CRD COMPUTATIONAL RESEARCH DIVISION

Exploring Post-Moore Microelectronics with HPC

Summer Program 2022
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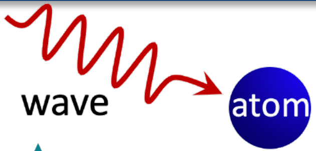
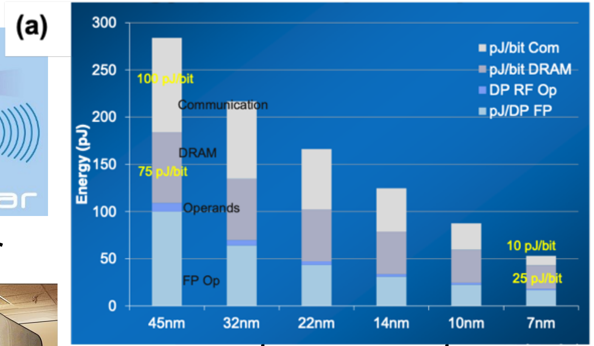
Next-gen microelectronics devices are crucial for energy/cost efficiency

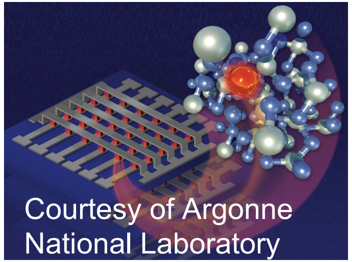


- Continuous miniaturization and integration of modern electronics drives people to utilize novel materials and new techniques

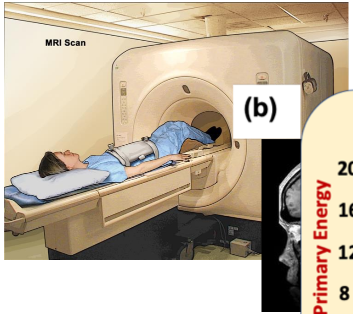
autonomous car



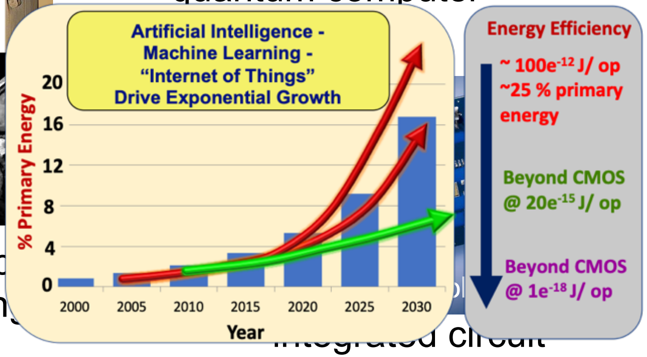
quantum computer



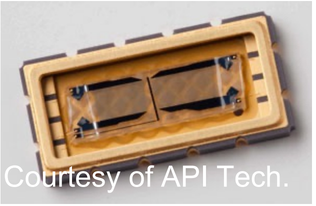
spintronic memory for computing applications



