TECH-X
SIMULATIONS EMPOWERING YOUR INNOVATIONS

VSim/Vorpal Updates

October 20, 2017

EASE AND PERFORMANCE

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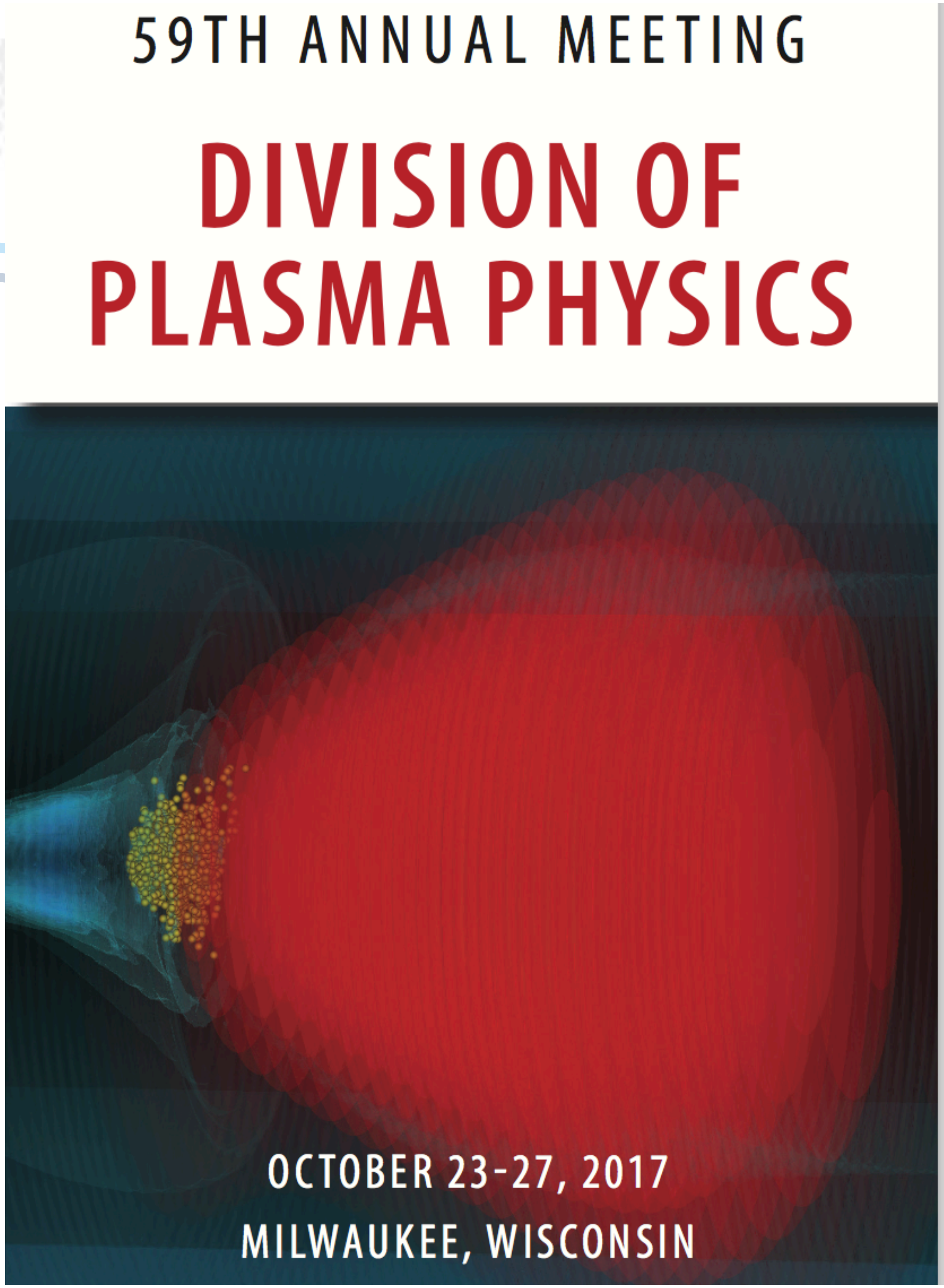


Shameless plug for AAC 2018

- 9600 feet
- 69% O_2
- Ben will lead jogs

Altitude (meters)	Altitude (feet)	Effective Oxygen %	Altitude Category	Example
0	0	20.9	Low	Boston, MA
500	640	19.6	Low	
1000	3281	18.4	Medium	
1500	4921	17.3	Medium	Boulder, CO
2000	6562	16.3	Medium	
2500	8202	15.3	High	Aspen, CO
3000	9843	14.4	High	
3500	11483	13.5	High	

It's been a while….

