



TECH-X
SIMULATIONS EMPOWERING
YOUR INNOVATIONS



Accelerator Computation: Fast, Cheap, and Easy

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Install VSim-11.0.1

- All: Copy VSim11EvalLicense.Exp19Sep2022.txlic
- Windows
 - ◆ Copy the installer, VSim-11.0.1-Win64.exe, to your machine
 - ◆ Run it
 - ◆ Run the application

- Mac
 - ◆ Copy the dmg to your machine and open it
 - ◆ Copy the application bundle to Applications

```
cd /Applications # or wherever one has installed VSim-11
xattr -rd com.apple.quarantine VSim-11.0
```

- ◆ Run the application
- Linux
 - ◆ Copy the tar ball to user local, untar it, and run it

```
tar xf VSim-11.0.1-Linux64.tar.gz
cd VSim-11.0.1
./VSimComposer.sh
```

Licensing

- Open Tools/Preferences→License Settings
- Click Add
- Navigate to USB, open VSim11EvalLicense.Exp19Sep2022.txlic

- Free 6 month licenses available by contacting sales@txcorp.com



Accelerator computation: (p)reproduce what will/did happen in the accelerator

- Charged particles (conventional)
 - ◆ Are generated in plasma sources
 - ◆ Are accelerated in cavities
 - ◆ Are transported through the machine
- Charged particles (plasma, advanced structures)
 - ◆ Are injected into the plasma
 - ◆ Into laser or beam generated plasma structures
 - ◆ Are accelerated
- Accelerator cavities
 - ◆ Oscillate at given frequencies
 - ◆ Heat due to EM absorption, cool by thermal transport
 - ◆ Transfer that heat/energy to the cooling system

Accelerator computation has multiple goals

- **Prediction**
 - ◆ How will this accelerator perform?
- **Diagnosis**
 - ◆ What is making this accelerator work?
- **Discovery**
 - ◆ Can one accelerate particles in plasmas?
 - ◆ What will the generated plasmas do
- **Design**
 - ◆ If we change some parameter, will the accelerator work better?
 - Use less power?
 - Have a lower-emittance beam?



Accelerator computation has moved towards increasing integration

- 60's-90's: Single physics
 - ◆ Tracking
 - ◆ Cavity calculations
 - ◆ Simplified loading calculations
- 90's-10's: Pair combined physics, but typically through files
 - ◆ EM + loading, multipacting
 - ◆ EM + thermal transport
- Future: full accelerator integration



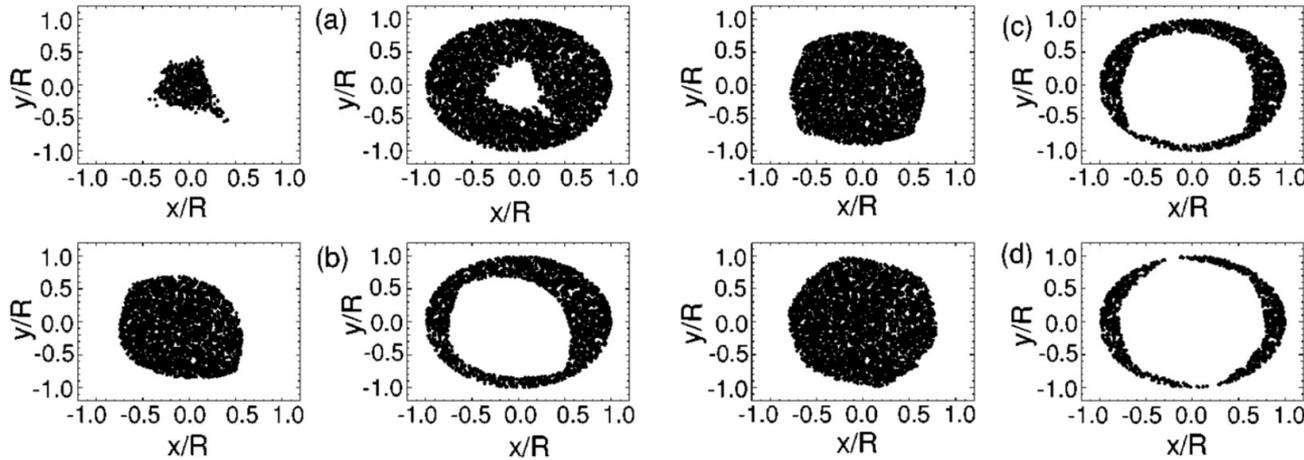
Accelerator modeling 60's-90's: mostly separated physics

- Tracking
 - ◆ Are the single-particle trajectories long-time confined?
 - ◆ At least one for every lab, and some had two (SixTrack+MAD at CERN)
 - ◆ Simple enough (few k lines) that many recreated rather than learn someone else's software
 - ◆ Invariants important! (symplectic integration)
- EM
 - ◆ MAFIA (10.1109/ICCEA.1999.825246)
 - ◆ CST: The interface is important!

PREDICTION

DESIGN

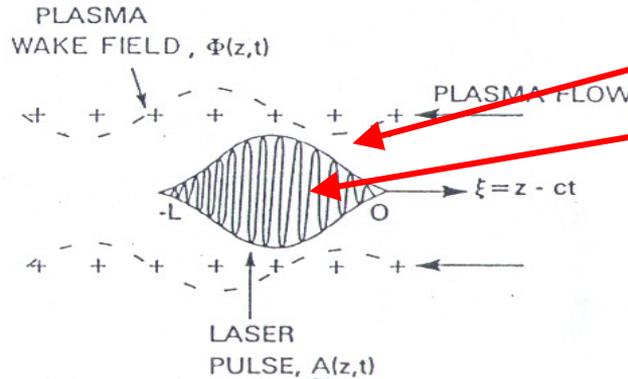
- Tracking shows improved lattices: <https://doi.org/10.1103/PhysRevE.69.056501>



DISCOVERY

The 2000's gave rise to self-consistent, distributed-memory, parallel computing

Motivation: plasma acceleration, 50x disparity causes 2500x computational requirements.



Plasma wavelength ~ group velocity

Laser wavelength

$$\gamma_L \equiv \omega_L / \omega_p$$

$$\gamma_F = 2\gamma_L^2$$

DISCOVERY

Computation used to determine what happened

- Like hitting a brick wall with a cannon ball and seeing a nice, coherent beam come out
- Theorem: uniformly moving wavepacket cannot trap particles (to accelerate them)
- Simulations showed that in initial evolution, the breathing of the pulse due to nonlinear laser-plasma interaction led to particle trapping.

