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Rocket Propulsion with Detonations: A Numerical Simulation Study

Sunil Bassi (SO-D, **Multidisciplinary Research Division, IPR**)
Email: sunil.bassi@ipr.res.in

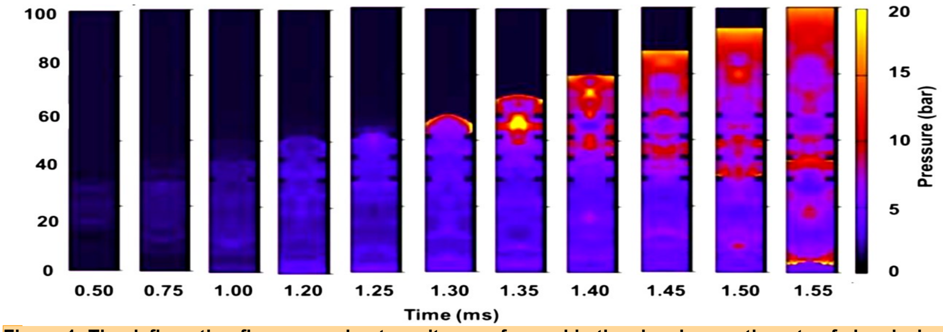


Figure 1: The deflagration flames accelerate as it move forward in the chamber, as the rate of chemical reactions increases with temperature. Further, the turbulences develop in the flow and they accelerate the flame propagation.

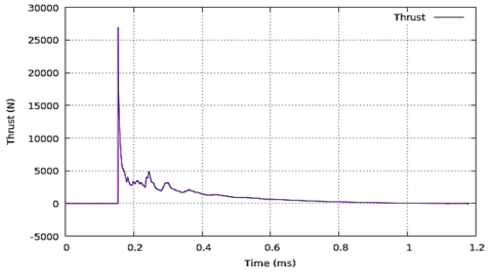


Figure 2: Magnitude of time dependent thrust during the exhaust process. Thrust remains zero till the detonation wave is away from the open end and then a sharp peak appears when shock front crosses the open end. Sharp peak also signifies that the shock front is spatially very thin.

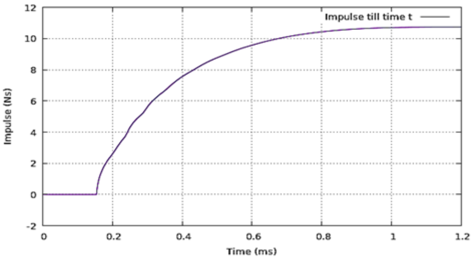


Figure 3. Impulse imparted to the rocket till time 't'. Impulse remains zero before the exhaust starts. It becomes constant when all the burnt products exit the chamber and chamber returns to initial ambient conditions of temperature and pressure.

The rising interest in space travel has resulted in an intensifying effort from the international community to develop robust rocket propulsion systems. Combustion flames, generally seen in daily life, progress via heat conduction and mass diffusion, and are called deflagration. A shock-driven mode (Detonations) of combustion is also possible, in which high-pressure shock compresses gases and dissociates the molecules of gases leading to the ignition of a combustible mixture that rapidly releases energy behind shock front and this energy sustains the shock wave . Detonation wave moves with supersonic speed, hence there is very little time for any motion making the process nearly isochoric. This is advantageous as isochoric processes are thermodynamically efficient. Pulse Detonation Engines (PDE) is a futuristic propulsion system [1], aimed to tap the higher thermo dynamical efficiency of the detonations. In PDE, detonations are formed in a pulsed manner by injecting a fuel-air mixture and igniting it repeatedly. Ignition is provided as a spark and detonation is formed by a process called Deflagration to Detonation Transition (DDT). With each pulse of detonation exhausting from the engine chamber, an impulse is imparted to the chamber and a push is provided to the rocket. With a high enough frequency of operation, a substantial thrust can be generated.

