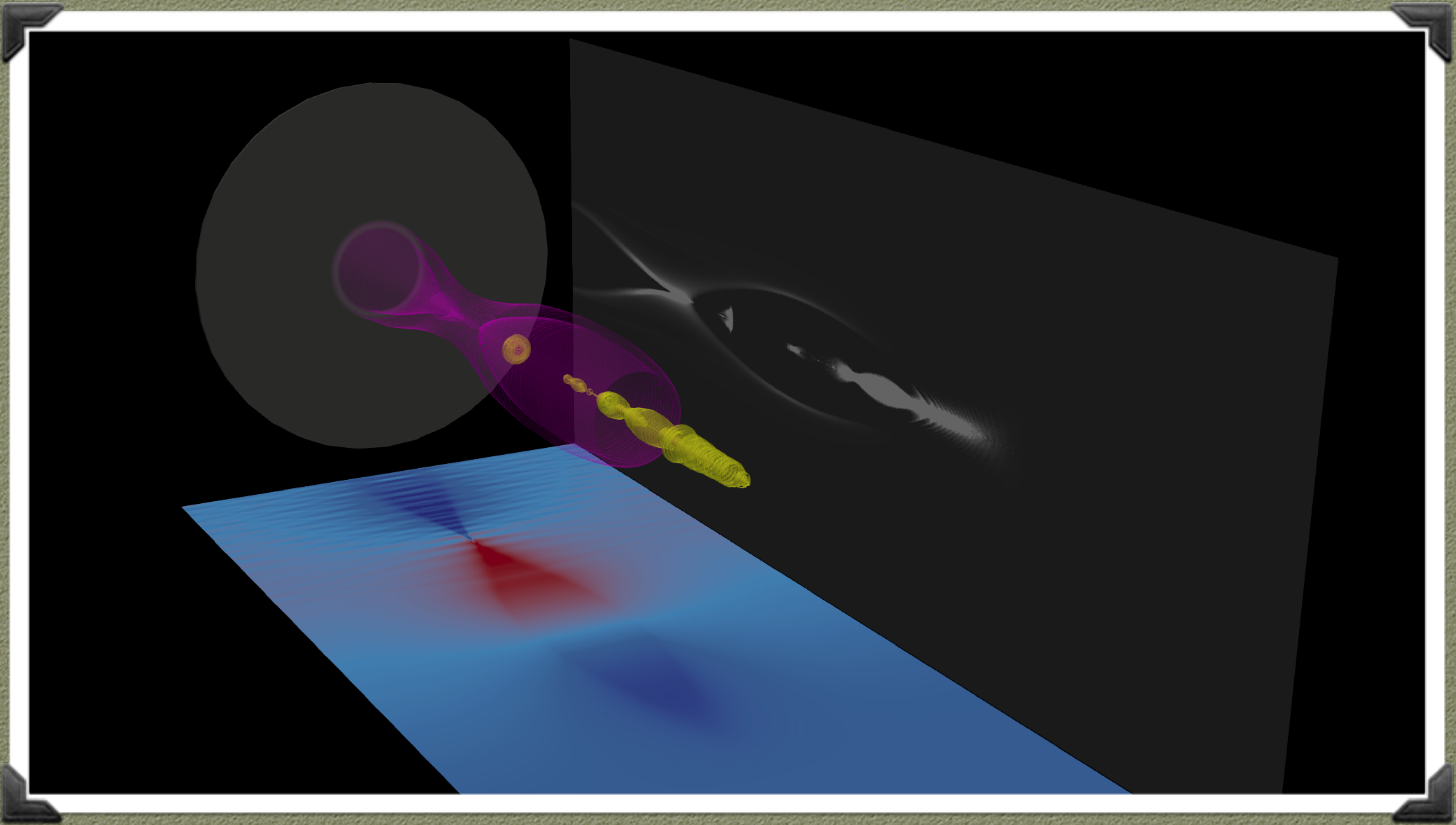


SUMMARY THEORY AND SIMULATIONS

topics - 4 sessions

1. Analytical models
2. Numerical Results
3. Numerical Methods
4. Scientific Computing

topics - 4 sessions

1. Analytical models
    - transverse bunch matching
2. Numerical Results
    - Code development
    - Code update
3. Numerical Methods
    - Cherenkov mitigation
    - Spectral methods PSATD
    - Adaptive Mesh Refinement (AMR)
    - Envelope
4. Scientific Computing
    - Dynamic load balancing
    - Data Reduction
    - In situ visalization
    - use of new libraries