portable magnetic resonance imaging



integrated circuit



acoustic filter

Miniaturization and integration

2022

2020

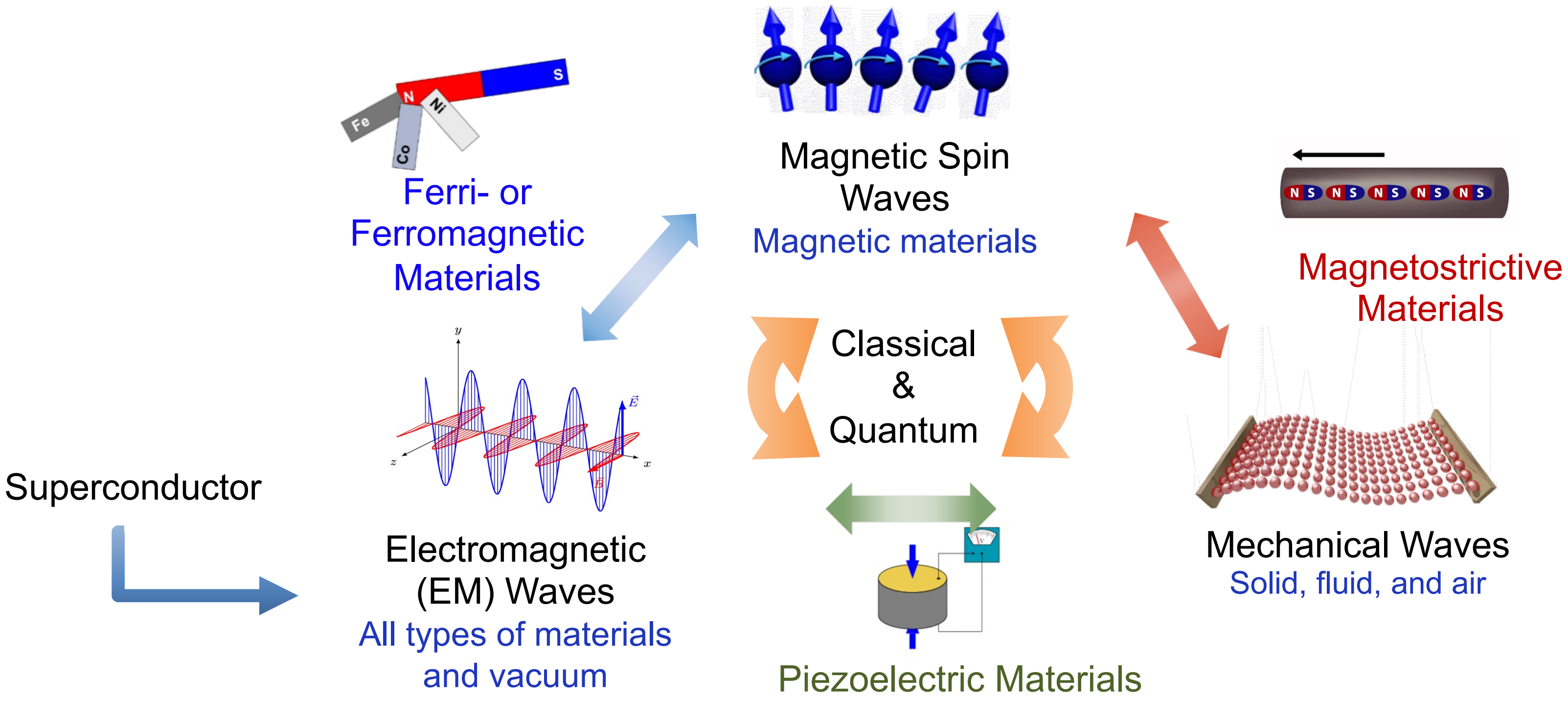
2018

2016

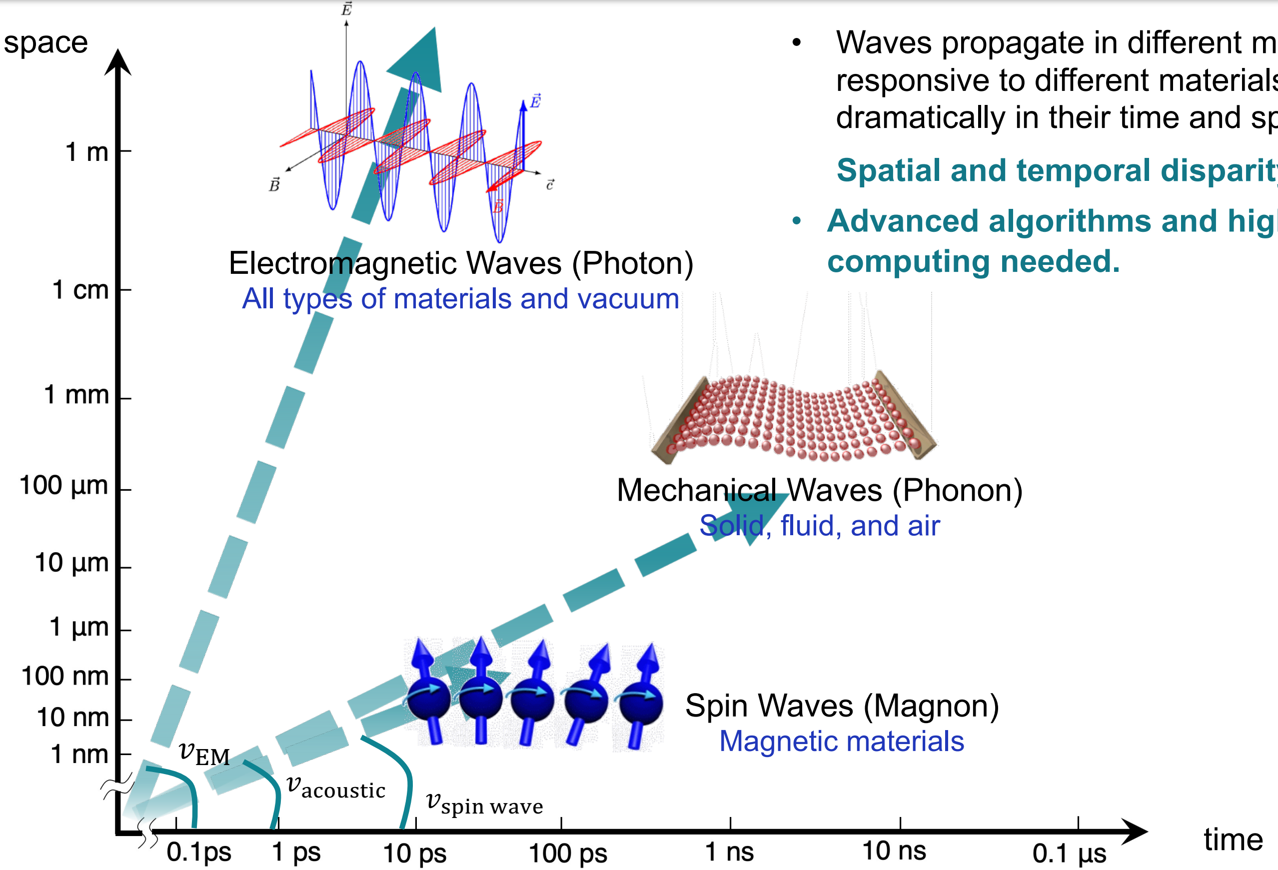
...

Multi-process coupling we focus on

- Complex physical coupling: Any wave interacting with any material, both classical and quantum
- Currently focused on EM and magnetization, expanding into superconductors and quantum applications



Waves' space and time disparity makes modeling challenging



- Waves propagate in different media, are responsive to different materials, and differ dramatically in their time and space dimensions:

  Spatial and temporal disparity

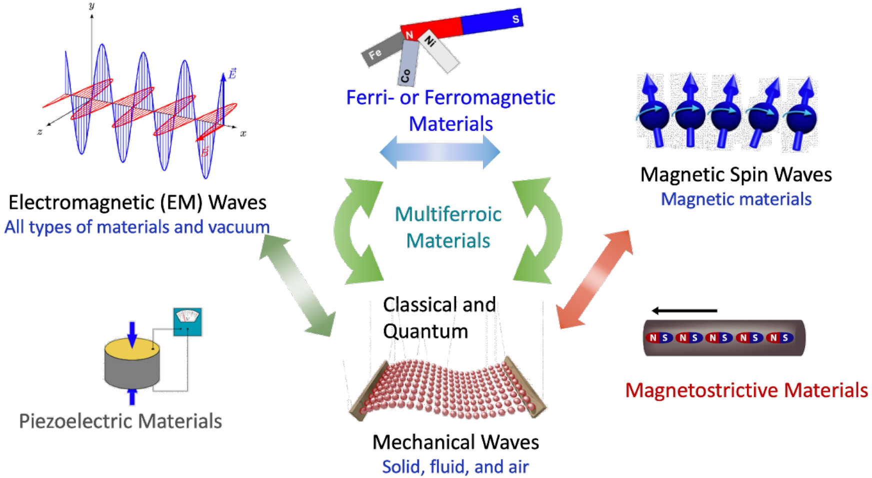
- **Advanced algorithms and high-performance computing needed.**

*Axes are not true to scale

Existing software are not capable of modeling such complicated problems

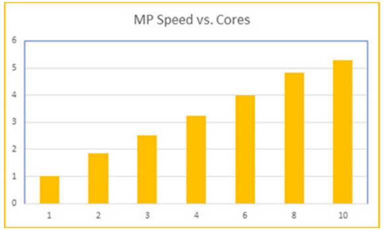
Current model limitations:

- Use the same single-physics model ; multiple physical coupling algorithm is not clear
- Treat sub-components as simplified black-boxes
- Typically limited to 1 level of magnification
- Proprietary commercial software (little to no customization of algorithm)
- Poor scaling & no GPU



Ansys HFSS

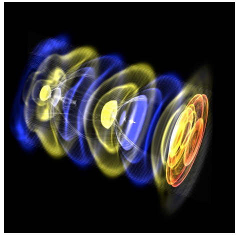
- Maximum scaling 2 nodes, 12 cores/node
- cannot use GPUs



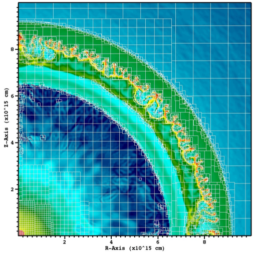
https://www.ansys.com/blog/how-to-optimize-speed-scalability-ansys-hfss-hpc

AMReX Framework provides exascale capability

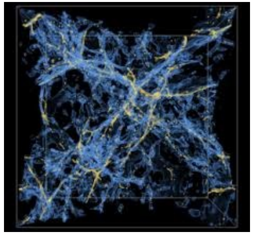
Exascale Computing application projects that partner with AMReX:



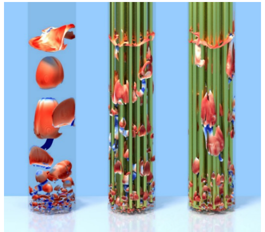
Accelerators



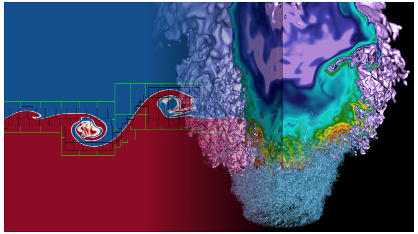
Astrophysics



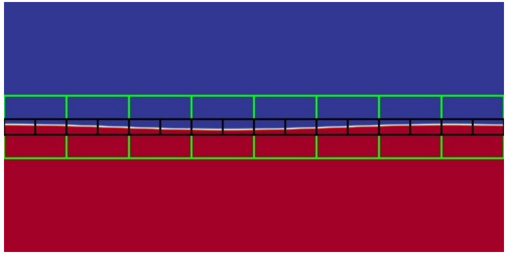
Cosmology



Multiphase flow



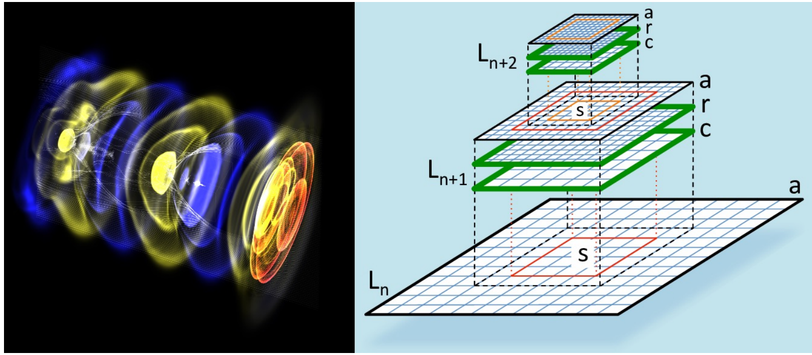
Combustion

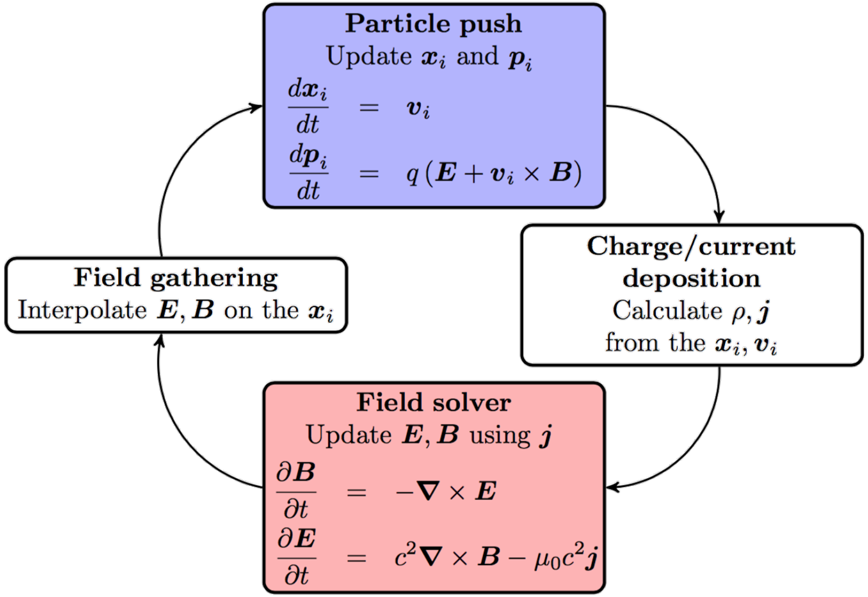


- AMReX is a block-structured Adaptive Mesh Refinement (AMR) framework for solving systems of nonlinear PDEs for a variety of US DOE applications.
  - DOE Exascale Computing Project (ECP) Co-Design Center
  - Performant on full HPC systems (multicore/GPU)
- Provides support for multiphysics modeling for time-dependent PDEs
  - Explicit & implicit mesh operations
  - Multilevel synchronization operations
  - Particle and particle/mesh algorithms
  - Solution of parabolic and elliptic systems using geometric multigrid
  - Embedded boundary (cut-cell) representation of geometry

Electromagnetic Particle-in-Cell code, WarpX, combines advanced numerics and multiphysics

- WarpX: Accelerator Division ECP application code for accelerators coupling particle-in-cell (PIC) electrons with Maxwell





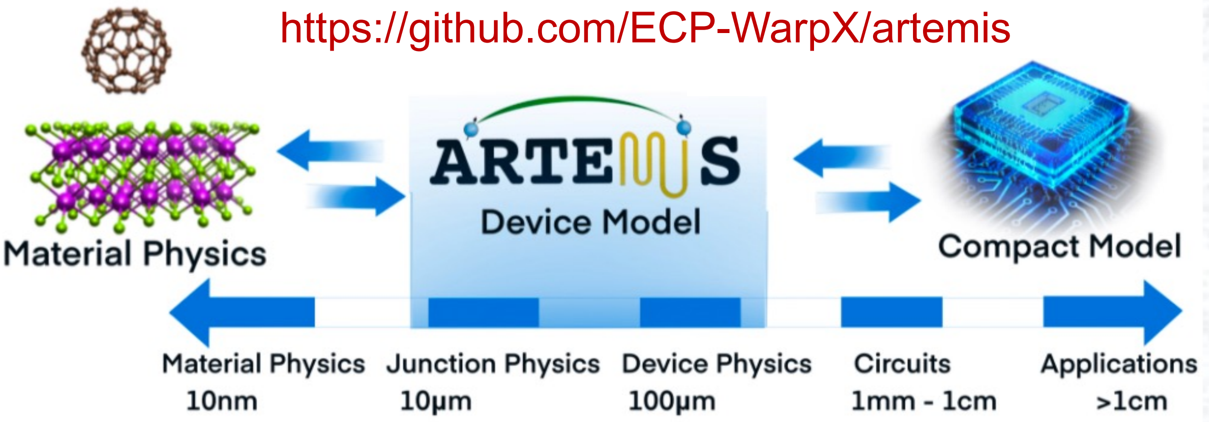
Advanced features:

Spectral Maxwell solver : High accuracy
Perfectly-Matched Layers : Wave absorption
Dynamic load-balancing : Efficient
Mesh refinement : multi-scale sans artifacts
Multi-physics: ionization

+ communications between sub-domains:
guard cell and particle exchanges handled using AMReX

ARTEMIS: Bridging the gap between material physics and circuit model

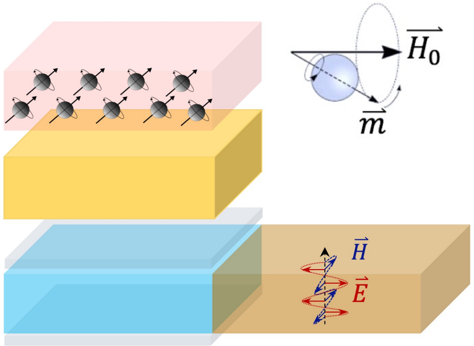
https://github.com/ECP-WarpX/artemis



- ARTEMIS bridges the gap between material physics and circuit model of PARADISE, by solving governing PDEs of the physics in devices such as MESO and NCFET.
- Based on two ECP codes, AMReX and WarpX
- Massively parallel, CPU and GPU support

Z. Yao, R. Jambunathan, Y. Zeng, and A. Nonaka, Int. J. High Perform. Comput. Appl., p. 10943420211057906, Jan. 2022.

Spintronic device modeling requires solving Maxwell's and LLG equation for magnetization



Landau-Lifshitz-Gilbert (LLG) equation

$$\frac{\partial \mathbf{M}}{\partial t} = \mu_0 \gamma (\mathbf{M} \times \mathbf{H}_{\text{eff}}) - \frac{\alpha}{|\mathbf{M}|} \mathbf{M} \times \frac{\partial \mathbf{M}}{\partial t}$$

$$H_{\text{eff}} = H + H_{\text{bias}} + H_{\text{ani}} + H_{\text{exch}} \ldots$$

Maxwell's equation

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$

$$\nabla \cdot \mathbf{D} = \rho \qquad \nabla \cdot \mathbf{B} = 0$$

- Algorithmically couple PDEs (LLG equation and Maxwell's equations)
- Solution procedure will evolve this coupling at each time step

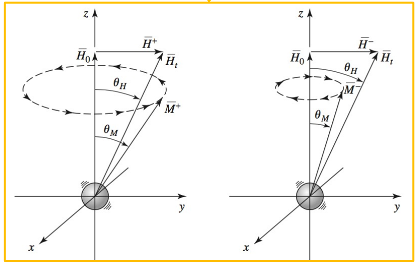
- $\boldsymbol{M}$: volume density of electron spins
- Continuum model that describes the evolution of $\boldsymbol{M}$ under the effective $\boldsymbol{H}$ and the torque

