

Accelerator Computation: Fast, Cheap, and Easy

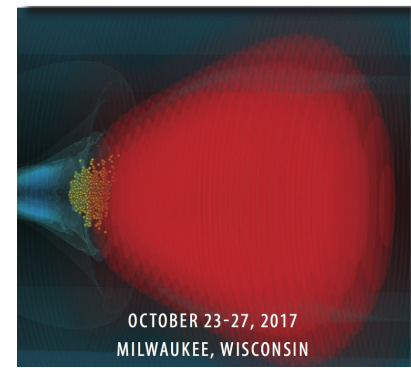
JOHN R CARY

TECH-X, U. COLORADO BOULDER

AUGUST 10, 2020

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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

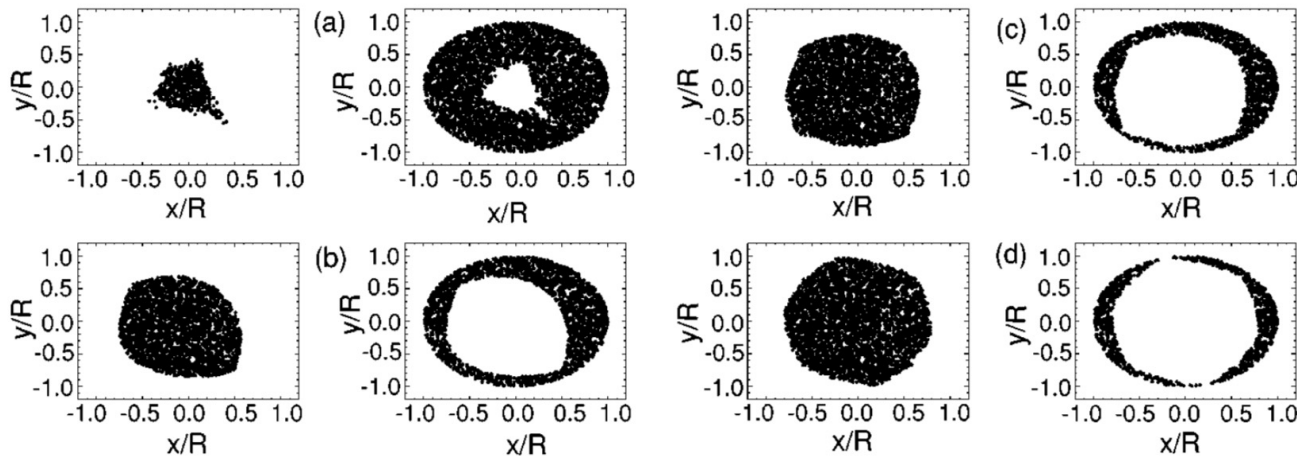
- Tracking
 - ◆ Are the single-particle trajectories long-time confined?
 - ◆ At least one for every lab, and some had two (SixTrack+MAD at CERN)
 - ◆ Simple enough (few k lines) that many recreated rather than learn someone else's software
 - ◆ Invariants important! (symplectic integration)
- EM
 -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

PREDICTION

DESIGN

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

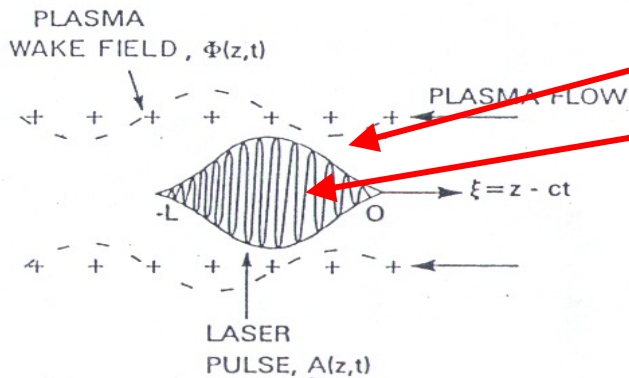
- Tracking shows improved lattices: <https://doi.org/10.1103/PhysRevE.69.056501>