High-quality electron beams from a laser wakefield accelerator using plasma-channel guiding

C. G. R. Geddes^{1,2}, Cs. Toth¹, J. van Tilborg^{1,3}, E. Esarey¹, C. B. Schroeder¹, D. Bruhwiler⁴, C. Nieter⁴, J. Cary^{4,5} & W. P. Leemans¹

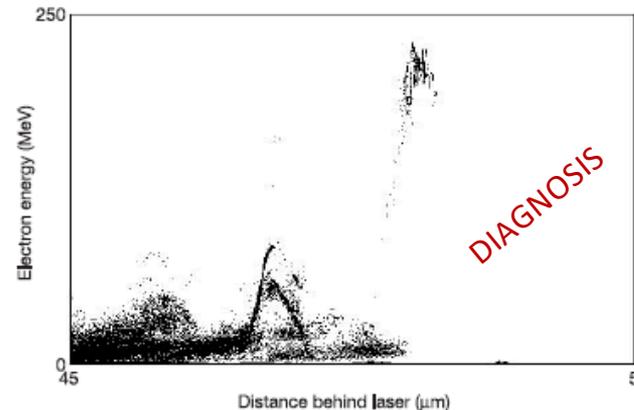
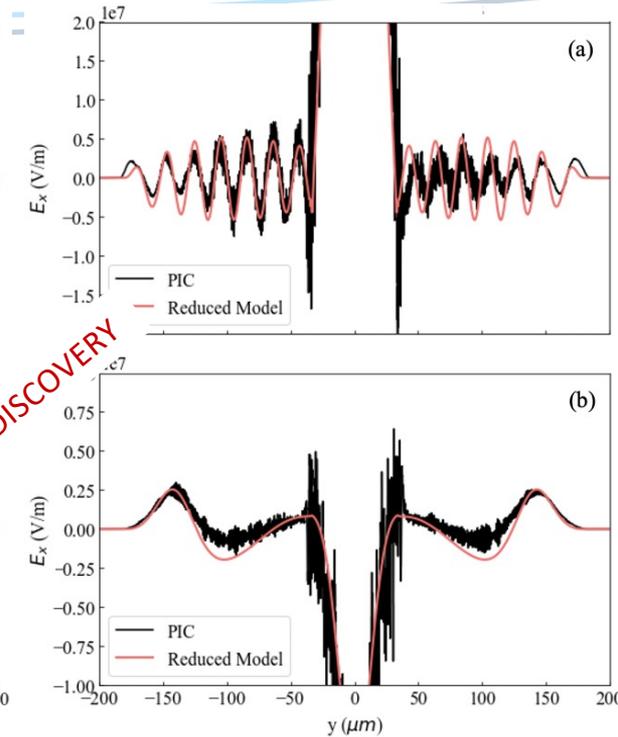
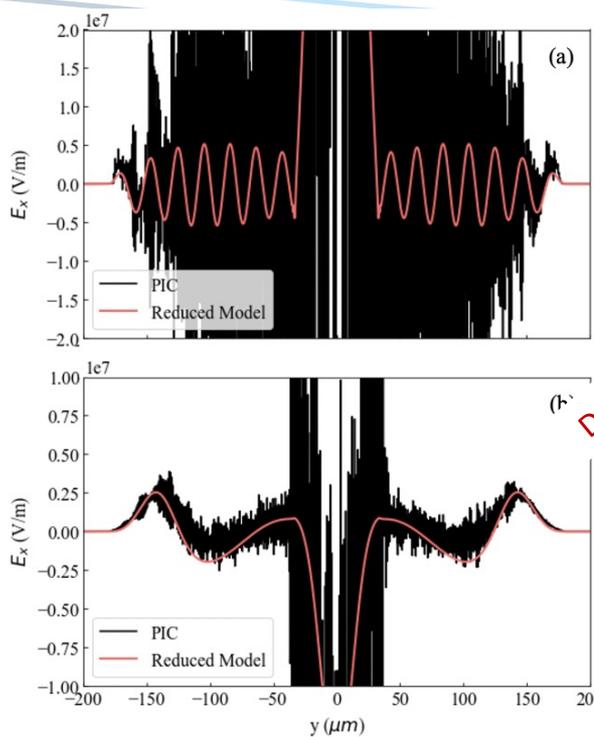
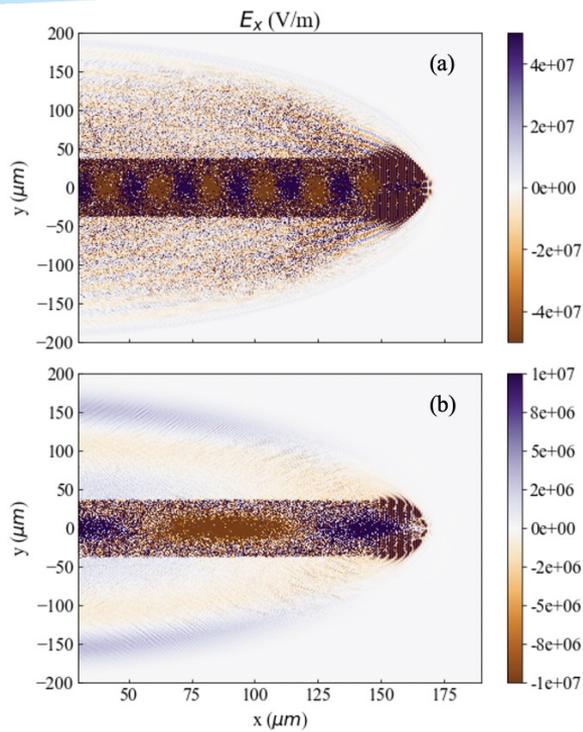


Figure 4 Particle in cell simulations, here displaying the phase space of the electrons, show an energy distribution similar to that in the experiments. A high-quality electron bunch is formed when the acceleration length is matched to the dephasing length, and when the laser strength is such that beam loading is sufficiently strong to turn off injection after the initial bunch of electrons is loaded. The peak energy observed in the simulations is 200 MeV, close to the experimental result.



TECH-X Laser production of plasma leads to Electromagnetic Pulses (EMPs, MOPA 48, Wolfinger)



- May be a diagnostic

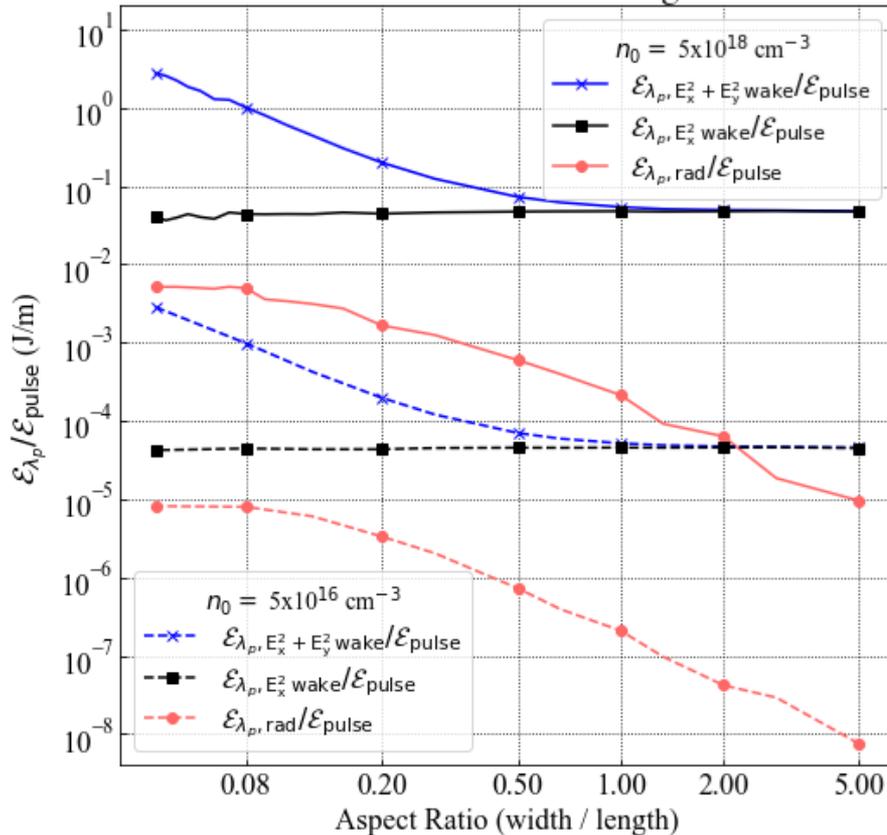
Constant trailing distance averaging pulls out the signal

