Predictive Simulation of Pattern Formation and Self-Organization in Plasmas

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Frontiers of Plasma Science Workshop

Virtual Town Hall Meeting - Plasma Self-Organization

August 12, 2015

Outline

1. **Research frontier**
   - Self-organization in Nature & Plasmas
   - Experimental & Computational

   Where we are

2. **Advancing the frontier**
   - Scope of advances needed:

     Mathematical, Computational, Experimental

   Where we need to go & how to get there

3. **Impact**
   - Scientific & Societal benefits

   Why it matters

1. Research Frontier

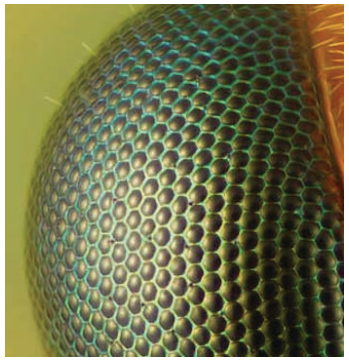
Simulation of Pattern Formation and Self-Organization: Capturing Nature with Confidence

S. Wolfram, A New Kind of Science (2002)

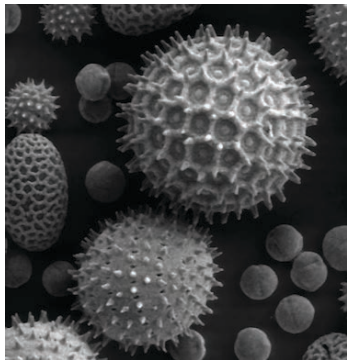
Pattern Formation & Self-Organization

- **Diverse manifestations:**
  - Biological, chemical, physical systems

wasp eye [1]



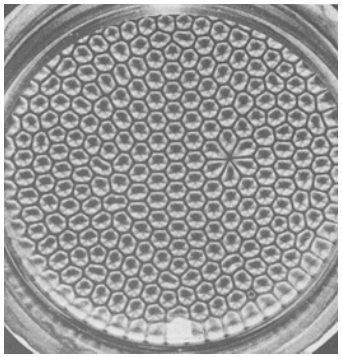
pollen [2]



snowflake [3]

chemical oscil. [4]

convection cells [5]

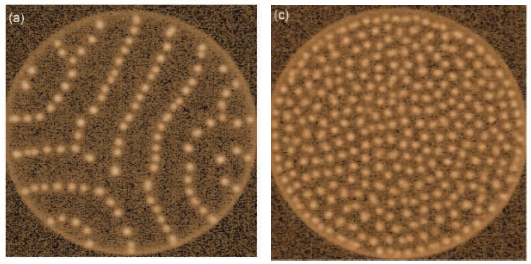


- **Competing effects:**
  - Transport/Dissipation vs. Forcing/Generation
- **Associated to:**
  - Instability, bifurcation, symmetry-breaking, dissipative structures, non-equilibrium, chaos …

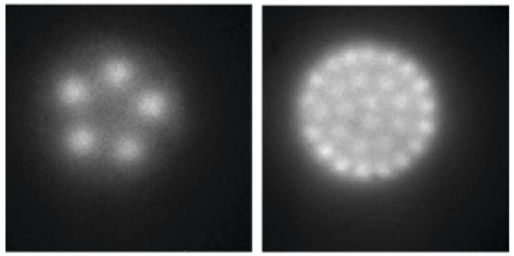
[1] www.telegraph.co.uk
[2] en.wikipedia.org/wiki/Pollen
[3] www.its.caltech.edu
[4] www.catea.gatech.edu/grade/mecheng/mod8/mod8.html
[5] www.dataisnature.com

Pattern Formation in Plasmas …

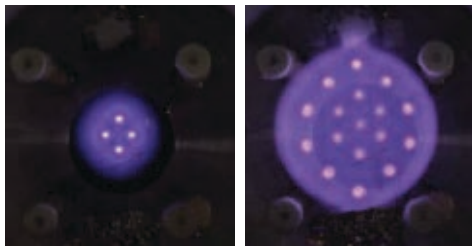
- **Found in diverse types of discharges:**
  - AC & DC, low & high pressure, high & low temperature, continuous & pulsed, uniform & dusty, solid & liquid surf., micro- & macroscopic, …

