Final Exam Solutions

Chris Weinberger and Wei Cai

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Problem F.1 (20') Orowan's equation
$\dot{\varepsilon} = \rho b v$ relates the plastic strain rate $\dot{\varepsilon}$ to the mobile dislocation density ρ, Burgers vector b and average dislocation velocity. To prove this equation (in a simple case), consider a planar closed dislocation loop in a finite, otherwise homogeneous linear elastic solid under zero tractions at the external surface. Let the area of the loop change by ΔA. As a result, the average strain of the body change by Δe_{ij}. Let the n_i be the normal vector of the plane.

Use Betti's theorem to show that

$$\Delta e_{ij} = -\frac{1}{2V}(n_i b_j + n_j b_i)\Delta A \tag{1}$$

[Hint: model the dislocation loop with an equivalent inclusion.]

Solution

First, we prove a general relationship between the average strain and the eigenstrain of an inclusion in a finite body under zero traction,

$$\overline{e^c_{ij}} = e^*_{ij}\frac{V_0}{V} \tag{2}$$

where $\overline{e^c_{ij}}$ is the averaged constrained strain field, e^*_{ij} is the eigenstrain, V_0 is the volume of the inclusion and V is the volume of the elastic body.

This relationship can be proved using Betti's theorem. Let field "1" be the constrained field, i.e. the field caused by applying force $t^{(1)}_j = \sigma^*_{ij} n_i$ on the surface S_0 of the inclusion, e.g. $u^{(1)}_j = u^c_j$. Let field "2" be a uniform field due to traction forces applied to the external surface S^{ext} of the elastic body, e.g. $\sigma^{(2)}_{ij} = \sigma^A_{ij}$.

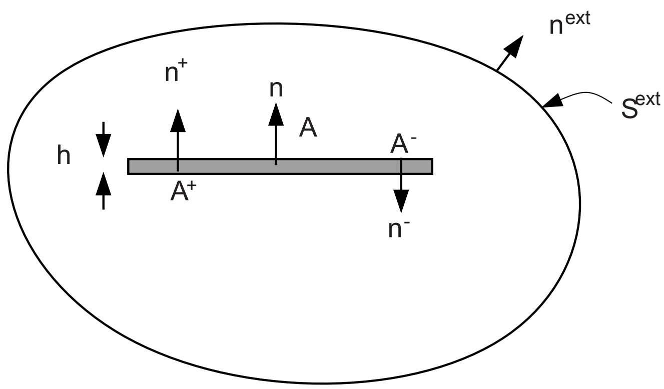

Figure 1: Equivalent inclusion model of a planar dislocation loop.

From Betti's theorem,

$$\int_{S_0} t_j^{(1)} u_j^{(2)} dS = \int_{S^{\mathrm{ext}}} t_j^{(2)} u_j^{(1)} dS \tag{3}$$

we have,

$$\begin{aligned}
\int_{S_0} \sigma_{ij}^* n_i u_j^{(2)} dS &= \int_{S^{\mathrm{ext}}} \sigma_{ij}^A n_i u_j^c dS \\
\sigma_{ij}^* \int_{V_0} u_{j,i}^{(2)} dS &= \sigma_{ij}^A \left(\int_{S^{\mathrm{ext}}} n_i u_j^c dS - \int_{S_0} n_i u_j^c dS \right) + \sigma_{ij}^A \int_{S_0} n_i u_j^c dS
\end{aligned}$$

Apply Gauss's theorem,

$$\begin{aligned}
\sigma_{ij}^* e_{ij}^A V_0 &= \sigma_{ij}^A \int_{V-V_0} u_{j,i}^c dV + \sigma_{ij}^A \int_{V_0} u_{j,i}^c dV \\
\sigma_{ij}^* e_{ij}^A V_0 &= \sigma_{ij}^A \int_V e_{ij}^c dV \equiv \sigma_{ij}^A \overline{e_{ij}^c} V \\
\sigma_{ij}^A e_{ij}^* V_0 &= \sigma_{ij}^A \overline{e_{ij}^c} V \qquad (4)
\end{aligned}$$

