High Performance Computing ICTP

Cairo University - Faculty of Science Department of Mathematics

EGYPT

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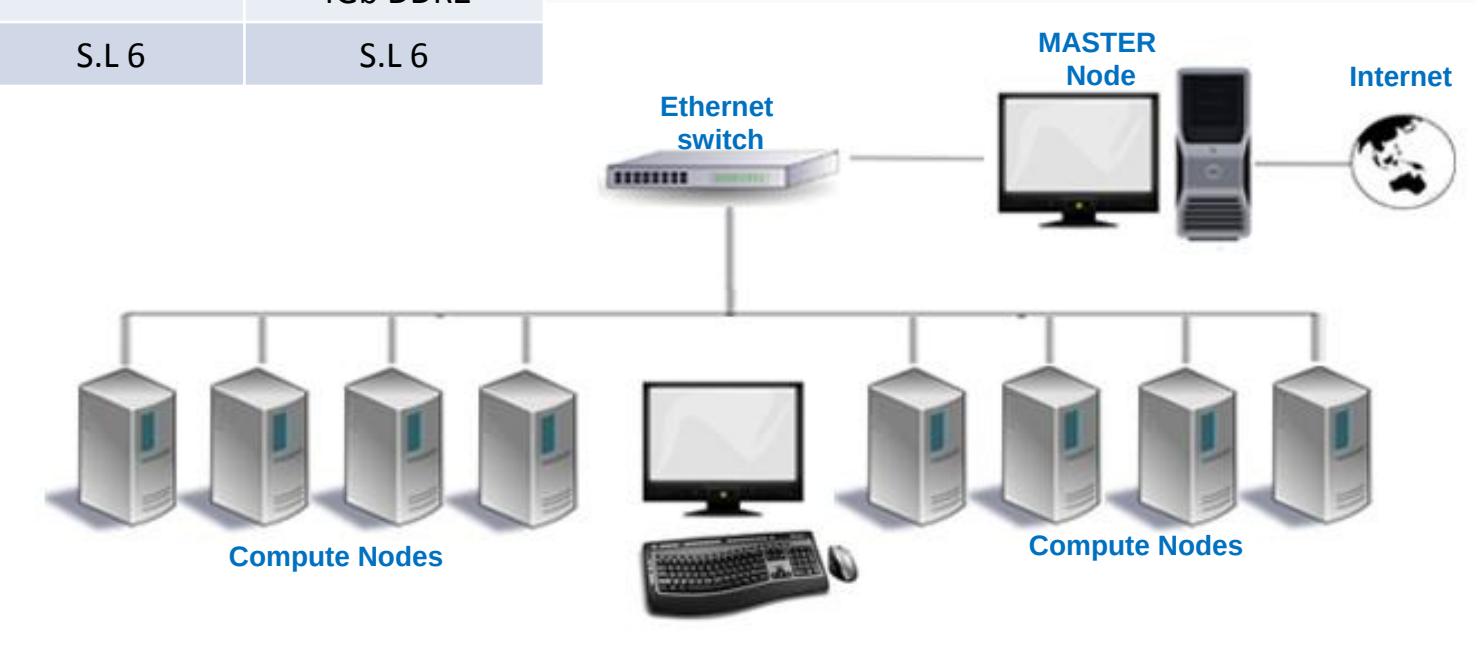
Lecturer Assistant

WORK EXPERIENCE

- Building a faculty of Science cluster with Scientific Linux “OS” and MPICH2.
- Presented a new algorithm “PIFD” for solving Some type of PDE with C++ and MPI.
- Developed a GUI application for simulate molecular dynamic using C++ , MPI , OpenGL

PC cluster description

	Master Node	Slave Node
CPU	Intel(R) core(TM)2 Quad CPU Q6700 2.66 GHz	Intel(R) core(TM)2 Duo CPU E7400 2.80 GHz
RAM	4Gb DDR2	4Gb DDR2
O.S	S.L 6	S.L 6



