Use of Computation for Understanding Plasmas, J. Cary, Tech-X, U. Colorado
Presented at Michigan Institute of Plasma Science and Engineering

June 18, 2018

Disaster is in the eye of the beholder!

ESPN.COM

On this date: Colorado's Miracle at Michigan - ESPN Video

On September 24, 1994, Kordell Stewart chucks a Hail Mary, which is...

Use of Computation for Understanding Plasmas

John R Cary

Tech-X, U. Colorado Boulder

June 25, 2018

Presented at Michigan Institute of Plasma Science and Engineering

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Acknowledgments: DOE, NSF over the years.
SLPIC recently: U.S. Department of Energy SBIR Phase I/II Award DE-SC0015762 and NSF award PHY1707430; GW also received partial support from the Institute for Modeling Plasma, Atmospheres, and Cosmic Dust (IMPACT) of NASA's Solar System Virtual Institute (SSERVI).

4 Big reasons to use computation

- Prediction and variation determination: Crab cavity
- Optimize configurations: Photonic crystal cavity
- Discovery: Electron Bernstein nonlinear processes
- Process elucidation: Laser wake-field acceleration

In each example, there is a result, and advance made to get that result.

Prediction and determination: what do I really have?

- It's tough to make **predictions, especially about the future**. (Danish parliament, 1936, https://quoteinvestigator.com/2013/10/20/no-predict/)

Olde Stage Fire, Boulder, Jan 2009
The Denver Channel

But before I start predicting, optimizing elucidating, discovering, how do I know I have it right?

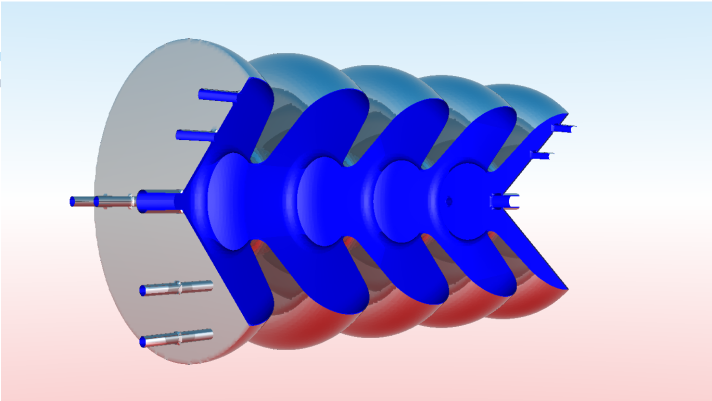
"No one believes in a theory except its author, whereas everyone relies on an experiment except the physicist who conducted it," Einstein

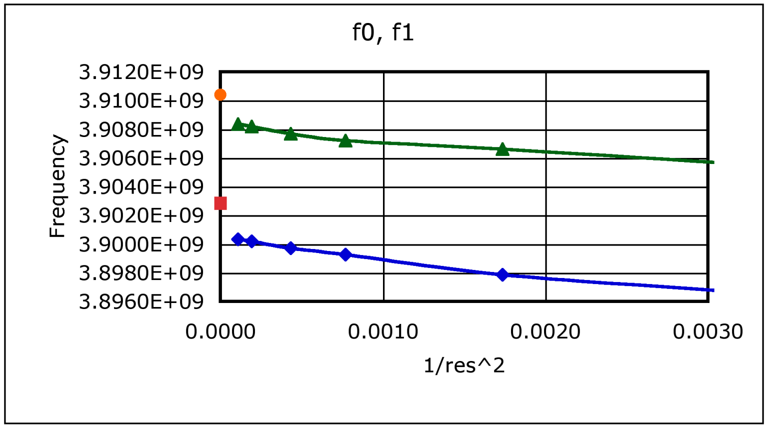
Where does the computationalist fit?

- Like the experimentalist
  - Error in putting system together
  - Error in data analysis
  - Error in calibration (switching units)
- Like the theorist
  - Might have the wrong model
  - Incorrect approximation

Validation: showing that the model is correct

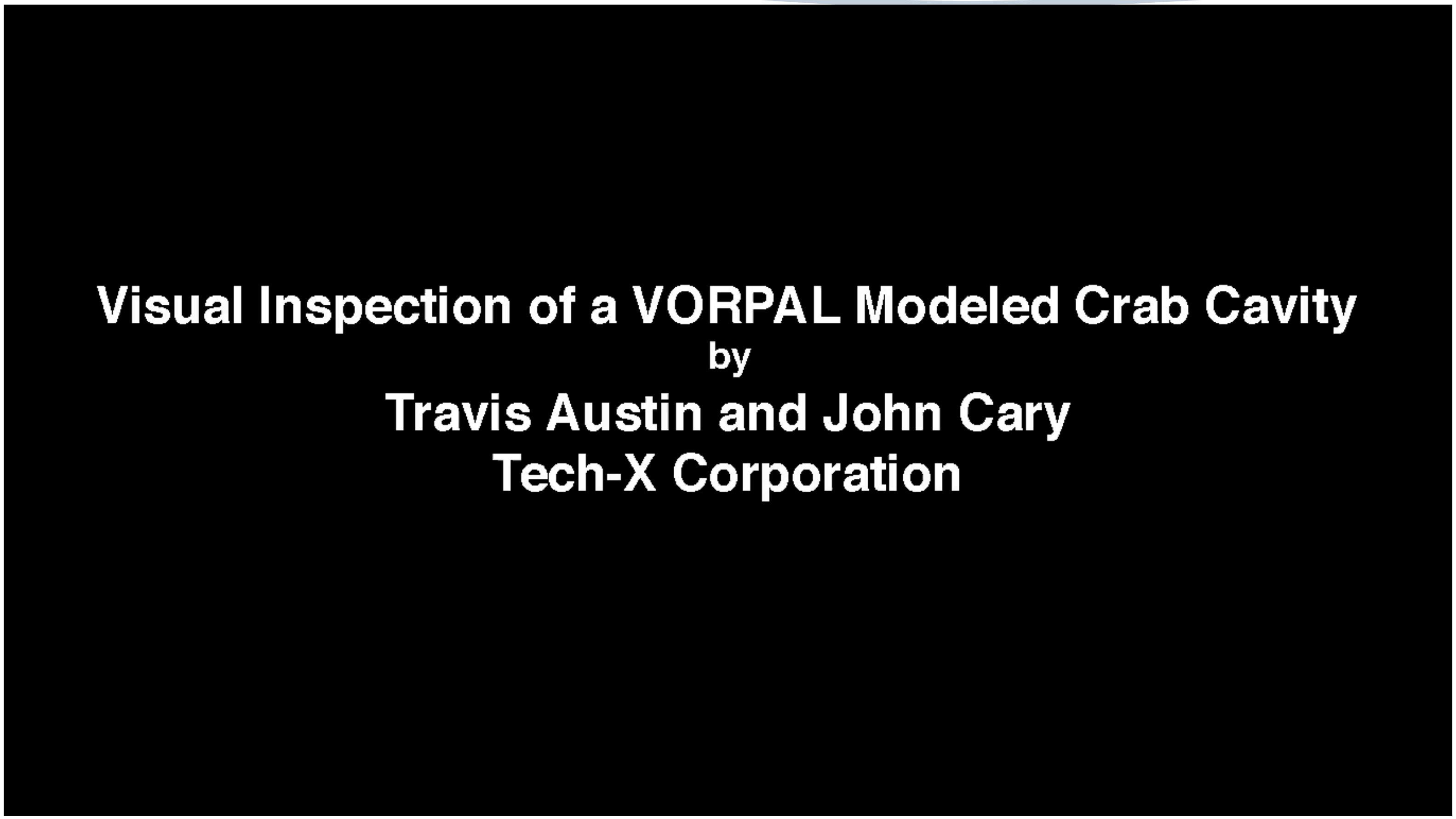
- Previous computations gave frequencies low by 5 MHz out of 4 GHz.
- Ours (improved algorithm and parallelism) were low by 2 MHz, yet we had verified against exact solutions!
- Model no holes? One? All?
- Correct for dielectric of air?





