PCRF Modeling Tools and Computational Resources

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http://pcrf.pppl.gov

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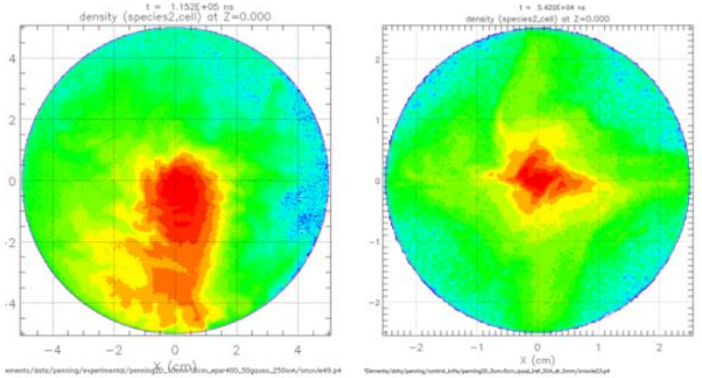
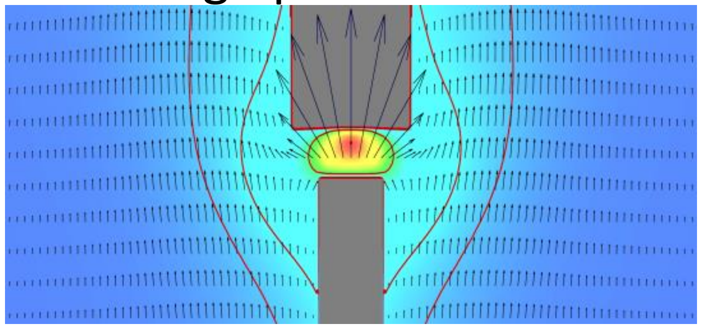
Computational Tools for LTP Modeling

- **Particle-in-cell codes (2D EDIPIC, 3D LTP PIC GPU/CPU, 3D PPPL-modified LSP)**
  - state of the art collision models and plasma-surface interaction, validated by numerous benchmarks
- **Fluid codes (3D ANSYS, OpenFoam)**
  - implemented sheath models, MHD effects, surface interface
- **Quantum Chemistry and Molecular Dynamics**
  - DFT codes: full and tight binding approximation, CMD (classical potentials), KMC –kinetic Monte Carlo, and thermodynamic code for chemical composition.