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

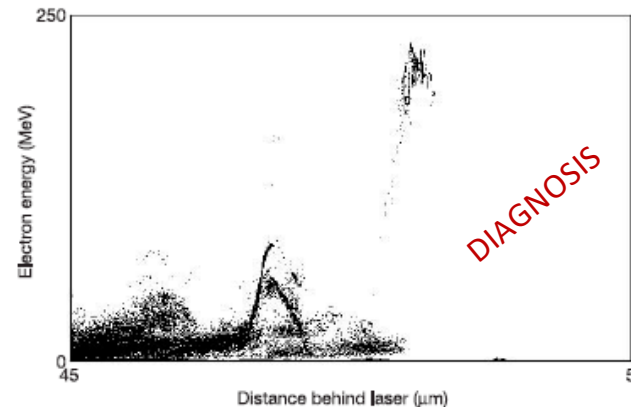
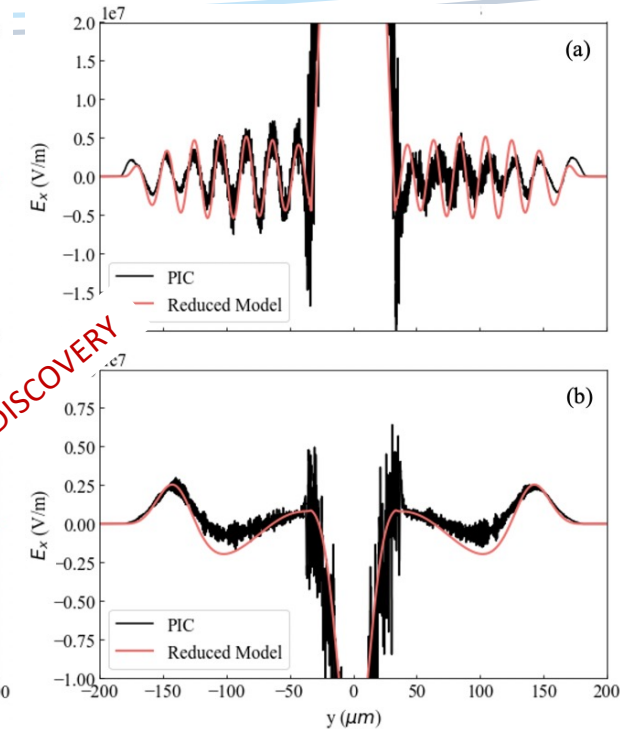
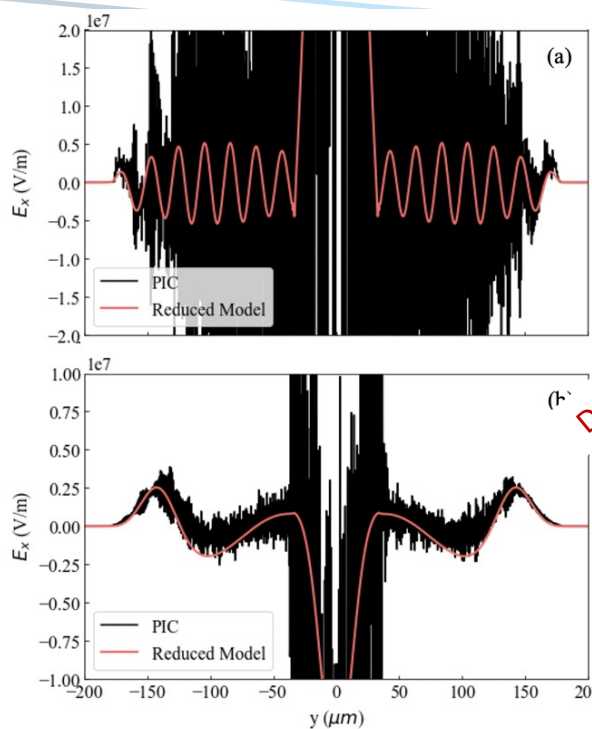
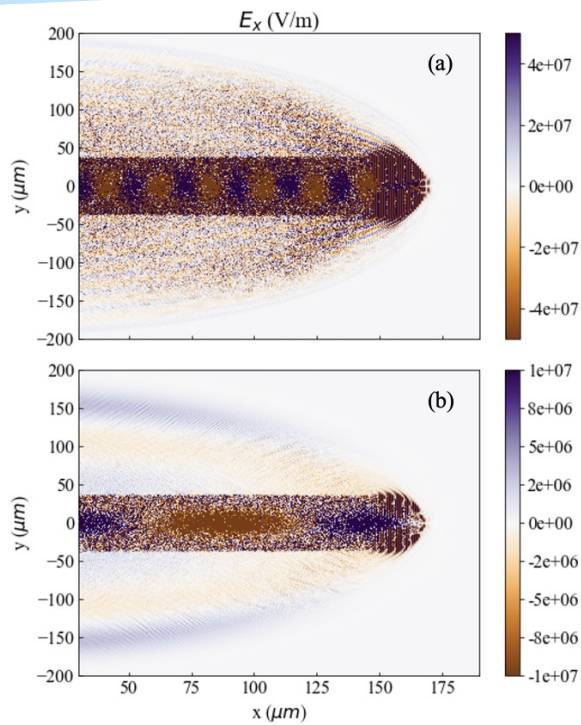


Figure 4 Particle in cell simulations, here displaying the phase space of the electrons, show an energy distribution similar to that in the experiments. A high-quality electron bunch is formed when the acceleration length is matched to the dephasing length, and when the laser strength is such that beam 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)



