Examples of Benchmarking and Validation for DC and RF discharges

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U.S. DEPARTMENT OF ENERGY | Office of Science

PPPL PRINCETON PLASMA PHYSICS LABORATORY

Why do Benchmarking and Validation?

- **Towards Predictive Modeling**
  - 2-3D PIC codes benchmarked and validated for simulations of plasma applications

- **Industry Collaboration: GE, Samsung.**
  - Need to debug codes, atomic physics and surface processes

- **Recent successes**:

  high-voltage breakdown simulations for GE plasma switch for electric grid,

  2D simulations of spoke in ExB devices;

  2D structure of arc

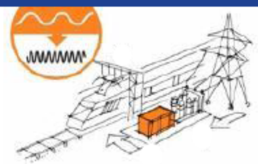
  Negative ion sources H^-.

PPPL Performed modeling of High Voltage Plasma Switch for General Electric and helped to understand operation of the device.

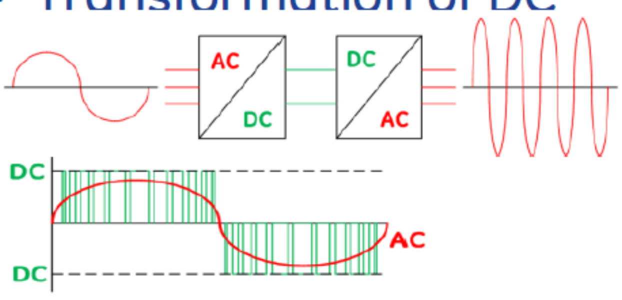
L. Xu, GI2.00006 Three regimes of high voltage breakdown in a high current plasma switch for modern electric grid, Tuesday, November 6, 2018, Ballroom 203, 12 pm

Technology Description

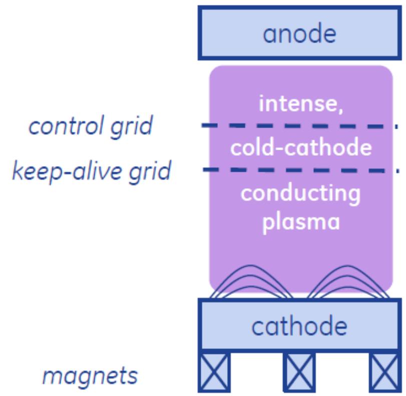
- Convert electricity into electricity

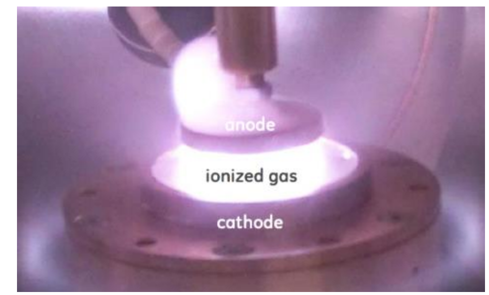


- Convert alternating current to direct current and vice versa
- Technology trends
  - Higher power & frequency
  - Large-scale PE systems
  - Transformation of DC