Because this is true for arbitrary applied stress σ_{ij}^A, then,

$$e_{ij}^* V_0 = \overline{e_{ij}^c} V \tag{5}$$

We model the dislocation loop as an equivalent inclusion as shown in Fig. 1. The inclusion has a plate-like shape around surface A with height h. The volume of the inclusion is $V_0 = Ah$. The positive side of the surface A^+ is displaced by b_j with respect to the negative side of the surface A^-. So that the eigenstrain for this equivalent inclusion is,

$$e_{ij}^* = -\frac{1}{2h}(b_i n_j + b_j n_i) \tag{6}$$

The average strain in the entire body is thus,

$$\overline{e_{ij}^c} = -\frac{V_0}{V}\frac{1}{2h}(b_i n_j + b_j n_i) = -\frac{A}{2V}(b_i n_j + b_j n_i) \tag{7}$$

When the area of the dislocation loop changes by ΔA, the change of total average strain is,

$$\Delta e_{ij} = -\frac{\Delta A}{2V}(b_i n_j + b_j n_i) \tag{8}$$

Problem F.2 (20') J-integral and Peach-Koehler force
Consider an infinite straight screw dislocation along z-axis with Burgers vector b_z in an infinite isotropic medium under uniform applied stress σ_{yz}^A.

(a) What is the driving force (per unit length) on this dislocation by Peach-Koehler formula?

(b) Compute the J-integral around this dislocation in both x and y directions, i.e., J_x and J_y, based on the known elastic field of the screw dislocation (Hirth and Lothe 1982). How do they compare with the Peach-Koehler force? Print results for both terms in the J-integral. Notice that in this case the J-integral is evaluated on a closed surface surrounding the dislocation.

Solution
(a) The Peach-Koehler force is

$$f_m = \epsilon_{inm}\sigma_{ij}b_j v_n$$

This results in

$$\begin{aligned} f_x &= \sigma_{yz}^A b_z \\ f_y &= 0 \\ f_z &= 0 \end{aligned}$$

(b) The J integral is

$$J_i = \int_S (w n_i - t_j u_{j,i})\, \mathrm{d}S$$

Choosing the coordinate system in Hirth and Lothe, we can write the stress tensor as

$$\sigma = \begin{bmatrix} 0 & 0 & -\frac{\mu b}{2\pi}\frac{y}{x^2+y^2} \\ 0 & 0 & \frac{\mu b}{2\pi}\frac{x}{x^2+y^2} + \sigma_{yz}^A \\ -\frac{\mu b}{2\pi}\frac{y}{x^2+y^2} & \frac{\mu b}{2\pi}\frac{x}{x^2+y^2} + \sigma_{yz}^A & 0 \end{bmatrix} \tag{9}$$

The strain can be written as

$$e = \frac{1}{2\mu}\begin{bmatrix} 0 & 0 & -\frac{\mu b}{2\pi}\frac{y}{x^2+y^2} \\ 0 & 0 & \frac{\mu b}{2\pi}\frac{x}{x^2+y^2} + \sigma_{yz}^A \\ -\frac{\mu b}{2\pi}\frac{y}{x^2+y^2} & \frac{\mu b}{2\pi}\frac{x}{x^2+y^2} + \sigma_{yz}^A & 0 \end{bmatrix} \tag{10}$$

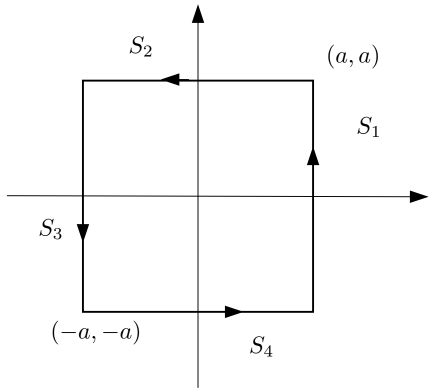

Figure 2: J-integral contour path Γ, consisting of four straight segments: S_1, S_2, S_3 and S_4.