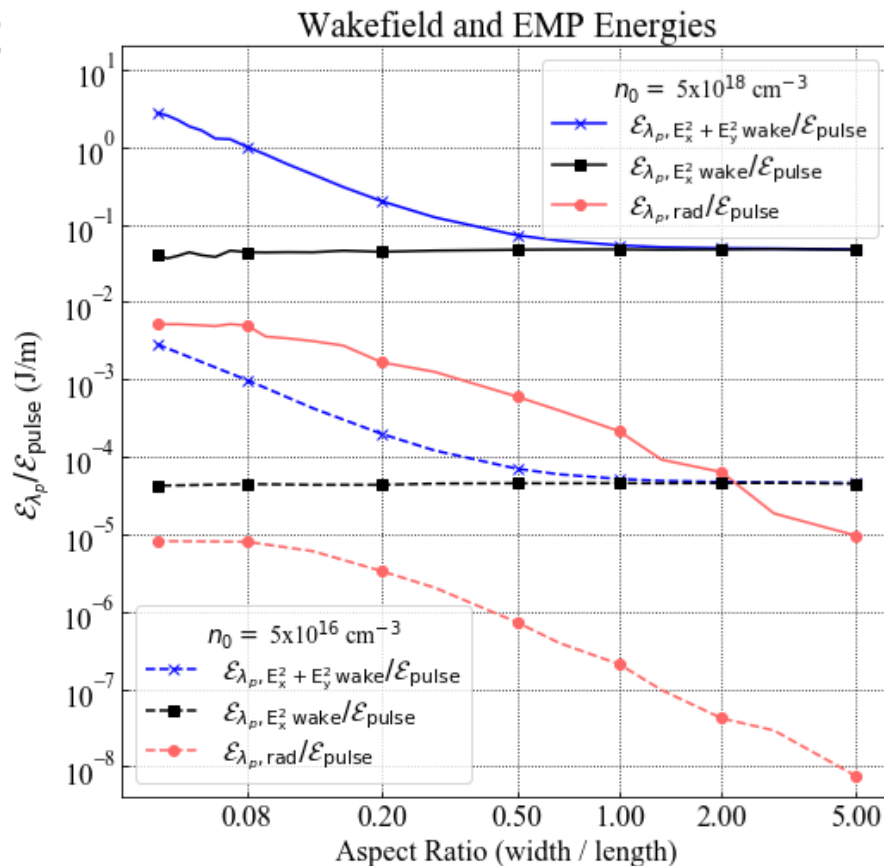
• May be a diagnostic

Constant trailing distance averaging pulls out the signal

Computations give behavior over wide range

- Cigars produce EMP, pancakes do not

DISCOVERY





TECH-X

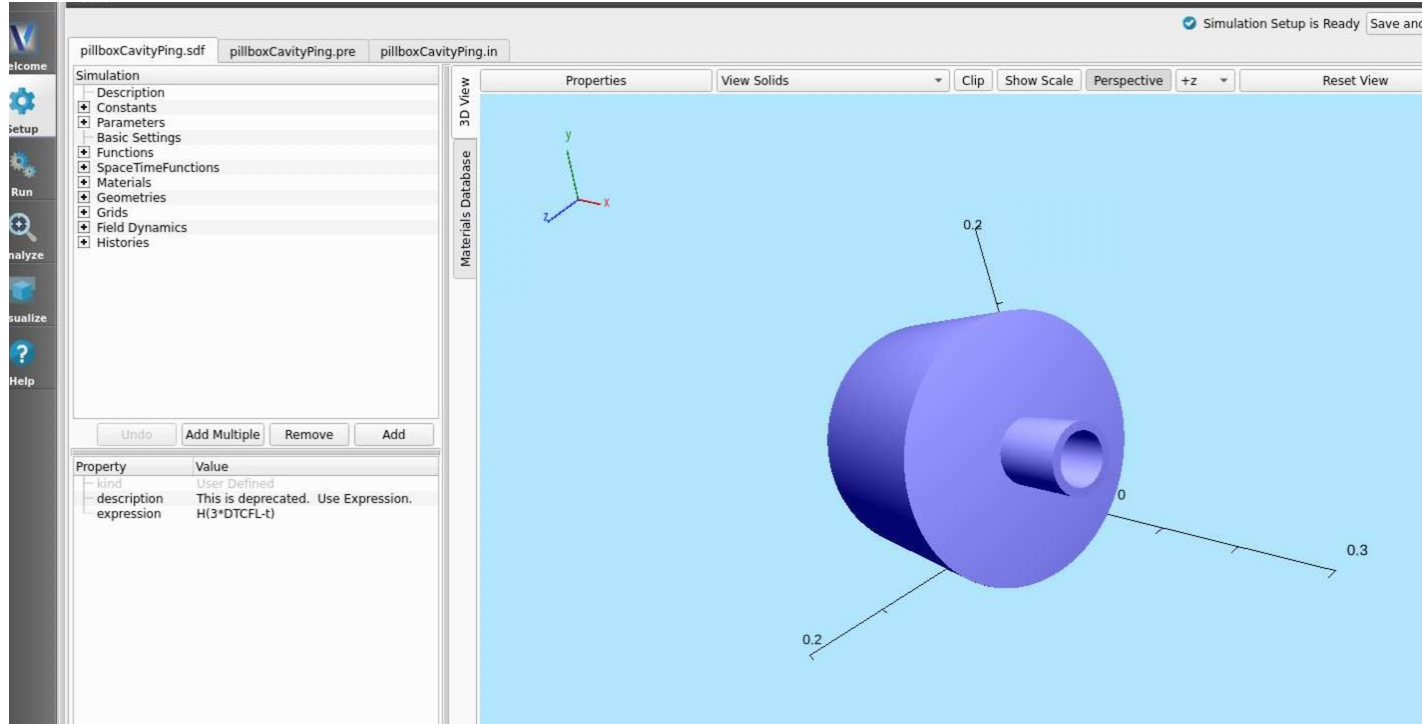
Vsim (<https://txcorp.com/vsim/>) self-consistently computes the evolution of charged particles and electromagnetic fields

- 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)