1 

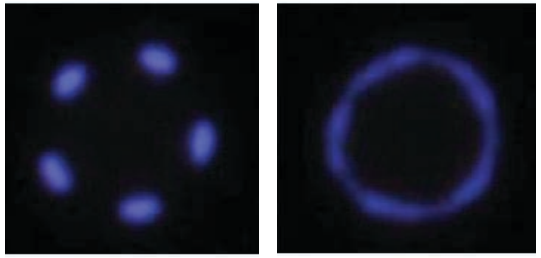
Low Temperature DC

2 

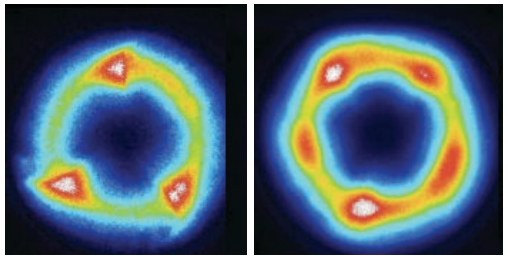
Microdischarges

3 

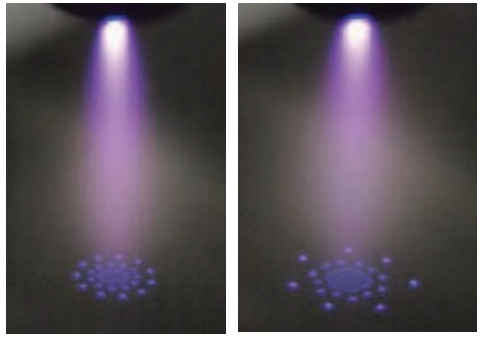
Dielectric Barrier Discharges

4 

Cathode discharges

5 

Magnetrons

6 

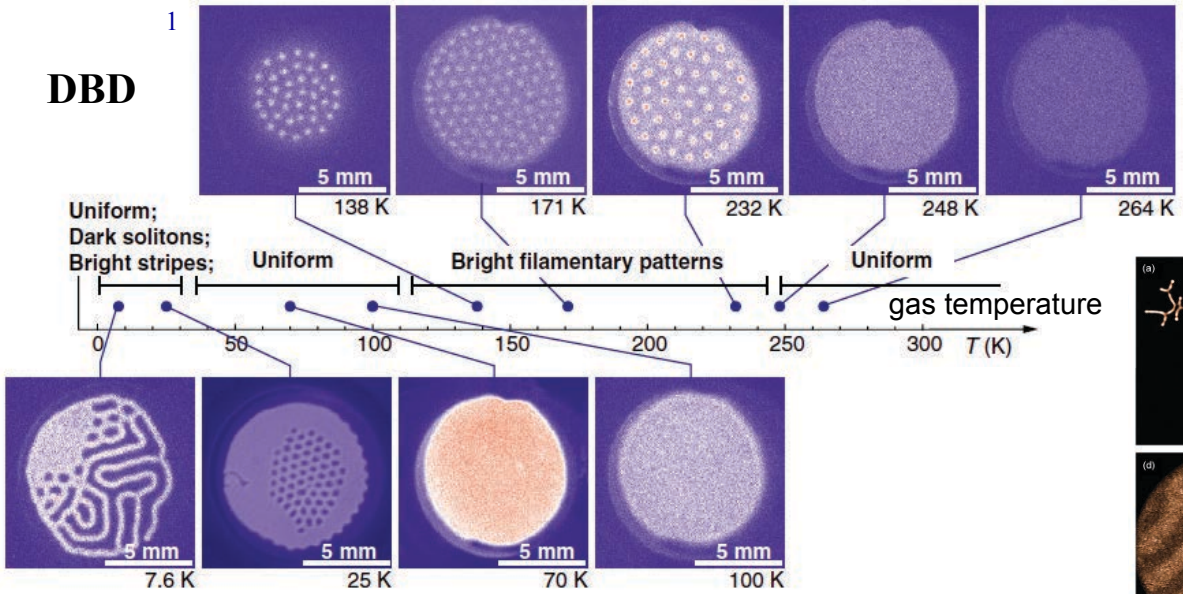
Glow

[1] Purwins H-G and Berlemeier J 2011 *IEEE Trans Plasma Sci* 39 11 2116
[2] Schoenbach K H, Moselhy M and Shi W 2004 *Plasma Sources Sci Technol* 13 177
[3] Abolmasov S P and Tachibana K 2011 *IEEE Trans Plasma Sci* 39 11 2090
[4] Zhu W-D, Niraula P, and Becker K H, 41ST ICOPS, Washington DC, May 27, 2014
[5] Yang Y, Tanaka K, Liu J, and Anders A 2015 *Appl Phys Lett* 106 124102
[6] Shirai N, Uchida S, Tochikubo F, and Ishii S 2011 *IEEE Trans Plasma Sci* 39 11 2652

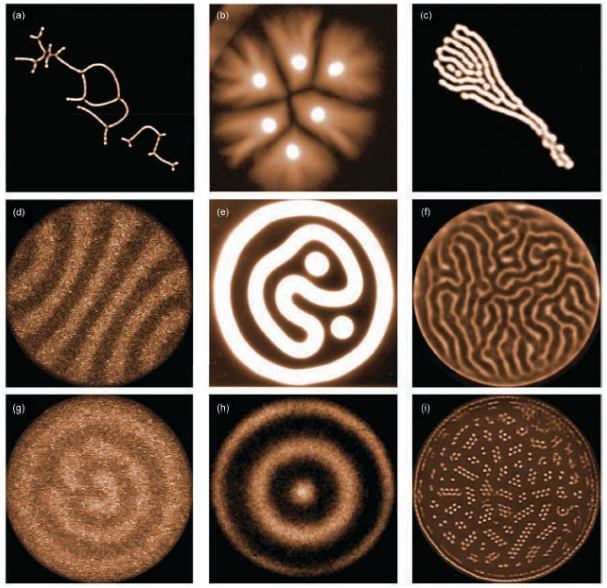
… an Exceedingly Wide Variety of Phenomena

- **Large variations depending on "a few" controlling parameters:**
  - pressure, temperature, composition, electrode spacing, frequency, …

DBD [1]



Low Temperature AC [2]



- Spots, stripes, rings, spirals, tessellations, clusters, …
- From static to dynamic

[1] Stauss, Muneoka, Ebato, Oshima, Pai and Terashima 2013 *Plasma Sources Sci Technol* 22 025021
[2] Purwins H-G 2011 *IEEE Trans Plasma Sci* 39 11 2112

Self-Organization Modeling: The Case of Biology

- Long trajectory (e.g. Turing (1952)) - good "qualitative" understanding
- E.g. activator–inhibitor system:

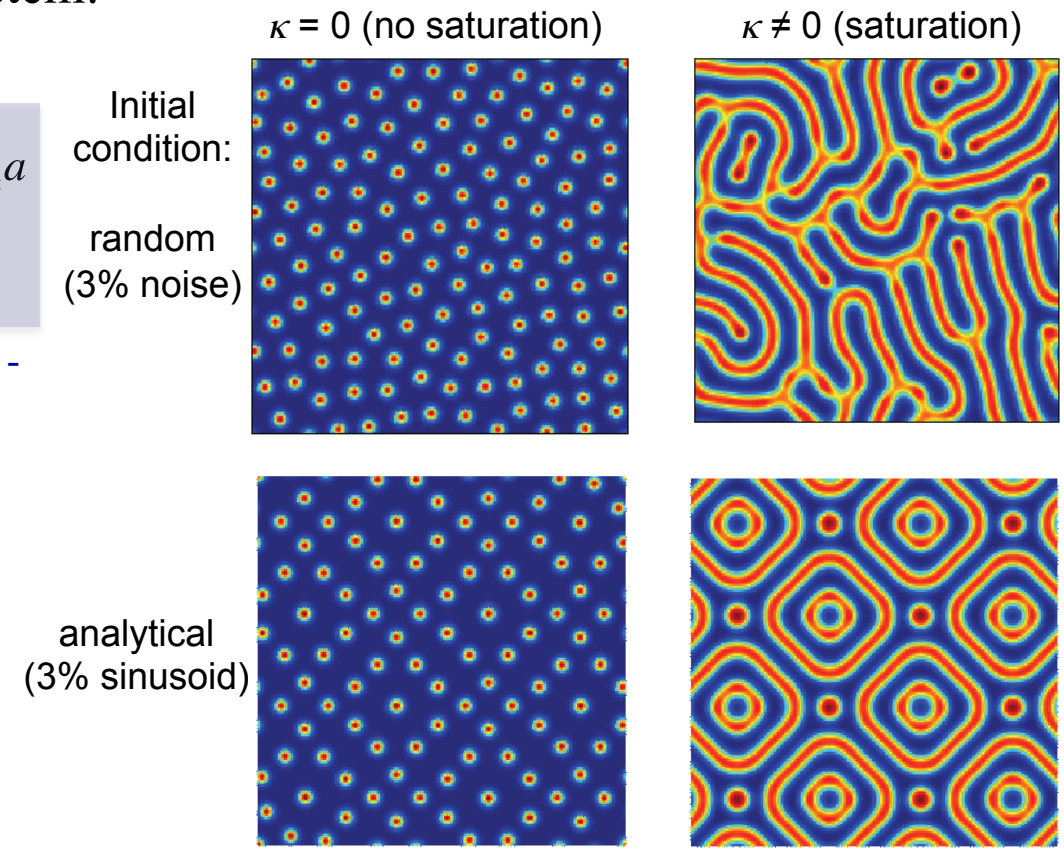
Parameters

$$\partial_t a = D_a \nabla^2 a + \rho_a \frac{a^2}{(1+\kappa_a a^2)h} - \mu_a a$$

$$\partial_t h = D_h \nabla^2 h + \rho_h a^2 - \mu_h h$$

Diffusive transport - dissipation (linear)

Reactive transport - equilibration (non-linear)



- … highly dependent on initial conditions

➢ Can we we achieve comparable understanding using state-of-the-art plasma models with <u>no</u> parameters (?)

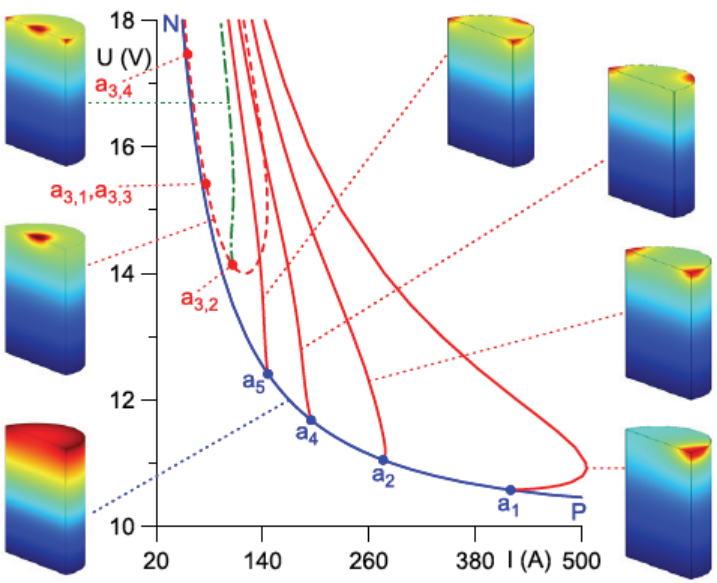
Computational Plasma Self-Organization

- Frontier Question:

Can current computational plasma tools "predict" pattern formation and self-organization reliably?

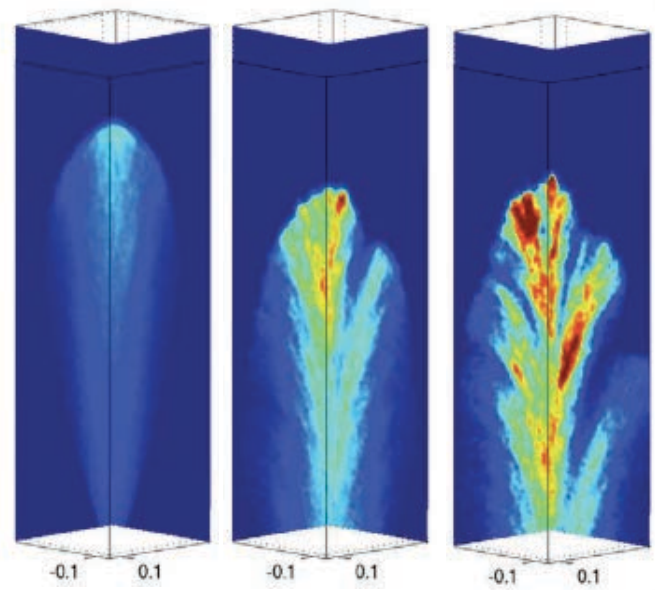
(no prior knowledge of solutions, no "tuning" parameters, suitable for applications)

