Working Group 2 Summary

Working Group 2 conveners –

David L. Bruhwiler (RadiaSoft)
Prof. Alexey Arefiev (UCSD)

radiasoft

AAC'22 Advanced Accelerator Concepts Workshop

November 6 - 11, 2022

Hyatt Regency Long Island, NY

Thematic distribution of WG2 presentations –

- Exascale PIC
    - WarpX
    - PIConGPU
- Integrated Infrastructure – Software and Facilities
    - virtual facilities / digital twins
    - integration with experimental facilities
    - synthetic diagnostics
    - machine learning
    - standards: code coupling, code integration, workflows, online models, ML
- Reduced models
    - quasi-static & cylindrical PIC
    - MHD for plasma channel formation
    - beam loading in TW linacs
- PIC algorithms
    - ionization physics
    - current deposition
    - particle pusher
    - moving towards strong-field QED
- Other algorithms
    - Vlasov with mesh refinement
    - differentiable computing
    - high-power laser amplifiers
- Simulation of experiments

Exascale PIC

Exascale PIC


From Compact Plasma Particle Sources to Advanced Accelerators with Modeling at Exascale

Axel Huebl

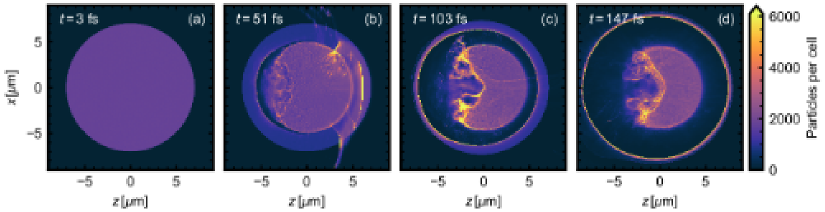
Lawrence Berkeley National Laboratory

On behalf of the AMP team (lead: J-L Vay @ LBNL)
LBNL, LLNL, SLAC, CEA, DESY, Modern Electron, CERN

with contributions by A Debus, BE Marré,
S Luedtke, WB Mori, A Beck et al.

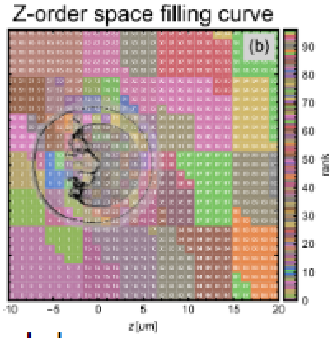
Selected Challenges for Exascale Modeling - Supercomputing

Exascale Needs Active Load Balancing and often **adaptive resolution**



Density fluctuations:
beams & particles move

- LPI: acceleration front
- PBA: injected beam


Z-order space filling curve

Open challenges:

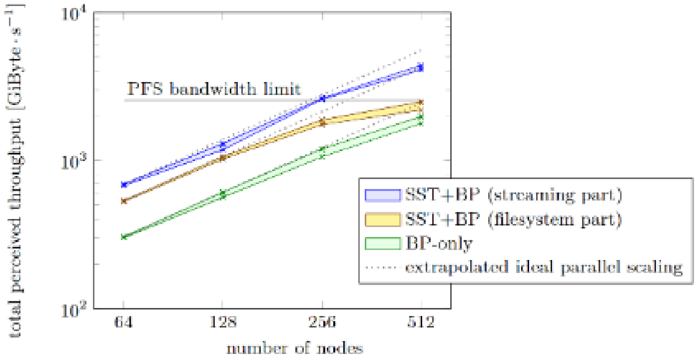
- communication cost model
- sub-step balancing

K Germaschewski et al., JCP ('16); J Derouillat et al., CPC ('18)
M Rowan et al., PASC21 ('21); K. G. Miller et. al., CPC ('21)

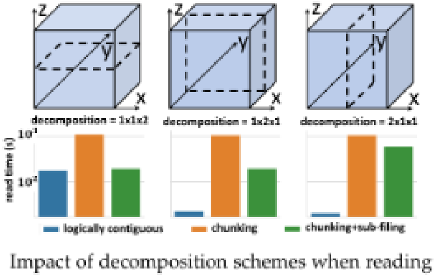
Concepts for PByte-Scale Data Analysis

main contributors: Axel Huebl, Franz Poeschel, Michael Bussmann, Norbert Podhorski, William Godoy, Lipeng Wang, Junmin Gu, Scott Klasky, et al.

Streaming Data Pipelines:



F Poeschel, A Huebl et al., SMC21 (2022)



Impact of decomposition schemes when reading

Online Data Layout Reorganization:
L Wan, A Huebl et al., TPDS (2021)

Exascale PIC

Jean-Luc Vay

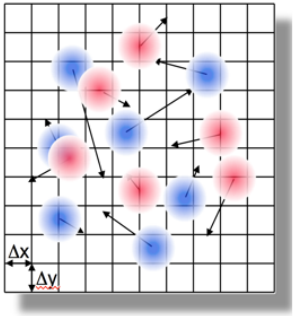
Lawrence Berkeley National Laboratory

On behalf of the WarpX team
LBNL, LLNL, SLAC, CEA, DESY, Modern Electron, CERN

Latest advances in the Particle-In-Cell code WarpX for efficient modeling of plasma accelerators at Exascale

WarpX: Multi-Physics Particle-in-Cell Code for Exascale

Particle-in-Cell



macro-
particles

electro-
magnetic (EM)
fields on a grid

Advanced Algorithms Pioneered by our Team

boosted frame, spectral solvers, Galilean frame, MR, …

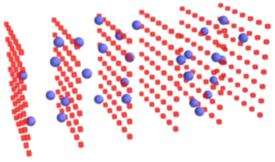
Multi-Physics Modules

field ionization of atomic levels, Coulomb collisions, QED processes (e.g. pair creation), macroscopic materials, embedded boundaries + CAD, …

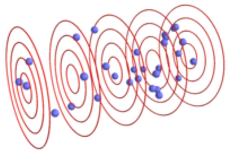
Open source ecp-warpx.github.io

Geometries

- 1D3V, 2D3V, 3D3V and RZ (quasi-cylindrical)



3D Cartesian grid



Cylindrical grid (schematic)

Multi-Node parallelization

- MPI: 3D domain decomposition
- dynamic load balancing

On-Node Parallelization

- GPU: CUDA, HIP and SYCL
- CPU: OpenMP

Scalable, Parallel I/O

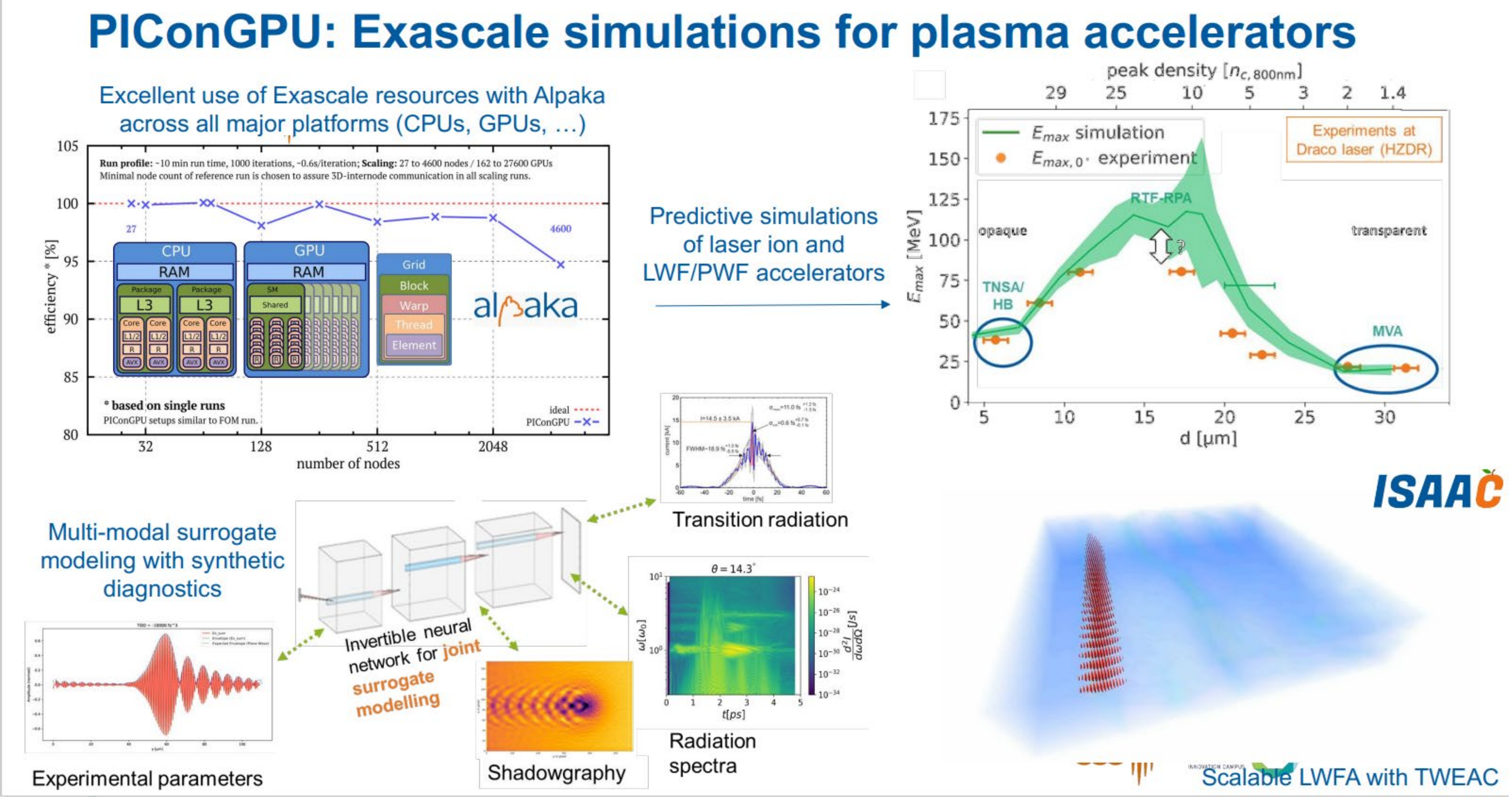
- AMReX plotfile and openPMD (HDF5 or ADIOS)
- in situ diagnostics

Exascale PIC

Now that we have Exascale, what can we do with it?
PIConGPU for next generation Accelerator Research

HZDR
HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

Michael Bussmann, Alexander Debus, Thomas Kluge, René Widera, Richard Pausch, Klaus Steiniger, Fin-Ole Carstens, Pawel Ordyna, Brian Marre, Ilja Göthel, Thomas Miethlinger, Anton Lebedev, Nico Hoffmann, Patrick Stiller, Anna Willmann, Franz Pöschel, Sergei Bastrakov, Bernhard Manfred Gruber, Jan Nikl, Marco Garten, Felix Meyer, Axel Huebl, Heiko Burau, Sunita Chandrasekaran, the experimental teams at HZDR, et al.!



PIConGPU: Exascale simulations for plasma accelerators

Excellent use of Exascale resources with Alpaka across all major platforms (CPUs, GPUs, …)

Run profile: ~10 min run time, 1000 iterations, ~0.6s/iteration; **Scaling:** 27 to 4600 nodes / 162 to 27600 GPUs
Minimal node count of reference run is chosen to assure 3D-internode communication in all scaling runs.

* based on single runs
PIConGPU setups similar to FOM run.

Predictive simulations of laser ion and LWF/PWF accelerators

Multi-modal surrogate modeling with synthetic diagnostics

Invertible neural network for joint surrogate modelling

Experimental parameters

Transition radiation

Shadowgraphy

Radiation spectra

Scalable LWFA with TWEAC

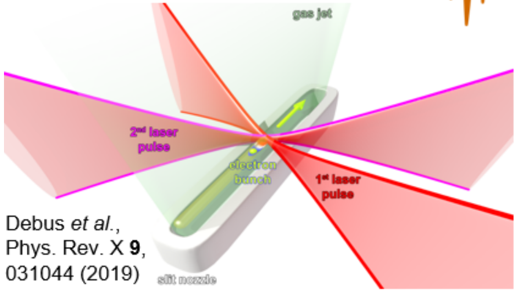
Exascale PIC

Alexander Debus[1], Klaus Steiniger[1], René Widera[1], Sergei Bastrakov[1], Finn-Ole Carstens[1], Felix Meyer[1], Richard Pausch[1], Marco Garten[1], Thomas Kluge[1], Jeffrey Kelling[1], Benjamin Hernandez Arreguin[6], Jeffrey Young[2,5], Franz Pöschel[2], Axel Hübl[4], David Rogers[6], Guido Juckeland[1], Sunita Chandrasekaran[2,3], Michael Bussmann[2,1], Ulrich Schramm[1]

PIConGPU

Traveling-wave electron accelerators

Towards scalable laser-plasma accelerators beyond 10 GeV



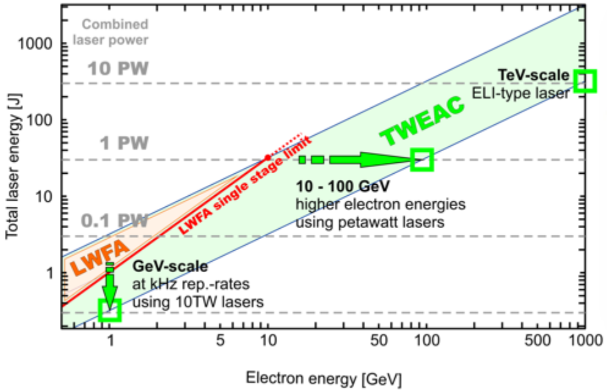
Debus *et al.*, Phys. Rev. X **9**, 031044 (2019)

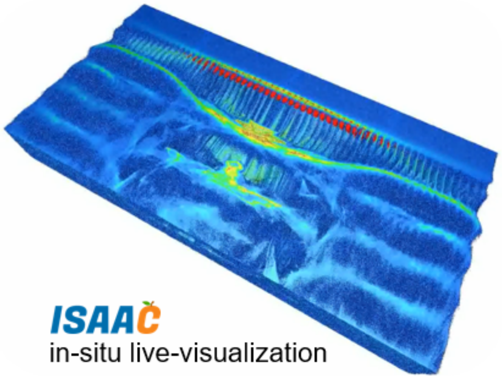
Traveling-wave electron acceleration (TWEAC)
Simultaneously circumvents the LWFA limitations of diffraction, dephasing and depletion **without staging**.

Single-staged TWEAC are in principle arbitrarily extendable in length, providing new avenues for energy-scalable LPAs.

Simulating TWEAC beyond 10GeV at high-fidelity require exascale resources.

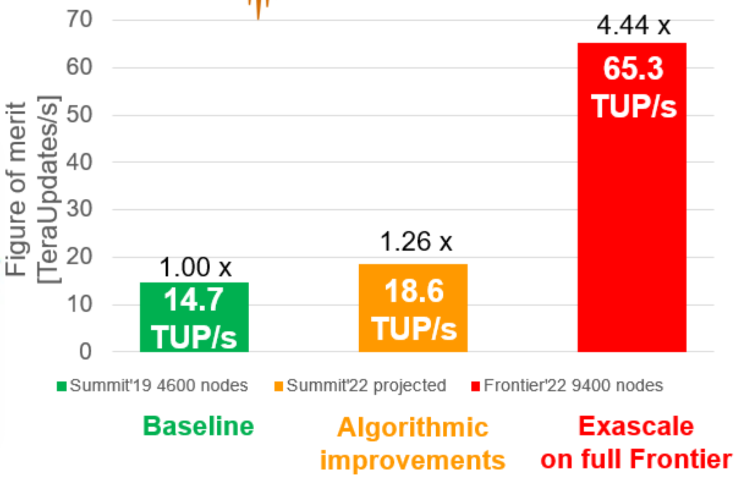
- Non-rotationally symmetric 3D geometry at high resolution.
- Long acceleration lengths far beyond LWFA depletion and dephasing need extended simulations over 10^6 - 10^7 timesteps at reasonable time to solution.