> ***"The modified CFD solver based on Conchas-Spray can be useful in the design and development of detonation-based rocket engines to harness the higher thermodynamical efficiency of detonations."***

Simulations are performed to study this process using an in-house modified CFD code based on Conchas-Spray. The additions in the code include the fuel models (Diesel, Propane, ATF Vapor, ATF Droplets), spark ignition mechanism, routine for time dependent thrust etc. Equations for mass, momentum, and energy conservation are solved by the finite difference method on a mesh in the 2D domain having azimuthal symmetry. A full set of the equations are reported in previous studies [2]. In this study, the fuel-air mixture is considered in stoichiometrically correct ratio inside a cylindrical chamber, and spark is provided as a heat source for a few microseconds at one end of the chamber. Deflagration is started by a spark ignition, which transfers into detonation after the DDT process. Turbulences in the flow accelerate the DDT process. To enhance the level of turbulence, some blockages are also used in the chamber, which are called DDT enhancement devices. As seen in the pressure plots (Fig. 1), initially flame (till 1.2 ms) propagates slowly and then the pressure at the flame front rises. The curved shock at the flame front is formed and quickly accelerates to form a fully developed detonation wave within 0.2 ms of the appearance of the shock front. After 1.55 ms, the detonation wave and burnt mixture behind it begin to exit the chamber. Detonation wave and burnt mixture behind it exits the chamber which produces the thrust. The time-dependent thrust produced during the exhaust is calculated at the open end by integrating the mass flow rate and adding pressure difference contribution into it. General thrust equation [3] is solved at the open end which is given by:

$$T = \dot{m}u + \left(P_f - P_o\right)A$$

$$T(t) = \sum_{i=1}^{i=n} 2\pi\rho_i u_i u_i + \sum_{i=1}^{n} \left(P_{if} - P_o\right) 2\pi r_i dr$$

Time average thrust of the engine is cal. by:

$$T_{avg} = \frac{1}{T_c}\int_0^{T_C} T\,(t)dt$$

The peak in the thrust-time (Fig. 2) graph appears when the detonation front just exits the chamber because pressure and fluid density are maximum at the detonation front. The total momentum imparted by the exhaust till time 't' is observed from the impulse time graph. As the thrust approaches zero at the end of the operation cycle, the impulse (Fig. 3) settles to a constant value. The net impulse produced in one cycle in the simulated operation cycle is 10.73 Ns. By dividing it by known weight of the fuel used in one cycle, fuel specific impulse if found to be 1960.3 s. The time averaged thrust T_{avg} produced by numerical engine for a frequency of operation 8 Hz (T_c = 125 ms) comes out to be 85.84 N approximately. These numbers match with reported experimental studies in literature [4].The geometry currently under investigation is for small prototypes and not much payload is expected. The thrust level is sufficient only for testing on ground tracks.

References:

1. *Kailasanath, K., "Review of Propulsion Applications of Detonation Waves," AIAA Journal, Vol. 39, No. 9, pp. 1698-1708, 2000.*
2. *Bassi, S., Soni, S., & Chaturvedi, S. (2019). Effect of Fuel Distribution on the Onset of Detonation in Gaseous Octane Air Mixture. Defence Science Journal, 69 (1), 31-36.*
3. *https://www.grc.nasa.gov/www/k-12/airplane/thrsteq.html.*
4. *E. Wintenberger, J.M. Austin, M. Cooper, S. Jackson, and J.E. Shepherd, Impulse of a Single-Pulse Detonation Tube, GALCIT Report FM 00-8, Graduate Aeronautical Laboratories California Institute of Technology Pasadena, CA 91125, U.S.A.*

Python Package Management Using Conda — Part-2
Creating Environments and Installing Packages

Rather than installing software system-wide, wouldn't it be great if we could install python package dependencies separately for each project. Conda environment allows us to have project-specific packages without having any conflict. One can create as many project-specific environments as needed in ANTYA in the user area without admin privileges and easily activate or deactivate environments to switch between them. In this part-2 of the Conda series, we will cover how you can create an environment and install packages inside that environment on ANTYA with an example.

