Dual Domain Material Point Method with Sub-points for Thermodynamic Nonequilibriums

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ABSTRACT

In this talk, we show a recent improvement [1] of the dual domain material point (DDMP) method [2] using sub-points and its application to multiscale calculations of thermodynamically nonequilibrium systems. In many cases, thermodynamic nonequilibriums are caused by significant strain rates that often result in extremely large material deformation. In these systems, traditional equation of state or constitutive relation is difficult to obtain, and the material response is usually history dependent. To bypass the need for the constitutive relations while computing continuum scale phenomena, we perform multiscale computations starting from the molecular scale. The Lagrangian capability of the material point method shows great advantage in tracking history of the material as it undergoes an extremely large deformation.

To perform such a numerical calculation for the continuum scale physics, multi-processing is invertible for a practical problem. Another significant advantage of the material point method is that there is no need for material points to communicate with each other directly. This property is very advantageous for parallel computing, because stresses on the material points can be calculated independently using different processors or threads.

Taking this advantage, in our multiscale calculation, we use the DDMP method to perform continuum level calculation, and use molecular dynamics (MD) simulations to calculate the stresses at the material points [3]. An MD system is setup for each material point, and its history is tracked throughout the entire calculation. The MD system communicates with the DDMP calculation through the strain rate and stress. The strain rate at a material point is communicated to the MD simulation, whereas the stress calculated from the MD simulation is used to drive the DDMP calculation. To accelerate, the MD calculations are performed in parallel in a GPU using CUDA. Examples of shock wave propagation in cerium and jet formation around copper notch are presented.

Work supported by the Next Generation Code Project.

REFERENCES

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