The energy density is,

$$w(x,y) = \frac{1}{2}\sigma_{ij}e_{ij} = \frac{\mu b^2}{4\pi^2}\frac{1}{x^2+y^2} + \frac{\sigma_{yz}^A b}{\pi}\frac{x}{x^2+y^2} + \frac{(\sigma_{yz}^A)^2}{\mu} \tag{11}$$

The displacement is,

$$u_z = \frac{b}{2\pi}\arctan\frac{y}{x} + 2ye_{yz}^A \tag{12}$$

$$u_x = u_y = 0 \tag{13}$$

so that,

$$u_{z,x} = -\frac{b}{2\pi}\frac{y}{x^2+y^2} \tag{14}$$

$$u_{z,y} = \frac{b}{2\pi}\frac{x}{x^2+y^2} + e_{yz}^A \tag{15}$$

The driving forces in x and y directions are

$$J_x = \int_S (wn_x - t_j u_{j,x})\,\mathrm{d}S = \int_\Gamma wdy - t_j u_{j,x} ds \tag{16}$$

$$J_y = \int_S (wn_y - t_j u_{j,y})\,\mathrm{d}S = \int_\Gamma -wdx - t_j u_{j,y} ds \tag{17}$$

where Γ is a contour going counter-clockwise around the dislocation, t_j is the traction force the material outside S exerts on the material inside. Notice that dx and dy can be either positive or negative depending on the local orientation of the contour Γ while ds is always positive.

Choose a square contour Γ as shown in Fig. 2. Let us evaluate the first integral in J_x (only S_1 and S_3 contribute).

$$\int_\Gamma wdy = \int_{-a}^{a} w(a,y)dy + \int_a^{-a} w(-a,y)dy = \frac{1}{2}\sigma_{yz}^A b \tag{18}$$

The second integral in J_x is,

$$\begin{aligned}
\int_\Gamma -t_j u_{j,x} ds &= \int_\Gamma -t_z u_{z,x} ds \\
&= -\int_{S_1} \sigma_{xz} u_{z,x} ds - \int_{S_2} \sigma_{yz} u_{z,x} ds + \int_{S_3} \sigma_{xz} u_{z,x} ds + \int_{S_4} \sigma_{yz} u_{z,x} ds \\
&= -\int_{-a}^{a} \sigma_{xz}(a,y) u_{z,x}(a,y) dy - \int_{-a}^{a} \sigma_{yz}(x,a) u_{z,x}(x,a) dx \\
&\quad + \int_{-a}^{a} \sigma_{xz}(-a,y) u_{z,x}(-a,y) dy + \int_{-a}^{a} \sigma_{yz}(x,-a) u_{z,x}(x,-a) dx \\
&= \frac{1}{2}\sigma_{yz}^A b \qquad (19)
\end{aligned}$$

Therefore,

$$J_x = \sigma_{yz}^A b \qquad (20)$$

The first integral in J_y is (only S_2 and S_4 contribute),

$$\int_\Gamma -w dx = \int_a^{-a} -w(x,a) dx + \int_a^{-a} -w(x,-a) dx = 0 \qquad (21)$$

The second integral in J_y is,

$$\begin{aligned}
\int_\Gamma -t_j u_{j,y} ds &= \int_\Gamma -t_z u_{z,y} ds \\
&= -\int_{S_1} \sigma_{xz} u_{z,y} ds - \int_{S_2} \sigma_{yz} u_{z,y} ds + \int_{S_3} \sigma_{xz} u_{z,y} ds + \int_{S_4} \sigma_{yz} u_{z,y} ds \\
&= -\int_{-a}^{a} \sigma_{xz}(a,y) u_{z,y}(a,y) dy - \int_{-a}^{a} \sigma_{yz}(x,a) u_{z,y}(x,a) dx \\
&\quad + \int_{-a}^{a} \sigma_{xz}(-a,y) u_{z,y}(-a,y) dy + \int_{-a}^{a} \sigma_{yz}(x,-a) u_{z,y}(x,-a) dx \\
&= 0 \qquad (22)
\end{aligned}$$

Therefore,

$$J_y = 0 \qquad (23)$$

Notice that the results are independent of a. These are consistent with the Peach-Koehler formula.

