Two-dimensional materials, Metamaterials & Machine Learning

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Rensselaer Polytechnic Institute
Colloquium, November 2019

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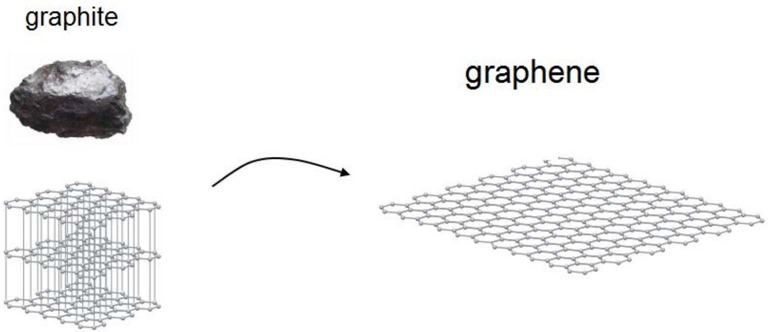
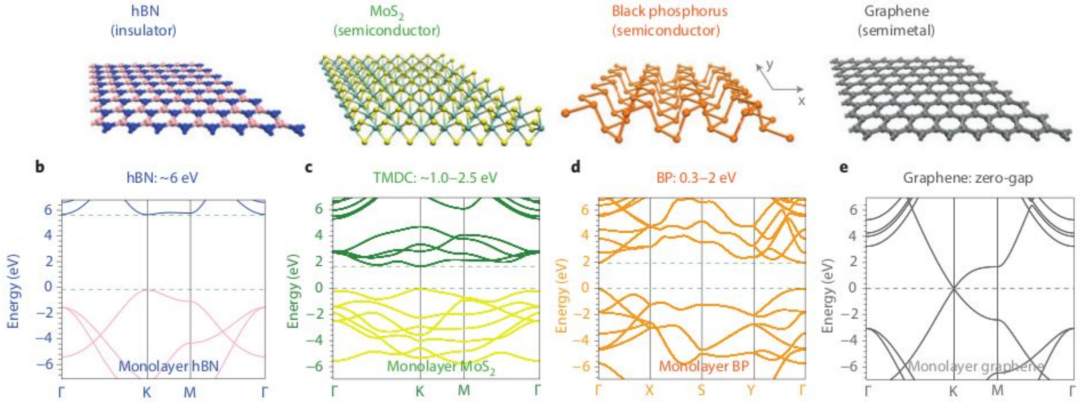
Two-dimensional materials

2D materials are crystals consisting of a single layer of atoms (typical thickness few nanometers)

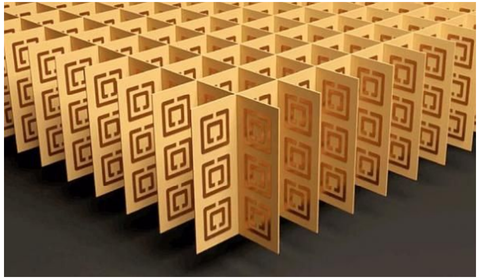
Properties change as move from 3 to 2 dimensions

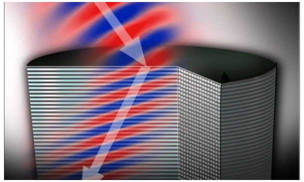


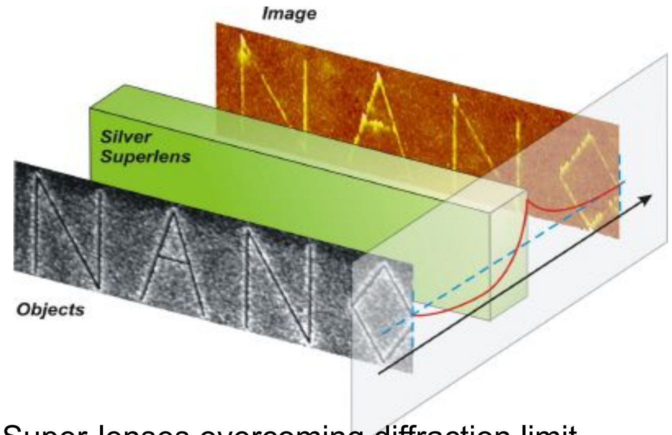


F. Xia et al., Nat. Phot. **8** 2014

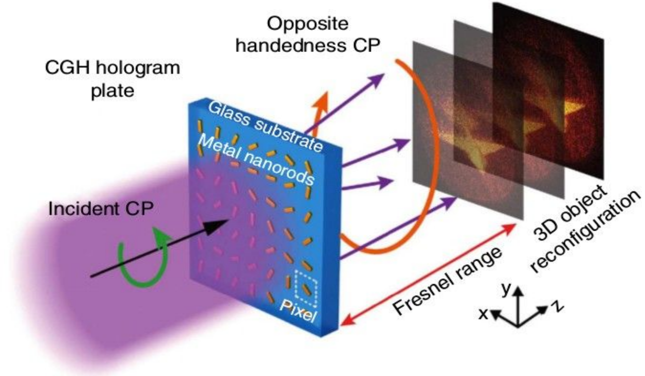
Metamaterials



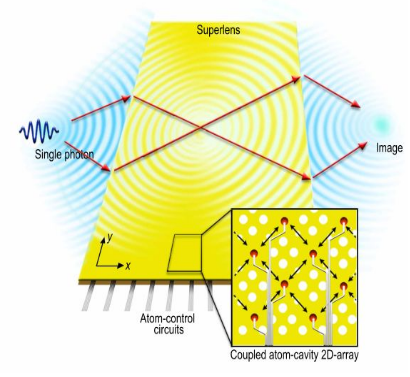




Super-lenses overcoming diffraction limit.
Nat. Mat. **7,** 2008

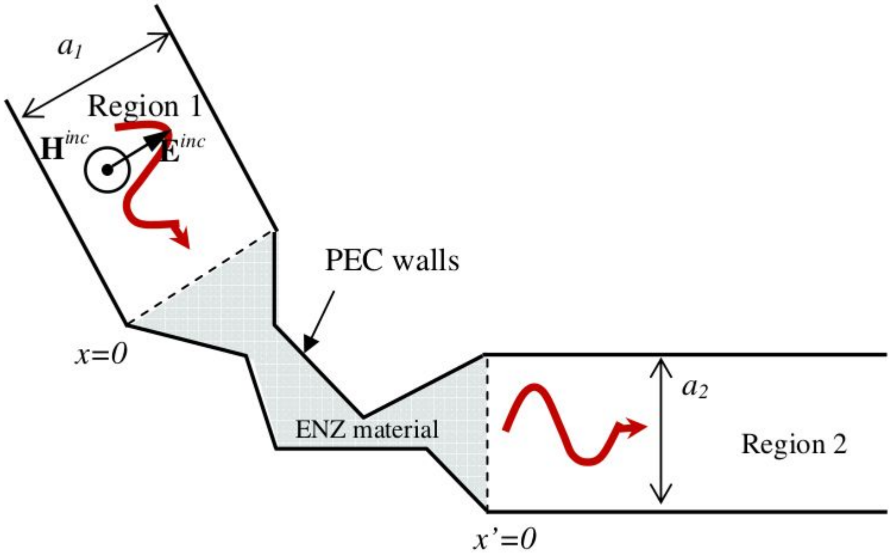


3D optical holography. Nat. Comm. **4,** 2013

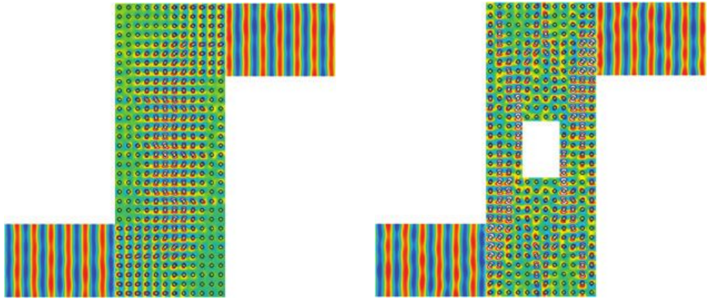


Quantum super-lens
Opt. Expr. **19,** 2012

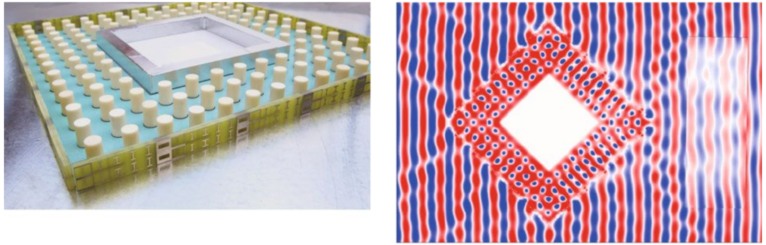
Epsilon-Near-Zero (ENZ)



Tunneling through narrow channels. PRL **97** 2006



Bending and Cloaking. Nat. Mat. **10** 2011



On-chip zero-index cloaking device.
Nat. Phot. **9** 2015; Nat. Light: Sc. & appl. **7**, 2018

Machine Learning

Handle big data

Regression/Classification

Dimensionality reduction

Optimization tasks

Predict new materials

Classify materials

Discover underlying laws

Forecast dynamics

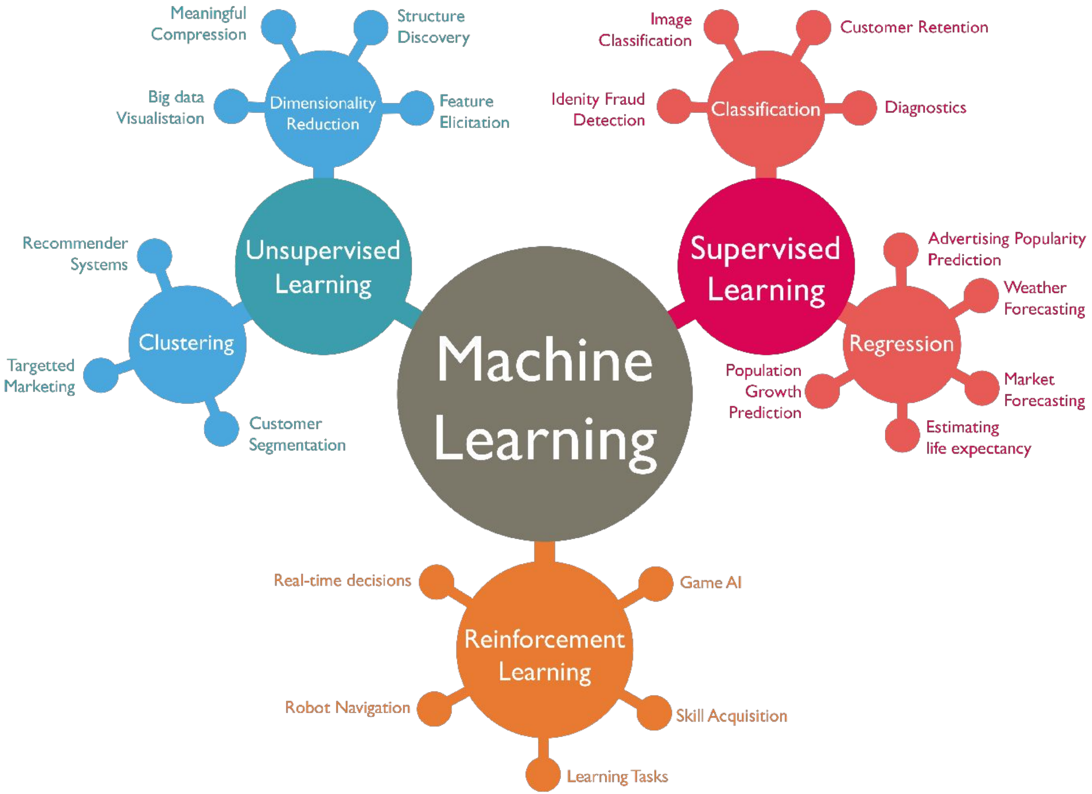
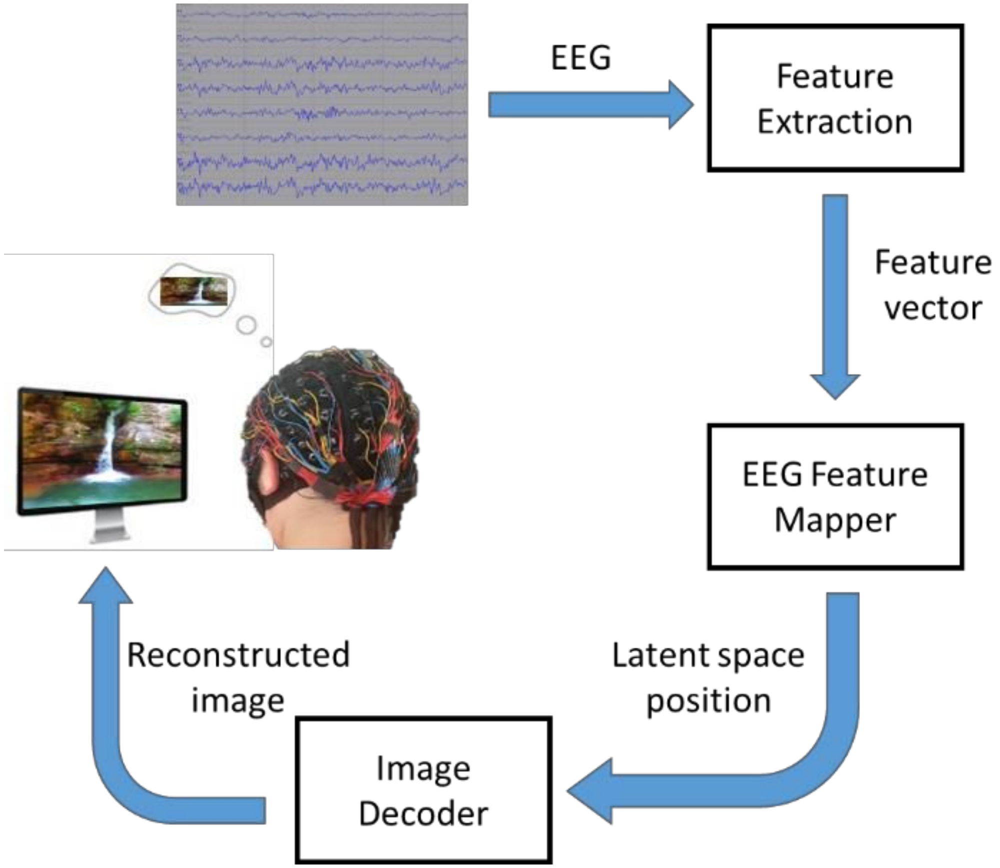


Image reconstruction from brain waves



bioArxiv 2019, 10.1101/787101
Posted Oct. 25, 2019

Outline

- Metamaterials based on graphene:
  - Epsilon-Near-Zero plasmonic nanocrystals
- Branched flow in random environments:
  - Electronic flow in graphene
- Machine Learning:
  - Forecast the electronic branching
  - Solve differential equations with Neural Networks

Graphene, the first semimetal

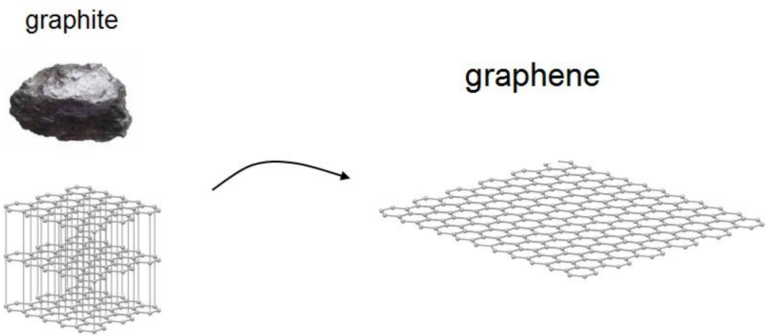
Hexagonal lattice of carbon atoms
(atomically thick material d = 0.32 nm)

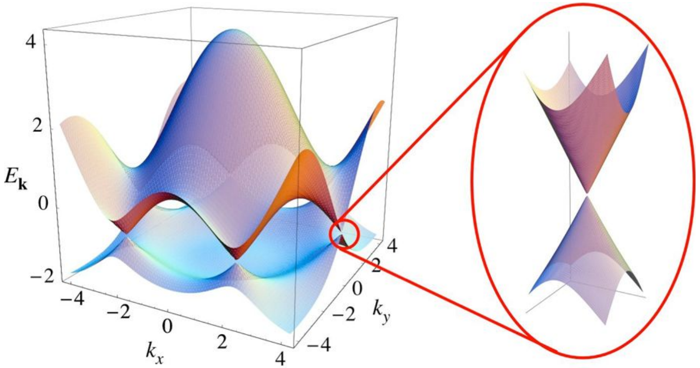
World’s highest electrical and thermal conductivity

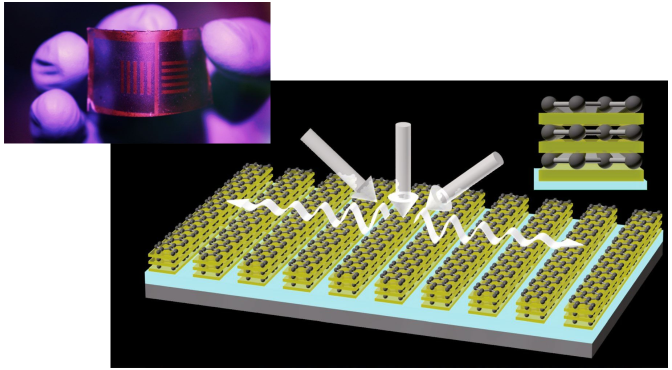
Much stronger than steel (huge in plane elastic constants)

