Simulating electron beams in RF cavities with beam loading

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

Sergey Kutsaev

Yury Eidelman

*bruhwiler@radiasoft.net

Advanced Accelerator Concepts (AAC) workshop

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Motivation

The HEPAP accelerator R&D subpanel recommended development of a roadmap for accelerator science and technology [1]. The community is developing one [2] based on four grand challenges –

GC #1: Beam Intensity – "How do we increase beam intensities by orders of magnitude?"

GC #2: Beam Quality – "How do we increase the beam phase space density by an order of magnitude, towards the quantum degeneracy limit?"

GC #3: Beam Control – "How do we measure and control the beam distribution down to the individual particle level?"

GC #4. Beam Prediction – "How do we develop predictive 'virtual particle accelerators'?"

In this proposal, we address primarily GC #4, but with relevance to the other three grand challenges.

For this effort to be sustainable upon the conclusion of an SBIR-funded project, our work must be applicable to industrial and medical linac design. Hence, we will leverage the open source Hellweg code [3–11], which is routinely used by the principal investigator for contract R&D work.

[1] B. Barletta et al. "Accelerating Discovery: A Strategic Plan for Accelerator R&D in the U.S." In: *Report of the Accelerator Research and Development Subpanel (HEPAP)*. 2015.

[2] S. Nagaitsev et al. "Accelerator and Beam Physics Research Goals and Opportunities". In: (2021). arXiv: 2101.04107 [physics.acc-ph].

[3] S. V. Kutsaev. "Electron dynamics simulations with Hellweg 2D code". In: *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 618 (2010), pp. 298–305.

[10] S. V. Kutsaev et al. "Ir-192 Radioisotope Replacement with a Hand-Portable 1 MeV Ku-band Electron Linear Accelerator". In: *Applied Radiation and Isotopes* 179 (2022), p. 110029.

[11] *The open source* `Hellweg` *repository*. URL: https://github.com/radiasoft/rslinac.

Hellweg – TW linacs

Contents lists available at ScienceDirect

Radiation Physics and Chemistry

journal homepage: www.elsevier.com/locate/radphyschem

Linear accelerator for security, industrial and medical applications with rapid beam parameter variation

S.V. Kutsaev[a,*], R. Agustsson[a], A. Arodzero[a,b], R. Berry[a], S. Boucher[a], A. Diego[a], D. Gavryushkin[a], J.J. Hartzell[a,1], R.C. Lanza[b], A.Yu. Smirnov[a], A. Verma[a,2], V. Ziskin[c,3]

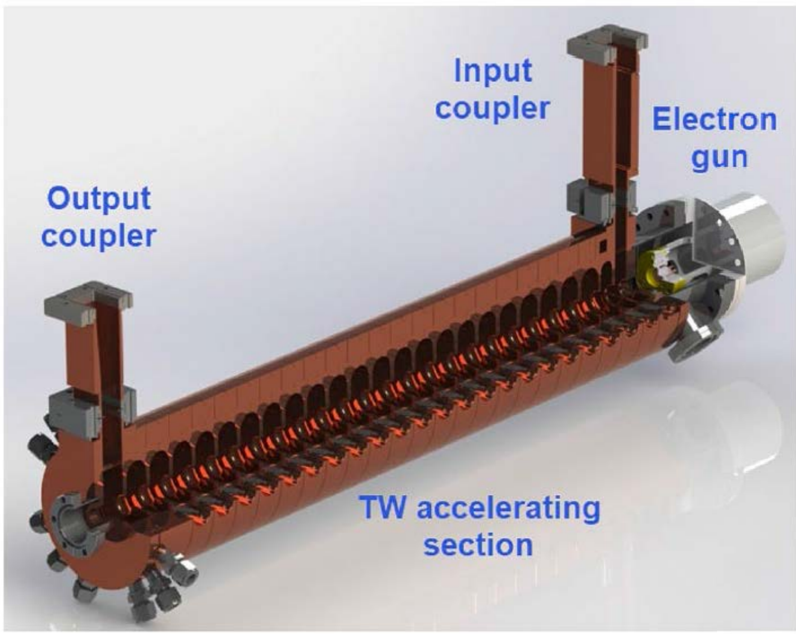
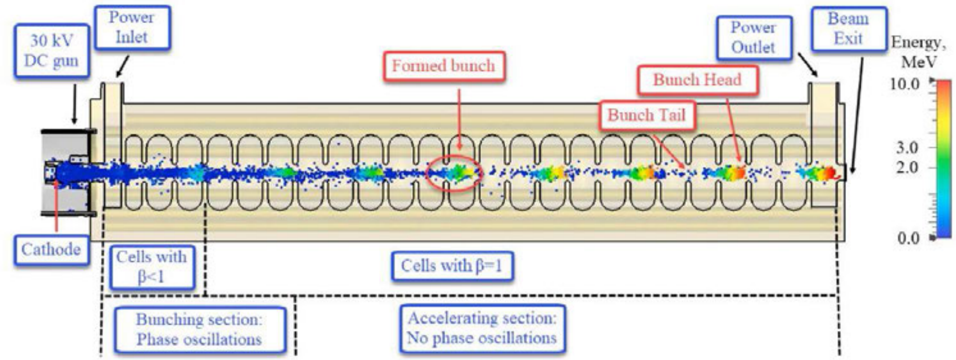


Fig. 3. Engineering design of a TW disk-loaded waveguide for the FLEX linac.