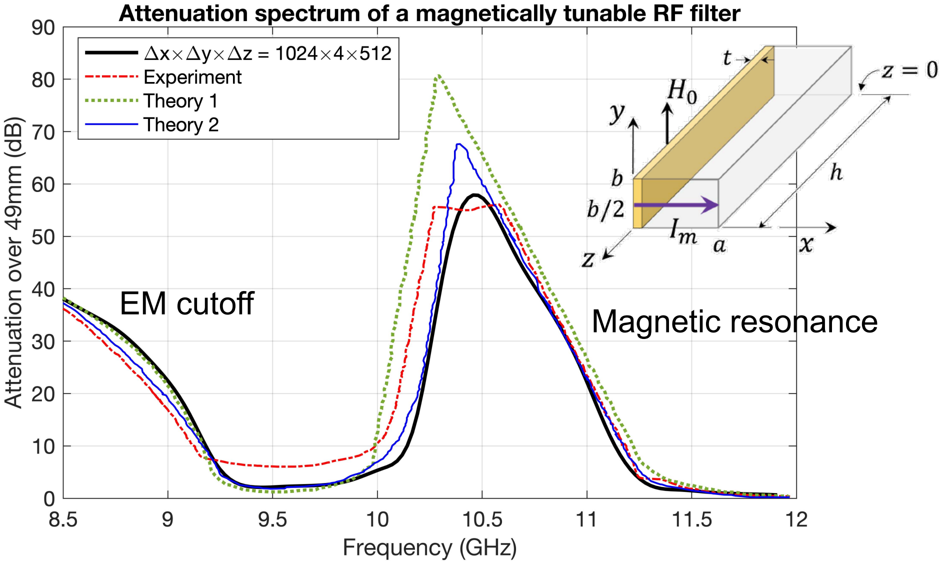
Magnetically Tunable Filter

$t = 0.45\ mm, a = 14.95\ mm$

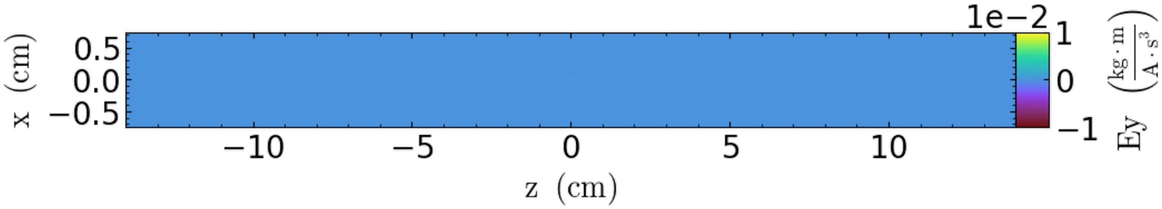
$4\pi M_S = 1750\ Gauss$

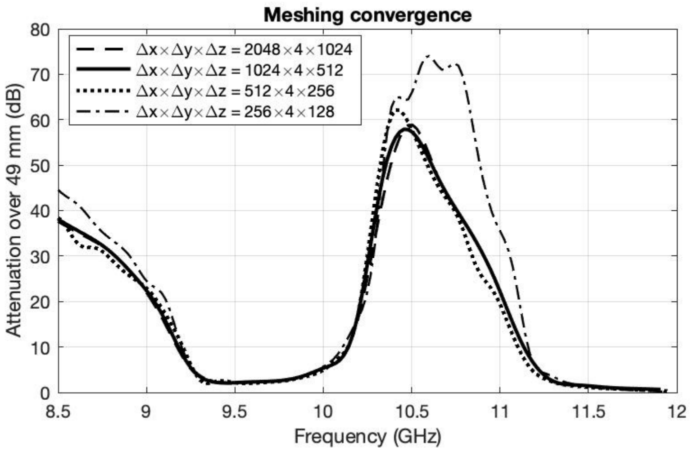
$H_i = 2890\ Oe, \Delta H = 35\ Oe$





- Demonstrated both EM propagation and the coupling between EM and other physical phenomena such as magnetic resonance.





Variable	E_{32}^{64}	E_{64}^{128}	Rate
E_x	1819.4	455.23	2.00
E_y	1820.5	455.04	2.00
E_z	1882.8	470.47	2.00
H_x	9.6659	2.4359	1.99
H_y	9.4752	2.3788	1.99
H_z	9.4590	2.3607	2.00
M_x	5.1343	1.2870	2.00
M_y	4.7851	1.1989	2.00
M_z	4.9642	1.2429	2.00

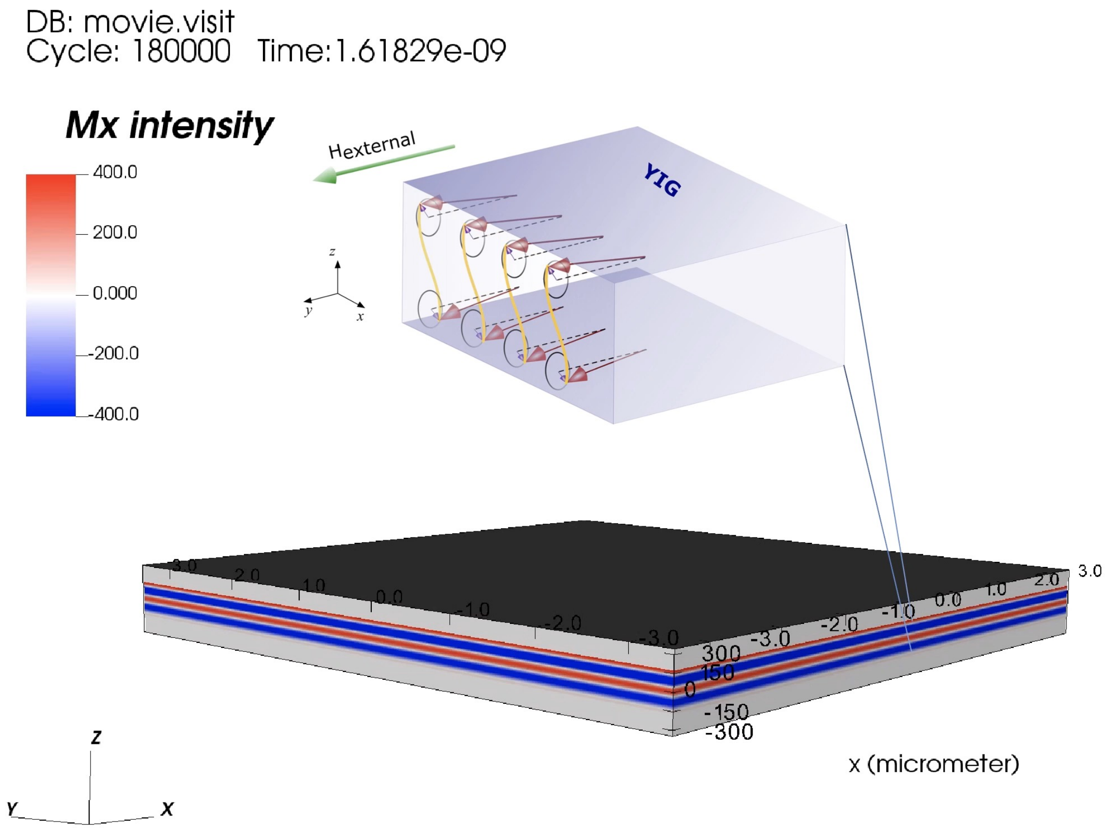
Table 1: Convergence rates in the L^1 norm for all field variables.