Semimetal with tunable electronic and optical properties

Linear band structure yields ultra-relativistic physics

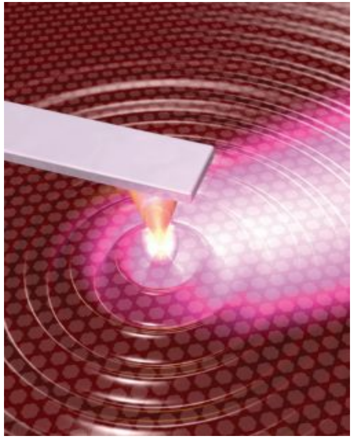




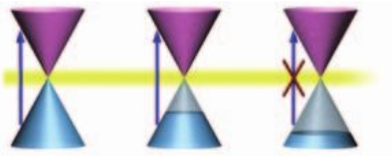


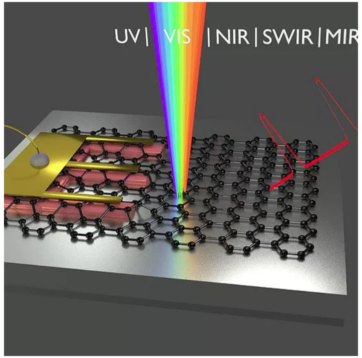
Graphene-based metamaterial broadband absorber
Nature Photonics **13,** 2019

Plasmons



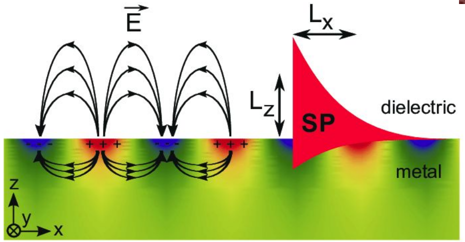
Gate field, chemical deposition



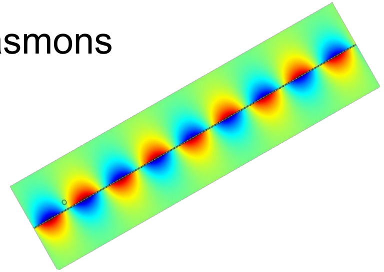


A. N. Grigorenko et al., Nat. Phot., **6** 2012

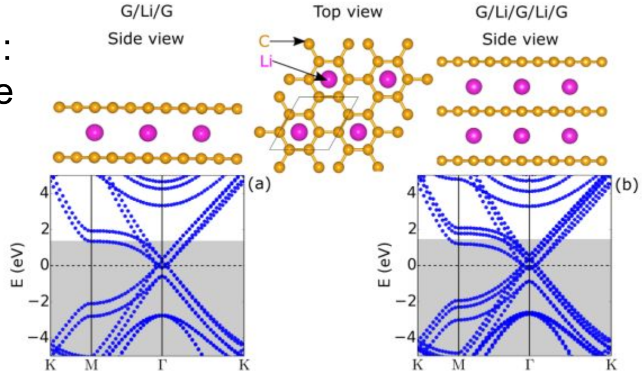
3D plasmons



2D plasmons

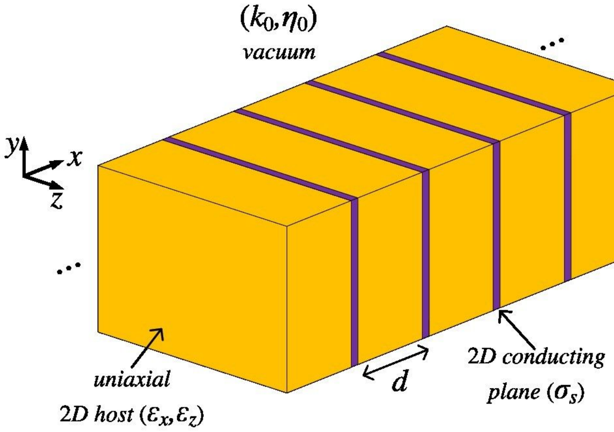


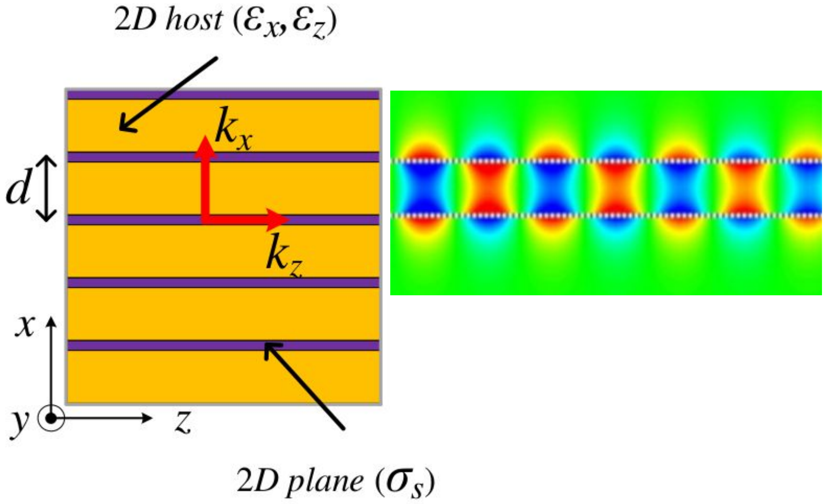
Li - Intercalation:
Visible graphene
2D plasmons



S. Shirodkar, MM et al., PRB **97**, 2018

Plasmonic nanocrystal





The 2D metals carry surface current

$$J = \sigma E_z$$

Maxwell Equations

Transversal Field

$$-\mathrm{i}\frac{\partial}{\partial z}\boldsymbol{\Psi} = \mathcal{M}\cdot\boldsymbol{\Psi} \Leftrightarrow$$

$$-\mathrm{i}\frac{\partial}{\partial z}\begin{pmatrix} E_x \\ H_y \end{pmatrix} = k_0\eta_0 \begin{pmatrix} 0 & 1+\frac{1}{k_0^2}\frac{\partial}{\partial_x}\frac{1}{\varepsilon_z}\frac{\partial}{\partial_x} \\ \frac{\varepsilon_x}{\eta_0^2} & 0 \end{pmatrix}\begin{pmatrix} E_x \\ H_y \end{pmatrix}$$

Longitudinal Field

$$E_z = \frac{\mathrm{i}\eta_0}{k_0\varepsilon_z}\frac{\partial H_y}{\partial x}$$

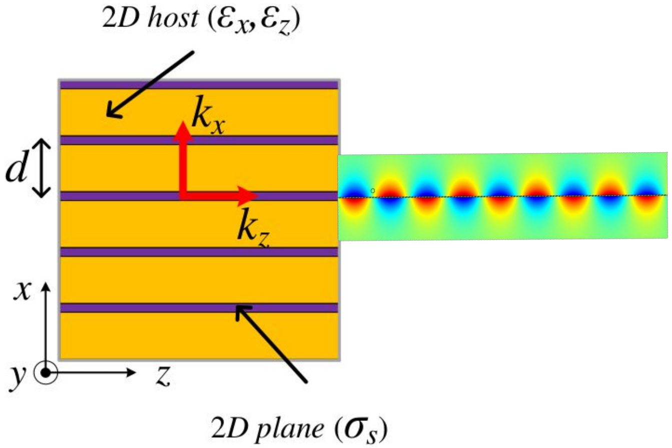
$$k_0 = \omega / c$$

$$\eta_0 = \sqrt{\mu_0/\varepsilon_0}$$

Plasmon and Bloch waves along z and x directions

$$\boldsymbol{\Psi}(x,z) = \boldsymbol{\Psi}(x)e^{\mathrm{i}k_z z},$$

$$k_z\boldsymbol{\Psi} = \mathcal{M}\boldsymbol{\Psi}$$



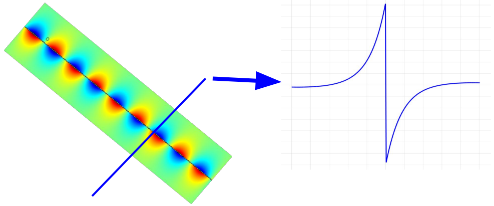
Metamaterial dispersion and band-structure

$$D\left(k_x, k_z\right) = \cos\left(k_x d\right) - \left[\cosh\left(\kappa d\right) - \frac{\xi\kappa}{2}\sinh\left(\kappa d\right)\right] = 0$$

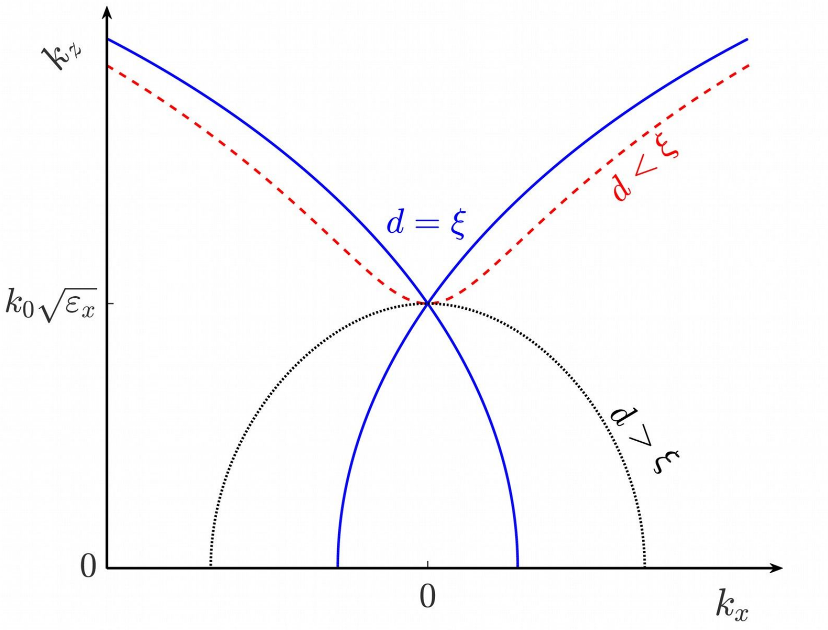
$$\kappa^2 = \frac{\varepsilon_z}{\varepsilon_x}\left(k_z^2 - k_0^2\varepsilon_x\right)$$

Plasmonic Thickness
(twice the decay length)

$$\xi = -\frac{i\sigma}{\omega\varepsilon_z}$$



Wang *et. al.* PRL **112** 2012



MM *et. al.* PRB **94**, 2016

Anisotropic ENZ effective medium

dense grid: $d \ll \lambda$

$$\frac{k_z^2}{\varepsilon_x} + \frac{d}{(d-\xi)\varepsilon_z} k_x^2 = k_0^2$$

effective medium

$$\frac{k_z^2}{\varepsilon_x^{\mathrm{eff}}} + \frac{k_x^2}{\varepsilon_z^{\mathrm{eff}}} = k_0^2$$

$\Rightarrow$

$$\varepsilon_x^{\mathrm{eff}} = \varepsilon_x$$

$$\varepsilon_z^{\mathrm{eff}} = \frac{d-\xi}{d}\varepsilon_z$$

ENZ condition in one direction

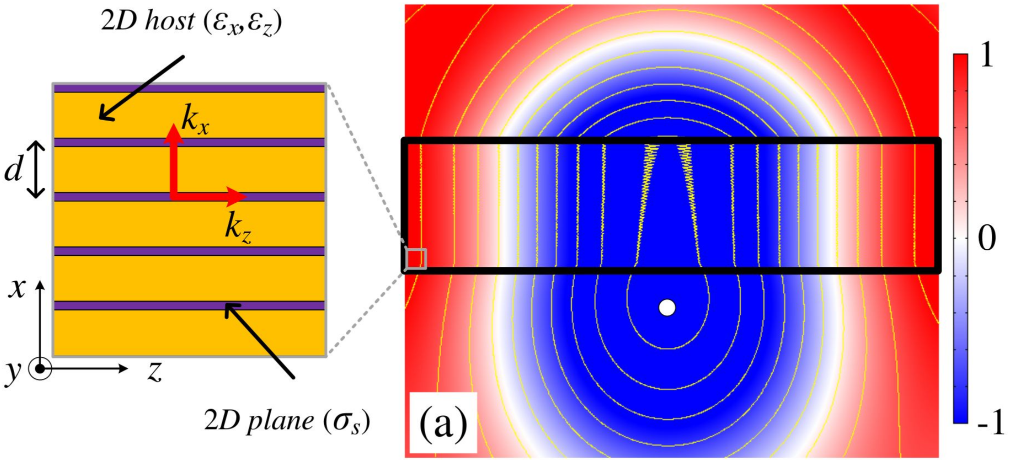
$$d = \xi \Rightarrow \varepsilon_z^{\mathrm{eff}} = 0$$

MM *et. al.* PRB **94**, 2016

ENZ behavior (simulation)

- 40 doped graphene layers in MoS_2 host (ε_x=3.5, ε_z=13, d=20.8 nm).
- Drude model for graphene conductivity.
- λ_0=12 μm (THz regime).
- 2D magnetic dipole source.

$$\sigma(\omega) = \frac{ie^2\mu_c}{\pi\hbar^2(\omega + i/\tau)}$$



Ultra fast phase transition

No dispersion

No phase delay

MM *et. al.* PRB **94**, 2016

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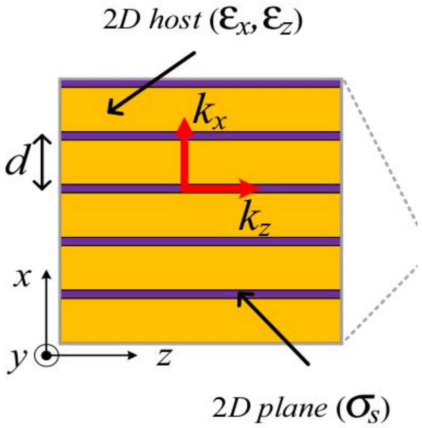
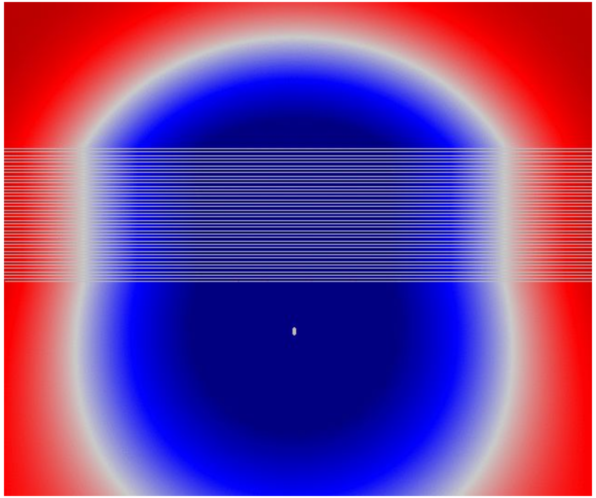




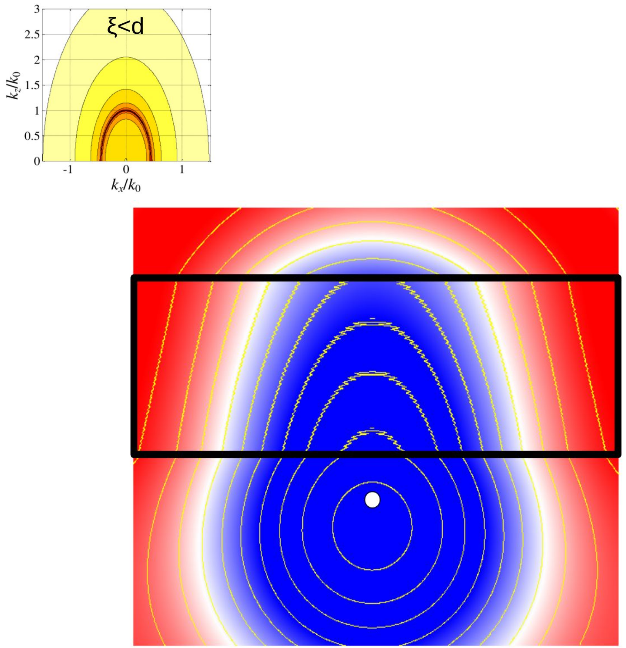
Ultra fast phase transition

No dispersion

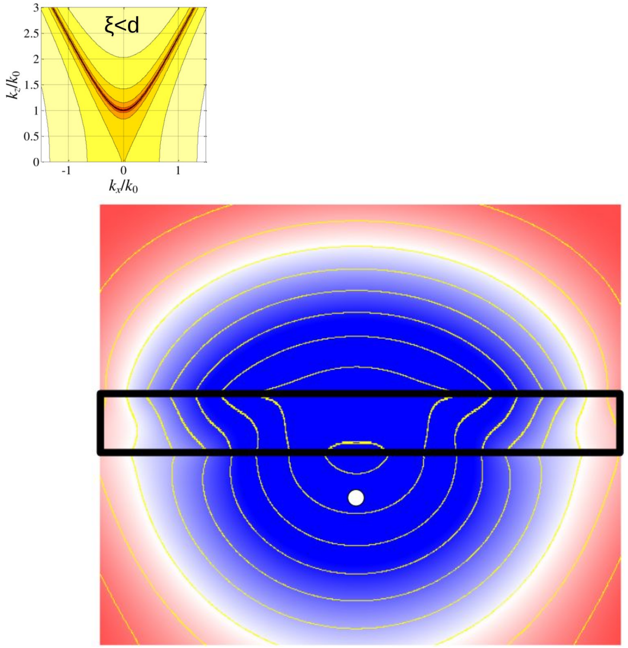
No phase delay

MM *et. al.* PRB **94**, 2016

Tunable optical properties



Weak plasmon coupling



Strong plasmon coupling

MM *et. al.* PRB **94**, 2016

General formulation for 2D plasmonic nanocrystals

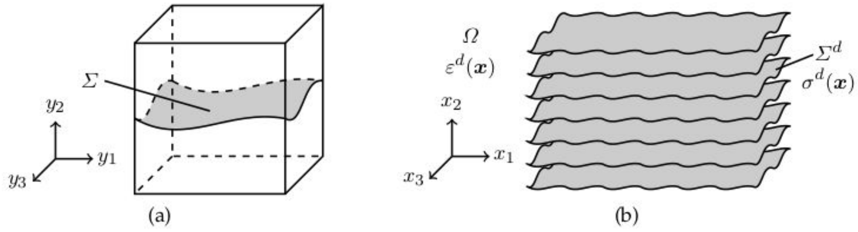
Arbitrary shape of a 2D material

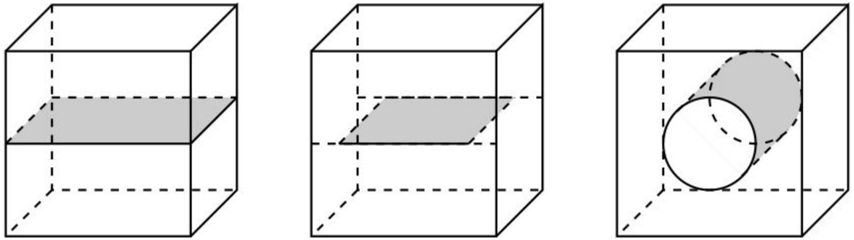
Spatial & frequency-dependent host permittivity