Matlab script used in this calculation.

```
%compute J-integral for screw dislocation

syms mu b SYZA x y a
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```
sxz = -mu*b/(2*pi) * y/(x^2+y^2);
syz = mu*b/(2*pi) * x/(x^2+y^2) + SYZA;

exz = sxz/(2*mu);
eyz = syz/(2*mu);
EYZA = SYZA/(2*mu);

u = b/(2*pi)*atan(y/x) + 2*EYZA*y;
uzx = b/(2*pi) * (-y)/(x^2+y^2);
uzy = b/(2*pi) *   x /(x^2+y^2) + 2*EYZA;

w = (2*sxz*exz + 2*syz*eyz)/2;

Jwx1 = int(subs(w,x,a), y, -a, a);
Jwx2 = 0;
Jwx3 = int(subs(w,x,-a), y, a,-a);
Jwx4 = 0;

Jtx1 =-int(subs(sxz*uzx,x,a), y, -a, a);
Jtx2 =-int(subs(syz*uzx,y,a), x, -a, a);
Jtx3 = int(subs(sxz*uzx,x,-a), y,-a, a);
Jtx4 = int(subs(syz*uzx,y,-a), x,-a, a);

Jwx = simplify(Jwx1 + Jwx2 + Jwx3 + Jwx4);
Jtx = simplify(Jtx1 + Jtx2 + Jtx3 + Jtx4);
Jx = simplify(Jwx+Jtx);

Jwy1 = 0;
Jwy2 = -int(subs(w,y,a), x, a, -a);
Jwy3 = 0;
Jwy4 = -int(subs(w,y,-a),x,-a,  a);

Jty1 =-int(subs(sxz*uzy,x,a), y, -a, a);
Jty2 =-int(subs(syz*uzy,y,a), x, -a, a);
Jty3 = int(subs(sxz*uzy,x,-a), y,-a, a);
Jty4 = int(subs(syz*uzy,y,-a), x,-a, a);

Jwy = simplify(Jwy1 + Jwy2 + Jwy3 + Jwy4);
Jty = simplify(Jty1 + Jty2 + Jty3 + Jty4);
Jy = simplify(Jwy+Jty);

%display result
Jx, Jy
```

Problem F.3 (40') Crack nucleation
(a) Consider cutting an isotropic solid into two halves by a mathematical plane and uniformly separating the two halves normal to the plane by u. Let the traction force $f(u)$ per unit area across the plane take the following form (universal binding curve),

$$f(u) = A\, u\, \mathrm{e}^{-\alpha u} \tag{24}$$

What is the surface energy per unit area $\gamma(u)$?

(b) Put the solid under plane strain condition. For a slit like crack with length $2a$ along x-axis under uniform applied stress σ_{yy}^A, what is the critical condition that the crack will grow according to Griffith's criteria? [Hint: you only need to figure out what γ value to use in the Griffith's criteria.]

(c) Suppose the stress distribution $\sigma_{yy}^A(x)$ in the absence of the crack on the x-axis is not uniform. Let $u(x)$ be the separation of the upper and lower halves of the solid across x-axis. Then the Gibbs free energy of the system can be written as,

$$\Delta G = -K \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho(x)\rho(x') \ln|x - x'| dx dx' + \int_{-\infty}^{\infty} \gamma(u(x)) dx - \int_{-\infty}^{\infty} \sigma_{yy}^A(x) u(x) dx \tag{25}$$

where $\rho(x) = du(x)/dx$, $K = \mu/(4\pi(1-\nu))$. The first term describes the elastic interactions in the absence of applied stress. The second term describes the surface energy and the third term describes the work done by the applied stress. The function $u(x)$ that minimizes ΔG corresponds to the physical separation of the planes under applied stress $\sigma_{yy}^A(x)$.

Write a Matlab program that can solve for $u(x)$ that minimizes ΔG for a given $\sigma_{yy}^A(x)$. Represent $u(x)$ by a piece-wise linear function on a uniform grid with size d: $u_i = u(id)$, $i = -N, -N+1, \cdots, N$. Apply boundary conditions: $\rho(x) = 0$, $x < -Nd$ or $x > Nd$. Express ΔG as a function of u_i. Starting with initial condition: $u_i = 0$. Compute derivative $g_i = \frac{\partial \Delta G}{\partial u_i}$. Update u_i by $u_i - g_i \cdot \delta$ with a small step size δ. Repeat the iteration until convergence has been reached.

Let

$$\sigma_{yy}^A(x) = B\mathrm{e}^{-\beta x^2} + C \tag{26}$$

$\mu = 1$, $\nu = 0.3$, $A = 0.1$, $\alpha = 1$, $B = 0.05$, $\beta = 0.01$, $C = 0$, $d = 1$, $N = 500$, $\delta = 0.1$.