ISAAC
in-situ live-visualization

PIConGPU scales to full Frontier!

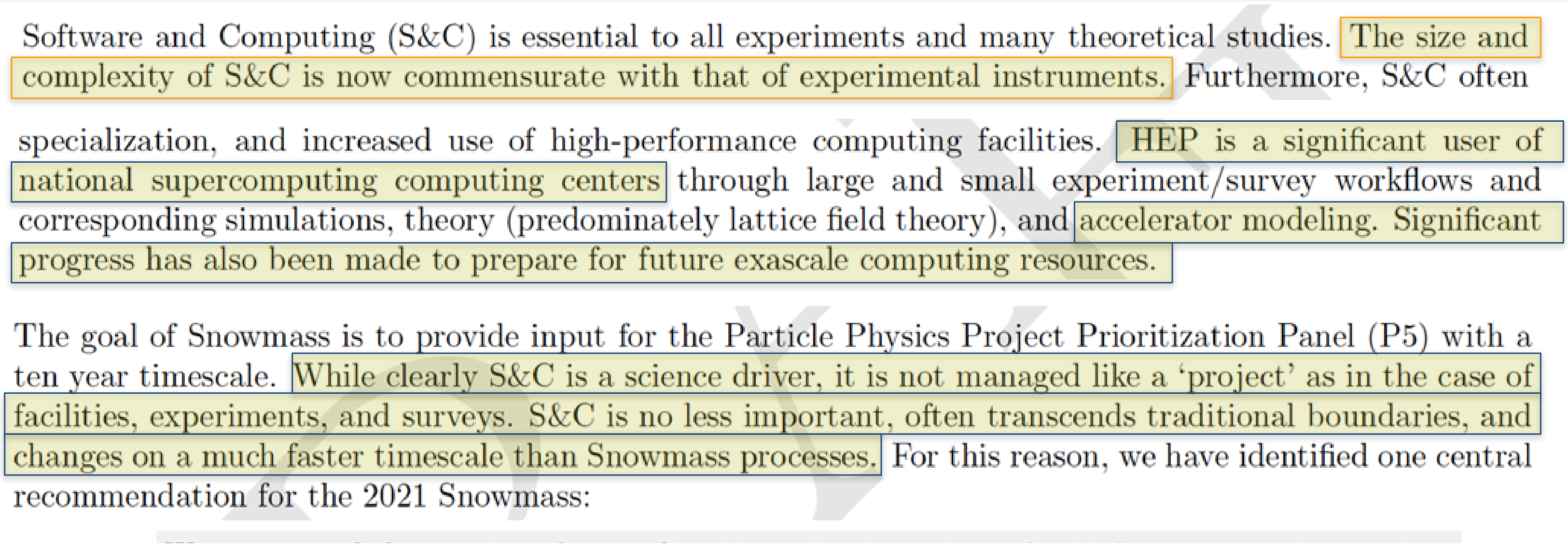


Dr. Alexander Debus | Advanced Accelerator Concepts Workshop 2022 | November 6 – 11, 2022 | Hyatt Regency Long Island, Hauppauge, NY, USA

HZDR

Integrated Infrastructure – Software and Facilities

Snowmass21: *Computational Frontier (CompF) report executive summary*



Software and Computing (S&C) is essential to all experiments and many theoretical studies. The size and complexity of S&C is now commensurate with that of experimental instruments. Furthermore, S&C often

specialization, and increased use of high-performance computing facilities. HEP is a significant user of national supercomputing computing centers through large and small experiment/survey workflows and corresponding simulations, theory (predominately lattice field theory), and accelerator modeling. Significant progress has also been made to prepare for future exascale computing resources.

The goal of Snowmass is to provide input for the Particle Physics Project Prioritization Panel (P5) with a ten year timescale. While clearly S&C is a science driver, it is not managed like a 'project' as in the case of facilities, experiments, and surveys. S&C is no less important, often transcends traditional boundaries, and changes on a much faster timescale than Snowmass processes. For this reason, we have identified one central recommendation for the 2021 Snowmass:

Integrated Infrastructure – workflows & standards

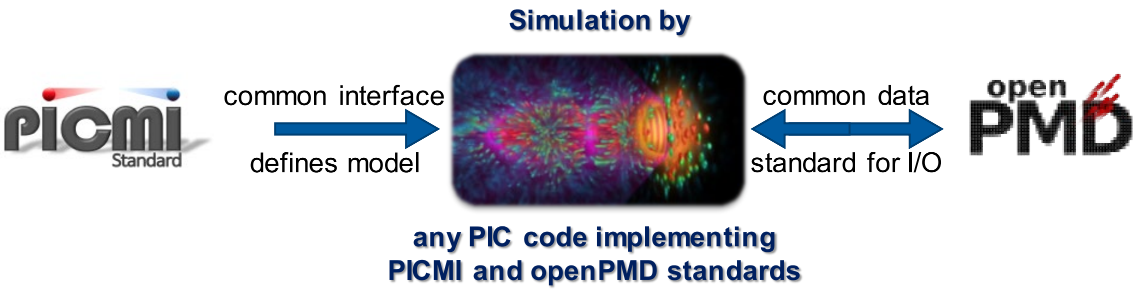
Now that we have Exascale, what can we do with it?
PIConGPU for next generation Accelerator Research

Michael Bussmann, Alexander Debus, Thomas Kluge, René Widera, Richard Pausch, Klaus Steiniger, Fin-Ole Carstens, Pawel Ordyna, Brian Marre, Ilja Göthel, Thomas Miethlinger, Anton Lebedev, Nico Hoffmann, Patrick Stiller, Anna Willmann, Franz Pöschel, Sergei Bastrakov, Bernhard Manfred Gruber, Jan Nikl, Marco Garten, Felix Meyer, Axel Huebl, Heiko Burau, Sunita Chandrasekaran, the experimental teams at HZDR, et al.!

More data
Digital
Twins

Standardization, testing and workflows

Challenges:
Standardization of Code architectures, implementation details and physics capabilities



Simulation by

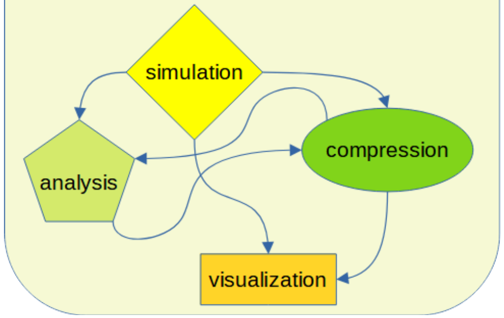
common interface
defines model

common data
standard for I/O

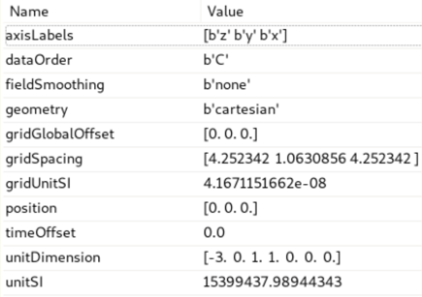
any PIC code implementing PICMI and openPMD standards

Complex workflows, streaming data

Interoperable:
Data exchange spans applications, platforms and teams



Reusable:
Rich and standardized description for physical quantities



Name	Value
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gridSpacing	[4.252342 1.0630856 4.252342]
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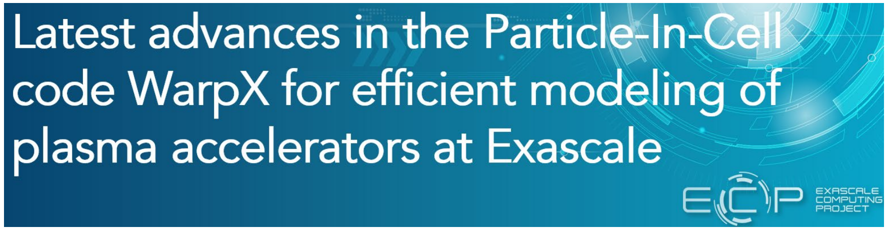
timeOffset	0.0
unitDimension	[-3. 0. 1. 1. 0. 0. 0.]
unitSI	15399437.98944343

Integrated Infrastructure – workflows & standards

Jean-Luc Vay

Lawrence Berkeley National Laboratory

On behalf of the WarpX team
LBNL, LLNL, SLAC, CEA, DESY, Modern Electron, CERN



Latest advances in the Particle-In-Cell code WarpX for efficient modeling of plasma accelerators at Exascale

Thoughts toward the establishment of a 10-year roadmap for advanced accelerator concepts computation

Proposal

- Ultimate goal: End-to-end Virtual Accelerators (EVA) with on-the-fly tunability from users of physics & numerics complexity
- Development and adoption of input/output standards as early activities of roadmap
- Development of workflows with plug & play swap of models/codes enabled by standards
- Development of EVAs and Virtual Test Stands (VTS) for various AAC thrusts (LWFA, PWFA, SWFA, DLA, …)
- Application of EVAs and Virtual Test Stands (VTS) for various AAC thrusts with milestones
    - E.g., for LWFA: model chain of 10 multi-GeV stages for HEP collider, maximizing beam charge and energy gain, and minimizing energy spread and emittance growth

Integrated Infrastructure – ML / synthetic diagnostics

Phase Space Reconstruction from Accelerator Beam Measurements Using Neural Networks and Differentiable Simulations

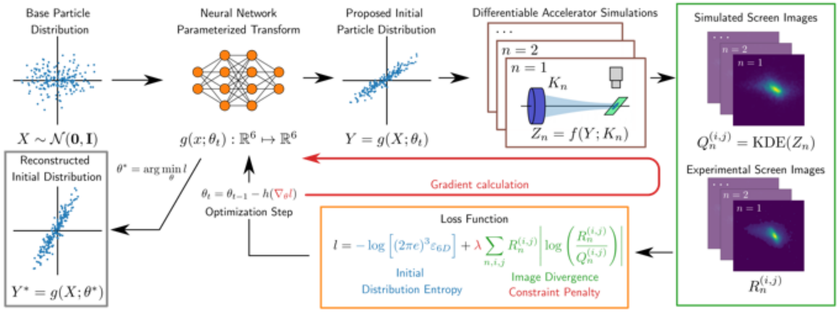
Ryan Roussel

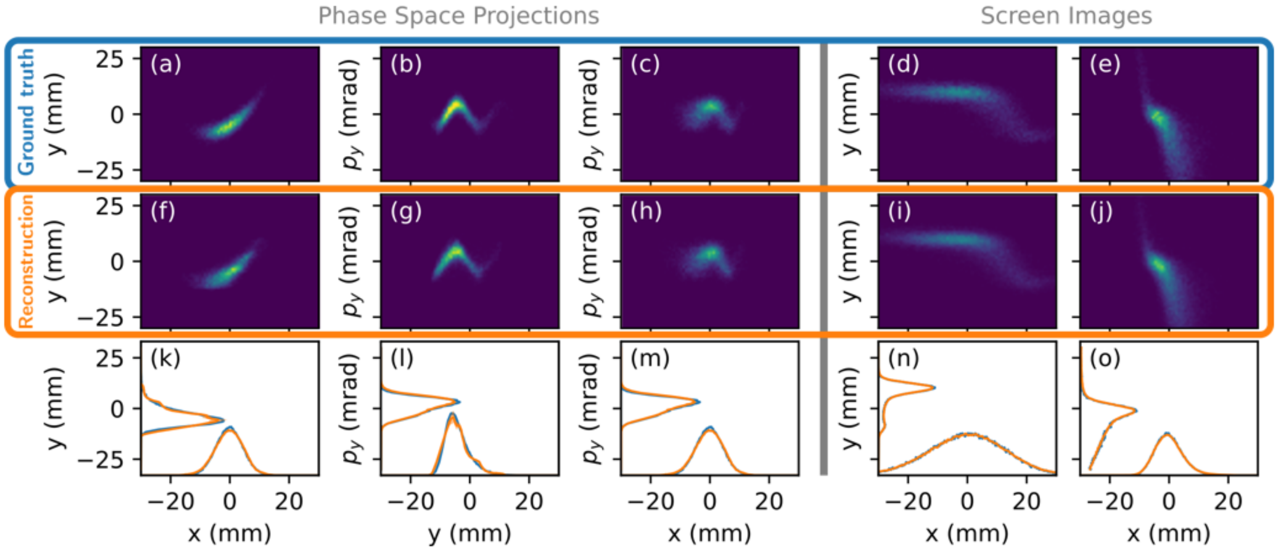
Phase Space Reconstruction from Accelerator Beam Measurements Using Neural Networks and Differentiable Simulations

SLAC

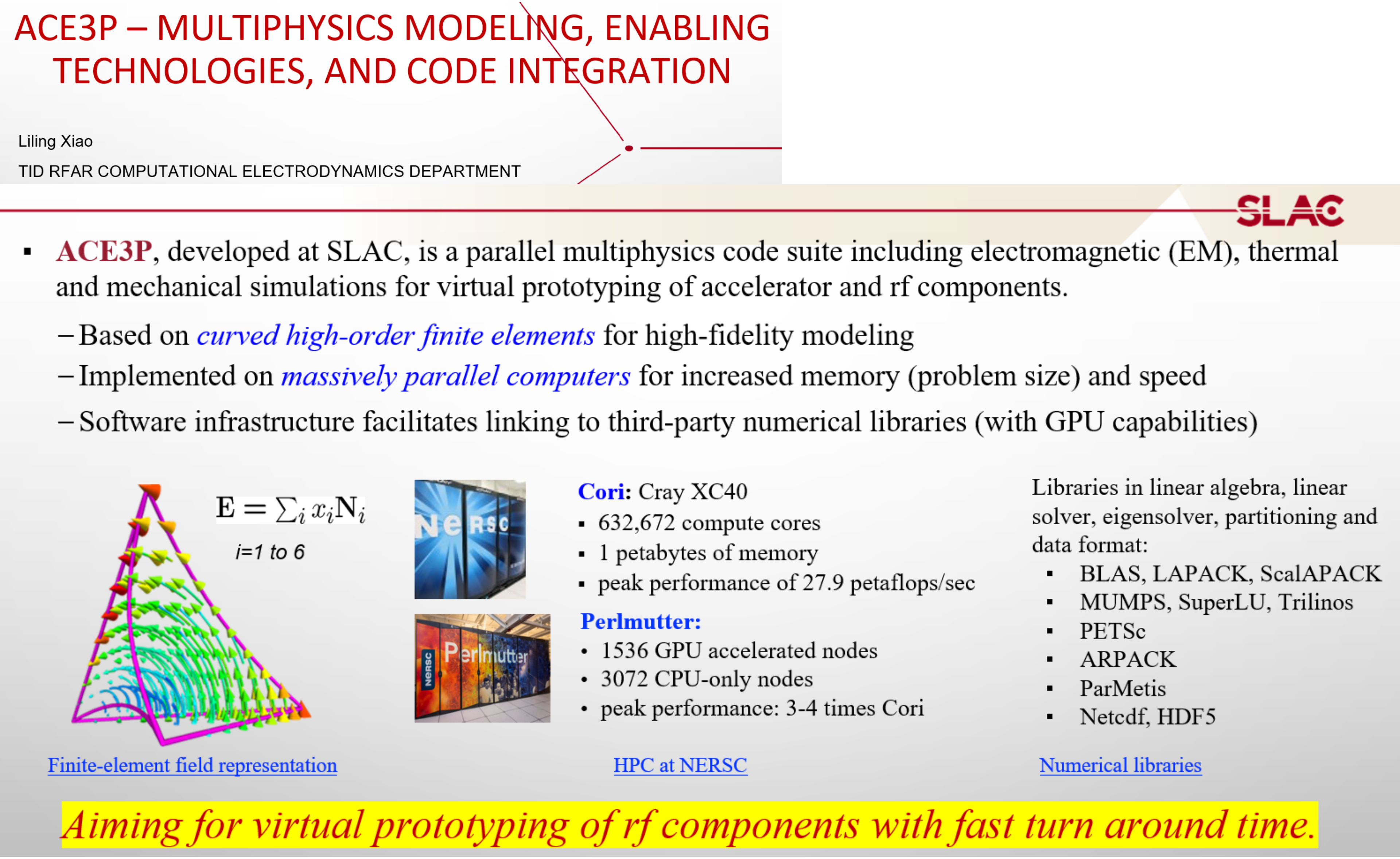
- We can create **detailed reconstructions of beam phase spaces** from simple tomographic accelerator measurements without special diagnostics