Periodicity along any direction

Finite number of structural periods

Finite and edge effects





Maier, MM, *et al*. RSPA 2019

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Branched Flow

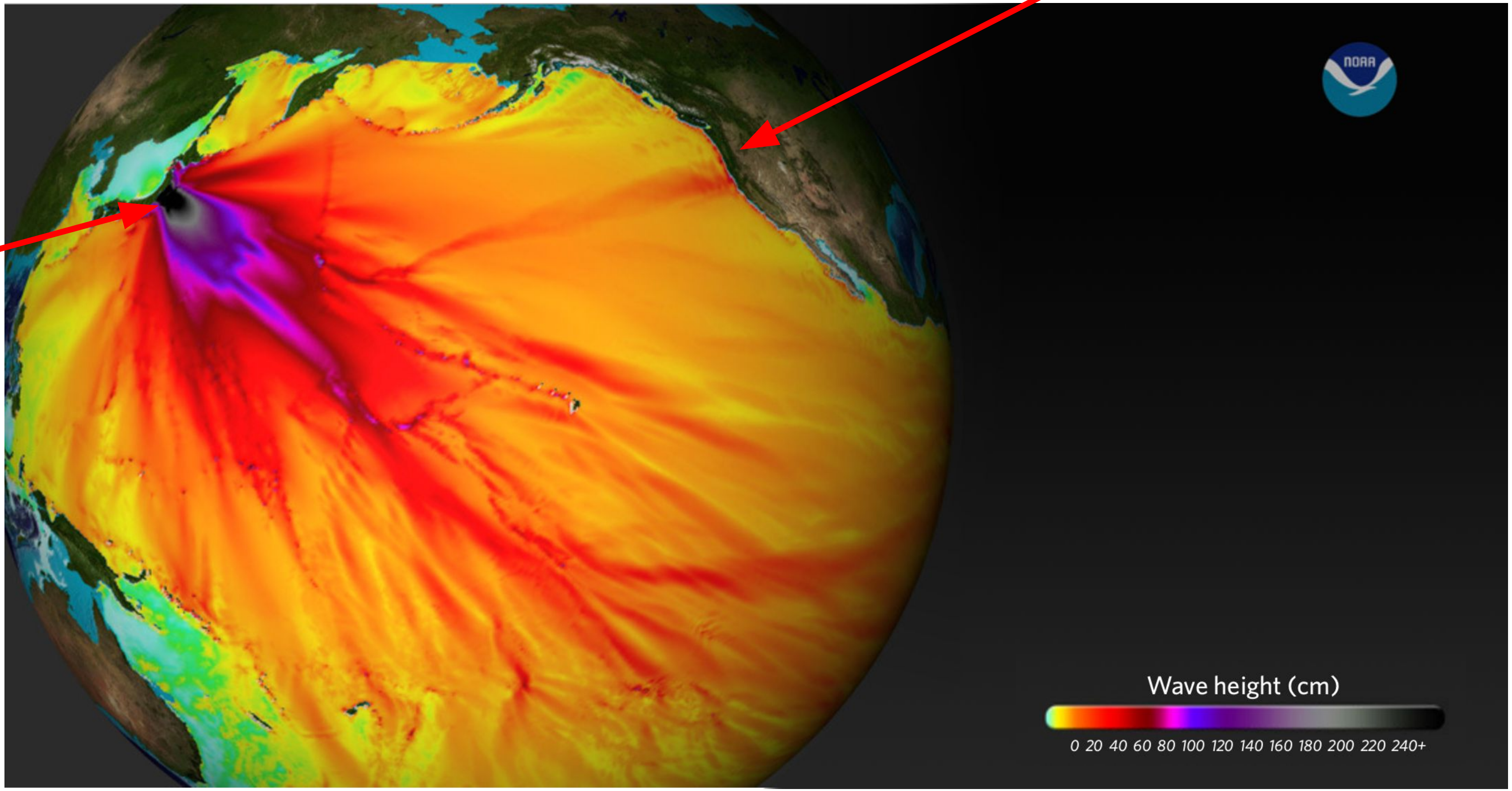
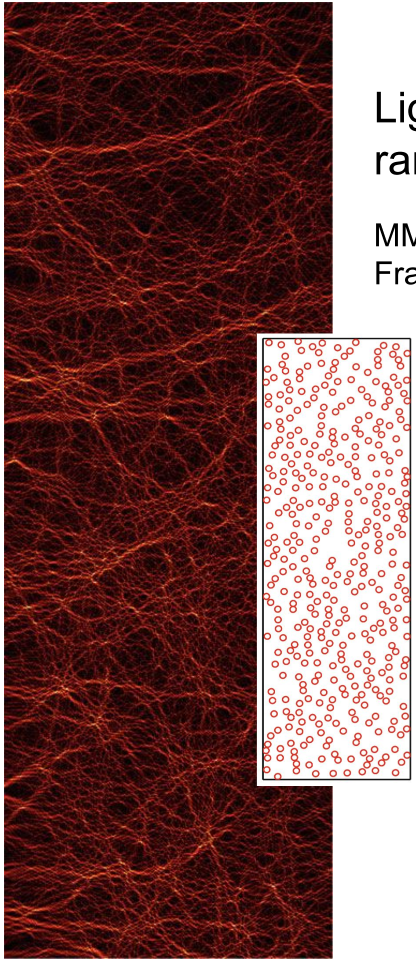


Figure 1 | Branched flow seen in a National Oceanic and Atmospheric Administration wave energy map produced after the 2011 Sendai earthquake in Japan. Note the strong branch heading for Crescent City in northern California.

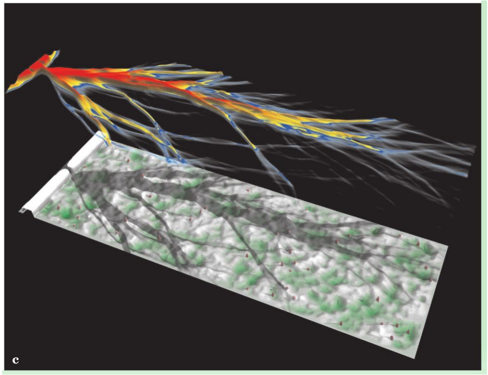
Heller, Nat. Phy. **12**, 2016



Light propagation in random refr. medium

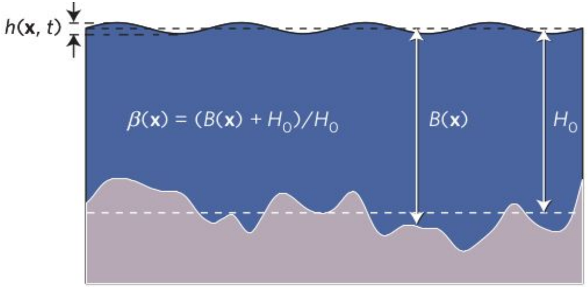
MM *et al.,* Chaos, Solitons & Fractals, **84**, 2016

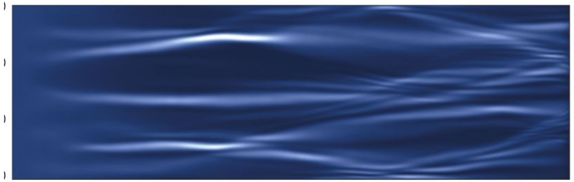
Electronic flow in 2DEG



Topinka *et al.,* Phys. Today **12**, 2003

Tsunami waves



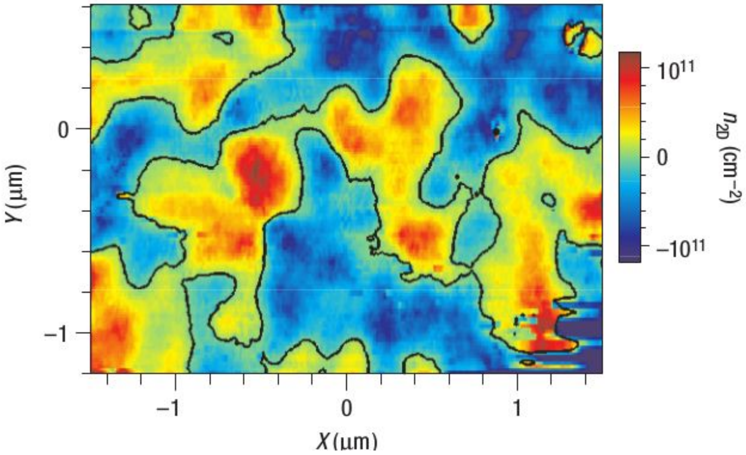


Degueldre, Nat. Phys. **12**, 2016

Substrates for graphene (experiments)

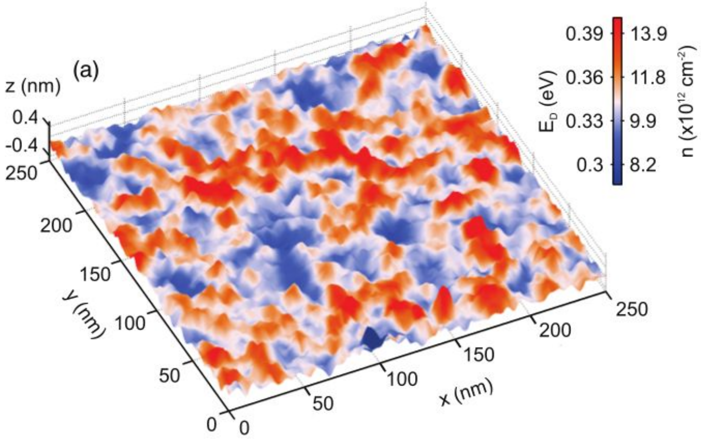
Charged impurities create disordered potential. Charge Puddles

graphene on hBN



Martin *et al.*, Nat. Phys. **4**, 2008

graphene on Ir(111)

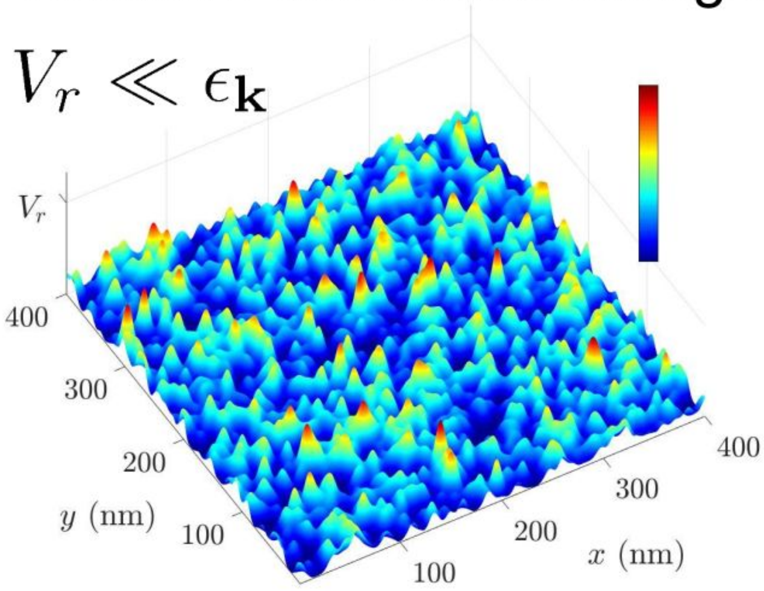


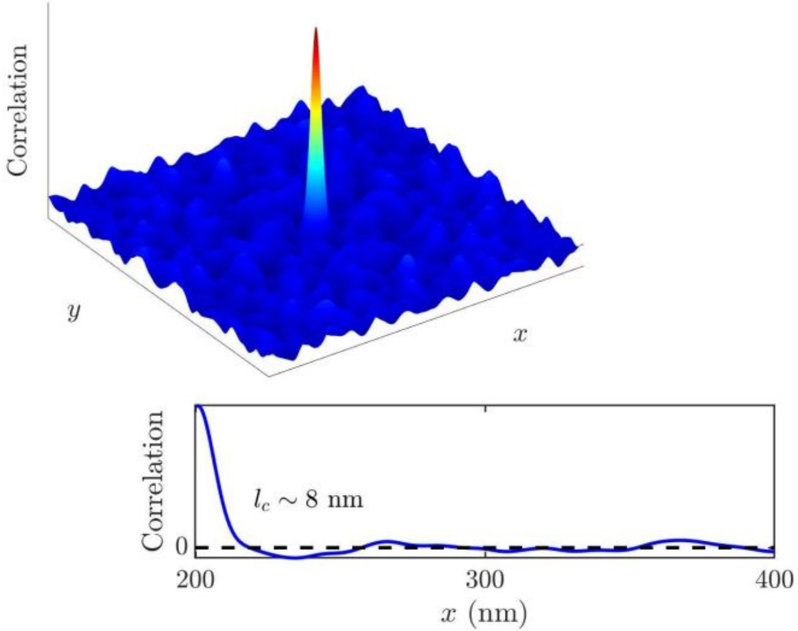
Samaddar *et al.*, PRL. **116**, 2016
Martin *et al.*, PRB. **91**, 2015

Disordered Potential (simulations)

Random distributed charge puddles of radius $\mathrm{R} = 4$ nm.

$V_r \ll \epsilon_{\mathbf{k}}$





MM *et al.,* EPL **122**, 2018

Relativistic electronic branching in graphene

Ultra-Relativistic Hamiltonian

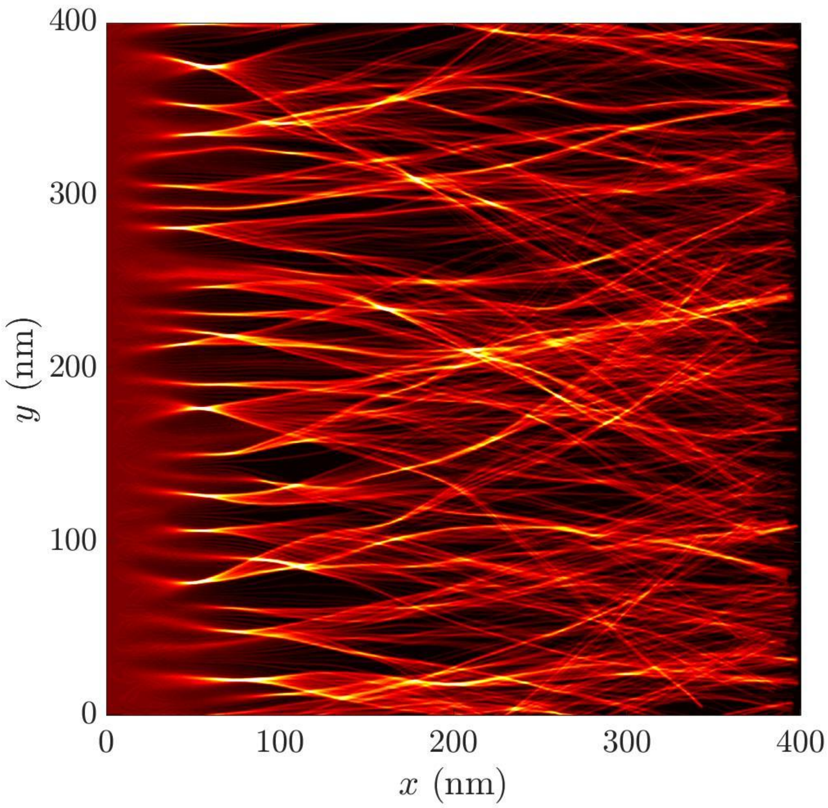
$$\mathcal{H} = v_F \sqrt{p_x^2 + p_y^2} - \alpha x + V_r(x, y)$$

$$p_x(0) = 1$$

$$p_y(0) = 0$$

Caustic is a singularity in the density of a classical electronic flow

MM *et al.*, EPL **122**, 2018



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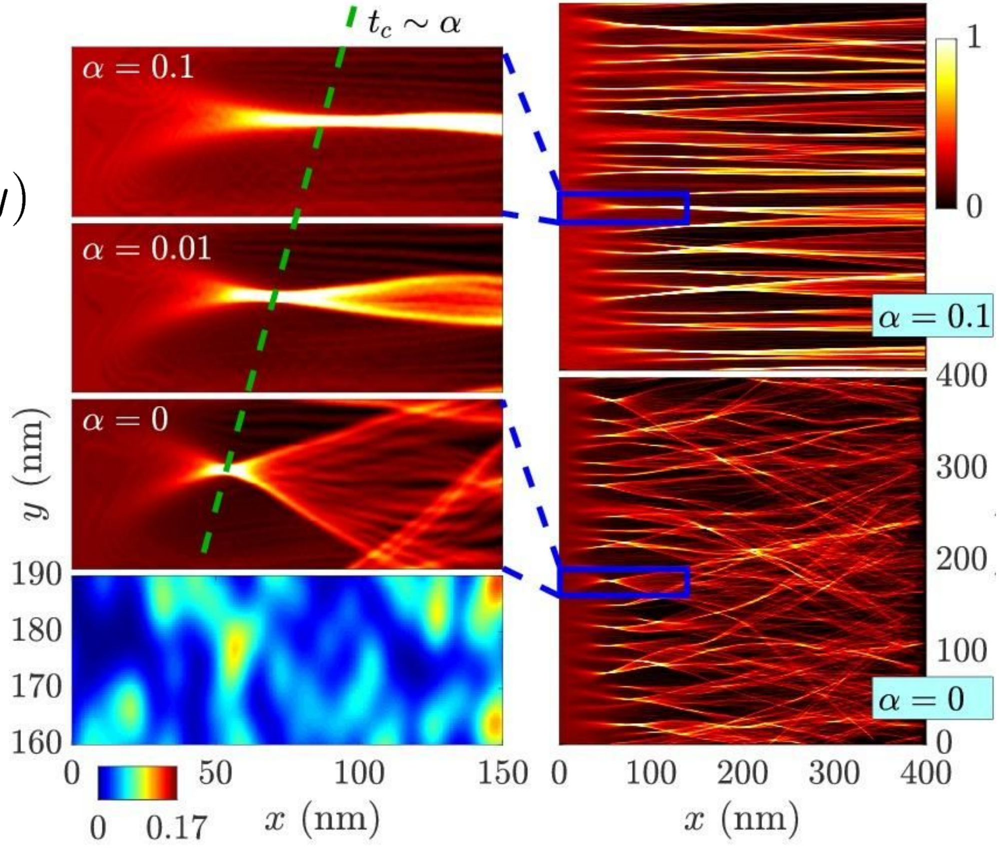