Plot the resulting $u(x)$.

(d) Increase the background stress C in step of 0.01 while keeping other parameters fixed. What is the critical value of C where the system is unstable against crack nucleation and propagation?

[Hint:

$$\int_0^d \int_{nd}^{(n+1)d} \ln|x - x'| dx dx' = \left[\ln d - \frac{3}{2} + f(n)\right] d^2 \tag{27}$$

where

$$f(n) = \frac{(n+1)^2}{2}\ln(n+1) - n^2 \ln n + \frac{(n-1)^2}{2}\ln(n-1) \tag{28}$$

for $n > 1$ and $f(1) = \ln 4$, $f(0) = 0$.]

Solution

(a) Given the restoring force

$$f(u) = Au \exp(-\alpha u)$$

the surface energy is

$$\begin{aligned}\gamma(u) &= \int_0^u f(t)\,\mathrm{d}t = \int_0^u At\exp(-\alpha t)\,\mathrm{d}t \\ &= \frac{A}{\alpha^2}\left[1 - (1+\alpha u)\exp(-\alpha u)\right] \end{aligned} \tag{29}$$

(b) The surface energy γ reaches its maximum when $u \to \infty$. Thus, $\gamma \equiv \gamma(u = \infty) = A/\alpha^2$. Using this value in the griffith criteria the critical stress is (for plane strain)

$$\sigma_{yy}^A = \sqrt{\frac{4\mu\gamma}{(1-\nu)\pi a}} = \sqrt{\frac{4\mu A}{(1-\nu)\pi a \alpha^2}} \tag{30}$$

(c) Let $u(x)$ be piecewise linear, thus ρ is piecewise constant. Let

$$\rho_i = \frac{u_{i+1} - u_i}{d} \tag{31}$$

The first integral in ΔG can be written as

$$\begin{aligned} & -K\int_{-\infty}^{\infty} \rho(x)\rho(x')\ln|x - x'|\,\mathrm{d}x\,\mathrm{d}x' \\ = & -K\sum_i\sum_j \rho_i\rho_j \int_{x_i}^{x_{i+1}}\int_{x_j}^{x_{j+1}} \ln|x - x'|\,\mathrm{d}x\,\mathrm{d}x' \\ = & -K\sum_i\sum_j \rho_i\rho_j \int_0^d \int_{nd}^{(n+1)d} \ln|x - x'|\,\mathrm{d}x\,\mathrm{d}x' \end{aligned}$$

where n is determined by the number of elements seperating x_j and x_i.

$$n = \frac{|x_j - x_i|}{d} = |j - i| \tag{32}$$

The second two integrals can be approximated using the trapezoidal rule

$$\int_{-\infty}^{\infty} \gamma(u(x))\,\mathrm{d}x = d \sum_i \frac{A}{\alpha^2}[1 - (1 + \alpha u_i)\exp(-\alpha u_i)]$$

and

$$\int_{-\infty}^{\infty} \sigma_{yy}^A(x) u_i \,\mathrm{d}x = d \sum_{i=1}^{2N+1} [B \exp(-\beta x_i^2) + C] u_i$$

Thus ΔG can be written as

$$\Delta G = -K \sum_i^{2N} \sum_j^{2N} \rho_i \rho_j R_{ij} + d \sum_{i=1}^{2N+1} \frac{A}{\alpha^2}[1-(1+\alpha u_i)\exp(-\alpha u_i)] - d \sum_{i=1}^{2N+1} [B \exp(-\beta x_i^2) + C] u_i$$

where

$$R_{ij} = \int_0^d \int_{nd}^{(n+1)d} \ln|x - x'| \,\mathrm{d}x\,\mathrm{d}x' \ , \qquad (n = |j - i|)$$

Next we compute $g_i = \partial \Delta G / \partial u_i$. Using the chain rule,

$$g_i = -2K \sum_k \sum_j \rho_k R_{jk} \frac{\mathrm{d}\rho_j}{\mathrm{d}u_i} + d[A u_i \exp(-\alpha u_i)] - d[B \exp(-\beta x_i^2) + C]$$

Notice that,

$$\frac{\mathrm{d}\rho_j}{\mathrm{d}u_i} = \frac{\delta_{j\,i+1} - \delta_{ij}}{d}$$

then g_i becomes

$$g_i = -2K/d \sum_k^{2N} \rho_k (R_{j+1\,k} - R_{jk}) + d[A u_i \exp(-\alpha u_i)] - d[B \exp(-\beta x_i^2) + C]$$

The numerical solution of u_i for $C = 0$ is plotted Fig. 3. This result is obtained after $N_{\mathrm{step}} = 5000$ steepest descent steps. ΔG has converged to within 10^{-13}.

