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# GAṆANAM (गणनम्)

HIGH PERFORMANCE *COMPUTING* NEWSLETTER

INSTITUTE FOR PLASMA RESEARCH, INDIA

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# Molecular Dynamics Simulation Study of Laser-Cluster Interactions Using In-house Developed Code

**Dr. Sagar Sekhar Mahalik** (PDF, BTS Division, IPR)

***Email: sagar.sekhar@ipr.res.in***

**C**lusters are finite aggregates of atoms/ molecules (few to several thousands) bound together via Van der Waals forces. Under specific conditions of pressure and temperature, their size may vary from sub-nanometer to a few tens of nanometers [1]. Clusters serve as an intermediate state between solid and gas since their average atomic density is typically of the order of the gas density while its local atomic density is close to the solid density. The localized solid-like atomic density of a cluster and its smaller size (of a few nanometers) than the wavelength of 800 nm laser pulse (typically used in experiments) allow full penetration of laser field without attenuation [Figure 1(a)], contrary to micron-sized solids, leading to nearly 90% laser absorption in clusters [2]. Thus an atomic cluster acts as a unique target for high-energy particle generation. As a cluster is irradiated by a laser, constituent atoms are ionized (called inner ionization) and a nano-plasma is formed. Subsequently, laser absorption by electrons and removal of those hot electrons from the transient cluster potential (called outer ionization) creates a local electrostatic field which, when added to the laser field, may create even higher charge states. Subsequent outer ionization of electrons leaves the cluster with a net positive charge which explodes due to inter-ionic Coulomb repulsion (cluster expansion) [Figure 1(b)]. Clusters irradiated with strong laser pulses can serve as efficient table-top radiation sources of x-rays, energetic KeV electrons, MeV ions and MeV neutrals. High neutron yield also has been found from fusion reaction in deuterium clusters. The energetic electrons and ions from laser irradiated clusters can be used in biological imaging as well as proton beam radiation therapy for cancer treatment. Therefore, the interaction of laser with atomic cluster has been the topic of considerable interest since the early nineties.

***"The current 3-D MD simulation code developed at IPR can be used in studying the dynamical behavior of Laser-Cluster Interactions."***

***Coupling of laser energy to cluster electrons can happen through collisional and collision-less processes***. However, the collisional process of absorption becomes inefficient for infrared lasers with intensities $I_0 = 10^{16}\ W/cm^2$ and can be neglected as it scales as ~ $I_0^{-3/2}$. On the other hand, the collisionless resonance absorption mechanism includes both linear resonance (LR) and anharmonic resonance (AHR). Resonance absorption processes are frequency-dependent phenomena and depend on the system's eigen frequency and the driver's frequency. For the spherical cluster, LR happens when Mie-plasma frequency ($\omega_m=\omega_p/\mathrm{sqrt}(3)$) matches with the laser frequency ($\omega$). LR occurs after a longer time (typically > 50fs) during the Coulomb expansion phase and many electrons collectively leave the cluster by absorbing a huge amount of laser energy. However, for very short infrared laser pulses of duration < 20fs, laser absorption by electrons mainly occur by AHR [3].

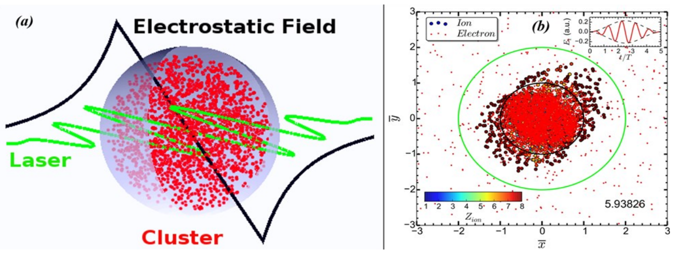



**Figure 1: (a) Schematic of laser interaction with a spherical argon cluster, (b) Dynamics of a laser-driven argon cluster shows inner ionization, outer ionization, and Coulomb explosion all happening simultaneously. Colorbar in (b) shows the different charge states of the argon.**