- Convergence on the result is observed in the mesh refinement process
- Adaptive Mesh Refinement (AMR) implementation is under progress

- Second-order accuracy is observed for all field variables

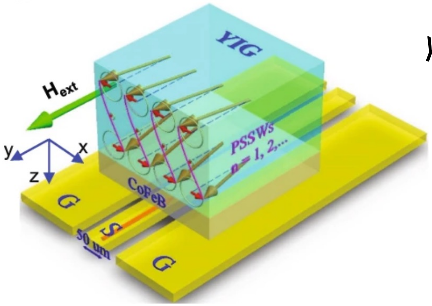
L_1 norm calculation $$E_c^f = \frac{1}{N_{\text{pts}}} \sum_{i,j,k} |\phi_f - \phi_c|$$

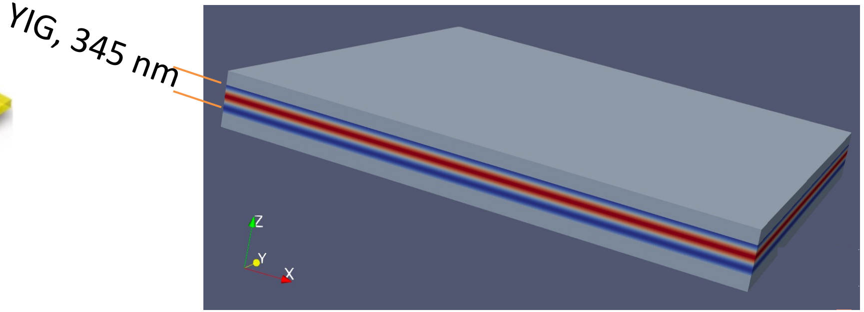
Case 2: Multi-spin interactions generate resonant modes matching theoretical predictions



Case 2: Multi-spin interactions generate resonant modes matching theoretical predictions

$$\boldsymbol{H}_{ex} = \frac{2A_{ex}}{\mu_0 M_s^2}\nabla^2 \boldsymbol{M}$$



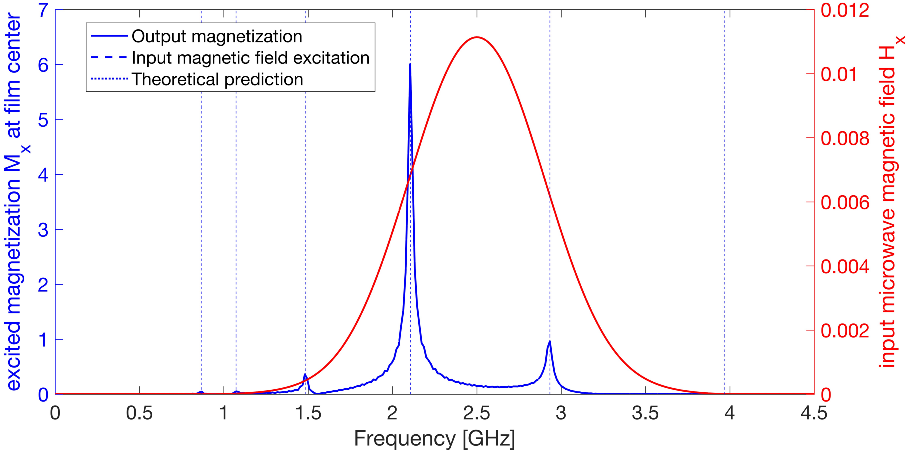


Boundary conditions at magnetic material interfaces:

- Pinned Boundary $\boldsymbol{M} = 0$
- Free Boundary $\frac{\partial \boldsymbol{M}}{\partial \boldsymbol{n}} = 0$

Excitation of perpendicular standing spin waves (PSSW)

$$f_{PSSW} = \frac{\gamma\mu_0}{2\pi}\sqrt{\left[H_{ext} + M_S + \frac{2A_{ex}}{\mu_0 M_s}\left(\frac{(2p+1)\pi}{2d}\right)^2\right] \times \left[H_{ext} + \frac{2A_{ex}}{\mu_0 M_s}\left(\frac{(2p+1)\pi}{2d}\right)^2\right]}$$



H. Qin, S. J. Hämäläinen, and S. Van Dijken, *Sci. Rep.*, vol. 8, no. 1, pp. 1–9, 2018.

Resonance frequencies as theoretically predicted

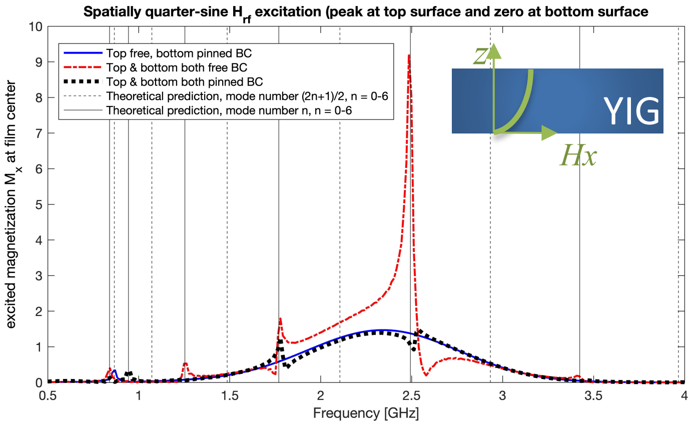
Odd mode:

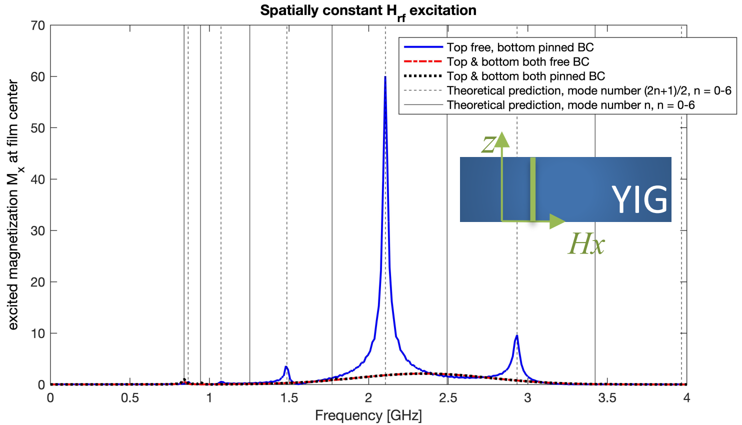
$$f_{PSSW} = \frac{\gamma\mu_0}{2\pi}\sqrt{\left[H_{ext} + M_S + \frac{2A_{ex}}{\mu_0 M_S}\left(\frac{(2p+1)\pi}{2d}\right)^2\right] \times \left[H_{ext} + \frac{2A_{ex}}{\mu_0 M_S}\left(\frac{(2p+1)\pi}{2d}\right)^2\right]}$$

Even mode:

$$f_{PSSW} = \frac{\gamma\mu_0}{2\pi}\sqrt{\left[H_{ext} + M_S + \frac{2A_{ex}}{\mu_0 M_S}\left(\frac{p\pi}{d}\right)^2\right] \times \left[H_{ext} + \frac{2A_{ex}}{\mu_0 M_S}\left(\frac{p\pi}{d}\right)^2\right]}$$

- Engineering EM field distribution in the coupled resonator leads to different magnetic resonance modes

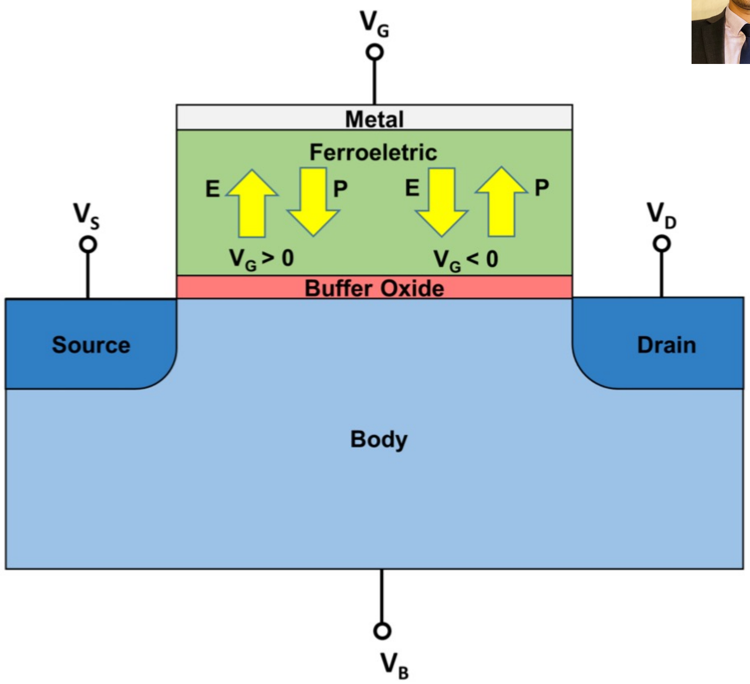




We are developing a 3D phase-field model to simulate ferroelectric based Field Effect Transistors