Details https://arxiv.org/abs/2209.04505





Integrated Infrastructure – multiphysics & code integration



ACE3P – MULTIPHYSICS MODELING, ENABLING TECHNOLOGIES, AND CODE INTEGRATION

Liling Xiao

TID RFAR COMPUTATIONAL ELECTRODYNAMICS DEPARTMENT

- **ACE3P**, developed at SLAC, is a parallel multiphysics code suite including electromagnetic (EM), thermal and mechanical simulations for virtual prototyping of accelerator and rf components.
  - Based on *curved high-order finite elements* for high-fidelity modeling
  - Implemented on *massively parallel computers* for increased memory (problem size) and speed
  - Software infrastructure facilitates linking to third-party numerical libraries (with GPU capabilities)

$\mathrm{E} = \sum_i x_i \mathrm{N}_i$

i=1 to 6

Finite-element field representation

Cori: Cray XC40
- 632,672 compute cores
- 1 petabytes of memory
- peak performance of 27.9 petaflops/sec

Perlmutter:
- 1536 GPU accelerated nodes
- 3072 CPU-only nodes
- peak performance: 3-4 times Cori

HPC at NERSC

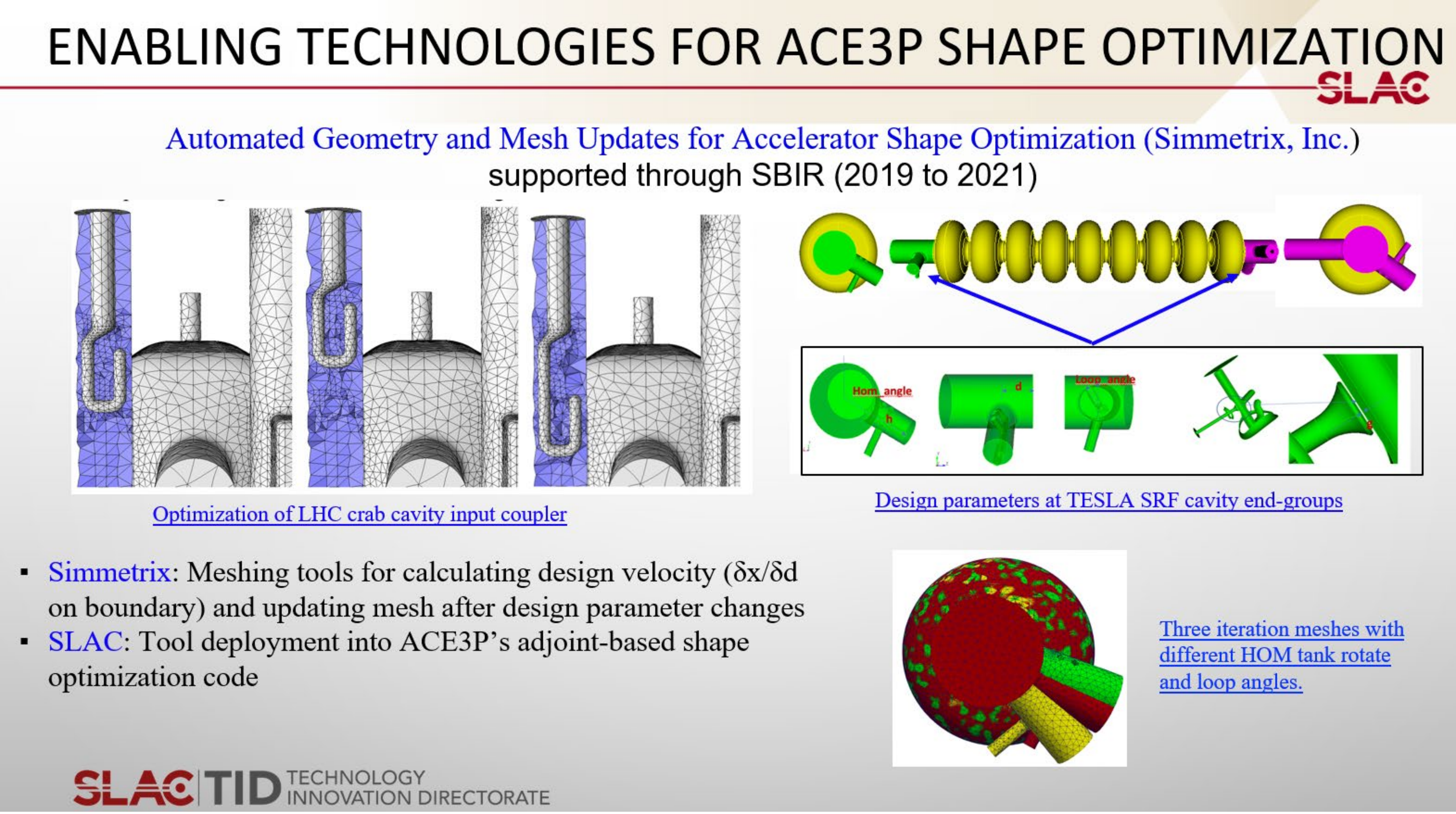
Libraries in linear algebra, linear solver, eigensolver, partitioning and data format:
- BLAS, LAPACK, ScalAPACK
- MUMPS, SuperLU, Trilinos
- PETSc
- ARPACK
- ParMetis
- Netcdf, HDF5

Numerical libraries

Aiming for virtual prototyping of rf components with fast turn around time.

Integrated Infrastructure – multiphysics & code integration

Liling Xiao



ENABLING TECHNOLOGIES FOR ACE3P SHAPE OPTIMIZATION

Automated Geometry and Mesh Updates for Accelerator Shape Optimization (Simmetrix, Inc.) supported through SBIR (2019 to 2021)

Optimization of LHC crab cavity input coupler

Design parameters at TESLA SRF cavity end-groups

- Simmetrix: Meshing tools for calculating design velocity (δx/δd on boundary) and updating mesh after design parameter changes
- SLAC: Tool deployment into ACE3P's adjoint-based shape optimization code

Three iteration meshes with different HOM tank rotate and loop angles.

PIC algorithms

PIC algorithms: ionization physics

Efficient algorithms for multi-level ionization of high-atomic-number gases and applications

Speaker: Aiqi Cheng[1]

Co-authors: Roman Samulyak[1], Rotem Kupfer[2], Navid Vafaei-Najafabadi[1]

This algorithm is able to

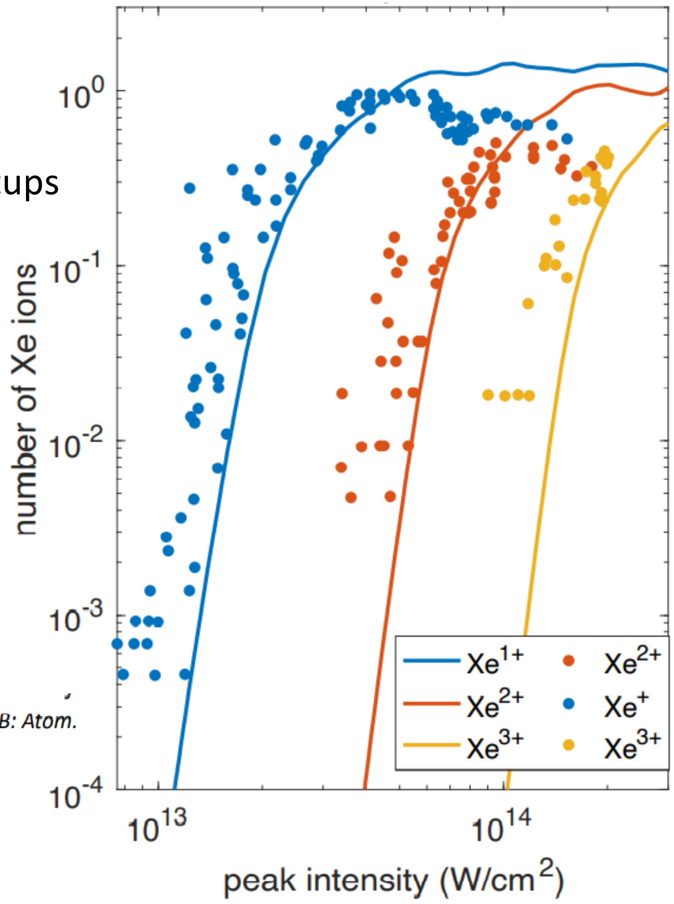
- resolve time scale difference between the ionization process and PIC computation time step by implementing analytical solution of the ionization dynamics
- reduce the memory allocation from recording number densities of different ion levels by solving 4-level ODE system, which greatly improves the efficiency of computation

Implementation into the 3D SPACE code enables some application including

- Computing ion yield from certain lasers from 3D
- Simulating ionization injection from high-Z gas in various experimental setups

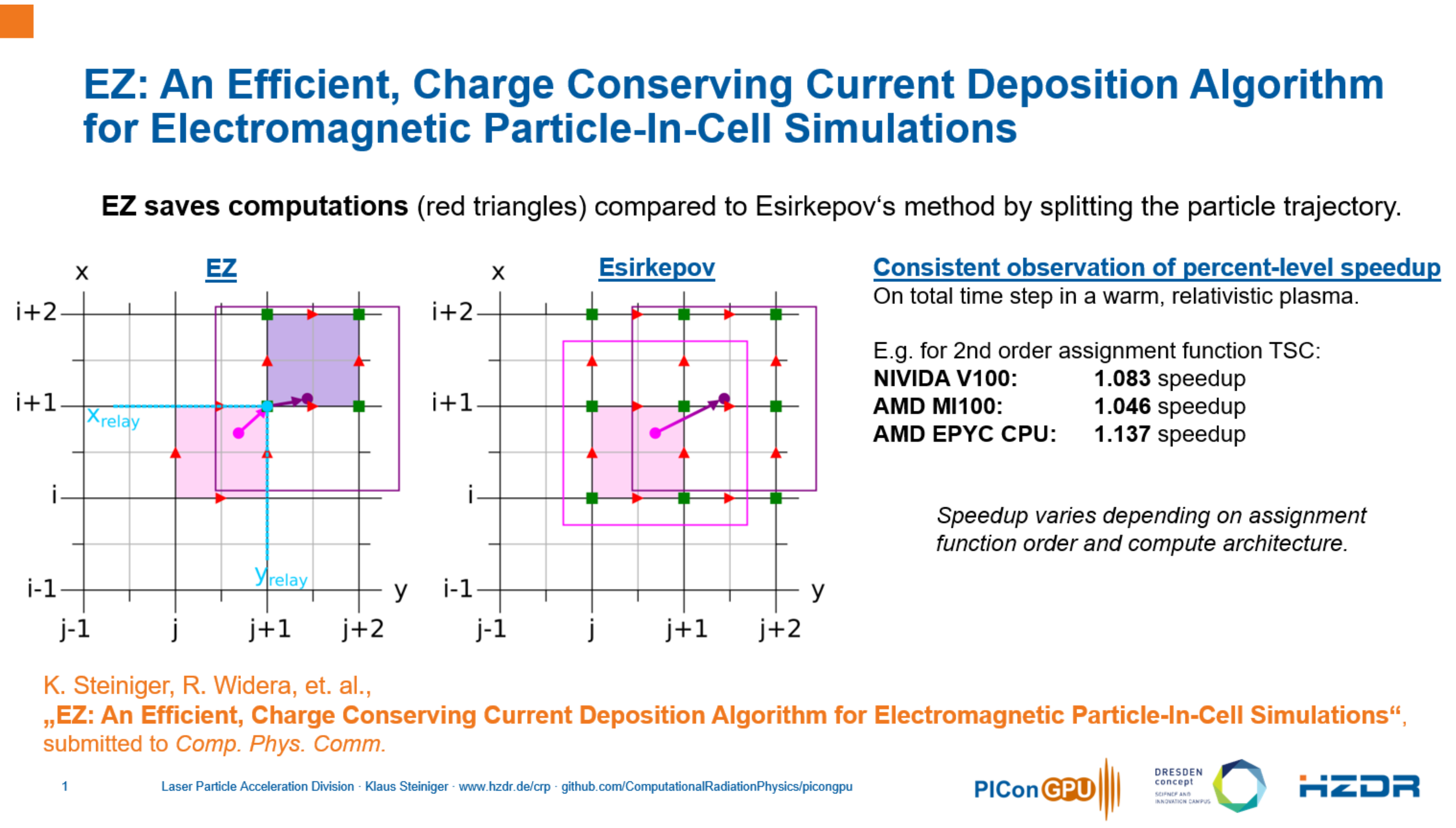
Future plans:

- reduced order models
- specialised MHD codes for long-time-scales
- novel methods for particle cooling
- integrated modeling and software



[3] F. Yergeau, S. L. Chin, and P. Lavigne, "Multiple ionisation of rare-gas atoms by an intense CO_2 laser (10^14W/cm^2)," *J. Phys. B: Atom. Mol. Phys.*, vol. 20, no. 4, pp. 723–739, Feb. 1987, doi: 10.1088/0022-3700/20/4/013.

PIC algorithms: current deposition



EZ: An Efficient, Charge Conserving Current Deposition Algorithm for Electromagnetic Particle-In-Cell Simulations

EZ saves computations (red triangles) compared to Esirkepov's method by splitting the particle trajectory.

Consistent observation of percent-level speedup
On total time step in a warm, relativistic plasma.

E.g. for 2nd order assignment function TSC:

NIVIDA V100:	**1.083** speedup
AMD MI100:	**1.046** speedup
AMD EPYC CPU:	**1.137** speedup

Speedup varies depending on assignment function order and compute architecture.