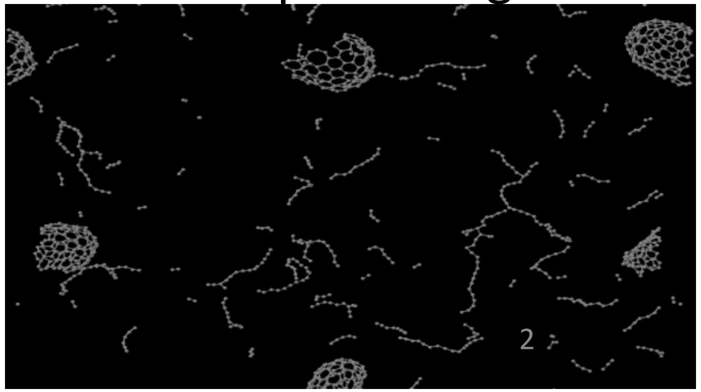
E-beam plasma



High pressure arc



Nanoparticles grow



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PPPL Modeling Team

Fluid Codes: Andrei Khodak, Alex Khrabry

Quantum Chemistry and Molecular Dynamics: Yuri Barsukov, Stephane Ethier

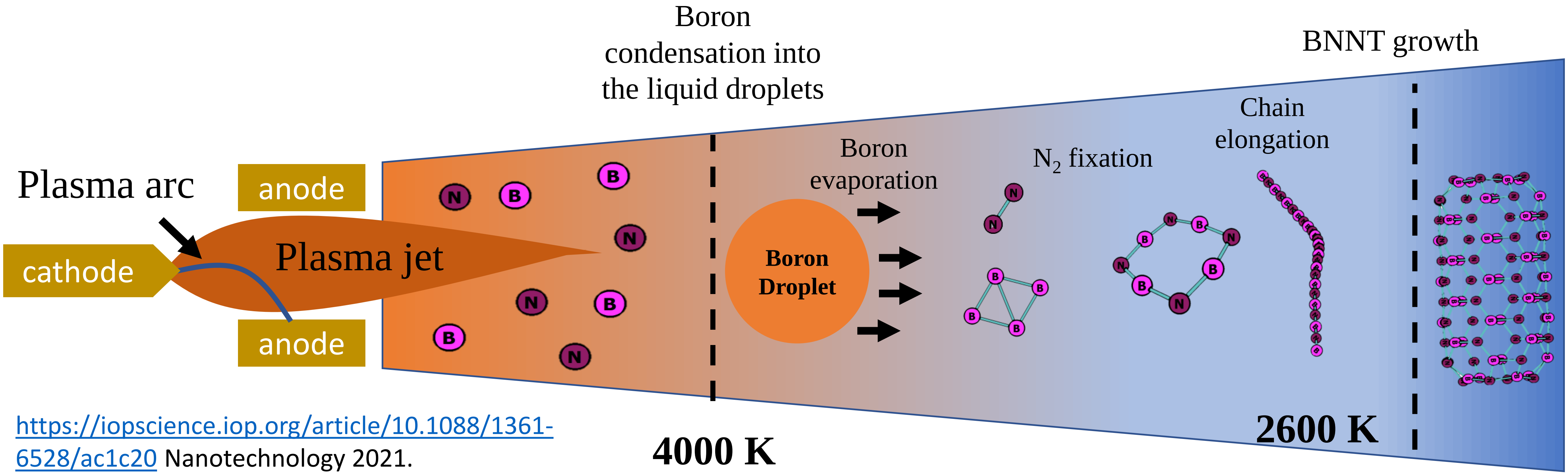
PIC simulations: Andrew (Tasman) Powis, Willca Villafana, Dmytro Sydorenko, Alex Khabrov, Stephane Ethier, Igor Kaganovich

Students: Sierra Jubin, Salman Sarwar, Haomin Sun, Michael May, Omesh Dwideli

Collaborators: Dmytro Sydorenko (U. Alberta, CA), Sarvesh Sharma (IPR, India), Liang Xu (Germany), Jian Chen (China).

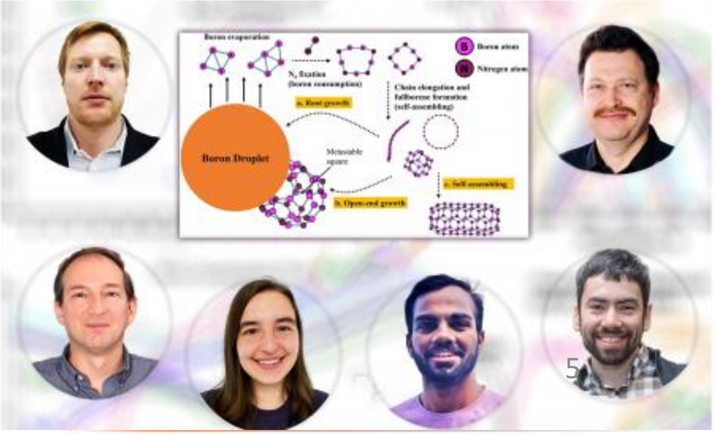
Toolbox Instead of Just One (favorite) Tool

Example of Quantum Chemistry Study: BNNTs Synthesis at High Temperature



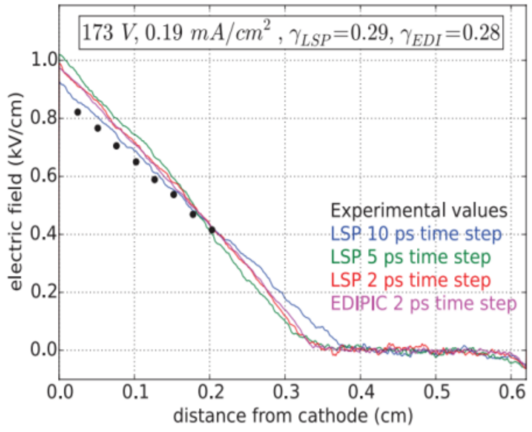
https://iopscience.iop.org/article/10.1088/1361-6528/ac1c20 Nanotechnology 2021.

We have proposed a chemical reaction pathway for precursor formation of boron nitride nanotubes (BNNT) growth. We showed that the critical step in BNNT synthesis is N_2 fixation, which occurs in the reaction of N_2 with small $B_{4,5}$ clusters, forming $B_{4,5}N_4$ chains. Subsequent chain elongation occurs via collisions of B_4N_4 and B_5N_4 with each other, and these larger chains are in turn precursors to fullborene and BNNT growth.