What is Conda Environment ?

A Conda environment is a directory that contains a specific collection of packages that you have installed and if you change one environment your other environments remain unaffected. Further we will see in the next issues how Conda environment files can be shared to recreate/reproduce an environment on a remote server.

Why use Conda Environment ?

It is often impossible to install different versions of the same python package in a single module or at the same time. One solution could be to have multiple modules for different versions of the packages but this would result in complex dependencies that should not really exist. Creating isolated Conda environments is the best practice we should follow.

Example Project: Implementation in ANTYA

Suppose you have a python code for a research problem that takes > 24 hours for a single run and you have explored that ***"numba—a python compiler"*** could help you in speeding up simulation. Now, you want to install numba without disturbing the existing packages which you are already using for the simulation.

 # Conda basic is available by default for all ANTYA Users and there is no need to load any module. Create the project name with Conda

```
[user@login1 ~]$ conda create --name numba-project
```

 # Now activate the created environment

```
[user@login1 ~]$ conda activate numba-project
```

 # This will activate the environment and your shell would show you are inside the environment. Now check the available packages in environment

```
(numba-project) [user@login1 ~]$ conda list
```

#Since there are no packages installed, this will not list any packages. Now install the required numba package (for a specific version, one can specify the version as, numba=version_no)

```
(numba-project) [user@login1 ~]$ conda install numba
```

 # This command will take few minutes to install numba alongwith the other dependencies of numba like python programming language latest release, numpy etc. Now to check the list of installed packages with version, use the following command

```
(numba-project) [user@login1 ~]$ conda list
```

 # To come out of the environment, deactivate the environment

```
(numba-project) [user@login1 ~]$ conda deactivate
[user@login1 ~]$
```

 # To see the list of all available/created environments. You can activate any of the listed environments using the "conda activate env-name" command and install/update any packages into the existing environment

```
[user@login1 ~]$ conda env list
```

 # Default location of the user installed environment

```
[user@login1 ~]$ ls /home/user/.conda/envs/
```

 # Deleting an environment and all its packages installed within

```
[user@login1~]$ conda remove --name numba-project --all
```

ANTYA UPDATES AND NEWS

1. New Packages/Applications Installed

⇒ **NVIDIA HPC SDK as nvhpc modules**

A Comprehensive Suite of Compilers, Libraries and Tools having both PGI and CUDA in one single package with OpenMPI support.

⇒ **OMFIT**

A modeling framework for integrated tokamak simulation tasks is available on user request.

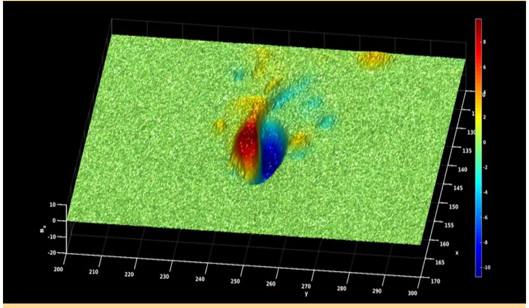
2. USER QUOTAS UPDATE

Updated User Default Quotas

/home — 200 GB
/scratch — 10 TB

Users can further request for increase in their default scratch quotas by sending an email to HPC Team for up to 50 TB.

B_z Profile of Current Vortices Formed During Intense Laser Plasma Interaction
(HPC Picture of the Month)



Pic Credit: **Devshree Mandal**

Coherent structures in plasma holds wide interest as they are robust and stable . One such coherent structure called "Current Vortices" are found to transport EM energy into denser plasma density where laser is not able to propagate while interacting with overdense plasma.

The image was generated in Matlab with data obtained from OSIRIS 4.0 simulation run on ANTYA (OSIRIS 4.0 used under UCLA/IST-IPR OSIRIS Agreement).