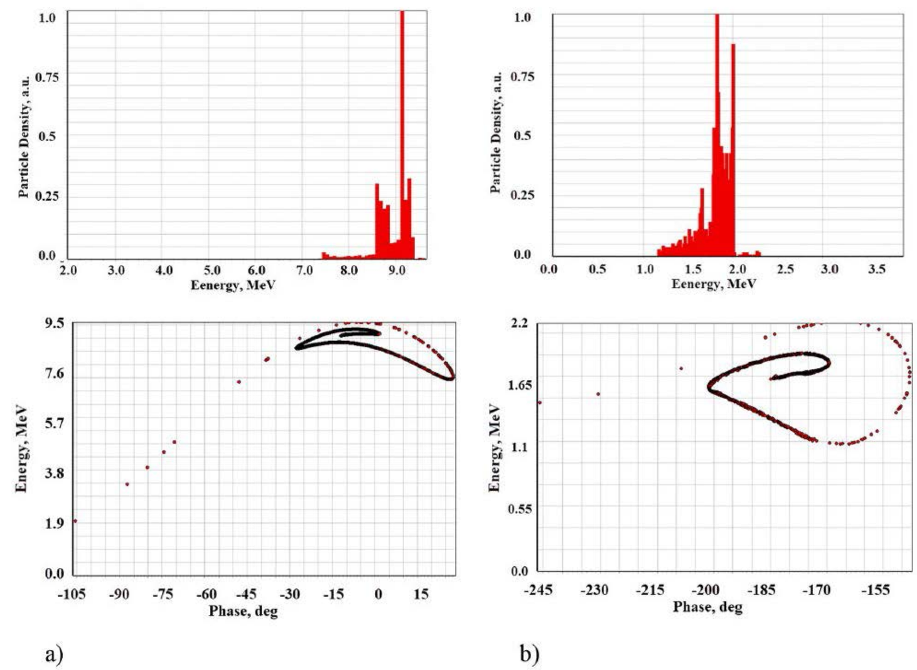


Fig. 4. Energy spectra (top) and phase portraits (bottom) of 9 MeV (a) and 2 MeV (b) bunches, simulated in Hellweg (Kutsaev, 2010; Kutsaev et al., 2019b). Note that 2 MeV bunch is in decelerating phase.

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Cloud-based design of high average power traveling wave linacs

S V Kutsaev[1], Y Eidelman[2], D L Bruhwiler[2], P Moeller[2], R Nagler[2] and J Barbe Welzel[2]

[1]RadiaBeam Technologies LLC, 1717 Stewart St, Santa Monica, CA 90403, USA,
[2]RadiaSoft LLC, 1348 Redwood Ave, Boulder, CO 80304, USA

kutsaev@radiabeam.com

Hellweg is 1000x faster than CST

Table 1. Comparison of Hellweg and CST simulations.

Code	Hellweg	CST
Input current	250 mA	250 mA
Output current	124 mA	115 mA
Beam energy	9.6 MeV	9.2 MeV
Input power	4.6 MW	4.6 MW
Output power	1.73 MW	1.72 MW
Simulation time	~30 sec	~8 hrs

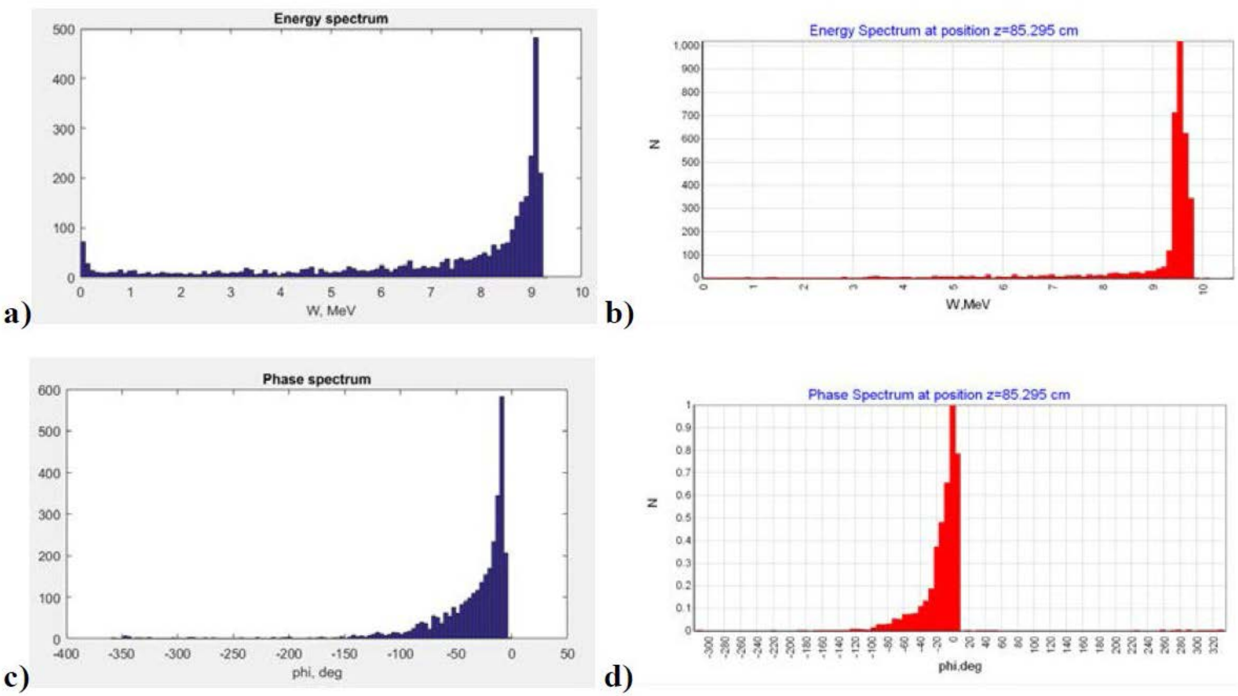

Figure 2. The simulated beam energy (a, b) and phase (c, d) spectra is presented, as generated by two codes: CST Particle Studio (a, c) and Hellweg (b, d)

Applied Radiation and Isotopes 179 (2022) 110029

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Applied Radiation and Isotopes

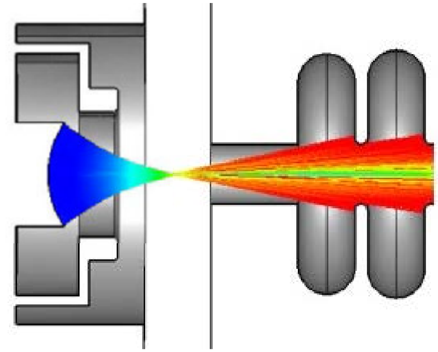
journal homepage: www.elsevier.com/locate/apradiso