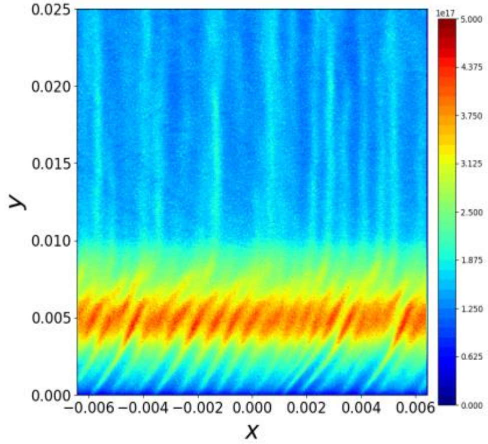


Computational Tools for LTP Modeling: PIC

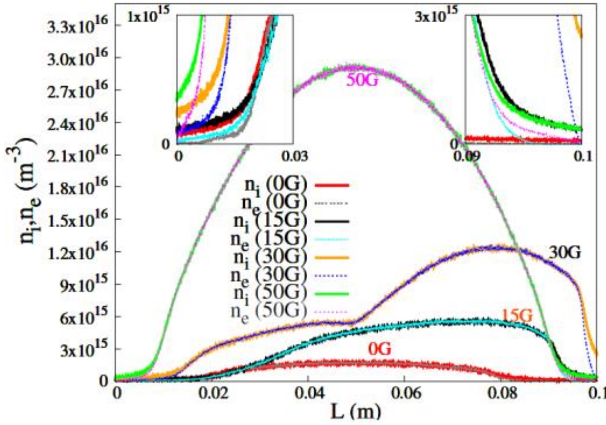
- **Particle-in-cell codes (2D EDIPIC, 3D LTP-PIC, PPPL-modified LSP)**



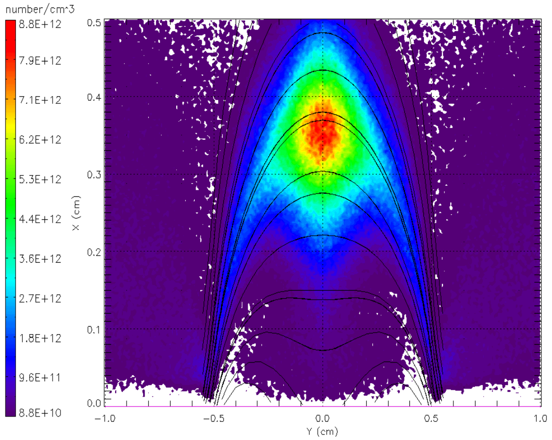
Benchmarking with a glow discharge [Carlsson *et al*, 2016]



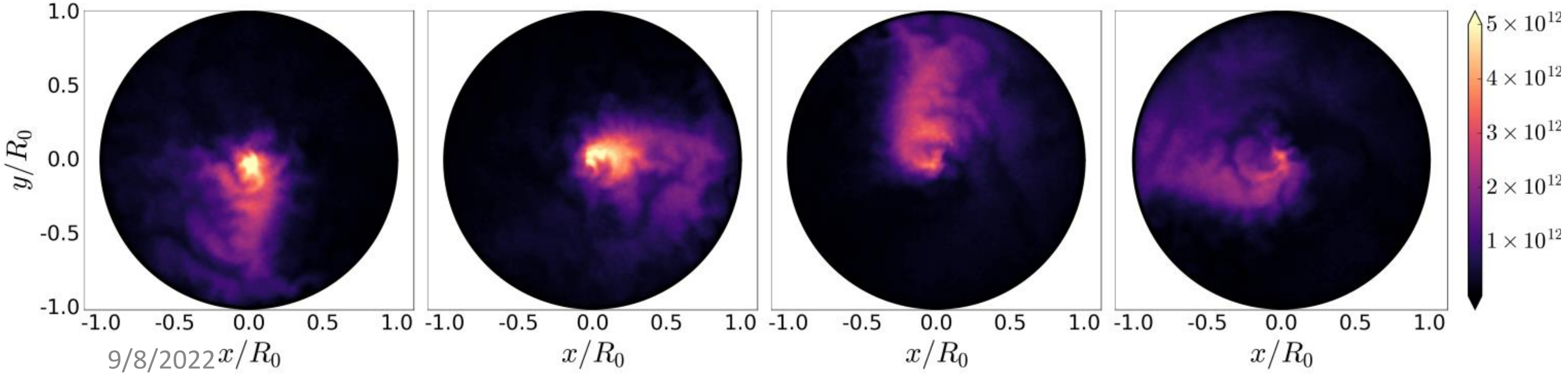
Benchmarking with a Hall thruster, Powis