Caustic is a singularity in the density of a classical electronic flow

MM *et al.*, EPL **122**, 2018

Theoretical Model

Approximate Hamiltonian for $p_x \gg p_y$

$$\mathcal{H} = p_x + \frac{p_y^2}{2p_x} - \alpha x + V_r(x,y) \qquad (v_F = 1)$$

Local curvature u equation in the quasi-2D approach $(x = t)$

$$\frac{du}{dt} + \frac{u^2}{1+\alpha t} + \frac{\partial^2}{\partial y^2} V_r(t,y) = 0 \qquad \text{where} \qquad u(t,y) = \frac{\partial p_y}{\partial y}$$

Caustics are areas with high intensity

$$|u(t_c)| \to \infty$$

MM *et al.*, EPL **122**, 2018

Scaling of the First Caustic

Random potential as a white noise

$$\frac{\partial^2}{\partial y^2} V_r(t, y) = \sigma^2 \xi(t) \qquad \text{with} \qquad \langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = 2\delta(t - t')$$

Langevin equation for the local curvature

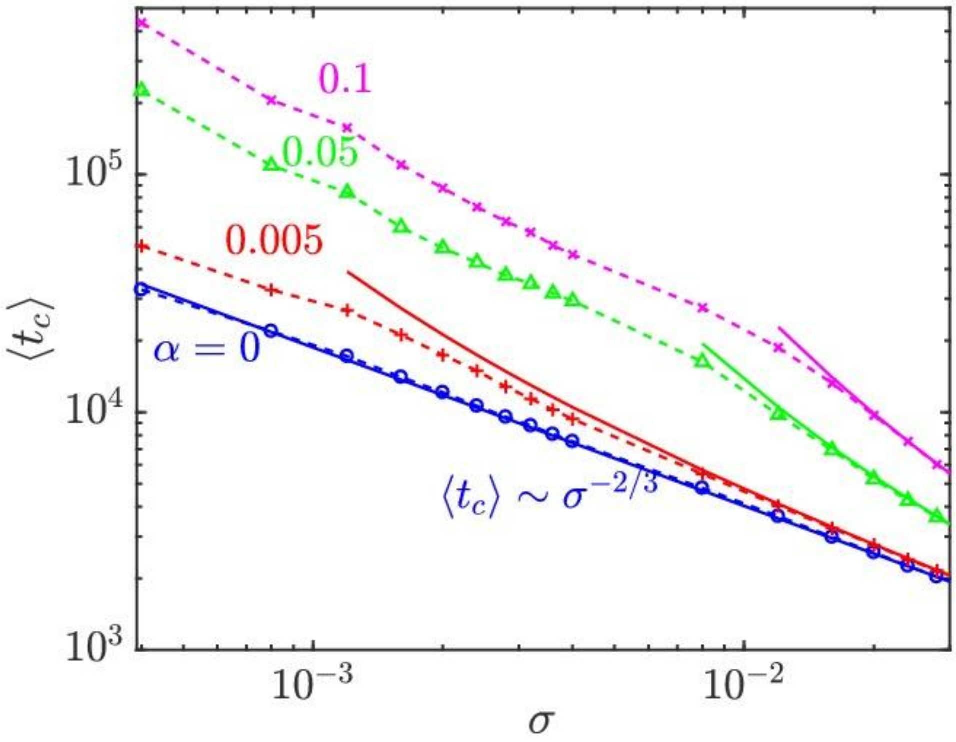
$$\dot{u} = -\frac{u^2}{1 + \alpha t} + \sigma^2 \xi(t)$$

First passage problem for $|u| \to \infty$ $\quad \left(\alpha\sigma^{-2/3} \ll 1\right)$

$$\langle t_c \rangle \sim \sigma^{-2/3}\left(1 + 2\tilde{\alpha} + 3\tilde{\alpha}^2 + \frac{10}{3}\tilde{\alpha}^3\right) \qquad , \qquad \tilde{\alpha} = 1.11\alpha\sigma^{-2/3}$$

MM *et al.*, EPL **122**, 2018

First Caustic Time



Points & Dashed lines:
Simulations

Solid lines:
Theoretical Prediction
up to $\alpha\sigma^{-2/3} < 1$

MM *et al.*, EPL **122**, 2018

Machine Learning

Can Neural Networks predict the onset of branching ?

… or can they predict singularities in dynamical systems ?

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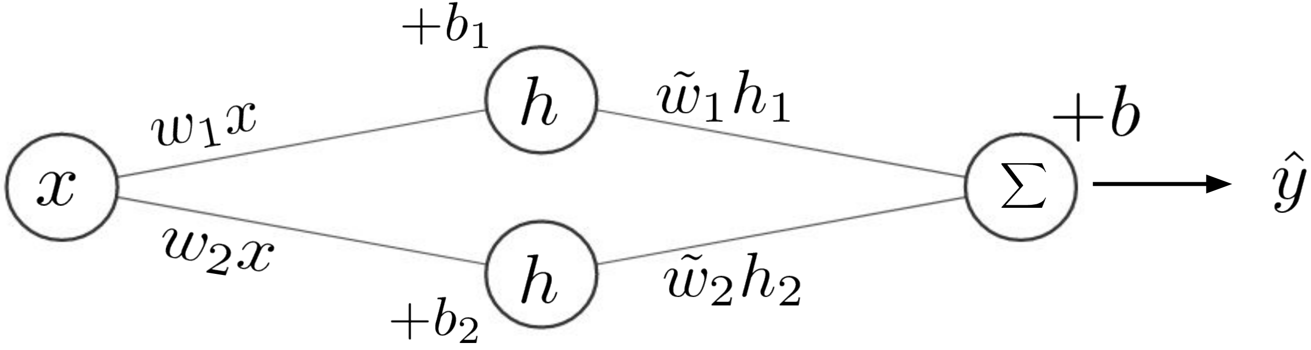
Neural Networks



$$h_i = h(w_i x + b_i)$$

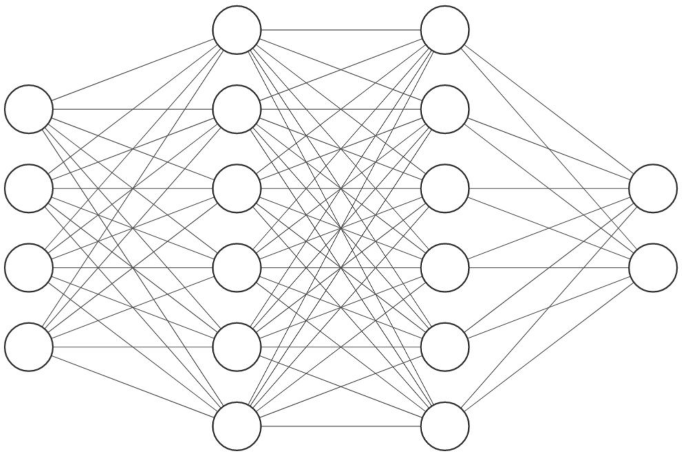
$$\hat{y} = \sum_i \tilde{w}_i h + b_i$$

Loss Function examples:

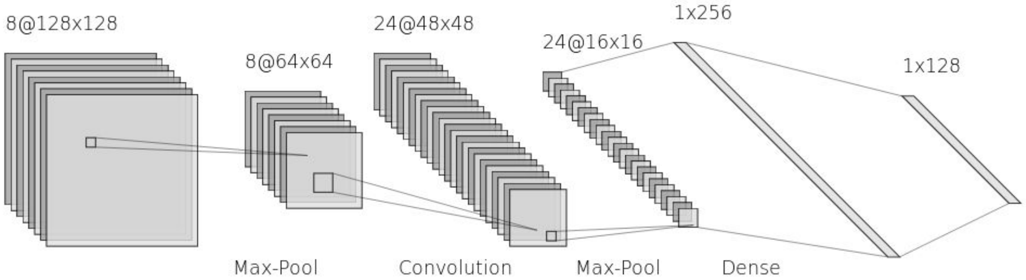
$$L = (\hat{y} - y)^2$$

$$L = \left(\frac{d\hat{y}}{dx} - f(\hat{y}) \right)^2$$

Deep Neural Networks

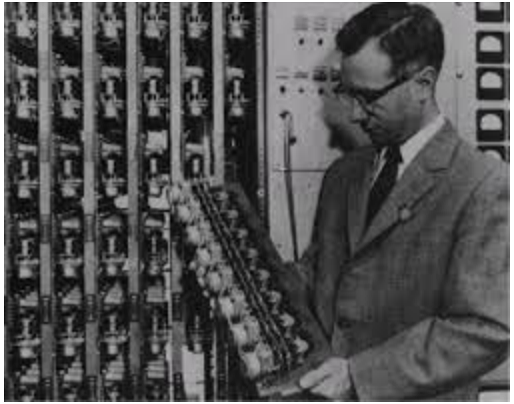


Input Layer ∈ $\mathbb{R}^4$ Hidden Layer ∈ $\mathbb{R}^6$ Hidden Layer ∈ $\mathbb{R}^6$ Output Layer ∈ $\mathbb{R}^2$

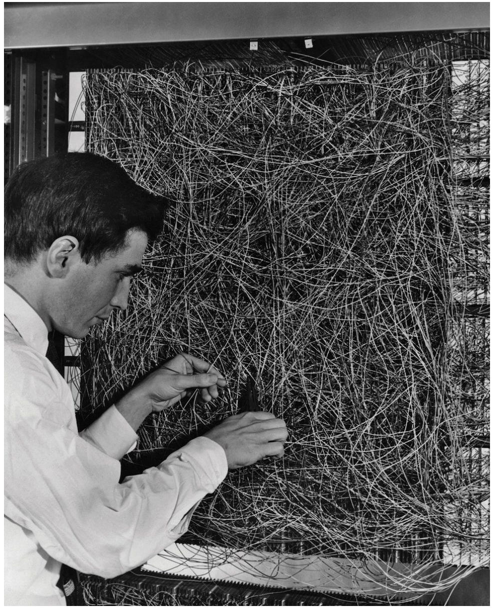


Perceptron: The early days

Training a perceptron



Debugging the network



Rosenblatt, F. (1958). "The Perceptron: A Probabilistic Model For Information Storage And Organization In The Brain". *Psychological Review*. **65** (6): 386–408.

Neural Networks

Can Neural Networks predict the onset of branching ?

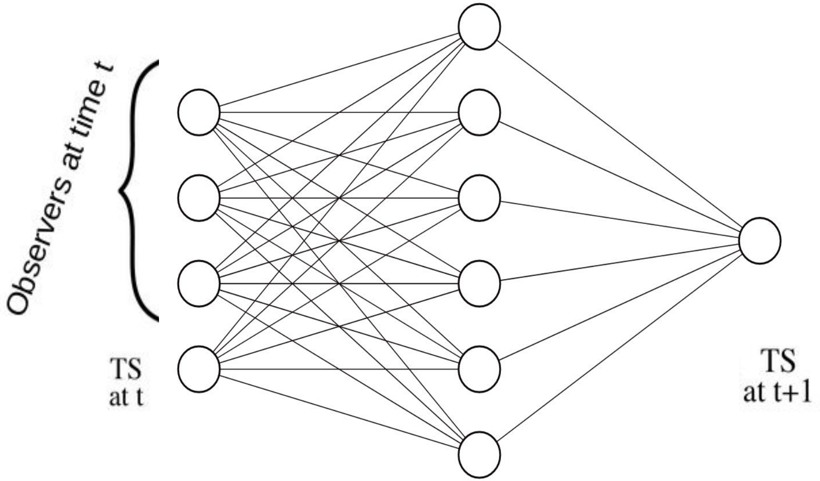
… or can they predict singularities in dynamical systems ?

Neural Networks

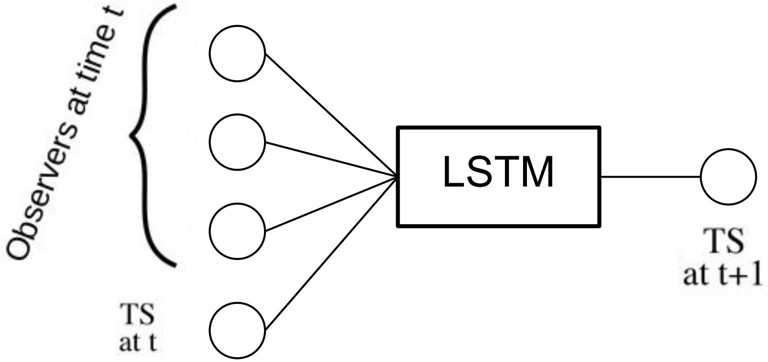
Can Neural Networks predict the onset of branching ?

… or can they predict singularities in dynamical systems ?

Forward Neural Network with Obsr. (OFNN)



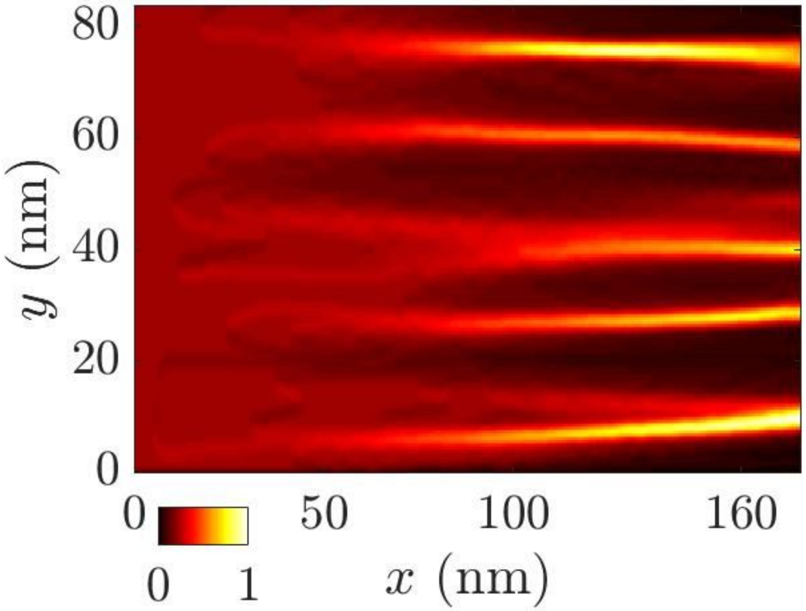
Long Short Term Memory with Obsr. (OLSTM)



Neofotistos *et al.,* Front. In Phys. **7**, 2019

A novel NN method on predicting branching

Predicting Singular events in wave dynamics



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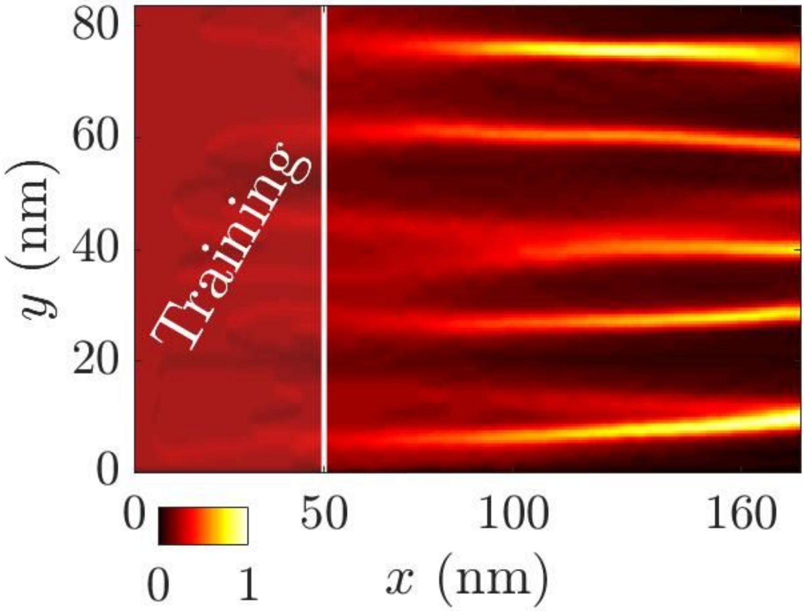

