A modular, GPU-based, direct-summation $N-$body integrator

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Introduction

Motivation

- Dynamical evolution of a dense stellar systems. (N-body Problem)
- Newtonian systems compounded by more than two stars, needs numerical approaches.
- Evolution of the High Performance Computing (HPC).

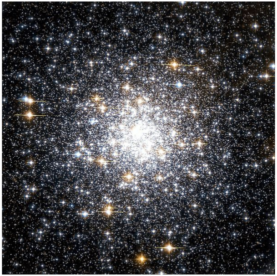


Figure : Globular cluster "Messier 69" in the constellation Sagittarius.

Introduction

N-body algorithms classification

Collision-less A star just sees the background potential of the rest of the stellar system. A model of this situation is the Barnes-Hut Treecode with a complexity $O(N \log N)$ [1] or the fast multipole method with $O(N)$ [2].

Collisional ("direct-summation") One star integrates all gravitational forces for all stars. This typically scale as $O(N^2)$. A well-known example is the family of algorithm of Aarseth the direct-summation NBODY integrator [3, 4, 5] or KIRA code [6].

Introduction

The computational challenge

- The N-body codes evolution is related to the available hardware in our time.
- The algorithms with a complexity of $O(N^2)$ require supercomputers.
  - e.g beowulf clusters, which require a parallelization of the code (NBODY6++ developed by Spurzem et al. [4]).
  - Special-purpose hardware, like the GRAPE (short for GRAvity PipE system [7, 8, 9, 10].
- The literature overview reveals a strong interest on porting the existing codes to the GPU architecture, like e.g. the work of [11, 12, 13] on single nodes or using large clusters [14, 15, 16].

The N-body problem

Definition

Purely dynamic problem, in which the bodies orbital evolution is determined exclusive by the gravitational interaction,

$$\ddot{\boldsymbol{r}}_i = -G \sum_{\substack{j=1 \\ j \neq i}}^{N} m_j \frac{(\boldsymbol{r}_i - \boldsymbol{r}_j)}{|\boldsymbol{r}_i - \boldsymbol{r}_j|^3}, \quad (1)$$

where G is the gravitational constant ($6.67384 \times 10^{-11} m^3 kg^{-1} s^{-2}$), m_j is the mass of the jth particle and $\boldsymbol{r}_j$ the position in *Cartesian* coordinates.

Note

We denote vectors by bold fonts.

The N-body problem

Checking the system evolution

- The initial condition are usually the masses, position and velocity.
- Chaotic nature, the evolution of this systems will depend of the initial parameters.
- The often invariant to check the integration of the system, is the system's energy,

$$E = \frac{1}{2}\sum_{i=1}^{N} m_i \boldsymbol{v}_i^2 - \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{G m_i m_j}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}, \tag{2}$$

where $\boldsymbol{v}_i$ is the velocity of the particle i.

The N-body problem

Particle's time steps

- The real scenario, individual time steps.
  - Hard scenario for parallel computing.
- Forming groups of particles, block time steps scheme [17].
  - This time step scheme is popular among N-body code, like Starlab [18, 19], Aarseth N-body codes [3, 5, 15], ϕGRAPE [20], which gives us the possibility to check our algorithm behavior.

GPU Computing

Introduction

- *“Using a GPU (Graphic Processing Unit) together with a CPU to accelerate scientific calculation operations or general purpose calculation”*

Figure : NVIDIA® GTX Titan

GPU Computing

Features

- CPU,
  - Designed to have a good performance in parallel and non-parallel scenarios.
  - Minimizes the latency experimented by a thread (large cache memory)
- GPU,
  - Designed to perform highly parallel work.
  - Maximizes the throughput of all the threads.

Performance

Capacity of perform individual instructions in a certain time.

Latency

Measure of time delay experienced in a system.

Throughput

Capacity of perform a whole task in a certain time.

GPU Computing

Architecture

Task parallelism

Each processor perform a different task.

Data parallelism

Each processor perform the same task, but not on the same data set.