Richardson Extrapolation (1911)

Visualization allowed checking the model in detail



Validation study showed that we had the wrong model

- Reduce the equator radius by 0.001 inch
- Get agreement
- Ask makers to measure their cavities
- Sure enough …

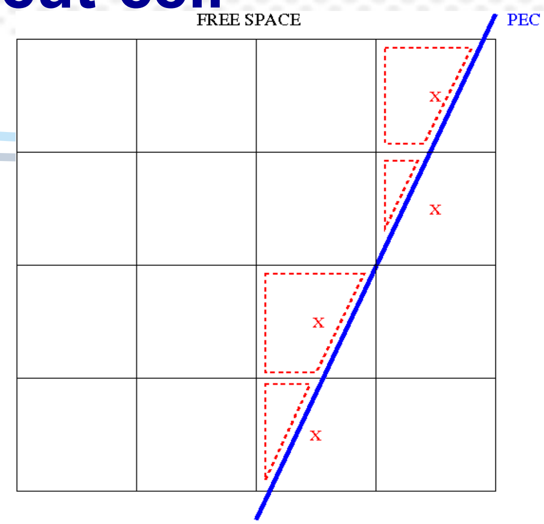
- To what extent can we determine the precise shape of objects by measuring their frequency spectra?

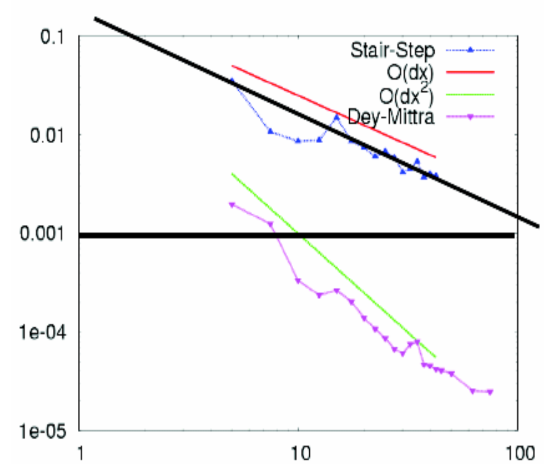
Needed advance: tunable cut-cell electromagnetics

- Dey-Mittra algorithm: Modify Faraday update at boundary cells.
- Get instability unless drop some cells
- Write magnetic update as a matrix multiply
- Gershgorin theorem says which cells have to be dropped for a given reduction of time step

Application of Dey–Mittra conformal boundary algorithm to 3D electromagnetic modeling, Journal of Computational Physics 228 (2009) 7902–7916

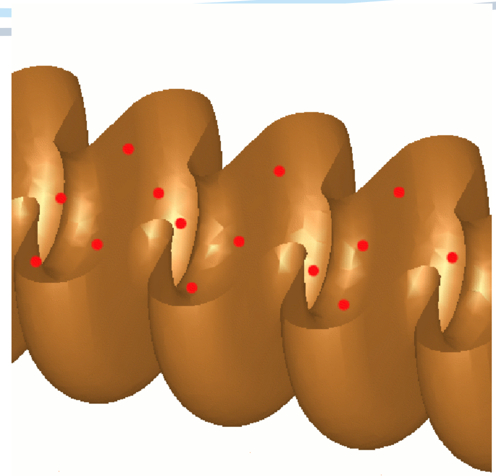
- Bad title! (Should have mentioned validation, time step limits)





Needed advance: mode extraction

- Turns any time-domain code into a frequency domain code
- Ring up finite bandwidth, compute time series in subspace
- Diagonalize subspace
- Multiple simulations if near degeneracies



G. R. Werner and J. R. Cary, “Extracting Degenerate Modes and Frequencies from Time Domain Simulations,” J. Comp. Phys. 227, 5200-5214 (2008)

Optimization: investigate how multiple configurations work, pick best

https://wright.nasa.gov/airplane/tunnel.html
At the end of 1901, the Wright brothers were frustrated by the flight tests of their 1900 and 1901 gliders. … Based on their measurements, the 1901 aircraft only developed 1/3 of the lift which was predicted by using the Lilienthal data. During the fall of 1901, the brothers began to question the aerodynamic data on which they were basing their designs. They decided to measure their own values of lift and drag with a series of wind tunnel tests

…

They made between one and two hundred models and made quick preliminary tests in October, 1901, to develop their test techniques and to investigate a wide range of design variables. ... Following the preliminary experiments, they chose about 30 of their best designs for more detailed parametric studies.

Wright brothers' wind tunnel, 1901

- Build small before building large
- Compute before building at all

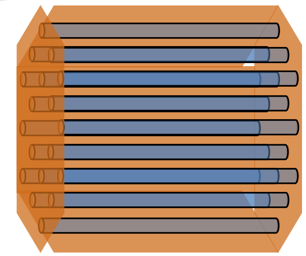
Optimization: What is the best photonic crystal cavity?

STUDY OF HYBRID PHOTONIC BAND GAP RESONATORS FOR PARTICLE ACCELERATORS

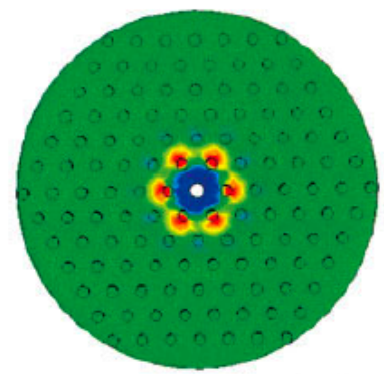
M. R. Masullo,[1] A. Andreone,[2] E. Di Gennaro,[2] S. Albanese,[3] F. Francomacaro,[3] M. Panniello,[3] V. G. Vaccaro,[3] and G. Lamura[4]

2486 MICROWAVE AND OPTICAL TECHNOLOGY LETTERS / Vol. 48, No. 12, December 2006 DOI 10.1002/mop

room temperature confirm the monomodal behavior, but the Q value is lower than expected (roughly 10^3). This is mainly due to



- Idea: put harmful modes (wake fields) in pass band of photonic crystal, and they leave.
- Thought that regular crystals would be best. How much error can be tolerated?
- Serendipitous observation: some slight movements led to increased Q

