

# Parallel computing activities at IPR: Experience and expectations from the grid infrastructure

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# Overview of the presentation

- Large scale computing in plasma physics
- Overview of computing resources at IPR
- Grid computing and IPR: Motivation and commitment
- Garuda Grid: Activities and experience so far
- Expectations and vision for the future

# Large scale computation in plasma physics

Major applications in laboratory plasmas and space physics

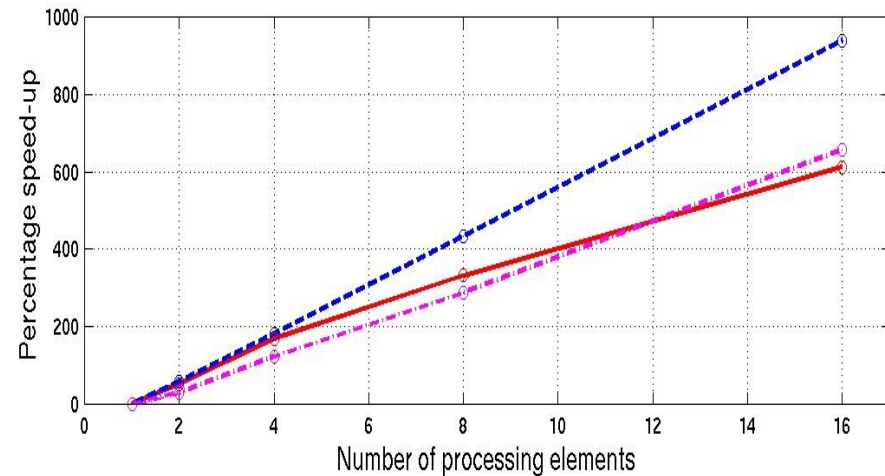
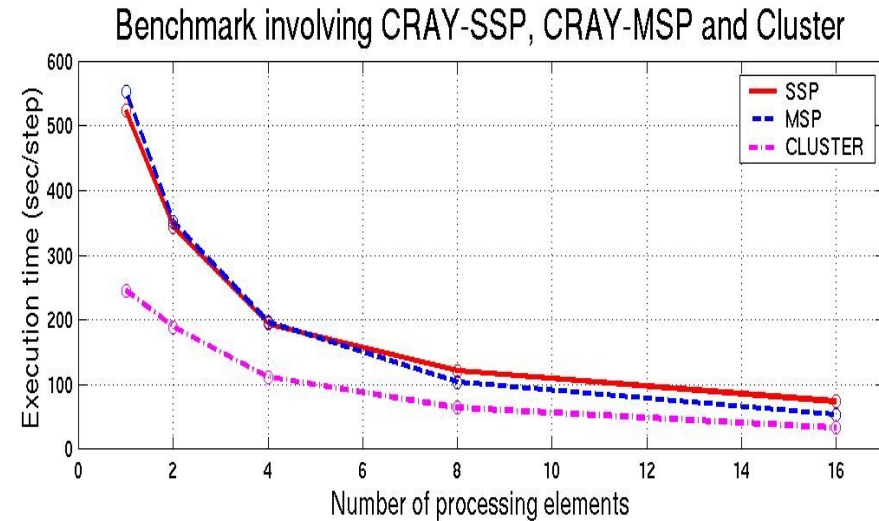
- **Multi-dimensional Magneto-Hydro-Dynamic (MHD) turbulence codes:** Multi-variable, Multi-scale; Involve complex computations, harder to parallelize
- **Particle-simulation codes:** Both deterministic and statistical techniques, Often involve tracing the trajectories of large number of interacting particles, Massive amount of simpler computations
- **Kinetic and Vlasov simulation codes:** Multi-dimensional, Require large degree of accuracy and resolution; use large, dense and multidimensional grids and complex computational methods, heavy post-processing requirements
- **Molecular-dynamics simulations:** Simulation of the dynamics at the scales of atomic and molecular sizes: Massive memory requirements

## High performance computing resources at IPR

- **CRAY-X1E supercomputer:** Combination of shared and distributed memory based parallel computing architectures, Multi-streaming vector processors
- **Clusters of machines running Linux OS:** Simple but fast, purely distributed memory parallel computing architecture
- **Access to the computing grid GARUDA**