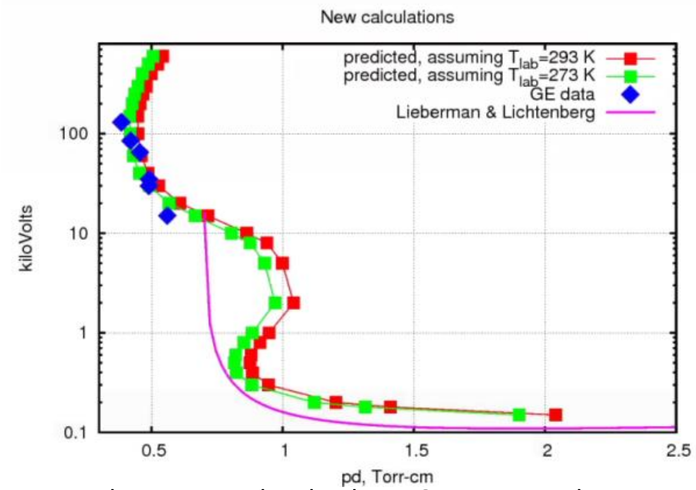
Effect of weak magnetic field in capacitively coupled discharge S. Sharma et al



Plasma switch, Carlsson, Khrabrov & Kaganovich



Rotating spoke in a Penning discharge [Powis *et al*, 2018]



Plasma switch, Khrabrov & Kaganovich

Our PIC Development Team

Igor D. Kaganovich, PI management, benchmarking, physics models.

2D EDIPIC:

Dmytro Sydorenko is a research scientist at Univ. of Alberta, main developer of EDIPIC since his Ph.D. thesis; recently working on upgrading 2D EDIPIC. **Willca Villafana** 1^{st} year postdoc, **Alex Khabrov** is a research scientist at PPPL with extensive experience in numerical theory and modeling of LTPs; benchmarking, physics models, state-of-the-art collision models.

Users: Haomin Sun, 2^{snd} year PPPL student; **Sarvesh Sharma** a research scientist at IPR India.

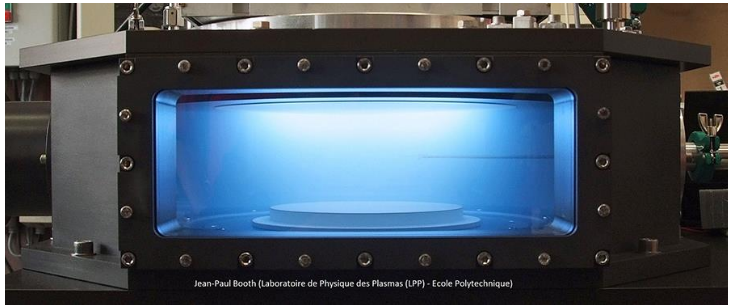
LTP-PIC:

Andrew (Tasman) Powis is 1^{st} year postdoc, main code developer.

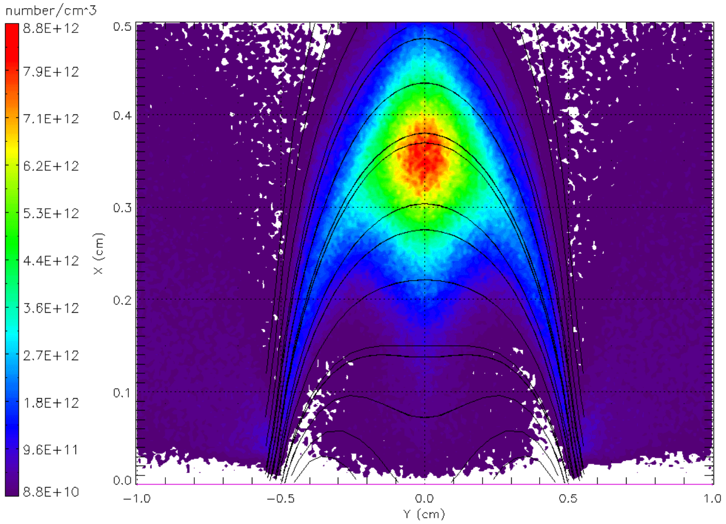
Stéphane Ethier, expert in high performance computing and heterogeneous CPU/GPU architectures.