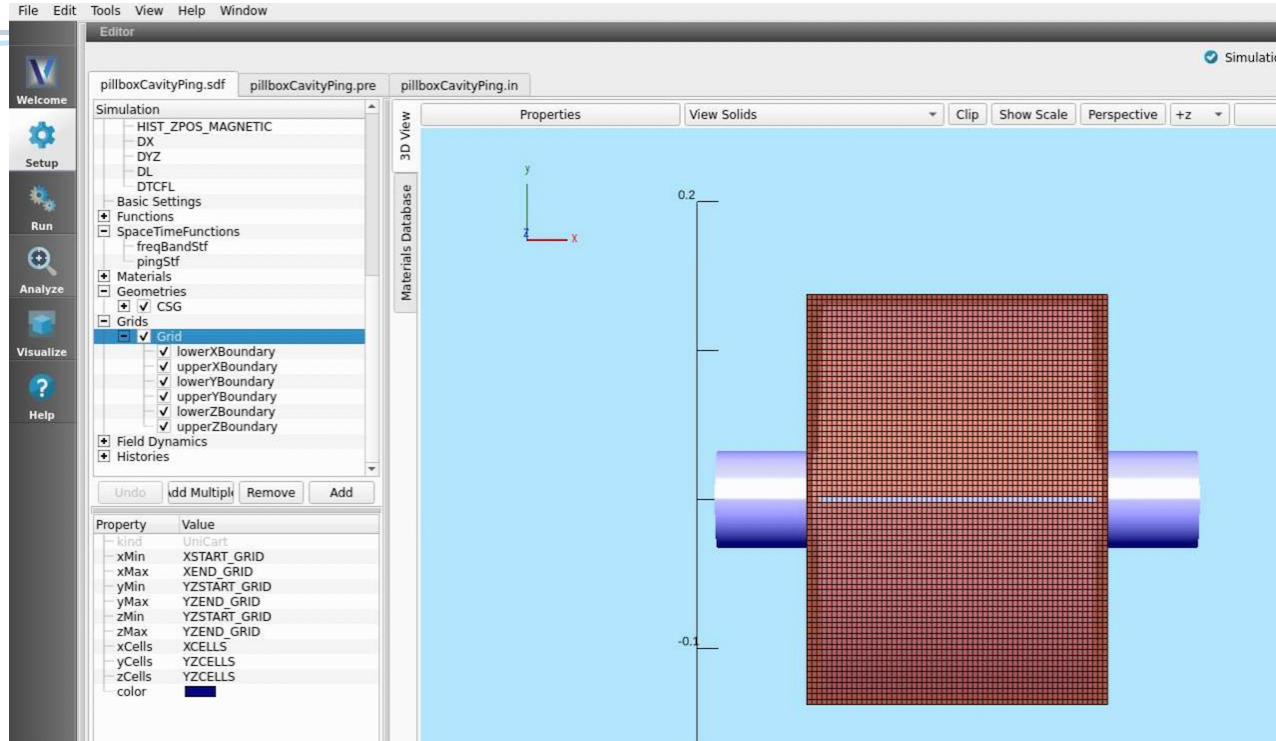
Example: compute the modes of a cavity

- 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



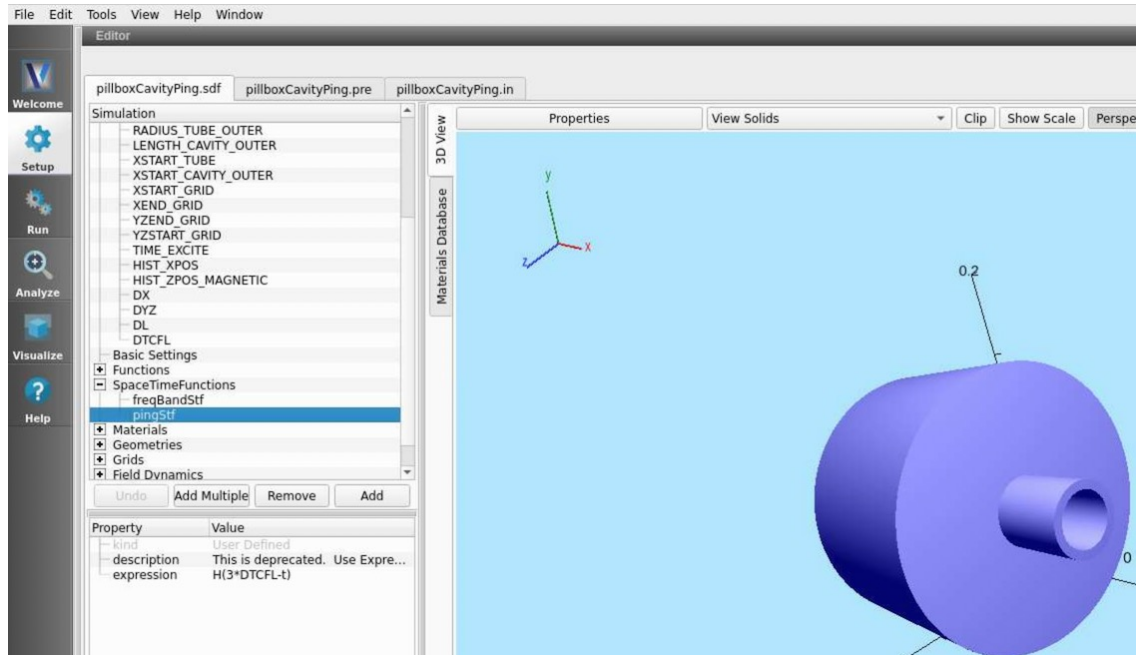
Mesh to accurately represent the system



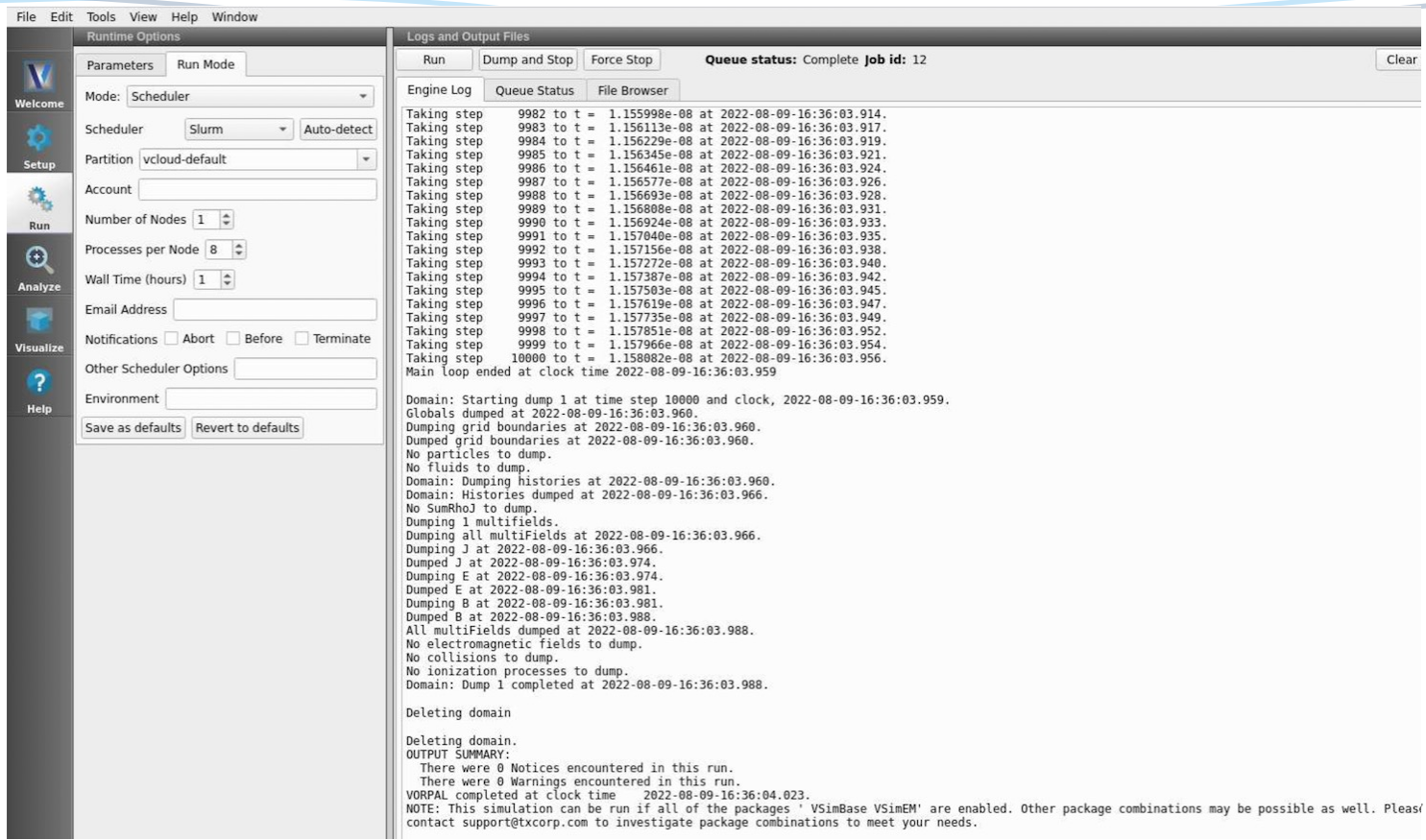
- 2nd order accurate, so 20 cells across give .25% accuracy

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 VORPAL simulation runtime interface. The left sidebar contains navigation buttons: Welcome, Setup, Run, Analyze, Visualize, and Help. The main window is divided into two panes. The left pane, titled 'Runtime Options', has tabs for 'Parameters' and 'Run Mode'. Under 'Parameters', the 'Mode' is set to 'Scheduler'. Below this, there are fields for 'Scheduler' (set to 'Slurm'), 'Partition' (set to 'vcloud-default'), 'Account' (empty), 'Number of Nodes' (set to 1), 'Processes per Node' (set to 8), 'Wall Time (hours)' (set to 1), 'Email Address' (empty), 'Notifications' (with checkboxes for 'Abort', 'Before', and 'Terminate'), 'Other Scheduler Options' (empty), 'Environment' (empty), and buttons for 'Save as defaults' and 'Revert to defaults'. The right pane, titled 'Logs and Output Files', has tabs for 'Run', 'Dump and Stop', and 'Force Stop'. The 'Run' tab is active, showing a table with columns 'Engine Log', 'Queue Status', and 'File Browser'. The table lists simulation steps from 9982 to 10000, each with a timestamp. Below the table, the 'Queue status' is 'Complete' and 'Job id' is '12'. The bottom of the right pane shows a log of simulation output, including domain starting, dumping grid boundaries, dumping histories, dumping all multifields, dumping J, E, B, and B at various times, dumping all multifields, dumping electromagnetic fields, collisions, and ionization processes, and finally deleting the domain.