Prabhat Kumar
(AMCR)

NC-FET structure

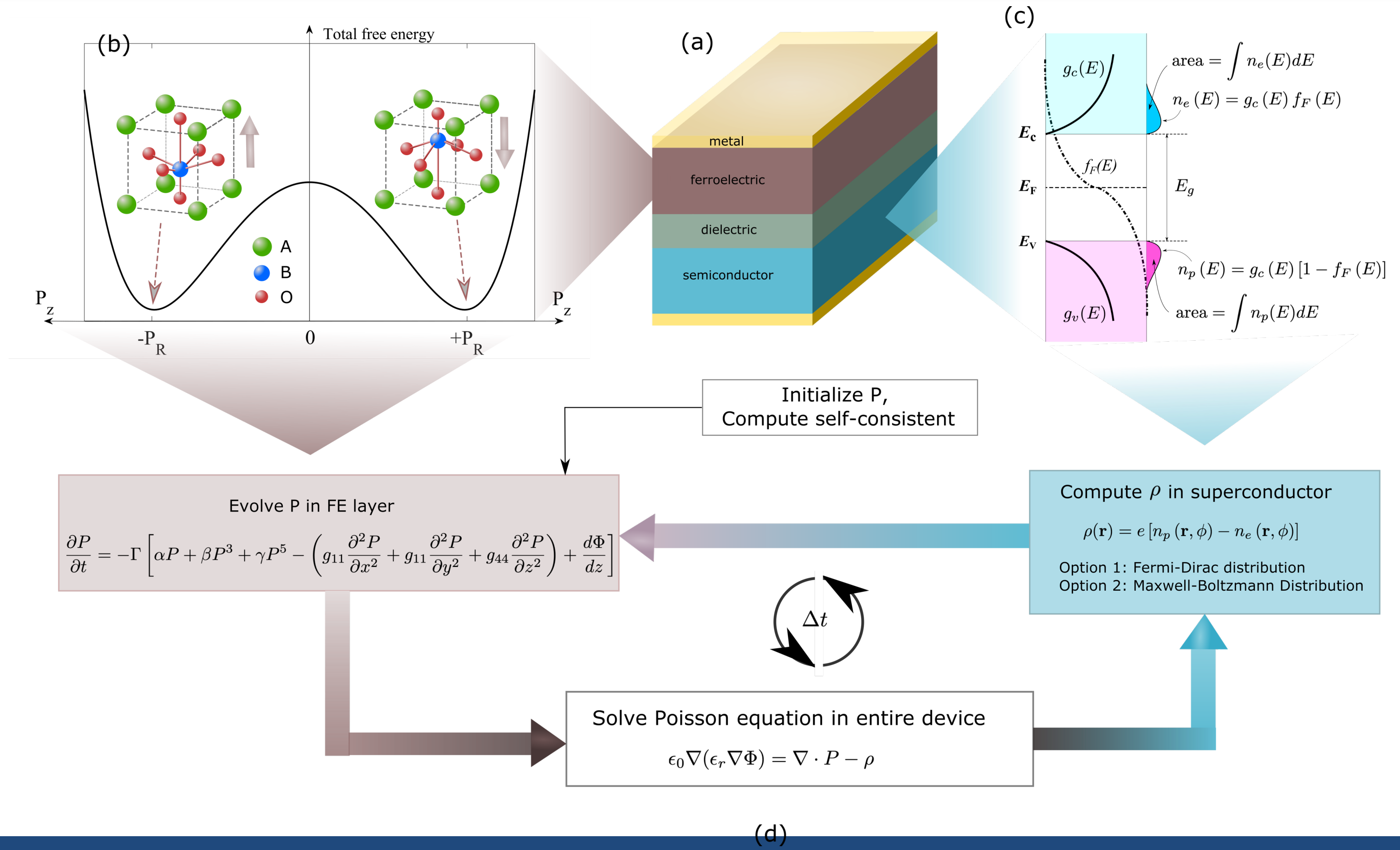


$$S = \frac{\partial V_G}{\partial \log_{10} I_D} = 60mV\left(1 + \frac{C_{dm}}{C_{ox}}\right)$$

- Negative capacitance effect of ferroelectrics can help breach the so-called Boltzmann Tyranny*
- Modeling challenges:
  - Ginzburg-Landau model for FE polarization
  - Poisson's equation across the gate stack
    Semiconductor charge transport in channel
- Need Boltzmann transport model to capture short-channel effects

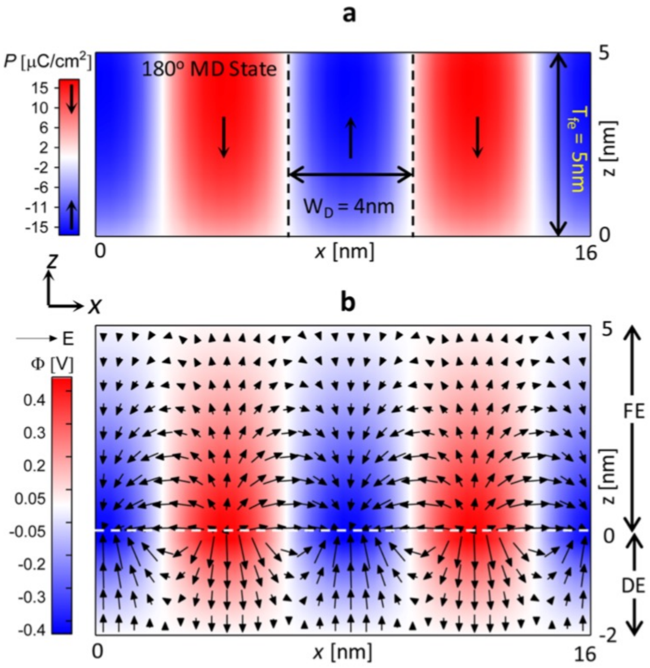
Salahuddin and Datta, Nano Lett. 2008, 8, 2, 405–410

Our model solves self-consistent solutions of coupled ferroelectric systems at every timestep

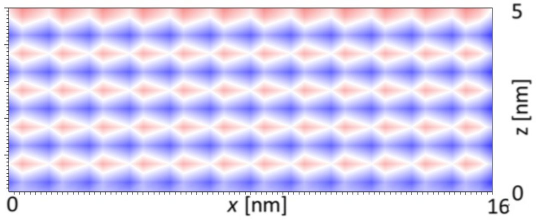


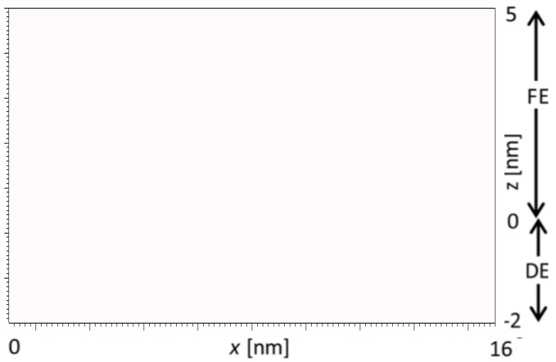
Our 3D model results agree well with existing 2D models for ferroelectrics