What We Plan to Model

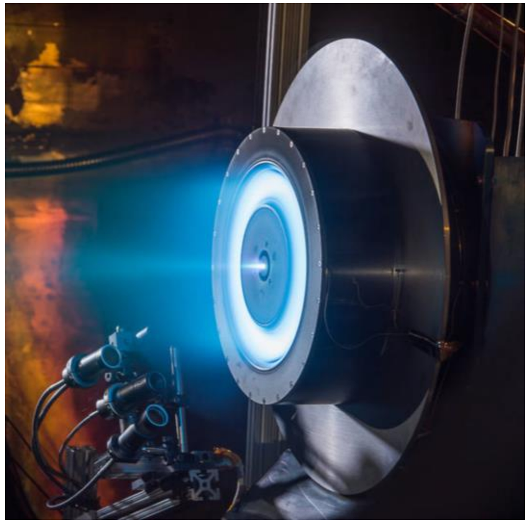
CCP cylindrical 2 and 3D, Amat



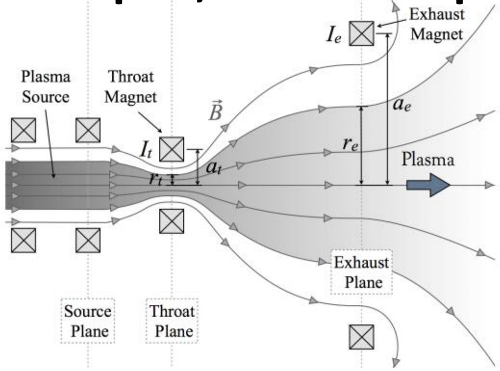
magnetron cylindrical 2 and 3D, Amat, GE



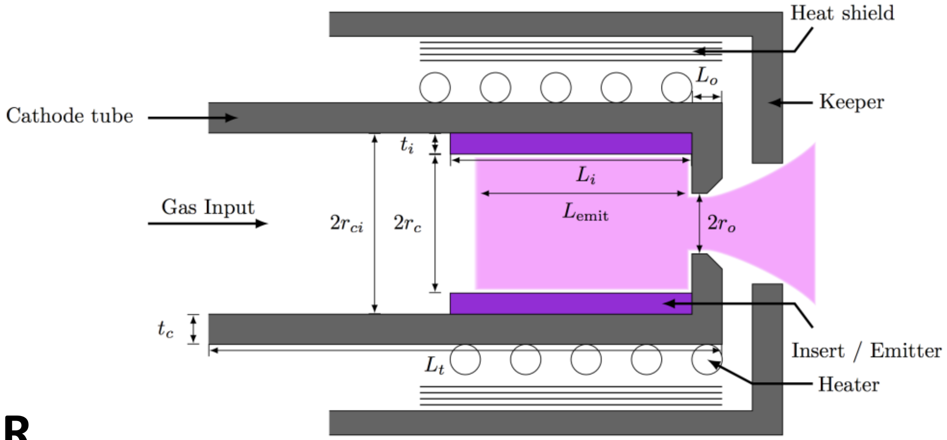
Hall Thruster 3D, AFSOR



Magnetic Nozzle 3D, AFSOR, Tri-alpha, UIUC user project



Hallow cathode with orifice for AFSOR, MI user project



Towards modelling large 2D and 3D plasmas

Better Software

- High performance on a single or multicore CPU
- Acceleration with GPUs
- Excellent parallelisation and load balancing
- Portability and extensibility
- Validation and verification
- Good documentation

Better Algorithms

- Allow for large cell sizes
- Allow for large time steps
- Explicit where possible
- Good long-term accuracy and stability

Introducing EDIPIC-2D

2d3v Particle-in-Cell

Designed from the ground up for performance on highly distributed computing systems

Multiple ion species. Walls may emit particles.