File Edit Tools View Help Window

Runtime Options

Parameters Run Mode

Mode: Scheduler

Scheduler Slurm Auto-detect

Partition vcloud-default

Account

Number of Nodes 1

Processes per Node 8

Wall Time (hours) 1

Email Address

Notifications ☐ Abort ☐ Before ☐ Terminate

Other Scheduler Options

Environment

Save as defaults Revert to defaults

Logs and Output Files

Run Dump and Stop Force Stop Queue status: Complete Job id: 12 Clear

Engine Log Queue Status File Browser

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.

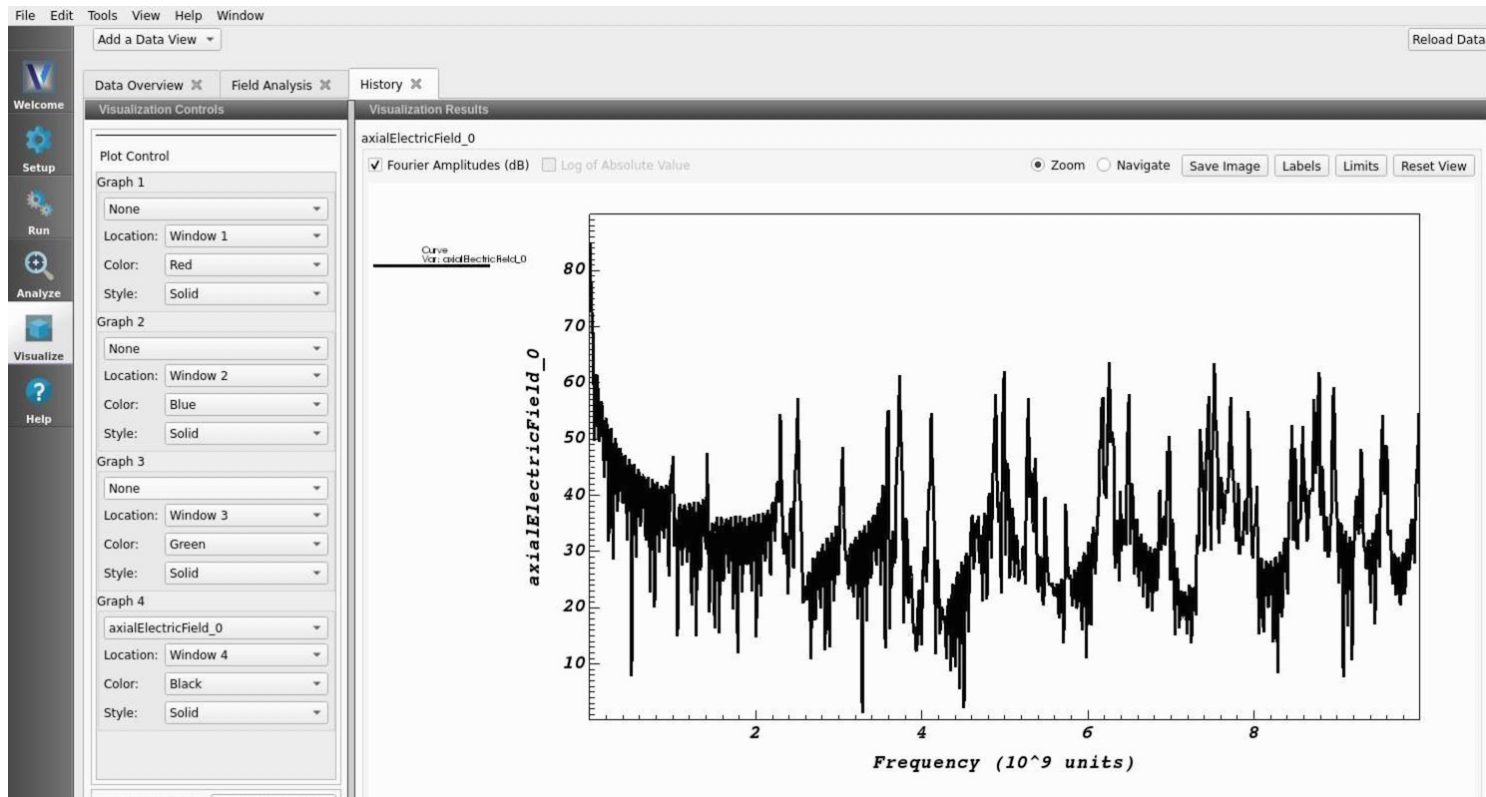
Domain: Starting dump 1 at time step 10000 and clock, 2022-08-09-16:36:03.959.
 Globals dumped at 2022-08-09-16:36:03.960.
 Dumping grid boundaries at 2022-08-09-16:36:03.960.
 Dumped grid boundaries at 2022-08-09-16:36:03.960.
 No particles to dump.
 No fluids to dump.
 Domain: Dumping histories at 2022-08-09-16:36:03.960.
 Domain: Histories dumped at 2022-08-09-16:36:03.966.
 No SumRhoJ to dump.
 Dumping 1 multifields.
 Dumping all multifields 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 multifields 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.