Computations give behavior over wide range

- Cigars produce EMP, pancakes do not

DISCOVERY

Wakefield and EMP Energies





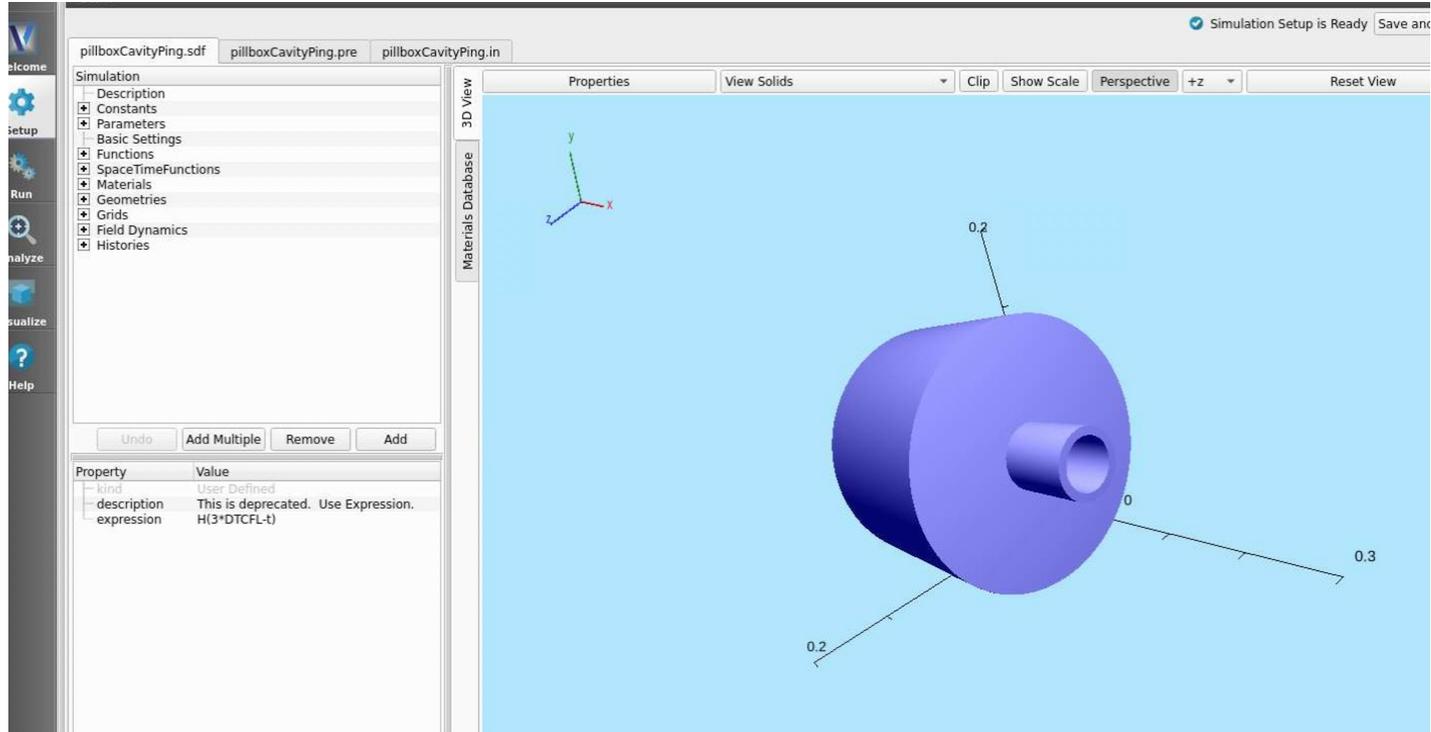
TECH-X Vsim (<https://txcorp.com/vsim/>) self-consistently computes the evolution of charged particles and electromagnetic fields

- Fields evolve according to Maxwell or Poisson
- Particles
 - ◆ Accelerate by interpolated E and B fields
 - ◆ Move
 - ◆ Deposit charge or current to be used as a source in Maxwell or Poisson
- Reactions treated as sub-time-step phenomena
 - ◆ 2-body collisions
 - ◆ decays
 - ◆ 3-body interactions (e.g., recombination)
 - ◆ field ionization
- VSim comes with many documented examples, open Help, external window
- Runs in cloud (demo)

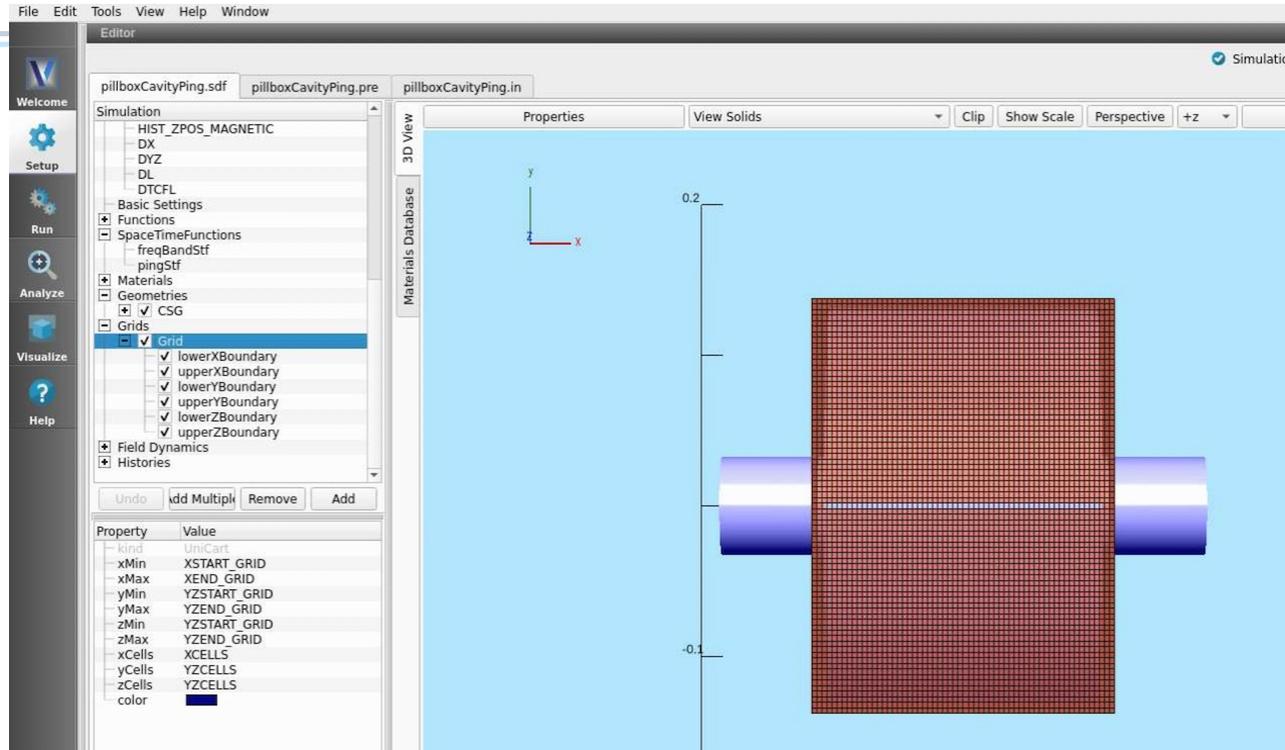
Example: compute the modes of a cavity

- Construct the cavity
 - ◆ CSG: parametric representation
 - ◆ CAD: import from mechanical design
- Excite the cavity
 - ◆ Current block
- Fourier analysis to get basic spectrum
- Selectively excite the cavity
- Filter Diagonalization to get the modes to high accuracy

