N-T-S MBFEA Code Consistency Study

Ahmed Elgailani - January, 17, 2020

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1 What is meant by "consistency"?

In short, it means the equivalence between the work done by/on the system and the associated total change of energy.
In other words, we need to verify that

$$f_{i\alpha}\delta r_{i\alpha} = -\Delta E \tag{1}$$

Where i is the node index, α is the coordinate, f is the force and ΔE is the change in the potential energy of the system.

2 The algorithm for checking the consistency

For any given configuration of the system (including the non-relaxed or non-stationary ones): loop over all the nodes while doing the following:

- For node i (while leaving all other nodes in their places), curPosX(i) += d, where d is any relatively small value (d = 0.00001 in this study)
- Calculate the forces and energy for the system in this state
- Calculate and store the consistency factor for node i in the x-direction as $f_x d/\Delta E$
- curPosX(i) -= d (returning the x position to its original value)
- do the same for the y-direction for node i

3 Internal forces only (no surface interactions)

First I checked for consistency when there is no contact between the meshes. As shown in figure 1 below, for almost all the nodes, the value $f_x d/\Delta E \approx 1$ with an error of the same order of magnitude of d. However, some nodes have a pathological value, with a factor of

around 2. This is attributed to inherent problems in the studied mesh. A similar result for the y-direction is also obtained.

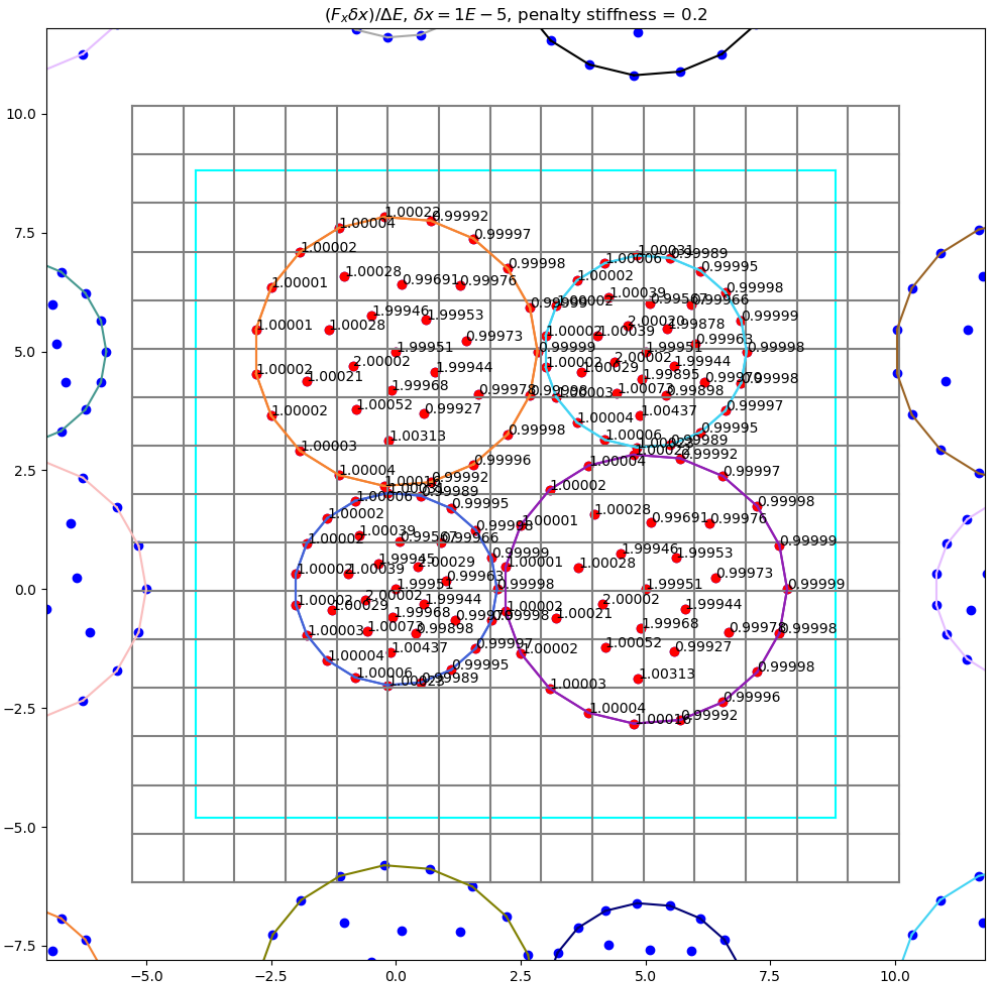

Figure 1: A plot for consistency factors in the x direction, $f_x d/\Delta E$, for the case where no interpenetration between the meshes. The meshes inside the cyanic box are part of the original image (red nodes); Everythnig else is a ghost image (blue nodes). The small squares defined by the grey grid are the Verlet cells. d = 1E-5.

