Quadruple arithmetic computation for FreeFEM with application to a semi-conductor problem

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For some semi-conductor problem it is known that double precision arithmetic computation is not sufficient, because the condition number of the stiffness matrix is extremely large, more than 1e+14. This is caused by an approximation of the drift terms in the current density of electron/hole by weighted exponential function with electrostatic potential. The range of the potential around 35 leads to 1e+16 in exponential weight.

Hence, it is mandatory to use quadruple precision arithmetic with 33 significant digits in both calculation of finite element matrix and linear solver. Thanks to "qd" library that is written by C++ for double-double data structure, such high precision computation is feasible in acceptable computational time.

The system for the current density of electron/hole is formulated by mixed type with the gradient of the density distribution of electron/hole and so-called Slotboom variable of them. This pair of unknowns can avoid extra error in discretization of exponential weight with electro-static potential and leads to a symmetric weak form. For discretized of divergence space for the gradient, Raviart-Thomas element is used and element stiffness matrix consists of element-wise mass matrix with exponential weight and divergence term.

For RT0 element, the element stiffens matrix can be computed by using exact formula or by numerical quadrature with table of integration points and weights in quadurple precision number, which is generated by numerical optimization procedure. Obtained linear system in nonlinear Newton iteration to resolve the coupling of electrostatic potential and electron/hole density is solved by "Dissection" sparse linear solver in quadruple precision, because the solver is also written by C++ template.

This work is supported by KIOXIA in Japan.