Accelerated PVT flash calculations using GPUs

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The numerical solution of the compositional model requires calculations of thermodynamic equilibrium between the phases of the system. For each time step the following unknowns are solved: pressure [P] (for oil and gas), temperature [T], velocity [u] and saturation [S] (for each phase). At an intermediate stage of the solution of these variables, the thermodynamic equilibrium of the system has to be updated performing flash calculations, establishing new mass balance among the phases. This operation must be performed for each node (control volume) of the mesh, with the new P and T updates at each time step [t]. The outputs of flash calculations for each phase are; molar fractions [z_i], molar volume [Vmix_i] and fugacity [Fc_i], necessary to proceed with the solution of the compositional equation system. The Flash calculations are modularized in a single class (C++ function), which includes one loop for error minimization and a nested Newton-Raphson loop, roughly this are the main operations and would be our Kernel in the GPUs. We benefit from the complete data independence between neighbor nodes and previous time steps. This way for every time step, each thread of the GPU performs a flash calculation per node of the mesh, updating into the GPU's memory its pressure and temperature of the corresponding node. Performance improvement will be sought by analyzing mesh access patterns and using the appropriate memory type in the CUDA memory hierarchy.