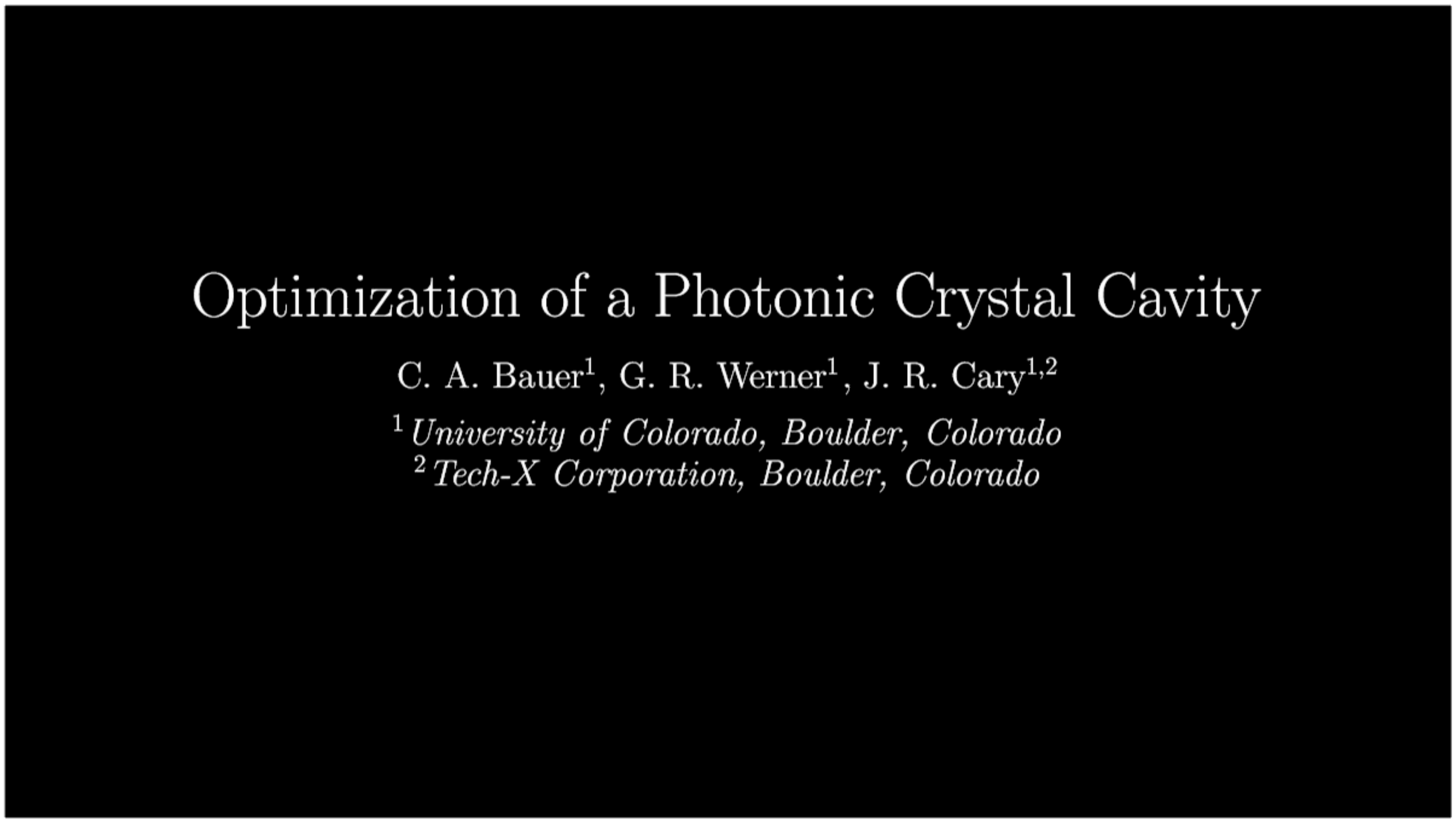


If a slight movement can make a better cavity, then maybe there is a better configuration?

- Wrap Vorpal in a python script
- For each value of parameters (locations of rods)
  - Ring up cavity
  - Extract frequencies and damping
  - Compute new positions using Nelder-Mead optimization (robust, best for computations with noise or errors).

Optimization found completely unexpected solution

- Constrained to be 6-fold periodic



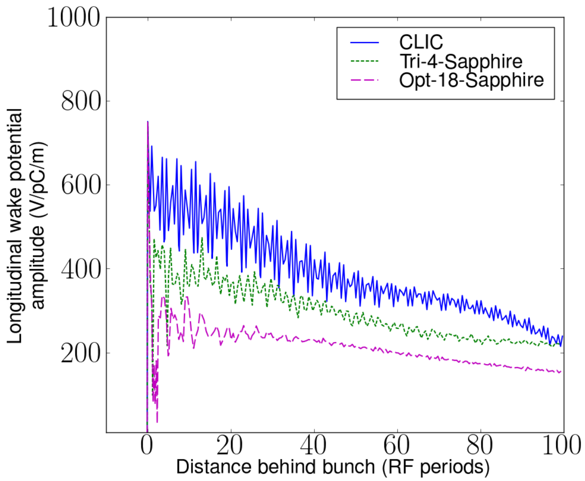
Optimization found

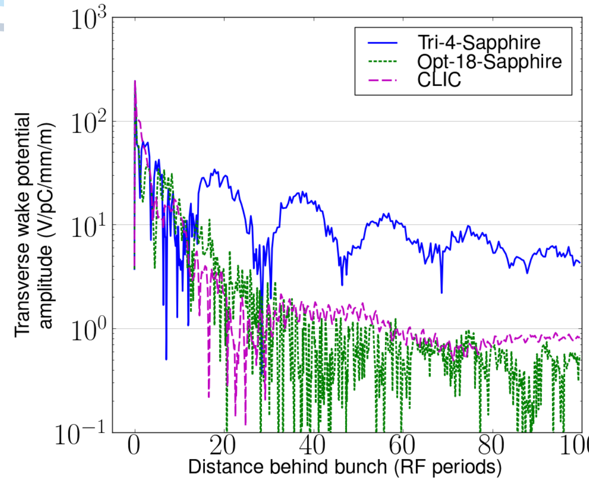
- 2 orders of magnitude improvement in Q (confinement)
- Asymmetric result

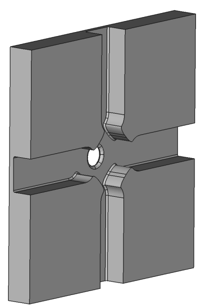
- Relied upon subscale algorithm for dielectrics

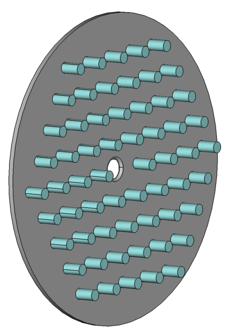
G. R. Werner and J. R. Cary, “A Stable FDTD Algorithm for Non-diagonal, Anisotropic Dielectrics,” J. Comp. Phys. **226,** 1085-1101 (2007), doi:10.1016/j.jcp.2007.05.008.
C. A. Bauer, G. R Werner, and J. R. Cary, “A second-order 3D electromagnetics algorithm for curved interfaces between anisotropic dielectrics on a Yee mesh,” J. Comput. Phys. **230**, 2060-2075 (2011), doi:10.1016/j.jcp.2010.12.005.

Hybrid, optimized cavities: lower longitudinal wake fields, comparable transverse

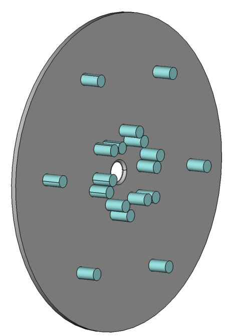








CLIC Team at CERN



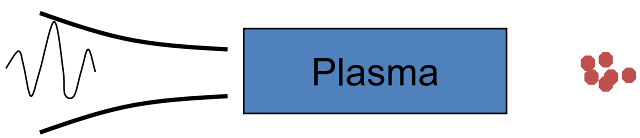
Graduate thesis at U. Colorado

Scientific discovery: what will nonlinearity do to electron Bernstein propagation?

- Resonant upshift of wave energy into second harmonics
- Nonlinear transfer of energy eliminates usage for frequency much larger than the electron cyclotron frequency
- Needed developments
  - Implicit electromagnetics
  - δf EMPIC for RF

Process identification: 2004 Nature Dream-Beam issue shows first exp. results for quality beams in LWFA

LWFA = Laser Wake Field Acceleration



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

C. G. R. Geddes[1,2], Cs. Toth[1], J. van Tilborg[1,3], E. Esarey[1], C. B. Schroeder[1], D. Bruhwiler[4], C. Nieter[4], J. Cary[4,5] & W. P. Leemans[1]

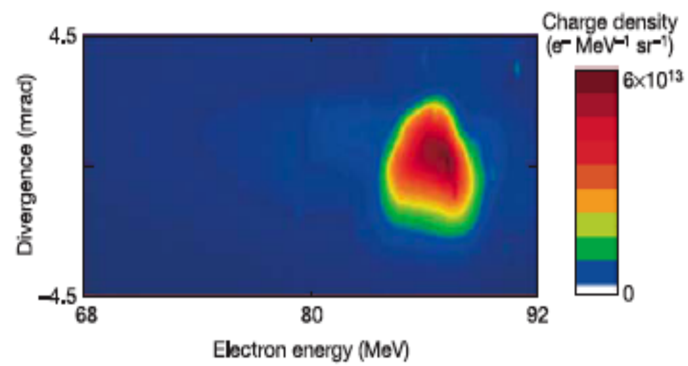


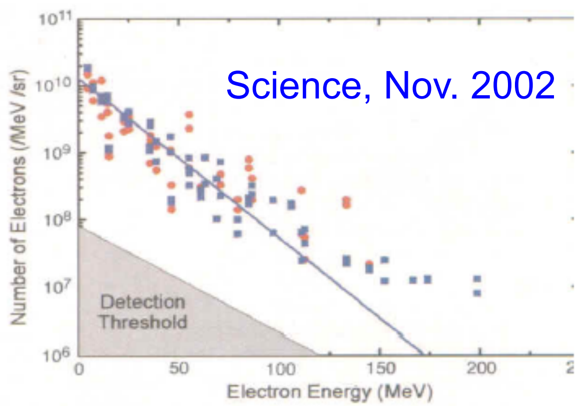
Figure 3 Single-shot electron beam spectrum and divergence of the channel-guided