- VSim/Vorpal basics: input file format, scaling
- Making VSim/Vorpal easier to use
- VSim/Vorpal applications
  - Plasma acceleration
  - Photonics
  - Plasma discharges
- Increasing Vorpal performance
- Working with the Vorpal team

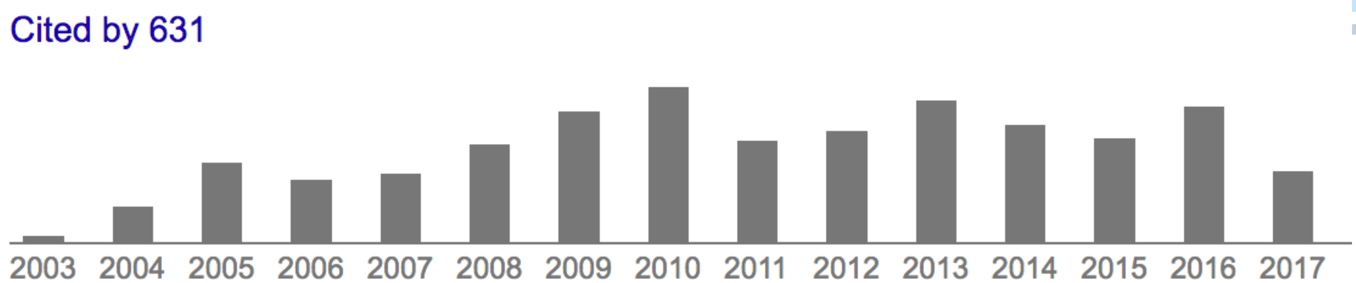
Terminology and support/access models

- Computational engine: Vorpal
- Full package: VSim
- Front end: VSimComposer
- VSim has a different business model

Code	Method of support	Access
WARP	DOE	FOSS
OSIRIS	DOE, NSF	MoU controlled
VSim	SBIR, Sales, Grants	Commercial or collaboration

There are others: EPOCH, Smilei, …

Advanced accelerator researchers are a part of Vorpal users



- Advanced accelerators
  - Litos group (CU)
  - UCLA (Majernik)
  - Strathclyde/Cockcroft (Hidding)
  - ELI/John Adams, Romanian National Institute of Laser, Plasma and Radiation Physics, other EU partners
  - TU-Darmstadt
- Available at NERSC (other labs by demand)
- But we are also responding to a much larger group of non-plasma accelerator users, who are driving ease of use:
  - ISIS/Rutherford
  - FNAL (SRF coatings)
- 173 licensing agreements since 2012

VSim/Vorpal has historically had great flexibility

- Input file can define problems down to the operator level
- Gives a physics-based language for simulation

```
<FieldMultiUpdater laserLauncher2>
  kind = STFuncUpdater
  operation = set
  velOverC = -1.0
  lowerBounds = [0  0]
  upperBounds = [1  190]
  components = [2]
  writeFields = [E]

  <STFunc stFunc>
    kind = expression
    expression =
(14127083706293.72*((t<2.8352948091842926e-14)*(0.5-0.5*cos(221606
1.0))*(cos(2354564459136066.5*t+((-6e-05*1768.3882565766146)*(8333
2/1.0112579092935932))))
  </STFunc>

</FieldMultiUpdater>

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  components = [0   1   2]
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  readFields = [B depField]
  writeFields = [E]
  lowerBounds = [0  0]
  upperBounds = [951  190]
</FieldMultiUpdater>
```
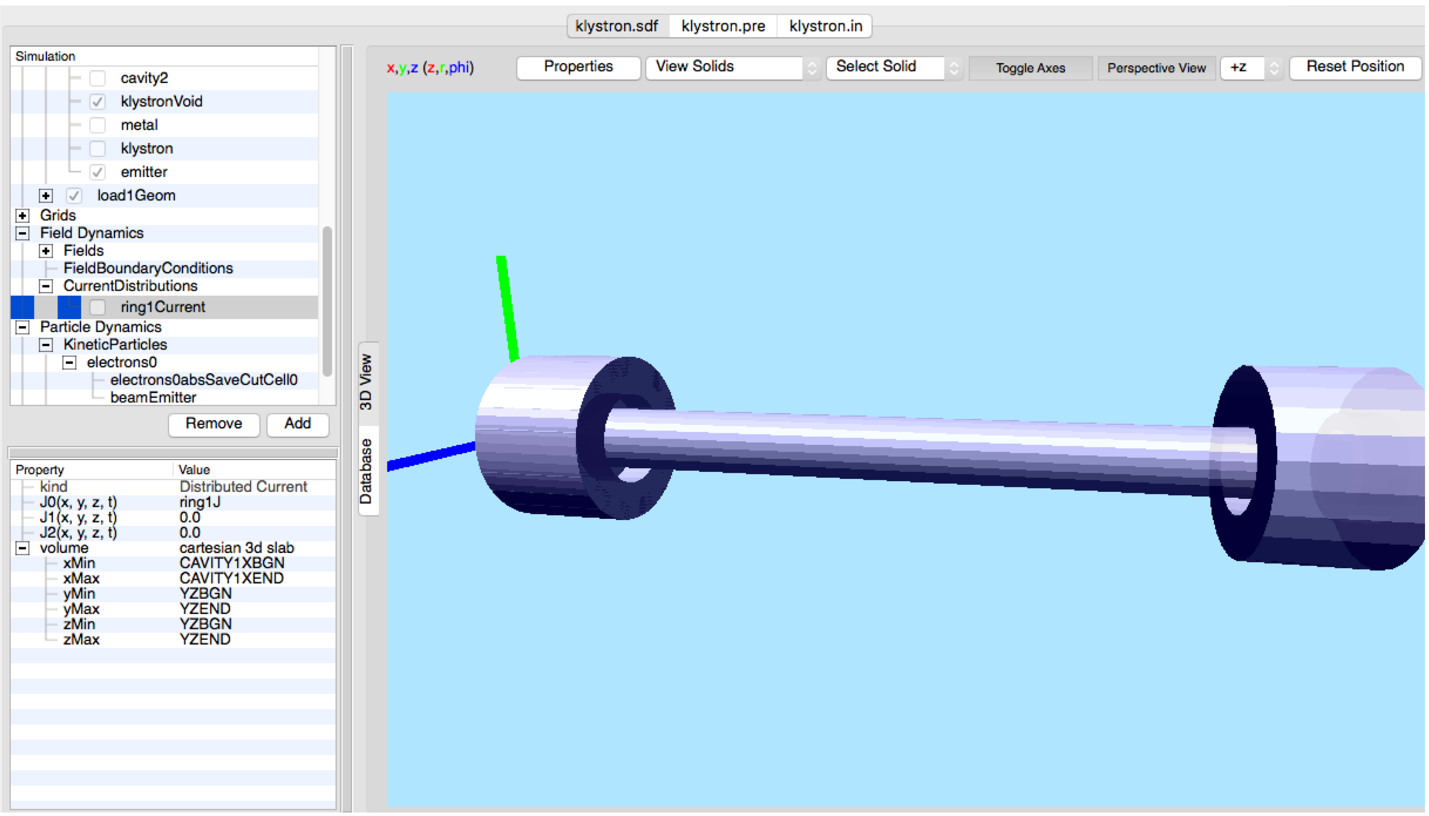