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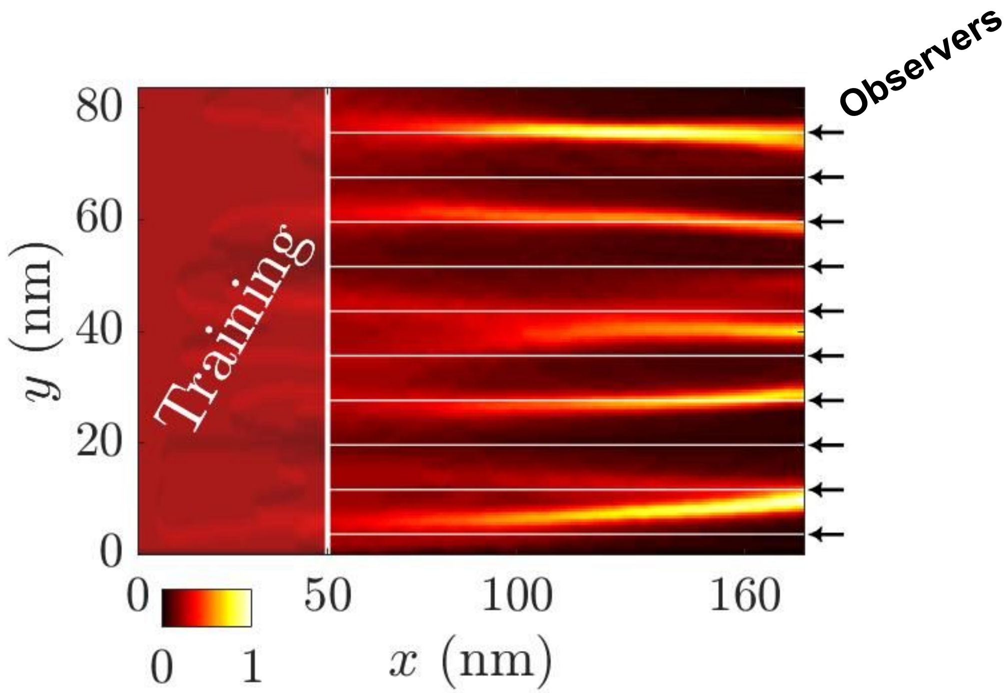
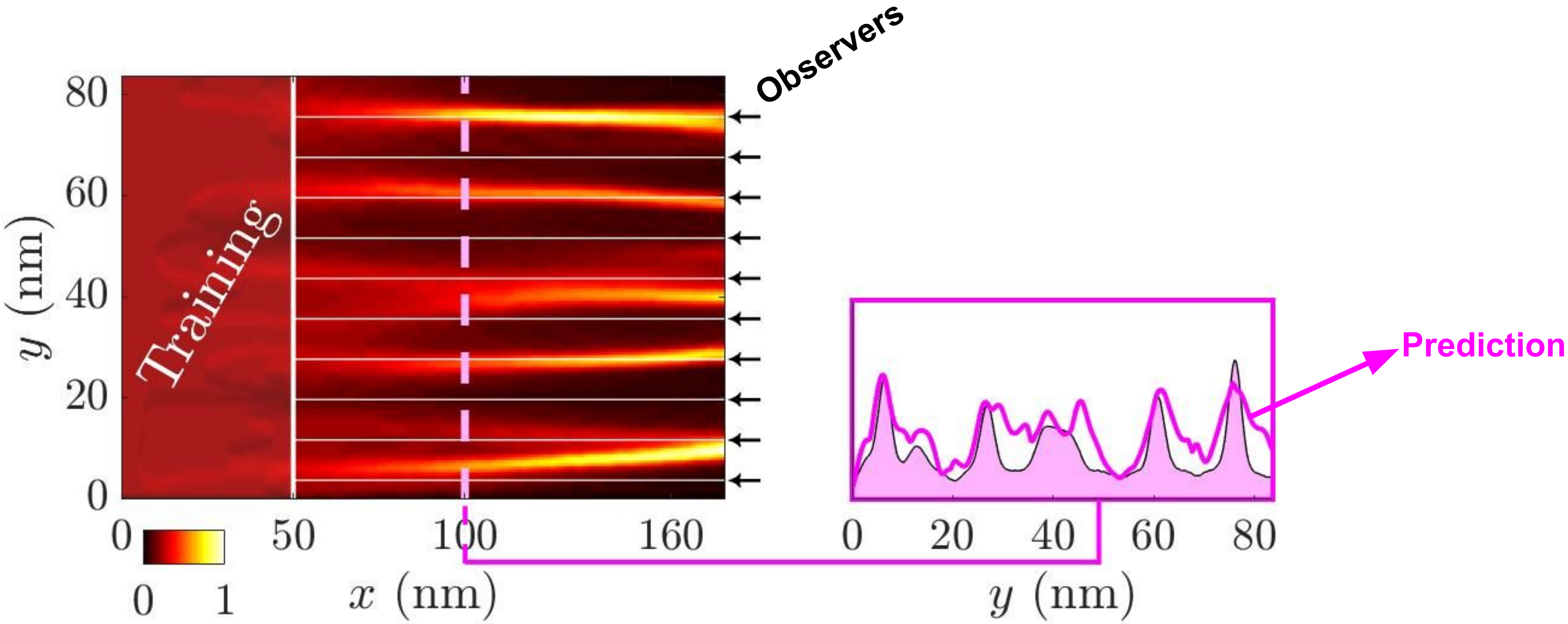
Predicting Singular events in wave dynamics



A novel NN method on predicting branching

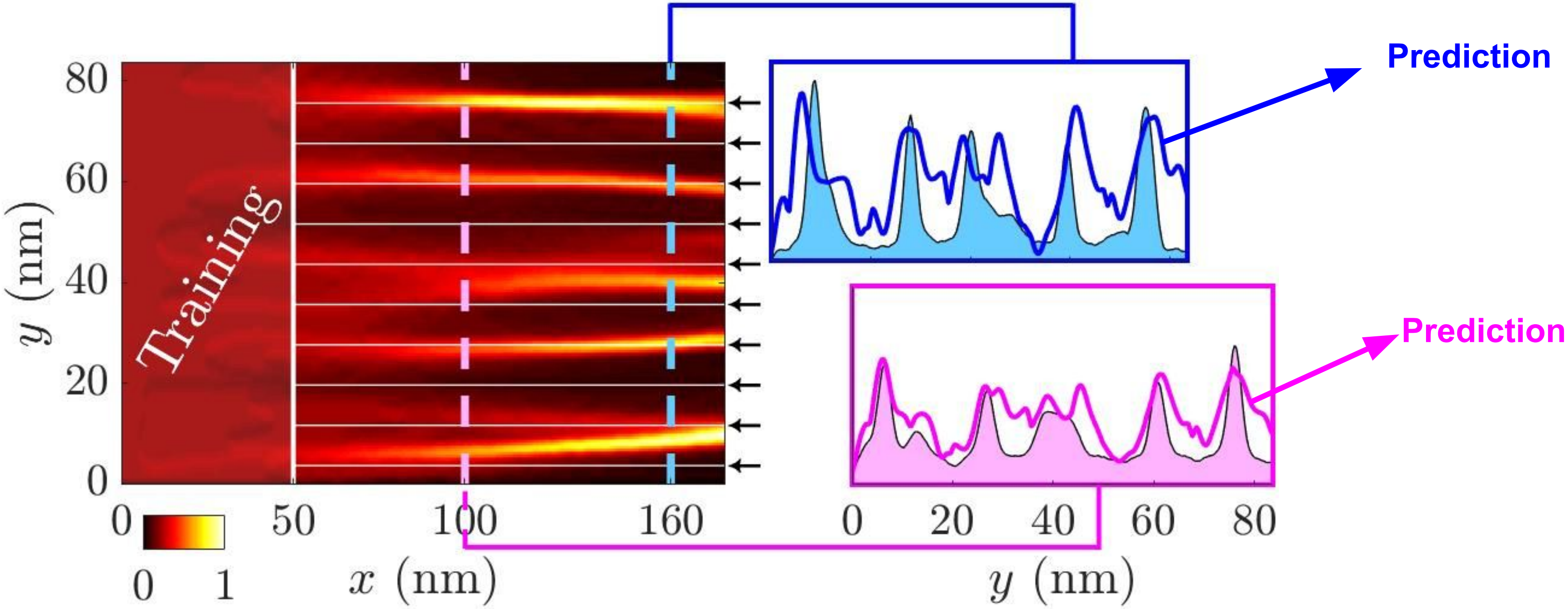
Predicting Singular events in wave dynamics



Neofotistos *et al.*, Front. In Phys. **7**, 2019

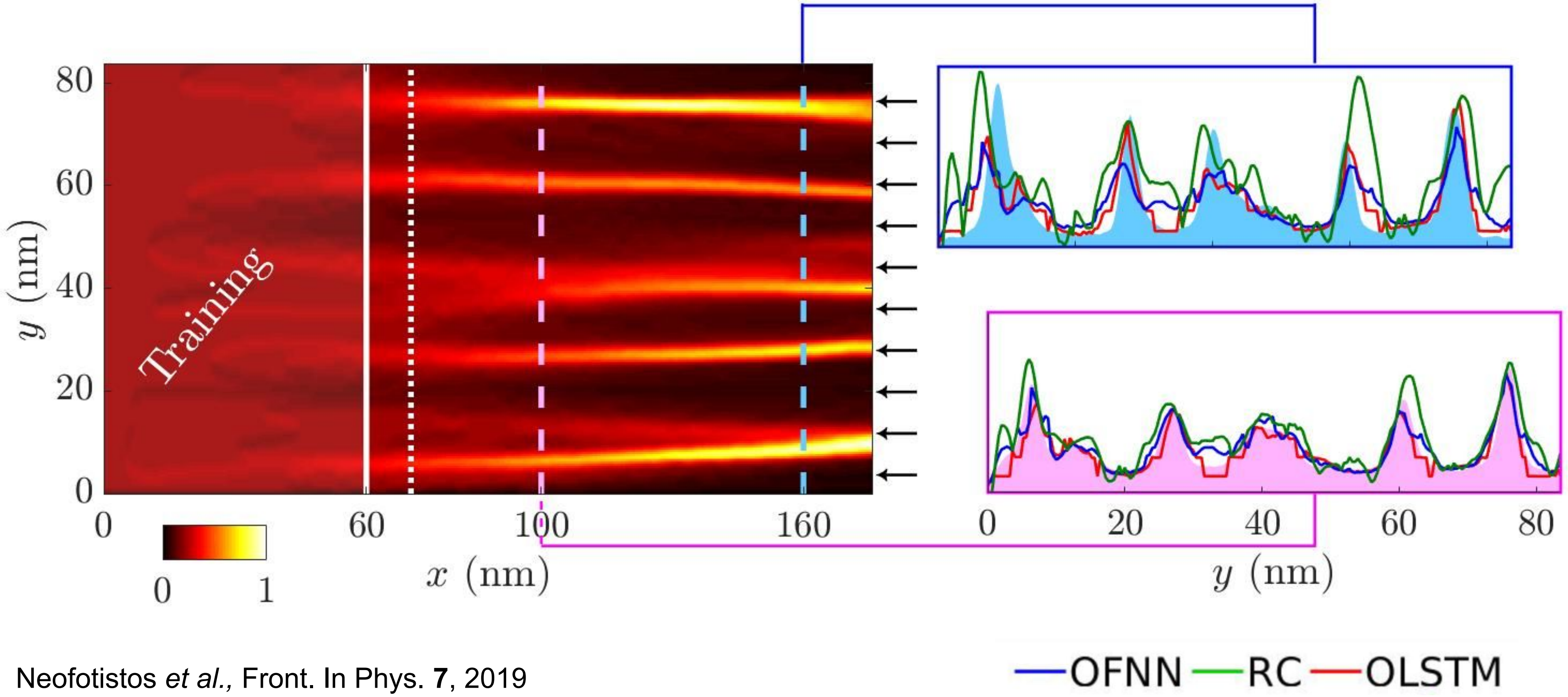
A novel NN method on predicting branching

Predicting Singular events in wave dynamics



Neofotistos *et al.,* Front. In Phys. **7**, 2019

Results of our novel NN architectures



Neofotistos *et al.,* Front. In Phys. **7**, 2019

Outline

- Metamaterials based on graphene:
  - Epsilon-Near-Zero plasmonic nanocrystals
- Branched flow in random environments:
  - Electronic flow in graphene
- Machine Learning:
  - Forecast the electronic branching
  - Solve differential equations with Neural Networks

Hamiltonian Dynamics (Conservative Systems)

Aiming to learn the position and momenta

$$\mathcal{H}(q_i, p_i) = K(p_i) + V(q_i)$$

by satisfying Hamilton's equations of motion

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i}.$$

Symplectic notation

$$\dot{\mathbf{z}} = \mathbf{J} \cdot \frac{\partial \mathcal{H}}{\partial \mathbf{z}}$$

with

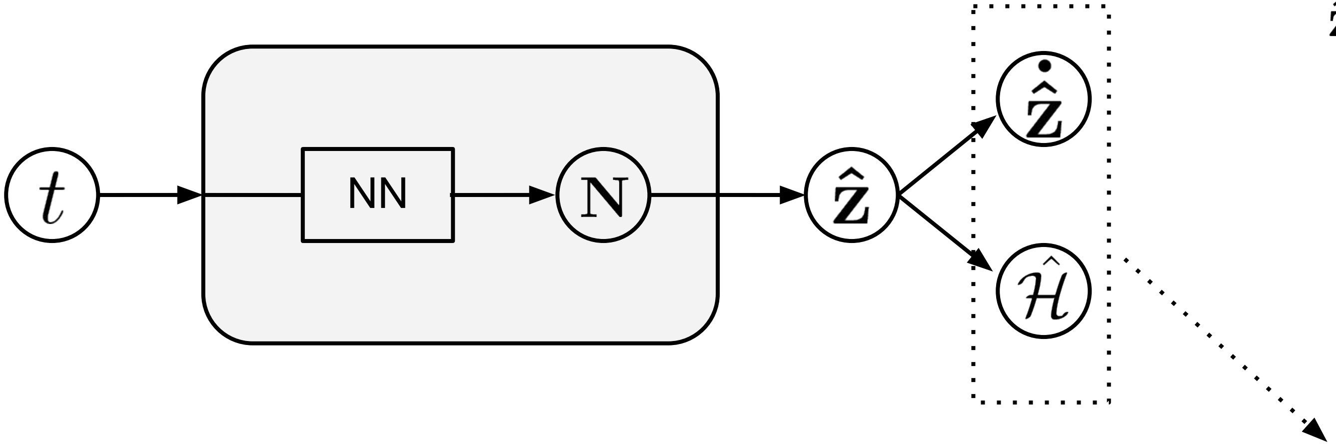
$$\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{1} \\ -\mathbf{1} & \mathbf{0} \end{pmatrix}$$

$$\mathbf{z} = (q_1, \ldots, q_\nu, p_1, \ldots, p_\nu)^T$$

Hamiltonian Neural Network

$$\hat{\mathbf{z}},\ \mathbf{N} \in \mathbb{R}^D$$

$$\hat{\mathcal{H}} \equiv \mathcal{H}(\hat{z})$$



$$\hat{\mathbf{z}}(t) = \mathbf{z}(0) + f(t)\mathbf{N}(t)$$

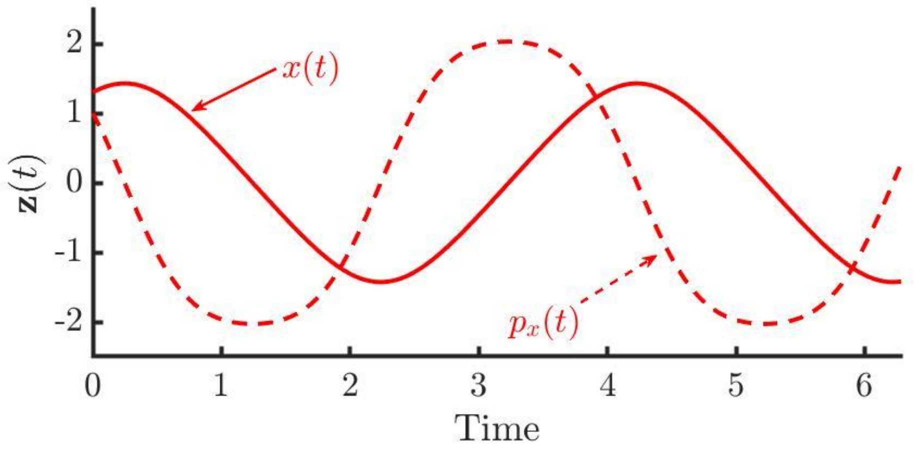
$$f(0) = 0$$

$$L = \left(\dot{\hat{\mathbf{z}}} - \mathbf{J} \cdot \frac{\partial \hat{\mathcal{H}}}{\partial \hat{\mathbf{z}}}\right)^2$$