Cathode Spots in Arcs:
Multiple solutions - bifurcation



Benilov, Plasma Sources Sci. Technol. 23 (2014) 054019

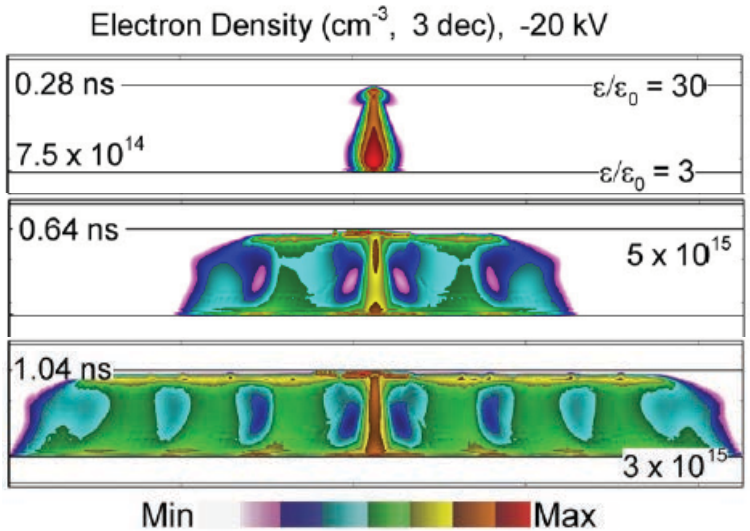
Streamers:
Symmetry-breaking



Li, Teunissen, Nool, Hundsdorfer, and Ebert, Plasma Sources Sci. Technol. 21 (2012) 055019

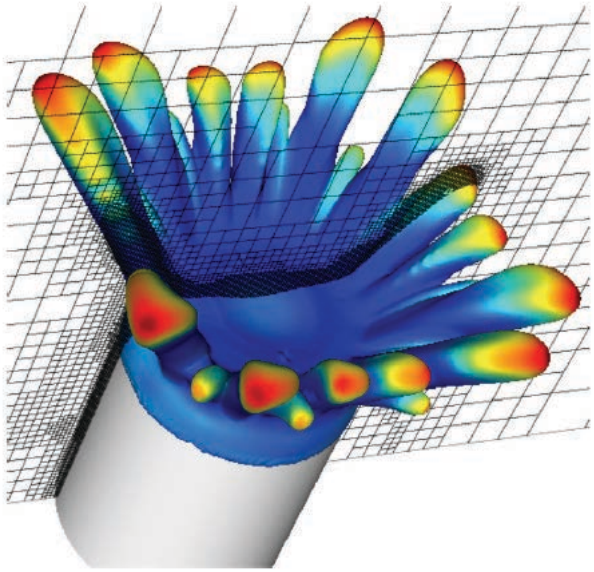
Computational Plasma Self-Organization (cont.)

DBD:
Filament formation



Babaeva and Kushner, Plasma Sources Sci. Technol. 23 (2014) 065047

Corona discharges:
Streamers formation



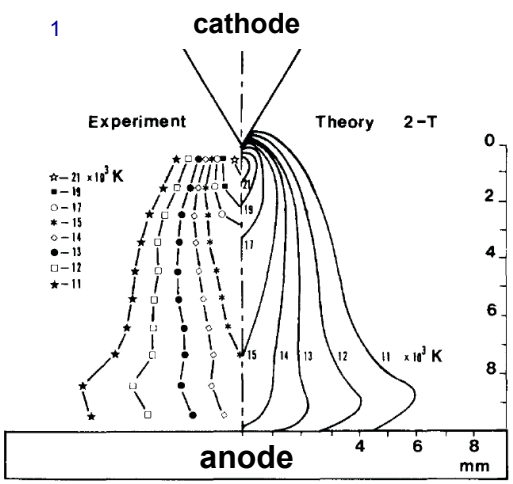
Nikandrov, Arslanbekov, Kolobov, IEEE TPS 36 (2008) 932

- Features of state-of-the-art simulations:
  - Deal with wide range of spatial & temporal scales
  - Computationally demanding, often trading detailed physics and dimensionality

A Specific Case: Anode Patterns in Arcs

- **Free-burning arc:** Canonical discharge & applications relevant (welding)
- **Extensively studied:** Experimentally & Numerically (benchmark)
- **Features:** Simple geometry, “steady”, “axi-symmetric”, “LTE”, … ???