VSim users demanding ease of setup: Geometries (CSG, CAD import), Grids

- Allow easy setup of beams, kickers, focusing



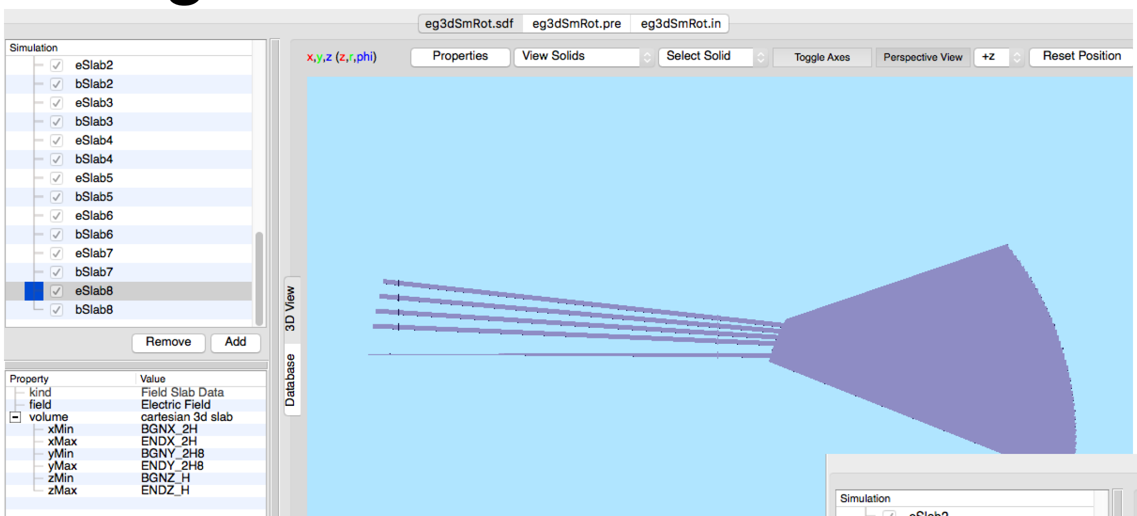
Addresses needs of vacuum electronics, plasma discharges, photonics