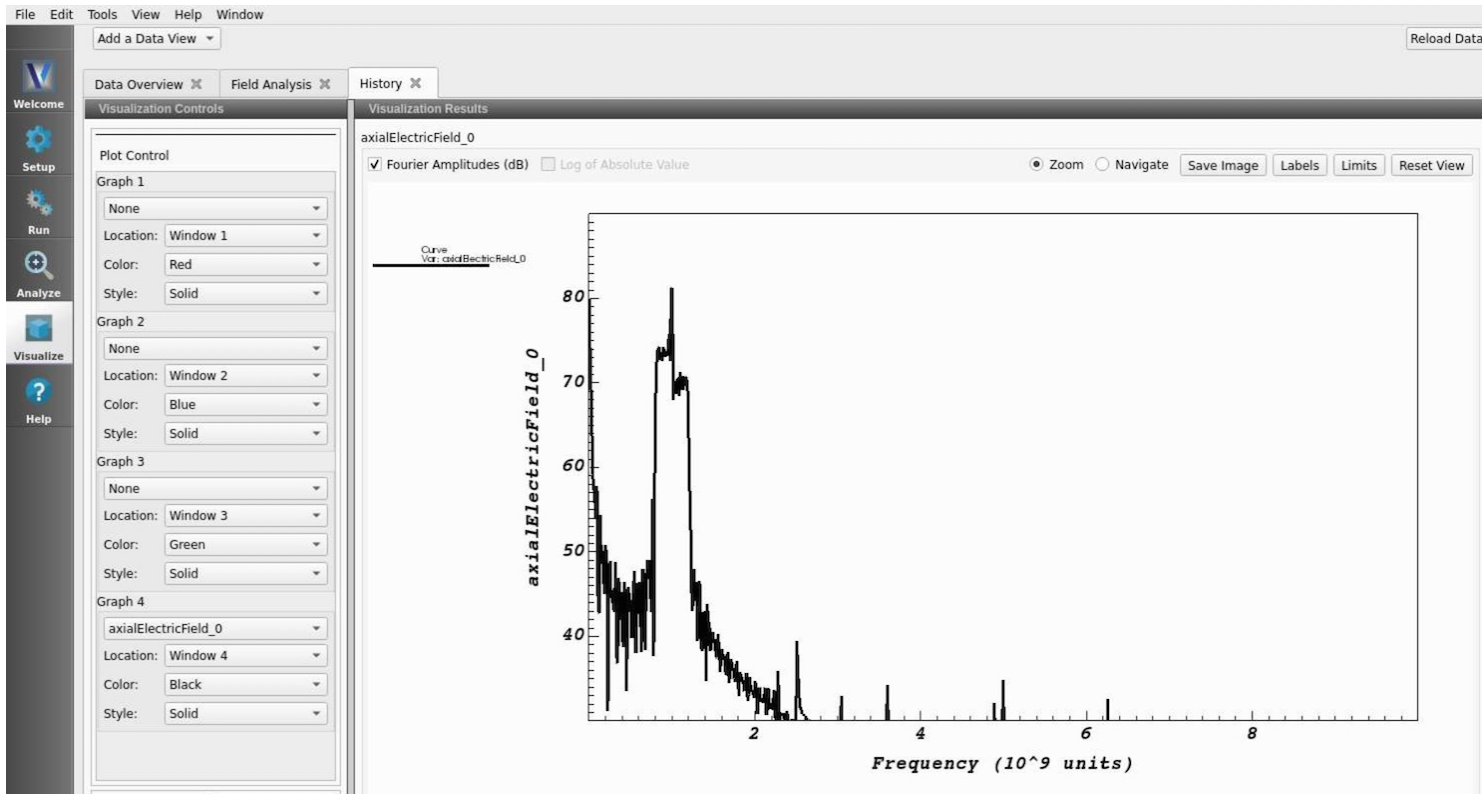
OUTPUT SUMMARY:
 There were 0 Notices encountered in this run.
 There were 0 Warnings encountered in this run.
 VORPAL completed at clock time 2022-08-09-16:36:04.023.
 NOTE: This simulation can be run if all of the packages 'VsimBase VsimEM' are enabled. Other package combinations may be possible as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

- 50k steps
- Fourier transform



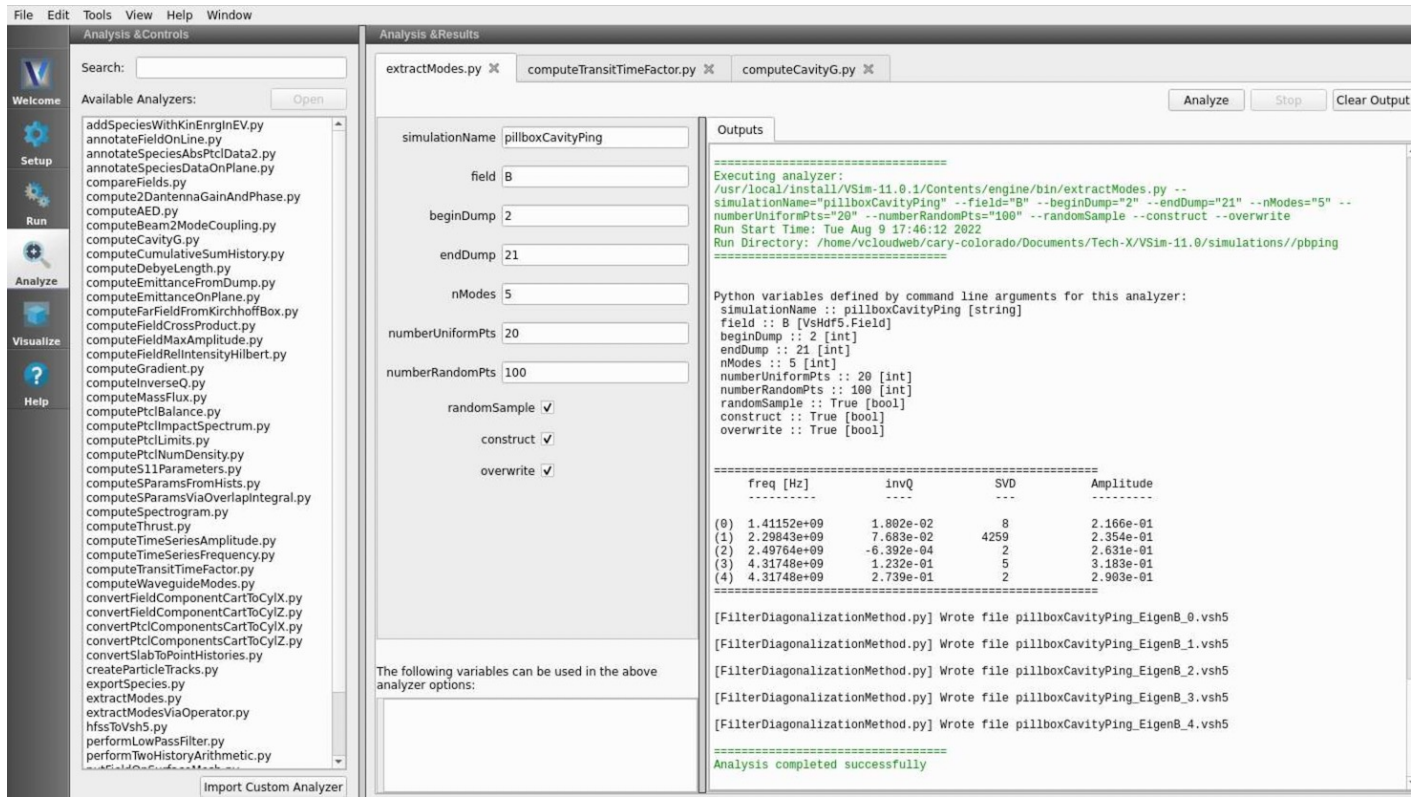
Excite the cavity over a range of frequencies