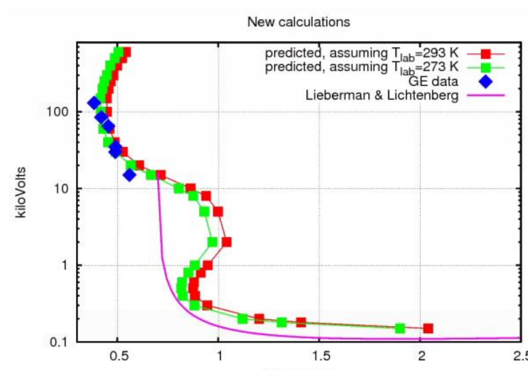


Schematics and image of plasma switch





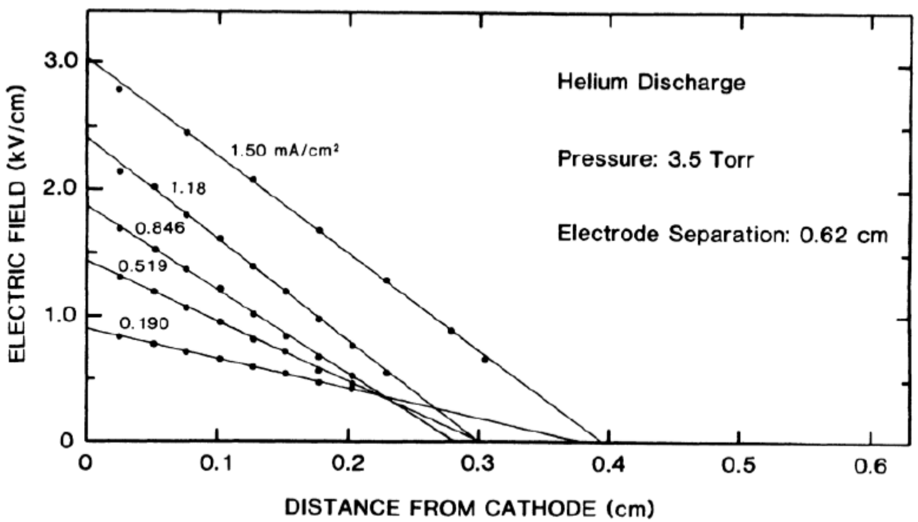
PIC modeling clarified the discharge parameters for high voltage breakdown and plasma fluxes to the electrodes.



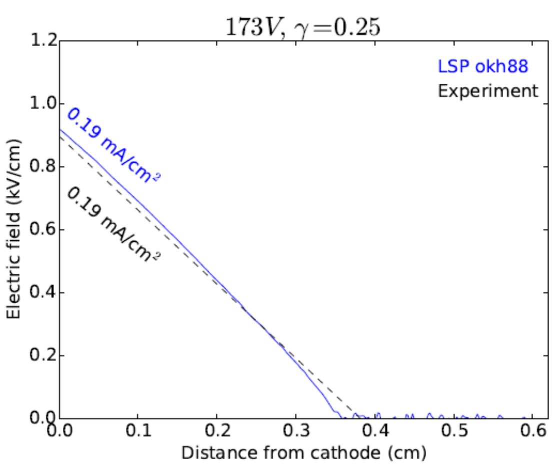
Simulated Voltage breakdown voltage as function of pressure and gap width

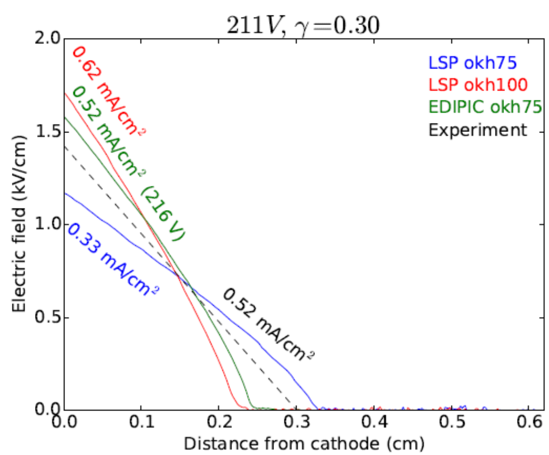
Benchmarking of 2 PPPL codes

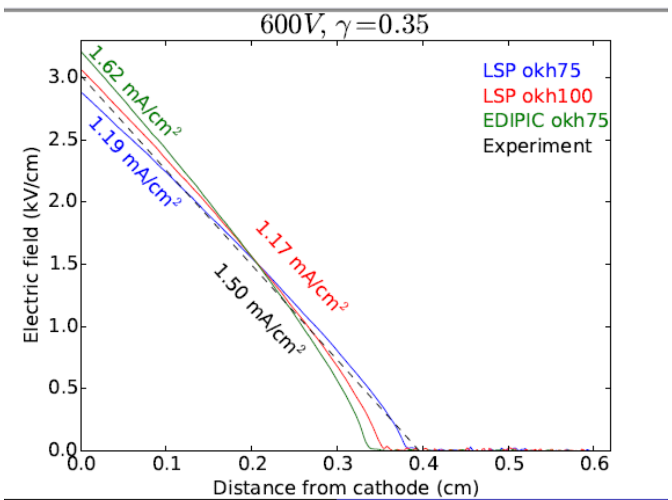
Johan Carlsson, Alexander Khrabrov, Igor Kaganovich, Timothy Sommerer and David Keating**, "***Validation and benchmarking of two particle-in-cell codes for a glow discharge***",** PSST **26,** 014003 (2017).