Like shooting a cannon ball through a brick wall and seeing a tightly correlated, monoenergetic group of bricks come out on the other side

Prior to 2004, one could get large gradients but only poor quality beams

Electron Acceleration by a Wake Field Forced by an Intense Ultrashort Laser Pulse

V. Malka,[1*] S. Fritzler,[1] E. Lefebvre,[2] M.-M. Aleonard,[3] F. Burgy,[1] J.-P. Chambaret,[1] J.-F. Chemin,[3] K. Krushelnick,[4] G. Malka,[3] S. P. D. Mangles,[4] Z. Najmudin,[4] M. Pittman,[1] J.-P. Rousseau,[1] J.-N. Scheurer,[3] B. Walton,[4] A. E. Dangor[4]



the electron density modulations in these plasma waves can reach a few tens of percent (9–13), which corresponds to electric fields on the order of 100 GV/m. The energetic

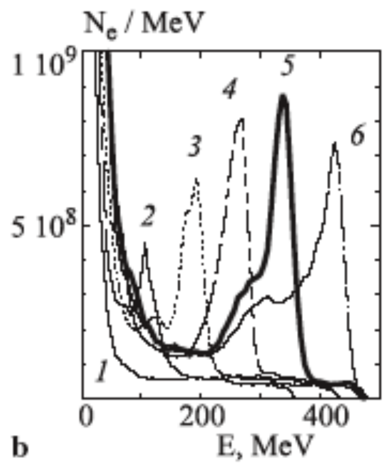
- Many proposals for injection were proposed, but simulation [Cary et al, Phys. Plasmas 12 (5), 056704 (2005)] did not bode well: 10-12 pC beams

Pukhov and Meyer-Ter-Vehn: existence of self-trapping in a "broken regime"

A. PUKHOV[1,✉]
J. MEYER-TER-VEHN[2]

Laser wake field acceleration: the highly non-linear broken-wave regime

Appl. Phys. B, Dec. 2002



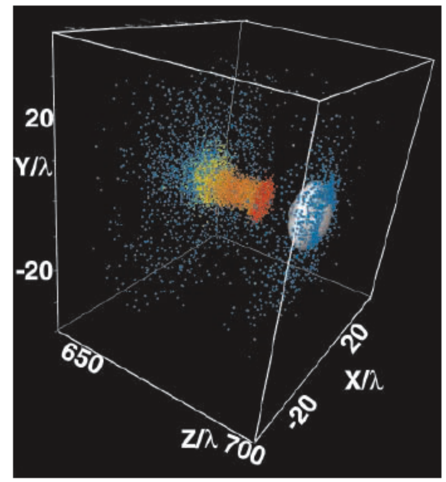


FIGURE 3 The case of a 12-J, 33-fs laser pulse after propagating $z/\lambda = 690$ in 10^{19} cm^{-3} plasma. 3D perspective view of hot electron distribution. Each 100th electron above 10 MeV is shown as a *dot* colored according to its energy. The *white disc* shows the laser-intensity surface at $I = 10^{19}$ W/cm^2

- 12 J, 33 fs, (360 TW) laser
- plasma density = 1.e25 m^{-3}

Could we believe these experiments of different regimes?

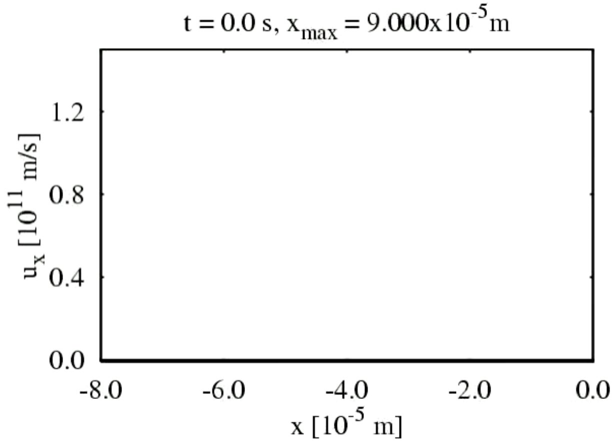
Author	Laser	Power	Plasma density (cm^{-3})
Pukhov et al	12 J, 33 fs	363 TW	1e19
Leemans et al	0.5 J, 55 fs	9 TW	4e19
Mangles et al	0.5 J, 40 fs	12.5 TW	2e19
Faure et al	1 J, 30 fs	32 TW	6e18

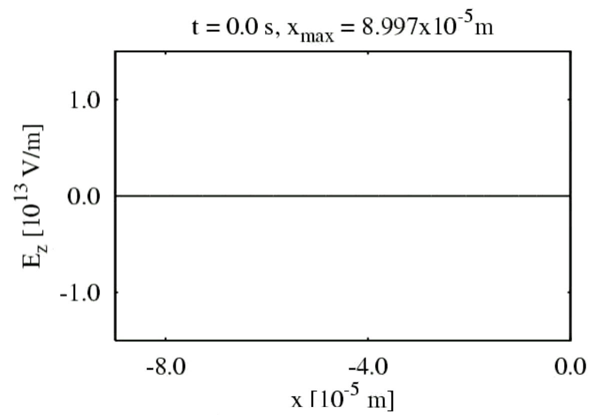
Different spot sizes, plasma profiles, …

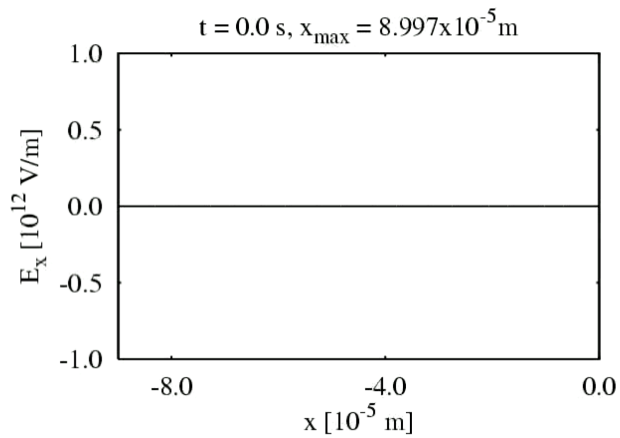
"No one believes in a theory except its author, whereas everyone relies on an experiment except the physicist who conducted it," Einstein

Computations elucidated the process

- Modulational instability to resonance (pulse length ~ c/f_p
- Peaking of accelerating field.
- Time variation cause bunch formation, rotation in phase space causes narrow energy spread







How?

How do we compute these systems?

- We know the fundamental equations
- Just write down the ODE's, put them into Matlab, Mathematica, …?
- Collisions occur on atomic length (10^{-10} m) and time (10^{-16} s), scales

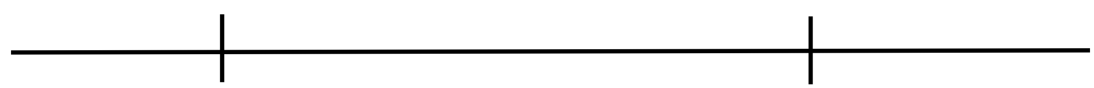
3 eV electron, v = 1e6 m/s
1 A = 10^{-10} m interaction distance, t = 10^{-16} s
Resolve or not?

- If the interaction dynamics is highly correlated, must resolve
- Liquids, solids,
- Strongly coupled plasmas

- If the interactions occur rarely (mean-free-path > separation), then can treat collisions probabilistically
- Gases, "usual" plasmas

Collisions uncorrelated: fluid or particles?

- Gas/Plasma dynamics separates on collisionality
- Knudsen number Kn is ratio of the molecular mean free path length to a representative physical length scale
- Small Kn: lots of collisions, Chapman-Enskog: fluid equations
- Large Kn: few collisions, follow macro-particles, collide rarely, known as Direct Simulation Monte Carlo
- Same applies to plasma: fluid versus Particle-In-Cell
- Combination is PIC-DSMC (Birdsall, Verboncoeur, …)



Where is the transition for typical plasmas?

