Exascale Predictive Simulation of Inductively Coupled Plasma Torches

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Milinda Fernando: Solving the Boltzmann Equation for Electron Kinetics using the Galerkin Approach

Ruairi O'Connor: Argon Kinetic Model Validation

Will Ruys: PARLA: Heterogeneous Tasking in Python

SOLVING THE BOLTZMANN EQUATION FOR ELECTRON KINETICS USING THE GALERKIN APPROACH

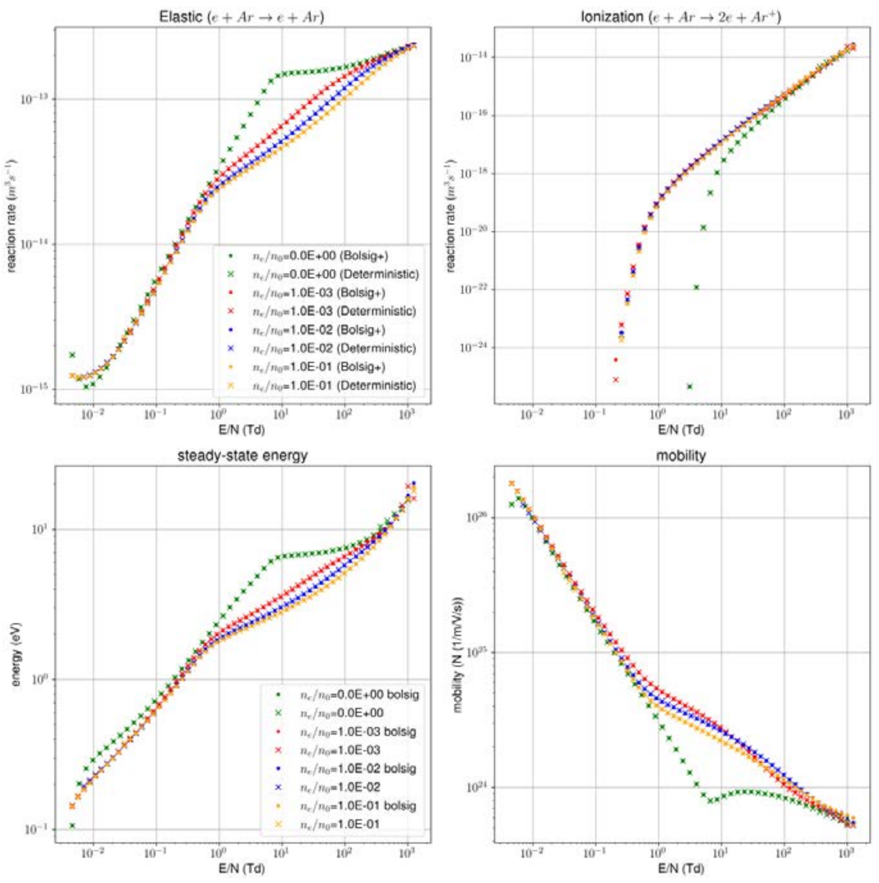
MILINDA FERNANDO , DANIIL BOCHKOV, TODD OLIVER , LAXMINARAYAN R AJA , PHILIP VARGHESE , ROBERT MOSER , AND GEORGE BIROS

• Goal: Develop scalable robust deterministic Boltzmann solver to determine species kinetics properties to enable accurate plasma simulations.

• Challenges: Dimensionality of the problem (6 + 1 dimensions), numerical + HPC challenges.

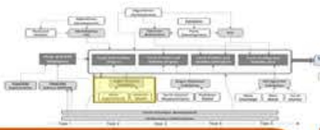
Contributions

- Presented framework goes beyond the traditional two-term approximation
- Ability to handle low-frequency oscillatory electric fields
- Verification with the state-of-the-art Bolsig + Solver
- Open-source implementation in Python



Argon Kinetic Model Validation

Ruairi O'Connor, Juan P. Barberena THE UNIVERSITY OF TEXAS AT AUSTIN



Predictive Engineering & Computational Science

Overview

Plasma chemistry and kinetic models are required for predictive simulations of an ICP at the UT PSAAP center

