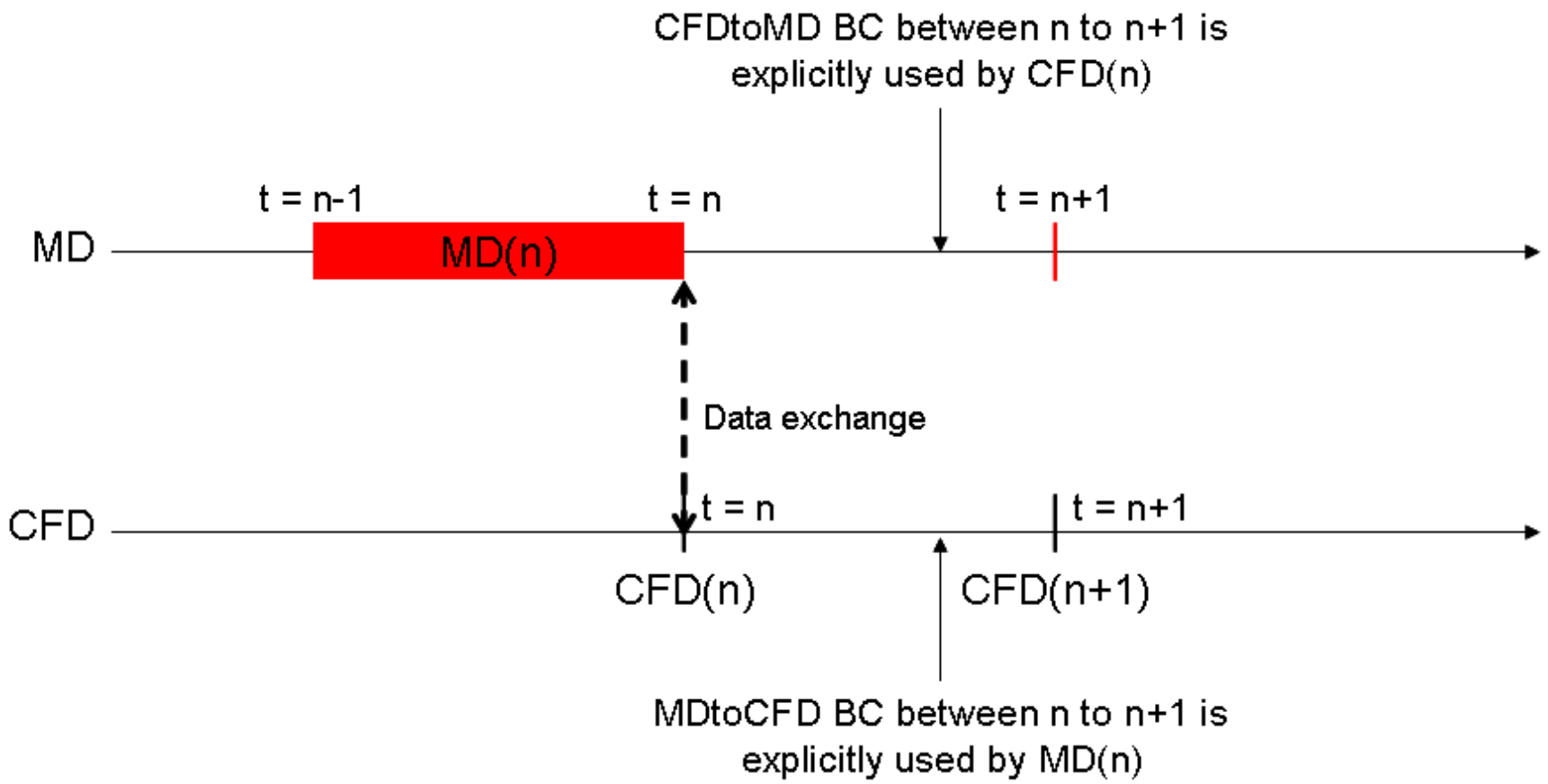
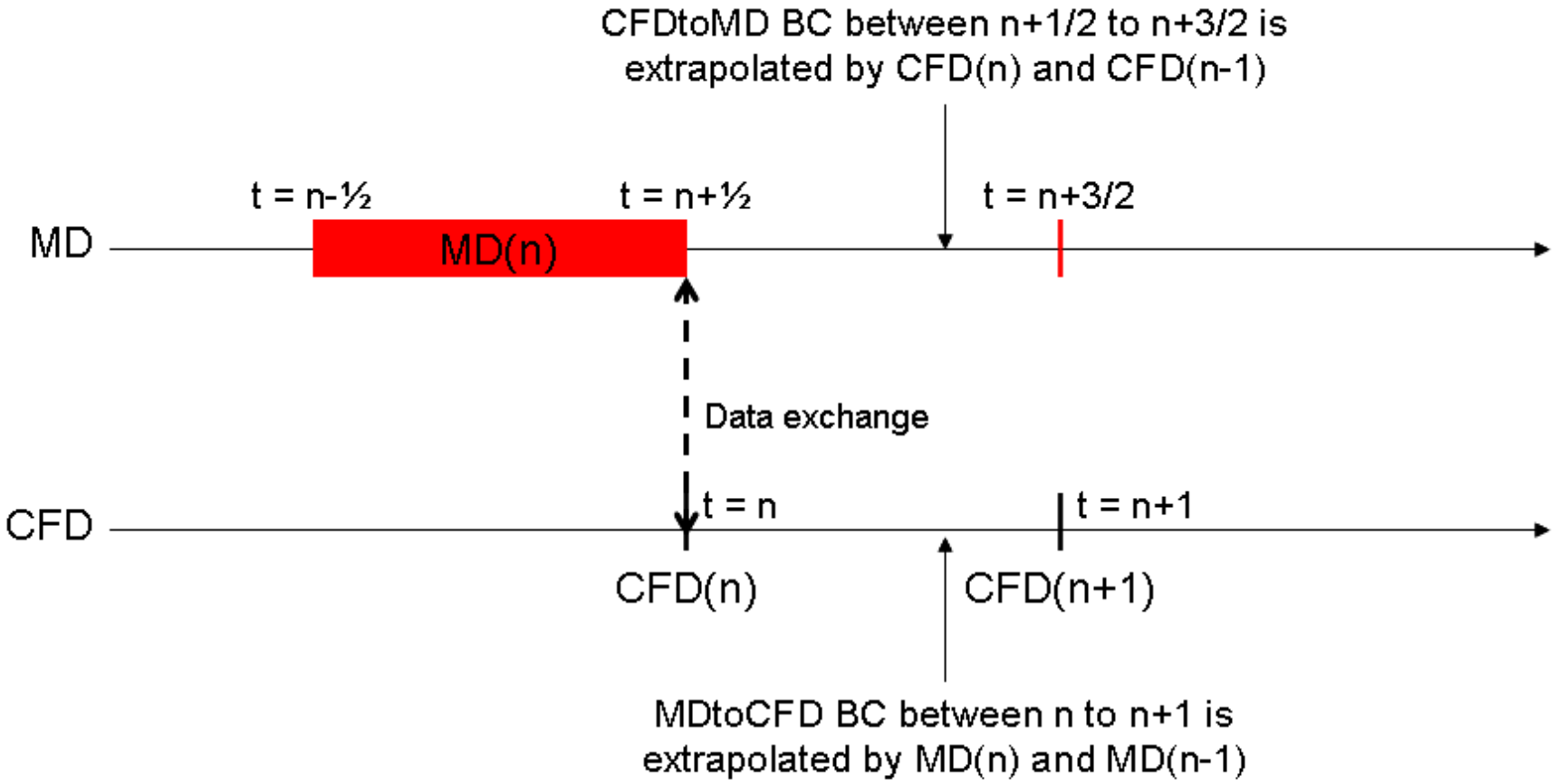
I have to agree that the current paper does not have something novel from scientific point of view.

