Special Program in Applied Mathematics and Applied Mechanics

Accurate Gradient Approximation for Complex Interface Problems in 3D by an Improved Coupling Interface Method

2013 - 09 - 11 (Wed.)
15:00 - 17:00
308, Mathematics Research Center Building (ori. New Math. Bldg.)

Most elliptic interface solvers become complicated for complex interface problems at those "exceptional points" where there are not enough number of neighboring interior points for high order interpolation. Such complication increases especially in three dimensions. Usually, the solvers are thus reduced to low order accuracy. In this paper, we make classification of these exceptional points and propose two recipes to maintain order of accuracy there. The proposed recipes are to improve our previous method, the coupling interface method, but the idea is also applicable to other interface solvers. The main idea is the follows. The goal is to have at least first order approximation for second order derivatives at those exceptional points. Recipe 1 is to use the finite difference approximation for the second order derivatives at a nearby interior grid, if it is available. Recipe 2 is to flip domain signatures and introduce a ghost state so that a second-order method can be applied. This ghost state is a smooth extension of the solution at the exceptional point from the other side of the interface. The original state is recovered by a post-processing using nearby states and jump conditions. The choice of recipes is determined by a classification of the exceptional points. The method renders the solution and its gradient uniformly second-order accurate in the entire computed domain. Careful numerical tests are performed to show second order accuracy for gradients for complex interface problems in two and three dimensions, including a real molecule (1D63) which is composed hundreds of atoms.