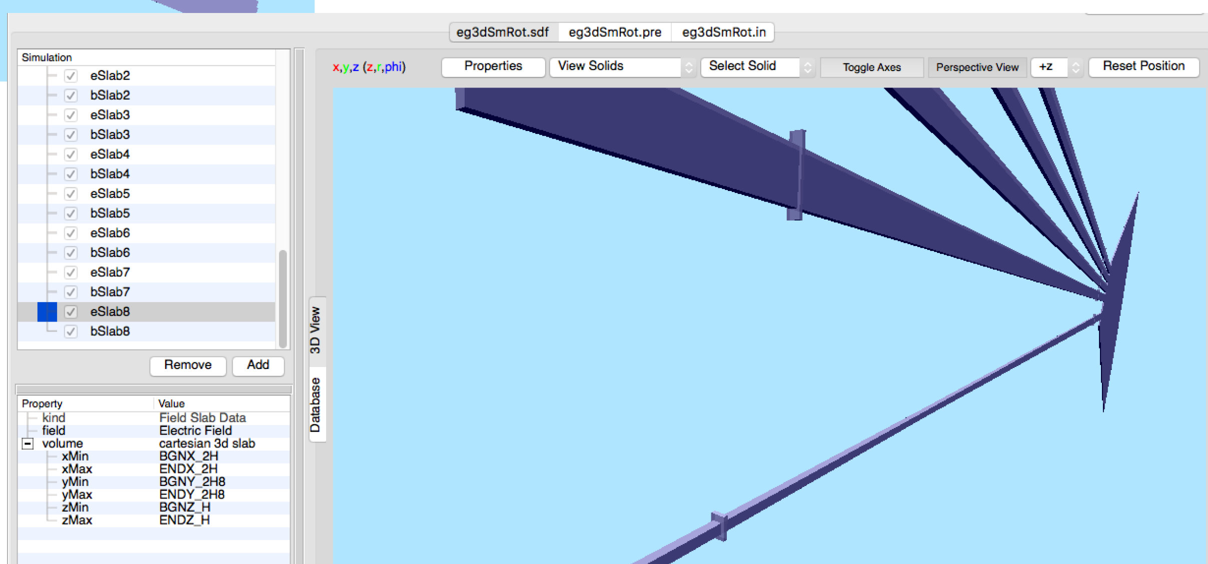
Conformal (cut-cell) boundaries

Primary and secondary emission

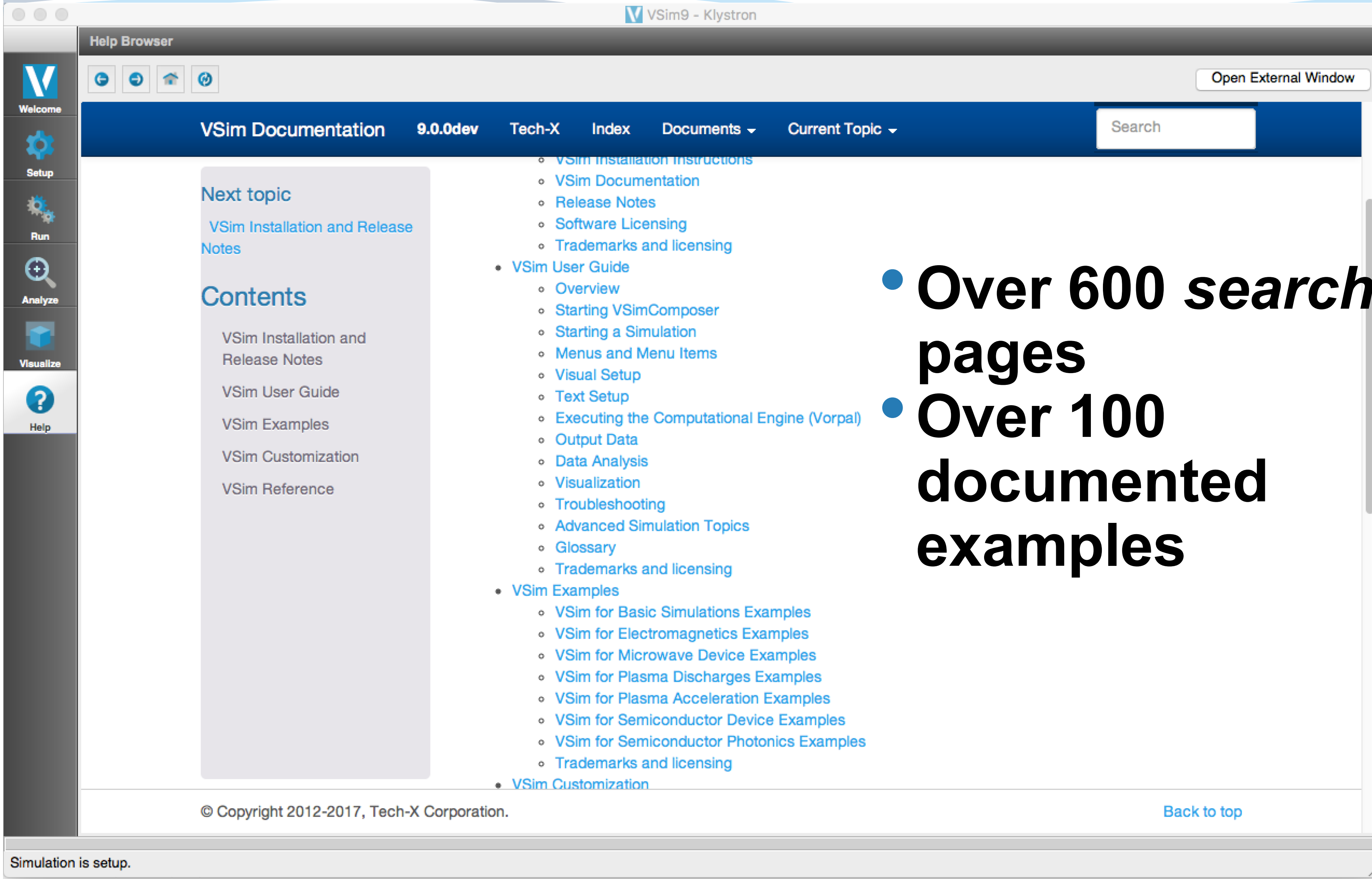
VSim users demanding ease of setup: Monitors