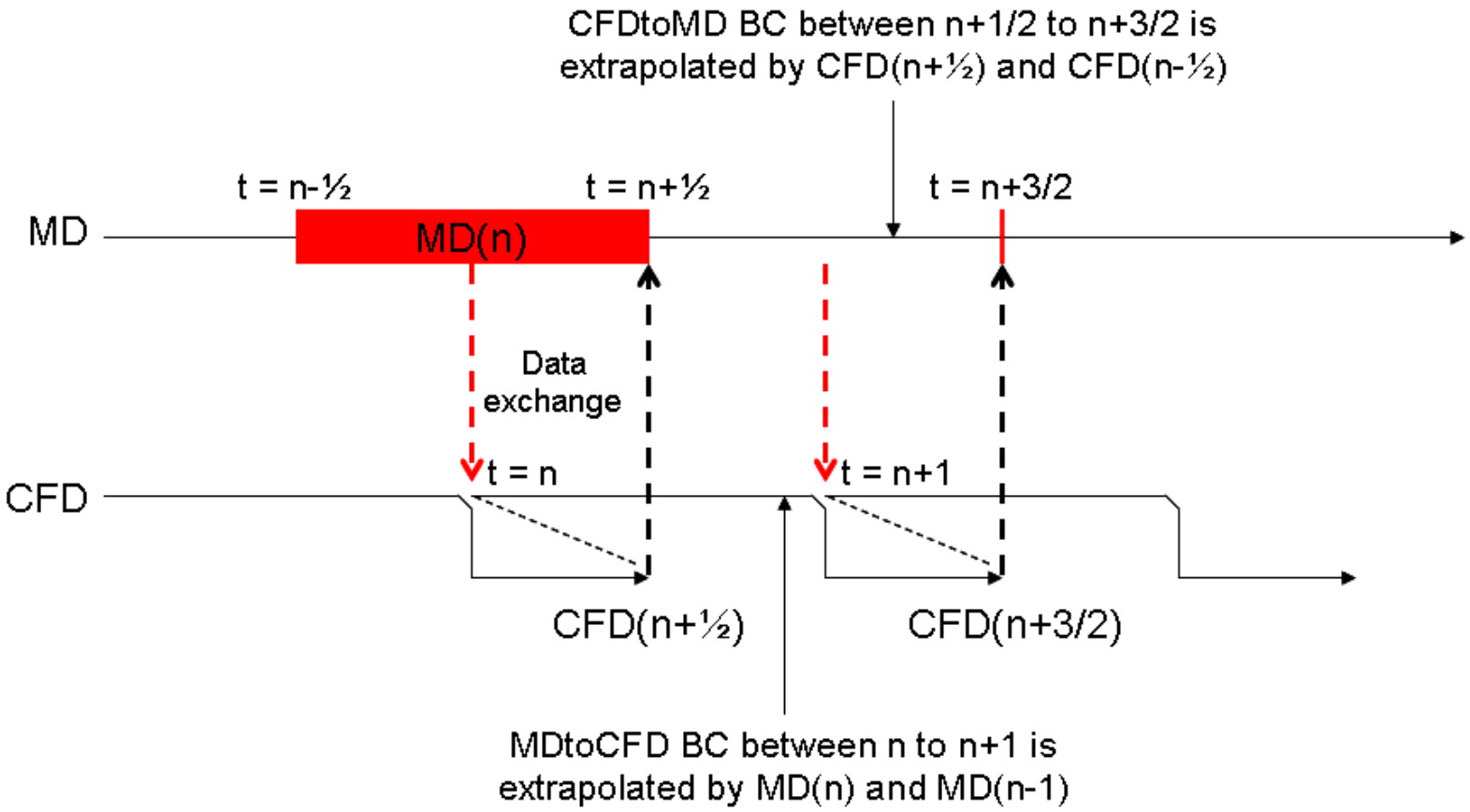
- Simulation cases (Couette and oscillating boundary) are already done by others (oscillating by Coveney, Ryu, others);
- system scale (10-7 meter system) has been solved by some (Yen, others);
- slower flow simulation (order of 1 meter per second level) was failed (due to far longer sampling time for statistical noise reduction in slow flow: statistical error is inversely proportional to the square of characteristic velocity);
- temporal scheme to get more accurate unsteady solution is not effective (better than the original but not clearly better than extrapolation, while having additional computational cost)