Handheld MeV linac

Ir-192 radioisotope replacement with a hand-portable 1 MeV Ku-band electron linear accelerator

S.V. Kutsaev [a,*], R. Agustsson [a], R. Berry [a], S. Boucher [a], D. Bruhwiler [b], K. Schulze [a], A. Yu. Smirnov [a], K. Taletski [a]

[a] RadiaBeam Technologies, LLC, Santa Monica, CA, 90404, USA
[b] RadiaSoft LLC, Boulder, CO, 80304, USA



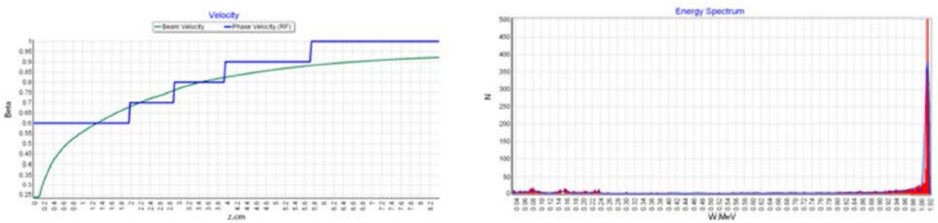


Fig. 6. Energy spectrum optimization procedure (left): beam (green) and phase (blue) velocity profile along the accelerating structure. Corresponding simulated beam energy spectra are shown on the right side. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

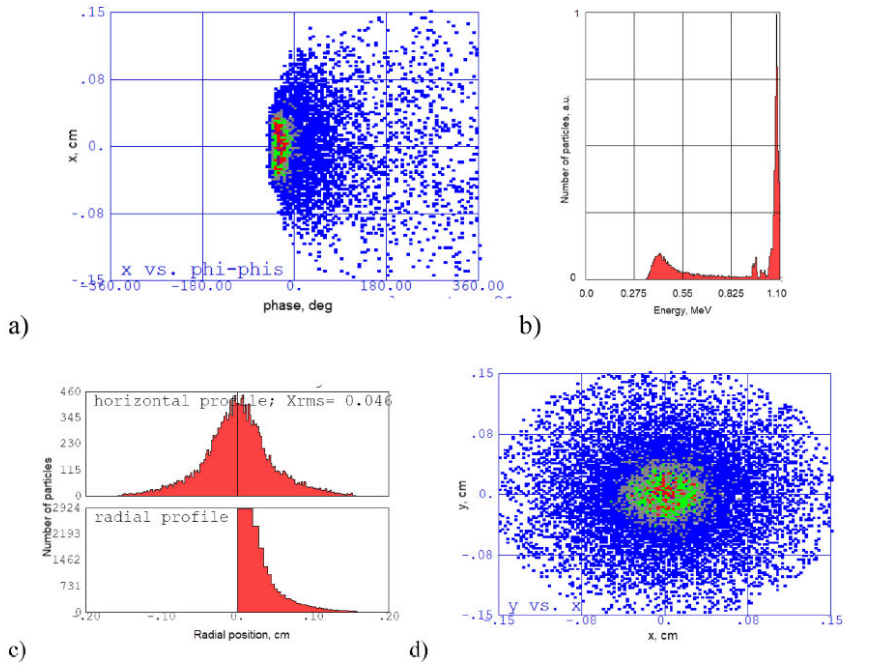


Fig. 8. Particle distribution at the end of the linac as simulated in Parmela: a) longitudinal beam profile, b) energy spectrum, c) radial distribution, d) transverse beam cross-section. Color represents particle density. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

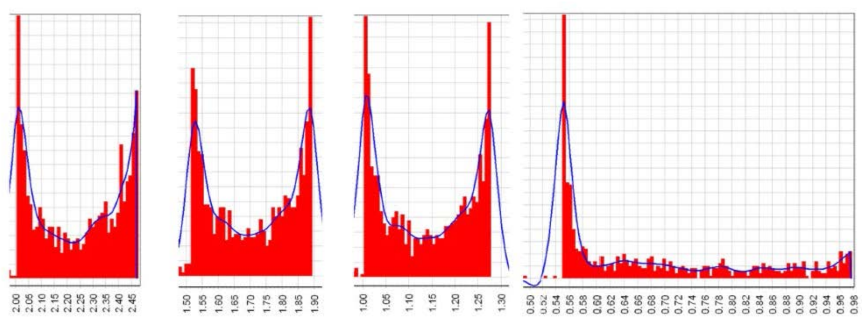


Fig. 9. The energy spectrum of the accelerated beam is shown for the nominal 2 MeV linac design, as the gun current is increased from 10 mA to 750 mA. The spectra (from left to right) correspond to the energies of 2.45 to 0.55.

Higher-energy photoinjector & TW linac with high phase space density

- Initial attempt to benchmark with SPARC linac design
  - photocathode gun is roughly approximated
  - we are working to generalize Hellweg for this application

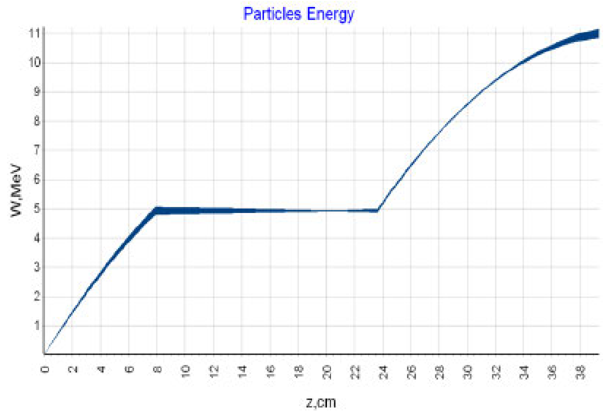


Figure 2: Electron energy vs position.