- 3 eV electron, v = 1e6 m/s
- electrons collide with He gas

$$\lambda = 1/n\sigma$$

$$\mathrm{n} = 1/\lambda\sigma$$

- λ = 1 mm, σ=5x10^{-20} m^2, n = 2x10^{22} m^{-3}, or 1 Torr
- ν = 1e9 s^{-1} = v/λ_{mfp}
- Ions? 1% ionization, 2x10^{14} cm^{-3}, 5e8 s^{-1}, λ = 2mm

TABLE II. Momentum-transfer cross section for electron-helium collisions.

ϵ (eV)	$q_m(\epsilon)$ (Å^2)
4.00	6.62
5.00	6.31
6.00	6.00
7.00	5.68
8.00	5.35
9.00	5.03
10.00	4.72
11.00	4.44
12.00	4.15

Milloy, Crompton PRA77

- **electron collision rate in completely ionized plasmas**:

$$\nu_e = 2.91 \times 10^{-6} n_e \ln\Lambda\, T_e^{-3/2}\,\mathrm{s}^{-1}$$

For Low Temperature Plasmas at low density need method which is "mostly" collisionless

Given particles, how to calculate?

- Coulomb interaction leads to N_p^2 force computations

$$\frac{d\gamma_i v_i}{dt} = \frac{q_i}{\epsilon_0 m_i} \sum_j q_j \frac{\mathbf{x}_i - \mathbf{x}_j}{\left|\mathbf{x}_i - \mathbf{x}_j\right|^3}$$

- Lenard-Weichert (retarded potentials) - worse due to need to keep history

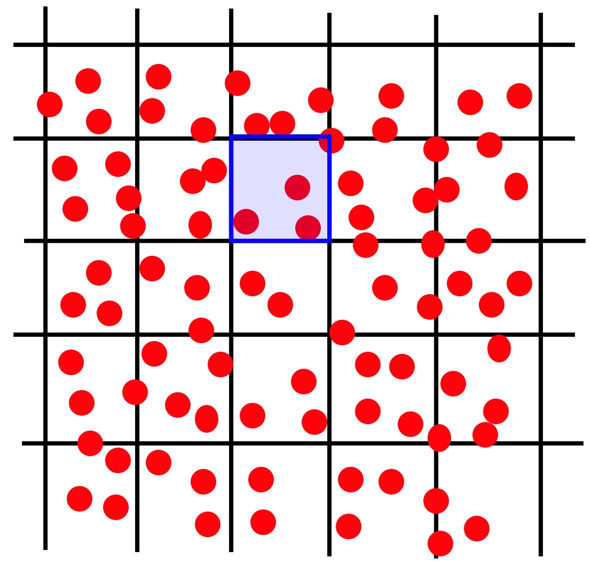
$$\frac{d\gamma_i v_i}{dt} = \frac{q_i}{\epsilon_0 m_i} \sum_j q_j F_{ij}(\mathbf{x}_i, \mathbf{x}_i(t-\tau))$$

- For 10^9 particles, compute 10^{18} interactions/step

Particle In Cell (PIC) reduces to N_p scaling

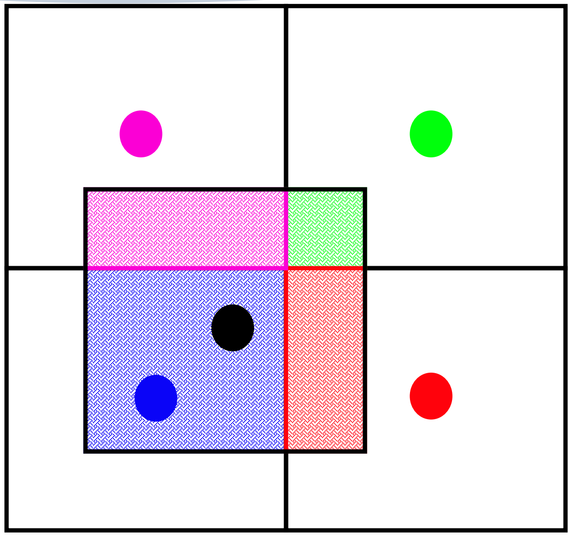
- Valid when short range forces can be treated probabilistically

- Particle contributions to charges and currents are added to each cell: $O(N_p)$ operations
- Forces on a particle are found from interpolation of the cell values: $O(N_p)$ operations



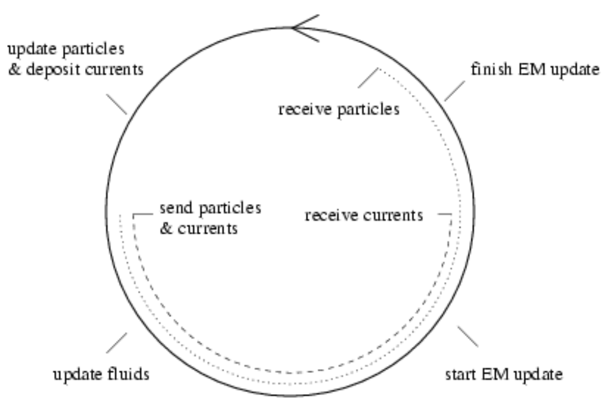
Finding the force: interpolation (gather)

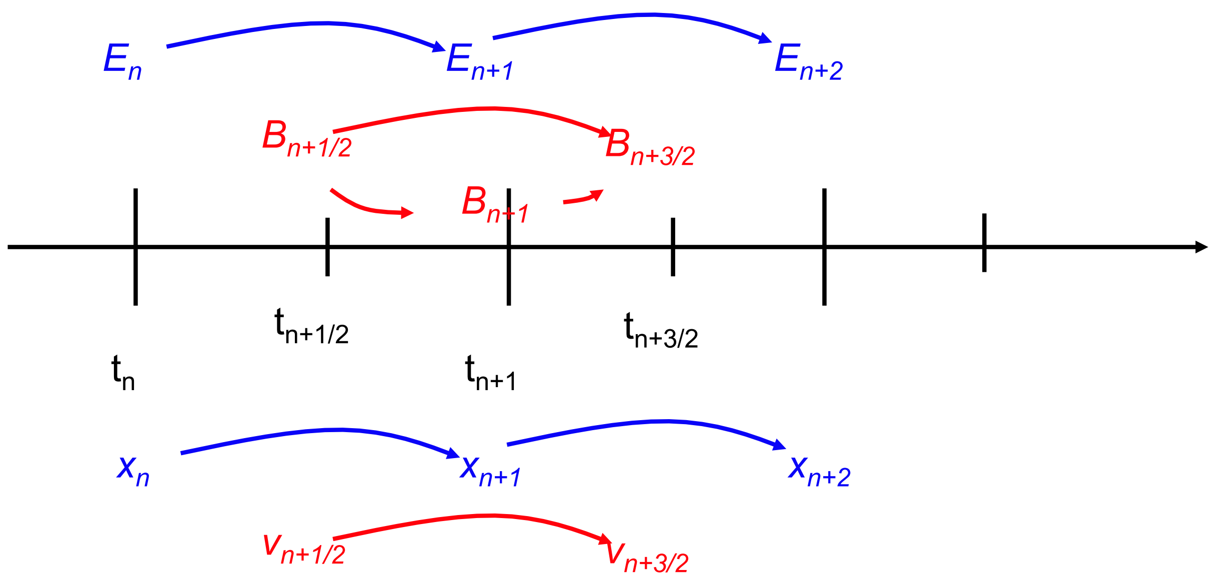
- Linear weighting for each dimension
  - 1D: linear
  - 2D: bilinear = area weighting
  - 3D: trilinear = volume weighting
- Force obtained through 1st order, error is 2nd order
- For simplicity, no loss of accuracy, weight first to nodal points



Full cycle: leap-frog

- General
- Electrostatic
- Electromagnetic



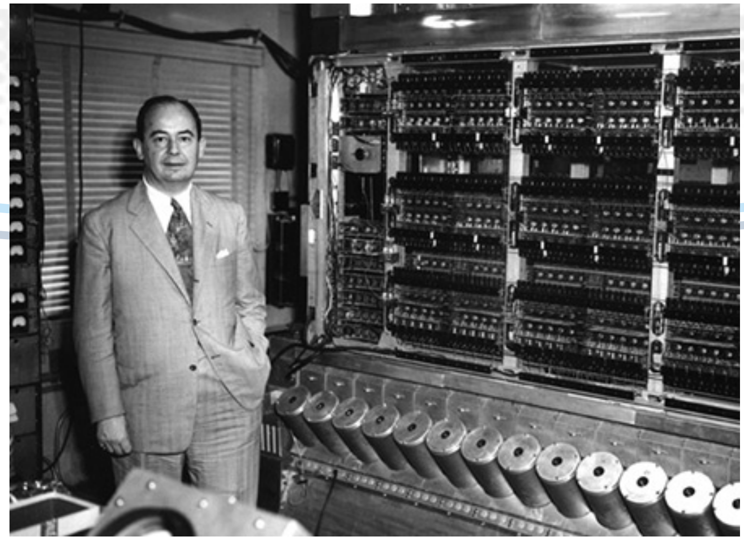


How can we get more computational results?