K. Steiniger, R. Widera, et. al.,
„EZ: An Efficient, Charge Conserving Current Deposition Algorithm for Electromagnetic Particle-In-Cell Simulations",
submitted to *Comp. Phys. Comm.*

1 Laser Particle Acceleration Division · Klaus Steiniger · www.hzdr.de/crp · github.com/ComputationalRadiationPhysics/picongpu

PIC algorithms: particle pusher at high fields

Daniel Gordon, Bahman Hafizi, Dan Younis

Special Unitary Particle Pusher

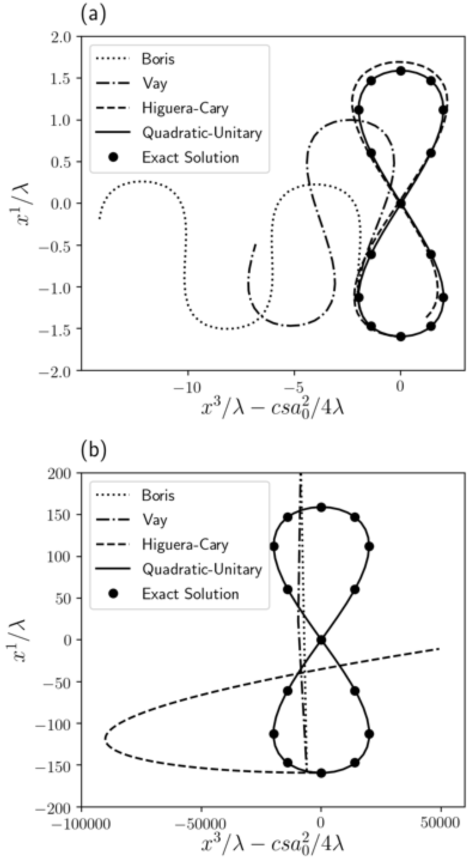
By making use of the spinor representation of a four-vector, an exact time translation in an arbitrary uniform field can be compactly written

$$\zeta = \begin{pmatrix} u^0 + u^3 & u^1 - iu^2 \\ u^1 + iu^2 & u^0 - u^3 \end{pmatrix}$$

$$\zeta(s+\Delta s) = \Lambda(\Delta s)\zeta(s)\Lambda^\dagger(\Delta s)$$

$$\boldsymbol{\Psi} = \frac{\Delta s}{2}\frac{e}{mc}(\mathbf{E} + i\mathbf{B})$$

$$\Lambda(\Delta s) = \cosh\Psi + \boldsymbol{\sigma}\cdot\frac{\boldsymbol{\Psi}}{\Psi}\sinh\Psi$$



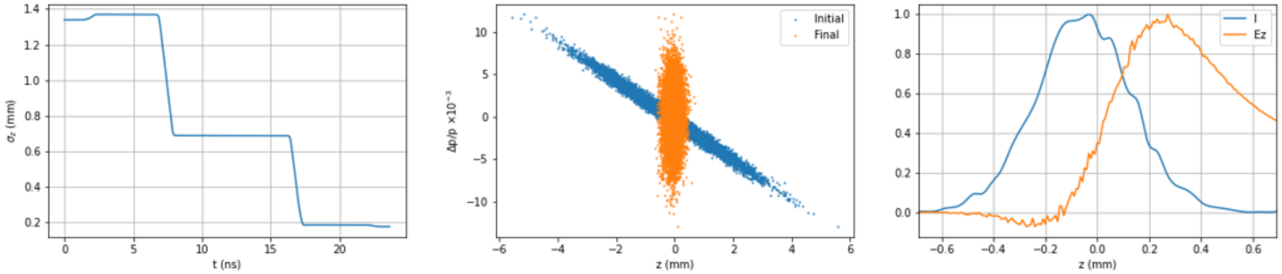
a=10

a=1000

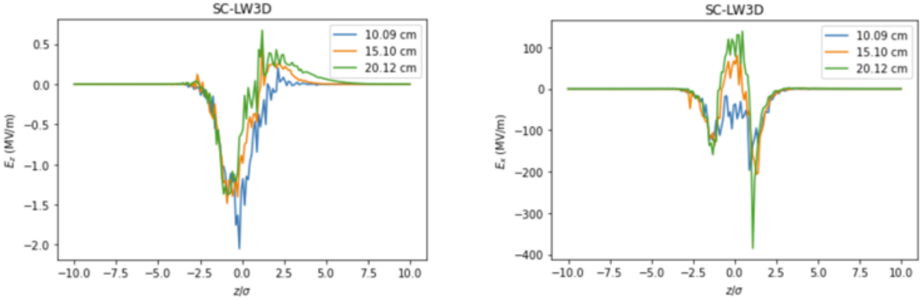
PIC algorithms: Lienard-Wiechert solver

First-Principle Simulations of Electron-Bunch Compression Using a Large-Scale Lienard-Wiechert Solver, *Afnan Al Marzouk, Northern Illinois University*

- Used the LW3D first-principle large-scale code (developed by R. Ryne) to perform simulations to the bunch compressor at AWA and showed compression by a factor of 7.5 and computed CSR through the process.

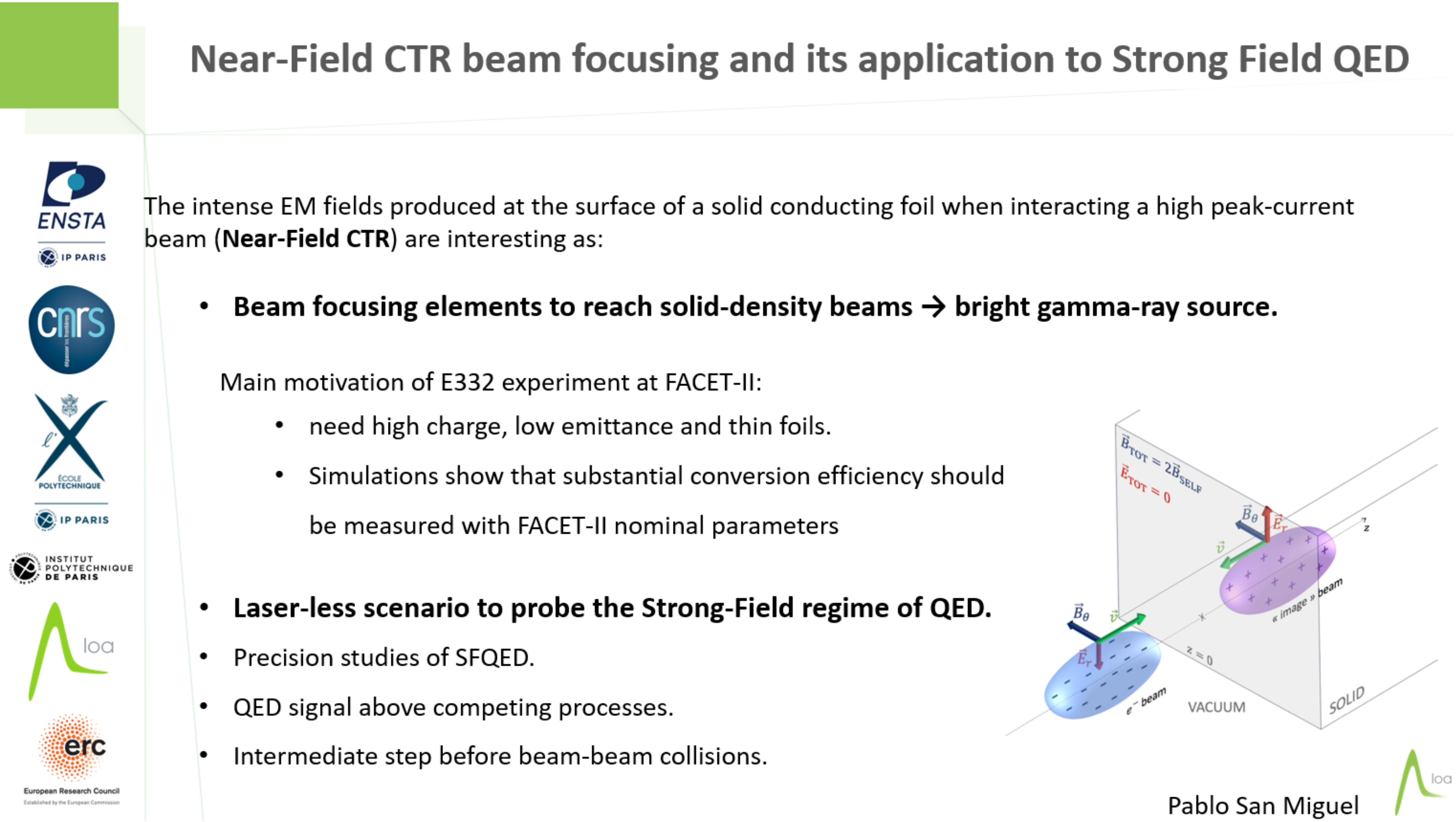


- We are on the process of developing a self-consistent version of the LW3D to study the impact of CSR on the beam, which will also help investigate possible CSR mitigations.
- We showed initial results of the longitudinal and transverse wakefields that are different from the non-self-consistent results.



Northern Illinois University

PIC algorithms: moving towards strong-field QED



Near-Field CTR beam focusing and its application to Strong Field QED

The intense EM fields produced at the surface of a solid conducting foil when interacting a high peak-current beam (**Near-Field CTR**) are interesting as:

- **Beam focusing elements to reach solid-density beams → bright gamma-ray source.**

Main motivation of E332 experiment at FACET-II:

  - need high charge, low emittance and thin foils.
  - Simulations show that substantial conversion efficiency should be measured with FACET-II nominal parameters

- **Laser-less scenario to probe the Strong-Field regime of QED.**
- Precision studies of SFQED.
- QED signal above competing processes.
- Intermediate step before beam-beam collisions.

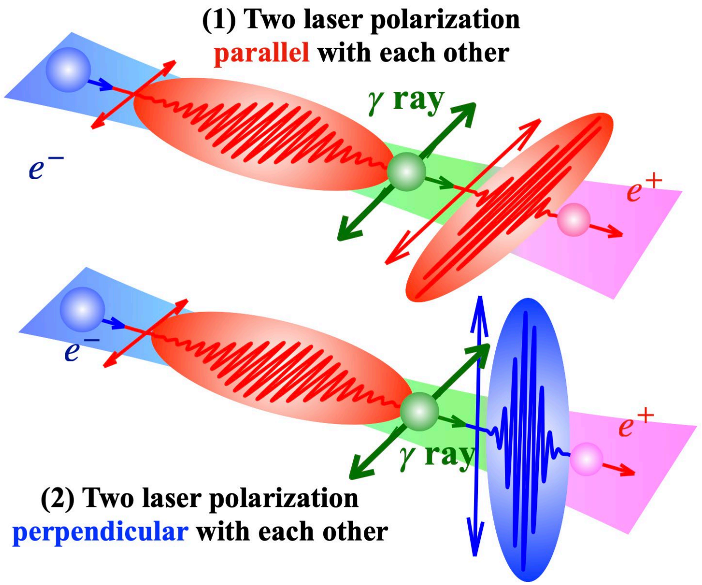
Pablo San Miguel

PIC algorithms: moving towards strong-field QED

Spin and polarization-dependent Osiris QED module for the future strong field QED laser-plasma experiment

Q. Qian,[1] D. Seipt,[2,3] M. Vranic,[4] T. Grismayer,[4] T. Blackburn,[5]
C. P. Ridgers,[6] A.G.R. Thomas[1]

[1] THE GÉRARD MOUROU CENTER FOR ULTRAFAST OPTICAL SCIENCE UNIVERSITY OF MICHIGAN
[2] HELMHOLTZ Helmholtz Institute Jena
[3] GSI Helmholtzzentrum für Schwerionenforschung GmbH
[4] ipfn INSTITUTO DE PLASMAS E FUSÃO NUCLEAR TÉCNICO LISBOA
[5] UNIVERSITAS GOTHOBURGENSIS 1891
[6] UNIVERSITY of York



- Including the lepton spin and photon polarization in the QED calculation of the PIC code is necessary. They strongly influence the NLC and NBW spectrum.

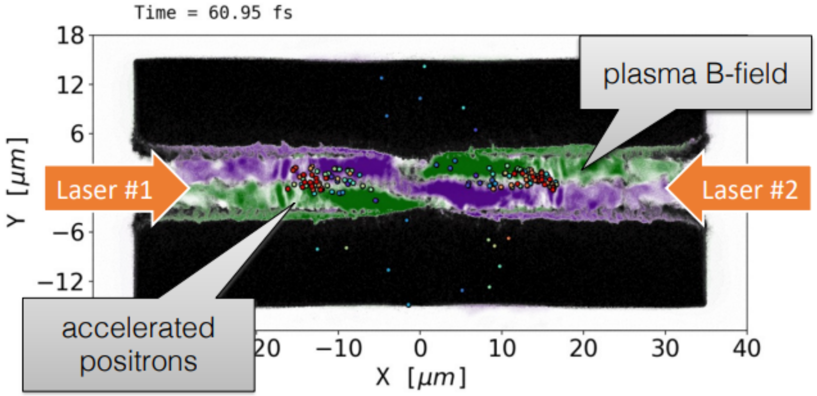
- Spin and polarization-resolved quantum radiation reaction module is now developed based on PIC code Osiris. The code passed the benchmark tests and could reproduce the published results.

- A two-pulses involved pair-production scheme is proposed. This scheme offers a controlled way to study how the photon polarization state will influence the NBW process and also provide proof for the spin and polarization-resolved NBW theory.

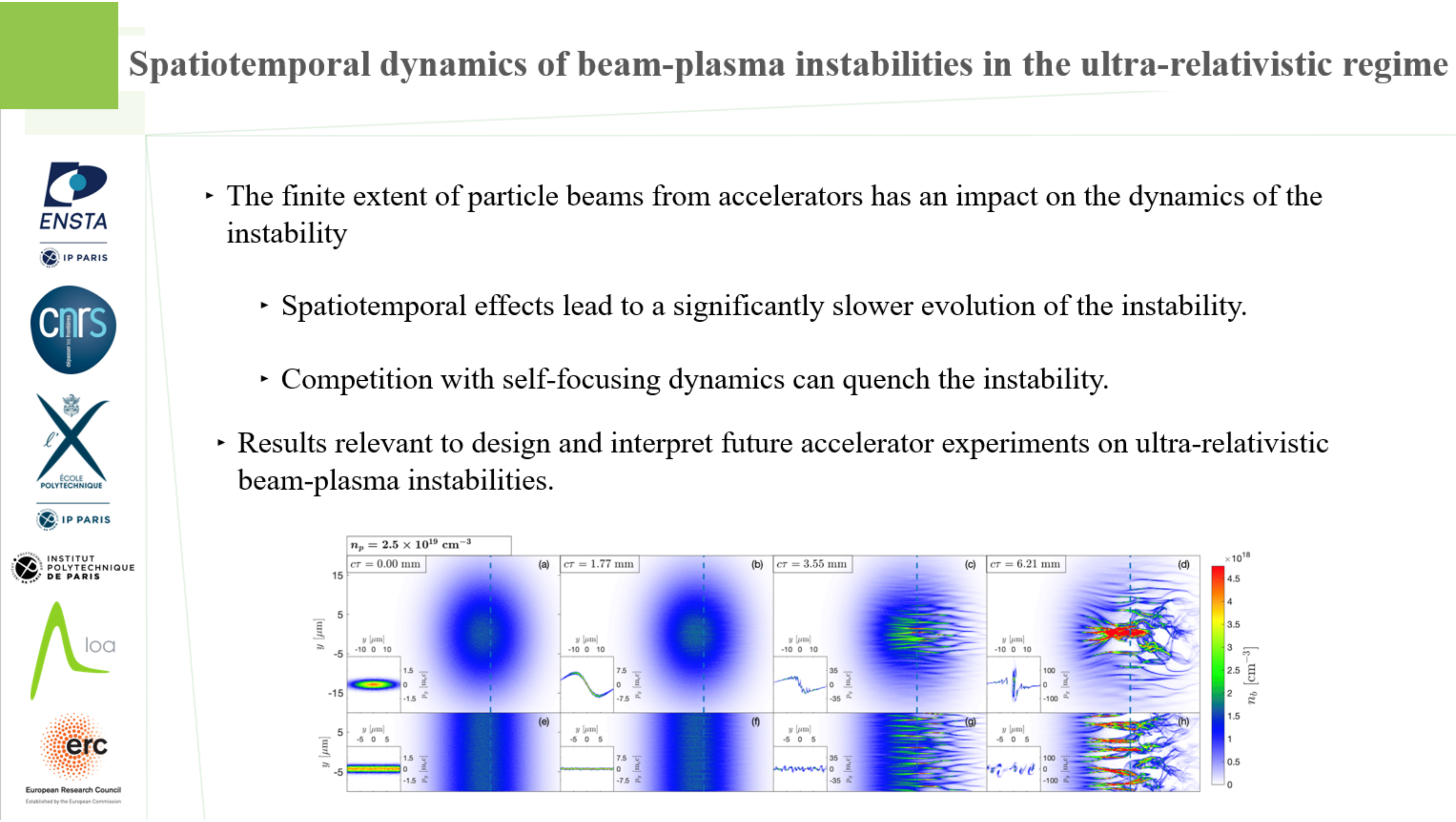
PIC algorithms: positron production

A. Arefiev (UCSD)

- Two-photon pair production inside a laser-irradiated plasma can be efficient even at currently available laser intensities.
- The plasma provides acceleration mechanisms that generate collimated beams of ultra-relativistic positrons.
- Positrons can be produced and accelerated using a single laser or two counter-propagating lasers.