MD(n): Solution averaged between n-1 to n
CFD(n): Instantaneous solution at n



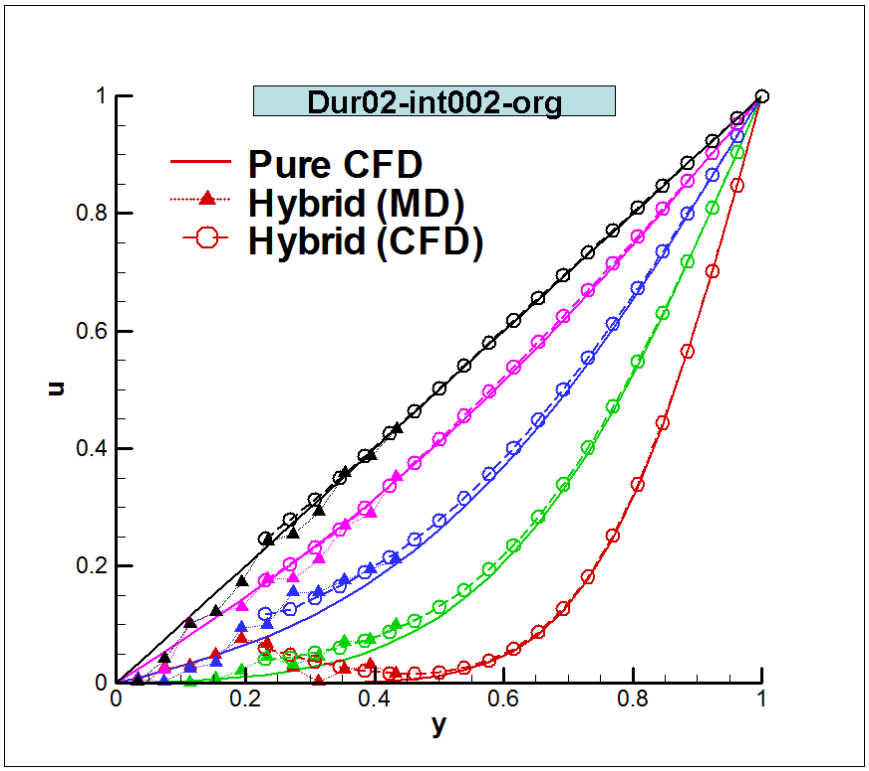
MD(n): Solution averaged between n-½ to n+½
CFD(n): Instantaneous solution at n