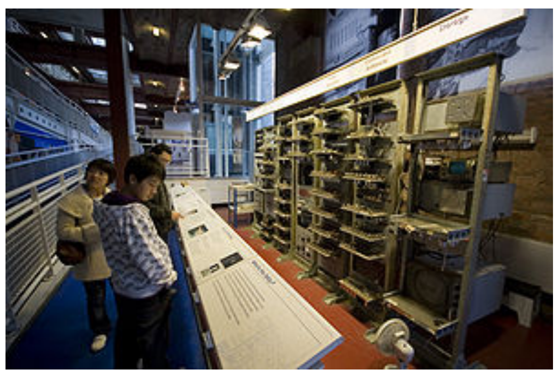
- Bigger/faster machines
- Better, perhaps more adapted, algorithms
- Use of new compute devices
- Make computation available to more people

We've been on the bigger-machine path for a long time

The Baby had a 32-bit word length and a memory of 32 words (1 kilobit) … The program consisted of 17 instructions and ran for 52 minutes before reaching the correct answer of 131,072, after the Baby had performed 3.5 million operations (for an effective CPU speed of 1.1 kIPS)



John von Neumann, 1945, IAS stored program computer. See *Turing's Cathedral*



Replica of Manchester Baby (Wikipedia), was the world's first stored-program computer. 1948

Kiloscale (1945?)
Megascale
Gigascale
Terascale
Petascale
Exascale (2023?)

Speed-Limited Particle-In-Cell: the better algorithm path

Basic PIC methods – solve for distribution function by method of characteristics

- Conservation form

$$\partial_t f(\mathbf{x},\mathbf{v},t) + \nabla_x[\mathbf{v} f(\mathbf{x},\mathbf{v},t)] + \nabla_v[\mathbf{a}(\mathbf{x},\mathbf{v},t) f(\mathbf{x},\mathbf{v},t)] = 0$$

- Advection form

$$\partial_t f(\mathbf{x},\mathbf{v},t) + \mathbf{v}\cdot\nabla_x[f(\mathbf{x},\mathbf{v},t)] + \mathbf{a}(\mathbf{x},\mathbf{v},t)\cdot\nabla_v[f(\mathbf{x},\mathbf{v},t)] = 0$$

- Solution:

$$f(\mathbf{x},\mathbf{v},t) = \sum_p w_p \delta\left(\mathbf{x}-\mathbf{x}_p(t)\right)\delta\left(\mathbf{v}-\mathbf{v}_p(t)\right)$$

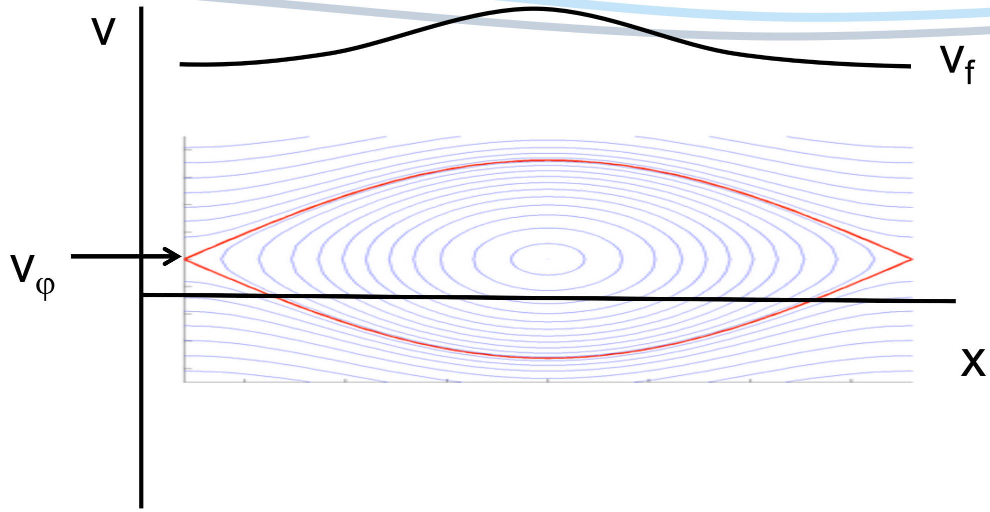
- w_p= particle weight
- x_p, v_p = particle trajectory, satisfying
- Discretize, put on grid, add fields…

$$\dot{\mathbf{x}}_p = \mathbf{v}_p \qquad \dot{\mathbf{v}}_p = \mathbf{a}(\mathbf{x}_p,\mathbf{v}_p,t)$$

Explicit particle in cell limited

- Solve harmonic oscillator by same method, find that time step must be smaller than $2/\omega_0$. Otherwise goes unstable.
- Also must limit time step so that particles do not cross more than about a cell per step. Otherwise inaccurate.
- These limitations are true even when the distribution not changing on relevant time scales:
  - Electron flow in gas
  - Quasineutral plasma expansion
  - Plasma thrusters

Fast electrons are in equilibrium with slow (ion-scale) dynamics



- Resonance moving slowly with respect to particles at some velocity
- Particles at that velocity essentially in equilibrium with the perturbation
- Time derivative can be ignored

SLPIC is based on a simple ansatz

$$f(\mathbf{x},\mathbf{v},t) = \beta(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)$$

$$\partial_t\left[\beta g(\mathbf{x},\mathbf{v},t)\right] + \nabla_x[\beta \mathbf{v} g(\mathbf{x},\mathbf{v},t)] + \nabla_v[\beta \mathbf{a}(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)] = 0$$

$$\partial_t\left[g(\mathbf{x},\mathbf{v},t)\right] + \nabla_x[\beta \mathbf{v} g(\mathbf{x},\mathbf{v},t)] + \nabla_v[\beta \mathbf{a}(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)] = \partial_t\left[(1-\beta)g(\mathbf{x},\mathbf{v},t)\right]$$

- Choose β such that
  - For slow particles, β = 1 (RHS vanishes)
  - For fast particles, β ➔0, RHS unimportant compared with phase space derivatives
  - In both cases, RHS can be neglected

$$\partial_t\left[g(\mathbf{x},\mathbf{v},t)\right] + \nabla_x[\beta \mathbf{v} g(\mathbf{x},\mathbf{v},t)] + \nabla_v[\beta \mathbf{a}(\mathbf{x},\mathbf{v},t)g(\mathbf{x},\mathbf{v},t)] = 0$$

- Distribution evolves as if velocity *and* acceleration reduced for fast particles

Significant freedom in the prefactor

- Choose β such that
  - For slow particles, β = 1 (RHS vanishes)
  - For fast particles, β ➔0, RHS unimportant compared with phase space derivatives

$$\beta(\mathbf{x},\mathbf{v},t) = \frac{v_0}{\sqrt{v_0^2 + v^2}} \qquad \beta\mathbf{v} = \frac{\mathbf{v}}{\sqrt{1+\left(v/v_0\right)^2}}$$

- Freedom to pick β to be a function of position
  - Variable grid: refine in plasma sheath, choose smaller β there
  - Increase β in time when faster phenomena appear

SLPIC equations can be solved in same way as original

$$g(\mathbf{x},\mathbf{v},t) = \sum_p w_p \delta\left(\mathbf{x} - \mathbf{x}_p(t)\right)\delta\left(\mathbf{v} - \mathbf{v}_p(t)\right)$$

$$\dot{\mathbf{x}}_p = \beta(\mathbf{x}_p,\mathbf{v}_p,t)\mathbf{v}_p \qquad \dot{\mathbf{v}}_p = \beta(\mathbf{x}_p,\mathbf{v}_p,t)a(\mathbf{x}_p,\mathbf{v}_p,t)$$

- Particle accelerate, move more slowly
- Follow same trajectories
- Transform back to get actual distribution function

$$f(\mathbf{x},\mathbf{v},t) = \beta(\mathbf{x},\mathbf{v},t)\sum_p w_p \delta\left(\mathbf{x} - \mathbf{x}_p(t)\right)\delta\left(\mathbf{v} - \mathbf{v}_p(t)\right)$$

- Slowing down the particles makes them more dense. The prefactor counteracts that.