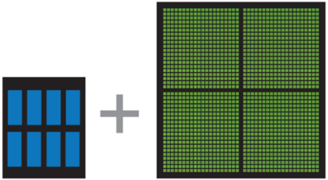


Figure : GPU and CPU core scheme

GPU Computing

Functionality

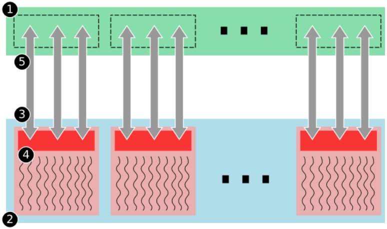


Figure : CUDA Programming strategy

1. CPU memory allocation,
2. GPU memory allocation,
3. Data copying, CPU $\rightarrow$ GPU,
4. Task execution on the data,
5. Data copying, GPU $\rightarrow$ CPU,

Implementation

Integrators details

- The code structure,
- Integration scheme,
- Parallelization scheme.

Implementation

The code

- Main goal in the development, legibility.
  - Easy to read, modify and understand,
- Balance between optimization and maintainability.

Implementation

The code

For the development of GRAVIDY , we have followed the next steps:

- Serial implementation,
- Profiling and performance assessment,
- Parallelization of the hot-spots,
- Optimization,

Note

The same as CUDA C Best Practices [21], called the APOD cycle, (Assess, Parallelize, Optimize and Deploy).

Implementation

The code

- OOP and SoA.
- Double-precision, importance of accuracy.
  - on GPU, this reach the half of the theoretical maximum performance peak.
  - NVIDIA Tesla C2050/M2050, single precision peak in GFLOPs is 1030.46, and only 515.2 with double precision.

Note

A posible future upgrade is to use mixed-precision [22], or pseudo double-precision [23] to achieve a better performance in our code.

Prediction-correction method

Introduction

In a *N*-body system

The force acting on each particle varies smoothly.

- Interpolation for the time interval extension (prediction).
- Reduce the amount of the force calculation.
- By finite differences it is possible to get the higher order derivatives of the force, which are used to add precision (correction).

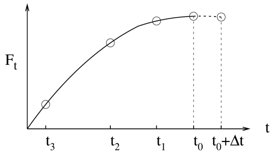


Figure : Polynomial fit of the gravitational force in function of time.

Prediction-correction method

Block time steps

- Reduce the amount of predictions,
- Enhance the parallelism,
- Based on an adaptive system.

$$\Delta t_i = \sqrt{\eta \frac{|\boldsymbol{a}_i||\boldsymbol{a}_i^{(2)}| + |\boldsymbol{a}_i^{(1)}|^2}{|\boldsymbol{a}_i^{(1)}||\boldsymbol{a}_i^{(3)}| + |\boldsymbol{a}_i^{(2)}|^2}}, \qquad (3)$$

Block definition

$2^n \Delta t_s \leq \Delta t_i < 2^{n+1} \Delta t_s$

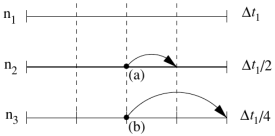


Figure : Time step hierarchical levels.

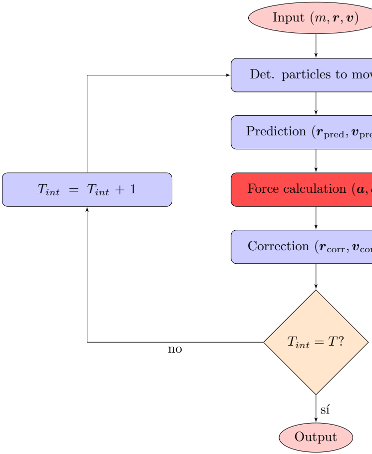
Prediction-correction method

Hermite scheme

Prediction

$$\boldsymbol{r}_{i,pred} = \boldsymbol{r}_{i,0} + \boldsymbol{v}_{i,0}\Delta t_i + \frac{1}{2!}\boldsymbol{a}_{i,0}\Delta t_i^2 + \frac{1}{3!}\dot{\boldsymbol{a}}_{i,0}\Delta t_i^3 \quad (4)$$

$$\boldsymbol{v}_{i,pred} = \boldsymbol{v}_{i,0} + \boldsymbol{a}_{i,0}\Delta t_i + \frac{1}{2!}\dot{\boldsymbol{a}}_{i,0}\Delta t_i^2 \quad (5)$$