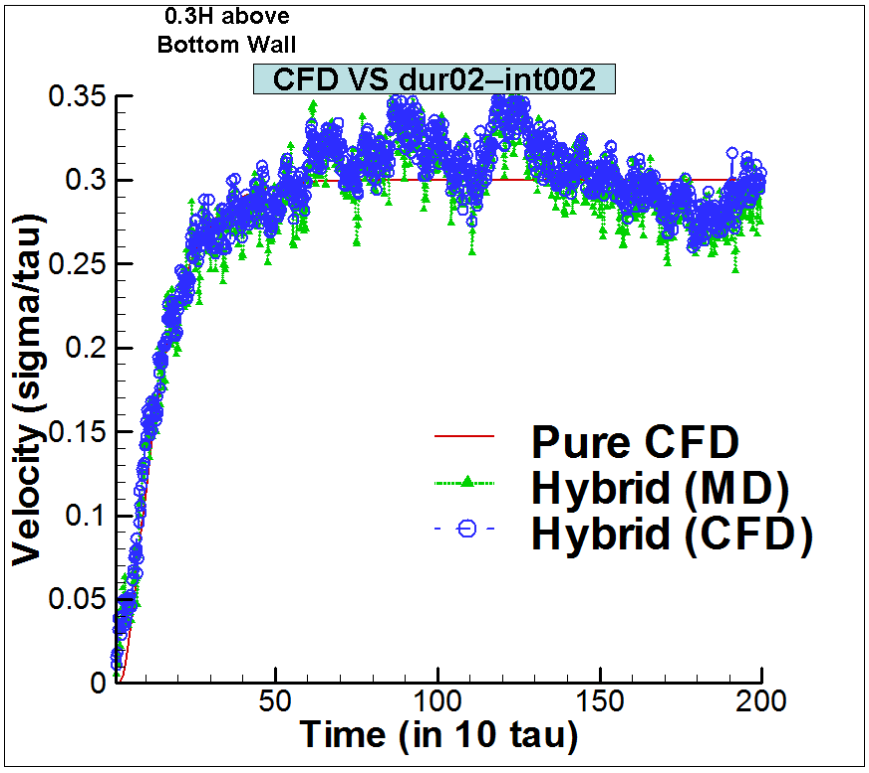


MD(n): Solution averaged between n-½ to n+½
CFD(n+½): Predicted solution at n+½

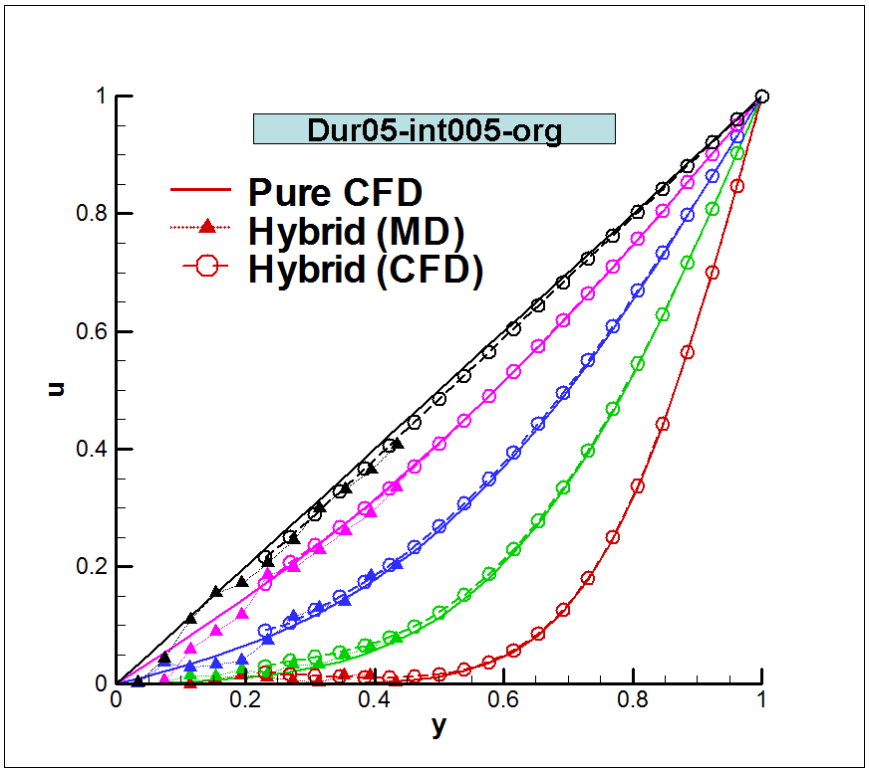
1. Couette flow

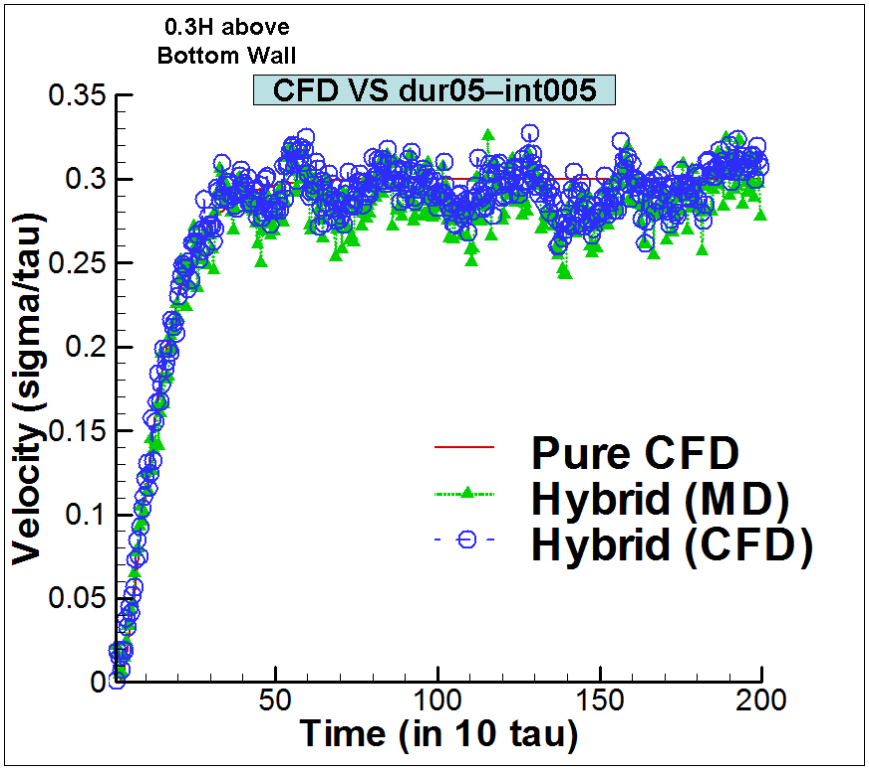
- Original (with extrapolation) + sampling duration 2 tau + sampling interval 2 tau