But, solving with particles not a requirement. Could use continuum methods on the speed limited equation

SLPIC is NOT

- A coordinate transformation (would not change the way particles move through space)
- A delta-f approach (the weight does not vary in time; not separation into two distributions)
- Even necessarily a PIC approach. One could use continuum methods.

SLPIC is simply an ansatz that allows one to treat fast particles as if in equilibrium while treating slow particles exactly

SLPIC fits easily into the PIC cycle

- Field solve (unchanged)
- Particles
  - Interpolate: same
  - Accelerate: modified acceleration, point-wise implicit algorithms solved by quartic for unmagnetized
  - Move: Just move less by β (could be implicit when β depends on x)
  - Deposit: only change from standard pic is the variation of β from one end to other. Treatment known from δf.

To determine the plasma oscillation stability need to know plasma frequency

- Standard analysis, 1D

$$-i(\omega - k\beta v)\tilde{g}_1 = -\tilde{a}_1 \partial_v [\beta g_0(v)] \qquad g_1 = \tilde{g}_1 \exp(ikx - i\omega t)$$

$$\tilde{n}_1 = \int dv \tilde{f}_1 = \int dv \beta \tilde{g}_1 = -ia_1 \int dv \frac{\beta}{\omega - k\beta v} \partial_v [\beta g_0]$$

$$\tilde{n}_1 = ia_1 \left\langle \partial_v \frac{\beta}{\omega - k\beta v} \right\rangle \qquad 1 - \frac{\omega_p^2}{\omega^2} \left\langle \frac{\beta^2 + \beta' \omega / k}{(1 - k\beta v/\omega)^2} \right\rangle = 0$$

$$\omega_s^2 \approx \omega_p^2 \frac{v_0^2}{v_e^2}$$

- Plasma frequency reduced by v_0/v_e
- Both Δt limits relaxed by same factor

Changes to stability?

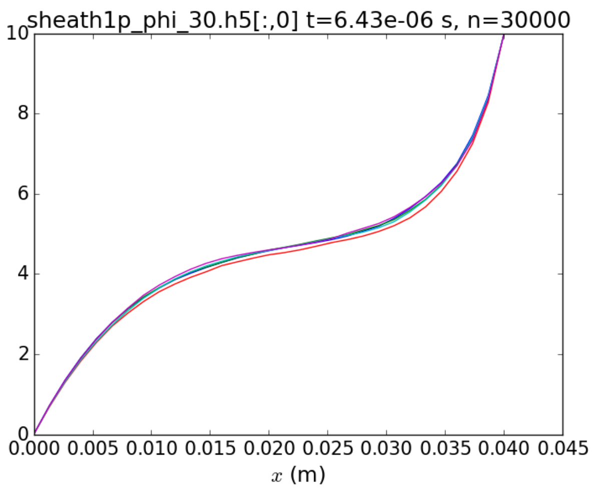
- $v_p \Delta t \leq \Delta x$: Relaxed by ratio of electron thermal velocity to perturbation velocity
- $\omega_e \Delta t \leq 1$: Relaxed by ratio of electron thermal velocity to perturbation velocity
- $\Delta x \leq \lambda_e$: Conjecture: much reduced
- EM CF (if relevant): the same

Expect big gains in computational speeds when

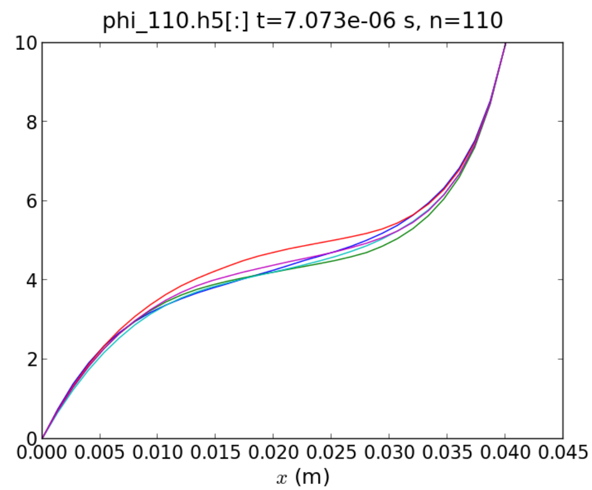
- $v_0 << v_e$
- Need not resolve electron plasma oscillations
- Especially good for
  - $T_e > T_i$
  - Large mass ions
- Examples
  - plasma sheath
  - free expansion
  - plasma thrusters

SLPIC finds sheaths in many fewer steps

- In sheath, electron velocity distribution critical
- But Boltzmann approximation not accurate near boundary: at best a clipped Maxwellian



Standard PIC, 30000 steps for stability



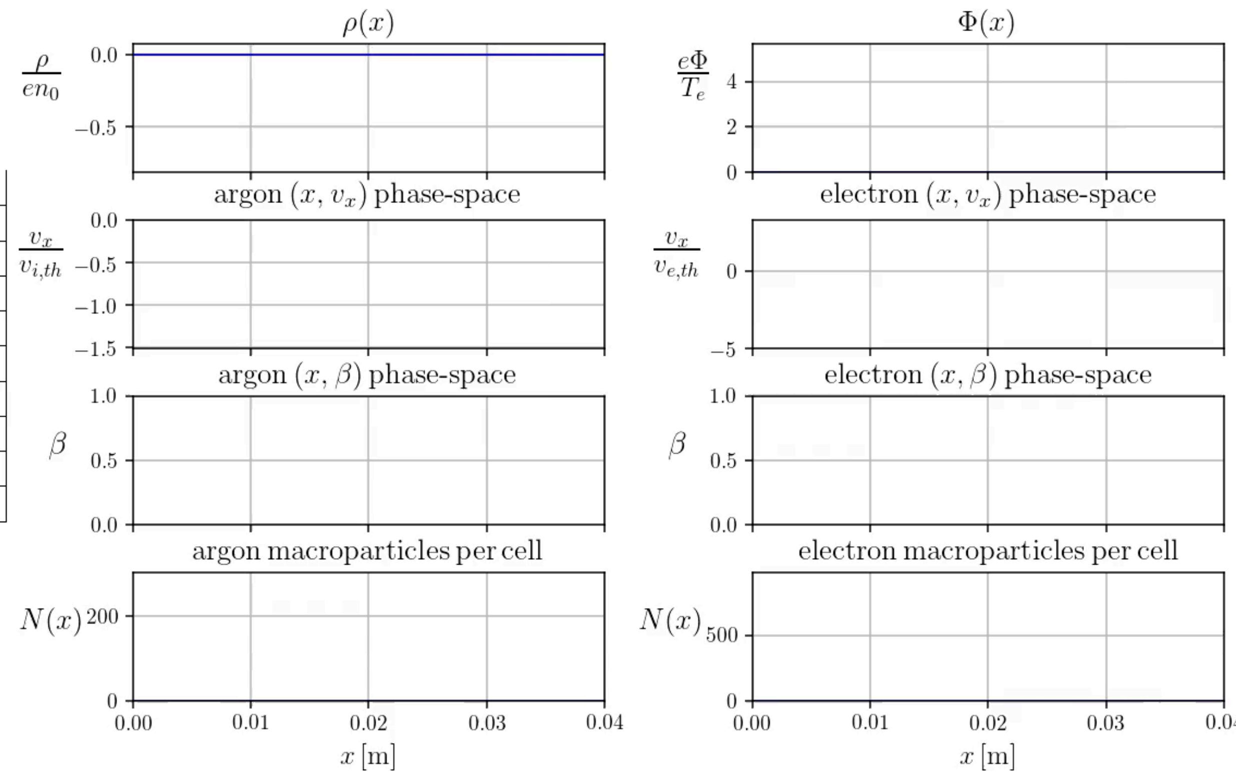
SLPIC, 110 steps for stability

SLPIC gets free expansion correct with much reduced computational requirements

- Argon; In free expansion, electrons held back by ions

VSim

	PIC	SLPIC
$\Delta t \frac{\omega_{pe}}{2\pi}$	0.0041	1.3
# steps	0	0
# electrons	0	0
# ions	0	0
m_i/m_e	$40 \cdot 1836$	
speed limit	N/A	$0.013\,v_{e,th}$
cpu time (h:m:s)	00:00:12	00:00:00
sim time t	0.00 μs	
speedup	886	