PIC algorithms: instability comparison with theory



Spatiotemporal dynamics of beam-plasma instabilities in the ultra-relativistic regime

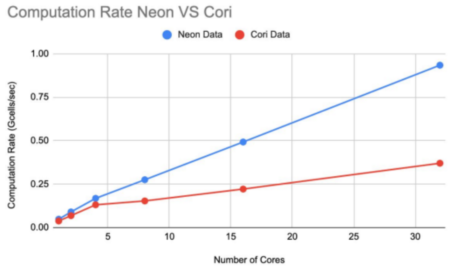
- The finite extent of particle beams from accelerators has an impact on the dynamics of the instability
  - Spatiotemporal effects lead to a significantly slower evolution of the instability.
  - Competition with self-focusing dynamics can quench the instability.
- Results relevant to design and interpret future accelerator experiments on ultra-relativistic beam-plasma instabilities.

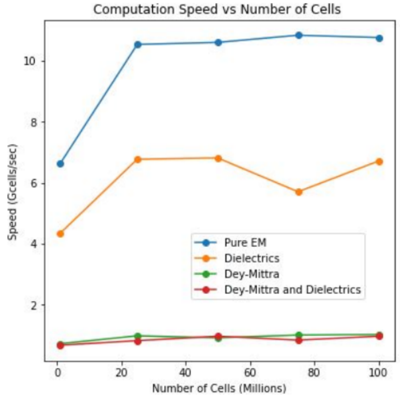
PIC algorithms: time-explicit PIC for plasma channel formation

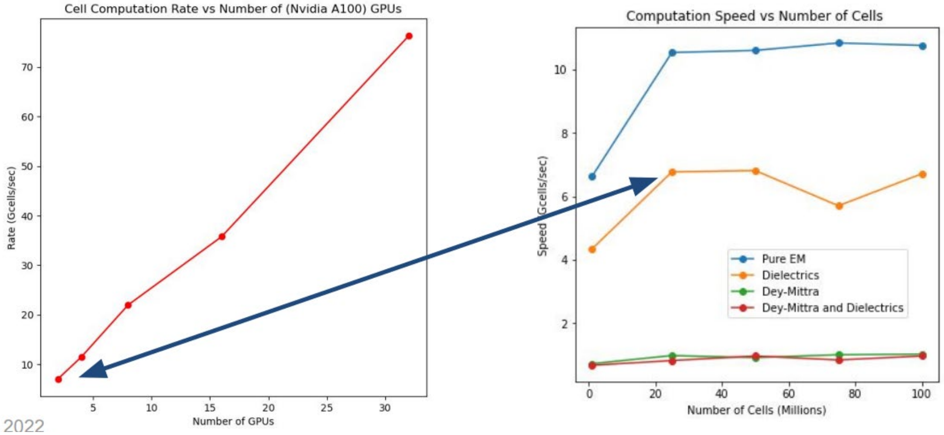
GPU Accelerated Simulations of Channel Formation for LWFA

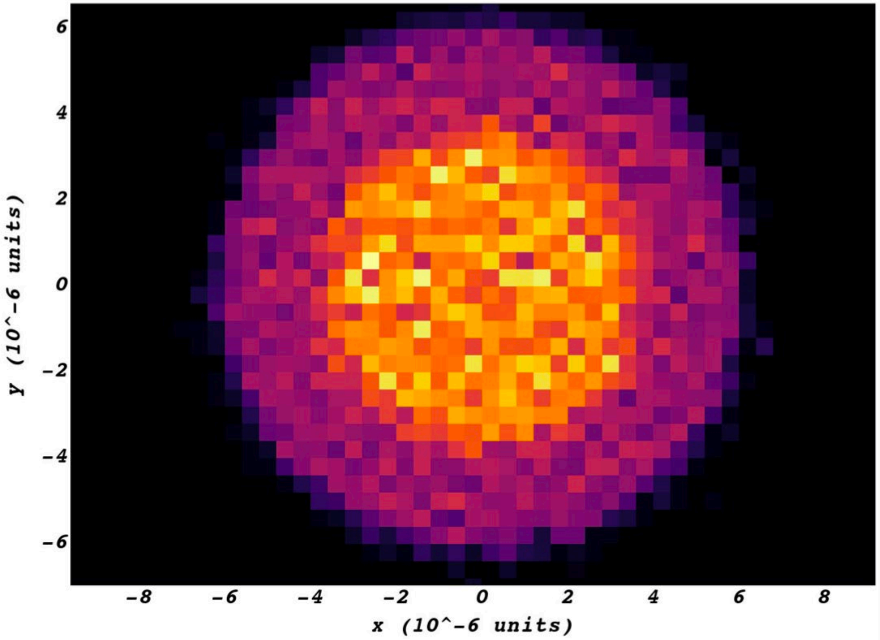
Jarrod Leddy[1], Steven Lanham[1], Scott Sides[1],
Kathryn Wolfinger[2], Ilya Zilberter[1], John Cary[1,2]

- CPU speeds up to 1 Gcell/s with 32 cores on Neon (AMD Epyc)
- A100 GPU speed >10 Gcell/s









- Laser interaction with fluid requires EM-PIC
- Setup:
  - ADK ionization model
  - Fluid Helium
  - Kinetic He^{+}, He^{2+}, e^{-}
- Helium neutral results in two ionization states after laser passthrough
- Creates electron density step down (see image)
- 4x faster on GPU than 32 core CPU, more optimization on the way

Reduced Models

Reduced models: quasistatic PIC

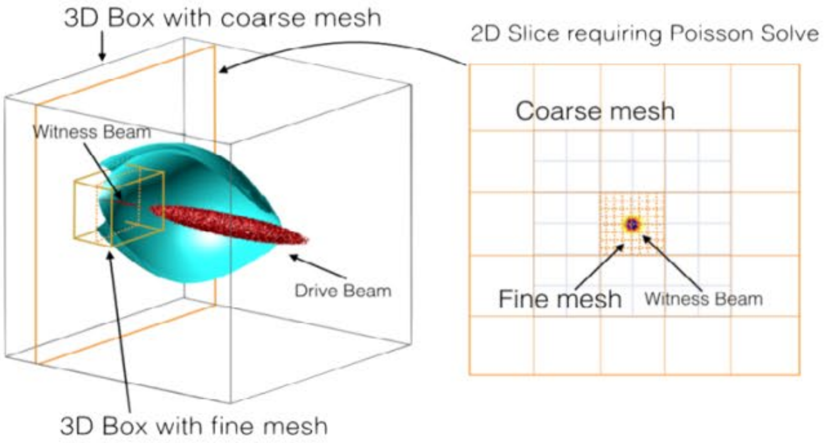
Qianqian Su[1], Fei Li[1], Weiming An[2], Yujian Zhao[1], Lance Hildebrand[1], Viktor Decyk[1], Paulo Alves[1], Ann Almgren[3], Warren Mori[1]

[1] University of California, Los Angeles, US
[2] Beijing Normal University, Beijing, China
[3] Lawrence Berkeley National Lab

UCLA

Electrical & Computer Engineering Department

Mesh refinement in QuickPIC



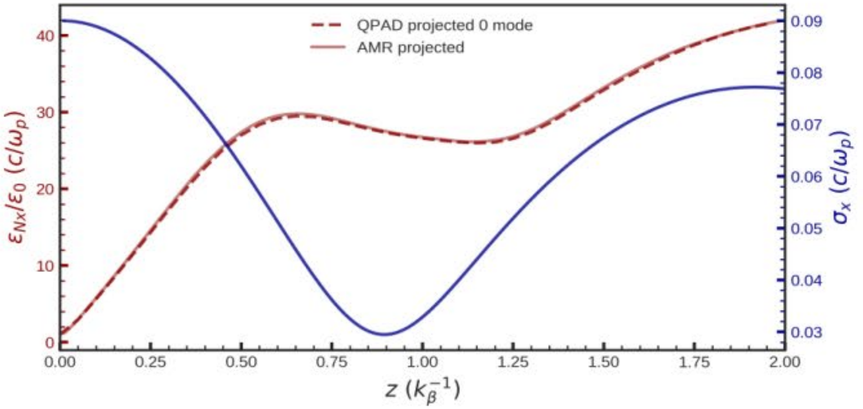
We have developed a MPI + OpenMP parallelized mesh refinement code based on QuickPIC

Estimation of roughly a thousand times speed-up compared to full QuickPIC with fine resolution everywhere

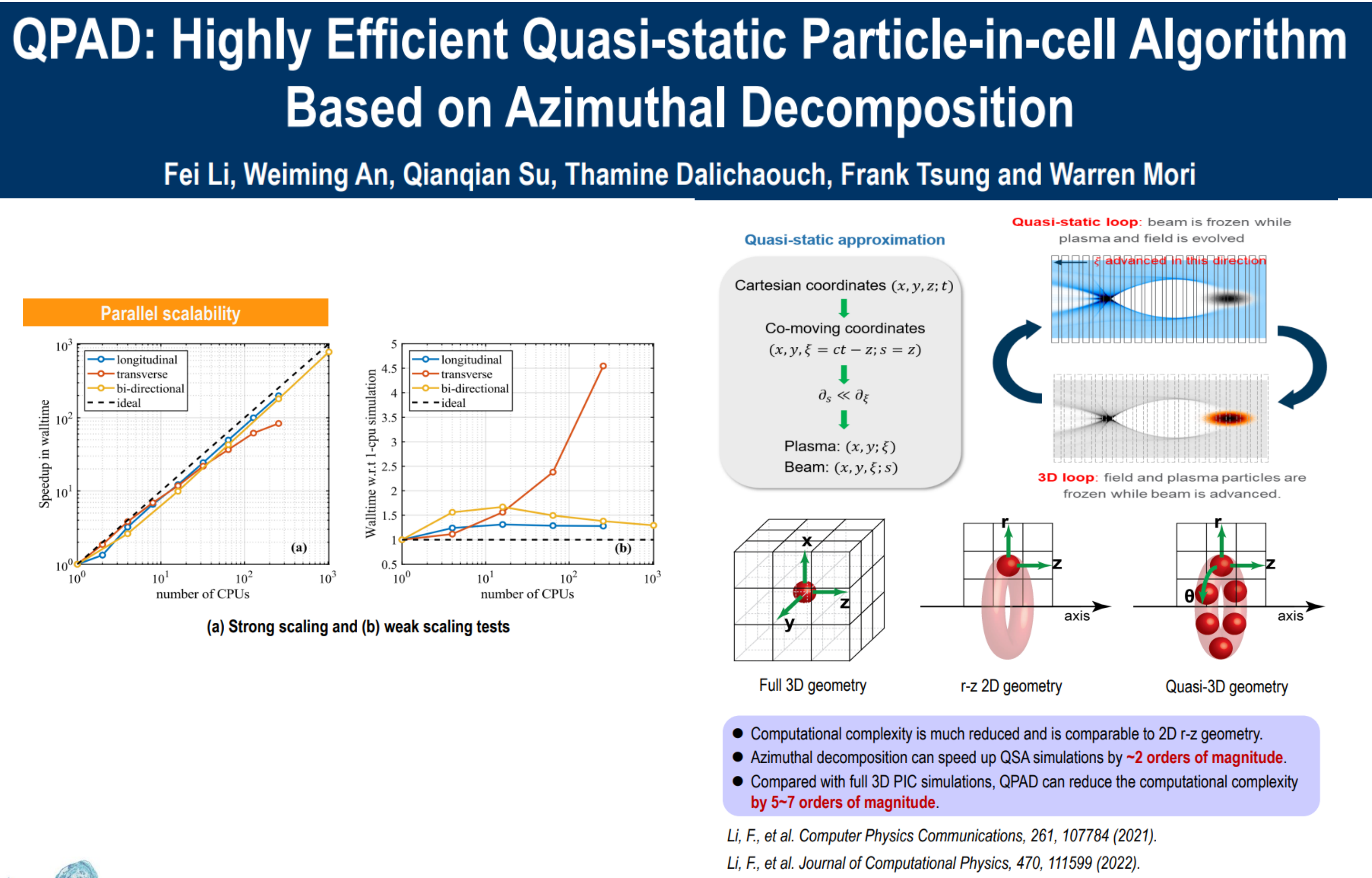
The scalability of the code has been improved by using pipelining and improving load balancing.

We also developed an adaptive mesh refinement option for an evolving beam and enables significant speed up.

Several benchmark cases have been tested and get consistent result as previously published papers and a Quasi-3d QS PIC code QPAD.



Reduced models: quasistatic PIC



QPAD: Highly Efficient Quasi-static Particle-in-cell Algorithm Based on Azimuthal Decomposition

Fei Li, Weiming An, Qianqian Su, Thamine Dalichaouch, Frank Tsung and Warren Mori

Parallel scalability

(a) Strong scaling and (b) weak scaling tests

Quasi-static approximation

Cartesian coordinates $(x, y, z; t)$

Co-moving coordinates $(x, y, \xi = ct - z; s = z)$

$\partial_s \ll \partial_\xi$

Plasma: $(x, y; \xi)$
Beam: $(x, y, \xi; s)$

Quasi-static loop: beam is frozen while plasma and field is evolved

3D loop: field and plasma particles are frozen while beam is advanced.

Full 3D geometry

r-z 2D geometry

Quasi-3D geometry

- Computational complexity is much reduced and is comparable to 2D r-z geometry.
- Azimuthal decomposition can speed up QSA simulations by **~2 orders of magnitude**.
- Compared with full 3D PIC simulations, QPAD can reduce the computational complexity **by 5~7 orders of magnitude**.

Li, F., et al. Computer Physics Communications, 261, 107784 (2021).

Li, F., et al. Journal of Computational Physics, 470, 111599 (2022).