Construct the cavity out of tubes, hollowing out



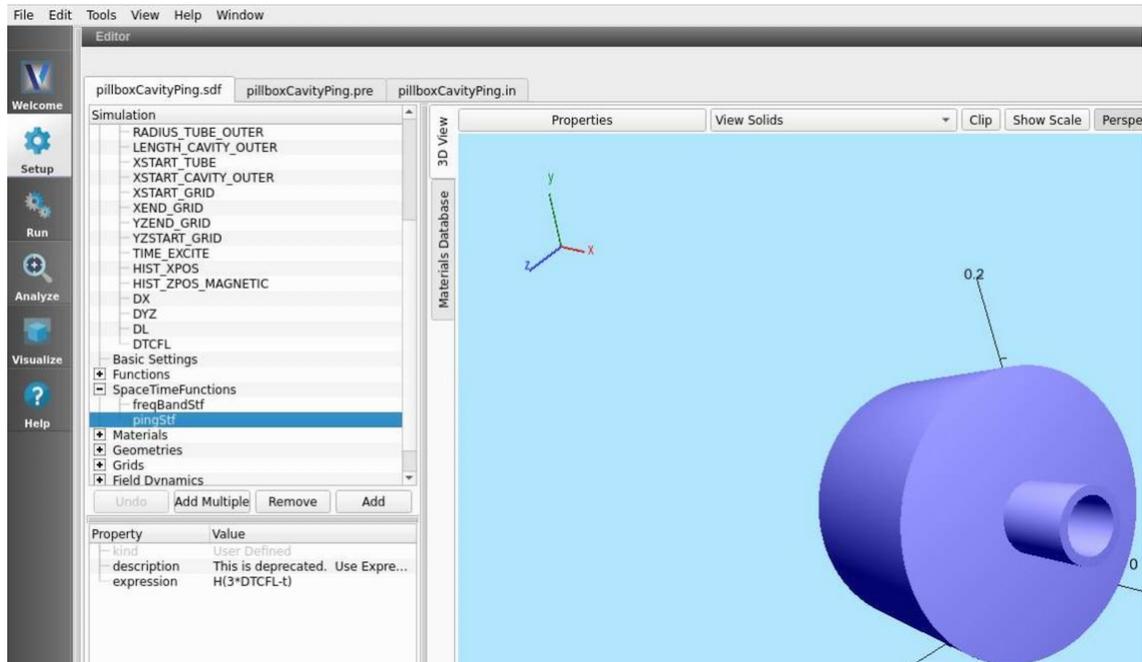
Mesh to accurately represent the system



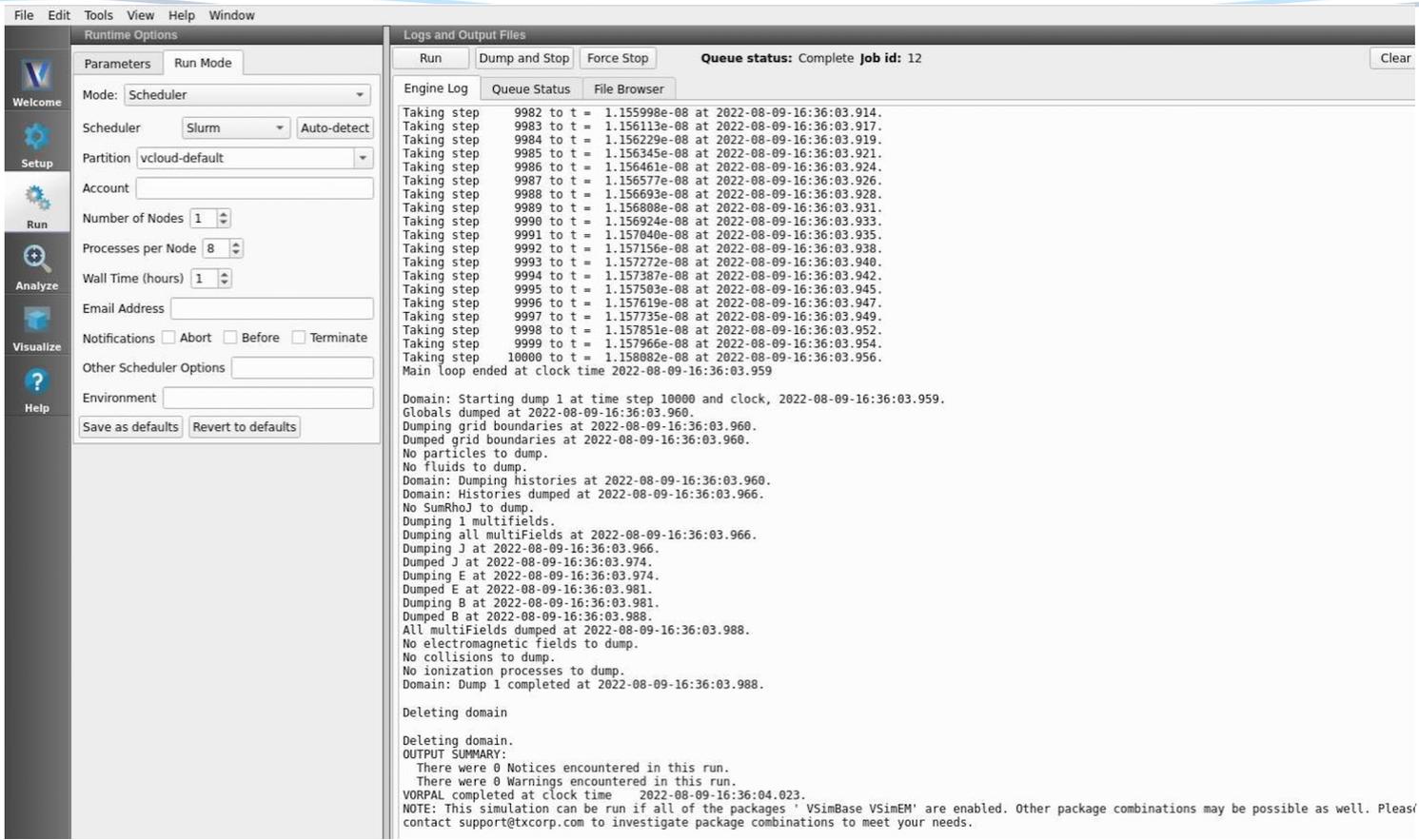
- 2nd order accurate, so 20 cells across give .25% accuracy

Create a temporal ping for exciting the cavity

- Add appropriate variables
- Use Heaviside function



- Choose
 - ◆ Number of steps
 - ◆ Parallel
 - ◆ through scheduler
- Hit Run



The screenshot shows the software interface with the following components:

- Runtime Options Panel:**
 - Mode: Scheduler
 - Scheduler: Slurm (Auto-detect)
 - Partition: vcloud-default
 - Account: [Empty]
 - Number of Nodes: 1
 - Processes per Node: 8
 - Wall Time (hours): 1
 - Email Address: [Empty]
 - Notifications: Abort Before Terminate
 - Other Scheduler Options: [Empty]
 - Environment: [Empty]
 - Buttons: Save as defaults, Revert to defaults
- Logs and Output Files Panel:**
 - Buttons: Run, Dump and Stop, Force Stop
 - Queue status: Complete Job id: 12
 - Engine Log, Queue Status, File Browser tabs
 - Log content:


```

          Taking step 9982 to t = 1.155998e-08 at 2022-08-09-16:36:03.914.
          Taking step 9983 to t = 1.156113e-08 at 2022-08-09-16:36:03.917.
          Taking step 9984 to t = 1.156229e-08 at 2022-08-09-16:36:03.919.
          Taking step 9985 to t = 1.156345e-08 at 2022-08-09-16:36:03.921.
          Taking step 9986 to t = 1.156461e-08 at 2022-08-09-16:36:03.924.
          Taking step 9987 to t = 1.156577e-08 at 2022-08-09-16:36:03.926.
          Taking step 9988 to t = 1.156693e-08 at 2022-08-09-16:36:03.928.
          Taking step 9989 to t = 1.156808e-08 at 2022-08-09-16:36:03.931.
          Taking step 9990 to t = 1.156924e-08 at 2022-08-09-16:36:03.933.
          Taking step 9991 to t = 1.157040e-08 at 2022-08-09-16:36:03.935.
          Taking step 9992 to t = 1.157156e-08 at 2022-08-09-16:36:03.938.
          Taking step 9993 to t = 1.157272e-08 at 2022-08-09-16:36:03.940.
          Taking step 9994 to t = 1.157387e-08 at 2022-08-09-16:36:03.942.
          Taking step 9995 to t = 1.157503e-08 at 2022-08-09-16:36:03.945.
          Taking step 9996 to t = 1.157619e-08 at 2022-08-09-16:36:03.947.
          Taking step 9997 to t = 1.157735e-08 at 2022-08-09-16:36:03.949.
          Taking step 9998 to t = 1.157851e-08 at 2022-08-09-16:36:03.952.
          Taking step 9999 to t = 1.157966e-08 at 2022-08-09-16:36:03.954.
          Taking step 10000 to t = 1.158082e-08 at 2022-08-09-16:36:03.956.
          Main loop ended at clock time 2022-08-09-16:36:03.959

          Domain: Starting dump 1 at time step 10000 and clock, 2022-08-09-16:36:03.959.
          Globals dumped at 2022-08-09-16:36:03.960.
          Dumping grid boundaries at 2022-08-09-16:36:03.960.
          Dumped grid boundaries at 2022-08-09-16:36:03.960.
          No particles to dump.
          No fluids to dump.
          Domain: Dumping histories at 2022-08-09-16:36:03.960.
          Domain: Histories dumped at 2022-08-09-16:36:03.966.
          No SumRhodJ to dump.
          Dumping I multifiFields.
          Dumping all multifiFields at 2022-08-09-16:36:03.966.
          Dumping J at 2022-08-09-16:36:03.966.
          Dumped J at 2022-08-09-16:36:03.974.
          Dumping E at 2022-08-09-16:36:03.974.
          Dumped E at 2022-08-09-16:36:03.981.
          Dumping B at 2022-08-09-16:36:03.981.
          Dumped B at 2022-08-09-16:36:03.988.
          ALL multifiFields dumped at 2022-08-09-16:36:03.988.
          No electromagnetic fields to dump.
          No collisions to dump.
          No ionization processes to dump.
          Domain: Dump 1 completed at 2022-08-09-16:36:03.988.

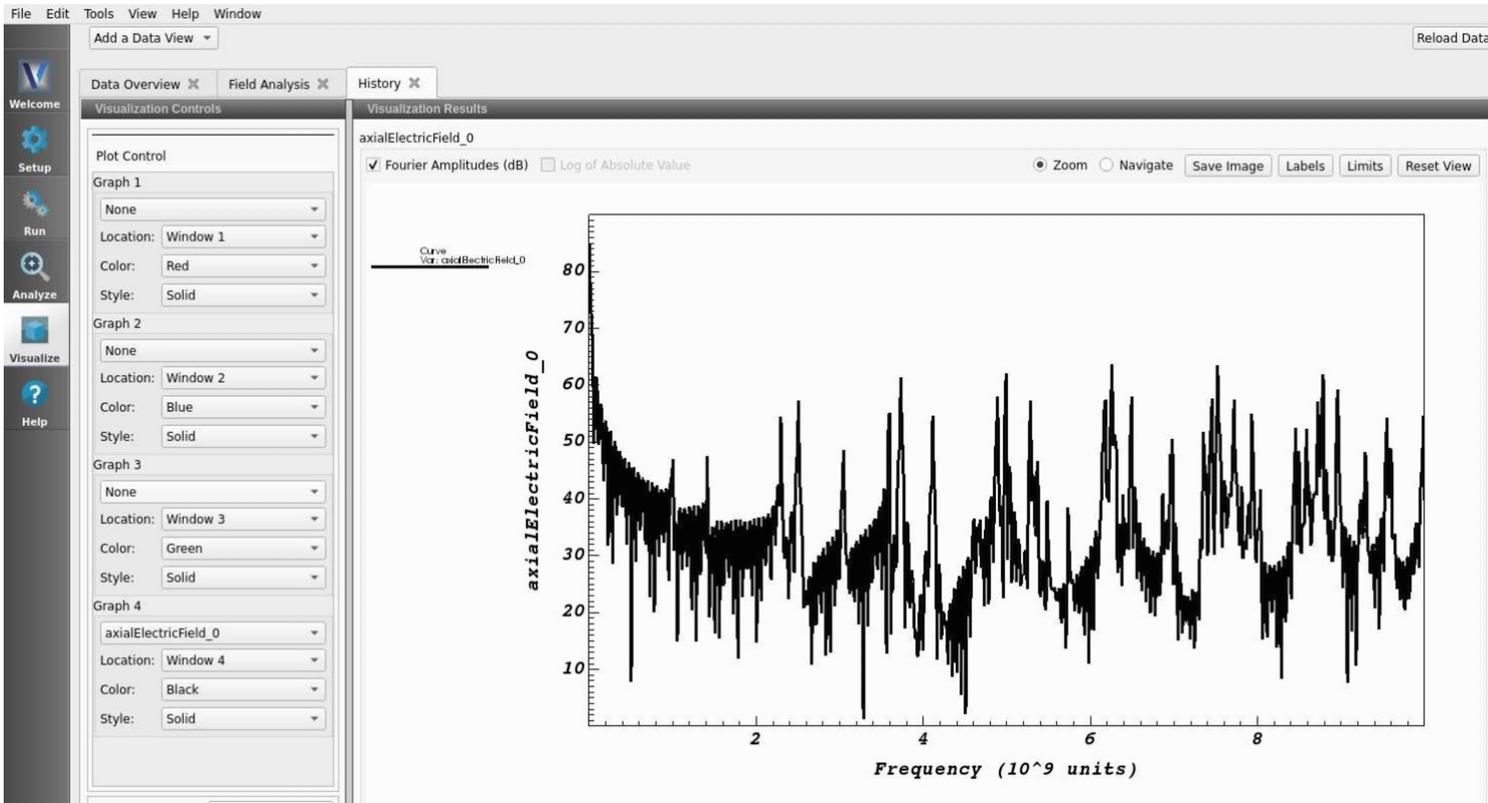
          Deleting domain

          Deleting domain.
          OUTPUT SUMMARY:
          There were 0 Notices encountered in this run.
          There were 0 Warnings encountered in this run.
          VORPAL completed at clock time 2022-08-09-16:36:04.023.
          NOTE: This simulation can be run if all of the packages ' VSimBase VSimEM' are enabled. Other package combinations may be possible as well. Please
          contact support@txcorp.com to investigate package combinations to meet your needs.
          
```