1



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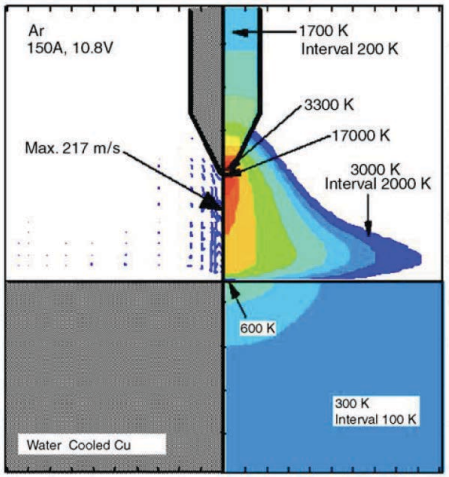
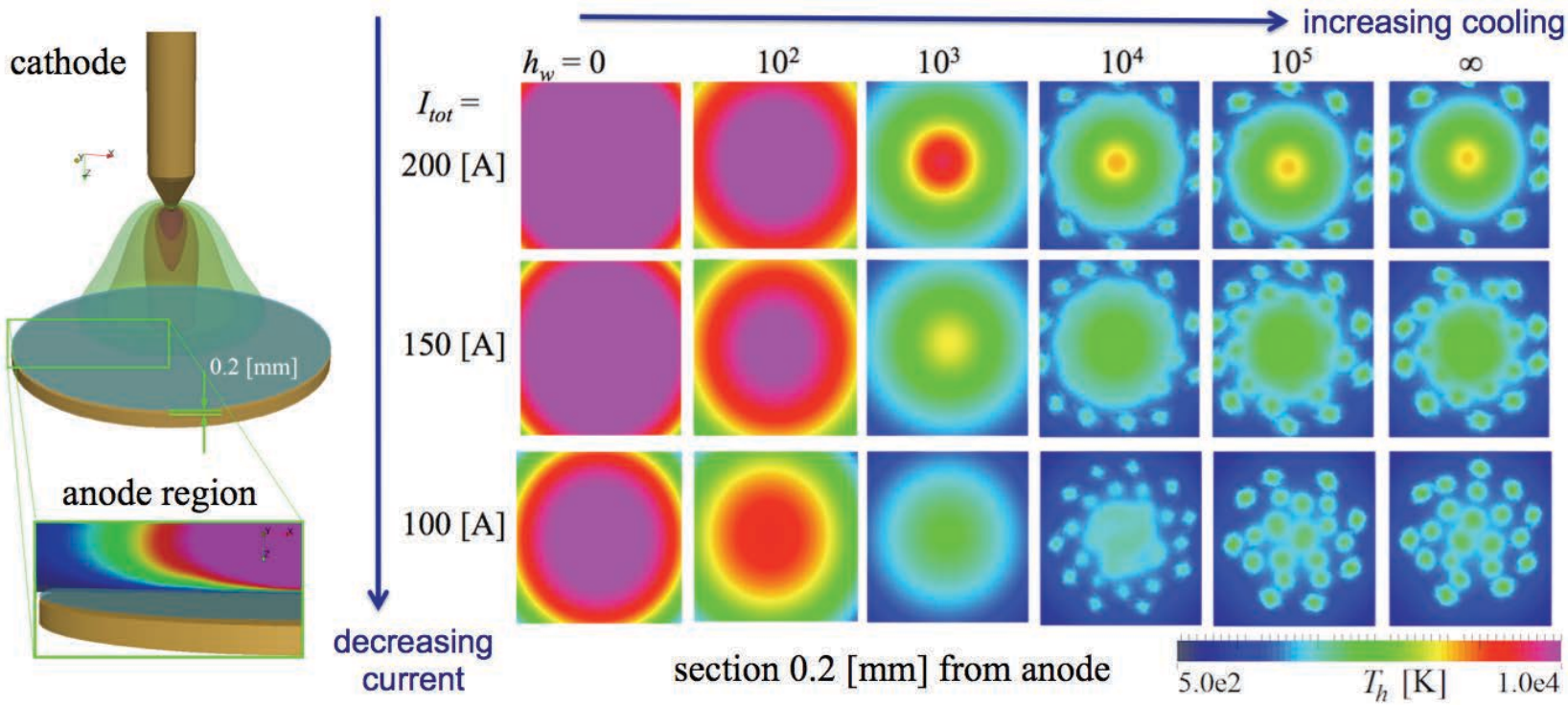


➢ Anode patterns?

[1] Hsu K C and Pfender E 1983 *J Appl Phys* 54 8 4359
[2] Murphy A B 1999 *IEEE Trans Plasma Sci* 27 1 30
[3] Tashiro S, Tanaka M, Ushio M, Murphy A B and Lowke J J 2006 *Vacuum* 80 1190

Plasma Flow Simulation: Pattern Capture

- 3D, time-dependent, non-equilibrium, "industrial-strength" solver [1, 2]
- Spontaneous (no forcing) pattern formation with current & cooling level

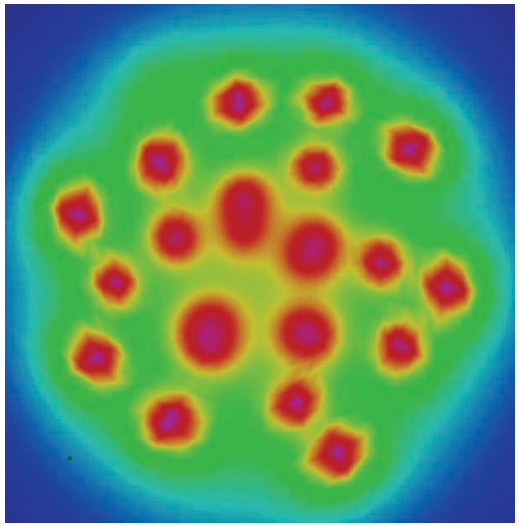


➢ Different solutions → underlying bifurcation phenomena (?)

[1] J. P. Trelles, Plasma Sources Sci. Technol. 22 (2013) 025017
[2] J. P. Trelles, Plasma Sources Sci. Technol. 23 (2014) 054002