Accurate and complete measurements of the plasma quantities: E(x), γ, J, U.
E. den Hartog, et al, Phys. Rev. A 38, 2471 (1988).

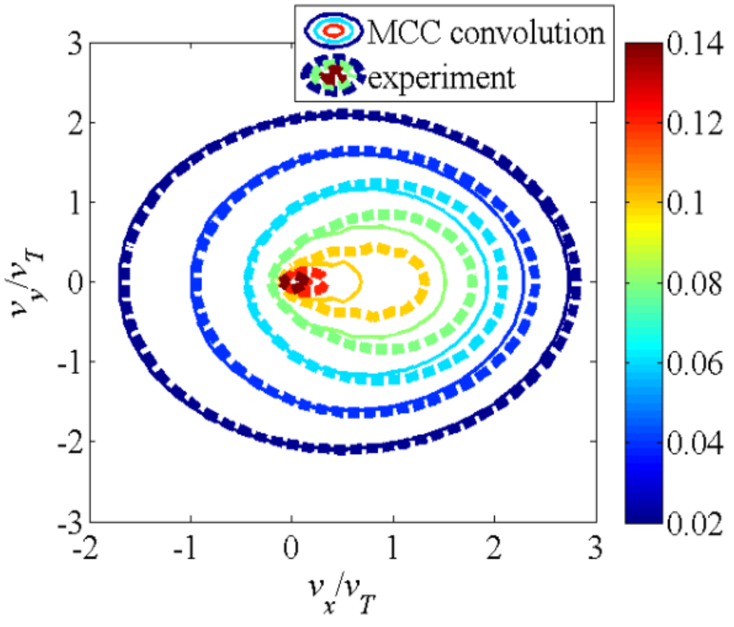


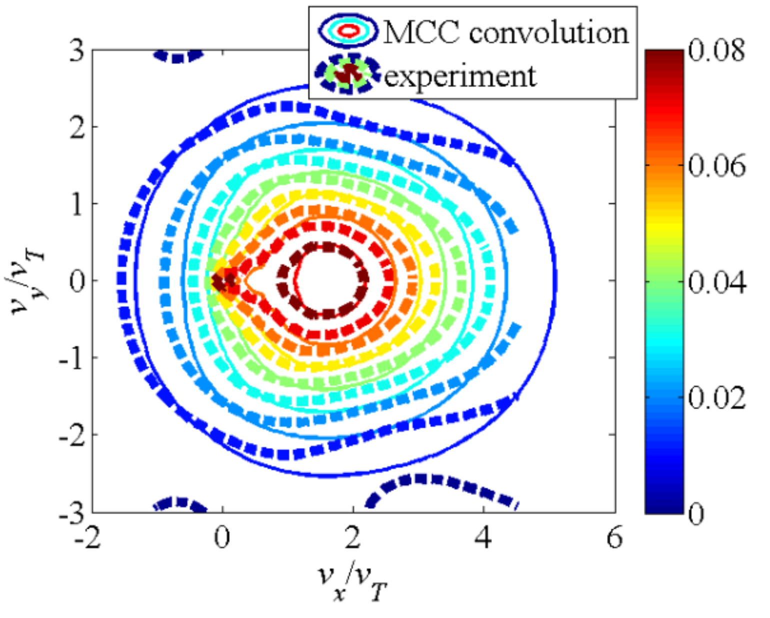




Validation of ion velocity distribution functions (ivdf) in argon and helium discharges.