4 NTS interactions with PBCs

Doing the same test here, things got interesting at the boundaries. As seen in figure 2 below, the consistency factor is very low at the boundary nodes. At first, I thought I made an error either in applying the PBCs or the NTS interactions. But I quickly exonerated the latter because NTS works fine for the internal contacts.
Eventually, it turned out that what happened at the boundary nodes is not a bug in the physics of the code but rather in the way I calculated the consistency factor at the boundaries. When a node at the boundary is moved slightly by a d amount in the x or y direction, its ghost images also are moved. The way I constructed the code is that if a ghost image is interacting with an original node then the energy associated with its interaction is added to the total energy of the system. So, while the force on the tested boundary node is correctly calculated by the code as the negative derivative of the energy with respect to the displacement at the node position, the difference in energy includes the energy difference caused by the movement of the ghost nodes as well; resulting in $fd < \Delta E$ yielding a consistency factor significantly less than unity. By reconstructing the code to only move the tested node when performing the consistency check I concluded that the code is doing the right thing and all the forces are derived from a potential with no "spurious" forces added to the system. Figure 3 shows the final results that I was looking for.

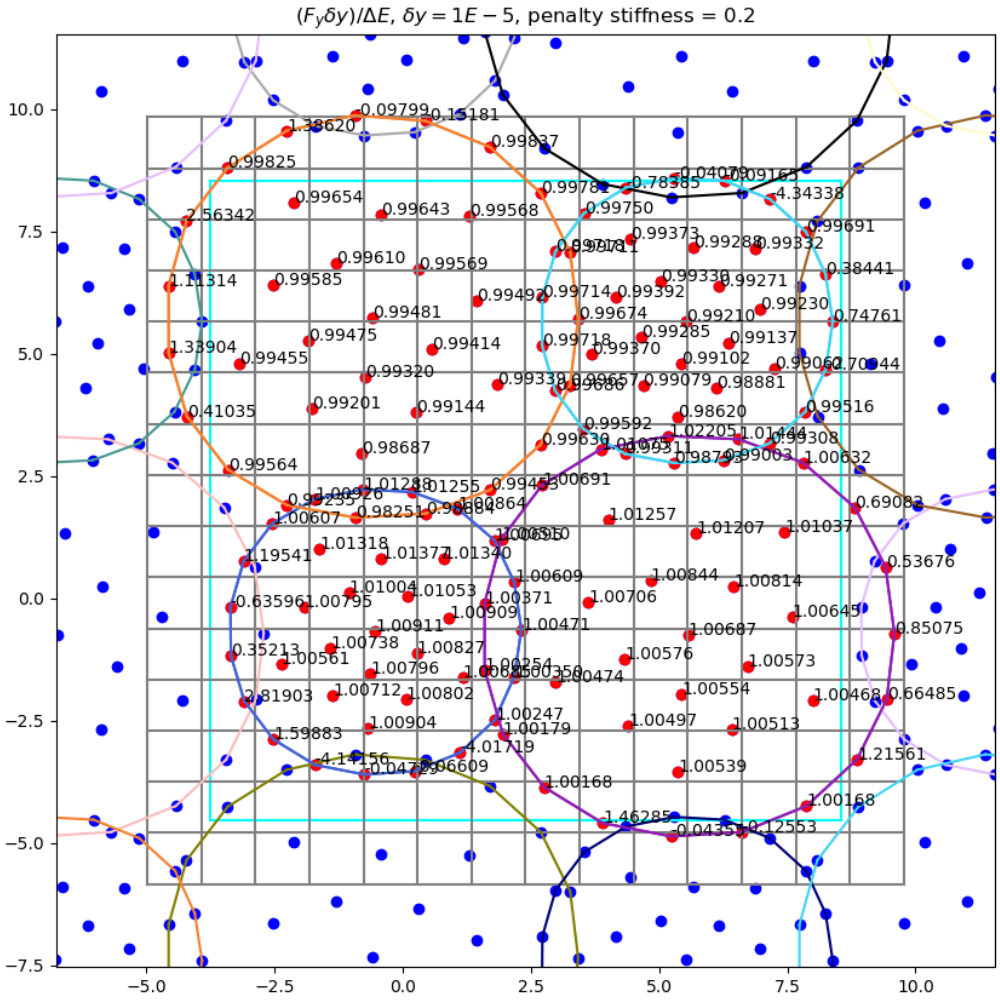

Figure 2: A plot for consistency factors in the y-direction, $f_y d/\Delta E$, for the case where there are interpenetrations between the meshes with PBCs. The meshes inside the cyanic box are part of the original image (red nodes); Everything else is a ghost image (blue nodes). The small squares defined by the grey grid are the Verlet cells. d = 1E-5. This is one of the "pathological" consistency results before debugging.