TO KNOW PATHS OF SPECIFIC MODULE INSTALLED IN ANTYA

```
$ module show modulename
```

ANTYA HPC Cluster Computational Resources

Resource Name	Total Nodes	Total Cores	Total GPU Cards	Remarks
CPU Nodes	236	9440	0	40 cores with 376 GB usable RAM /node
GPU Nodes	22	880	44	40 cores with 376 GB usable CPU RAM /node 2xP100 GPU cards (16GB GPU RAM/card) /node
High Memory Nodes	02	160	0	80 cores with 1 TB usable RAM/node
Visualization Node	01	40	02	40 cores with 376 GB usable CPU RAM /node 2xP40 GPU cards (24 GB GPU RAM/card) /node
Total (Nodes, Cores, Cards)	**261**	**10520**	**46**	

ANTYA HPC USERS' STATISTICS—JULY

♦ **2934 Successful Jobs**

♦**Top User: CPU Cores (cumulative)**

Swapnali Khamaru

♦**Top User: GPU Cards (cumulative)**

Suruj Kalita

♦**Top User: Walltime (cumulative)**

Swapnali Khamaru

♦**Top User: Jobs (cumulative)**

Anshika Chugh

Other Recent Work on HPC (Available in IPR Library)

Unstable evolution of electron holes and their effect on plasma turbulence	**DEBRAJ MANDAL**
Blob Formation Mechanism from 3D Plasma Simulation in Scrape-off Layer Tokamak Plasmas	**NIRMAL K BISAI**
Emergent dynamics of a cellular automata model for excitable media	**PROMIT MOITRA**
Design and analysis of a 100 W at 77 K Gamma-type Reverse Stirling Cycle based Cryocooler for Cryopumps	**ROHAN DUTTA**
Quasi-Recurrence: a new novel feature observed in 3D-Magnetohydrodynamic plasmas	**SHISHIR BISWAS**
Variation of turbulent spot structure with aspect ratio in a 3D Yukawa liquids – A Molecular Dynamics Study	**SURUJ JYOTI KALITA**
Asymptotic diffusion limits of Yukawa particles on periodic potentials	**ANSHIKA CHUGH**
Discovery of a quiescent toroidal nonneutral plasma state at small aspect ratios	**SWAPNALI KHAMARU**
Magnetic island coalescence problem in the presence of in-plane shear flow	**JAGANNATH MAHAPATRA**
Effect of Enclosure Geometries on the Performance of Plasma-based Microwave Absorber	**HIRAL B JOSHI**
Kinetic trapped particle instability in homogeneous and inhomogeneous 1D Vlasov plasmas	**SANJEEV KUMAR PANDEY**
Rayleigh-Benard convection in 2D Yukawa liquids under an extreme temperature gradient and external forcing : A molecular dynamics study	**PAWANDEEP KAUR**
Finite size effects on the dynamics of long wavelength modes in inhomogeneous one dimensional Vlasov plasmas	**SANJEEV KUMAR PANDEY**
Effect of controlled ion population on the evolution of a quiescent low aspect ratio toroidal pure electron cloud : A 3D PIC approach	**SWAPNALI KHAMARU**
Resonant absorption of laser energy in X-mode configuration of magnetised plasma	**AYUSHI VASHISTHA**
Terahertz radiation generation by a soliton in a laser-plasma system	**DEEPA VERMA**
Electromagnetic Transparency in strongly magnetized plasmas	**DEVSHREE MANDAL**
Simulation of electrode biasing in the edge and scrape-off layer regions of a Tokamak	**VIJAY SHANKAR**
Impact of gravity on dynamics of seeded impurity ions in tokamak plasma	**SHRISH RAJ**
Numerical Simulation of An Expanding Magnetic Field Plasma Thruster	**VINOD SAINI**

Acknowledgement

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

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

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