Fig. **Angular distribution of ion velocity distribution function simulated by PIC and measured by flat probe. Left: Argon, Right: Helium.**





H. Wang, V. S. Sukhomlinov, I. D. Kaganovich, and A. S. Mustafaev, "*Simulations of Ion Velocity Distribution Functions Taken into Account Both Elastic and Charge Exchange Collisions*", PSST **26**, 024001 (2017).

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Negative hydrogen ion sources

- **Electron impact induced processes**

$$R_1:\ H_2(\upsilon) + e \rightarrow H_2(\upsilon') + e\ \text{(via resonant } H_2^-)$$

$$R_2:\ H_2(\upsilon) + e \rightarrow H_2(\upsilon') + e + h\nu\ \text{(via } B^1\Sigma_u^+,\ C^1\Pi_u)$$

$$R_3:\ H_2(\upsilon) + e \rightarrow 2H + e$$

$$R_4:\ H_2(\upsilon) + e \rightarrow H_2^+ + 2e$$

$$R_5:\ H_2(\upsilon) + e \rightarrow H + H^+ + 2e$$

$$R_6:\ H_2(\upsilon) + e \rightarrow H^- + H$$

- **Vibrational-translational relaxation**

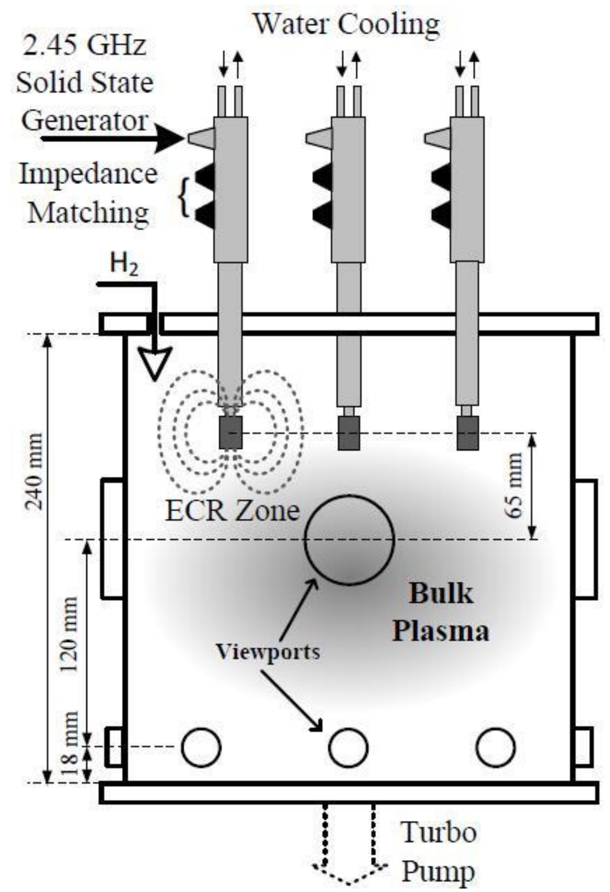
$$R_7:\ H_2(\upsilon) + H \rightarrow H_2(\upsilon') + H$$

$$R_8:\ H_2(\upsilon) + H_2(\omega) \rightarrow H_2(\upsilon \pm 1) + H_2(\omega)$$

$$R_9:\ H^- + H_2(\upsilon) \rightarrow H + H_2(\upsilon - 2) + e$$

- **Wall relaxation**

$$R_{10}:\ H_2(\upsilon') + \text{wall} \rightarrow H_2(\upsilon)\ (\upsilon < \upsilon')$$

