CUDA IMPLEMENTATIONS FOR THE ACCELERATION OF MICRORHEOLOGY MODELS

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1. Abstract

- Complex fluids are characterized with both solid and fluid proprieties by their elasticity and viscosity, or **rheological properties**.
- Recently, **microrheology** has been developed as an accurate technique to obtain rheological properties (i.e. friction coefficient) in soft matter from the microscopic motion of colloidal tracers used as probes.
- A drawback for these techniques is their **high computational cost → High Performance Computing** is mandatory to develop the fastly computed microrheology models (see Figure 1).
- **OBJECTIVE:** **To accelerate existing microrheology models based on simulations of a tracer in a bath of Brownian quasi-hard spheres using GPU computing, and evaluate performance on a modern GPU.**

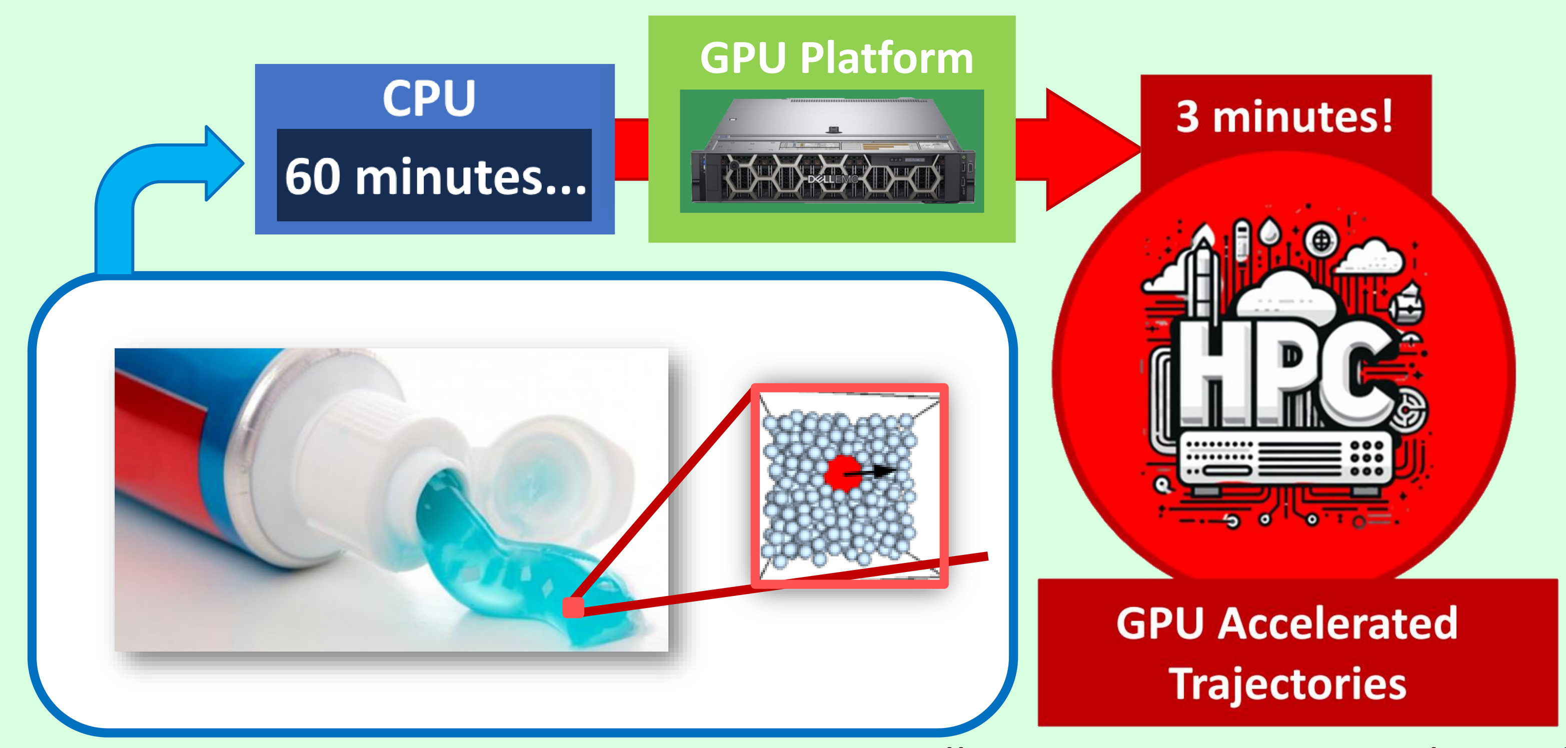

Figure 1*: Illustrative GPU accelerated microrheology model example*

2. Description of the models

The problem of microrheology in colloidal systems of hard spheres was confronted through particle simulations.
In the simulation of Brownian systems, a friction force with the solvent and a random force must be considered in addition to the direct interaction forces. The friction force is proportional to the particle velocity, and the random force is linked to the friction coefficient via the fluctuation dissipation theorem. The final equation for particle *j* reads,

$$m\frac{d^2\mathbf{r}_j}{dt^2} = \sum_i \mathbf{F}_{ij} - \gamma_0\frac{d\mathbf{r}_j}{dt} + \boldsymbol{\eta}_j(t) \quad (+\mathbf{F}_{\text{ext}})$$