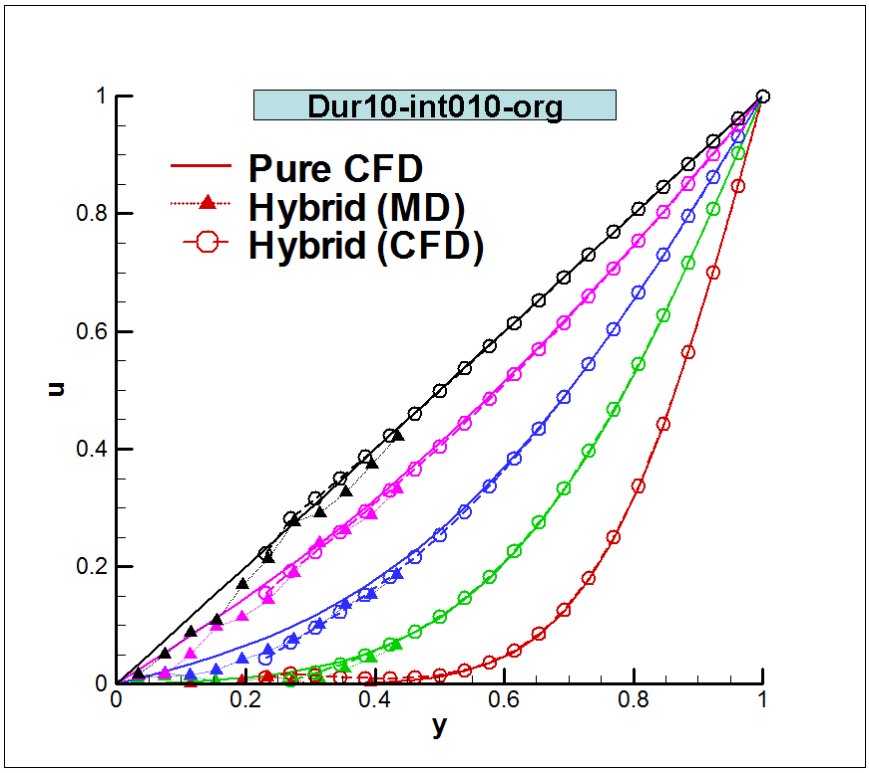


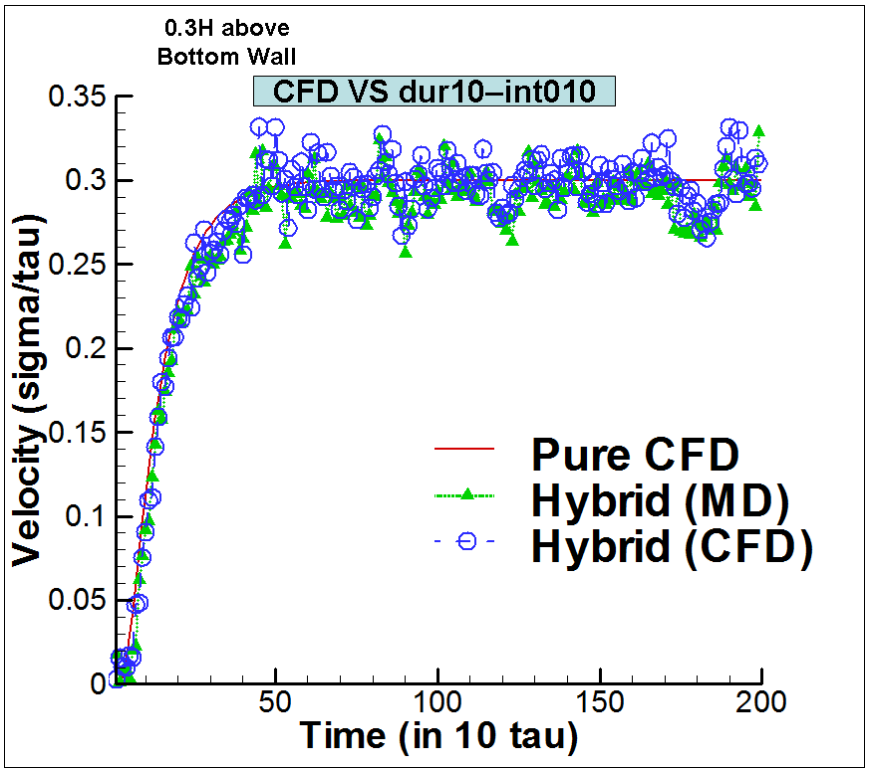
- Original (with extrapolation) + sampling duration 5 tau + sampling interval 5 tau



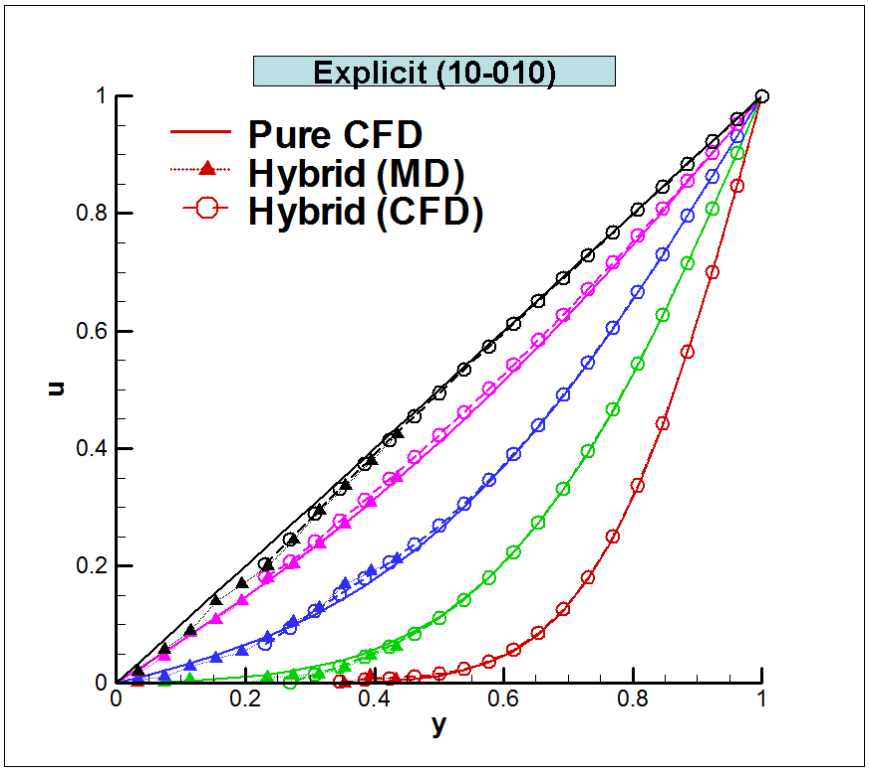


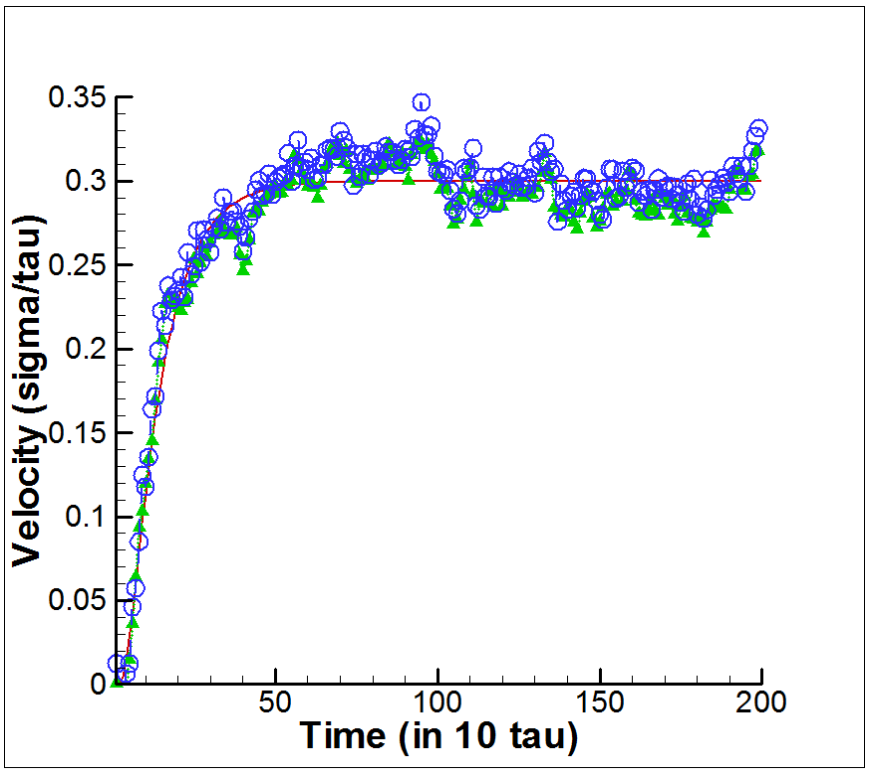
- Original (with extrapolation) + sampling duration 10 tau + sampling interval 10 tau