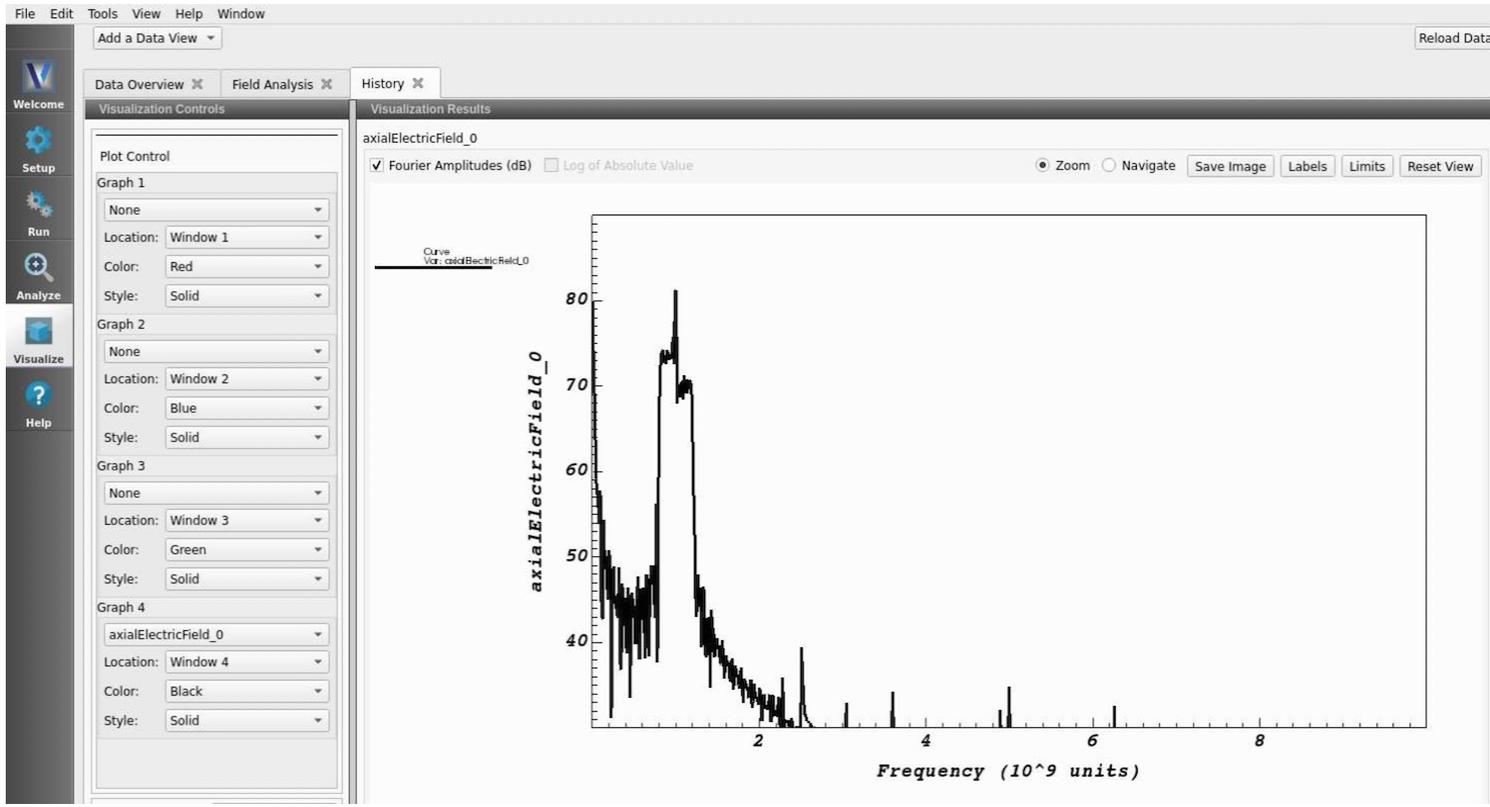
Visualize history

- 50k steps
- Fourier transform



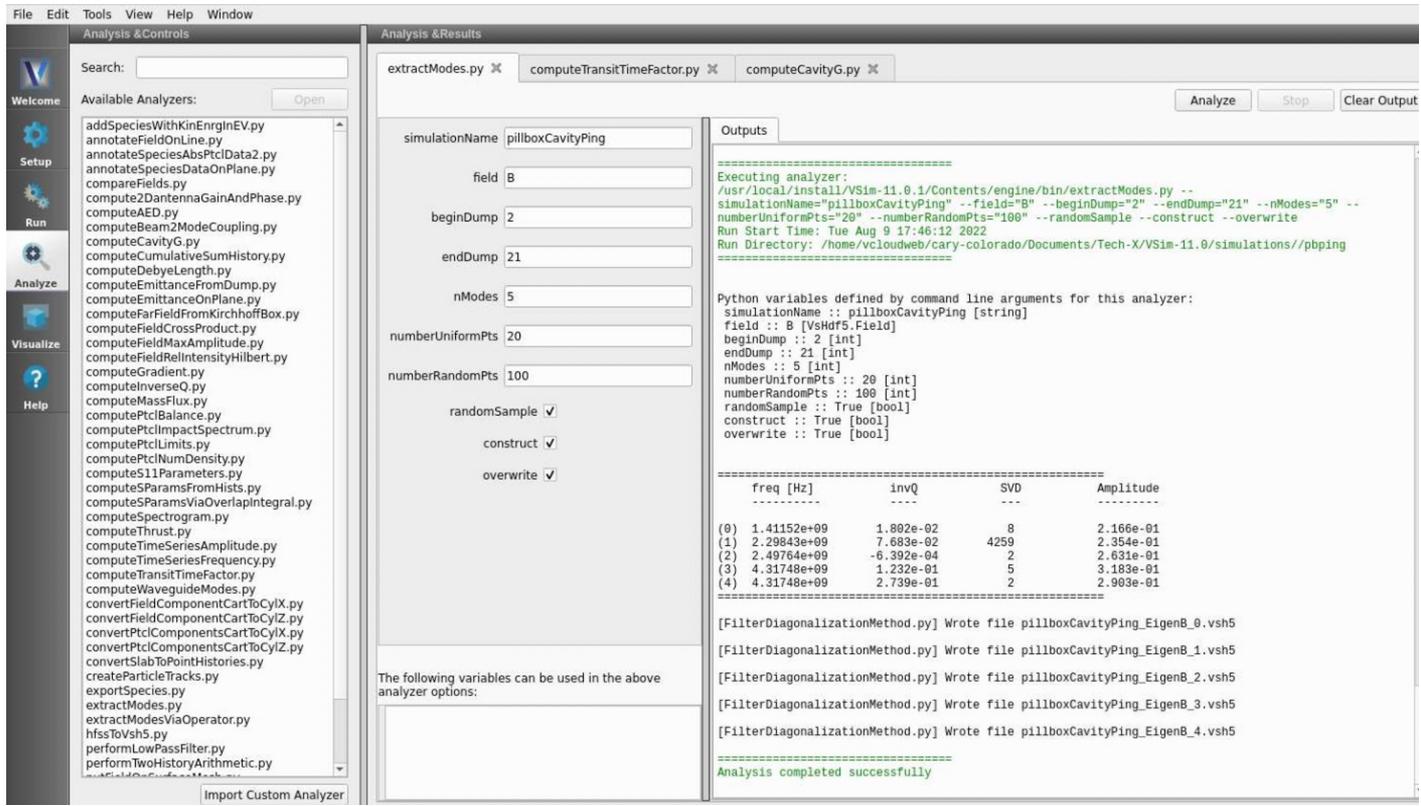
Excite the cavity over a range of frequencies

- Use freqBandStf
- 0.8-1.2 GHz



Use extractModes to get frequency to high accuracy

- An SVD fit to a number of sinusoids



The screenshot shows the Analysis & Controls software interface. The left sidebar contains navigation buttons for Welcome, Setup, Run, Analyze, Visualize, and Help. The main window is divided into two panes: Analysis & Controls and Analysis & Results.