$\mathbf{F}_{ext}$ is a constant external force that is applied only to the tracer particle (all particles undergo Brownian motion, but only the tracer is pulled). The simulations are run in a cubic box, with *N* particles and periodic boundary conditions.

In previous simulations of microrheology, the system with the (large) tracer particle is equilibrated, and at time *t=0* the tracer starts to be pulled with a constant force through a dense bath of hard colloids. However, as part of this research work, **a second generic model was developed**, where the time during which the force is exerted on the tracer called t_{off}, starting at time *t=0* can be defined (see Figure 2).

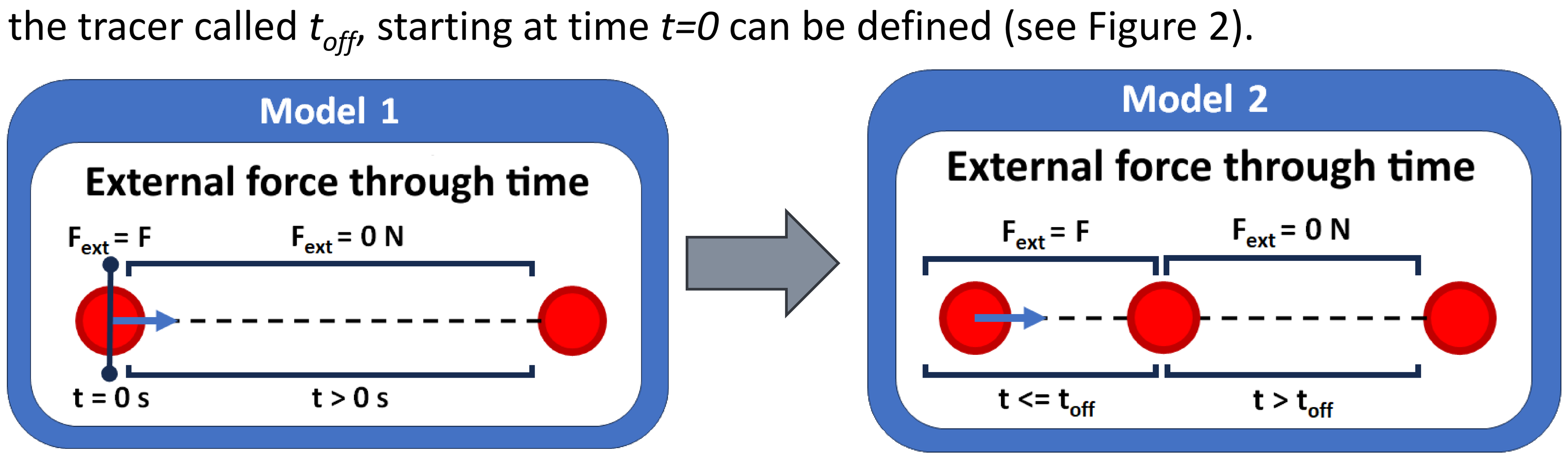

Figure 2*: Original microrheology model (Model 1), and newly developed model where the force is temporarily and constantly exerted (Model 2).*

In either model, the main **output** of the simulation is **the trajectory of the tracer**, that yields the **effective friction coefficient from its average velocity**, using the relation $\mathbf{F}_{ext} = \gamma_{eff}$ (**v**), valid for the stationary regime (see Figure 3). To obtain an accurate friction coefficient, it is necessary to run many simulations in a reasonable time.