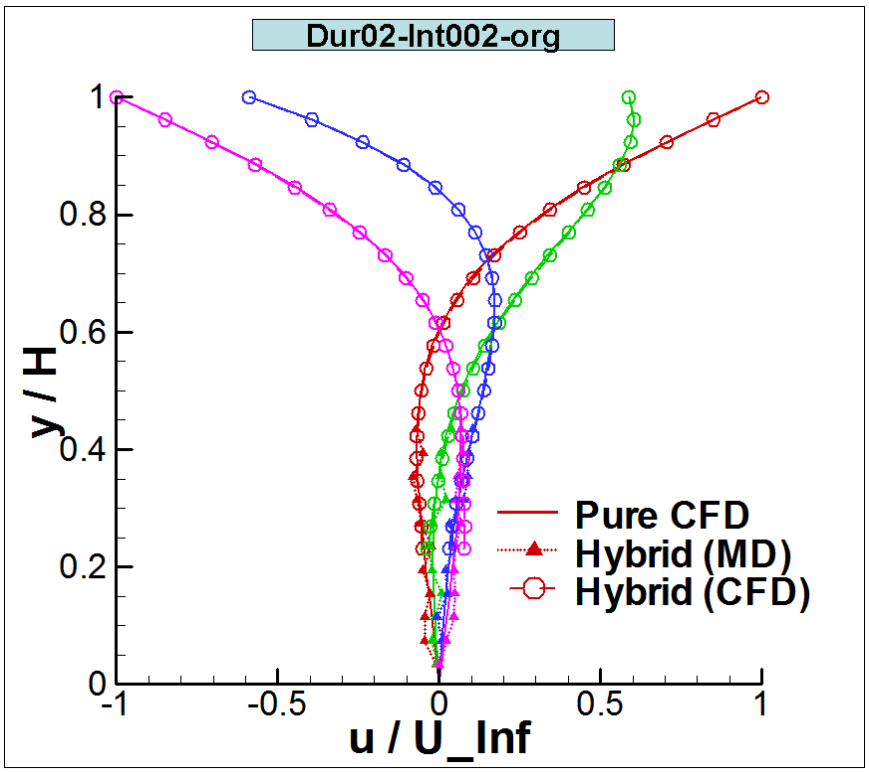
- Modified + sampling duration 10 tau + sampling interval 10 tau