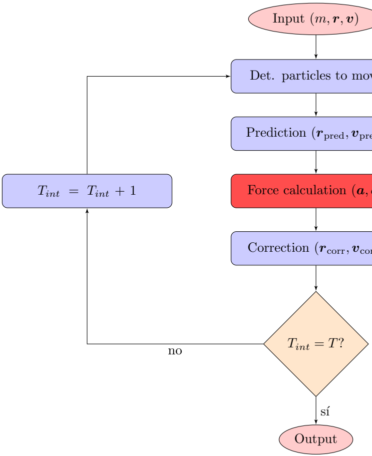
Prediction-correction method

Hermite scheme

Force calculation

$$\boldsymbol{a}_{i,1} = \sum_{\substack{j=0 \\ j \neq i}}^{N} G m_j \frac{\boldsymbol{r}_{ij}}{(r_{ij}^2 + \epsilon^2)^{\frac{3}{2}}}, \tag{6}$$

$$\dot{\boldsymbol{a}}_{i,1} = \sum_{\substack{j=0 \\ j \neq i}}^{N} G m_j \left[\frac{\boldsymbol{v}_{ij}}{(r_{ij}^2 + \epsilon^2)^{\frac{3}{2}}} - \frac{3(\boldsymbol{v}_{ij} \cdot \boldsymbol{r}_{ij})\boldsymbol{r}_i}{(r_{ij}^2 + \epsilon^2)^{\frac{5}{2}}} \right], \tag{7}$$



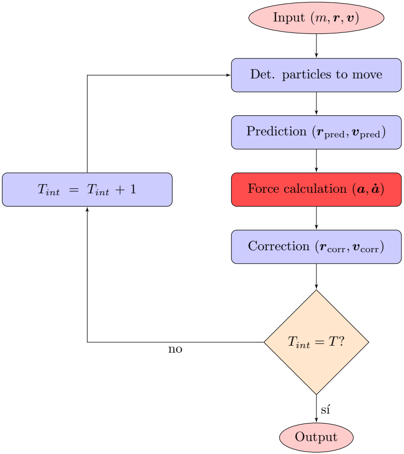
Prediction-correction method

Hermite scheme

Correction

$$\boldsymbol{r}_{i,1} = \boldsymbol{r}_{i,pred} + \frac{1}{24}\Delta t_i^4 \boldsymbol{a}_{i,0}^{(2)} + \frac{1}{120}\Delta t_i^5 \boldsymbol{a}_{i,0}^{(3)} \tag{8}$$

$$\boldsymbol{v}_{i,1} = \boldsymbol{v}_{i,pred} + \frac{1}{4}\Delta t_i^3 \boldsymbol{a}_{i,0}^{(2)} + \frac{1}{24}\Delta t_i^4 \boldsymbol{a}_{i,0}^{(3)} \tag{9}$$



Parallelization scheme

Force calculation

for i in $N_{act}[\,]$

  for j in $N[\,]$

    force_calculation(i,j)

Figure : Force calculation code illustration. The process itself belongs to a second level `for` loop. Thanks to the integrator scheme, we have a reduction of the step complexity from $O(N^2)$ to $O(N_{act}N)$

Parallelization scheme

Calculation relations

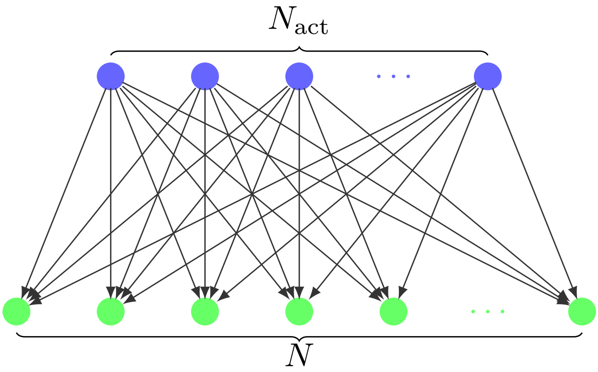


Figure : Relation between the particles which will be updated in a certain integration time (N_{act}) and the whole set of particles (N). The relation between the active particles and the others is $N_{\mathrm{act}} << N$