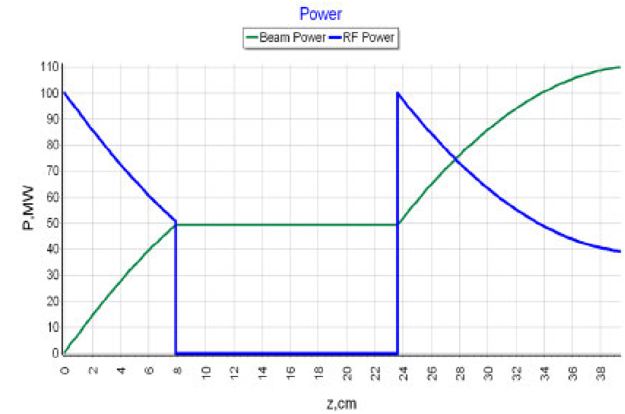


Figure 3: Beam (green) & RF (blue) power.

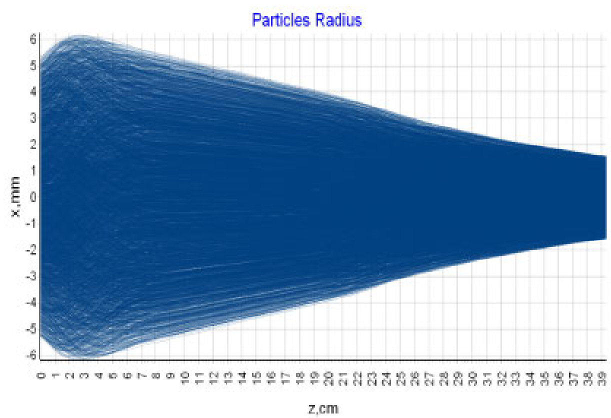


Figure 4: Horizontal electron trajectories.

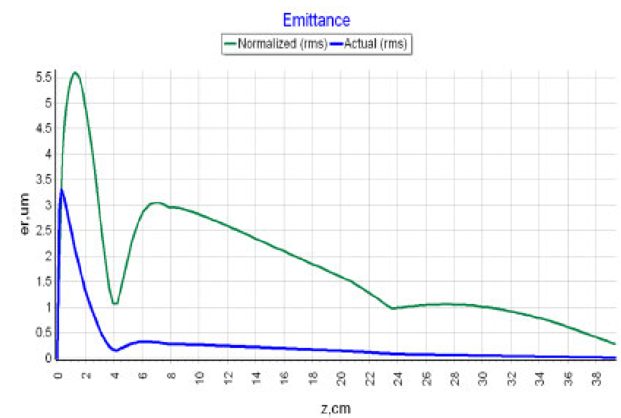


Figure 5: Normalized and geometric emittance.

D. Alesini et al. "The SPARC project: a high-brightness electron beam source at LNF to drive a SASE-FEL experiment". In: *Nucl. Instrum. and Methods in Physics Res. A* 507.1 (2003). Proc. 24th Int. Free Electron Laser Conf., p. 345. ISSN: 0168-9002.

M. Ferrario et al. "Experimental Demonstration of Emittance Compensation with Velocity Bunching". In: *Phys. Rev. Lett.* 104 (5 Feb. 2010), p. 054801.