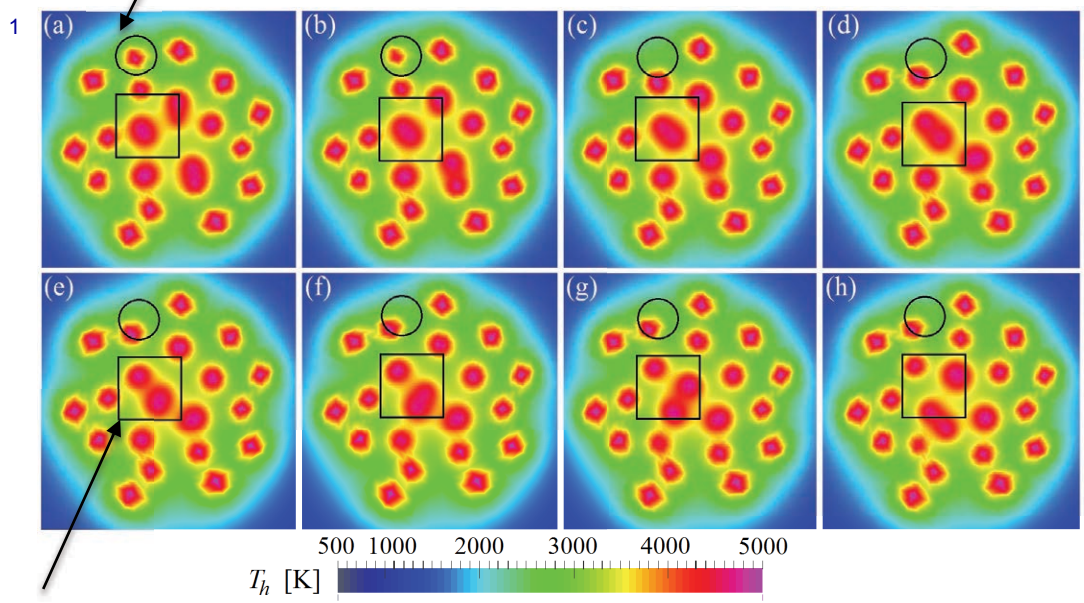
Pattern Dynamics

- Static to dynamic spots transition: large transport / equilibration imbalance



Spot formation, splitting, movement, disappearance

movement towards boundary, disappears



Spot forms in plasma center, splits, moves away

➢ Symmetric behavior ~ expected
→ Higher accuracy needed (?)

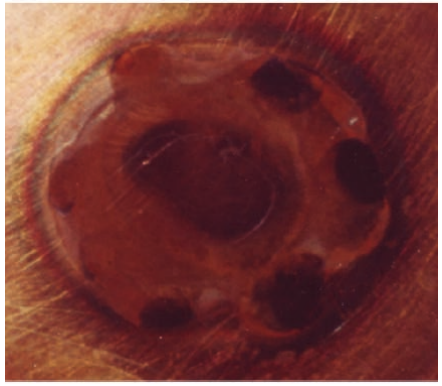
[1] J. P. Trelles, Plasma Sources Sci. Technol. 23 (2014) 054002

Experimental Validation

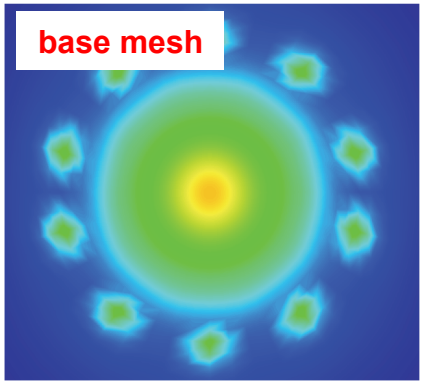
Experimental:
Erosion pattern

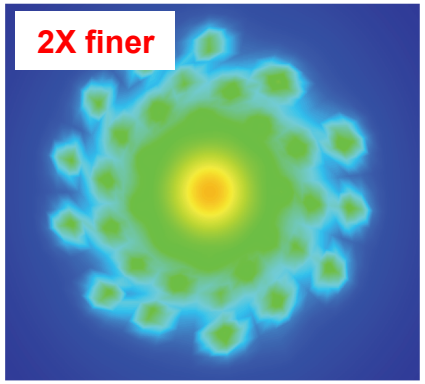
Computational:
Temperature dist.

[1]



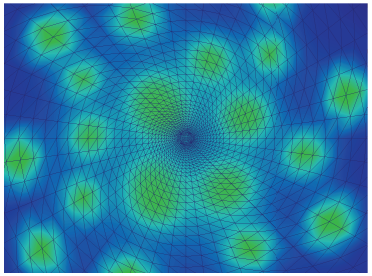
[2]