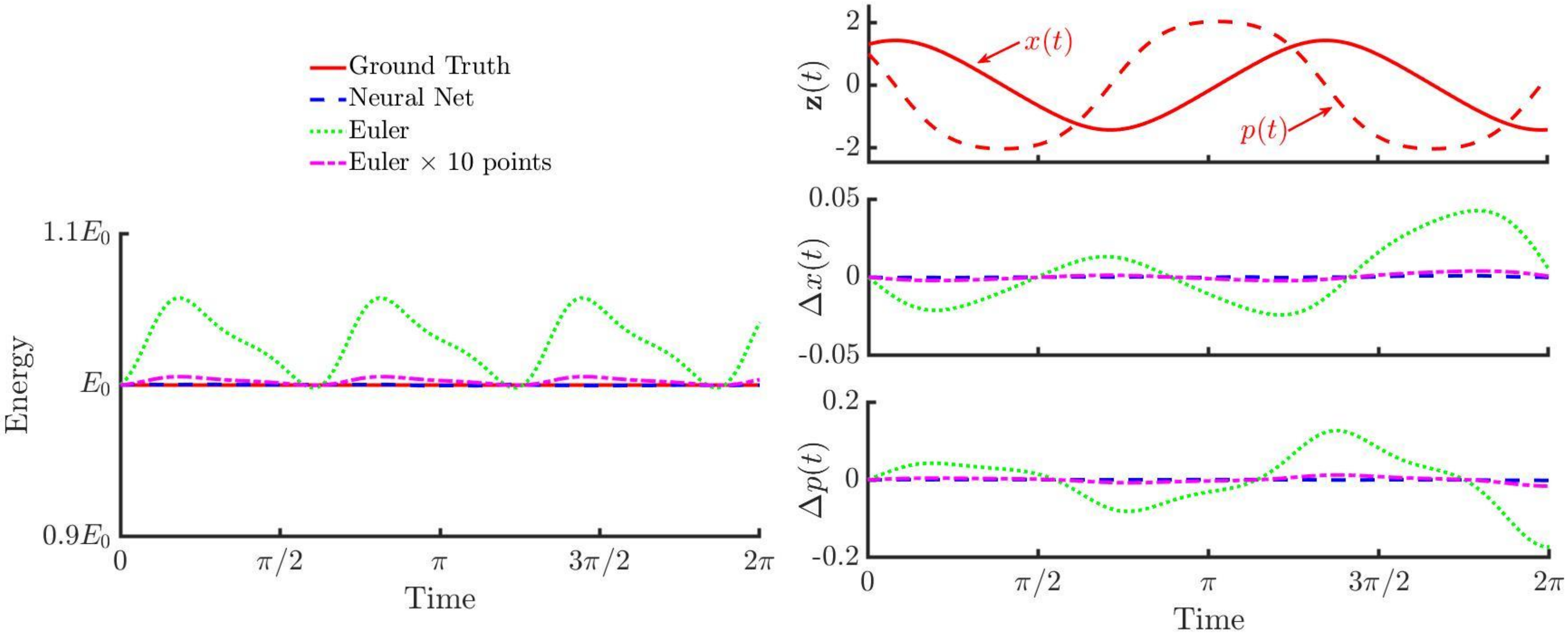
Nonlinear Oscillator

$$\mathcal{H}(q,p) = \frac{p^2}{2} + \frac{x^2}{2} + \frac{x^4}{4}$$

$$\dot{x} = p$$
$$\dot{p} = -(x + x^3)$$



NNs' solutions conserve the energy



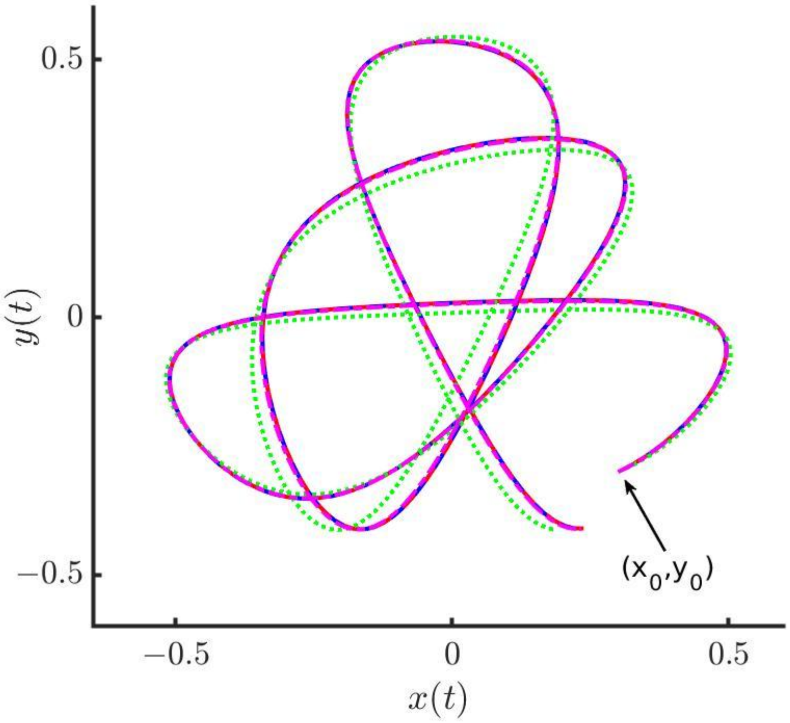
Henon-Heiles

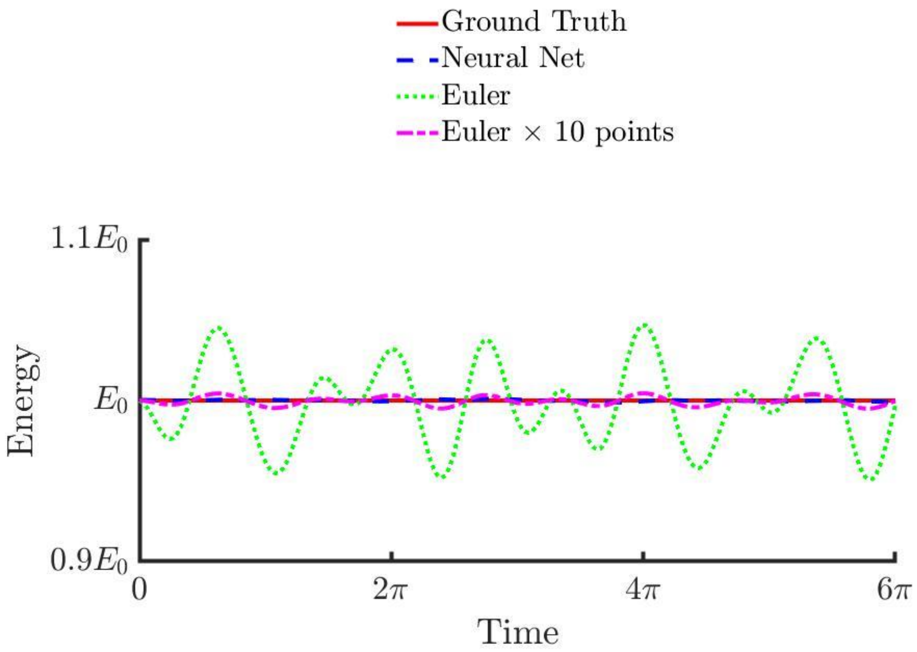
$$\mathcal{H} = \frac{p_x^2 + p_y^2}{2} + \frac{x^2 + y^2}{2} + x^2 y - \frac{y^3}{3}$$

$$\dot{x} = p_x\,, \qquad \dot{y} = p_y\,,$$

$$\dot{p}_x = -\left(x + 2xy\right), \qquad \dot{p}_y = -\left(y + x^2 - y^2\right)$$

Henon-Heiles

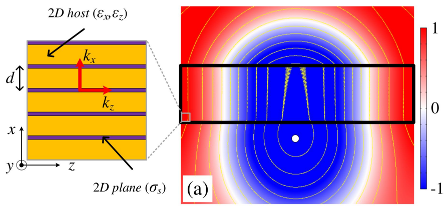




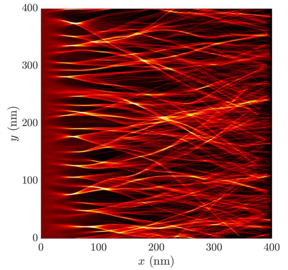
1.12 Lyapunov times

Conclusion

- Tunable metamaterials
  - Combination of 2D material layers
  - A systematic method for designing ENZ metamaterials



- Branched Flow
  - Universal wave phenomenon in random environments
  - Ultra-relativistic flow in graphene
  - Scaling law for electronic branching

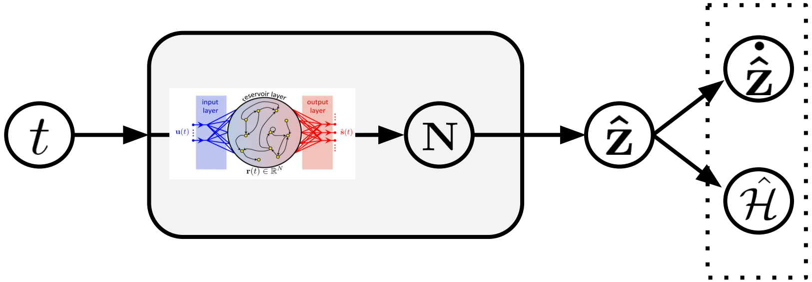


- Machine Learning
  - Forecasting branching
  - Solve ODEs with energy conservation

mariosmat@g.harvard.edu
https://scholar.harvard.edu/marios_matthaiakis

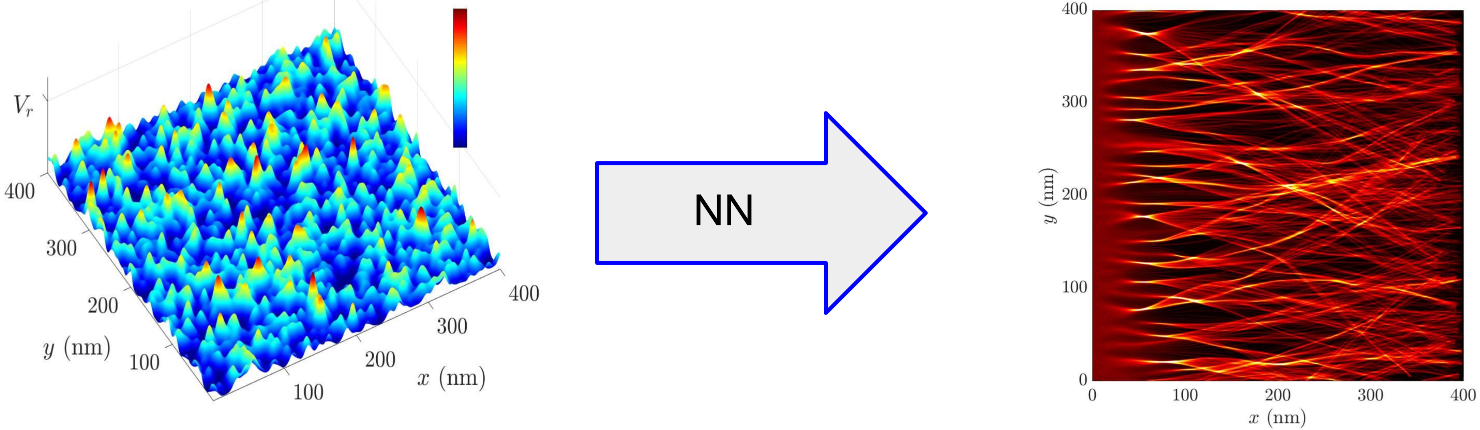
Future Directions

Hamiltonian Networks



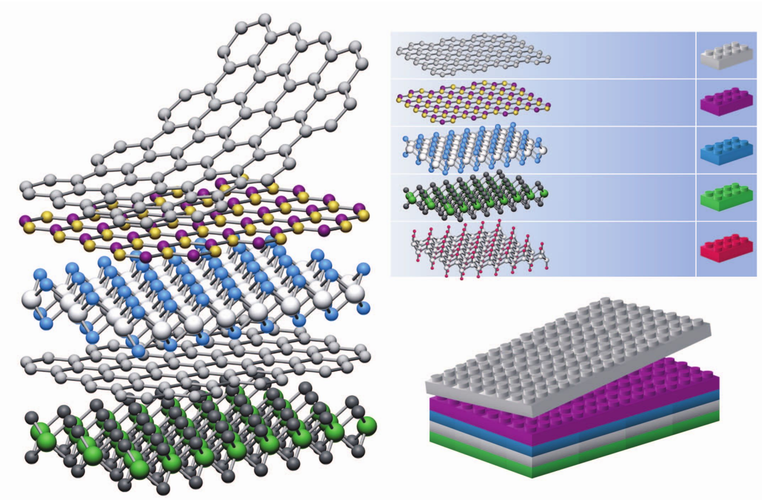
$$L = \left(\dot{\hat{\mathbf{z}}} - \mathbf{J} \cdot \frac{\partial \hat{\mathcal{H}}}{\partial \hat{\mathbf{z}}} \right)^2 + \text{constraints}$$

Predict branching from the potential

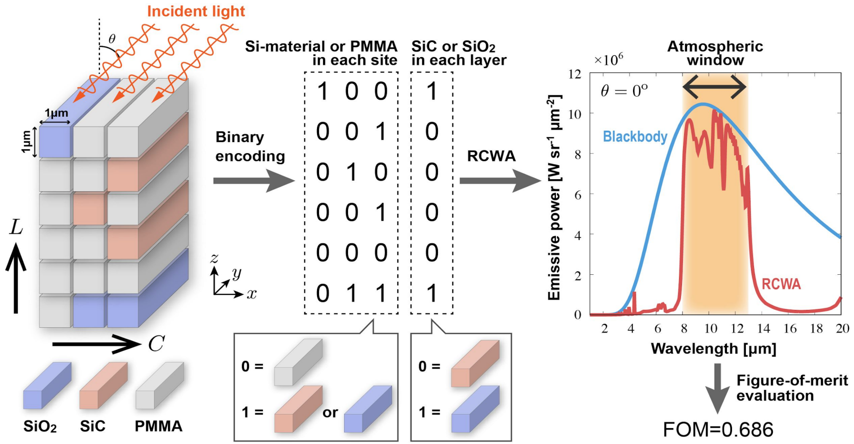


ML for designing quantum metamaterials

2D multilayer heterostructures



Geim *et al*. Nature **499** 2019



Kitai et al. ArxiV 1902.06573

Scheme:

Set target properties

Define a periodic structure

Choose the building elements

Let ML to design the optimal configuration

Acknowledgments

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AT HARVARD UNIVERSITY

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Selected Publications:

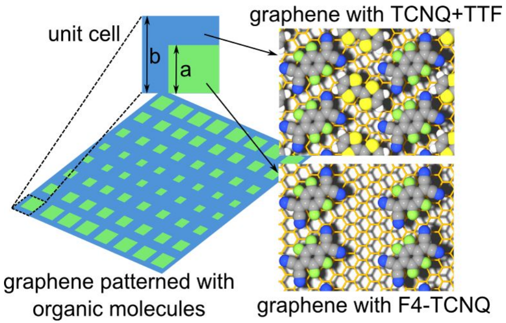
M. Mattheakis *et al.* PRB **94**, 201404(R) (2016)
M. Mattheakis *et al.* EPL **122**, 27003 (2018)
G. Neofotistos, MM *et al.,* Front. In Phys. **7**, 24 (2019)
M. Maier, MM et *al.*, Soc. A **475**, 20190220 (2019)
M. Mattheakis *et al.* arXiv 1904.08991 (2019)

mariosmat@g.harvard.edu
https://scholar.harvard.edu/marios_matthaiakis

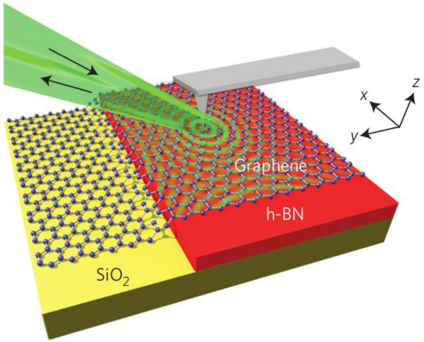
Thank you …

Supplementary Material

Graphene metamaterials

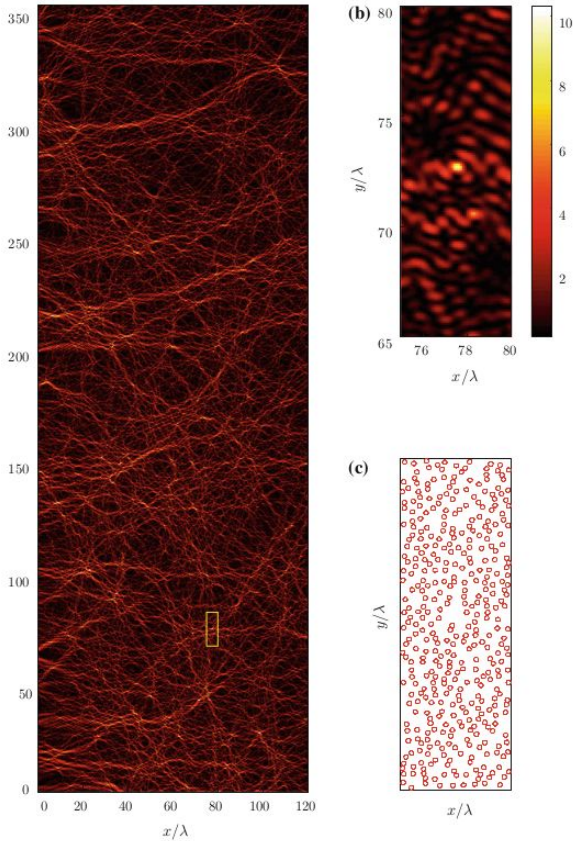


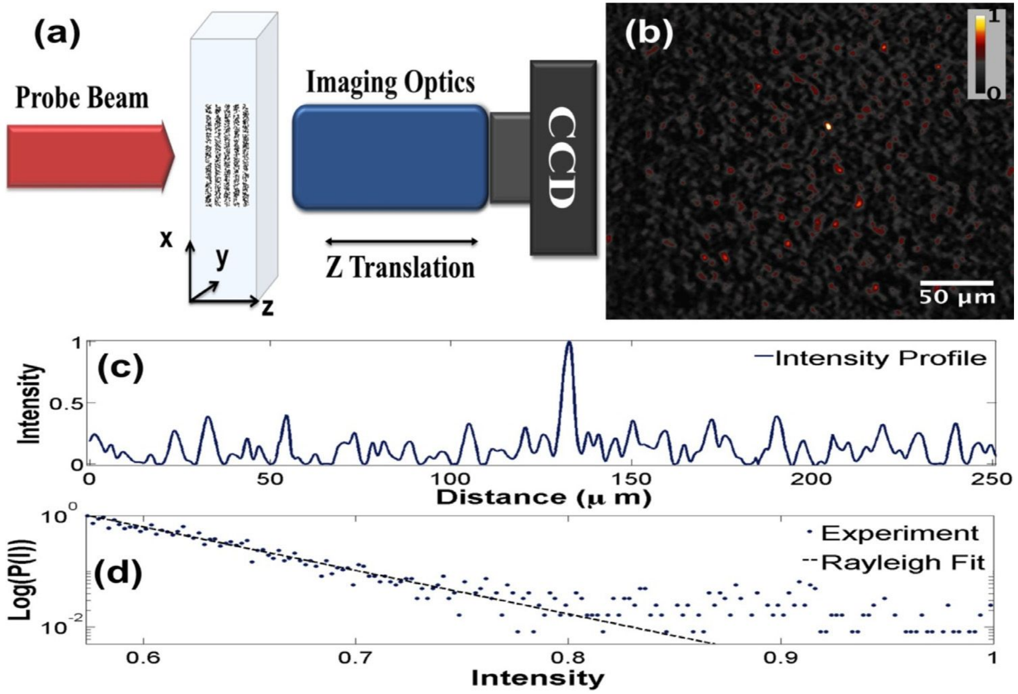
Nanoscale organic meta-lens. Nano Lett. **14** 2014



Tunable hyperbolic media. Nat. NanoTech. **10** 2015

Rogue Waves





M. Mattheakis et al. / Chaos, Solitons and Fractals 84 (2016) 73–80

Effective mass

Structural defects and doping create a small effective mass m

Relativistic Hamiltonian

$$\mathcal{H} = \pm v_F \sqrt{p_x^2 + p_y^2 + m^2} + V(x,y)$$

Effective Hamiltonian for $p_x \gg p_y \quad \& \quad p_x \gg m$

$$\mathcal{H} = p_x + \frac{p_y^2 + m^2}{2p_x} + V(x,y)$$

Langevin Curvature Equation

$$\frac{du}{dt} + \frac{u^2}{p_0 + \alpha t} + \partial_{yy} V_r(t,y) = 0$$

MM *et al.,* EPL **122**, 2018

Neural Networks

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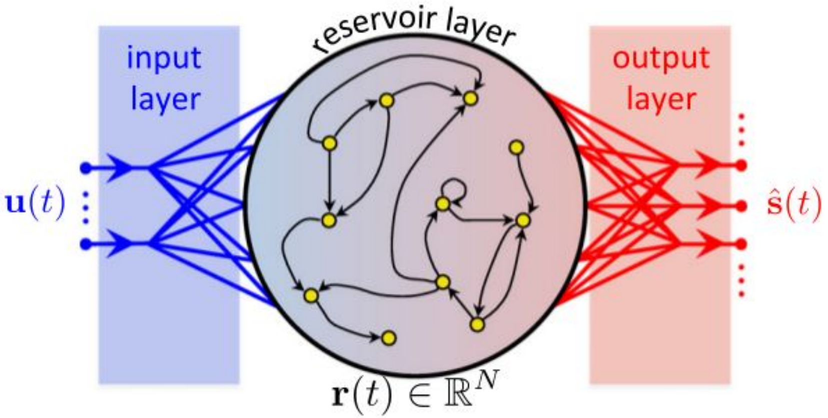
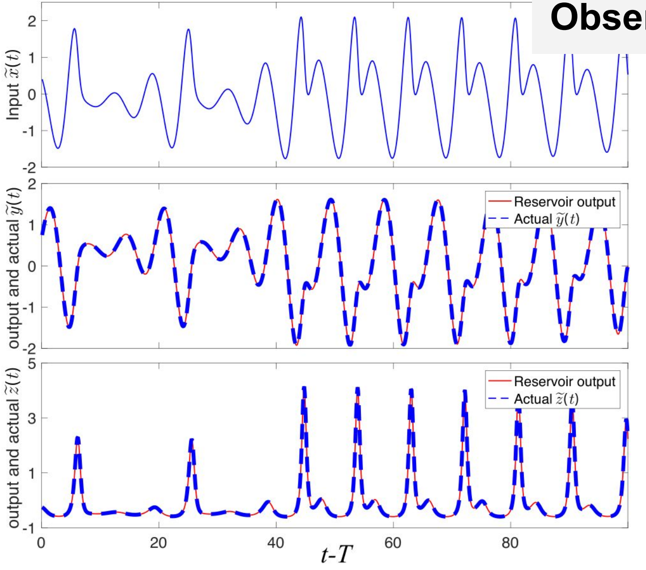
Reservoir Computing: Echo State Recurrent Network