- Place visually
- Align with other elements in the simulation





VSim continues to provide extensive documentation



- **Over 600 *searchable* pages**
- **Over 100 documented examples**

Tech-X has training sessions in both US and EU

Tech-X 2017 Worldwide Simulation Summit

Boulder, Colorado - July 7, 2017:

Tech-X will hold its 2017 TWSS VSim training session September 12-14, 2017 at Tech-X headquarters in Boulder, CO.

Learn how to use VSim FDTD (finite difference time domain) PIC (particle-in-cell) simulation software. Acquire knowledge and gain insights from world class experts about:

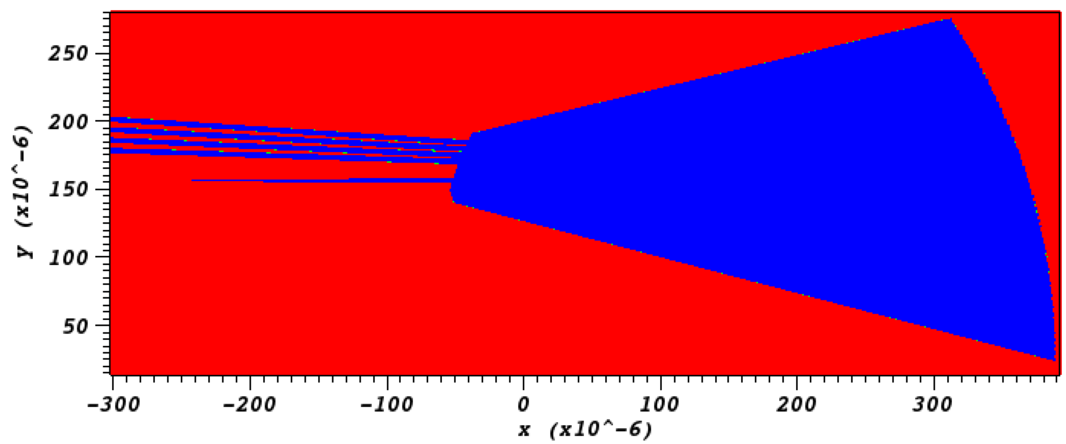
- Plasma physics simulation
- Microwave vacuum device design (e.g. helix TWT amplifiers, klystrons, and magnetrons)

- Typically UK in Spring, US in Fall
- Full set of course notes available

Vorpal directions: photonics, algorithms, reactions/collisions, performance

- Photonics: large problems for a critical industry, relevant to AA, direct and upstream (interconnects)
- Algorithms: improving relativistic dynamics
- Reactions/collisions: Trojan horse and modeling plasma targets
- Performance: a complete refactoring for GPU and Phi

- $\lambda = \lambda_0/n = 1310/1.914 = 684$ nm
- Device is 783k λ^2, 6M λ^3
- At 20 cells/λ, this is 49e9 cells and requires 300k steps
- Limitation: no business case for $(2)50k simulations (1M core-hours)

