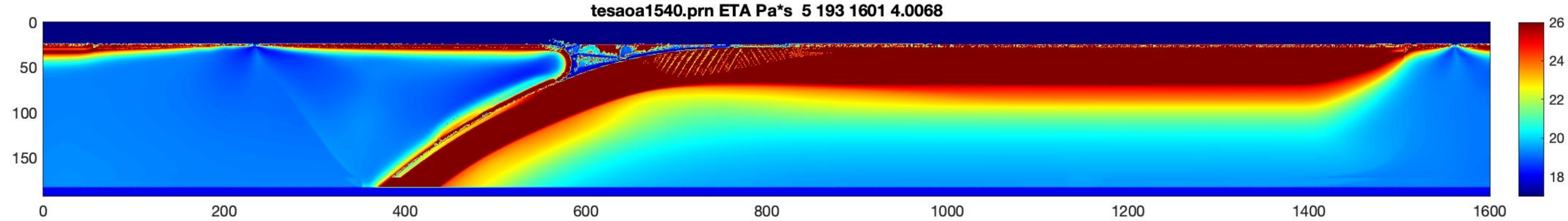
log viscosity
tesaoa2.prn
0
50
100
150
0
200
400
600

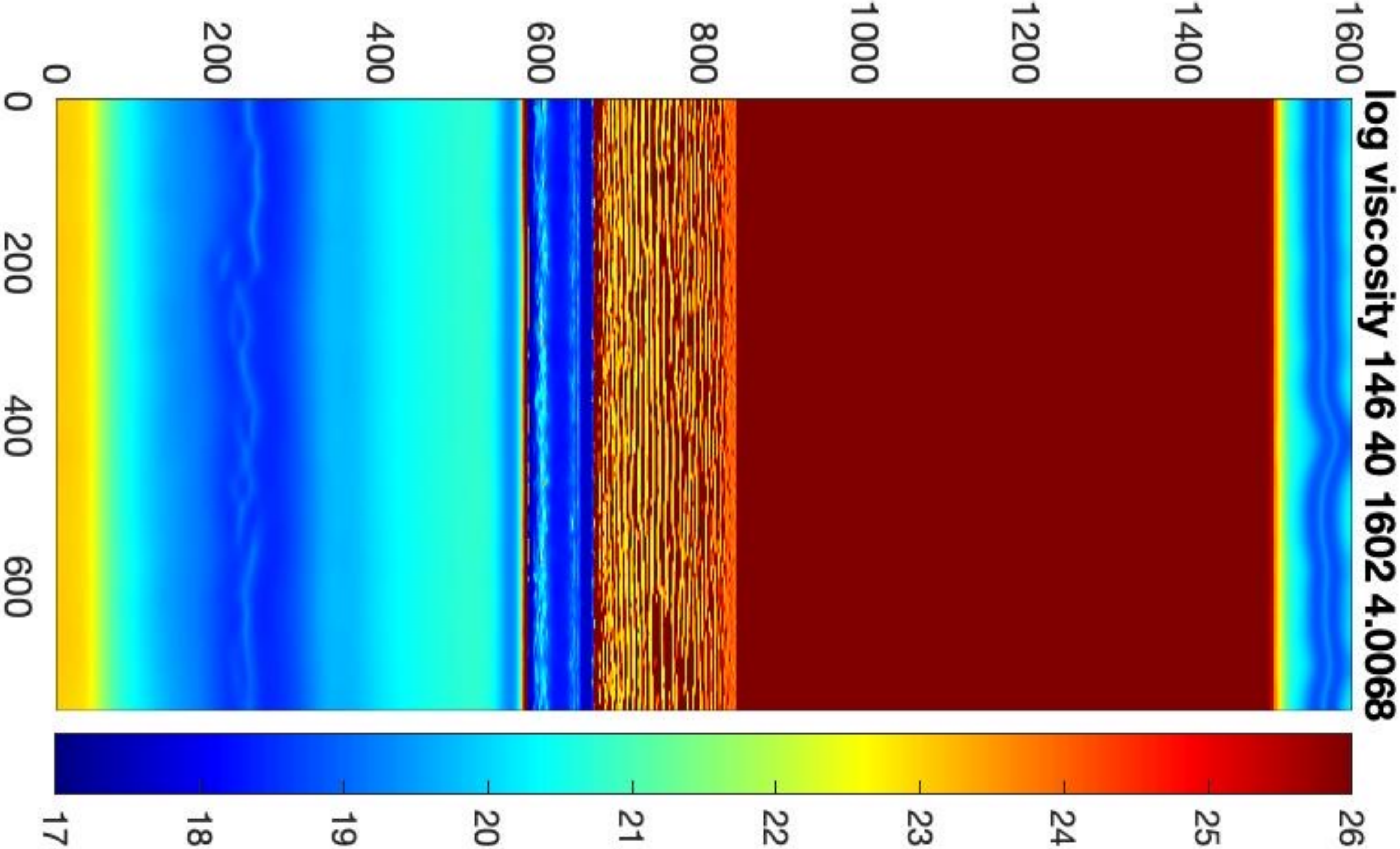


grain size
tesaoa2.prn Gr
0
50
100
150
0
200
400
600


log viscosity
tesaoa1540.prn ETA
0
50
100
150
0
200
400
600


grain size
tesaoa1540.prn Grain s
0
50
100
150
0
200
400
600


tesaoa1540.prn ETA Pa*s 5 193 1601 4.0068


log viscosity 146 40 1602 4.0068

Conclusions

New I3ELVIS is ready for use

Parallelization is still OpenMP and requires fat nodes

I3ELVIS Outlook

Planetary - Adding self-gravitation should be straigth forward

STM - Adding inertia and Rate- and State Friction should be straigth forward

HTM - Adding poroelasticity and two-phase flow should be straigth forward

Landscape - Adding coupling to surface processes should be straigth forward