Parallelization scheme

Threads task

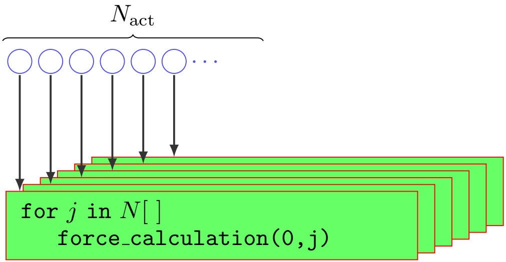


Figure : For each $i-$particle in N_{act} a `for` will be through the whole set of particles and perform the calculation of the gravitational interaction between i and N particles. The scheme could be know as $i-$parallelization, since it assumes that each thread will be one N_{act} particle.

Parallelization scheme

Tiles scheme

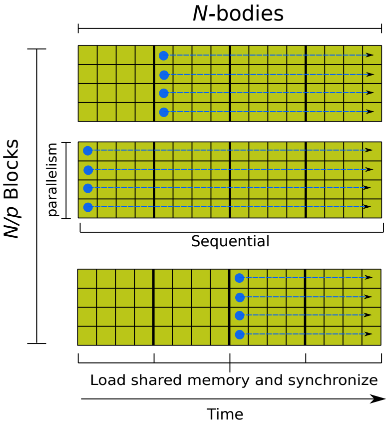


Figure : Grid configuration using the *tiles* approach (This figure is based on [24])

Parallelization scheme

$j-$parallelization scheme

Our configuration is based in the idea presented in [15],

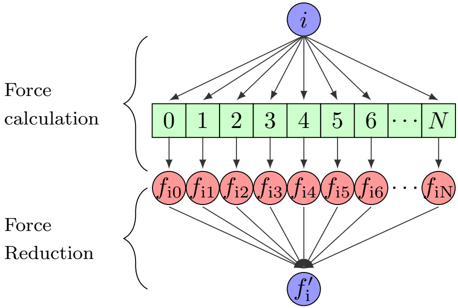


Figure : Parallelization scheme to split the $j-$loop instead of the $i-$loop. In this case, we have two sections, the first is to calculate the force interactions of the $i-$particle with the whole system but by different threads. Then a reduction (sum) is necessary to get the new value for the $i-$particle force.

Experiments

Computational specs

UTFSM Cluster, GPU node. (Chile)

CPU	Intel(R) Xeon(R) CPU X5650 @ 2.67GHz (24 cores)
GPU	Tesla M2050 @ 575 Mhz (448 cores).
RAM	24 GB
OS	Scientific Linux release 6.4

Table : Hardware and Software settings.

Experiments

Units and systems

- Equal-mass Plummer sphere [25].
- Standard N-body units for the calculations and resulting output of the code [26, 27],

N-body Units

- Total mass, $\sum_{\mathrm{i=0}}^{N} m_i = 1$.
- Gravitational constant, $G = 1$.
- Total energy, $E_{\mathrm{tot}} = K + U = -0.25$,

Experiments

η and the energy conservation

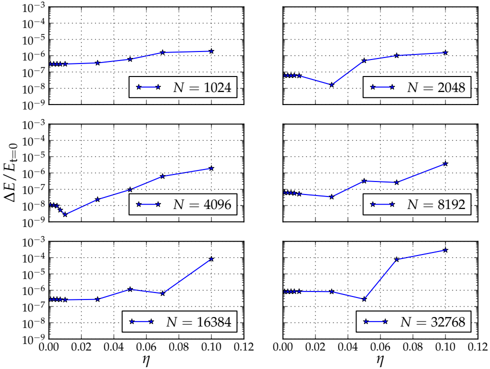


Figure : Cumulative energy error up to $t = 1$ NBU as a function of η. All the plots represent Plummer spheres with different amount of particles.