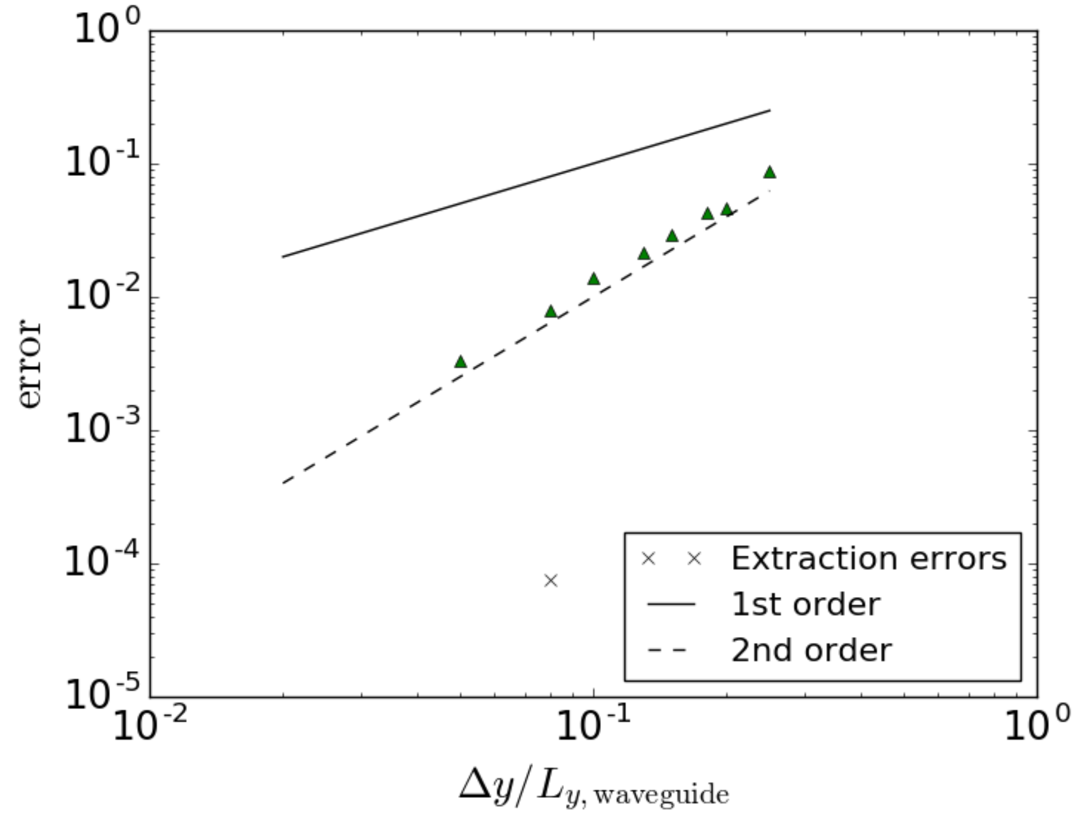


Recent addition: second-order-behaving dielectric updaters relevant to

- 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.



Improvements to the engine: the Boris Push

- Boris, 1971: Strang splitting allowing direct calculation of particle acceleration
  - Extremely good. Penn et al for muon cooling. Qin: volume preservation (weak symplectic integration)
- Vay, 2008: Improve Boris to have particle ExB equilibrium
- Cary-Higuera, 2017: ExB equilibrium and volume preservation
- Use
  - Texeira
  - Ryne

Allows explicit update

Single-particle equilibrium

Distribution equilibrium

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 relativistic Boris Push only in the method for calculating the Lorentz factor. This is shown to have the same second-order accuracy in time as that found by splitting the electric acceleration and magnetic rotation (Boris Push) and that found by averaging the velocity in the magnetic rotation term (Vay's method) [J.-L. Vay, Physics of Plasmas (1994-present) 15, 056701 (2008)]. All three

Vorpal addressing performance

- Best approach to performance changed
  - 2000: optimize cache use by component proximity
  - 201X: optimize vectorization by aligning data with similar operations (oh, and cache too)
- DARPA funded project to move all performance operations to GPUs
  - Grids
  - Fields
  - Particles
  - Reactions (collisions, field ionization, …)
  - + Implicit EMPIC

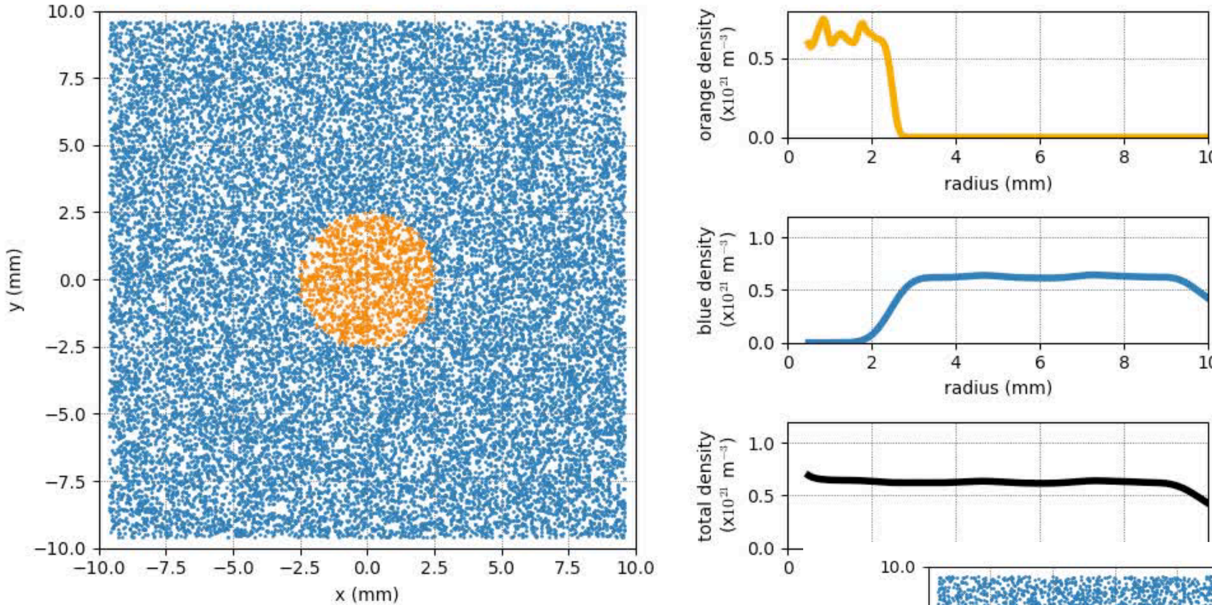
This move has allowed a general refactor