Major center spot, satellite minor spots ✓

Different pattern for finer mesh ✗

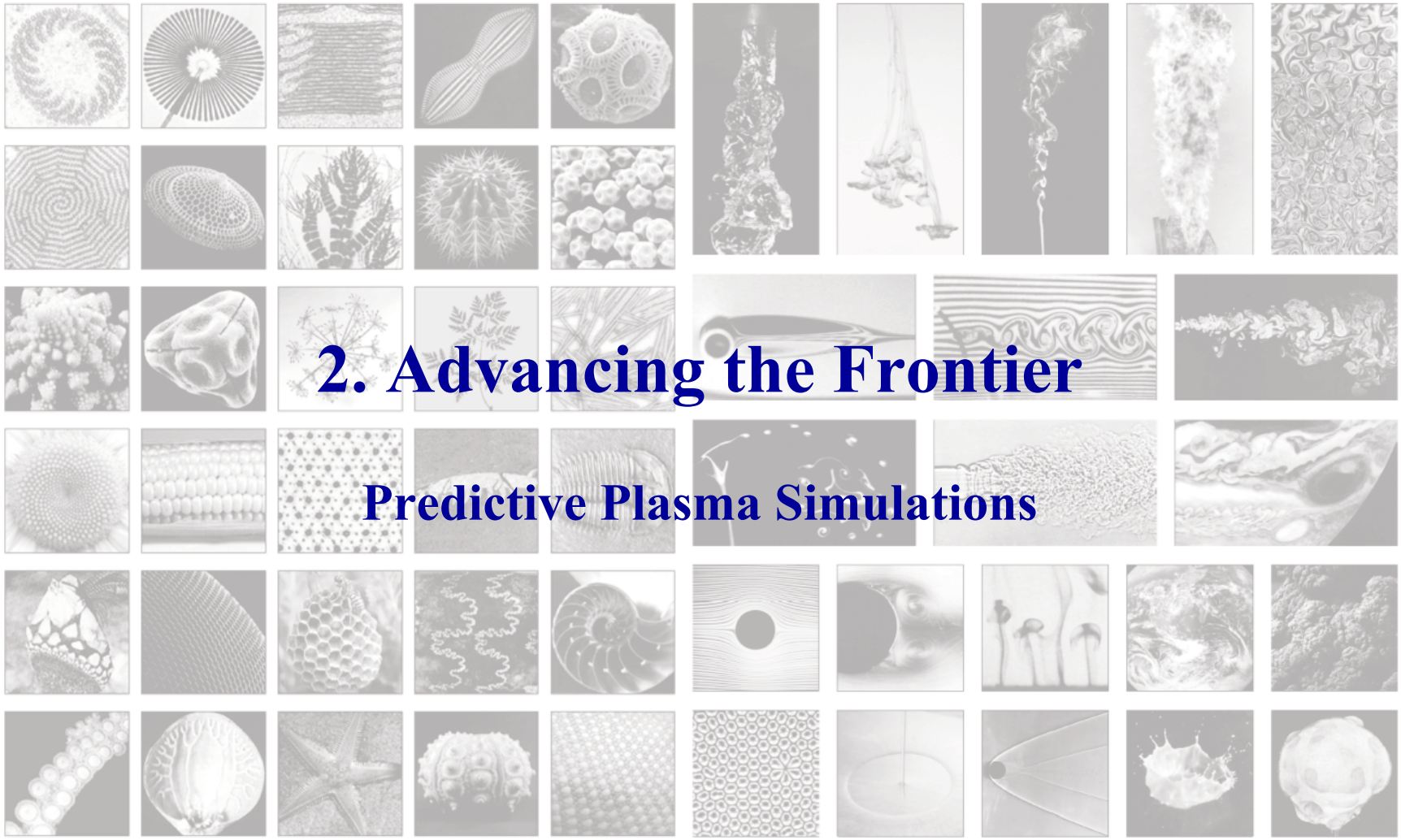


- Solution is discretization dependent!
  (despite spots encompass several nodes)

[1] Yang and Heberlein, Plasma Sources Sci. Technol. 16 (2007) 765
[2] J. P. Trelles, Plasma Sources Sci. Technol. 22 (2013) 025017

2. Advancing the Frontier

Predictive Plasma Simulations



S. Wolfram, A New Kind of Science (2002)

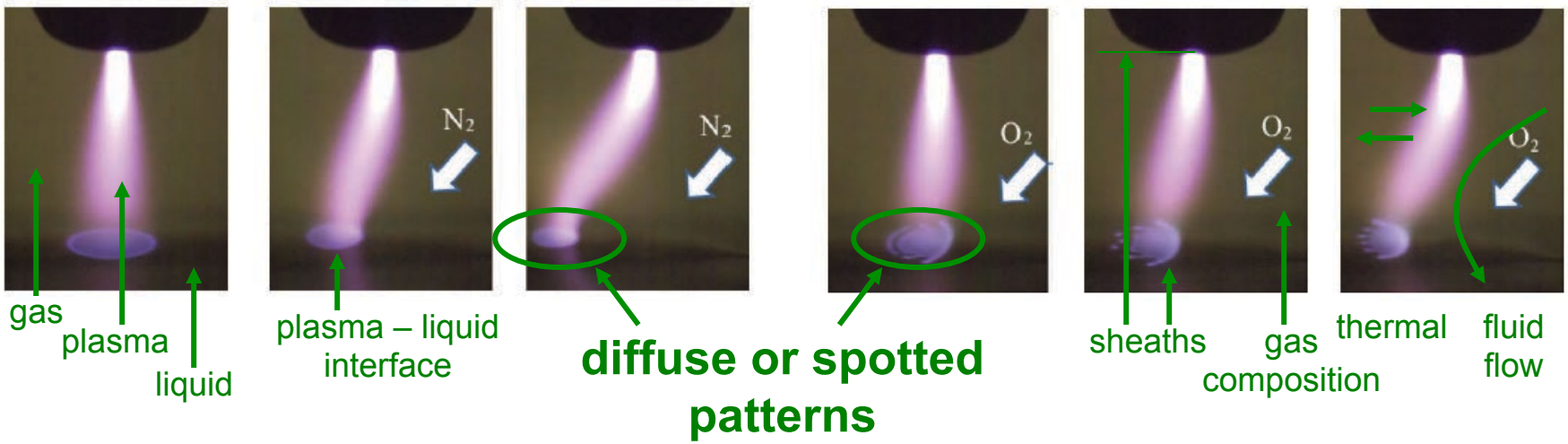
Beyond The Frontier (Where We Need To Go)

- **Example:** Glow discharge on liquid interface interacting with a gas stream

N_2: Smooth deflection, no patterns

O_2: Plasma-liquid interface pattern

[1]