Reduced models: quasistatic PIC

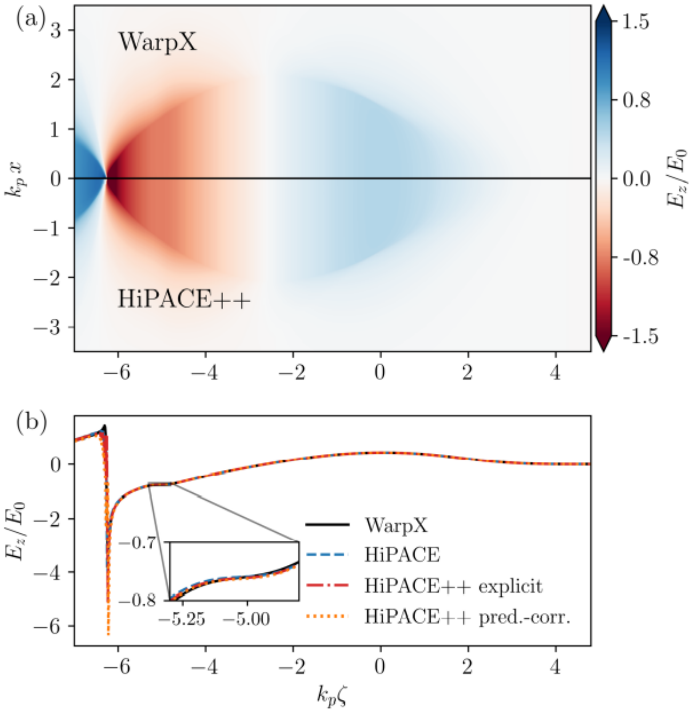
HiPACE++: a portable, 3D quasi-static Particle-in-Cell code

S. Diederichs,[1,2,3] C. Benedetti,[2] A. Huebl,[2] R. Lehe,[2]
A. Myers,[2] A. Sinn,[1] J.-L. Vay, [2] W. Zhang, [2] and M. Thévenet [1]

[1] Deutsches Elektronen-Synchrotron DESY, Germany
[2] Lawrence Berkeley National Laboratory, USA
[3] University of Hamburg, Germany

Single GPU easily outperforms many CPU cores

Benchmark and performance

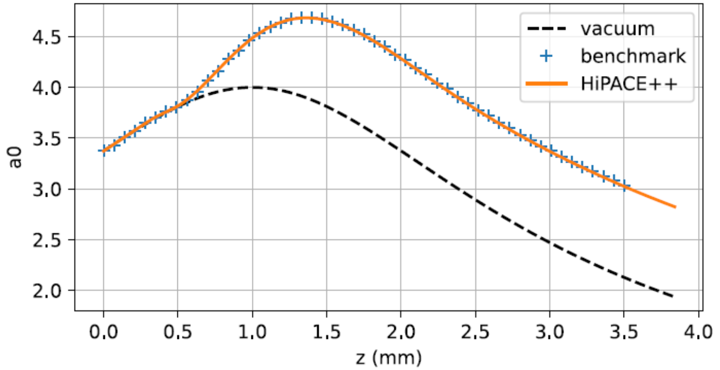


Laser envelope solver

Implemented the INF&RNO laser envelope model from Benedetti et al. PPCF 2018

- also implemented in Wake-T

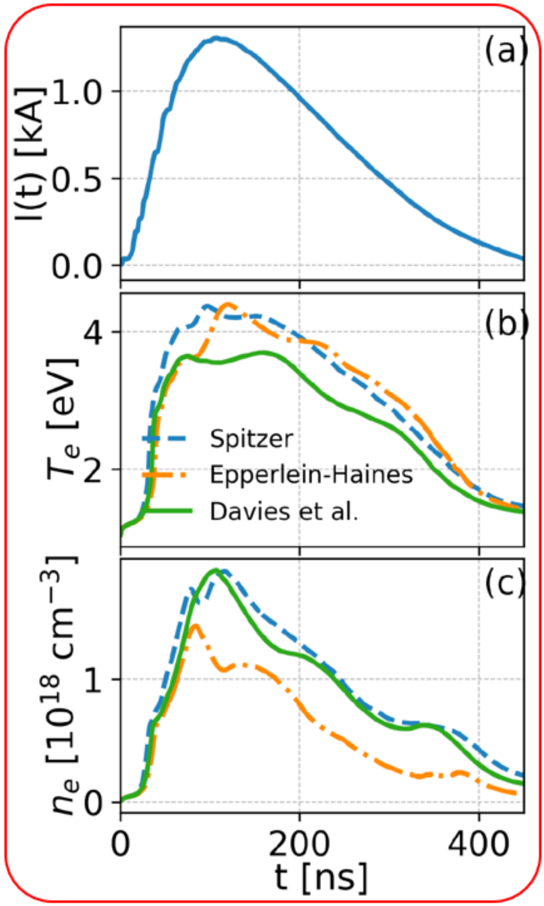
Benchmark vs Wake-T

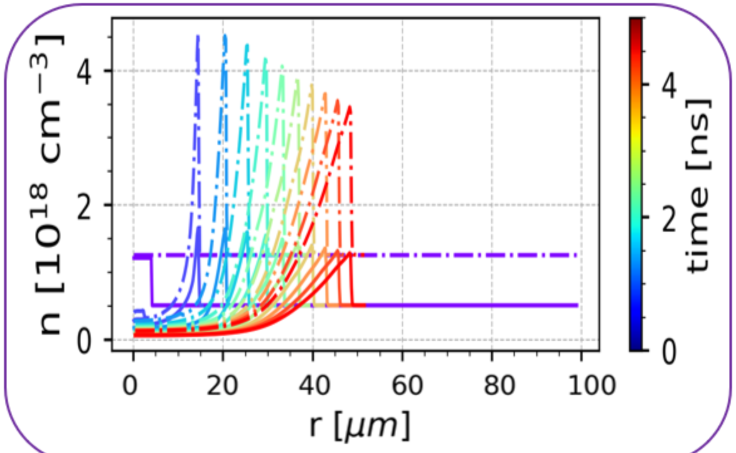


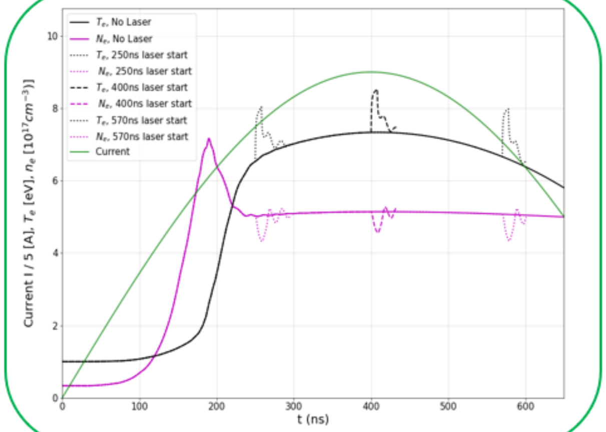
Reduced models: MHD simulation of plasma channel formation

FLASH simulations enable MHD study of structured plasmas

- Developed 2D and 3D simulations of a variety of AAC plasma systems
  - Capillary discharge plasmas for active plasma lens applications
  - Laser-heated capillary discharges for high intensity laser waveguides
  - Hydrodynamic optically-field-ionized plasmas for meter-scale channels
- Specific efforts explore impact of underlying models and assumptions
  - Anisotropic transport models reduce steady state temperature and density
  - Equation-of-state and opacities influence early time-scales of channel formation
- Simulation tools are accessible through publicly-available *Sirepo.com* portal







"Magnetohydrodynamic Modeling of Plasma Channels for Acceleration and Beam Transport"

Reduced models: MHD simulation of plasma channel formation

SIMULATIONS OF HYDRODYNAMIC OPTICAL-FIELD-IONISED PLASMA CHANNELS

Mathis Mewes, Rob Shalloo, Gregory Boyle, Jens Osterhoff, Maxence Thévenet
Deutsches Elektronen-Synchrotron DESY

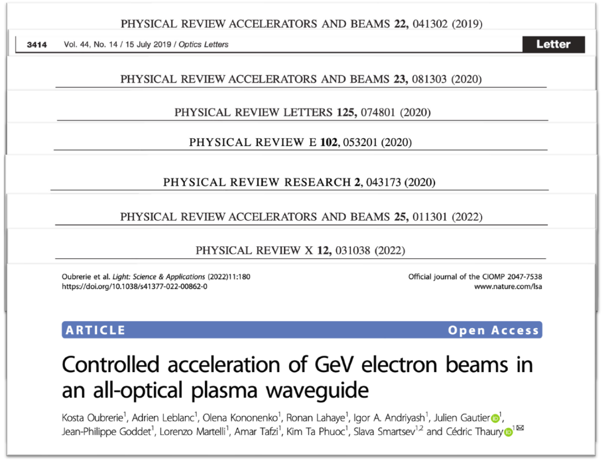
Christopher Arran
University of York

Laura Corner
University of Liverpool

Roman Walczak, Simon Hooker
University of Oxford

EXPERIMENTAL PROGRESS HAS BEEN QUICK

BUT SIMULATIONS PROVE TRICKY



PHYSICAL REVIEW ACCELERATORS AND BEAMS **22,** 041302 (2019)

3414 Vol. 44, No. 14 / 15 July 2019 / *Optics Letters* **Letter**

PHYSICAL REVIEW ACCELERATORS AND BEAMS **23,** 081303 (2020)

PHYSICAL REVIEW LETTERS **125,** 074801 (2020)

PHYSICAL REVIEW E **102,** 053201 (2020)

PHYSICAL REVIEW RESEARCH **2,** 043173 (2020)

PHYSICAL REVIEW ACCELERATORS AND BEAMS **25,** 011301 (2022)

PHYSICAL REVIEW X **12,** 031038 (2022)

Oubrerie et al. *Light: Science & Applications* (2022)11:180
https://doi.org/10.1038/s41377-022-00862-0

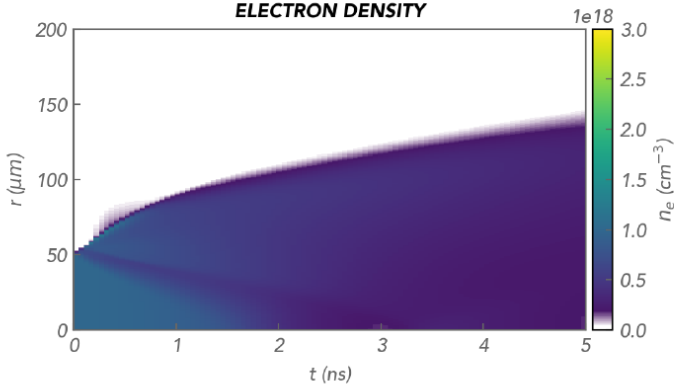
Official journal of the CIOMP 2047-7538
www.nature.com/lsa

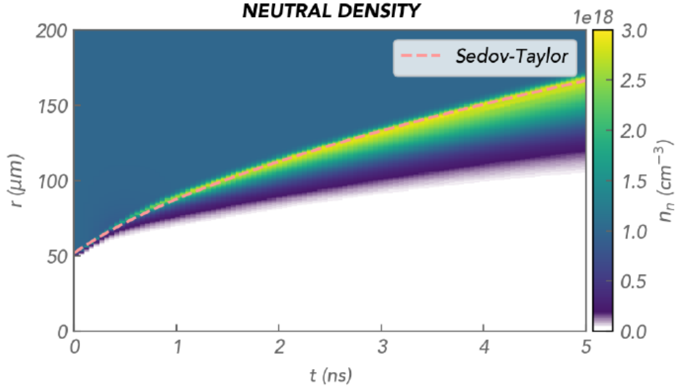
ARTICLE Open Access

Controlled acceleration of GeV electron beams in an all-optical plasma waveguide

Kosta Oubrerie[1], Adrien Leblanc[1], Olena Kononenko[1], Ronan Lahaye[1], Igor A. Andriyash[1], Julien Gautier[1], Jean-Philippe Goddet[1], Lorenzo Martelli[1], Amar Tafzi[1], Kim Ta Phuoc[1], Slava Smartsev[1,2] and Cédric Thaury[1]

- ✓ High-intensity guiding
- ✓ New plasma channel optics
- ✓ Meter-scale plasma channels
- ✓ Improved guiding confinement
- ✓ kHz Formation of plasma waveguides
- ✓ >GeV electron acceleration





THE HYDRODYNAMIC PLASMA MODEL

AN OVERVIEW OF KEY PHYSICS

- Single, quasi-neutral fluid
- Two temperatures (2T), separate for electrons from heavy particles (ions, atoms, molecules)
- Ionization state tracked via collisional reaction rates and diffusion
- **No explicit EM** fields required

Flow

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot(\rho\vec{v}) = 0$$

$$\frac{\partial \rho\vec{v}}{\partial t} + \vec{\nabla}\cdot(\rho\vec{v}\vec{v}) = -\vec{\nabla}p - \vec{\nabla}\cdot(\eta\vec{\nabla}\vec{v})$$

Electron energy

$$\frac{\partial C_e T_e}{\partial t} + \vec{\nabla}\cdot[(C_e T_e + p_e)\vec{v}] - \vec{v}\cdot\vec{\nabla}p_e - \vec{\nabla}\cdot(\lambda_e\vec{\nabla}T_e)$$
$$= -k_{e-h}(T_e - T_a) - \sum_{j,\alpha}\Delta E_j r_j$$

Similar for Atoms

Species α

$$\frac{\partial n_\alpha}{\partial t} + \vec{\nabla}\cdot(n_\alpha\vec{v}) + \vec{\nabla}\cdot\vec{d}_\alpha = \sum_j c_{j\alpha} r_j$$

Key

ρ: mass density
v: flow velocity
p: pressure
B: magnetic field
τ: viscous stress tensor
n: number density
c: stoichiometric const.
r: reaction rate
C: heat capacity
T: temperature
λ: thermal conductivity
k_{e-h}: collisional energy transfer
ΔE: reaction energy
d: diffusion flow
Transport Coefficients

COMSOL MULTIPHYSICS®

SIMULATION PARAMETERS

Dimension:	1D Radial
Species:	atomic hydrogen
Run Time:	~10 mins on PC ~500 grid points ~100 timesteps