- Vorpal has had piecemeal GPU support
- Grids: variable compatible throughout
- Fields, particles exist across CPU and devices (make use of all available power)
- Data structures are structures of arrays of structures (tiles)
- Hybrid (MPI/OpenMP) parallelism
- Auto-detection of available devices with auto-allocation
- Contiguous direction of all data selectable at compile time
- All algorithms coded in a way that works on GPU or with vector instructions on a CPU (multi- or many-core)
- Heart surgery on a walking patient

Variable grids to span spatial scale

- Driving beams: 100 nm radius, 10 nm cells
- System (wake): 200 μm diameter
- 20,000 cells each transverse direction, 400M in per transverse plane
- Exponential mesh is provably 2nd order
- Crosses simulation in $60\ln_{10}(200\mu/10n) = 260$ cells, or 70k per transverse plane, savings of 6,000
- Time stepping solved by implicit EM (ICOPS 2015)
- Variable grids now exist in VSim/Vorpal, but not across all objects
- Now being implemented everywhere (as a runtime option)

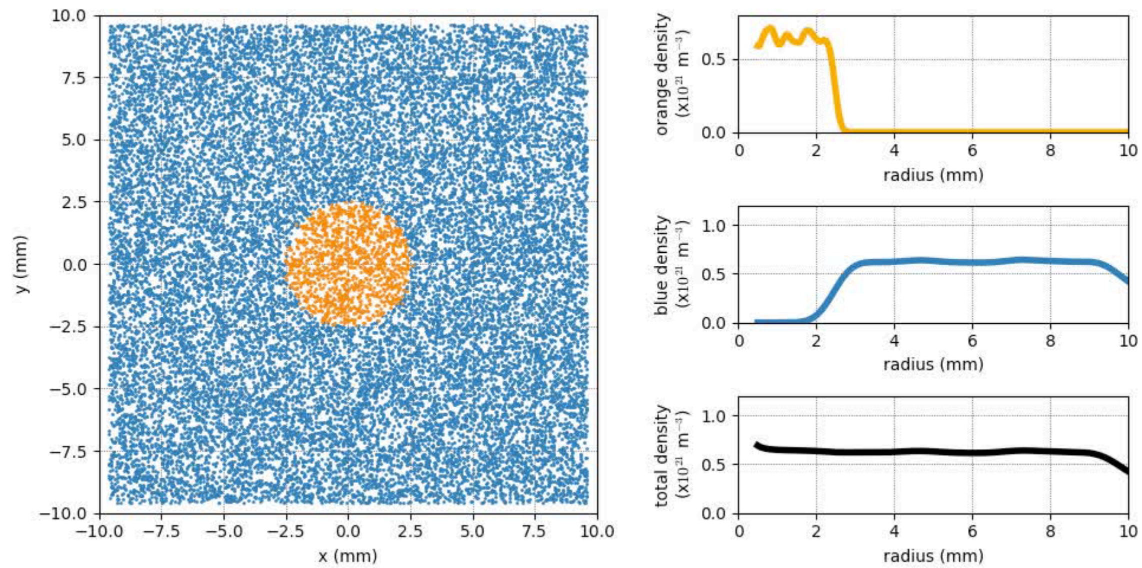
Reactions tested on plasma target-like device