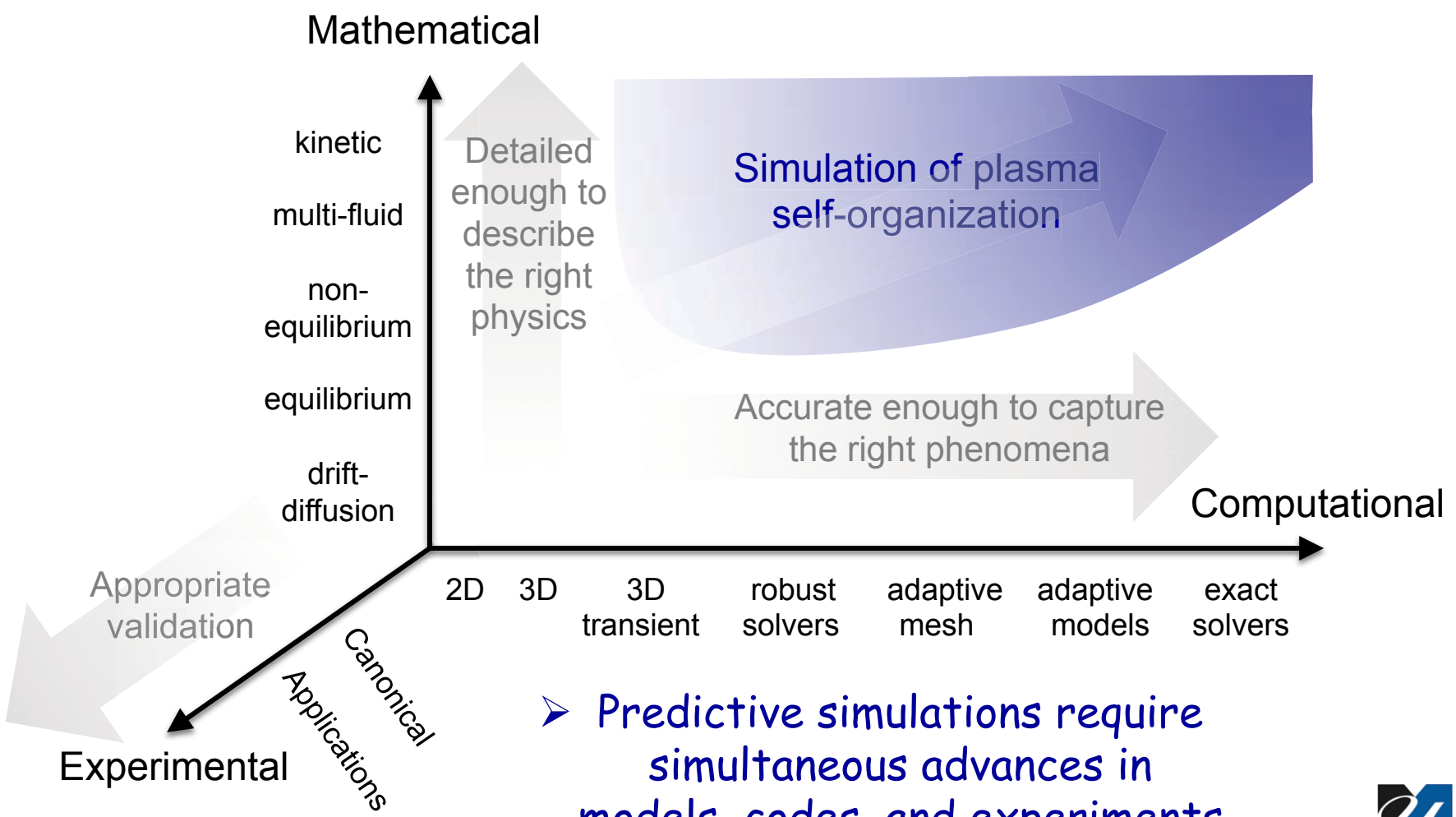
- **Patterns at plasma-liquid interface:** Fine balance between dissipation and forcing (fluid flow, chemistry, thermal, electromagnetic, multi-phase, …)

➢ Whole set of simulation capabilities needed to simulate this system is not yet available (as a single unit)

[1] Shirai, Uchida and Tochikubo, Plasma Sources Sci. Technol. 23 (2014) 054010

Advancing Towards Predictive Simulations

- **Plasma modeling & simulation panorama:**



➢ Predictive simulations require simultaneous advances in models, codes, and experiments

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Approach to Advancing the Frontier (1/3)

- **Integration of hierarchy of mathematical models**
  - A-priori or automatic model selection to provide adequate description of underlying physics in each part of the domain
  - E.g. from detailed kinetic model at a plasma interface to fluid flow in bulk
  - See V. Kolobov's talk on adaptive kinetic-fluid models

- **Comprehensive numerical methods**
  - Comprehensive: Consistent (satisfy original PDEs, kinetic model) & Complete (no tuning parameters)
  - Capable of handling complex geometries, large gradients, stiffness with minimal/selective "numerical stabilization" (slope limiters, upwinding)
  - Suitable for describing instability formation & growth (even turbulence)

- **Tools for studying bifurcation phenomena**
  - Continuation methods to track solutions while using adequate mathematical models, numerical approaches, and simulation accuracy

Approach to Advancing the Frontier (2/3)

- **Controllable, high-order accurate solutions**
  - Need high-order discretization and solution methods (e.g. spectral basis, NURBS), potentially locally (time & space) adaptive, non-conforming
  - E.g. NIMROD code for toroidal plasmas

- **Robust computational solvers**
  - Inexact (iterative) solvers (e.g. Newton-Krylov, Jacobian-free) may lead to artificial forcing for the formation of patterns
  - Challenge for parallel large-scale & scalable solvers
  - Need "exact" or "adaptively-accurate" solvers (e.g. direct linear solvers) adequately characterized and validated for plasma simulation

- **Discretization-independent simulations**
  - 3D & time-dependent simulations are "almost" mandatory to avoid limiting number of solutions – specially challenging for applications
  - Need spatial & temporal mesh refinement – sequential or locally adaptive, potentially using local error estimators

Approach to Advancing the Frontier (3/3)

- **Canonical experimental tests**
  - Need to identify and define experimental configurations with high controllability and relevance to fundamental studies and applications
  - Suitable for validation of computational models

- **Multi-resolution concurrent diagnostics**
  - High temporal and spatial resolution required to capture onset of instabilities and the dynamics of self-organization and patterns
  - Concurrent probing: optical (emission, spectroscopy), electrical (current, voltage), thermal (electron and gas temperature), fluid-dynamic (pressure and density) characteristics
  - Challenge for non-equilibrium, atmospheric-pressure, and multi-phase (e.g. plasmas on liquids) plasmas

3. Impact

Greater Understanding & Use of Nature and Plasmas

S. Wolfram, A New Kind of Science (2002)

Scientific & Societal Benefits

- **Fundamental understanding of pattern formation and self-organization**
  - Test and/or reveal universal underlying physics connecting plasmas to other fields (biology, fluid instabilities, flame development, phase-change, …)

- **Enable computational experiments**
  - Enhanced exploration that may lead to new plasma discoveries (e.g. unobserved patterns, new mechanisms) potentially prior to experimental tests

- **Process optimization and control**
  - Simulations can lead to approaches for suppressing or enhancing self-organization towards desired goals (e.g. uniformity of surface treatments, discrete surface functionalization)

- **Novel processes and applications**
  - Plasma medicine, materials synthesis, surface modification, etc. that may exploit the occurrence or suppression of patterns (e.g. signal transfer by transporting plasma "spots")

Thank You!