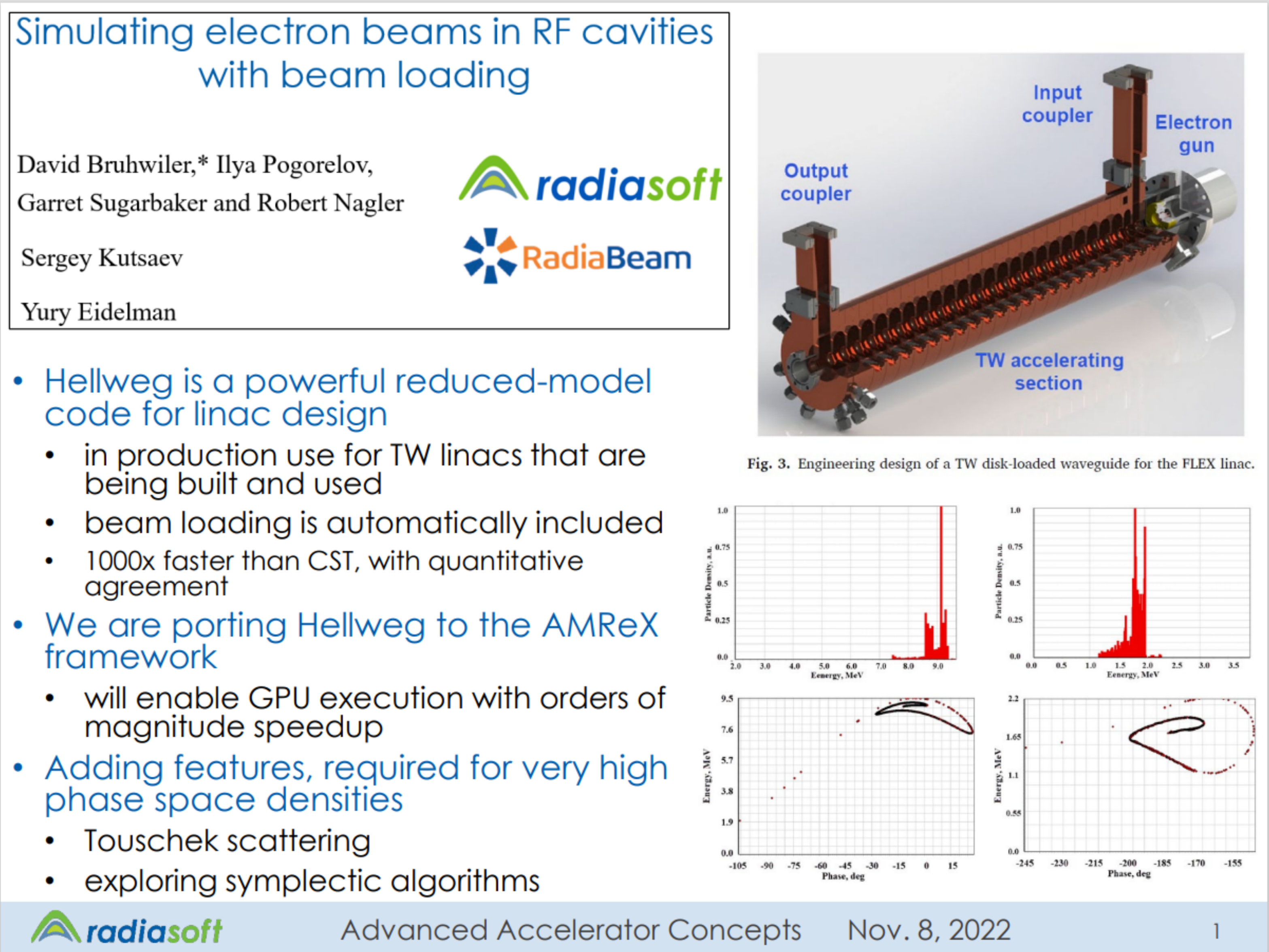
RESULTS

Channel formation on ns timescales

Good agreement with Sedov-Taylor

Neutrals play a key role in expansion

Reduced models: beam loading in TW electron linacs



Simulating electron beams in RF cavities with beam loading

David Bruhwiler,* Ilya Pogorelov,
Garret Sugarbaker and Robert Nagler

Sergey Kutsaev

Yury Eidelman

- Hellweg is a powerful reduced-model code for linac design
  - in production use for TW linacs that are being built and used
  - beam loading is automatically included
  - 1000x faster than CST, with quantitative agreement
- We are porting Hellweg to the AMReX framework
  - will enable GPU execution with orders of magnitude speedup
- Adding features, required for very high phase space densities
  - Touschek scattering
  - exploring symplectic algorithms

Fig. 3. Engineering design of a TW disk-loaded waveguide for the FLEX linac.

radiasoft   Advanced Accelerator Concepts   Nov. 8, 2022   1

Other algorithms

Other algorithms: Vlasov with mesh refinement

Eulerian Finite-Difference Vlasov Solver with a Non-Uniform Momentum Grid

Vlasov–Maxwell Equation

1-1/2 D

Prof. B. A. Shadwick (Univ of Nebraska - Lincoln)

- Transformation between the logical and physical momentum:

$$p_x = P_x(\xi) \quad \text{and} \quad p_z = P_z(\eta)$$

- Transform the Vlasov–Maxwell equation:

$$f(z, p_x = P_x(\xi), p_z = P_z(\eta), t) = F(z, \xi, \eta, t)$$

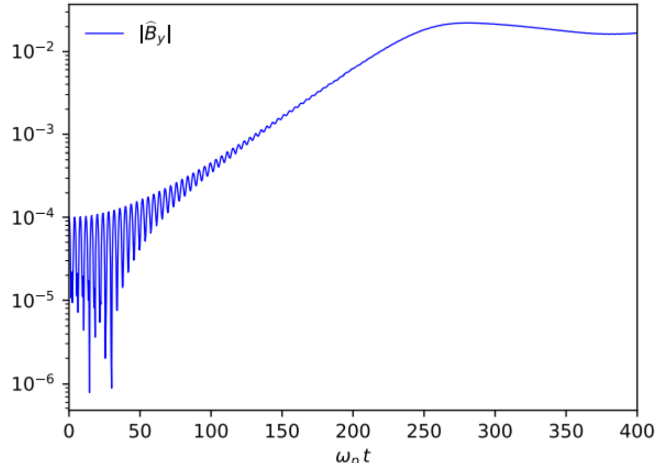
where

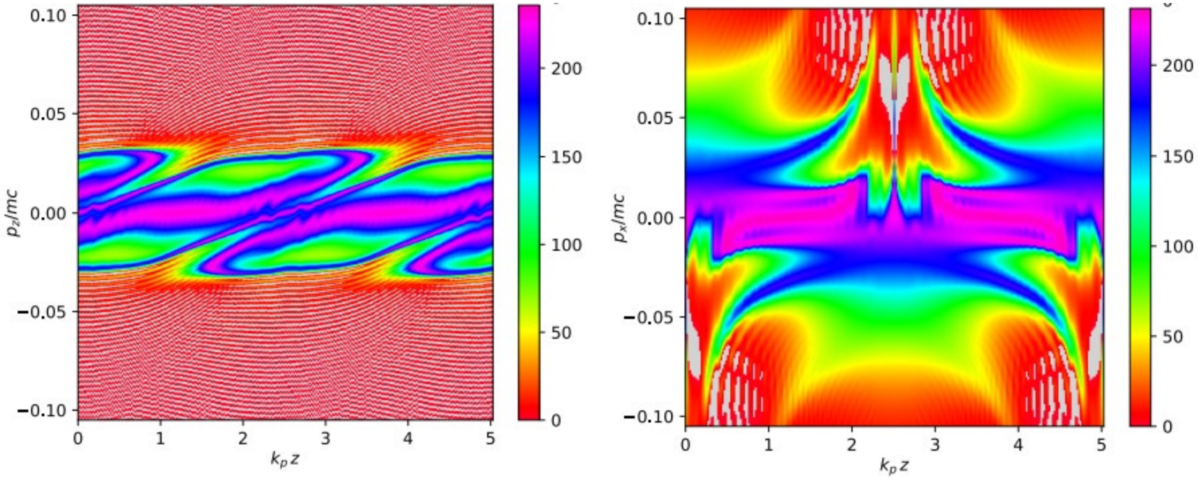
$$\frac{\partial F}{\partial t} + P_z(\eta)\,\frac{\partial F}{\partial z} + q\,\frac{E_x - P_z(\eta)\,B_y}{P_x'(\xi)}\,\frac{\partial F}{\partial \xi} + q\,\frac{E_z + P_x(\xi)\,B_y}{P_z'(\eta)}\,\frac{\partial F}{\partial \eta} = 0$$

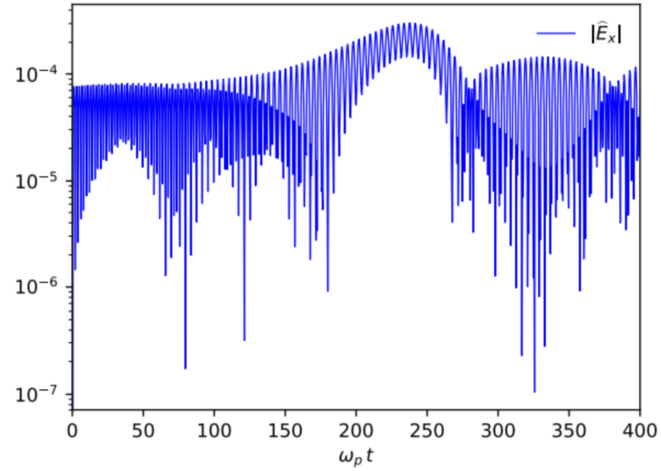
and

$$J_x = q\int d\xi\, d\eta\, P_x'(\xi)\, P_z'(\eta)\, P_x(\xi)\, F$$

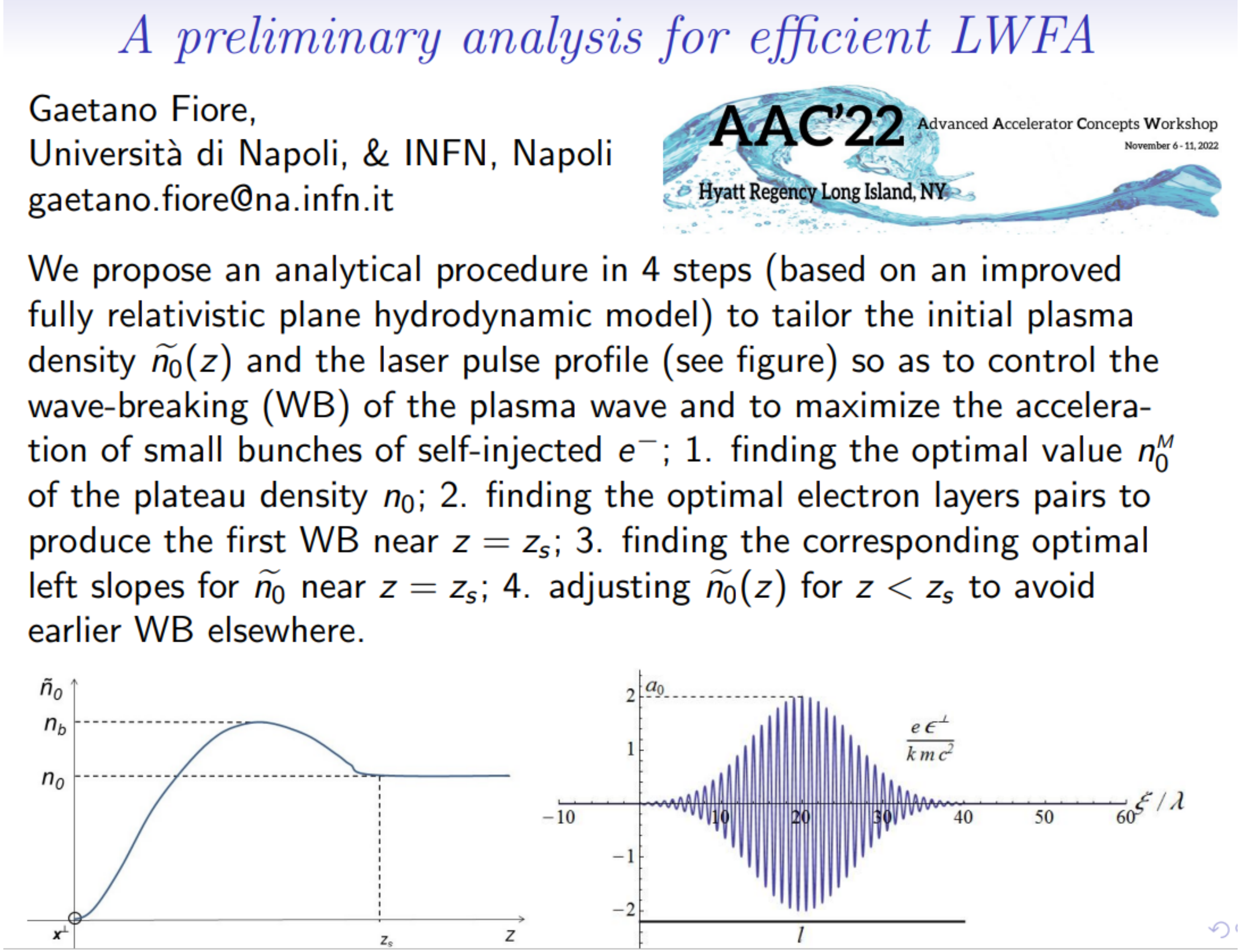
$$J_z = q\int d\xi\, d\eta\, P_x'(\xi)\, P_z'(\eta)\, P_z(\eta)\, F$$







Other algorithms: 1D semi-analytic approach with wavebreaking



A preliminary analysis for efficient LWFA

Gaetano Fiore,
Università di Napoli, & INFN, Napoli
gaetano.fiore@na.infn.it

AAC'22 Advanced Accelerator Concepts Workshop
November 6 - 11, 2022
Hyatt Regency Long Island, NY

We propose an analytical procedure in 4 steps (based on an improved fully relativistic plane hydrodynamic model) to tailor the initial plasma density $\widetilde{n}_0(z)$ and the laser pulse profile (see figure) so as to control the wave-breaking (WB) of the plasma wave and to maximize the acceleration of small bunches of self-injected e^-; 1. finding the optimal value n_0^M of the plateau density n_0; 2. finding the optimal electron layers pairs to produce the first WB near $z = z_s$; 3. finding the corresponding optimal left slopes for $\widetilde{n}_0$ near $z = z_s$; 4. adjusting $\widetilde{n}_0(z)$ for $z < z_s$ to avoid earlier WB elsewhere.

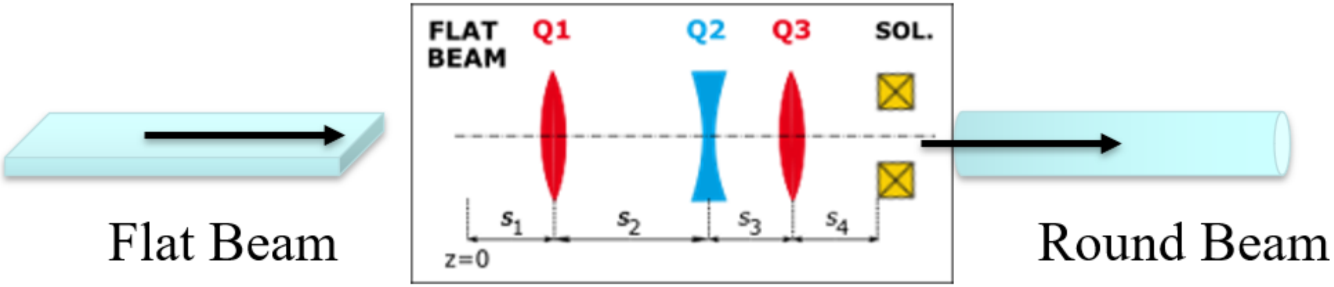
Other algorithms: differentiable computing

ADJOINT OPTIMIZATION OF CIRCULAR LATTICES

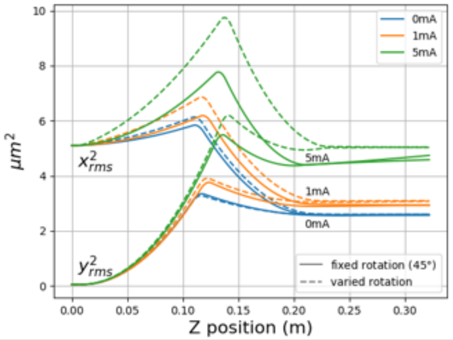
UMD Team

Efficient calculation of $\frac{dF(\mathbf{a})}{d\mathbf{a}}$ Where F is a Figure of Merit and where $\mathbf{a}$ is a vector of parameters

N – Dimensional gradient calculated with one additional pass through lattice.

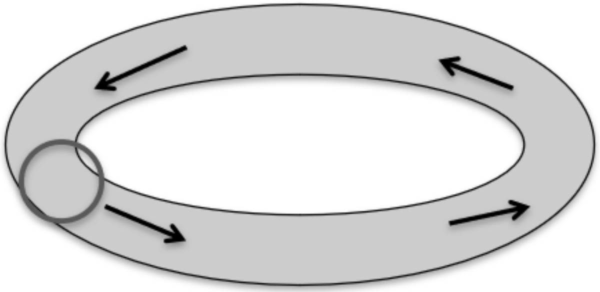


Optimization of Flat to Round Transformers Using Adjoint Techniques*
L. Dovlatyan, et al., Phys Rev Accel and Beams V25, 044002 (2022).

