

MULTI-SCALE SIMULATIONS IN ENERGY AND ENVIRONMENTAL ENGINEERING

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PROPOSAL

Scope of the minisymposium: Almost all problems have multiple scales in nature . Because of the limitation in computer resources in the past we mainly concentrated our attention at the individual level. In recent years numerical approaches at different geometric levels have been developed very fast: FVM and FEM for macroscale level, LBM and DSMC for mesoscale, and MDS for microscale. In spite of the tremendous successes achieved the three-level numerical approaches have their own limitations. For the macro-type method, the major limitation is the complete neglect of microscopic mechanism and hence the introduction of some empirical parameters or ad hoc assumptions. On the other hand, the meso-scale or micro-scale methods, even though can reveal the details of a complex meso-scale or micro-scale process, usually require enormous computer resources. One very useful approach is: only flow regions that require molecular resolution are treated by MDS, DSMC/LBM are adopted for regions which require mesoscale resolution, and a continuum simulation method everywhere else. This is the multiscale simulation. The major issue is how to transfer the information at the coupling interface to make the entire simulation stable and efficient. In this minisymposium different coupling methods will be presented.

Importance and applications. The importance of the multiscale simulation can be well understood from following two examples. The launching process of a spacecraft provides an example where the fluid flow around the spacecraft experiences from continuum to rarefied gas flow regimes and different numerical approaches should be used in different regimes. The 2nd example is the transport process in a proton exchange membrane fuel cell, where the fuel gas flow in polar plate channels, the diffusion process in the gas diffusion layer and the reaction at the catalyst layer occur at the geometric scales of millimeters, micrometers and nanometer respectively. Present numerical simulations are based on the macroscale method by including more than ten empirical parameters whose values are selected with great uncertainty. Only multiscale simulation may avoid such unpleasant situation.

REFERENCES

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