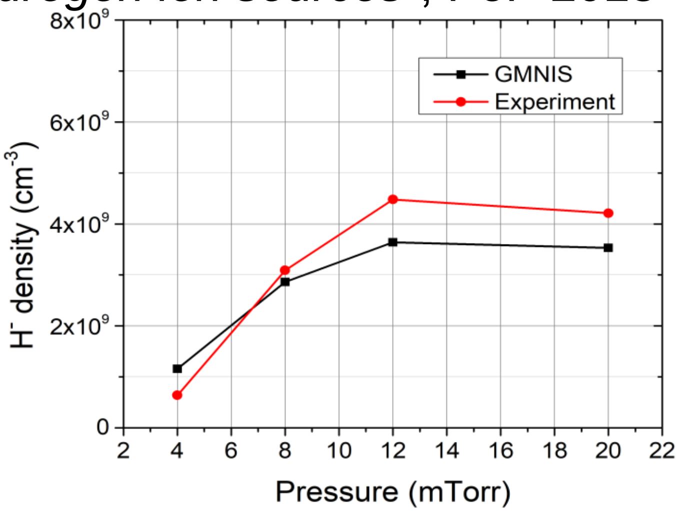


- **Experimental setup of the source**

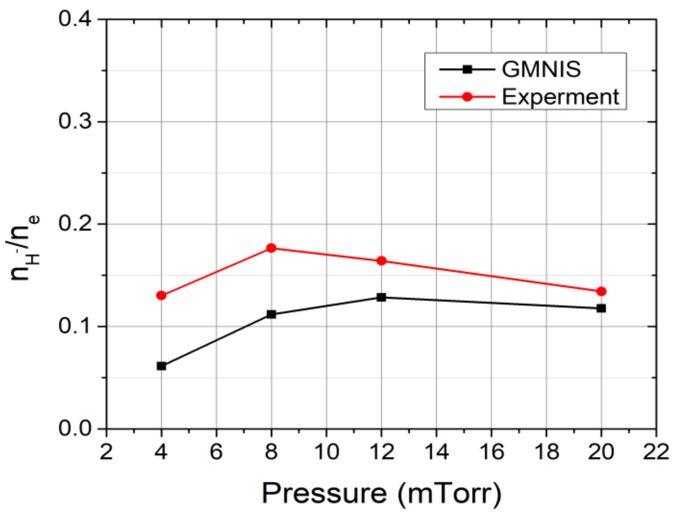
P. Svarnas, S. Aleiferis, Greece

Validation for ECR discharge

W. Yang et al, "*Benchmarking and validation of global model code for negative hydrogen ion sources*", PoP 2018



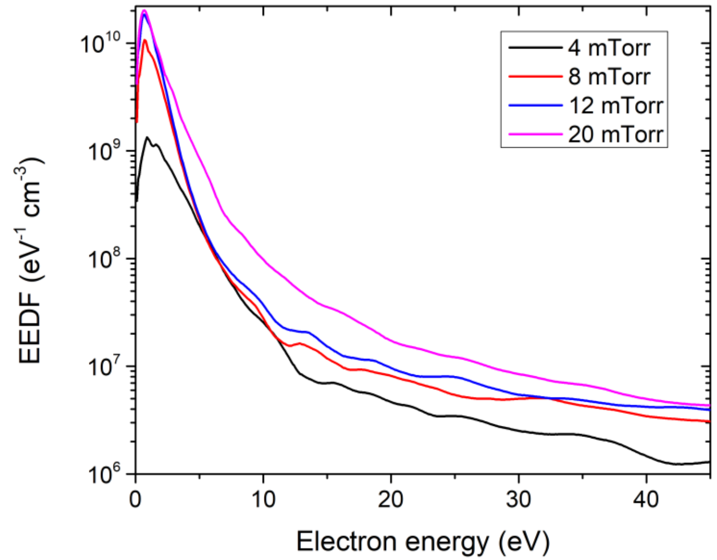
- **H^- density as a function of pressure.**



- **n_H-/n_e ratio as a function of pressure.**

Negative ion density is calculated based on measured EEDF:

$$n_{H^-} = \frac{\sum_{v=0}^{14} n_{H_2(v)} n_e \left\langle \sigma_{DA}(\varepsilon), \varepsilon \right\rangle}{k_{MN} n_+ + k_{AD} n_H + n_e \left\langle \sigma_{ED}(\varepsilon), \varepsilon \right\rangle + k_{MD} n_{H_2(v)}}$$



