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Application of GPU-Based Computation in Chemical and Safety Engineering

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Keywords: GPU acceleration; vapor-liquid equilibrium; reaction-diffusion systems; CSTR modeling; global sensitivity analysis; numerical methods

The work is focused on investigation of the possibilities of using GPU-accelerated computations in chemical and safety engineering, with an emphasis on evaluating their practical applicability for solving computationally demanding problems and on comparing different approaches to parallelization. The study considers implementations in MATLAB using the Parallel Computing Toolbox as well as lower-level approaches based on the ILGPU library in C#.

As a first part of the solution, a mathematical model describing vapor-liquid equilibrium (VLE) for a binary ethanol-benzene system was developed. The model is based on a modified Raoult's law combined with the NRTL activity coefficient model and requires repeated numerical solution of a nonlinear equation for equilibrium temperature. Due to the large number of independent evaluations, the problem was suitable for parallelization. Sequential, vectorized, and GPU-based implementations were created and compared. The results showed that GPU acceleration provides a significant reduction in computation time, achieving a speed-up of up to 140× times, compared to the sequential CPU implementation.

In the second part, a custom numerical solver for systems of ordinary differential equations based on an adaptive Runge-Kutta method was developed and applied to a dynamic model of a continuous stirred tank reactor (CSTR). The model including reaction kinetics, heat balances and mass balances, was used to perform large sets of independent simulations with randomly generated input parameters. These simulations were further analyzed using Monte Carlo methods and the Morris method for global sensitivity analysis. In this case, GPU acceleration

enabled efficient processing large number of simulations, achieving a 74× times speed-up compared to sequential implementation.

Third part of the work focused on a two-dimensional reaction-diffusion model describing the coupled transport of chemical species and heat with an exothermic reaction. The model is formulated as a system of nonlinear partial differential equations and solved using an explicit finite difference method on a spatial grid. In contrast with previous cases, parallelization was applied within a single simulation by distributing computations across spatial grid points. The results demonstrated that this type of data-parallel problem is also suited for GPU acceleration, with a speed-up of approximately 26×.

The obtained results indicate that GPU-based approaches can significantly reduce computational time across a wide range of problems in chemical and safety engineering.