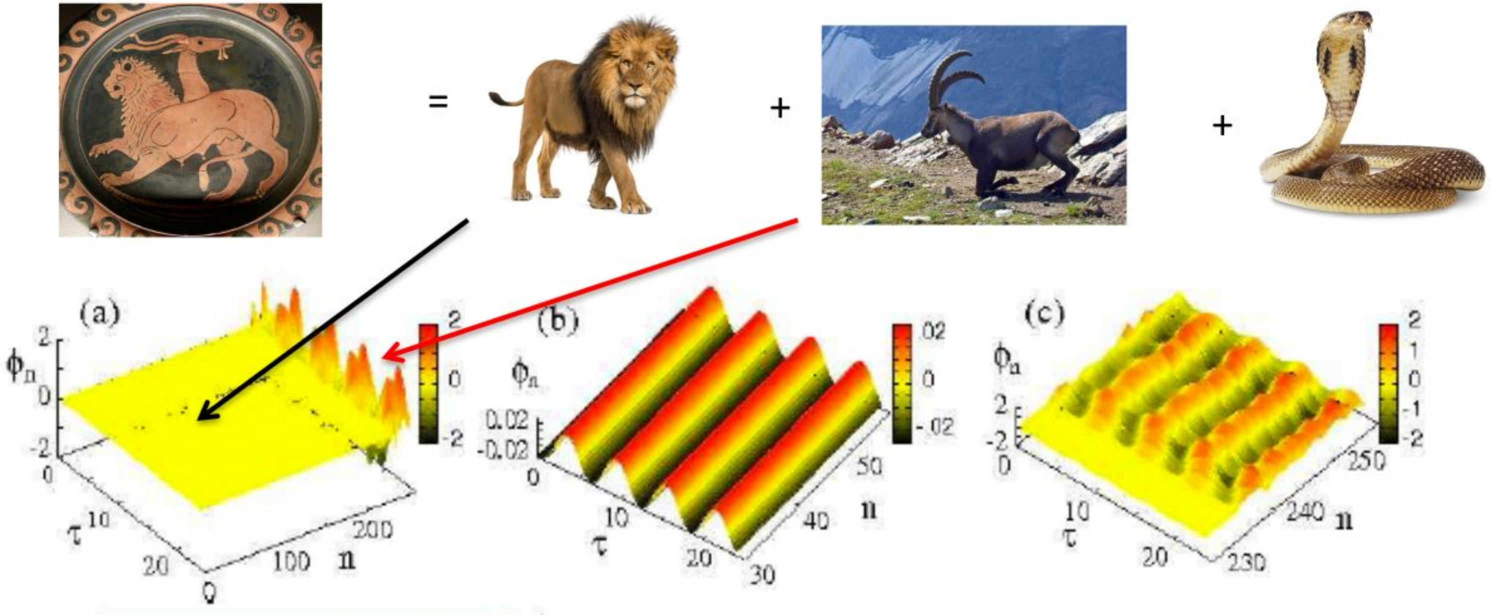
Lu *et al.*, Chaos **27**, 2017

Observer

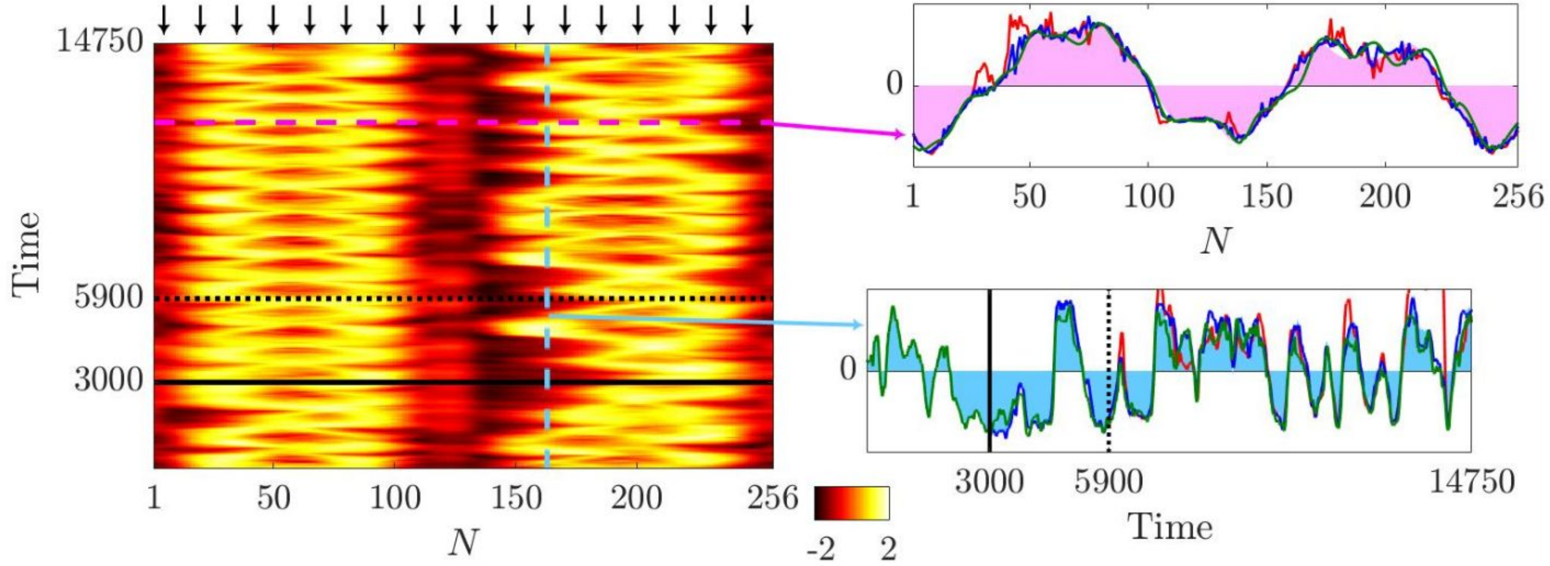


Chimeras:
Another study of spatiotemporal complexity

Coexisting of different states: Coherent and incoherent



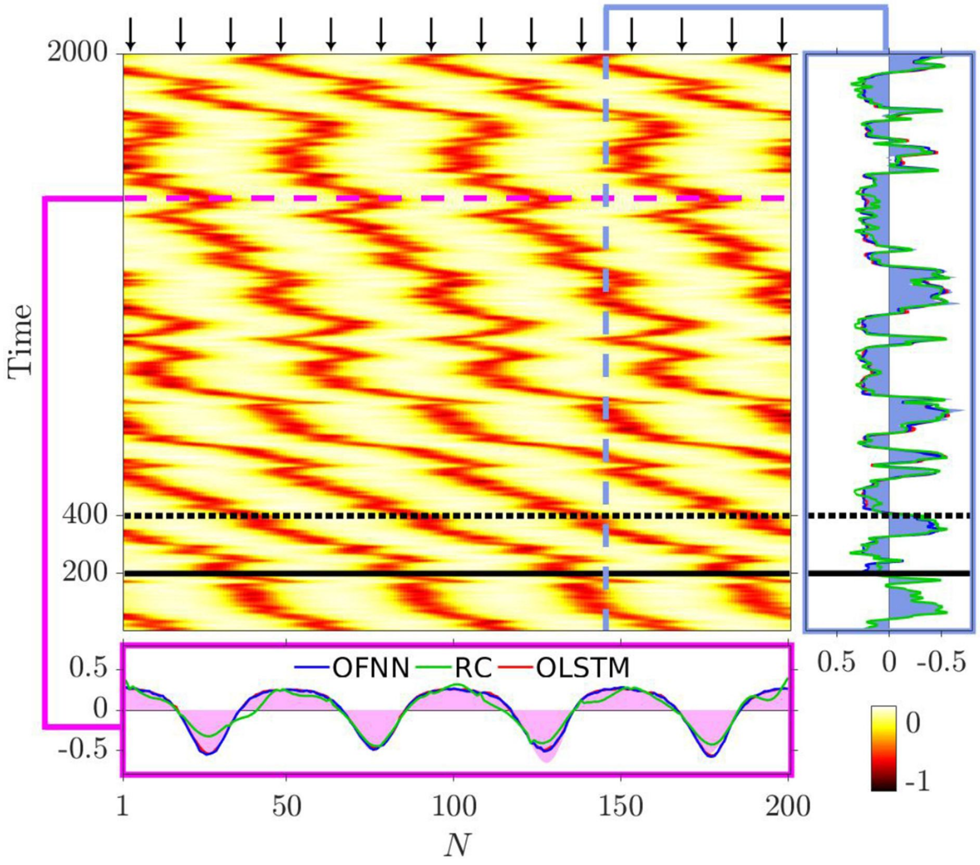
ML results: Chimeras



SQUID Chimera

Data from: Hizanidis et al, Eur. Phys J. (2016)

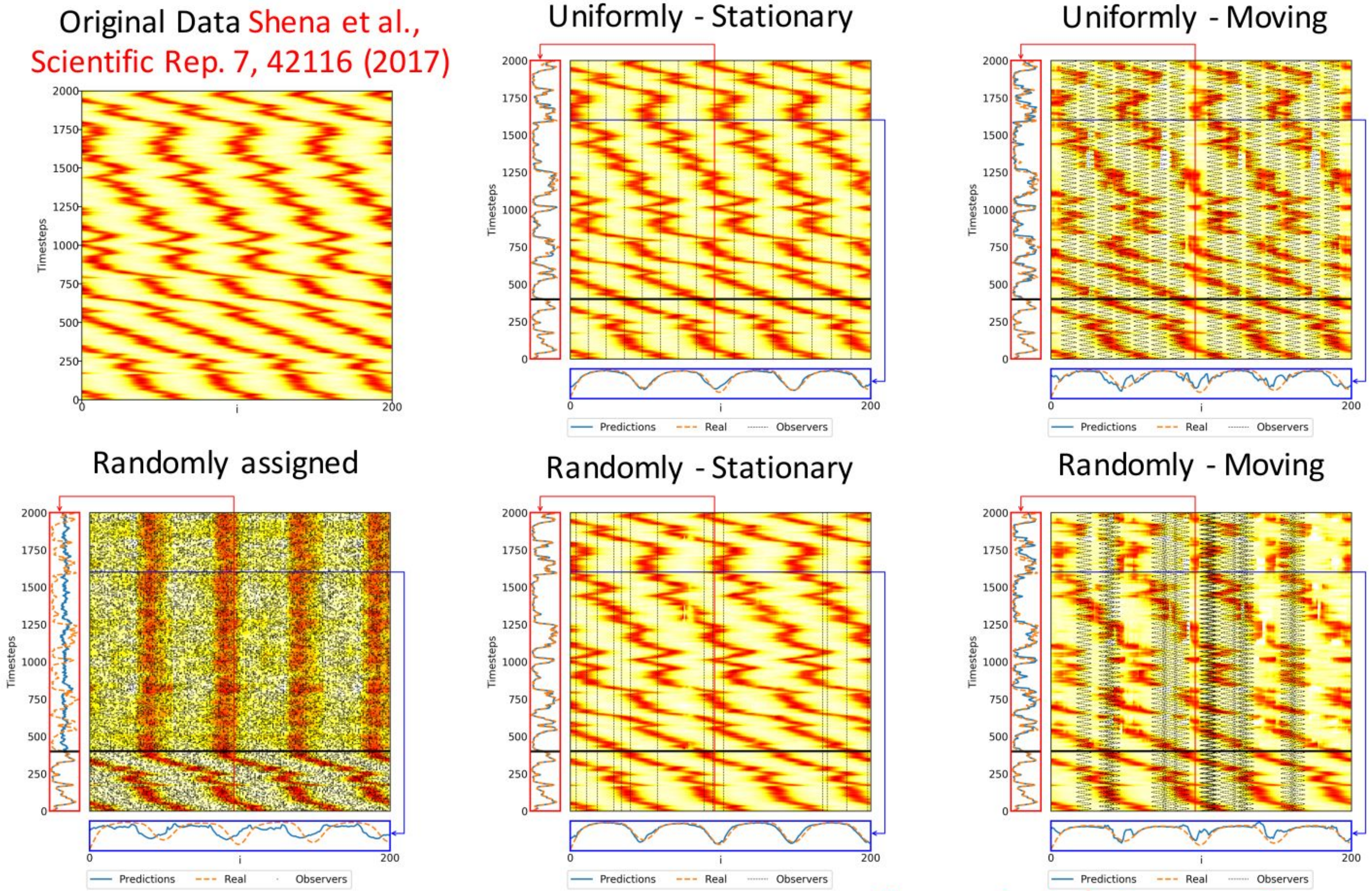
Predicting turbulent chimeras



Data: Semiconductor coupled lasers array
Shena, *et al.,* Sci. Rep. **7**, 2017

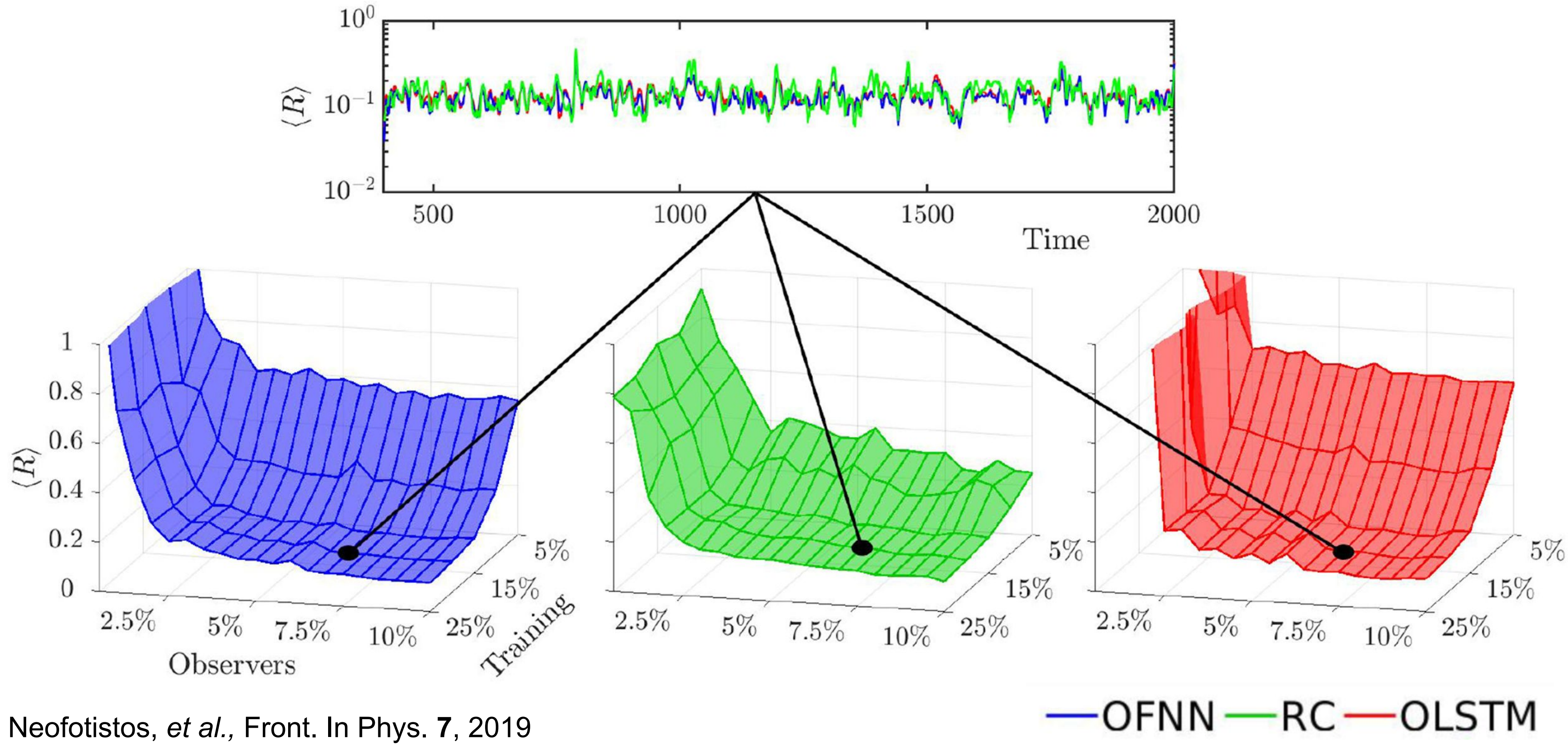
Neofotistos *et al.,* Front. In Phys. **7**, 2019