Monte-Carlo model of electron-neutral collisions:

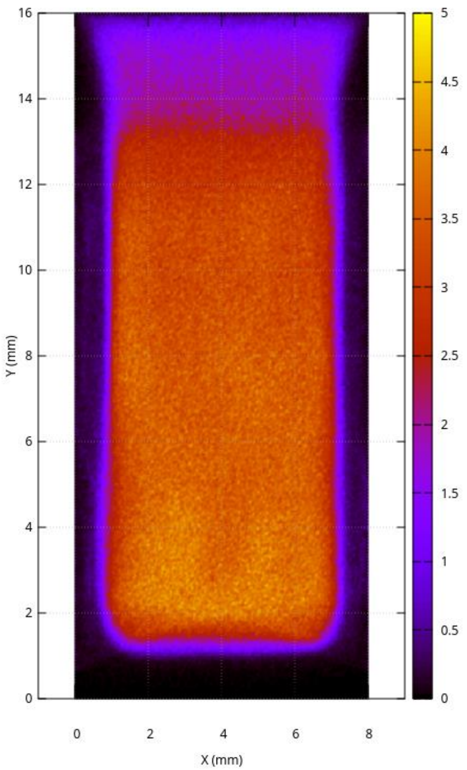
Multiple neutral species with nonuniform density

Code works on CPUs, is written in Fortran 90, parallelized with MPI.

The code combines domain decomposition and particle sharing.

Special methods ensure even particle load between CPU cores.

Abundant diagnostics output



2D Simulations of a hollow cathode DC system for GE.

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EDIPIC-2D Summary

- Includes external magnetic field, collisions, and SEE emission from walls which makes it suitable for simulations of dc and rf discharges.
- The code is parallelized with MPI and shows linear scaling in performance. The algorithm ensures even particle load between CPU cores.
- The code was validated in numerous benchmarks involving multiple other codes.
- **Source files are free:** github.com/PrincetonUniversity/EDIPIC-2D
  - together with a sample set of input data files, description of input and output data files, several programs for processing the output, compilation instructions.
- **Used by industry: Applied Material, GE, Tri-alpha,**
- **Internationally: Germany, China, India**
- PPPL, Universities: Purdue, U. of Saskatchewan, Alberta

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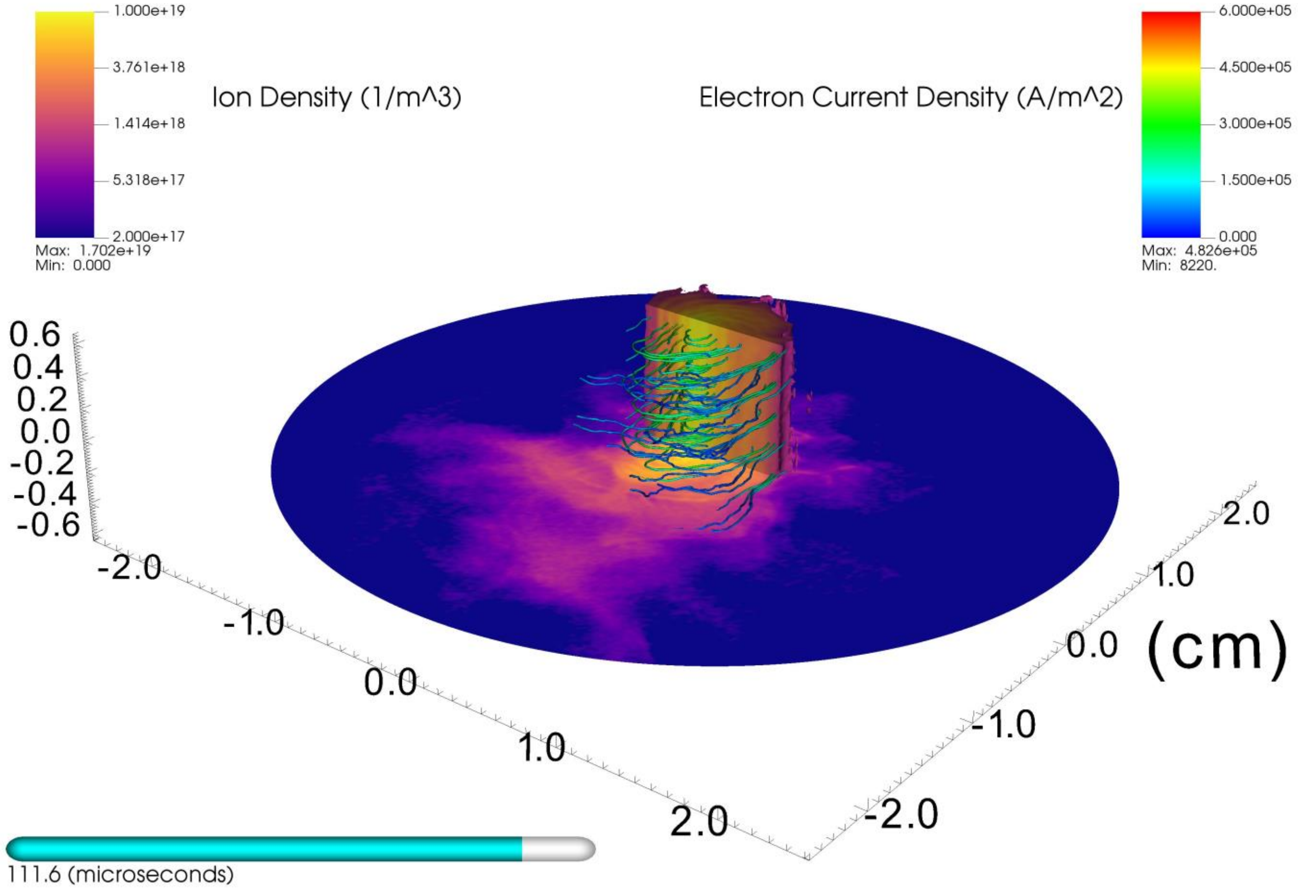
Introducing 3D LTP-PIC on CPU/GPU

