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The Application of High-dimensional Sparse Grids in Flash Calculations: from Theory to Realisation

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Abstract

Flash calculations are a performance bottleneck of compositional flow simulations. Some work has demonstrated the feasibility of using sparse grid techniques to remove the bottleneck, but a complete realisation of the idea is still not available. Thus, this work fills the niche. By introducing a new concept of layer to sparse grid points, the sparse grid construction can become much efficient. As a result, a much easier data structure the array can be used to store the sparse grids. Compared with the popular data structures to store the sparse grids such as the hash table and the tree, the array can minimize the space size and the traversing time, and at the same time reduce the number of points in the sparse grids by removing the architecture ancestors in the tree, which in turn makes parallelization of flash calculations come true. All of them are not only contributions to flash calculations, but also contributions to existing sparse grid techniques. Moreover, both of the sparse grid construction and interpolation algorithms can be done in parallel. Different from the former parallel algorithms in sparse grid techniques, which have troubles in decomposing the domain equally and keeping load balance among the processors, our parallel algorithm can achieve load balance easily among the threads for any sparse grid configurations. Lastly, multicomponent experiments are also carried out to demonstrate the accuracy, correctness and efficiency of the algorithms.

Introduction

A flash calculation is an important computing routine in compositional flow simulations ([1][2][3][4]). According to different conditions, flash calculations can be classified as P-T, P-H, P-S, U-V, S-V and V-T flash calculations ([5][6][7][8][9]). Traditionally, it is P-T flash calculations that are used in compositional flow simulations. Therefore, in this work, P-T flash calculations are discussed, and the work on the other flash calculations will be left to the further work. The concept of P-T flash calculations can be stated as this: given pressure p and temperature T, a mixture of c components with the molar fraction of each component being z_m can be divided into the oil phase and gas phase, in which the molar fraction of each component is x_m and y_m, respectively, $m = 1, \dots, c$. In other words, a P-T flash calculation is a routine to compute x_m and y_m, given p, T and z_m. However, in compositional flow simulations, usually T is constant, and p and z_m are changed with the progress of simulations. Moreover, there is $\sum_{m=1}^{c} z_m = 1$, which means z_c can be derived from $z_m, m = 1, \dots, c-1$. Thus, in compositional flow simulations, P-T flash calculations can be expressed as

$$(x_1, \dots x_c, y_1, \dots, y_c) = f(p, z_1, \dots, z_{c-1}), \tag{1}$$

but the expression of f is unknown. The main issue of P-T flash calculations in compositional flow simulations is that the time to finish the routine is huge and it often accounts for more than 70% of total simulation time [10]. When c is larger, the percentage can be more, which hints that P-T flash calculations have become a bottleneck of compositional flow simulations. More notes on P-T flash calculations can be referenced to [11]. Below, P-T flash calculations are called flash calculations for short.

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