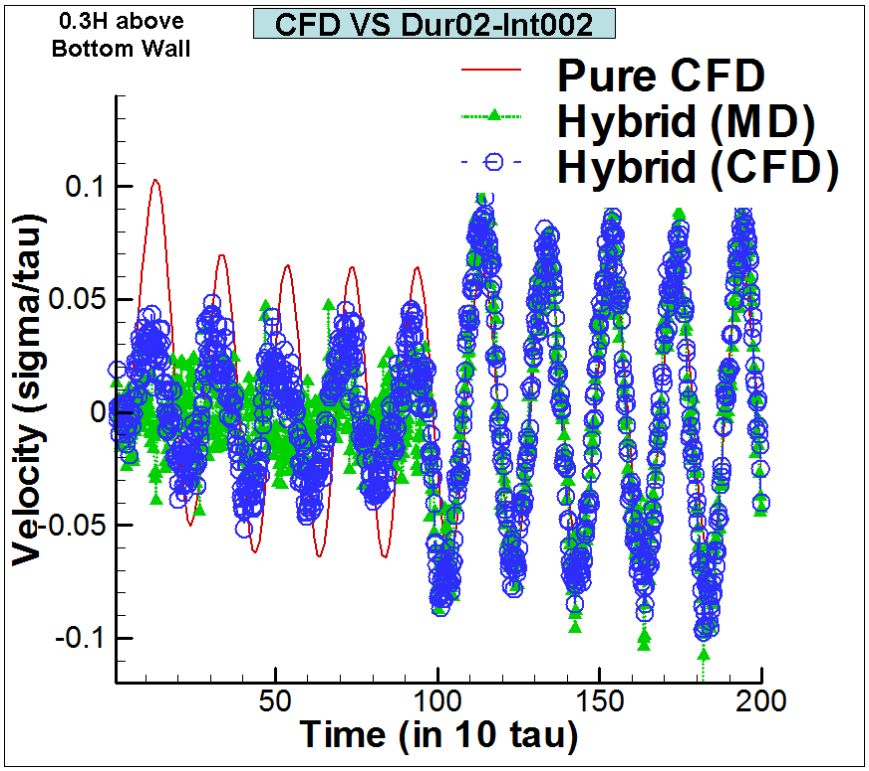




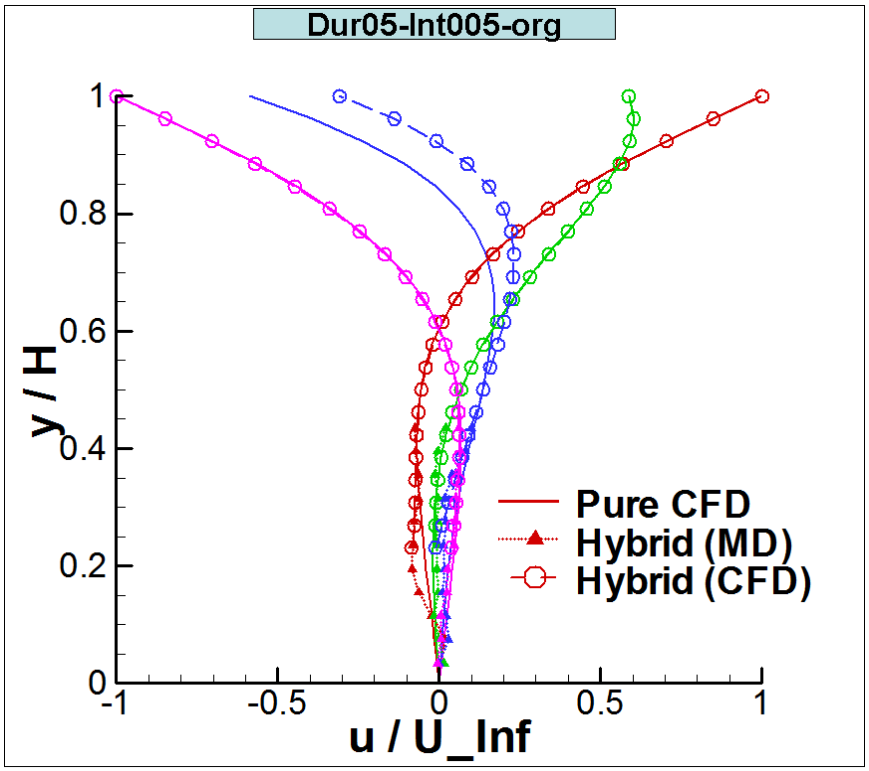
2. Oscillating boundary

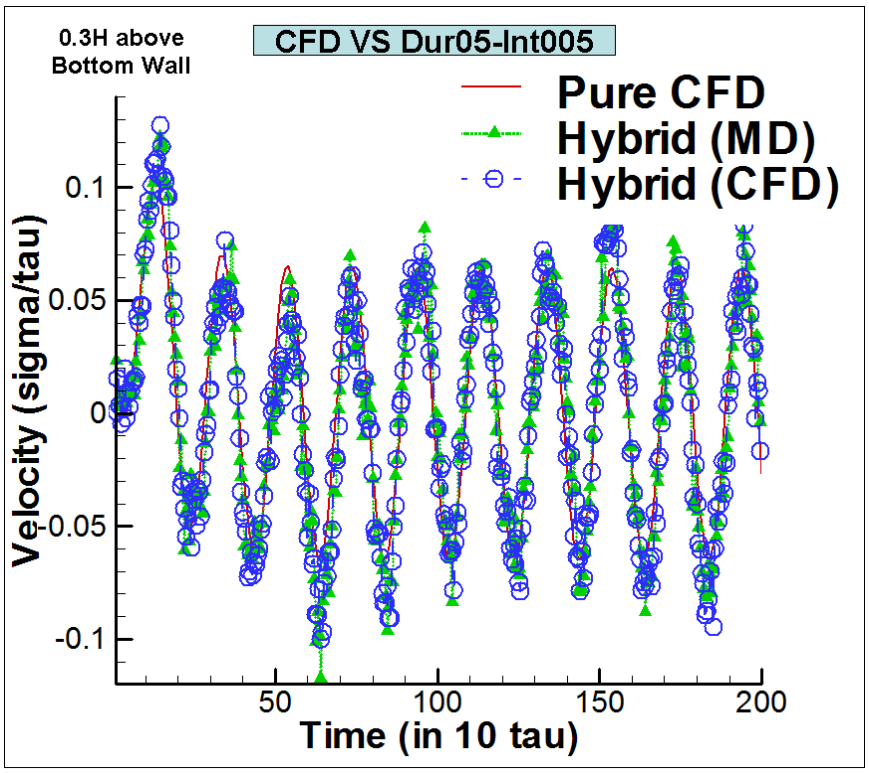
- Original (with extrapolation) + sampling duration 2 tau + sampling interval 2 tau



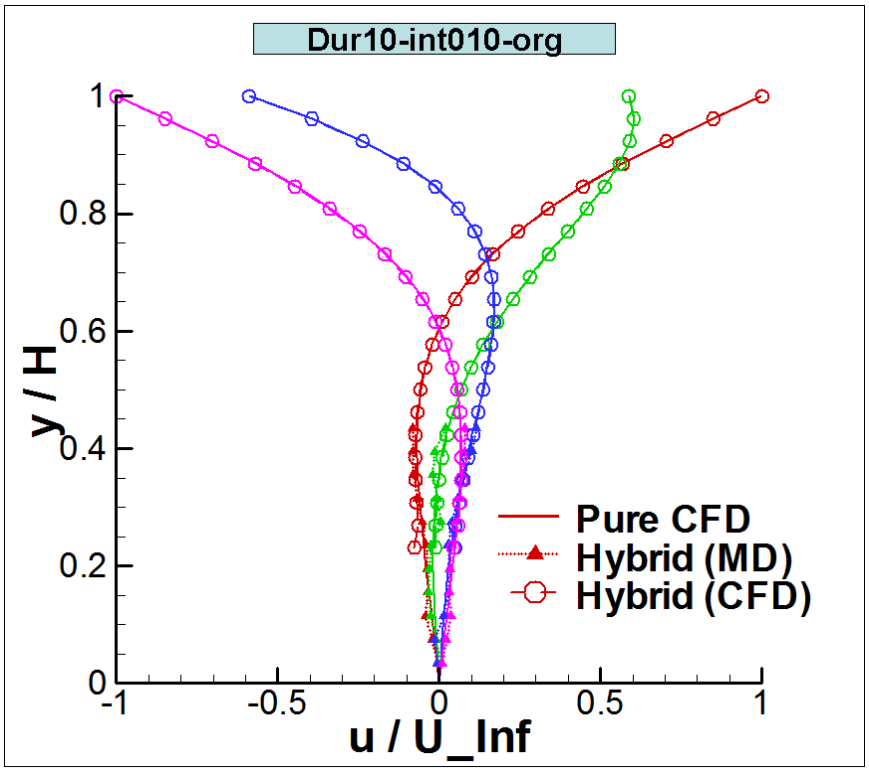


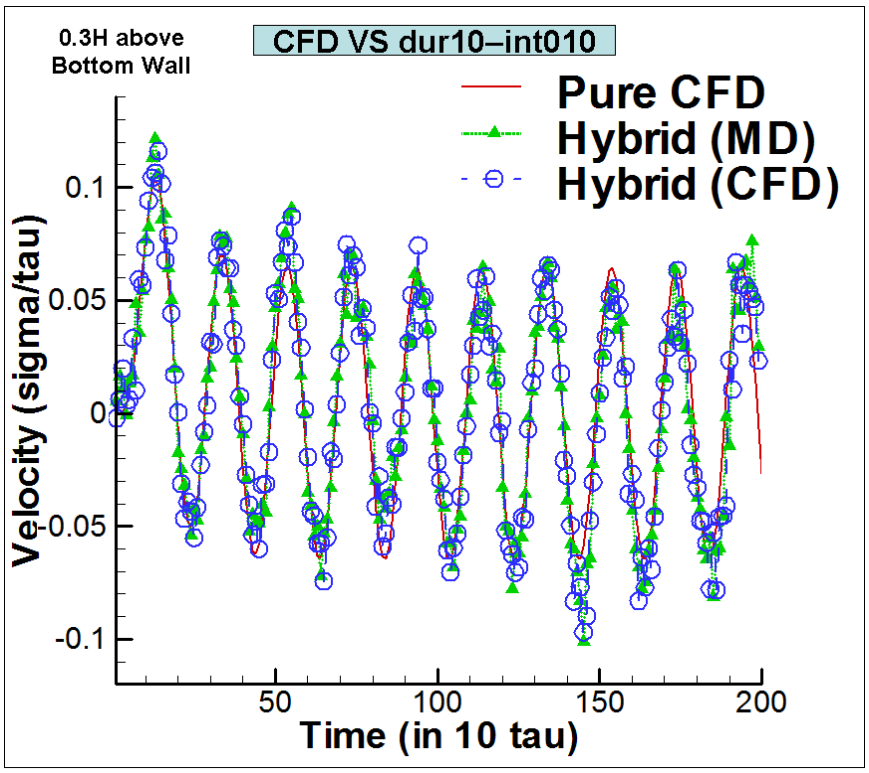
- Original (with extrapolation) + sampling duration 5 tau + sampling interval 5 tau