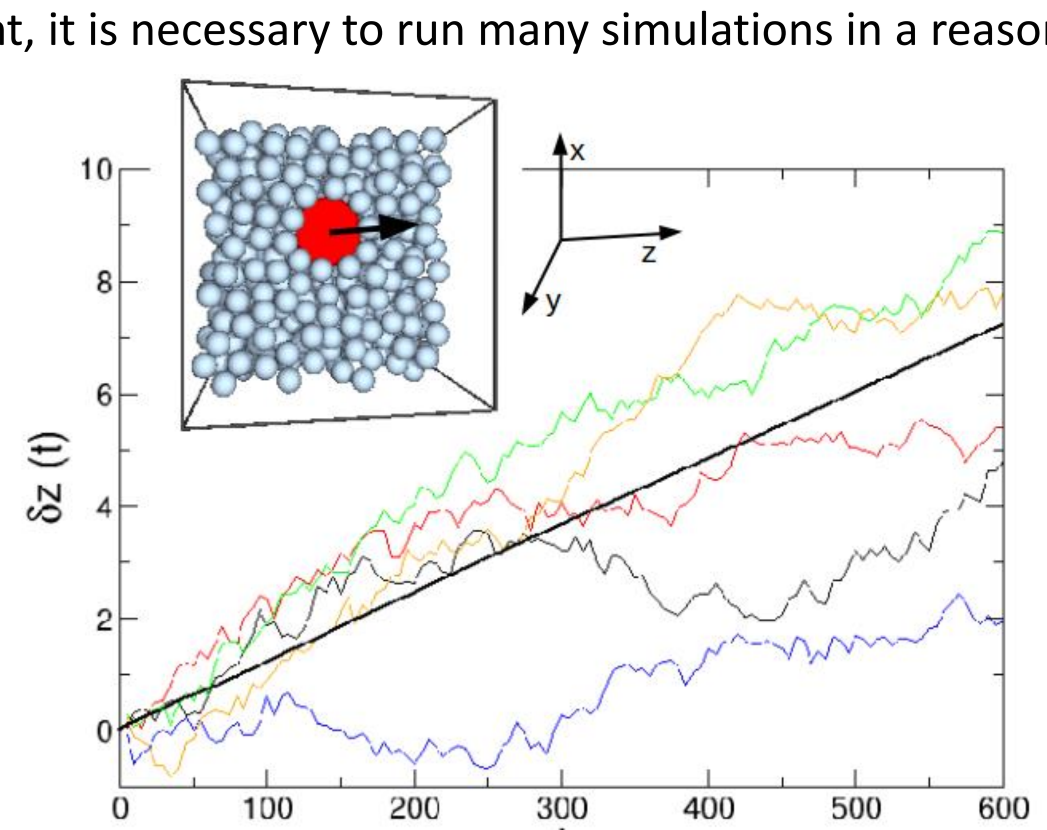

Figure 3*: Five trajectories of the tracer (thin lines) and average trajectory (thick line). δz(t) axis represents the tracer advance in the* $\mathbf{F}_{ext}$ *direction at the instant t.*

To obtain γ_{eff} **the following nested iterative procedures** in bottom-up order have to be computed, from which only **Level 1 was parallelized by means of a GPU**:

- A tracer trajectory in the $\mathbf{F}_{ext}$ direction, referred to as T_i for a specific number of bath particles and its corresponding system size, *L(N)*. (Level 1)
- The recording of *ntraj* trajectories (T_i) and calculation of their average, *T*, for a specific value of *L(N)*. (Level 2)
- The computation of *T* for several values of *L(N)*. (Level 3)

3. Evaluation and results

Microrheology problems have been executed and evaluated on platforms with a GPU using CUDA (11.0) and C as interfaces. Due to their various factors, two evaluation sets were created to correctly evaluate them, **the first one evaluating different particle amounts**, and the **second different tracer radiuses** (see Figure 4). The number of **trajectories and the total time steps of every trajectory are 5 and 50**, respectively.