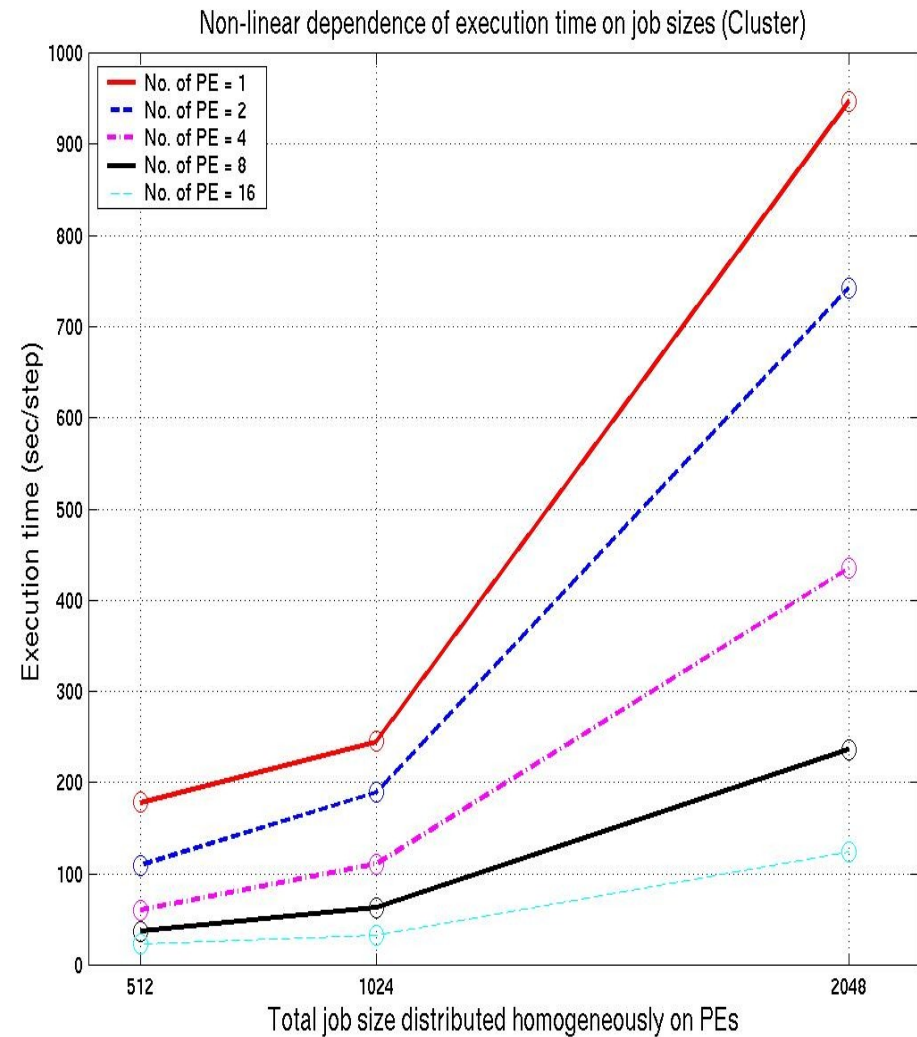
# Garuda Grid and IPR: Motivation and Commitment

- **Simple cluster based architecture ideal for normal parallel applications**
- **Recent benchmarks validate the capability of cluster based computing structured, largely offered by the grid computing infrastructure**
- **Accessibility to a variety of parallel computing platforms and resources**