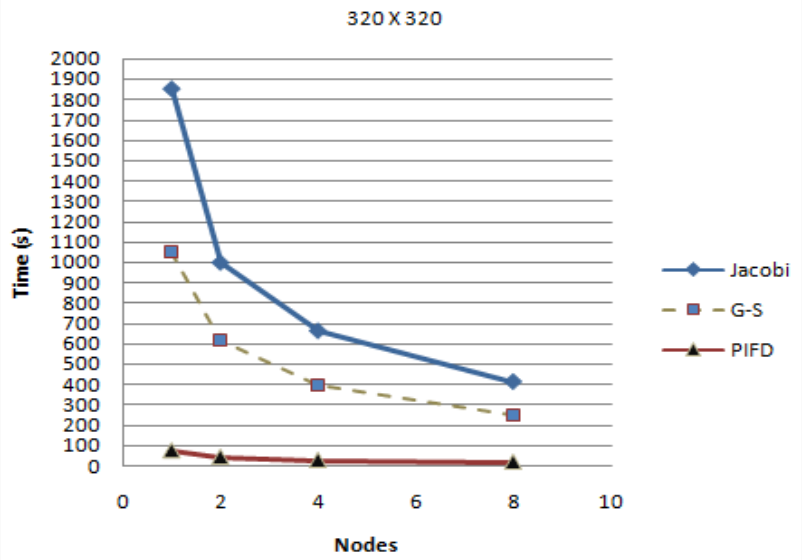
PC cluster description

software
MPICH
AMBER: is a popular software application for analyzing large-scale molecular dynamics (MD) simulation trajectory data.
DL_POLY: is a package of subroutines, programs and data files, designed to facilitate molecular dynamics simulations of macromolecules, polymers, ionic systems and solutions on a distributed memory parallel computer

	Master Node	Slave Node
CPU	core(TM) i7 CPU 2600 3.40 GHz	core(TM) i7 CPU 2600 3.40 GHz
RAM	8Gb DDR3 RAM	8Gb DDR3 RAM
O.S	S.L 6	S.L 6

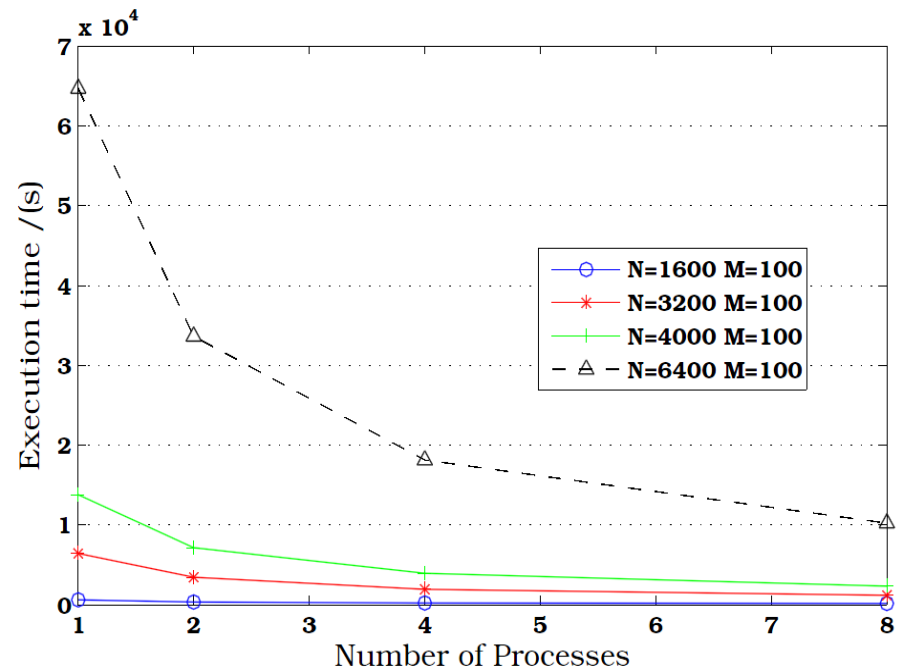
Numerical Results

C++ is selected in combination with the message passing interface library MPICH2.