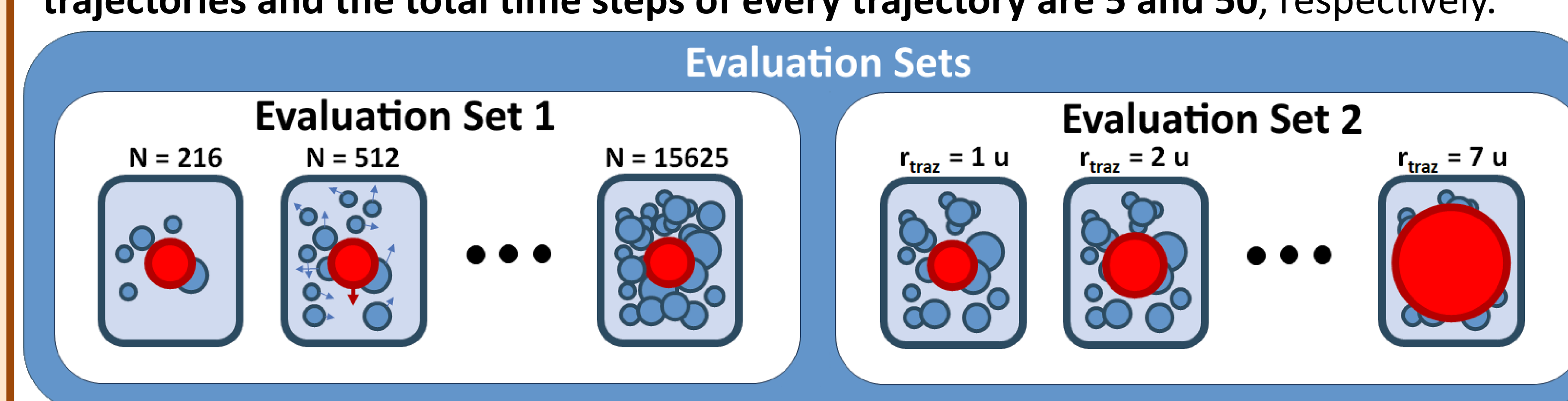

Figure 4*: Evaluation sets used in the simulations of the models.*

The modern computational architecture is: *Dell PowerEdge R7425 AMD EPYC 7301 (32 CPU-cores, 64-GB RAM), with a Volta V100 GPU*. The previous computational architectures are: *(1) Bullx R421-E4 Intel Xeon E5 2620v2 (12 CPU-cores, 64-GB RAM) with a NVIDIA K80 GPU (Kepler GK210) and (2) Bullx R424-E3 with a Tesla M2070 GPU.*

The first evaluation set's results showed improvements of the modern computation architecture over the previous ones, showing speedup factors up to **29x against the NVIDIA K80 GPU**, and up to **33x against the Tesla M2070 GPU** (see Figure 5). Additionally, a speedup factor of **30x was made against the sequential version** in the modern one. The second evaluation set was **only computed on the modern one,** as it was found early that **the tracer radius did not influence performance.**

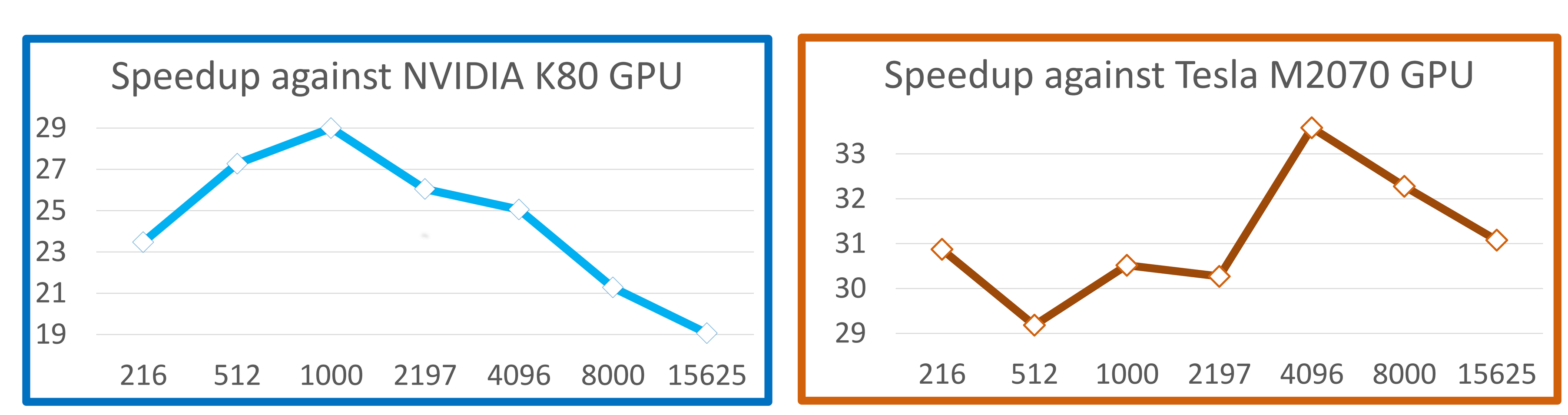

Figure 5*: First evaluation set's speedup factor of the Volta V100 architecture over the previous ones. The versions used are the GPU-accelerated ones.*

Conclusions

- An improved microrheology model has been developed and described.
- The new model has been shown to produce accurate values of the friction coefficient of colloidal systems if the number of particles is large.
- Significant hardware-based improvements have been proven thanks to new GPU architectures.
- The tracer radius has been proven not to have an influence on performance.
- Futures works are related to the exploitation of the computational resources of a multi-GPU cluster in order to obtain a faster output of microrheology models of interest, or the development of a web application to ease the process of trajectory visualization as well as the uploading or downloading of input and output files.

Acknowledgements

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