Vision – incorporate Hellweg into the AMReX ecosystem

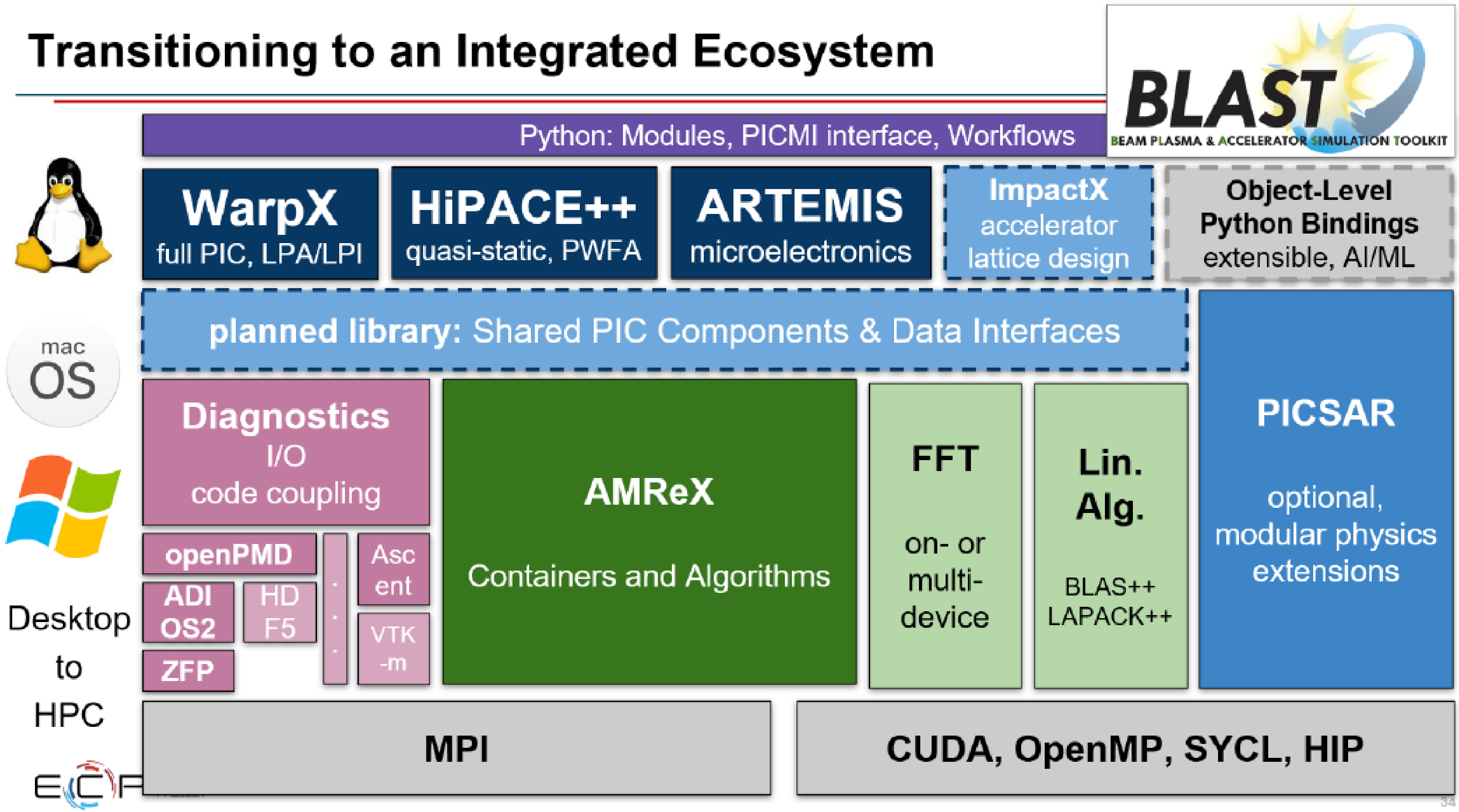


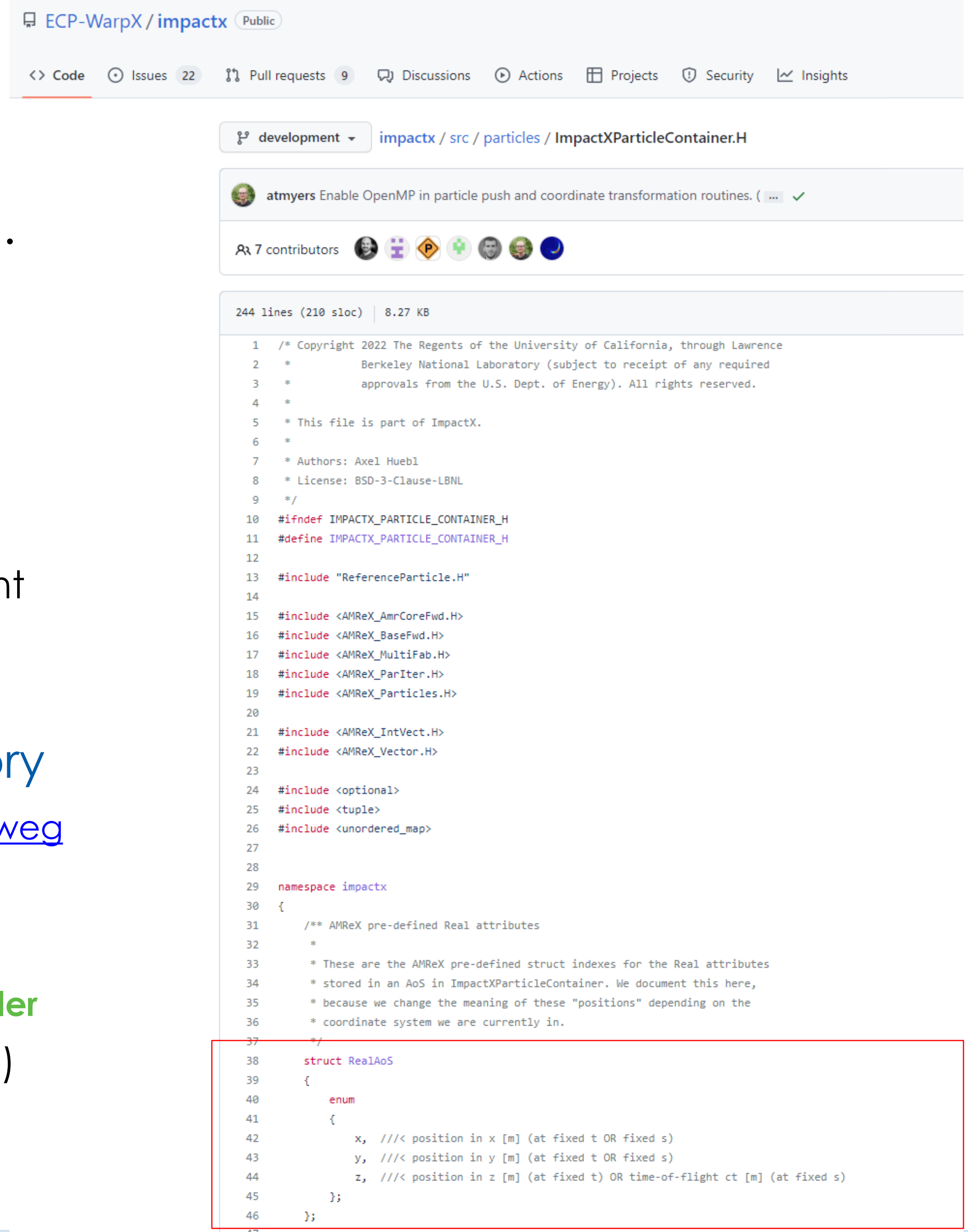
Figure 1. *Schematic of the integrated ecosystem that is envisioned for AMReX-based software to support the particle accelerator community and related applications.*

Porting Hellweg to AMReX

- *We are just getting started…*

- The ImpactX code base is very relevant to this project
  - Hellweg & IMPACT share some high-level commonalities
  - the algorithms are very different

- We're developing in the `rshellweg` GitHub repository
  - https://github.com/radiasoft/rshellweg
  - physics algorithms, in C++
  - C++ MS Windows GUI
    - **requires Embarcadero compiler**
  - Linux-only build system (no GUI)
    - **Python API for C++ library**
  - TBD – new AMReX version



Implementation of regression testing and benchmarking on CPU & GPU

- Python testing utility `pytest` is being used to develop unit & regression tests
- Tests are being developed for the existing code base
  - S. Kutsaev is compiling on MS Windows with Embarcadero
  - RadiaSoft team is compiling on Linux with g++
  - Special care is required to manage simultaneous development for both environments
- The AMReX version is not ready for testing
  - Hence, we're not yet running tests on GPUs
- In the future, we'll test for speed, as well as correctness

The 2D Hellweg equations of motion

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

ELSEVIER

Electron dynamics simulations with *Hellweg 2D* code

Sergey V. Kutsaev

Moscow Engineering Physics Institute (State University), Kashirskoe Sh., 31, 115410 Moscow, Russian Federation