Models for argon are being developed through a 1D (axial) computational model and validated in a sub-scale glow discharge facility

Rigorous UQ efforts are propagated through both experimental measurements and computational models

Future work will focus on molecular nitrogen and air plasmas

Objectives

1. Develop and validate electron kinetics models for low-temperature argon plasmas
2. Construct glow discharge facility with suite of plasma diagnostics
3. Determine minimum fidelity argon chemistry for LTPs

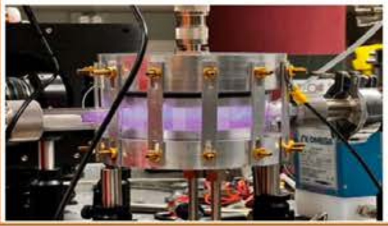
Glow Discharge Experiments

A CCP glow discharge facility has been built to provide key validation data for plasma models

Diagnostics include:

- RF Measurements (V, I, θ, P)
- Langmuir Probe $(n_e, T_e, EEDF)$
- Emission Spectroscopy $(n_{Ar(4p)})$
- Absorption Spectroscopy $(n_{Ar(m,r)})$

Validation to date has been with Ar(4p) density measurements as function of pressure, voltage
Langmuir probe and absorption spectroscopy measurements are in progress



Pressure:
0.1 – 10 Torr

Voltage:
0 – 500 V

Glow Discharge Facility

Results: 6-Species Model Validation

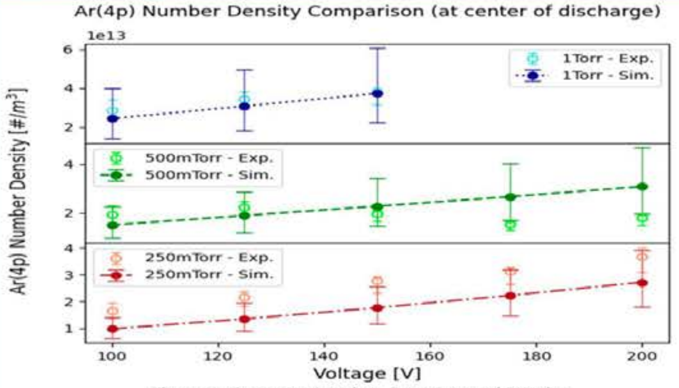


Figure 1: Computational vs. Experimental Results

Comparison shows excellent agreement between the computational model and experimental data in the 1 Torr pressure regime. At lower pressures, there is a partial validation success at certain voltage conditions.
However, it will be necessary to understand where the discrepancies in all other cases come from, and how to address them.

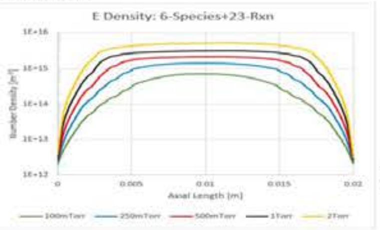
Computational Model

A 1-D (axial) simulations of argon CCP discharge are performed using purpose-built ***glowDischarge*** code

The kinetic model consists of 6 species (E, Ar^+, Ar_m, Ar_r, Ar_{4p}, Ar) and 34 reactions. Nominal values for the rate coefficients were obtained either from the literature (heavy-heavy reactions) or from cross-section data found in the LxCat databases

Uncertainties were quantified in all reaction rate coefficients, as well as electron transport properties, and propagated through the model. Experimental uncertainties in the voltage amplitude were also added to the model.

6-species, 34 reaction model has been validated against experimental data. 5-species model is believed to be minimum model required to capture relevant kinetics. This model is under development



Sample Simulation Result

Conclusion

- A kinetic model for argon was developed to simulate a 1-D glow discharge in the 0.1-10 Torr pressure regime. The uncertainties for the inputs (reaction rate coefficients and electron transport properties) were quantified and propagated through the model.
- A glow discharge validation facility was developed with a range of optical, electrical and probe-based diagnostics
- The model was validated with uncertainty against experimental observations. The agreement is good at the higher-pressure case, but some discrepancies are noticeable at lower pressures, which will need to be addressed.