Analysis & Controls Pane:

- Search: []
- Available Analyzers: [Open]
- List of analyzers including:
 - addSpeciesWithKinEngrInEV.py
 - compute2DantennaGainAndPhase.py
 - computeCavityG.py
 - extractModes.py
 - extractModesViaOperator.py

Analysis & Results Pane:

- Open tabs: extractModes.py, computeTransitTimeFactor.py, computeCavityG.py
- Buttons: Analyze, Stop, Clear Output
- simulationName: pillboxCavityPing
- field: B
- beginDump: 2
- endDump: 21
- nModes: 5
- numberUniformPts: 20
- numberRandomPts: 100
- randomSample:
- construct:
- overwrite:

Outputs Pane:

```

Executing analyzer:
/usr/local/install/VSim-11.0.1/Contents/engine/bin/extractModes.py --
simulationName="pillboxCavityPing" --field="B" --beginDump="2" --endDump="21" --nModes="5" --
numberUniformPts="20" --numberRandomPts="100" --randomSample --construct --overwrite
Run Start Time: Tue Aug 9 17:46:12 2022
Run Directory: /home/vcloudweb/cary-colorado/Documents/Tech-X/VSim-11.0/simulations/pbping
  
```

Python variables defined by command line arguments for this analyzer:

```

simulationName :: pillboxCavityPing [string]
field :: B [Vshd5.Field]
beginDump :: 2 [int]
endDump :: 21 [int]
nModes :: 5 [int]
numberUniformPts :: 20 [int]
numberRandomPts :: 100 [int]
randomSample :: True [bool]
construct :: True [bool]
overwrite :: True [bool]
  
```

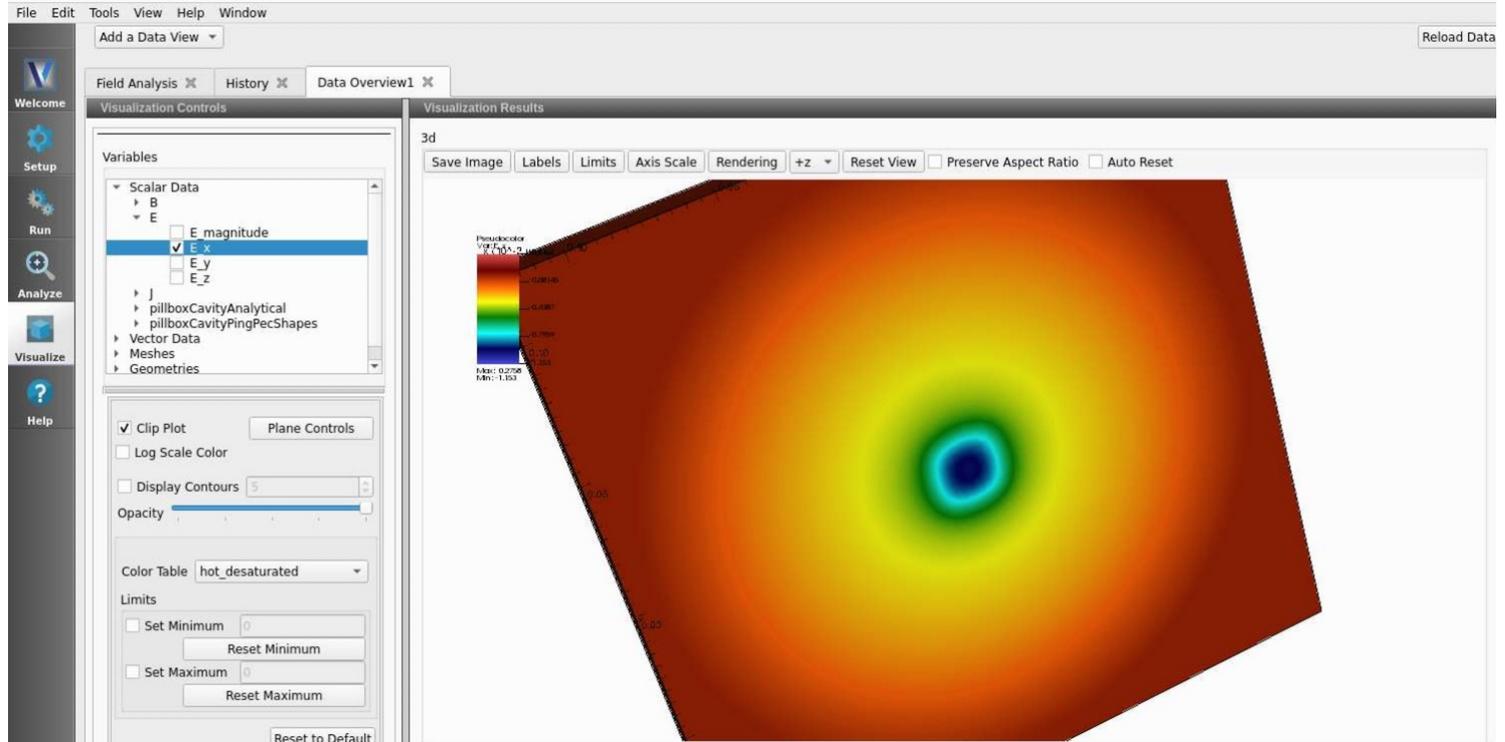
	freq [Hz]	invQ	SVD	Amplitude
(0)	1.41152e+09	1.802e-02	8	2.166e-01
(1)	2.29843e+09	7.683e-02	4259	2.354e-01
(2)	2.49764e+09	-6.392e-04	2	2.631e-01
(3)	4.31748e+09	1.232e-01	5	3.183e-01
(4)	4.31748e+09	2.739e-01	2	2.903e-01

The following variables can be used in the above analyzer options:

```

[FilterDiagonalizationMethod.py] Wrote file pillboxCavityPing_EigenB_0.vsh5
[FilterDiagonalizationMethod.py] Wrote file pillboxCavityPing_EigenB_1.vsh5
[FilterDiagonalizationMethod.py] Wrote file pillboxCavityPing_EigenB_2.vsh5
[FilterDiagonalizationMethod.py] Wrote file pillboxCavityPing_EigenB_3.vsh5
[FilterDiagonalizationMethod.py] Wrote file pillboxCavityPing_EigenB_4.vsh5
Analysis completed successfully
  
```

See modes in the viz panel



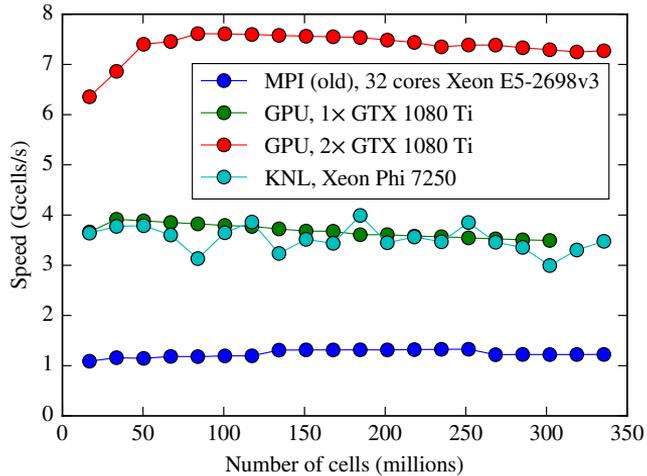


**Some things to think about moving forward
(what I am excited about)**

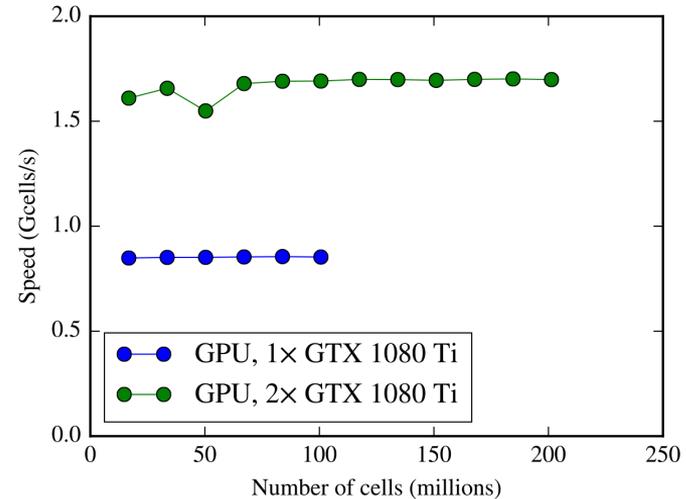
Heterogeneous Computing
Algorithms
Increasing integration