Moving observers



Barmparis et al., in preparation

Error in prediction for laser chimera case



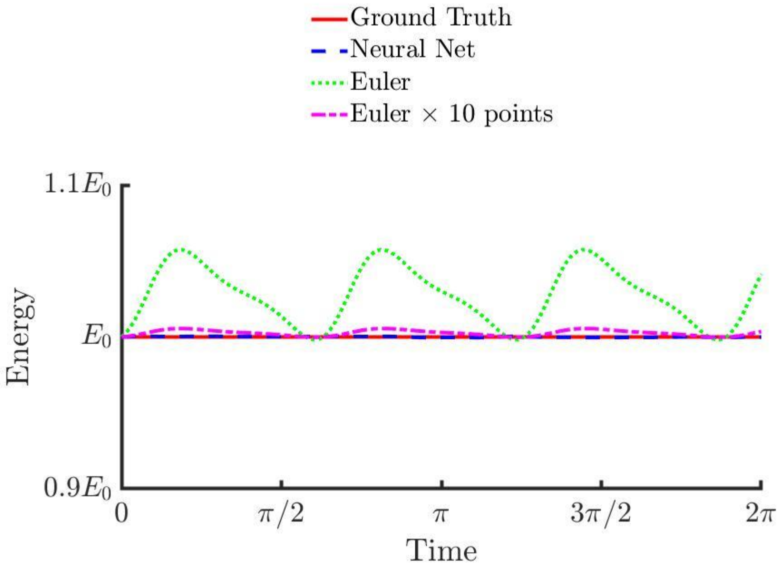
Neofotistos, *et al.,* Front. In Phys. **7**, 2019

NNs' solutions conserve the energy

$$q_i^{n+1} = q_i^n + \frac{\partial \mathcal{H}^n}{\partial p_i^n}\Delta t,$$

$$p_i^{n+1} = p_i^n - \frac{\partial \mathcal{H}^{n+1}}{\partial q_i^{n+1}}\Delta t$$

Symplectic Integrator



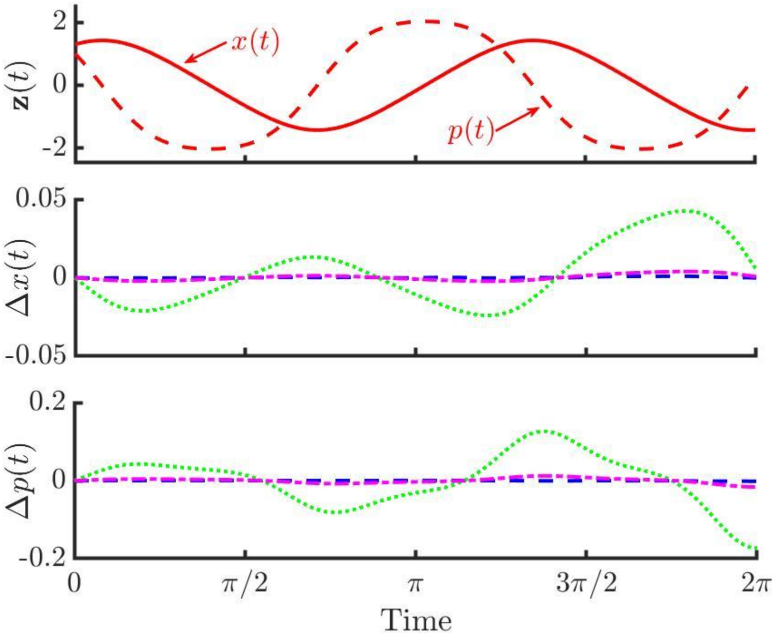
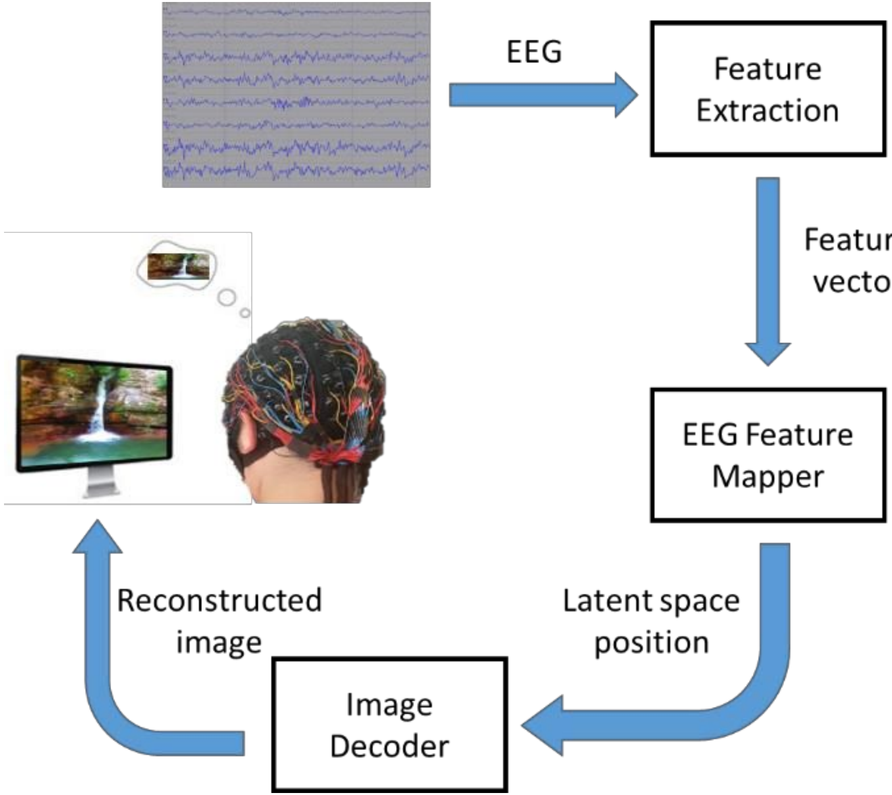


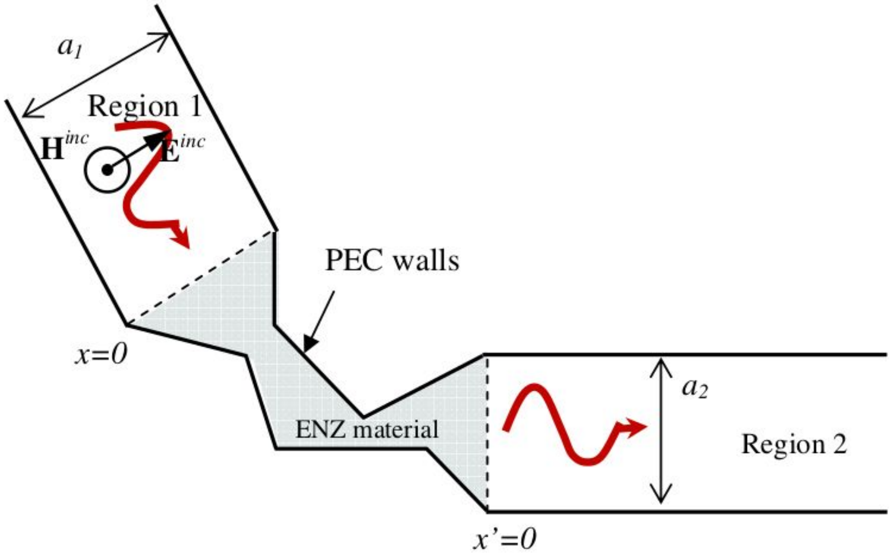
Image reconstruction from brain waves



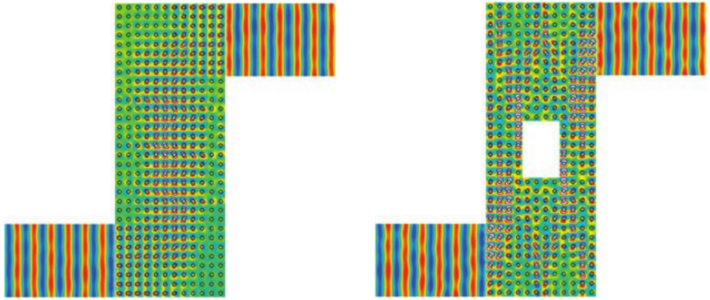
bioArxiv 2019, 10.1101/787101
Posted Oct. 25, 2019

https://www.youtube.com/watch?v=mJct6RUETh0&feature=youtu.be

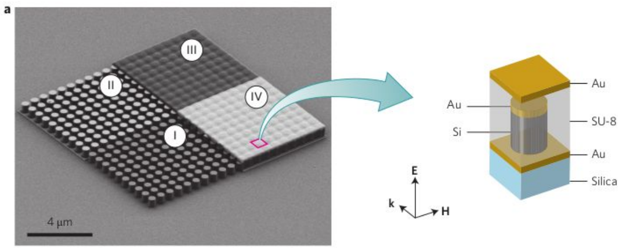
Epsilon-Near-Zero (ENZ)



Tunneling through narrow channels. PRL **97** 2006

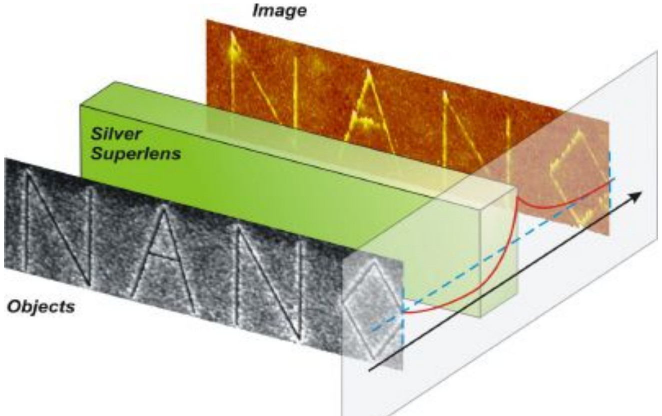


Bending and Cloaking. Nat. Mat. **10** 2011

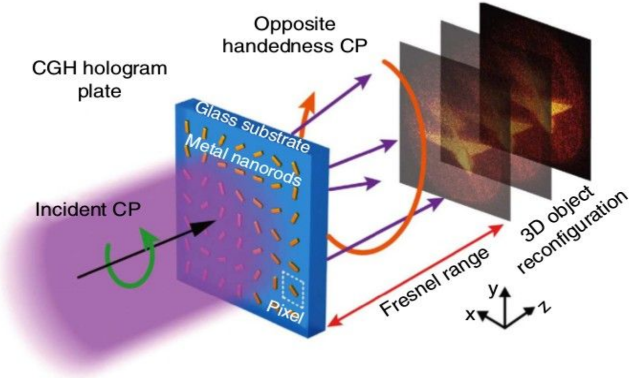


On-chip zero-index. Nat. Phot. **9** 2015

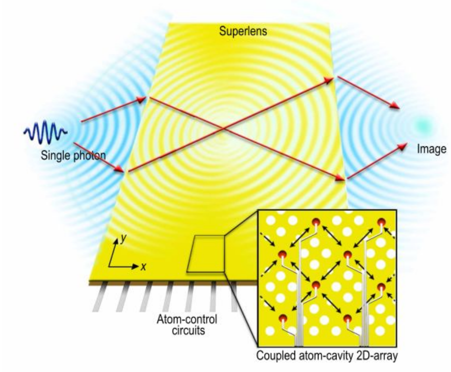
Metamaterials



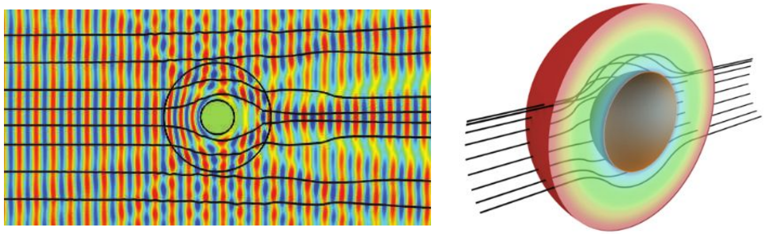
Super-lenses overcoming diffraction limit.
Nat. Mat. **7,** 2008



3D optical holography. Nat. Comm. **4,** 2013

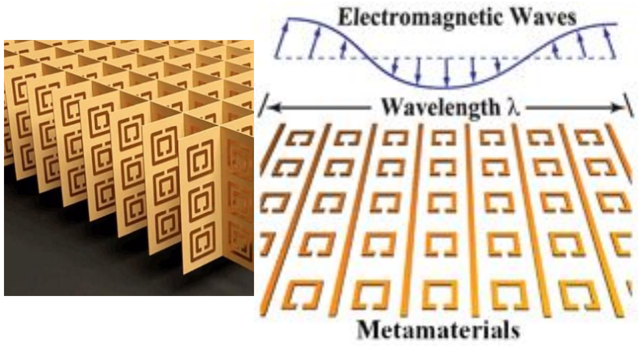


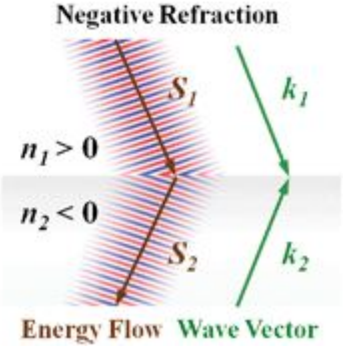
Quantum super-lens
Opt. Expr. **19,** 2012

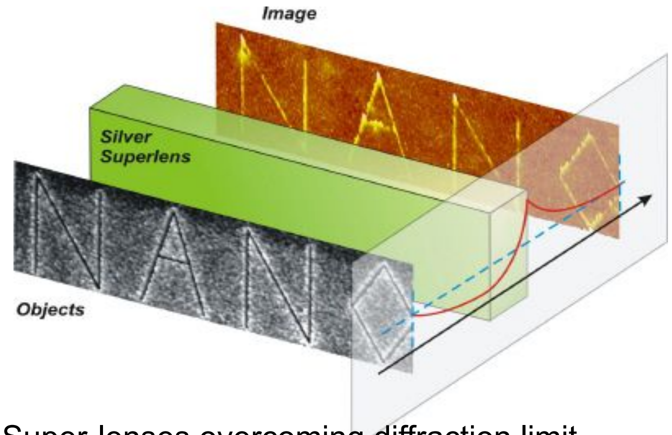


Cloaking devices.
Nat. Phot. **1**, 2007; Nat. Light: Sc. & appl. **7**, 2018

Metamaterials







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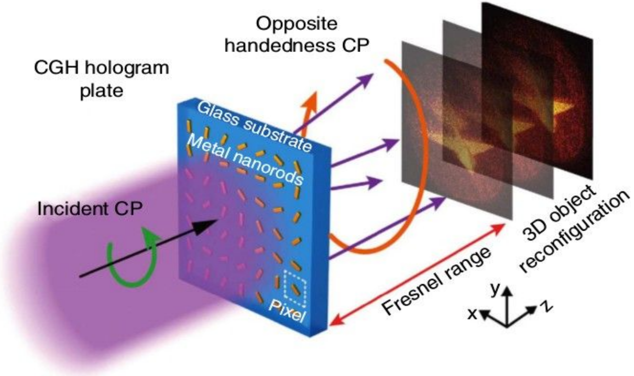

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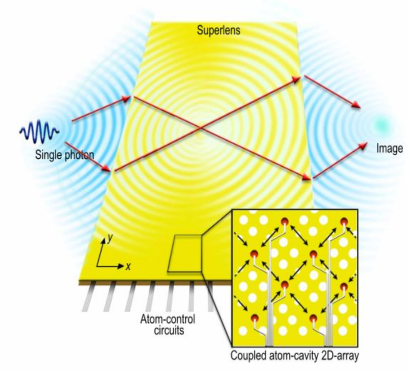


Quantum super-lens
Opt. Expr. **19,** 2012

Graphene, the first semimetal

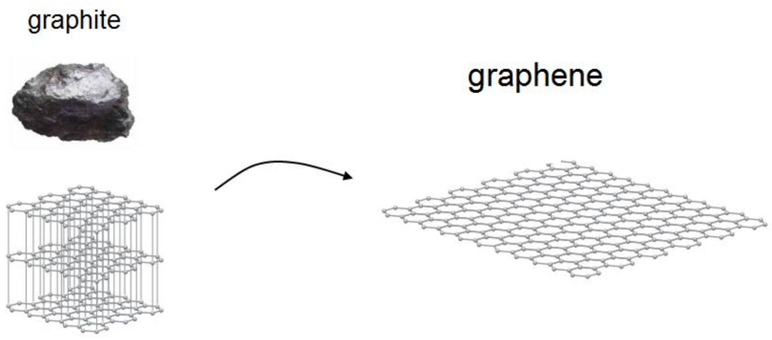
Hexagonal lattice of carbon atoms
(atomically thick material d = 0.32 nm)

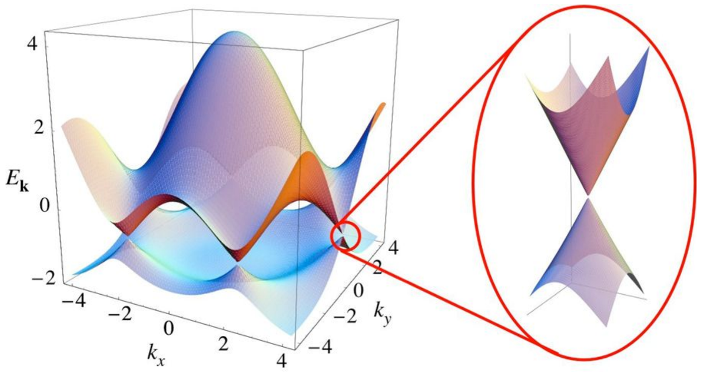
World's highest electrical and thermal conductivity

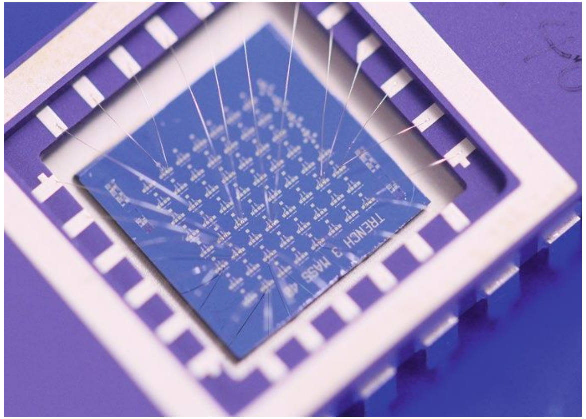
Much stronger than steel (huge in plane elastic constants)

Semimetal with tunable electronic and optical properties

Linear band structure yields ultra-relativistic physics







Integrated nanoelectromechanical accelerometer
Nature Electronics **2,** 2019