Designed from the ground up for performance on highly distributed computing systems

Designed to be portable and extensible

Special focus on performance of the electrostatic field solver and implementation of low-temperature specific collision algorithms



3D collisionless simulation of the Penning discharge with density contours and electron current streamlines

https://www.youtube.com/watch?v=Qlz3-by63yw

LTP-PIC Features

- Explicit momentum-conserving PIC with geometric multigrid electrostatic field solver
- Uniform Cartesian mesh in 2/3D with complex geometry
- Collisions with a fixed neutral background:
  - Electron/ion-neutral elastic, inelastic (excitation) and ionization
  - Ion-neutral charge-exchange
- Hybrid Domain and particle decomposition for improved load balancing
- 15,000+ lines of C code, parallelised via MPI and OpenMP
- Accelerated on GPUs with OpenACC

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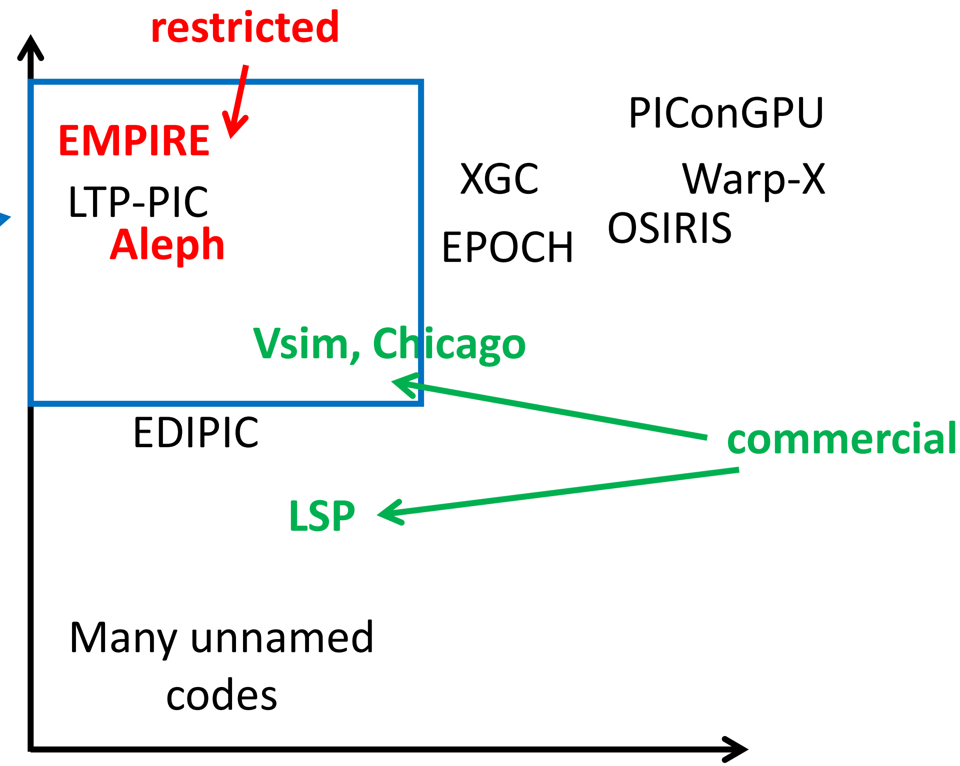
Why a new code?