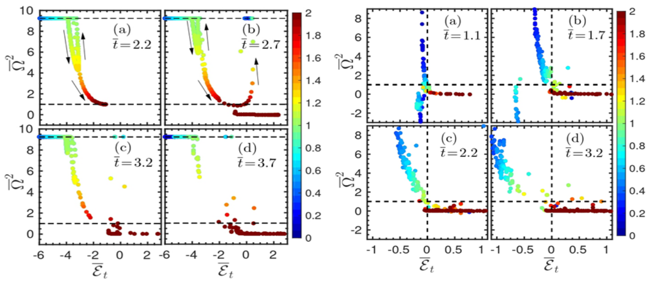


**Figure 2: Electrons undergoing AHR at different times in the energy versus frequency domain, obtained by RSM (left panel) and MD simulation (right panel).**

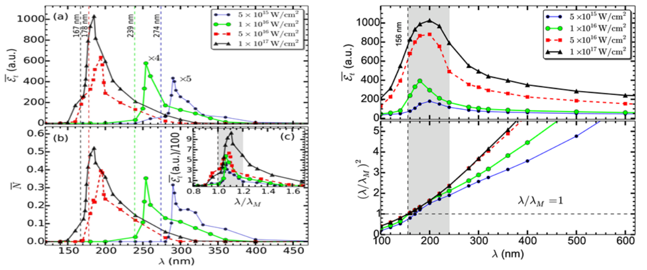


**Figure 3: Left panel: (Top) RSM results for average total absorbed energy and, (Bottom) fraction of outer ionization versus λ after the laser pulses of different peak intensities. Right panel: (Top) MD results for average total absorbed energy and, (Bottom) an approximate $(\lambda/\lambda_M)^2 = (\omega_M/\omega)^2$ for the same intensities. The shaded bar highlights that absorption maxima are red-shifted in the marginally over-dense regime of $\lambda/\lambda_M \approx 1$–1.5.**

For the detailed understanding of different absorption mechanisms by electrons in a laser-driven atomic cluster, a *3-D molecular dynamics (3D-MD) code* [4] with soft-core Coulomb interaction among the charged particles has been developed from scratch. Using this newly developed 3D-MD code in HPC clusters of IPR (UDAY and ANTYA) we study the dynamical behavior of deuterium and argon clusters irradiated by different peak intensities at different laser wavelengths. We identify anharmonic resonance absorption (AHR) mechanism as a universal dominant collisionless mechanism of absorption in the short pulse regime or in the early time of longer pulses in an over-dense pre-ionized deuterium cluster using MD simulations and rigid sphere model (RSM). Figure 2 shows electrons undergoing AHR at different times in the energy versus frequency domain, obtained by RSM and MD simulation. By analyzing trajectories of individuals and extracting their time dependent frequencies in the self-generated time-varying nonlinear plasma potential, we find that electrons become free from the cluster potential when the AHR condition is met i.e., when the dynamical frequency of an electron matches with the driving laser frequency. Again by performing RSM and MD simulations of an argon cluster, irradiated by short laser pulses we find out the optimal regime of laser wavelengths for an argon cluster to attain maximum absorption of laser energy at a given intensity and pulse energy [5]. Our results shown in figure 3 reveal that, for a given peak intensity and a plasma density, the efficient coupling of laser energy does not happen at the well-known linear resonance (LR) wavelength instead it happens at a red-shifted wavelength in the marginally over-dense regime of wavelength. This new finding in laser atomic cluster study may be useful to guide an optimum control experiment in the short-pulse regime where maximum energy is required to transfer from laser fields to charge particles and/or radiations.

**References:**

1. *O. F. Hagena and W. Obert, Journal of Chem. Phys., 56, 1793 (1972).*
2. *T. Ditmire, et al., Phys. Rev. A 53, 3379 (1996).*
3. *M. Kundu and D. Bauer, Phys. Rev. Lett., 96, 123401 (2006).*
4. *S. S. Mahalik and M. Kundu, Phys. Plasmas 23, 123302 (2016).*
5. *S. S. Mahalik and M. Kundu, Phys. Rev. A, 97, 063406 (2018).*

## Availing the Various Software Using the Environment Modules on ANTYA

Module is a Linux shell utility and allows to dynamically modify the user shell environment with the ability to reverse the changes by a single command using pre-defined module files. It helps in setting up the environment variables by just loading and unloading the modulefiles that one might traditionally do manually by exporting the commands either in bashrc or job scripts. HPC system ANTYA, having more than 10000 cores and 44 GPU cards, is serving as a shared platform for around 200 HPC Users where the users can run applications, both commercially licensed (ANSYS, COMSOL, CST, MATLAB, IDL) and open-source (LAMMPS, PLUTO, OpenFOAM, paraview, visit, etc.) as well as libraries and toolkits (intel, pgi, cuda, fftw, openmpi, gcc etc.). The number of installed software on ANTYA spans numerous applications from various domains in different versions and is installed at a shared location that is accessible to all the users. Modules facilitate the use of different versions of applications, libraries, and toolkits which enables the support of multiple package versions concurrently. The list of modulefiles of the applications is maintained by the HPC Team and updated regularly based on the user requests as well as system requirements.