If we consider the part of the beam with a wavelength width divided by N "large" particles, the dimensionless RF-filed amplitude $A = eE\lambda/W_0$ affecting each particle and the particle's phase, the ψ in this field can be calculated using the following formulae:

$$\frac{dA}{d\xi} = A\left\{\frac{1}{2}\frac{d}{d\xi}(\ln R_b) - w\right\} - \frac{2B}{N}\sum_{n=1}^{N} I_0\left(\frac{2\pi}{\beta_w}\sqrt{1-\beta_w^2}\eta_b\right)\cos\psi_n, \quad (2a)$$

$$\frac{d\psi}{d\xi} = 2\pi\left(\frac{1}{\beta_w} - \frac{1}{\beta_\xi}\right) + \frac{2B}{AN}\sum_{n=1}^{N} I_0\left(\frac{2\pi}{\beta_w}\sqrt{1-\beta_w^2}\eta_b\right)\sin\psi_n \quad (2b)$$

The components of the dimensionless electric A and magnetic $H = ecB_m\lambda/W_0$ field amplitudes that affect each particle can be found using the formulae:

$$A_\xi = A(\xi) I_0\left(\frac{2\pi}{\beta_w}\sqrt{1-\beta_w^2}\eta\right)\cos\psi + A_\xi^{coul} \quad (4a)$$

$$A_\eta = -\frac{\beta_w}{2\pi\sqrt{1-\beta_w^2}} I_1\left(\frac{2\pi}{\beta_w}\sqrt{1-\beta_w^2}\eta\right) \times \left\{\frac{dA}{d\xi}\cos\psi - \left[\frac{2B}{N}\sum_{n=1}^{N} I_0\left(\frac{2\pi}{\beta_w}\sqrt{1-\beta_w^2}\eta_n\right)\sin\psi_n + \frac{2\pi}{\beta_w}A(\xi)\right]\sin\psi\right\} + A_\eta^{coul} \quad (4b)$$

$$H_\theta = \frac{\beta_w A(\xi)}{\sqrt{1-\beta_w^2}} I_1\left(\frac{2\pi}{\beta_w}\sqrt{1-\beta_w^2}\eta\right)\sin\psi \quad (4c)$$

Apart from RF field, these expressions also consider a space charge field. To simulate the self-consistent dynamics of the particles, it is necessary to insert the expressions (4) in the equations of motion:

$$\frac{d\beta_\xi}{d\xi} = \frac{1}{\gamma\beta_\xi}\left((1-\beta_\xi^2)A_\xi + \beta_\eta(H_\theta - \beta_\xi A_\eta) - \beta_\theta H_\eta^{EXT}\right) \quad (5a)$$

$$\frac{d\beta_\eta}{d\xi} = \frac{1}{\gamma\beta_\xi}\left(A_\eta - \beta_\xi H_\theta - \beta_\eta(\beta_\xi A_\xi + \beta_\eta A_\eta)\right) + \frac{\beta_\theta}{\beta_\xi\gamma}H_\xi^{EXT} + \frac{\eta\theta^{\bullet 2}}{\beta_\xi} \quad (5b)$$

$$\eta^2\gamma\beta_\xi\frac{d\theta}{d\xi} = \frac{1}{2}\left(C - \eta^2 H_\xi^{EXT}\right) \quad (5c)$$

Here the constant C determines the initial conditions of the injected beam. In case of electron gun without magnetic field $C = 0$.

The 3D Hellweg equations of motion

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Nuclear Inst. and Methods in Physics Research, A

journal homepage: www.elsevier.com/locate/nima

Generalized 3D beam dynamics model for industrial traveling wave linacs design and simulations

Sergey V. Kutsaev [a,*], Yury Eidelman [b], David Bruhwiler [b]

[a] RadiaBeam Technologies LLC, 1717 Stewart St, Santa Monica, CA 90404, USA
[b] RadiaSoft LLC, 1348 Redwood Ave, Boulder, CO 80304, USA

$$\frac{d\beta_\zeta}{d\zeta} = \frac{1}{\gamma\beta_\zeta}\Big[(1-\beta_\zeta^2)A_\zeta + \beta_\eta\left(H_\theta - \beta_\zeta A_\eta\right) - \beta_\theta\left(H_\eta + \beta_\zeta A_\theta\right) + \beta_\eta H_\theta^{ext} - \beta_\theta H_\eta^{ext}\Big]$$

$$\frac{d\beta_\eta}{d\zeta} = \frac{1}{\gamma\beta_\zeta}\Big[(1-\beta_\eta^2)A_\eta + \beta_\theta\left(H_\zeta - \beta_\eta A_\theta\right) - \beta_\zeta\left(H_\theta + \beta_\eta A_\zeta\right) + \beta_\theta H_\zeta^{ext} - \beta_\zeta H_\theta^{ext}\Big] + \frac{\beta_\theta^2}{\eta\beta_\zeta}$$

$$\frac{d\beta_\theta}{d\zeta} = \frac{1}{\gamma\beta_\zeta}\Big[(1-\beta_\theta^2)A_\theta + \beta_\zeta\left(H_\eta - \beta_\theta A_\zeta\right) - \beta_\eta\left(H_\zeta + \beta_\theta A_\eta\right) + \beta_\zeta H_\eta^{ext} - \beta_\eta H_\zeta^{ext}\Big] - \frac{\beta_\theta\beta_\eta}{\eta\beta_\zeta}$$

$$\frac{dA}{d\zeta} = A\left\{\frac{1}{2}\frac{d}{d\zeta}\left(\ln R_b - w\right)\right\} - \frac{2B}{N}\sum_{n=1}^{N} I_0\left(\frac{2\pi}{\beta_{ph0}}\sqrt{1-\beta_{ph0}^2}\,\eta_n\right)\cos\psi_n$$

$$\frac{d\psi}{d\zeta} = 2\pi\left(\frac{1}{\beta_{ph0}} - \frac{1}{\beta_\zeta}\right) + \frac{2B}{AN}\sum_{n=1}^{N} I_0\left(\frac{2\pi}{\beta_{ph0}}\sqrt{1-\beta_{ph0}^2}\,\eta_n\right)\sin\psi_n$$

$$A = \frac{E\lambda}{W_o}$$

$$H = c\frac{B\lambda}{W_o}$$

Generalizing the Hellweg equations of motion

- Generalized from electrons only to handle arbitrary charge-to-mass ratio
  - ion linacs can be simulated in the future
- The velocity-like dynamical variables are being changed to momentum
  - enables accurate modeling of ultra-relativistic electrons
- Identified a strategy to develop a phase space preserving version of the eqn's
  - necessary for work in the future with very high phase space densities
  - otherwise, it is challenging to know if phase space dilution is physical or numerical

