GPUE: Graphics Processing Unit Gross-Pitaevskii Equation solver

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Summary

Bose–Einstein Condensates (BECs) are superfluid systems consisting of bosonic atoms that have been cooled and condensed into a single, macroscopic ground state (Pethick & Smith, 2008, Fetter (2009)). These systems can be created in an experimental laboratory, and allow for the the exploration of many interesting physical phenomenon, such as superfluid turbulence (Roche & Barenghi, 2008, White, Anderson, & Bagnato (2014), Navon, Gaunt, Smith, & Hadzibabic (2016)), chaotic dynamics (Gardiner, 2002, Kyriakopoulos, Koukouloyannis, Skokos, & Kevrekidis (2014), Zhang (2017)), and as analogues of other quantum systems (Dalibard, Gerbier, Juzeli|unas, & Öhberg, 2011). Numerical simulations of BECs allow for new discoveries that directly mimic what can be seen in experiments and are thus highly valuable for fundamental research. In practice, the dynamics of BEC systems can often be found by solving the non-linear Schrödinger equation known as the Gross–Pitaevskii Equation (GPE),

$$\frac{\partial \Psi(x,t)}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial}{\partial x^2} + V(x) + g|\Psi(x,t)|^2 \right)\Psi(x,t),$$

where $\Psi(x,t)$ is the one-dimensional many-body wavefunction of the quantum system, m is the atomic mass, $V(\mathbf{r})$ is a potential to trap the atomic system, $g = \frac{4\pi\hbar^2 a_s}{m}$ is a coupling factor, and a_s is the scattering length of the atomic species. Here, the GPE is shown in one dimension, but it can easily be extended to two or three dimensions. Though there are many methods to solve the GPE, one of the most straightforward is the split-operator method, which has previously been accelerated with GPU devices (Ruf, Bauke, & Keitel, 2009, Bauke & Keitel (2011)); however, there are no generalized software packages available using this method on GPU devices that allow for user-configurable simulations and a variety of different system types. Even so, there are several software packages designed to simulate BECs with other methods, including GPELab (Antoine & Duboscq, 2014) the Massively Parallel Trotter-Suzuki Solver (Wittek & Cucchietti, 2013), and XMDS (Dennis, Hope, & Johnsson, 2013).

GPUE is a GPU-based Gross-Pitaevskii Equation solver via the split-operator method for superfluid simulations of both linear and non-linear Schrödinger equations, with an emphasis on Bose–Einstein Condensates with vortex dynamics in 2 and 3 dimensions. GPUE provides a fast, robust, and accessible method to simulate superfluid physics for fundamental research in the area and has been used to simulate and manipulate large vortex lattices in two dimensions (O'Riordan, White, & Busch, 2016, O'Riordan & Busch (2016)), along with ongoing studies on vortex turbulence in two dimensions and vortex structures in three dimensions.

For these purposes, GPUE provides a number of unique features: 1. Dynamic field generation for trapping potentials and other variables on the GPU device. 2. Vortex tracking in 2D and vortex highlighting in 3D. 3. Configurable gauge fields for the generation of artificial magnetic fields and corresponding vortex distributions (Dalibard et al., 2011,Ghosh & Sachdeva (2014)). 4. Vortex manipulation via direct control of the wavefunction phase (Dobrek et al., 1999).

All of these features enable GPUE to simulate a wide variety of linear and non-linear (BEC) dynamics of quantum systems. The above features enable highly configurable physical system parameters, and allow for the simulation of state-of-the-art system dynamics. GPUE additionally features a highly performant numerical solver implementation, with performance greater than other available suites ("Comparing three numerical solvers of the gross-pitaevskii equation," n.d., O'Riordan (2017)). All GPUE features and functionalities have been described in further detail in the documentation (Schloss & O'Riordan, n.d.).

Acknowledgements

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