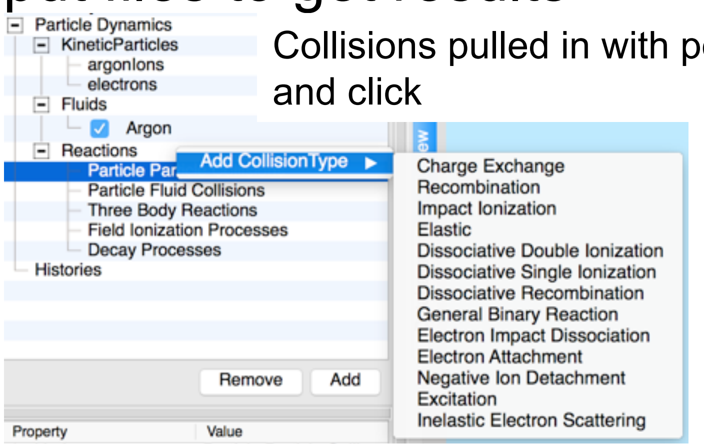
Multiple directions for SLPIC

- Applications
- Combine with implicit (energy conserving?)
- Use in continuum codes
- Inclusion of strong magnetic fields ($\omega_e \leq \Omega_e$)
- Collisions
- Spatial variation of β
- Combine with advanced computational devices (GPU, multi-/many core, AVX)

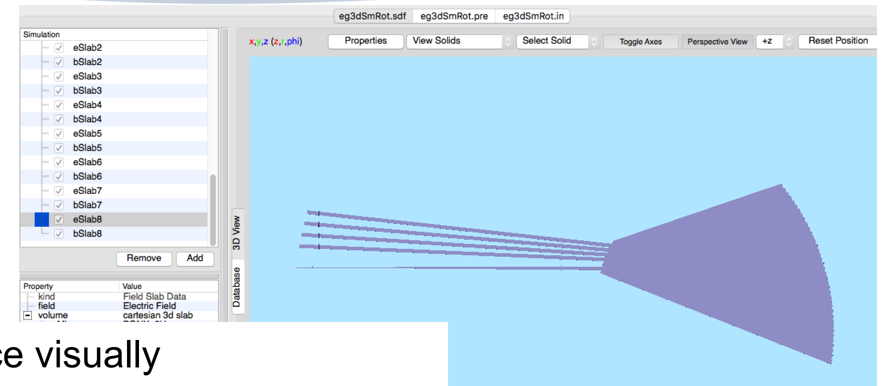
Democratization: let anyone participate

Democratization of computation requires ease of use

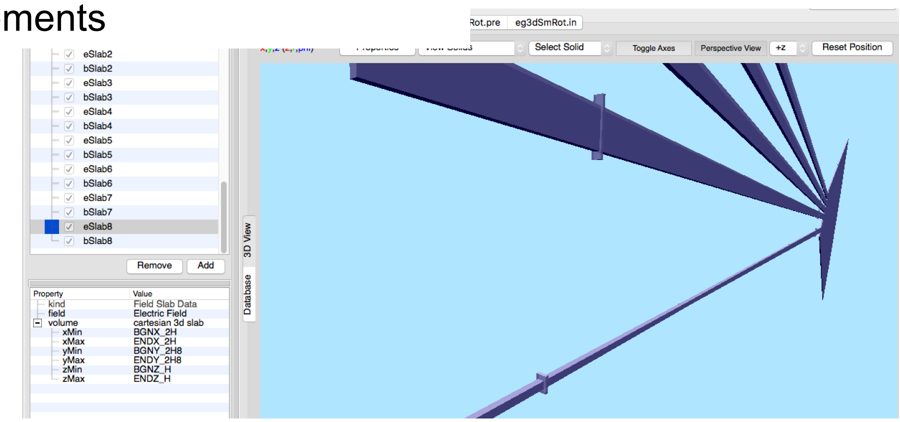
- Democratization
  - Any physics knowledgeable research can set up a problem easily
  - Any engineer with an undergraduate degree can use the code rapidly in design
- Should not be forced to build, learn input files to get results



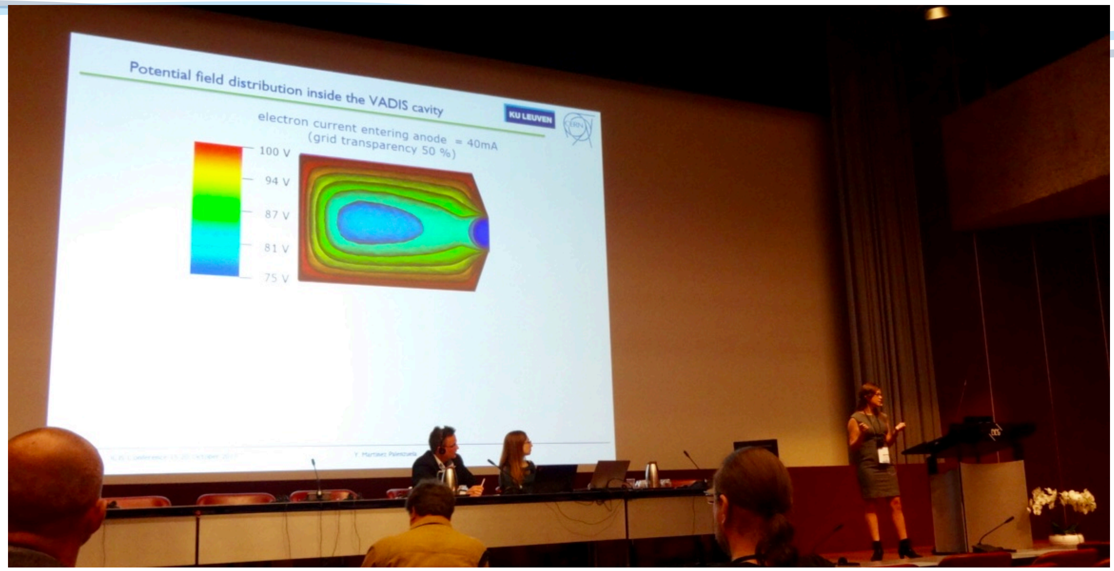
Collisions pulled in with point and click



Place visually
Line up with other simulation elements



Democratization: Yisel Martinez Palenzuela (CERN, KU Leuven) wins multiple awards using VSim



- Poster award: https://fys.kuleuven.be/iks/newsitems/yisel-martinez-awarded-poster-prize-at-the-eurisol-df-conference
- Young scientist award: https://fys.kuleuven.be/iks/newsitems/yisel-martinez-palenzuela-was-awarded-the-medicis-promed-funded-young-scientist-award-for-the-best-presentation-at-the-icis2017

Democratization: Nathan Hicks U Alaska Anch, uses VSim, gets NSF funding

Summary

- Computation has much to contribute to plasma physics
  - Elucidation
  - Prediction
  - Optimization
  - Discovery
- Getting to the level: pursue multiple fronts
  - Bigger/faster machines
  - New algorithms
  - Software/abstraction
  - Ease of use