(d) The solution of u_i for $C = 0.01, 0.02, 0.03$ and 0.04 are plotted in Fig. 3(b). At $C = 0.04$, the crack is unstable in that the relaxation does not converge – the plotted curve for $C = 0.04$ is the result after $N_{\mathrm{step}} = 2000$ relaxation steps. It goes unbounded as N_{step} increases.

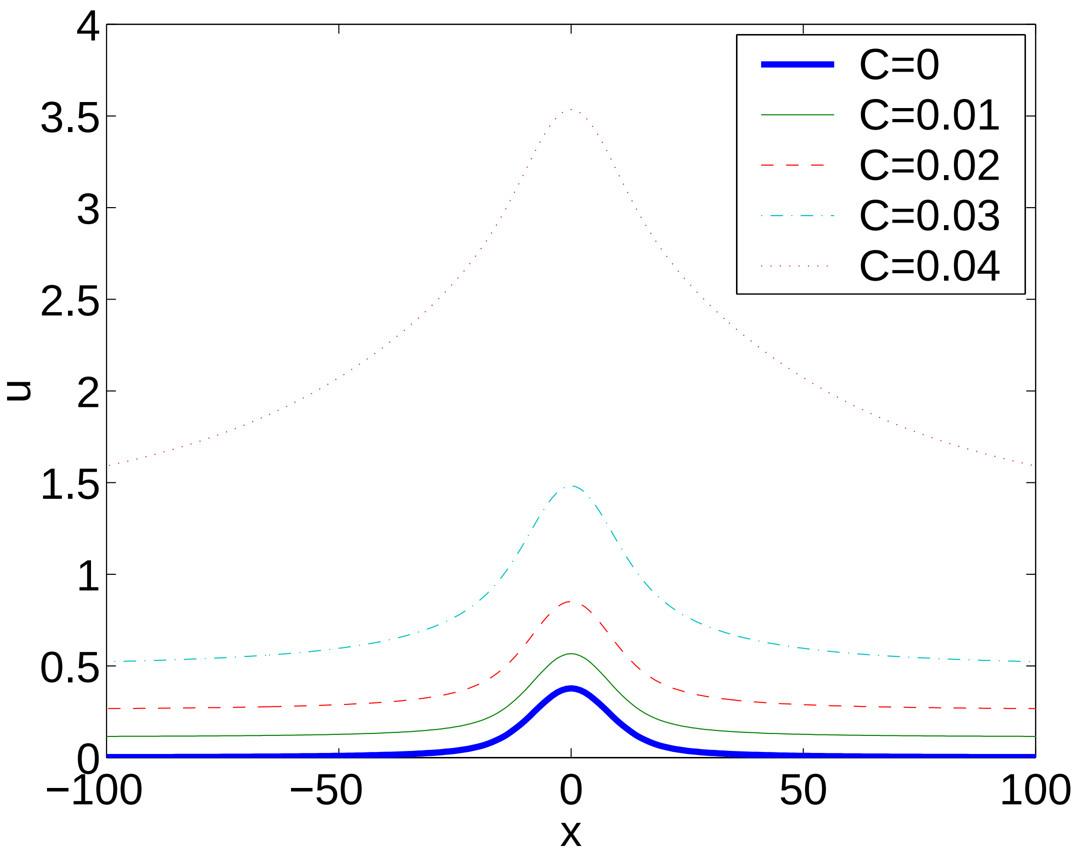

Figure 3: Crack opening displacement at $C = 0$, 0.01, 0.02, 0.03 and 0.04. The relaxation for $C = 0$, 0.01, 0.02, and 0.03 have converged after $N_{\text{step}} = 5000$ steepest descent steps. The relaxation for $C = 0.04$ does not converge – the plotted curve is the instantaneous result at $N_{\text{step}} = 2000$.