Future Research

1. Address discrepancies in the 6-Species model at some plasma conditions
2. Perform validation assessments with electron density, $Ar_{m,r}$ density.
3. Use statistical tools (Sobol Sensitivity Analysis & Mutual Information) to assess the quality of the validation efforts, and to aid in the detection of discrepancies in the models.
4. Implement laser absorption and Langmuir probe diagnostics

References

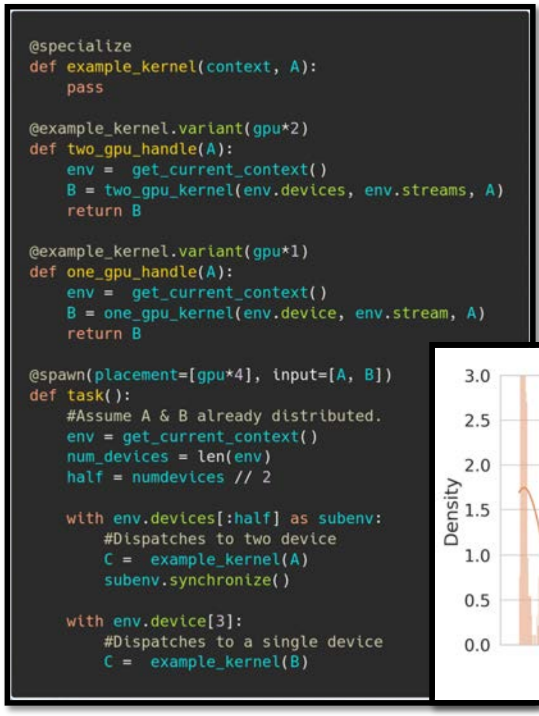
[1] Gudmundsson & Thortsteinsson, PSST 16, 399 (2007)
[2] Cheon et al, Plasma Process & Polymers 19, 2100251 (2022)
[3] Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2022). NIST Atomic Spectra Database

PARLA: Heterogenous Tasking in Python

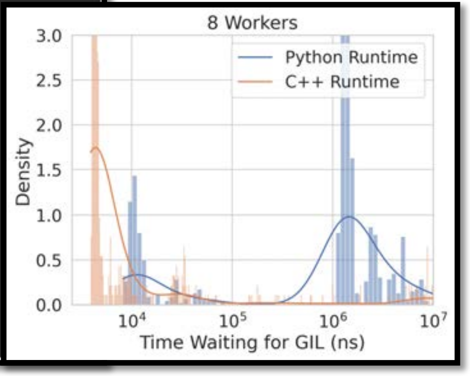
WILLIAM RUYS, HOCHAN LEE, YINENG YAN, BOZHI YU

Parla is a Python library for task based parallel programming that aims to make coordinating heterogenous systems simple, portable, & performant.

- Updates:
  - Runtime optimizations (alleviate GIL contention)
  - Adding multi-gpu tasks and function variants
  - Distributed Arrays (CrossPy)
  - Refactoring for future extensions in Task Mapping



```
@specialize
def example_kernel(context, A):
    pass

@example_kernel.variant(gpu*2)
def two_gpu_handle(A):
    env =  get_current_context()
    B = two_gpu_kernel(env.devices, env.streams, A)
    return B

@example_kernel.variant(gpu*1)
def one_gpu_handle(A):
    env =  get_current_context()
    B = one_gpu_kernel(env.device, env.stream, A)
    return B

@spawn(placement=[gpu*4], input=[A, B])
def task():
    #Assume A & B already distributed.
    env = get_current_context()
    num_devices = len(env)
    half = numdevices // 2

    with env.devices[:half] as subenv:
        #Dispatches to two device
        C =  example_kernel(A)
        subenv.synchronize()

    with env.device[3]:
        #Dispatches to a single device
        C =  example_kernel(B)
```



H. Lee *et al.*, "Parla: A Python Orchestration System for Heterogeneous Architectures," *SC22: International Conference for High Performance Computing, Networking, Storage and Analysis*, Dallas, TX, USA, 2022