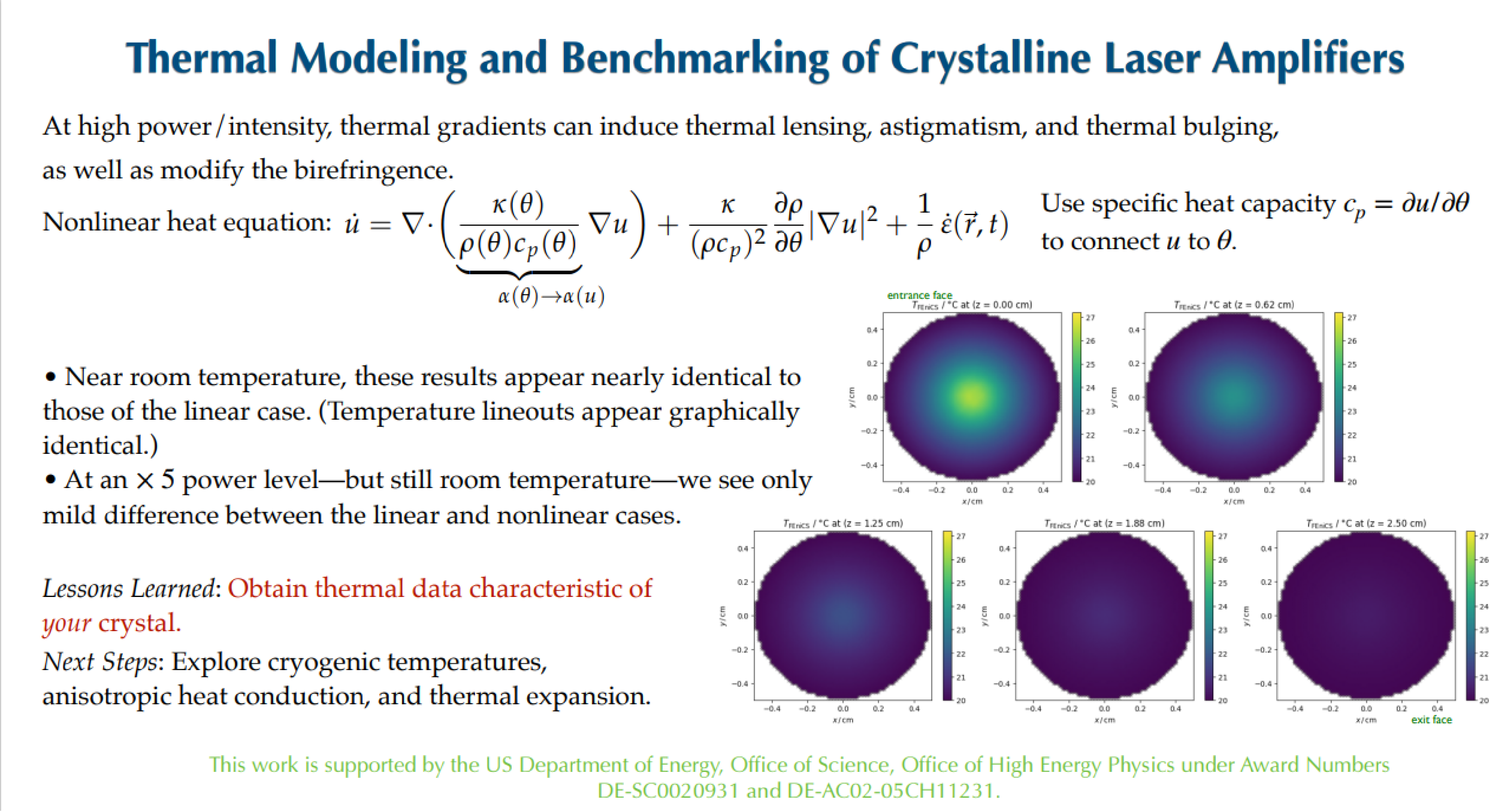


Optimization with strong self fields

Next up circular lattices



Other algorithms: High-power, high-rep-rate lasers



Thermal Modeling and Benchmarking of Crystalline Laser Amplifiers

At high power / intensity, thermal gradients can induce thermal lensing, astigmatism, and thermal bulging, as well as modify the birefringence.

Nonlinear heat equation: $\dot{u} = \nabla\cdot\left(\underbrace{\frac{\kappa(\theta)}{\rho(\theta)c_p(\theta)}}_{\alpha(\theta)\to\alpha(u)}\nabla u\right) + \frac{\kappa}{(\rho c_p)^2}\frac{\partial\rho}{\partial\theta}|\nabla u|^2 + \frac{1}{\rho}\dot{\varepsilon}(\vec{r},t)$

Use specific heat capacity $c_p = \partial u/\partial\theta$ to connect u to θ.

- Near room temperature, these results appear nearly identical to those of the linear case. (Temperature lineouts appear graphically identical.)
- At an × 5 power level—but still room temperature—we see only mild difference between the linear and nonlinear cases.

Lessons Learned: Obtain thermal data characteristic of *your* crystal.

Next Steps: Explore cryogenic temperatures, anisotropic heat conduction, and thermal expansion.

This work is supported by the US Department of Energy, Office of Science, Office of High Energy Physics under Award Numbers DE-SC0020931 and DE-AC02-05CH11231.

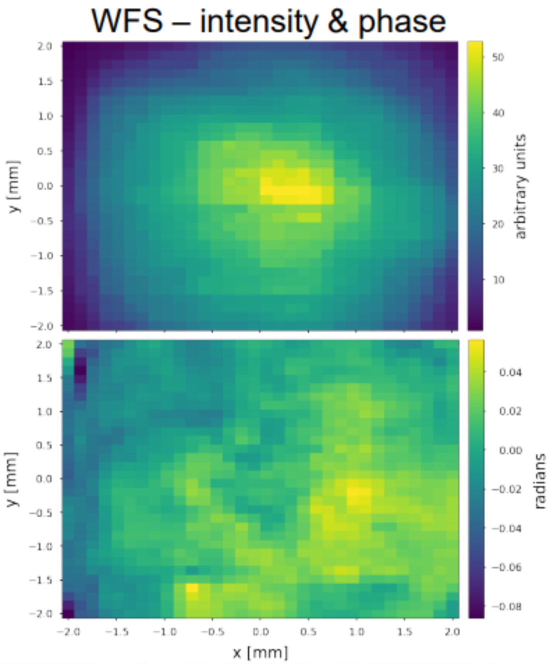
Other algorithms: High-power, high-rep-rate lasers

Simulation of electromagnetic pulses through high-power solid state laser amplifiers

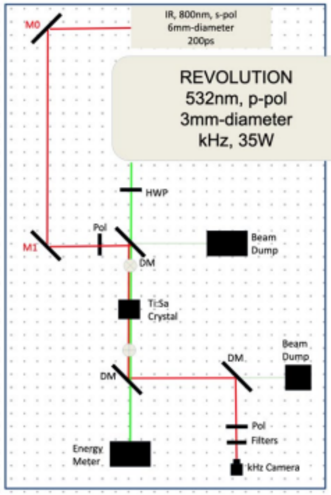
David L. Bruhwiler,* Boaz Nash, Dan T. Abell,
Gurhar Khalsa and Robert Nagler (RadiaSoft)

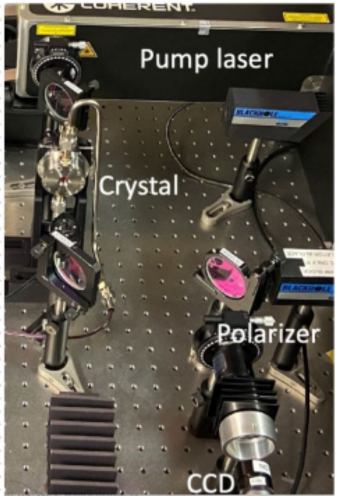
Jeroen van Tilborg, Qiang Chen, Csaba Tóth,
and Cameron G.R. Geddes (LBNL)

Nicholas B. Goldring (STATE33 Inc.)



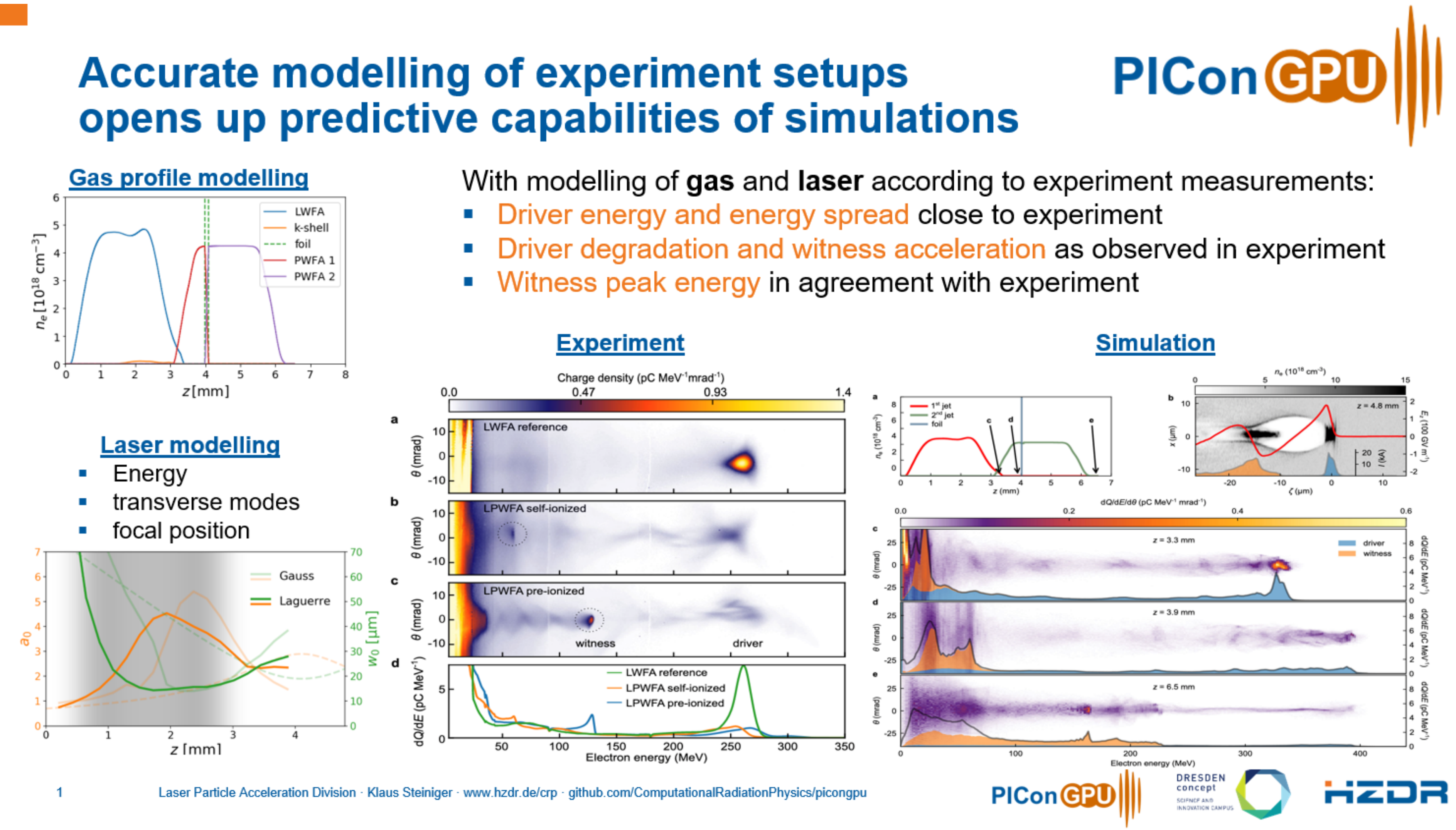
- PW lasers are moving toward KHz rep rates
  - software is needed for crystal amplifiers
  - Python library, https://github.com/radiasoft/rslaser/
  - Sirepo.com UI is being developed to support these capabilities
- Experiments at the BELLA Center enable validation
  - experimentally observed thermal focusing at 1 KHz is stronger than expected
  - possible explanations are being explored





Simulation of experiments *(one example of many)*

Simulation of experiments



Accurate modelling of experiment setups opens up predictive capabilities of simulations

Gas profile modelling

Laser modelling
- Energy
- transverse modes
- focal position

With modelling of **gas** and **laser** according to experiment measurements:
- Driver energy and energy spread close to experiment
- Driver degradation and witness acceleration as observed in experiment
- Witness peak energy in agreement with experiment

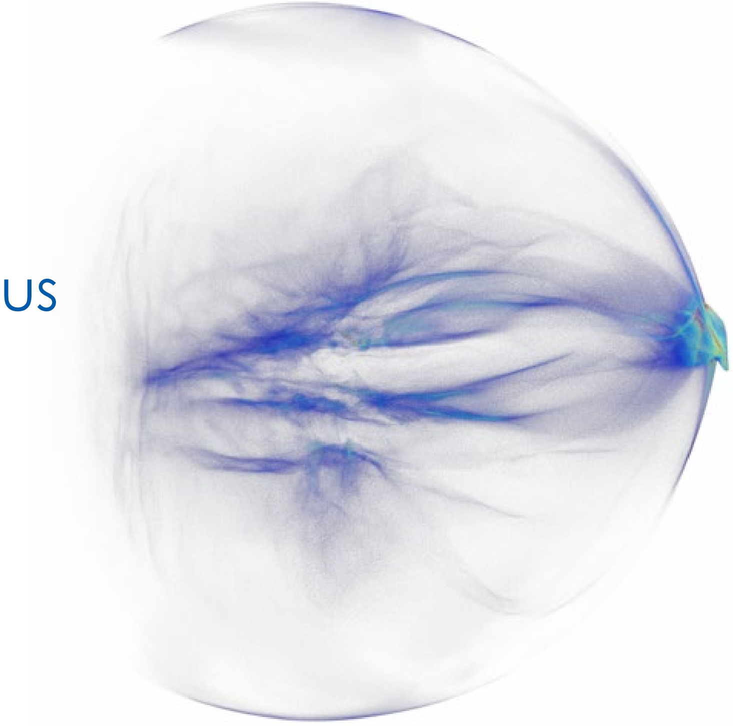
Experiment

Simulation

1 Laser Particle Acceleration Division · Klaus Steiniger · www.hzdr.de/crp · github.com/ComputationalRadiationPhysics/picongpu

Summary

- 2 plenary talks – Huebl & Xiao
- 2 invited talks – Bussmann & Debus
- 8 sessions
  - 2 joint sessions with WG1
  - 1 joint session with WGs 4, 5, 7, 8
- 30 contributed orals
  - including all those in joint sessions
- 9 contributed posters
  - 5 student posters
  - 4 others



3D visualization of the plasma proton density during the acceleration process of a few-fs, 1.15nC beam
Hilz, Ostermayr, Huebl et al.; Nat. Comm. **9**.432, 2018

Acknowledgements

The contributions of author D.L.B. are supported in part by RadiaSoft LLC and in part by the U.S. Department of Energy, Office of Science, Office of High Energy Physics, under Award Numbers DE-SC0020931 and DE-SC0022799.

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