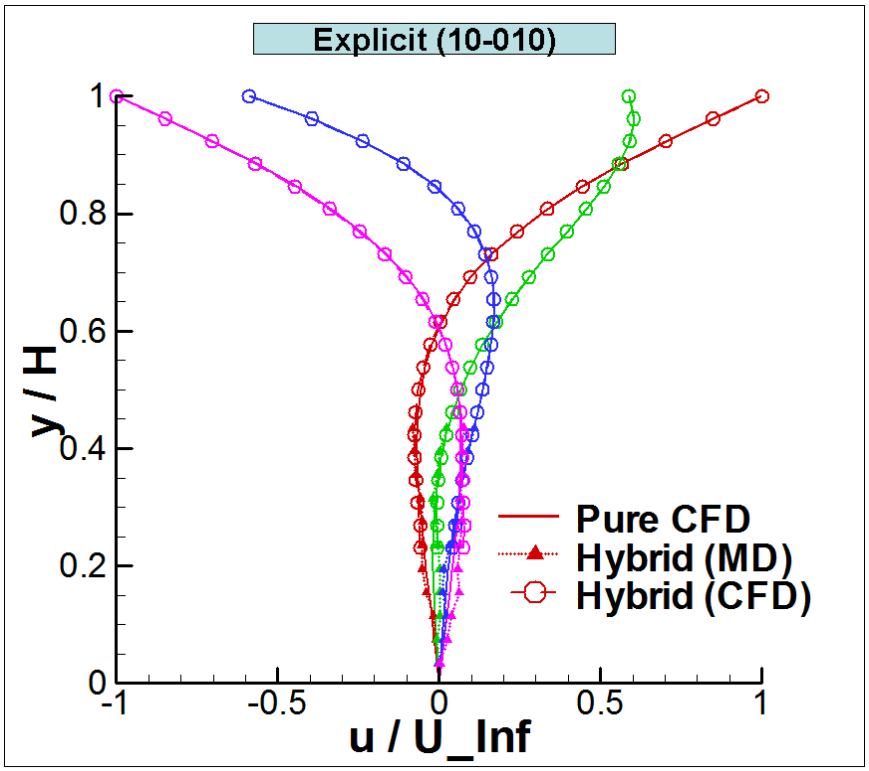


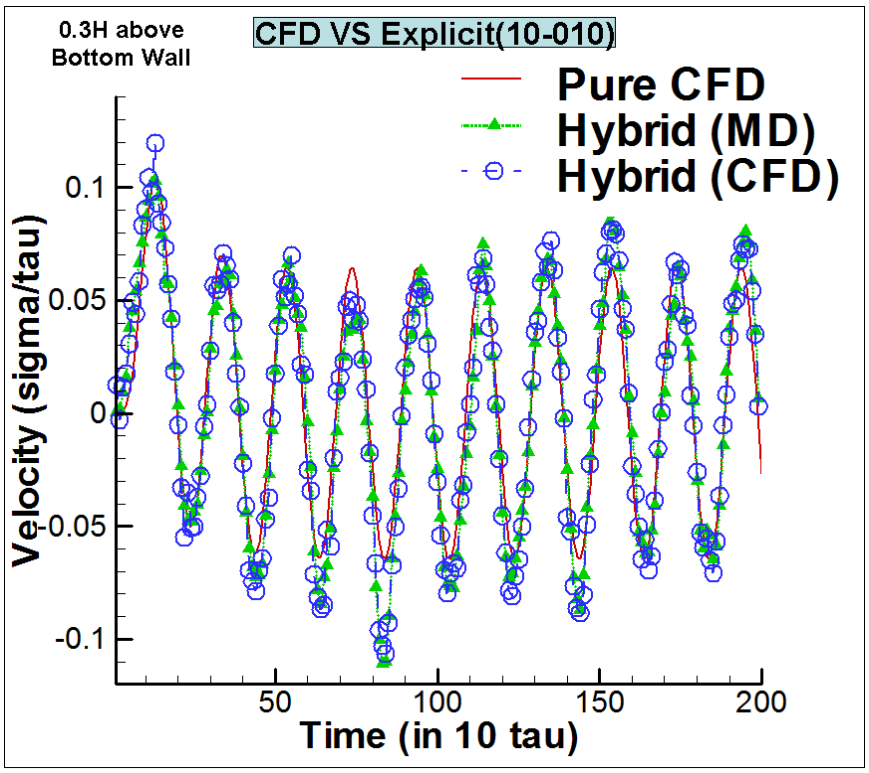
- Original (with extrapolation) + sampling duration 10 tau + sampling interval 10 tau





- Modified + sampling duration 10 tau + sampling interval 10 tau





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So, I'd like to discuss on what we shall emphasize in this paper.

What we have now is

1. how to determine the sampling condition (sampling duration) by pure MD simulation: it could be an item on the paper, not a standalone. To be a standalone, computation of error on various system sizes shall be conducted and it should be functioned (also mathematical investigation should be added) Also, this shall include which problems can be solved by hybrid CFD-MD, which problem is effective.

2. temporal coupling scheme: find out in which condition this technique is producing better solution by changing oscillating amplitude and frequency. This requires more experiments with various physical conditions and it is uncertain whether we can find good test problems.

3. water simulation: can be a standalone paper if some discussion is included on constrained Lagrangian dynamics. But a lot of change and inclusion on water modeling, simulation, etc. needs to be included.

4. BigJob for co-scheduling and load balancing: more discussion on 'generic interface' and 'load balancing capability' needs to be included. Also more experiments need to be included.