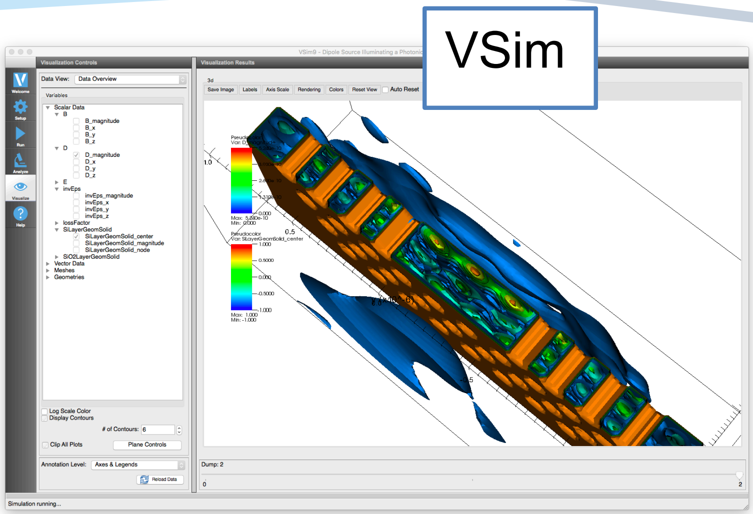
- Thanks to Jarrod Leddy, Scott Sides, Ben Cowan, Greg Werner
- Rayleigh-Taylor

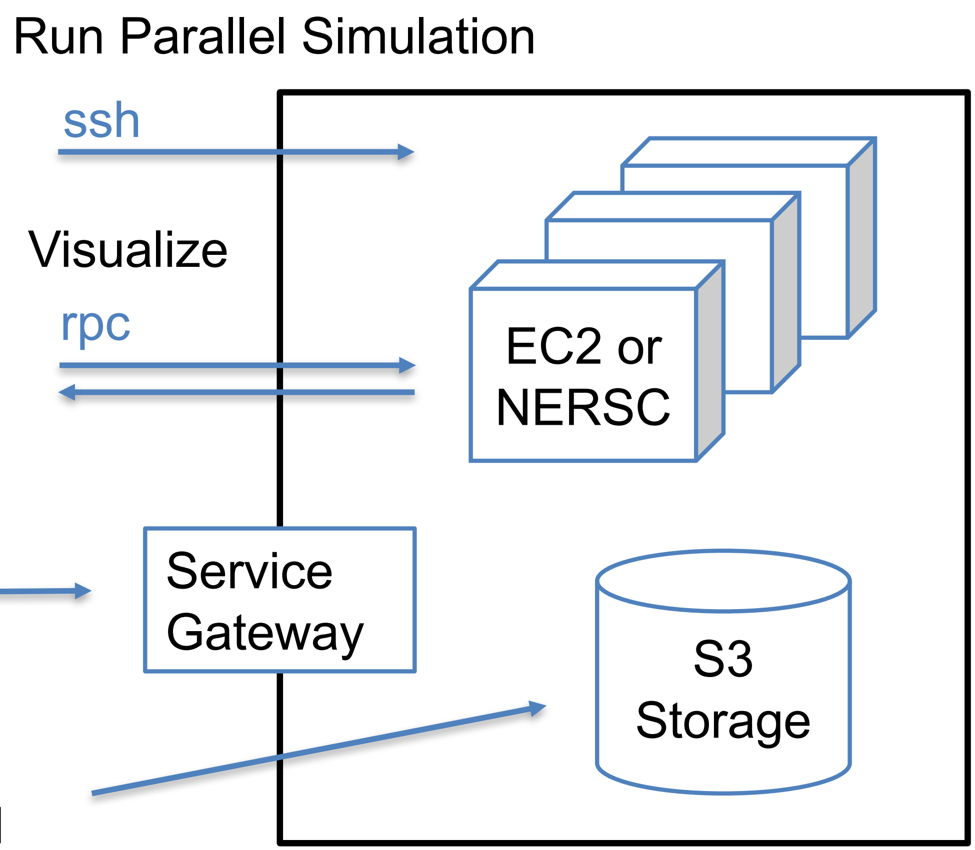
Collisionless

Collisional:



VSim will soon be available by cloud/remote submission through VSimComposer





Web Service Calls to spin up collection of nodes, setup them up for running

Some software must be installed on space that will become shared on collection nodes

How to work with Tech-X? There is a path for everyone…

- Why bother? (Ease of use combined with scalability)
- Join U. Colorado
- Piggyback
  - Many labs (e.g., FNAL) and universities (UCLA) have purchased a VSim license
  - Others could replace existing software (CST, HFSS)
  - Small/zero increment to use in another area
- Collaborate
  - Pursue joint funding
- Purchase
  - Deep University (WVa, UCD/CS) discounts, can get slides for computational physics class

Summary

- VSim in use in multiple AA projects (Strathclyde, ELI, …)
- VSim has synergistic wide use (photonics, plasma discharges)
- VSim recently made much easier to use, will continue in this direction with cloud approach (fire up GUI locally, use a supercomputer)
- VSim undergoing complete refactor for GPU, many-core (DARPA)
- Grids completed, first collisions showing up, fields done in library, particles done in prototype