Apart from using the applications installed at the shared location, Users can also install some specific applications in their home and can create custom module files for such specific applications. These custom module files can also be shared with your colleagues. The details about creating custom module files and sharing will be provided in the next issue. Following commands show how to use the existing modules on ANTYA:

**1. Show the available software**
The following command is used to check what are software and their versions currently available on ANTYA:

```
$ module avail
```

**2. Show the available versions of a software**
The following command is used to check the python versions currently available on ANTYA:

```
$ module avail python
```

**3. Load the specific versions of a software from the available list**
The following command is used to load the python version 3.8.5:

```
$ module load python385
```

**4. Switch to other version of a software**
The following command is used to switch from the python version 3.8.5 to python version 3.7.1:

```
$ module switch python385 python371
```

**5. Show the Content of a modulefile and what changes it does in user shell environment**
The following command is used to show content of python version 3.7.1:

```
$ module show python371
```

## ANTYA UPDATES AND NEWS

1. New Software Installed

⇒ petsc-3.14.0 module

⇒ visit-3.2.0 module

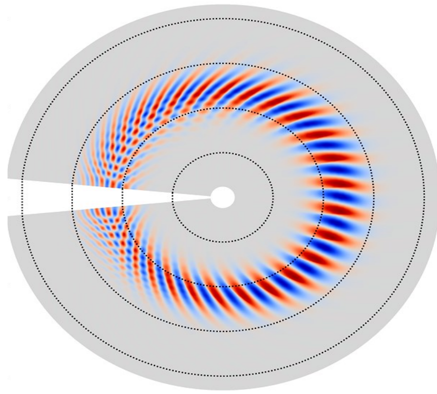
⇒ QGIS singularity container image now available

⇒ Licensed new and old versions (used in UDBHAV) of NAG compilers and libraries are now available in ANTYA as modules.

2. Phase-1 of firmware upgrade on compute nodes

**Parallel Computing Workshop at IPR**
Registration link
Last date to register 11th April 2021

## Ion-Temperature Gradient (ITG) Driven Instability
(HPC Picture of the Month)



Pic Credit: **Dr. Arkaprava Bokshi**

**The ITG mode driven turbulence is considered to be the primary mechanism for ion temperature loss in tokamak plasmas. The image shows the structure of the fluctuating ITG electrostatic potential in the poloidal plane.**
Simulated on ANTYA using a gyrofluid model in open source code, BOUT++. Simulation took ~1 min on 128 cores.

## Other Recent Work on HPC (Available in IPR Library)

| | |
|---|---|
| Thermo-fluid MHD analysis of a Circular U-bend | ANITA PATEL |
| Performance assessment of a compact volumetric neutron source as breeder | VINAY MENON |
| Numerical Simulation Of A Bi-directional Plasma Thruster For Space Debris Removal | VINOD SAINI |
| Collective excitations of rotating dusty plasma under quasilocalized charge approximation of strongly coupled systems | PRINCE KUMAR |
| RCS Reduction using Resistive-Ink based Metasurface Absorber | PRIYANKA TIWARI |
| Design, development and characterization of Broadband Polarization-Insensitive Metasurface Absorber using four Γ-shaped Resistive Arms for RCS reduction | PRIYANKA TIWARI |
| Emergence of directed motion in a 2D system of Yukawa particles on 1D asymmetric ratchet | ANSHIKA CHUGH |
| Design, Simulation, Fabrication and Testing of Linear Induction Motor for Electromagnetic Launchers (EML) | PEDADA PRASADA RAO |
| FEA Investigations of the Support Structures for the Magnet Test Facility | MAHESH M GHATE |


**TO CHECK THE FULL DETAILS OF A RUNNING JOB**

```
$ qstat -f jobid
```

## Acknowledgement

The HPC Team, Computer Division IPR, would like to thank all Contributors for current issue of GAṆANAM.

**On Demand Online Tutorial Session on HPC Environment for New Users Available**
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