Experiments

η and the clock time

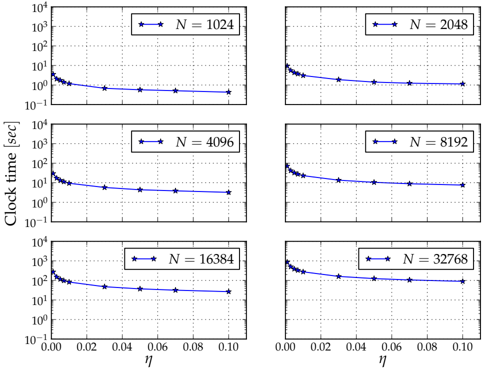


Figure : Clock time up to $t = 1$ NBU as a function of η. All the plots represent Plummer spheres with different amount of particles.

Experiments

Integrator scaling

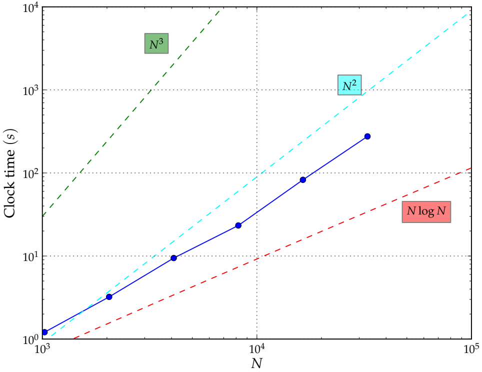


Figure : Clock time of integration up to $t = 1$ NBU using $\eta = 0.01$ and $\epsilon = 10^{-4}$ using different amount of particles.

Experiments

Clock time comparison

N	CPU (single thread)	CPU + OpenMP (many threads)	CPU + GPU (mixed approach)	GPU (multi threads)
1k	12.98 [s]	8.19 [s]	3.57 [s]	1.21 [s]
2k	61.32 [s]	34.94 [s]	13.42 [s]	3.22 [s]
4k	282.98 [s]	162.64 [s]	54.28 [s]	9.45 [s]
8k	1227.40 [s]	682.56 [s]	208.91 [s]	23.31 [s]
16k	5542.35 [s]	3227.91 [s]	904.82 [s]	82.63 [s]
32k	26383.71 [s]	15076.40 [s]	3722.92 [s]	275.53 [s]

Table : Clock time foreach integrator version.

Experiments

Clock time comparison

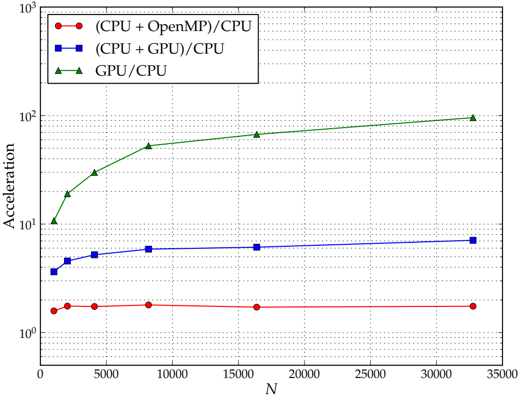


Figure : Acceleration between the implementations described in Table 2

Experiments

Integrator Performance

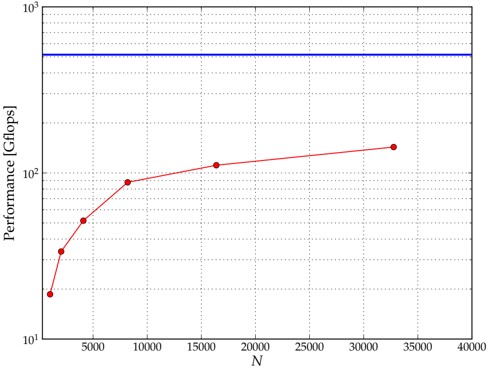


Figure : GPU gravitational interactions performance in GFLOPS for different amount of particles.