Existing 2D model (Saha & Gupta, Sci Rep 2020)



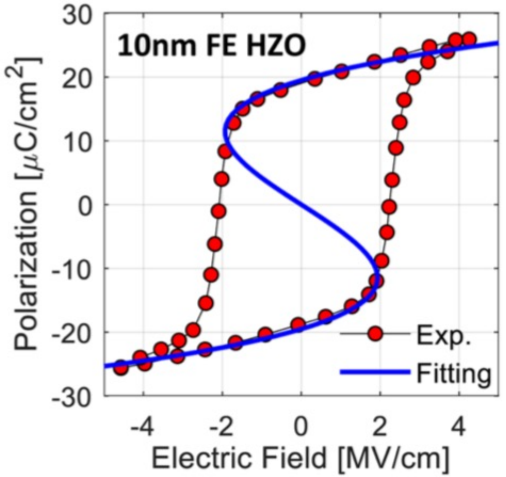
Results Using Our 3D model



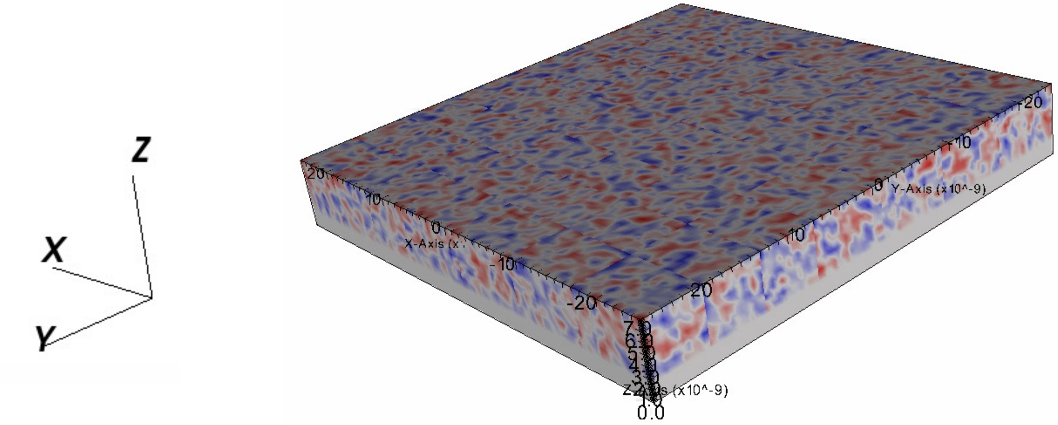


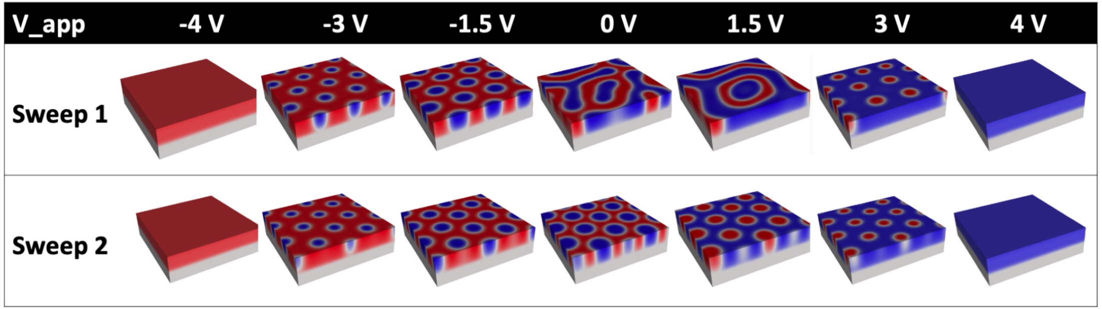
Material Parameters

$\alpha, \beta, \gamma, g_{11}, g_{44}, \epsilon_x, \epsilon_y, \epsilon_z$



3D models are needed to capture surface effects

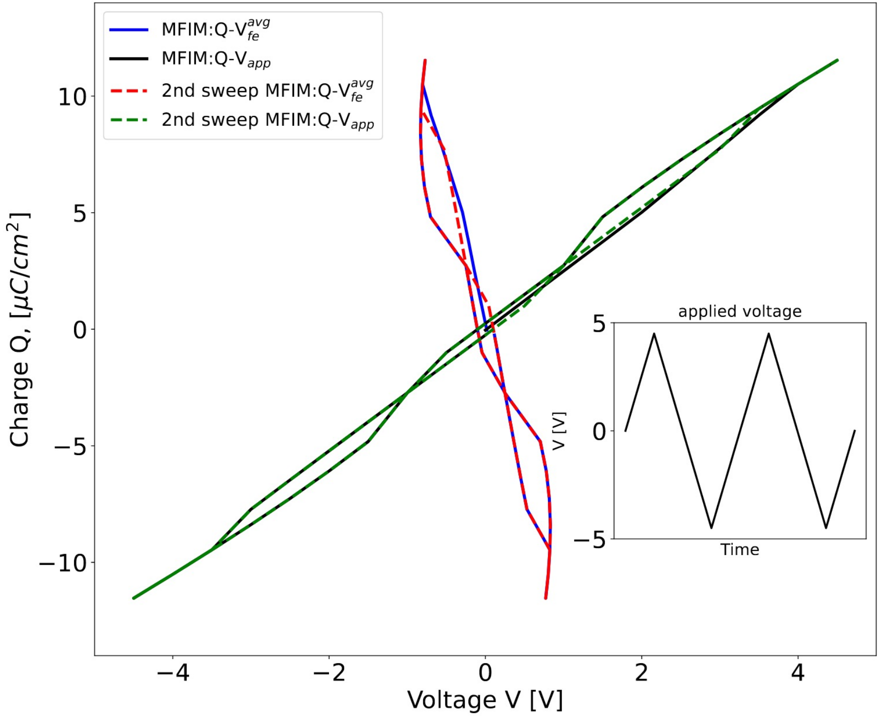




(b) Polarization switching dynamics

Negative capacitance predicted of MFIM stack using the 3D model

Prabhat Kumar
(AMCR)



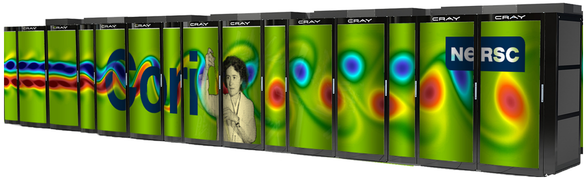
(a) Q-V Characteristics

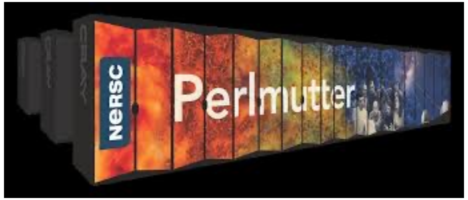
- The slope of Q-V curve indicates the value of the capacitance
- Hysteresis relation observed, indicating the memory feature of ferroelectric materials
- Except for the 1st sweep, repeated sweeps of voltage can generate identical initial states, and thus resulting in repeated Q-V curves.