- Near term plans –
  - treat half-cell rf cavities
  - include cathode emission
  - treat standing wave as well as TW

Future plans: modify the EOM to preserve phase space area

PHYSICAL REVIEW ACCELERATORS AND BEAMS **20,** 052002 (2017)

Symplectic modeling of beam loading in electromagnetic cavities

Dan T. Abell,* Nathan M. Cook, and Stephen D. Webb
RadiaSoft, LLC, 1348 Redwood Ave., Boulder, Colorado 80304, USA
(Received 3 November 2016; published 22 May 2017)

If we neglect the beam space charge, and consider only the cavity eigenmodes, then $\phi = 0$. Furthermore, our beam has $|d\mathbf{x}_\perp/d\tau| \ll dz/d\tau \sim 1$, while $|\mathbf{A}_\perp| \sim A_z$. We therefore choose to neglect the transverse coupling terms. We do not *have* to do this: all the algorithms and computational results described in this paper can be (and is some cases have been) done without making this simplification; but doing so leaves us with what we call the *beam electromagnetic Low Lagrangian*:

$$\mathcal{L}\left(\mathbf{x}, \frac{d\mathbf{x}}{dt}, \mathbf{A}, \frac{\partial \mathbf{A}}{\partial t}\right) = \int d\mathbf{x}_0 d\mathbf{v}_0 \left[-mc^2\sqrt{1-\left(\frac{d\mathbf{x}}{d\tau}\right)^2} + q\frac{dz}{d\tau}A_z(\mathbf{x},t)\right] \times \psi(\mathbf{x}_0,\mathbf{v}_0) + \frac{1}{8\pi}\int d\mathbf{x}\left[\left(\frac{\partial \mathbf{A}}{\partial \tau}\right)^2 - (\nabla \times \mathbf{A})^2\right]. \qquad (2)$$

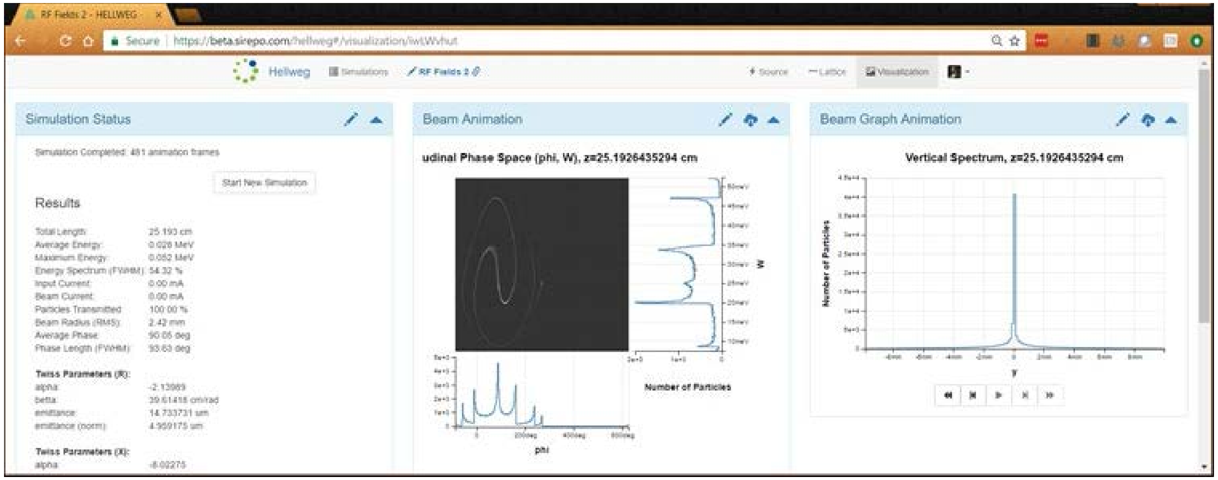
$$\psi(\mathbf{x}, \dot{\mathbf{x}}) = \sum_{j=1}^{N_{\mathrm{macro}}} w_j \Lambda(\mathbf{x} - \mathbf{x}^{(j)})\delta(\dot{\mathbf{x}} - \dot{\mathbf{x}}^{(j)})$$

$$F_\ell(\mathbf{x}^{(j)}) = \mathbf{z} \cdot \int d\mathbf{x}\, \mathbf{f}_\ell(\mathbf{x})\Lambda(\mathbf{x} - \mathbf{x}^{(j)})$$

$$\mathcal{H} = \underbrace{\sum_j c\sqrt{(\mathbf{p}_\perp^{(j)})^2 + \left(p_z^{(j)} - w_j\frac{q}{c}\sum_\ell Q_\ell F_\ell(\mathbf{q}^{(j)})\right)^2 + w_j^2 m^2 c^2}}_{\mathcal{H}_{\mathrm{pc}}} + \underbrace{\frac{1}{2}\sum_\ell\left[\frac{P_\ell^2}{C_\ell} + \frac{1}{L_\ell}Q_\ell^2\right]}_{\mathcal{H}_{\mathrm{f}}}$$