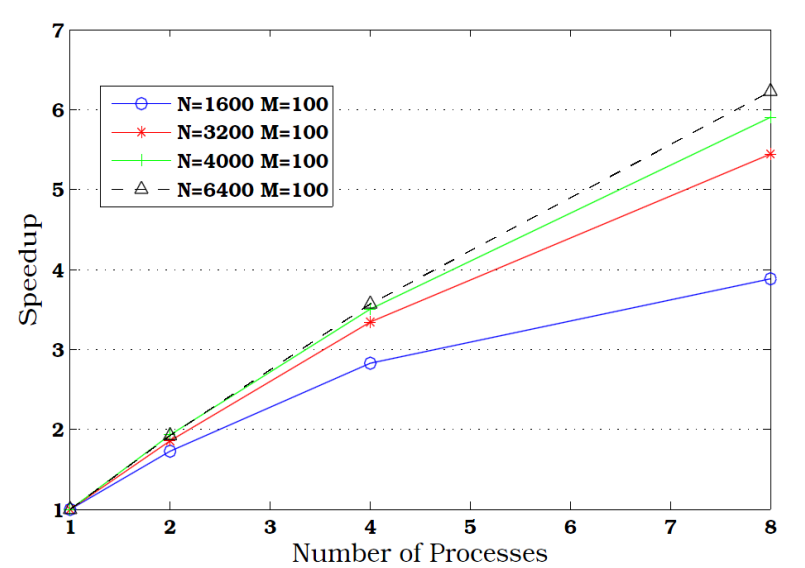


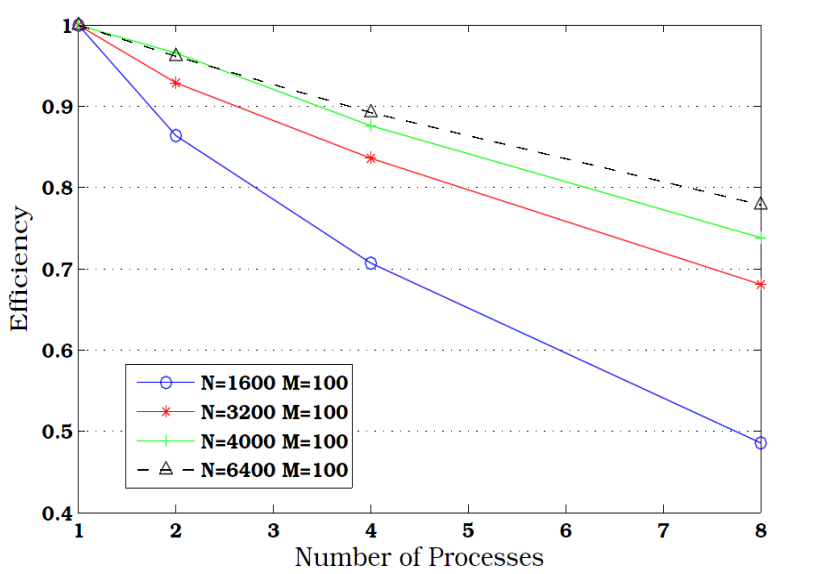
The execution time of PIFD, Jacobi and Gauss-Seidel on different number of computer nodes and w_{opt}=1.95.

C-N-FDM for solving time-fractional diffusion equation



C-N-FDM for solving time-fractional diffusion equation





PUBLICATION

Sweilam, N. H., H. M. Moharram, and Sameh Ahmed. "On the parallel iterative finite difference algorithm for 2-D Poisson's equation with MPI cluster." *Informatics and Systems (INFOS), 2012 8th International Conference on*. IEEE, 2012.

Kholmirzo Kholmurodov, Ermuhammad Dushanov, Kenji Yasuoka, Hagar Khalil, Ahmed Galal, Sameh Ahmed, Nasser Sweilam, Hatem Moharram, Molecular dynamics study of ethanol solvated by water on the Pt (1 1 1) surface, Chemical Physics, Volume 402, 19 June 2012, Pages 41-47, ISSN 0301-0104, 10.1016/j.chemphys.2012.04.002.

Thank You for Attention