Overview of ARTEMIS Features

- Portable to different platforms

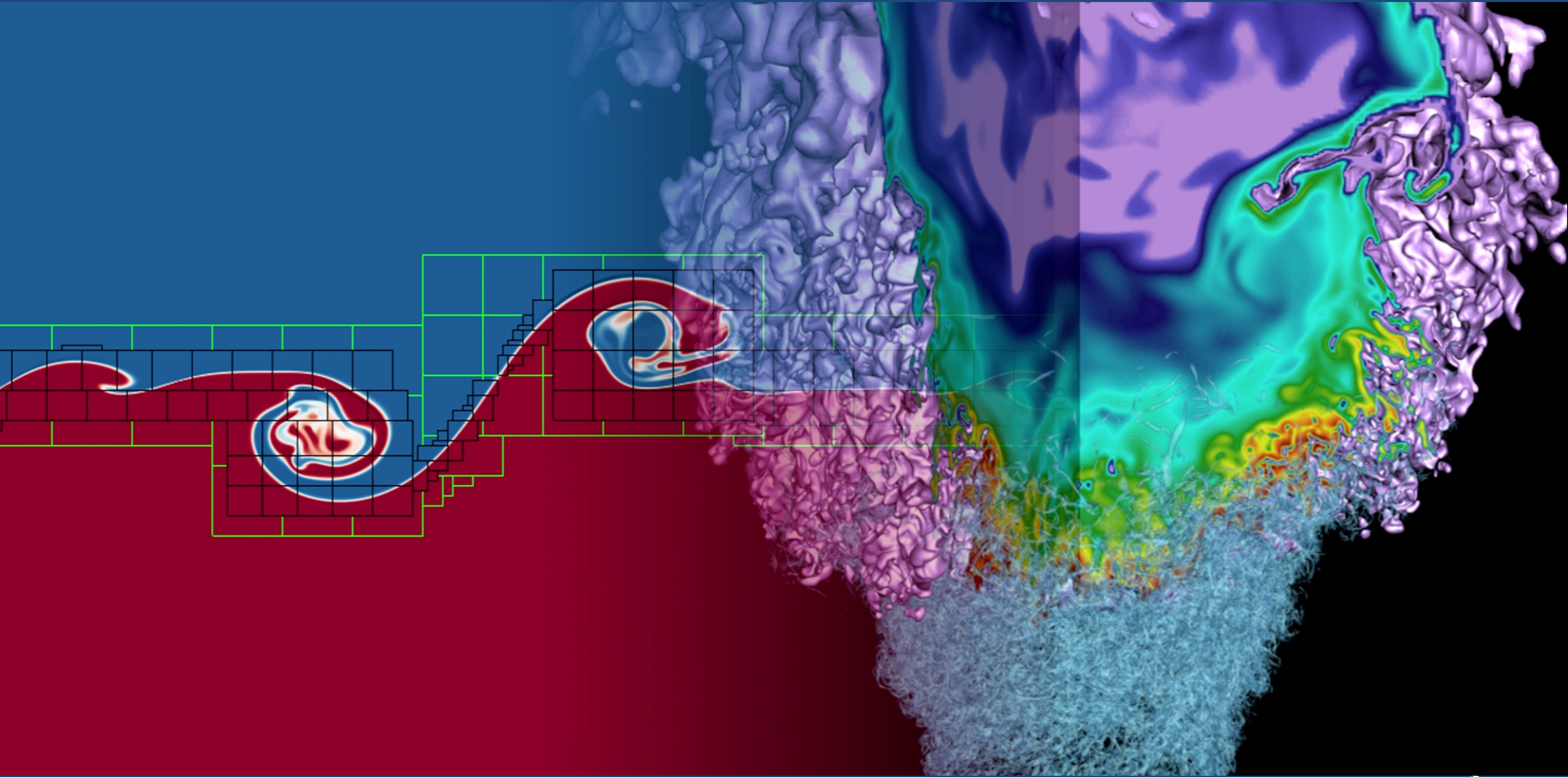
  laptops – leadership class multicore/GPU supercomputers





- Flexible to add “improvised” physical algorithms

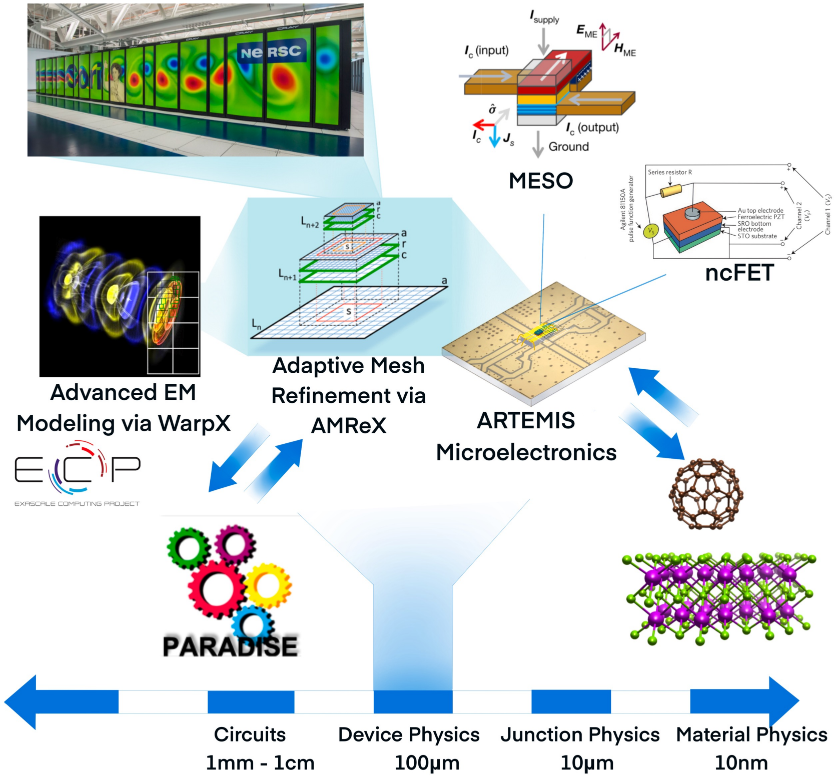
  - Adaptive mesh refinement (AMR) to increase the scale-disparity



Future Works

1. Couple (anti)ferromagnetic and ferroelectric phases for the design of magnetoelectric devices

2. Explore device input/output characteristics for larger-scale circuit design



Thanks to --- AMReX + WarpX + ARTEMIS Team

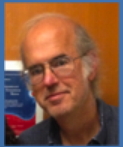
Ann Almgren (AMCR)

Jean-Luc Vay (ATAP)

Axel Huebl (ATAP)

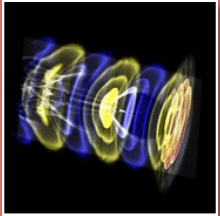
Rémi Lehe (ATAP)

John Bell (AMCR)



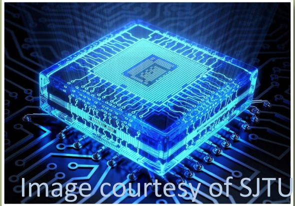
Weiqun Zhang (AMCR)

AMReX



Andrew Nonaka (AMCR)

Zhi (Jackie) Yao (AMCRD)



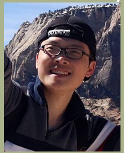
ARTEMIS (Adaptive mesh Refinement Time-domain Elec-trodynaMIcs Solver)

Revathi Jambunathan (AMCR)

Prabhat Kumar (AMCR)

Saurabh Sawant (AMCR)

Yadong Zeng (U. of Minnesota)



Ramamoorthy Ramesh (MSE, UC Berkeley)

Maurice Garcia-Sciveres (Physics, LBL)

DOE Micro-electronics Co-design Program

Sinéad Griffin (Molecular Foundry, LBL)

Quantum chip design

Thank You !

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John Shalf, CRD Computer Science
Ramamoorthy Ramesh, MSE, UC Berkeley
Maurice Garcia-Sciveres, Physics, LBL
Sinéad Griffin, Molecular Foundry, LBL
Jonathan Carter, CS
Peter Nugent, CRD Computational Science
Weiqun Zhang, CRD CCSE
Jean-Luc Vay, ATAP
Rémi Lehe, ATAP
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