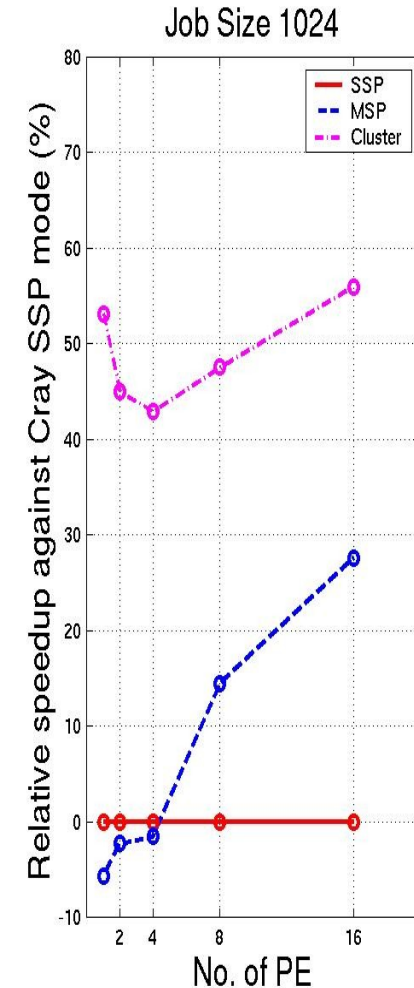
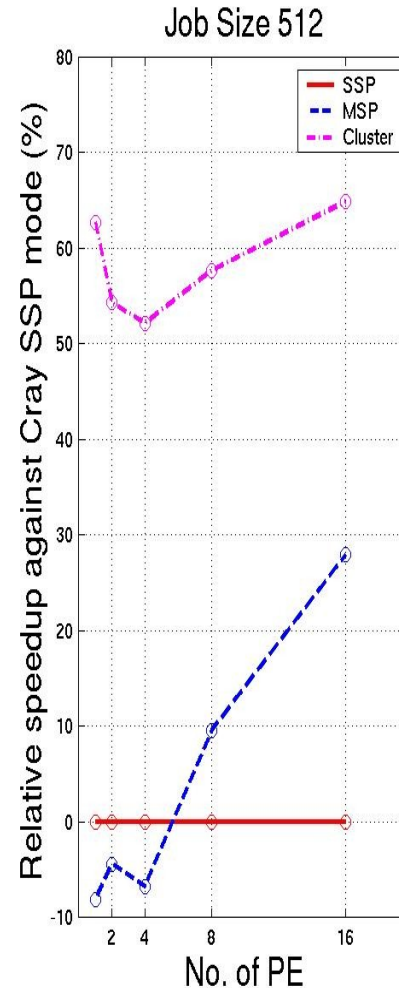
# Garuda Grid and IPR: Motivation and Commitment (cont.)

- Characteristics of the Kinetic-Vlasov code KSLab application, distributed homogeneously on the IPR Linux cluster
- Considerable non-linear overhead up on increasing the job-size
- The application is suitable as a tool to characterize and analyze the performance of available parallel architectures



# Garuda Grid and IPR: Motivation and Commitment (cont.)

- Normal parallel application show an excellent speed up on ordinary distributed memory clusters
- Speed up on switching to the Linux cluster exceeds that to the Cray-MSP, for any available number of processing elements
- The Cray-MSP should be an advantage for extraordinarily large jobs on a relatively larger size Cray
- Execution on clusters offered by grid infrastructure could be ideal for normal user applications



## Garuda Grid: Experience and activities so far

- The web based utility for precompiled job submission and execution tested successfully for small serial applications
- Precompiled parallel applications return errors following execution due to issues related with linking and appropriate setting of path/environment for corresponding MPI libraries (rt-tickets #4933, #4937)
- Alternatively, attempt are made to use GIDE utility to build the applications on the respective cluster in order to avoid the difficulties in linking with the local versions of MPI resources
- Initial problems with opening and running GIDE utility were solved with the help of GARUDA colleagues (rt ticket#6099)

## Garuda Grid: Experience and activities so far (cont.)

- A way to successfully access the GIDE, from the terminals other than the “iprgarudahnode”, was managed by setting up a user access to the vncserver in “gridfs”, allowing the export of “gridfs” display to user terminals across the interface of GARUDA and IPR networks
- GIDE is found to do the desired job, namely, the packaging and export of job resources to the target computing cluster (ch0x), across the GARUDA network
- Attempts to successfully build and execute a distributed test project are on in collaboration with colleagues at GARUDA (rt-ticket #6099, still open)
- The possible solution could be a universal path and environment settings for FORTRAN version of MPI on the target computing clusters, where the project is to be finally built and executed

# Expectations and vision for the future

- **A larger pool of dedicated clusters installed at various sites**
- **A standard and uniform resource structure, in order to minimize various initial technical issues while getting the projects work successfully**
- **Alternate versions of the utilities like GIDE for the users connected using Unix/Linux platforms**
- **We remain committed to contribute and support the activities of GARUDA in all possible ways**

**Thanks for your attention**