Future: Relaunch Sirepo/Hellweg app with targeted beta testing effort

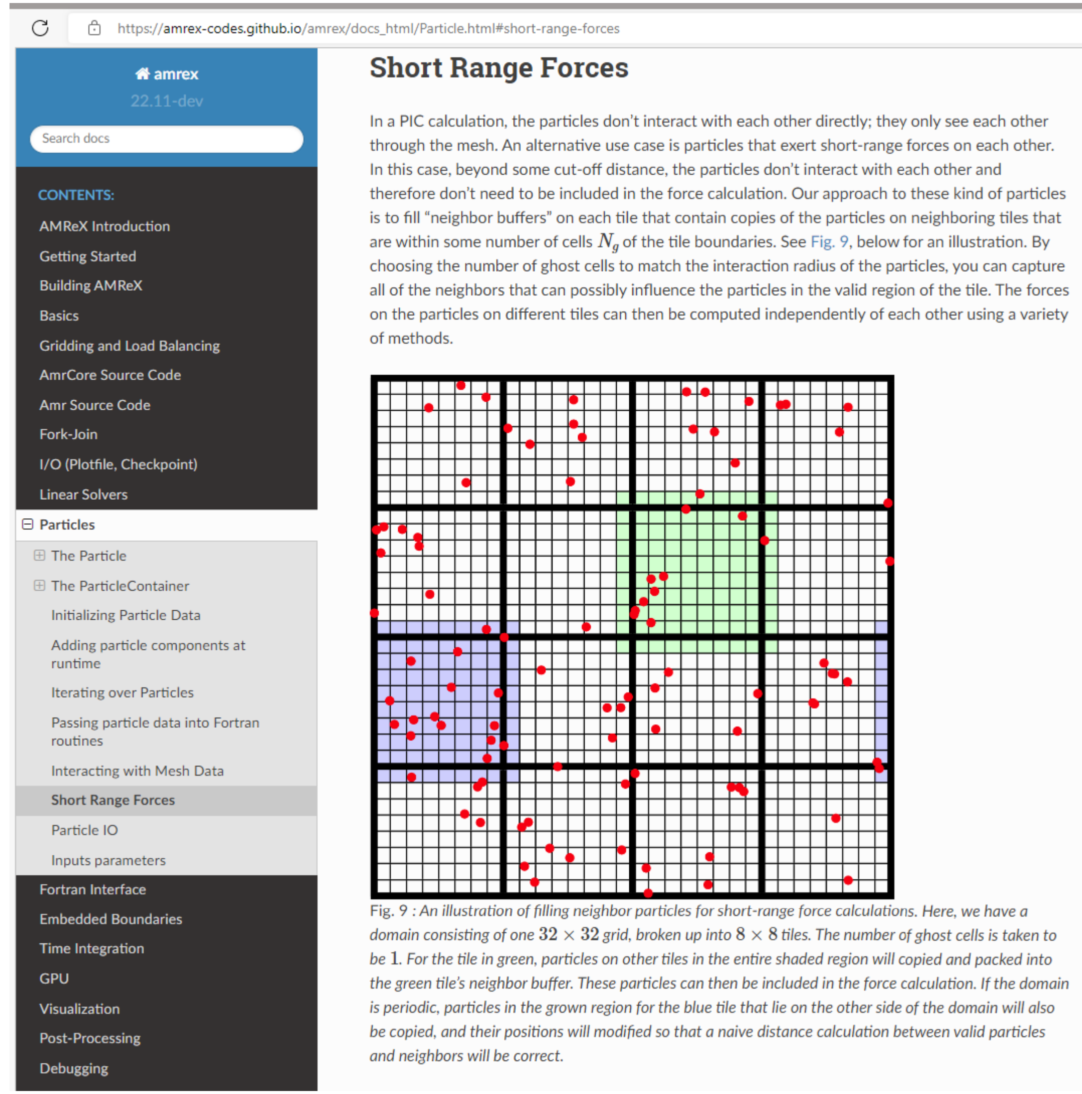
- We implemented an 'alpha' quality Hellweg app for `Sirepo.com`
  - funded by Phase 1 DOE/HEP SBIR; later removed due to lack of funding
- `Sirepo` is presently undergoing a major upgrade for the future
  - The GUI framework, originally written in `AngularJS` is being rewritten in `React`
    - `metaprogramming techniques are being used to simplify future app development`
  - The Python server, originally based on `Flask` is being rewritten to use `Tornado`
- We will relaunch the app in early 2023, using the new version of `Sirepo`
  - on the server, Sirepo will invoke the Hellweg Linux library via the Python API



S. V. Kutsaev et al. "Cloud-based design of high average power traveling wave linacs". In: *Journal of Physics: Conference Series* 941 (2017), p. 012106.

Future: Develop a strategy to model strong particle-particle scattering

- Touschek effect is essential at high phase space density
- AMReX provides capabilities for near-particle interactions
  - will only be implemented in the new version of Hellweg



https://amrex-codes.github.io/amrex/docs_html/Particle.html#short-range-forces

amrex
22.11-dev

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Short Range Forces

In a PIC calculation, the particles don't interact with each other directly; they only see each other through the mesh. An alternative use case is particles that exert short-range forces on each other. In this case, beyond some cut-off distance, the particles don't interact with each other and therefore don't need to be included in the force calculation. Our approach to these kind of particles is to fill "neighbor buffers" on each tile that contain copies of the particles on neighboring tiles that are within some number of cells N_g of the tile boundaries. See Fig. 9, below for an illustration. By choosing the number of ghost cells to match the interaction radius of the particles, you can capture all of the neighbors that can possibly influence the particles in the valid region of the tile. The forces on the particles on different tiles can then be computed independently of each other using a variety of methods.

Fig. 9 : An illustration of filling neighbor particles for short-range force calculations. Here, we have a domain consisting of one 32×32 grid, broken up into 8×8 tiles. The number of ghost cells is taken to be 1. For the tile in green, particles on other tiles in the entire shaded region will copied and packed into the green tile's neighbor buffer. These particles can then be included in the force calculation. If the domain is periodic, particles in the grown region for the blue tile that lie on the other side of the domain will also be copied, and their positions will modified so that a naive distance calculation between valid particles and neighbors will be correct.

Summary

- 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
  - space charge included approximately via quasistatic envelope model
  - 2D and 3D dynamics
  - 1000x faster than CST, with quantitative agreement
- We are porting Hellweg to the AMReX framework
  - will enable GPU execution with orders of magnitude speedup
  - growing suite of AMReX based codes: WarpX, ImpactX, others…
- We are generalizing the equations of motion
  - support ion linac design, as well as very high energy electron linacs
  - support standing wave structures and photocathode e- guns
- Adding new features, required for very high phase space densities
  - Touschek scattering
  - exploring phase space conserving algorithms