- Use freqBandStf
- 0.8-1.2 GHz



Use extractModes to get frequency to high accuracy

- An SVD fit to a number of sinusoids



File Edit Tools View Help Window

Analysis & Controls

Search:

Available Analyzers:

- addSpeciesWithKinEngrInEV.py
- annotateFieldOnLine.py
- annotateSpeciesAbsPtcData2.py
- annotateSpeciesDataOnPlane.py
- compareFields.py
- compute2DantennaGainAndPhase.py
- computeAED.py
- computeBeam2ModeCoupling.py
- computeCavityG.py
- computeCumulativeSumHistory.py
- computeDebyeLength.py
- computeEmittanceFromDump.py
- computeEmittanceOnPlane.py
- computeFarFieldFromKirchhoffBox.py
- computeFieldCrossProduct.py
- computeFieldMaxAmplitude.py
- computeFieldRelIntensityHilbert.py
- computeGradient.py
- computeInverseQ.py
- computeMassFlux.py
- computePtcBalance.py
- computePtcImpactSpectrum.py
- computePtcLimits.py
- computePtcNumDensity.py
- computeS11Parameters.py
- computeSParamsFromHists.py
- computeSParamsViaOverlapIntegral.py
- computeSpectrogram.py
- computeThrust.py
- computeTimeSeriesAmplitude.py
- computeTimeSeriesFrequency.py
- computeTransitTimeFactor.py
- computeWaveguideModes.py
- convertFieldComponentCartToCylX.py
- convertFieldComponentCartToCylZ.py
- convertPtcComponentsCartToCylX.py
- convertPtcComponentsCartToCylZ.py
- convertSlabToPointHistories.py
- createParticleTracks.py
- exportSpecies.py
- extractModes.py
- extractModesViaOperator.py
- hfsToVsh5.py
- performLowPassFilter.py
- performTwoHistoryArithmetic.py

Analysis & Results

extractModes.py ☒ computeTransitTimeFactor.py ☒ computeCavityG.py ☒

simulationName

field

beginDump

endDump

nModes

numberUniformPts

numberRandomPts

randomSample ☒

construct ☒

overwrite ☒

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

Outputs

```

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

```

	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

[FilterDiagonalizationMethod.py] Wrote file pillboxCavityPing_EigenB_0.vsh5

[FilterDiagonalizationMethod.py] Wrote file pillboxCavityPing_EigenB_1.vsh5

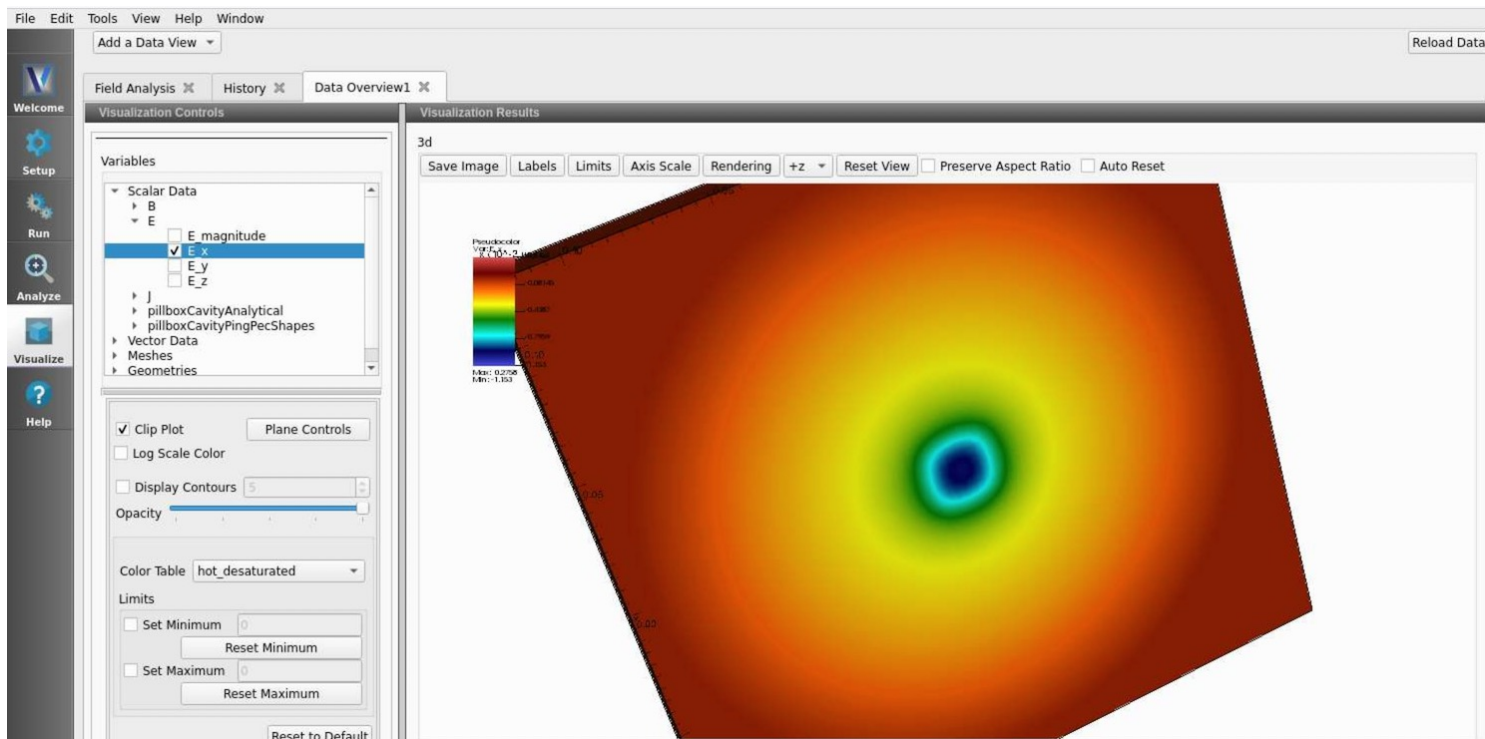
[FilterDiagonalizationMethod.py] Wrote file pillboxCavityPing_EigenB_2.vsh5