- **Measured EEDF as a function of electron energy.**

Validation of codes for CCP discharge

Miles M Turner, *"Uncertainty and sensitivity analysis in complex plasma chemistry models*", Plasma Sources Science and Technology **25**, 015003 (2016)

M. M. Turner, A. Derzsi, Z. Donkó, D. Eremin, S. J. Kelly, T. Lafleur, and T. Mussenbrock, "*Simulation benchmarks for low-pressure plasmas: Capacitive discharges*", Physics of Plasmas **20**, 013507 (2013) 64 citations

Z Donkó, A Derzsi, I Korolov, P Hartmann, S Brandt, J Schulze, B Berger, M Koepke, B Bruneau, E Johnson, T Lafleur, J-P Booth, A R Gibson, D O'Connell and T Gans, "*Experimental benchmark of kinetic simulations of capacitively coupled plasmas in molecular gases*", Plasma Phys. Control. Fusion **60**, 014010 2018.

M Daksha, A Derzsi, S Wilczek, J Trieschmann, T Mussenbrock, P Awakowicz, Z Donkó and J Schulze, "*The effect of realistic heavy particle induced secondary electron emission coefficients on the electron power absorption dynamics in single- and dual-frequency capacitively coupled plasmas*", Plasma Sources Sci. Technol. **26**, 085006 (2017).

Workshop on High Performance Computing for Plasma Applications

Monday November 5th, GEC 2018, Portland,

Organizers: Igor D. Kaganovich (PPPL), Douglas Keil (Lam Research Corporation), Tom Kirchner (York University)

9:30AM - 10:00	**Future of High Performance Particle-in-cell codes computing Invited Speaker: J. Carlsson with contributions from: G.- L. Delzanno, J-L Vay, Tech-X, Voss Scientific (LSP and Chicago codes), ICEPIC AFOSR**
10:00AM - 10:30AM	Efficient use of GPUs in PIC and associated issues Invited Speaker: P. Messmer (NVIDIA) with contributions from: H.J. Lee, D. Eremin, Voss Scientific (Chicago code), S. Ethier, PPPL
10:30AM - 11:00AM	3D Fluid simulations of discharges Invited Speaker: G. Hagelaar with contributions from: M. Kushner, L. Raja, D. Curreli, A. Smolyakov, Applied material, TEL, N. Babaeva
11:00AM - 11:30AM	3D Fluid simulations of arcs Invited Speaker: M. Benilov, with contributions from: M. Baeva, PPPL, CFDRC, Sandia, J. Trelles
11:30AM - 12:00PM	Atomistic simulations of plasma-surface interaction for ALD and ALE processes, Invited Speaker: S. Hamagushi, with contributions from: E. Neyts, D. Graves, P. Moroz TEL
12:00PM - 12:30PM	Dataset for cross sections , Invited Speaker: J. Tennyson (London) , with contributions from: R.K. Janev, K. Bartschat, T. Kirchner
Lunch	
2:00PM - 2:30PM	Mullti-scale methods for plasma chemistry, Invited Speaker: D. Curreli, with contributions from: Y. Omelchenko, J. Verboncoeur, L. Raja, Dutch groups, ChemKin
	High level HPC examples from MFE and IFE
2:30PM - 3:00PM	Update on Code Validations and Verifications , Invited Speaker: M. Turner with contributions from: A. Khrabrov, MIT DOE paper, OSCAR Applied Math approaches
3:00PM - 3:30PM	Laser plasma interaction, Invited Speaker: J.L. Vay with contributions from: W. Mori, A. Pukhov, G. Shvets
3:30PM - 4:00PM	MFE HPC PIC , Invited Speaker: CS Chang with contributions from: W.W. Lee, Z. Lin, W. Wang
4:00PM - 4:30PM	PSI modeling, Invited Speaker: Longtao Han (Stony Brook) with contributions from: E. Carter, A. Pigarov, P. Krstic
4:30PM - 5:00PM	Adaptive Kinetic – Vlasov methods, Invited Speaker: V. Kolobov, with contributions from: G. Hammett, F. Jenko, LLNL, GA