Proper restructuring shows near-perfect scaling

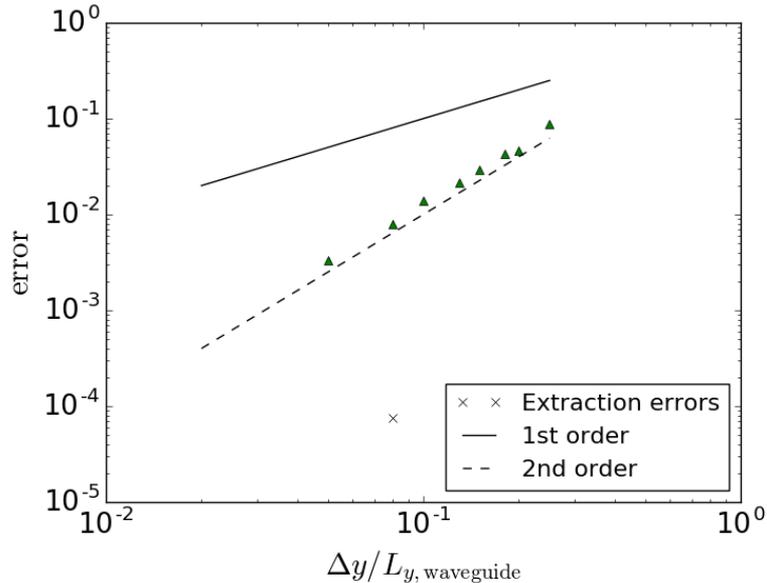


Vacuum FDTD updater



Cut-cell dielectric updater
(applied everywhere)

Algorithms: second-order dielectric updaters



- ACHIP
- THz at FLASHForward
- Dielectric lined wakefield accelerators
- BELLA Dielectric kicker

G. R. Werner and J. R. Cary, "A Stable FDTD Algorithm for Non-diagonal, Anisotropic Dielectrics," *J. Comp. Phys.* **226**, 1085-1101 (2007), doi:10.1016/j.jcp.2007.05.008.

Bauer, Carl A., Gregory R. Werner, and John R. Cary. "A second-order 3D electromagnetics algorithm for curved interfaces between anisotropic dielectrics on a Yee mesh." *Journal of Computational Physics* 230.5 (2011): 2060-2075.



Algorithms: structure-preserving particle pushes

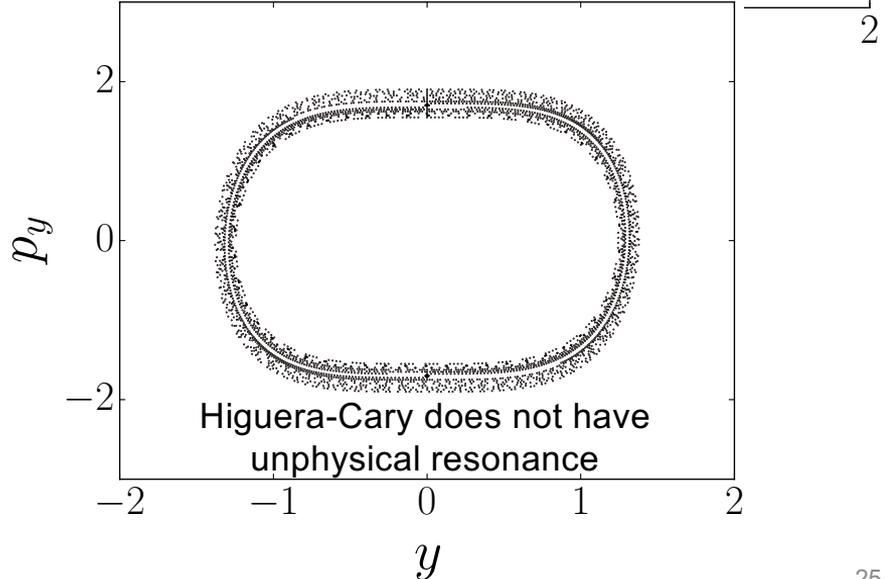
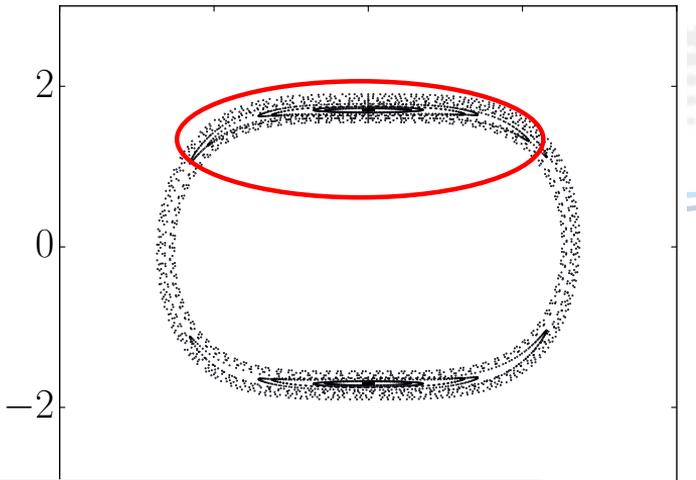
Structure-preserving second-order integration of relativistic charged particle trajectories in electromagnetic fields

A.V. Higuera* and John R. Cary†
*University of Colorado at Boulder and
Tech-X Corporation*

Time-centered, hence second-order, methods for integrating the relativistic momentum of charged particles in an electromagnetic field are derived. A new method is found by averaging the momentum before use in the magnetic rotation term, and an implementation is presented that differs from the

- Accelerators long known about importance of symplectic integration
- Symplectic not known for simulation, where one does not have easy access to potentials
- Next best: preserve the last Liouville invariant (phase-space volume): Higuera-Cary push.
- Eliminates unphysical resonance

p_y



To become a computational accelerator physicist

- Talk for students
- About the **use** of simulations, **not** the generation of simulation codes, **not** the development of algorithms, **not** the development of solvers or infrastructure
- We will do simulations here in class
- You will see examples of what can be good about simulation
- You will see what can go wrong

Computer scientists
are here

Infrastructure, e.g.,
MPI

Applied Mathematicians
are here

Applied Math, e.g.,
Linear solvers

Computation application
developers are here

Physics-based
algorithms, e.g., PIC

Physics code
development and
integration

Discovery, design are
here

Use of simulations

- Computational accelerator physics has evolved
- FAST: Use of parallelism and device based computing
- CHEAP: Cloud allows a single instance of the code to serve many users
- EASY: GUIs make computing intuitive