Experiments

Lagrange radii

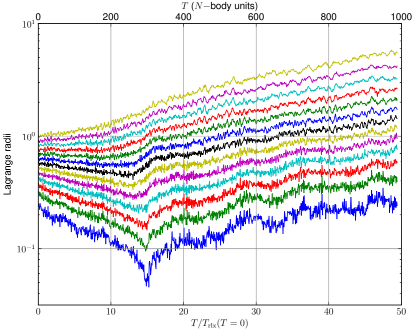


Figure : Lagrange radii of an N-body system with 1024 particles. The radii distribution are $5\%, 10\%, 15\%, \ldots, 65\%$ of the total mass. The core collapse is reached at $T_{\rm cc} \approx 15\,T_{\rm rh}$. The half-mass relaxation time is $T_{\rm rh} = 20.24[nbu]$

Experiments

Core radius and density evolution

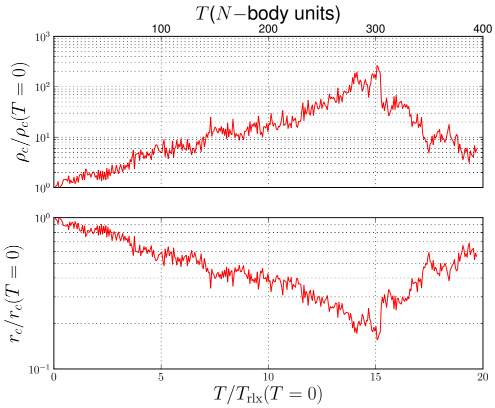


Figure : Evolution of the core radius and core density until core collapse in a system with $N = 1024$

Experiments

Long term integration

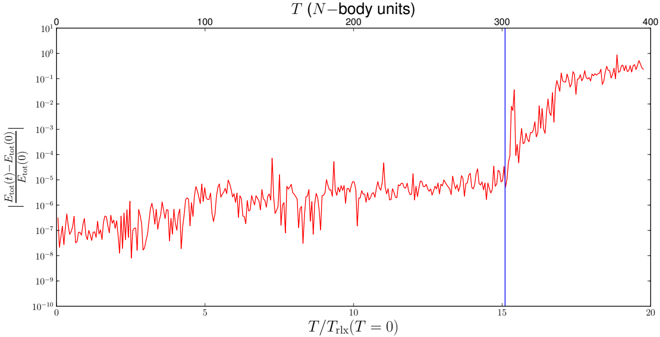


Figure : Energy conservation in a long time integration of a system with $N = 1024$

Challenges and future work

We presented a first version of our new N-body code, written purely in C/C++ and CUDA, called GRAVIDY .

- The current version of our code,
  - evolves a globular cluster, using and Hermite 4th order integration scheme, using block time steps.
  - has a suitable in the energy conservation, reaching errors around $\approx 10^{-9}$ and $\approx 10^{-7}$-

Challenges and future work

Features

- Iterative and incremental development (APOD cycle),
- Modular code,
- Documentation,
- Hermite 4th order integrator scheme,
- Block time steps,
- GPU computing to improve the hot-spots,

challenges and future work

the next steps (1/2)

- Continue the research on N-body integrators, like higher order Hermite schemes.
- More physical phenomena treatments,
  - Neighbors treatment, to handle the binary formation, This has been proved by using a time-symmetric integration scheme for the binary system, which is described in the work of [28].
  - Handle semi-Keplerian systems, N-body systems with a central massive particle [29], like a massive black hole (MBH) in the galactic center, or a star in a protoplanetary system, etc.
  - Post-Newtonian terms into the acceleration and its derivatives.

challenges and future work

the next steps (2/2)

- Porting the code towards large GPU clusters, multi-GPU environment.
- Studying new computational improvements,
  - Numerical precision,
  - Mixed-parallel schemes,
  - Different architectures,
- Use GPU Computing to solve additional Astrophysical problems,
  - Smoothed-particle hydrodynamics (SPH).

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