

Evaluating large scale particle simulations with OpenACC

Status Update

Samuel A. Cruz Alegría, Alessandra M. de Felice, Hrishikesh R. Gupta

(University of Lugano)

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Accomplishments thus far

Our accomplishments thus far include the following:

- Encoding particle movement in three dimensions.
- Using ParaView for visualizing our results.
- Including OpenACC parallel loops in the code.

Furthermore, an attempt has been made at simulating realistic particle interactions.

Serial code

The code mainly performs the following tasks:

- 1 Initializing particle positions.
- 2 Updating particle details such as position and velocity.
- 3 Writing particle details to a file in every time step.

Serial code

Demo at the end...

Visualization tools

In order to facilitate visualization of the particle simulation, we have decided to use *ParaView*.

Visualization tools

ParaView [2].

- Used at the CSCS (Swiss National Supercomputing Centre) [1].
- Open source, used for visualizing two and three-dimensional data sets.
- Platforms supported range from single-processor workstations to multiple-processor distributed-memory supercomputers or workstation clusters.
- Many file formats supported.

Visualization tools

We are using the VTK file format, which consists of the following header

```
1 ^I# vtk DataFile Version 1.0
2 ^I3D triangulation data
3 ^IASCII
4
5 ^^IDATASET POLYDATA
6 ^^IPOINTS N float
7 ^^I
```

and the following body

<i>x-coordinate</i>	<i>y-coordinate</i>	<i>z-coordinate</i>
$p0_x$	$p0_y$	$p0_z$
\vdots	\vdots	\vdots
pN_x	pN_y	pN_z

Visualization tools

Using the VTK file format, we create a file for each time step. In each file, we write the position of each particle in the given time step.

- positions_0.txt
- positions_1.txt
- positions_2.txt
- And so on...

Parallelization methods

Preliminary benchmarks made for comparing execution time of `update_particles()` function using serial version and parallel version (OpenACC).

Parallelization methods

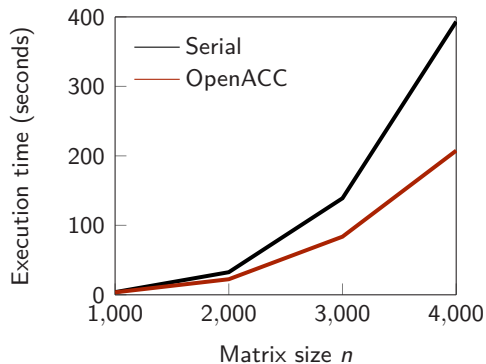


Figure: Matrix–matrix multiplication: execution time comparison.

Project plan

Show current project calendar...

References



CSCS. *ParaView*. URL: https://user.cscs.ch/scientific_computing/supported_applications/paraview/.



ParaView. *The ParaView Tutorial*. Nov. 2017. URL: https://www.paraview.org/Wiki/The_ParaView_Tutorial.

Questions

Thank you for your attention!
Any questions?