Software Performance

Required for multi time and length scale low-temperature plasma simulations



Codes in this region include

- Efficient algorithms which can target modern CPUs
- Parallelisation to 100's of nodes
- Acceleration on GPUs

Codes in this region include

- Electrostatic field solver
- Extensive suite of Monte-Carlo collision algorithms
- Surface interaction physics
- Complex geometry
- Kinetic neutral treatment

Plasma Temperature

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PCRF 2020, 2021 Accomplishments

- **Home Research**, 2 papers on collisionless turbulence submitted to PRL, 1 to PRE.
- UIUC group project was interested in excitation of electrostatic solitary waves during beam neutralization. They used their group code Chaos to perform 2D and 3D PIC simulations. **PPPL provided theory support weekly**. Extended verification of results was performed, new modes were discovered and are being analyzed. **3 papers submitted.**
- Perdue University is given 1D EDIPIC to simulate RF and MW discharges.1 paper submitted, 2 more in preparation. **PPPL provided code and theory support monthly**
- Sandia group applied ML to problem of hydrogen negative ions formation, a global model code was given to them for study of reaction pathways, paper in preparation.
- Tri-alpha is given EDIPIC code to simulate plasma spin up by the DC electrodes.
- LANL and LBNL user proposals were funded, started work in 2021.
- Seoul University group started using EDIPIC code and obtained first results.

Summary: Toolbox Instead of One Tool

Particle-in-cell codes (2D EDIPIC, 3D LTP PIC GPU/CPU, 3D PPPL-modified LSP)

state of the art collision models and plasma-surface interaction, validated by numerous benchmarks

Fluid codes (3D ANSYS)

implemented sheath models, MHD effects, surface interface

Quantum Chemistry and Molecular Dynamics

LAMMPS, DFT-TB, DFT: Gaussian, GAMESS, Orca, Firefly, CRYSTAL, VASP, Quantum Espresso (PU), Thermodynamics, KMC.

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PCRF Theoretical and computational Resources
(Mikhail Shneider, MAE Department, Princeton University)

study of a physical problem → formulation of mathematical model → estimates and analytical theory → numerical simulation → validation on known etalon experiment → interpretation of observations

Our codes:

- Fluid (diffusion-drift); hybrid, for example, ions are considered in the diffusion-drift approximation, and electrons are considered based on the solution of the non-local kinetic equation + Poisson equation for field
- Equilibrium and non-equilibrium weakly ionized plasma.
- In a molecular plasma translational, rotational, and vibrational degrees of freedom
- Radiative transfer

Possibilities for calculating various types of discharge

- DC Glow, Capacitive coupled RF in planar or cylindrical geometry
- DBD in planar geometry or asymmetric, Pulsed arcs
- Microwave breakdown

Laser induced plasma

- Nanosecond laser pulses – avalanche breakdown; femtosecond – Multi Photon Ionization (MPI)
- Resonance Enhanced MPI plasma generation and evolution in inert gases
- Laser-induced filament evolution
- Double laser or hybrid laser-microwave induced plasma

Detailed weakly-ionized plasma chemistry Air, Ar, Xe, Ar-Xe, Ar-N_2

Different kinds of MHD generators

MHD with alkali metal seeding or ionization by electron beams or nanosecond pulses

Users:

1. Prof. Xuewei Zhang, TAMUK

X. Zhang, M.N. Shneider, Electron generation and multiplication at the initial stage of nanosecond breakdown in water, J. Appl. Phys. 129, 103302 (2021)

2. Prof. Alexandros Gerakis, Luxemburg

M. Mokrov, M.N. Shneider, A. Gerakis, Analysis of coherent Thomson scattering from a low temperature plasma, Phys. Plasmas 29, 033507 (2022)

3. Prof. Alexander Fridman, Drexel University

Effects of plasma on physical properties of water: nanocrystalline-to-amorphous phase transition and improving produce washing, (submitted); arXiv:2204.05888, 2022