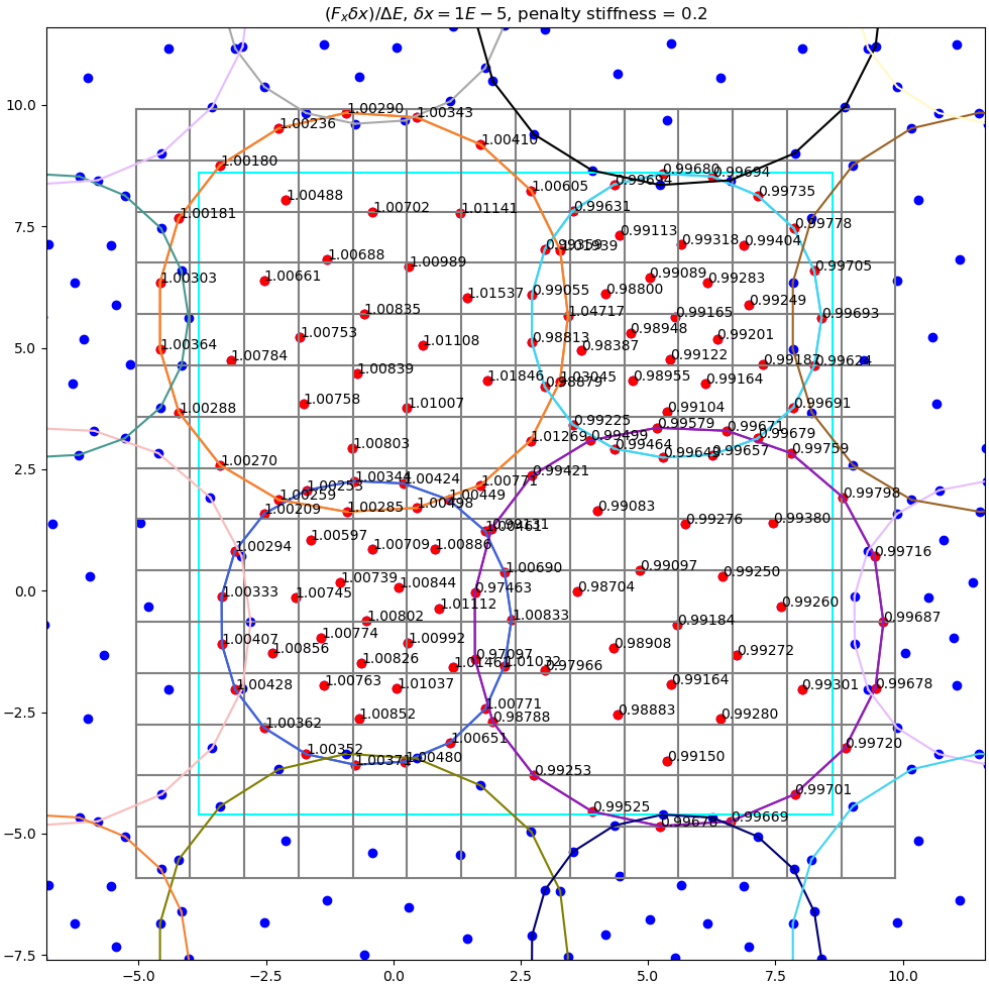

Figure 3: A plot for consistency factors in the x direction, $f_x d/\Delta E$, for the case where there are interpenetrations between the meshes with PBCs. The meshes inside the cyanic box are part of the original image (red nodes); Everythnig else is a ghost image (blue nodes). The small squares defined by the grey grid are the Verlet cells. d = 1E-5. This is consistency result after debugging.

5 Conclusion

The NTS and the PBC are working fine in MBFEA code. All forces are derived from associated energies.

A For future refernces

The code version used in this study is the branch named "improving_interaction_performance_3". The folder that contains all the runs and outputs of this study is :
"Research/Hydrogel/workspace/code_consistency_check"