[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





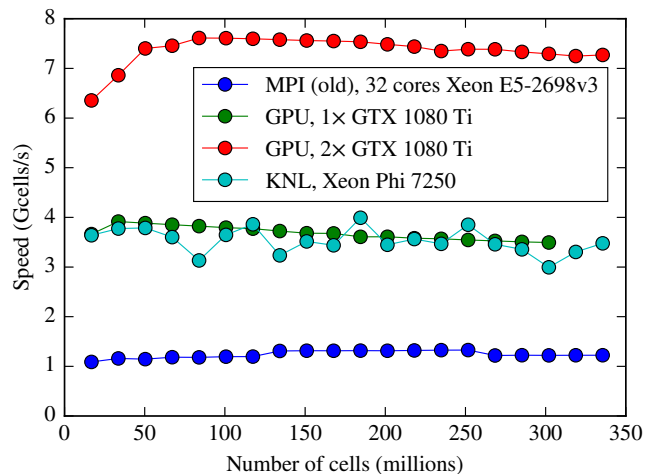
Some things to think about moving forward (what I am excited about)

Heterogeneous Computing
Algorithms
Increasing integration

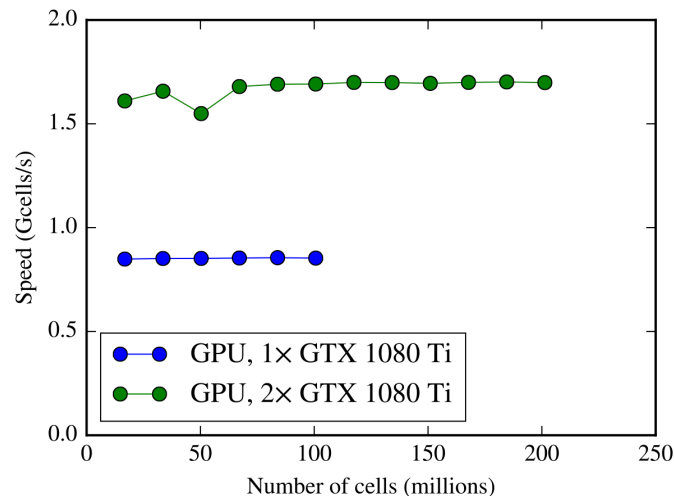


TECH-X

Proper restructuring shows near-perfect scaling

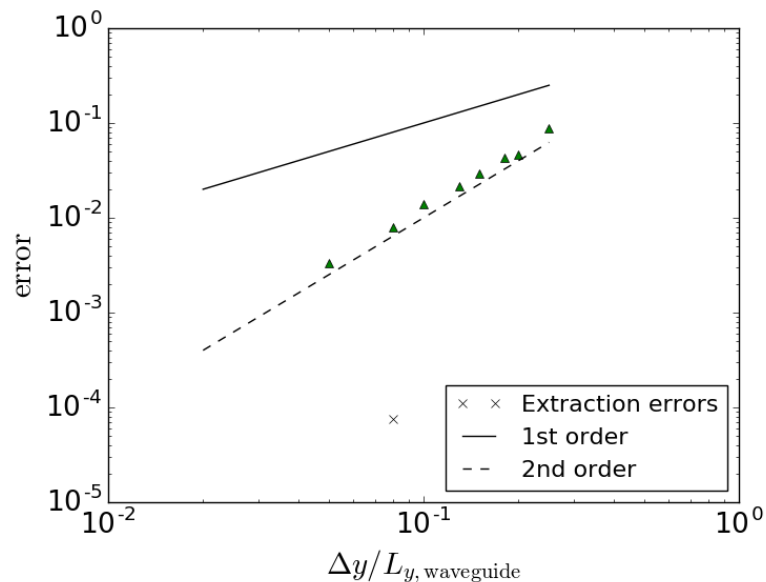


Vacuum FDTD updater



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.



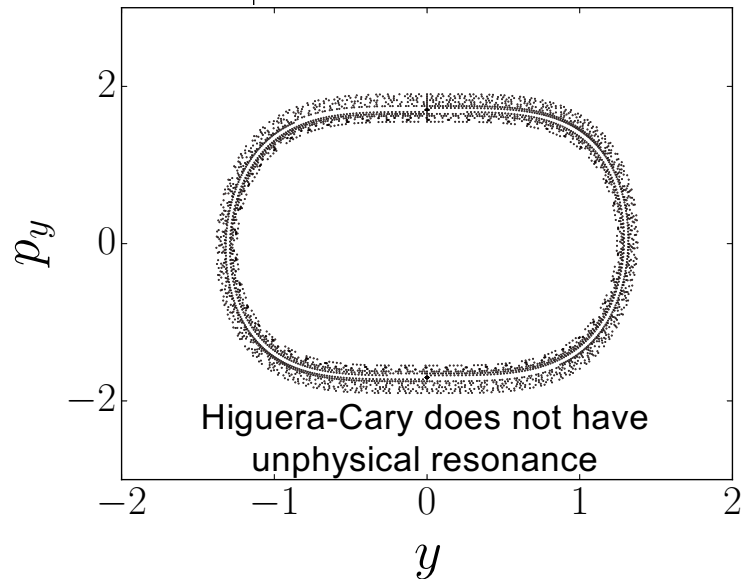
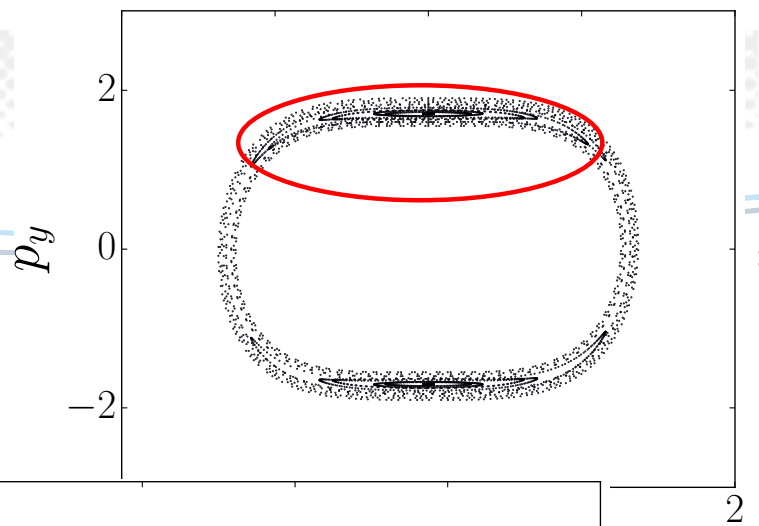
Algorithms: structure-preserving particle pushes

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



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