150 years of Maxwell's (other) equations and application to plasma acceleration

Robert Robson[1], Timon Mehrling[2] and Jens Osterhoff[2]

[1]James Cook University and Griffith University, Australia
[2]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

An approach invented by Maxwell exactly 150 years ago is until today important in science

- Maxwell's original "equations of matter" (velocity moment equation)

$$\boxed{\frac{\partial\left(n\overline{Q}\right)}{\partial t} = -\nabla\cdot\Gamma_Q + \frac{n}{m}\overline{\boldsymbol{F}\cdot\nabla_{\mathrm{v}}Q(\mathbf{v})} + n\overline{\left.\frac{\partial Q}{\partial t}\right)}_{col}}$$

J.C. Maxwell, Phil. Trans. Roy. Soc. London 157, 49 (1867)

$$Q = 1 \rightarrow \quad \frac{\partial n}{\partial t} + \nabla\cdot n\overline{\mathbf{v}} = 0$$

$$Q = m\mathbf{v} \rightarrow \quad \frac{\partial(nm\overline{\mathbf{v}})}{\partial t} = -\nabla\cdot(nm\,\overline{\mathbf{vv}}) + n\boldsymbol{F} - n\mu\nu_m\overline{\mathbf{v}}$$

etc.

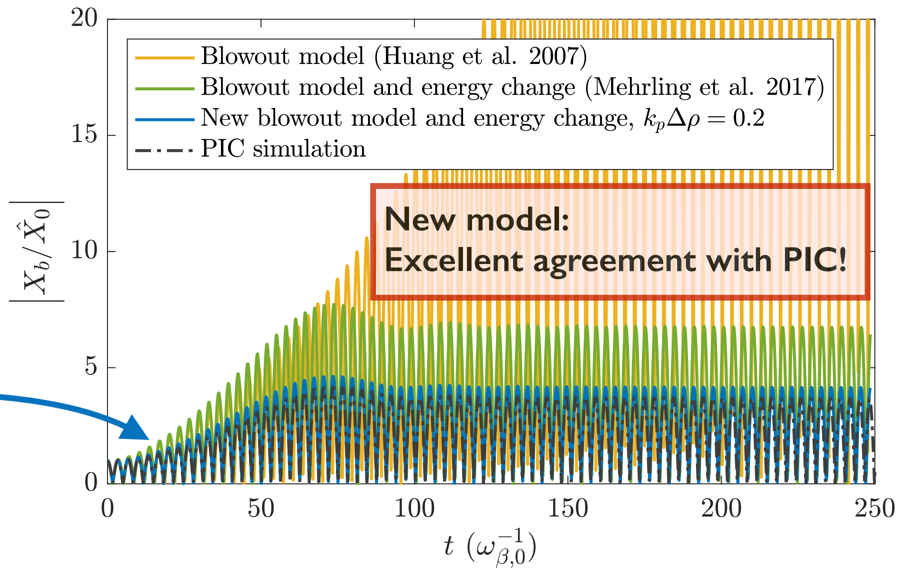
- This moment approach can be used to model the channel centroid in hosing in PWFAs

Moment equation for sheath electrons in the quasi-static approximation:

$$\partial_\xi\langle\Phi\rangle = \left\langle\frac{p_r}{1+\psi}\partial_r\Phi\right\rangle + \left\langle\frac{\gamma\dot{\theta}}{1+\psi}\partial_\theta\Phi\right\rangle + \left\langle\frac{\gamma F_r}{1+\psi}\partial_{p_r}\Phi\right\rangle + \left\langle\frac{\gamma F_\psi}{1+\psi}\partial_\psi\Phi\right\rangle$$

Setting. $\Phi = x$, etc. $\Rightarrow$ new channel centroid equation:

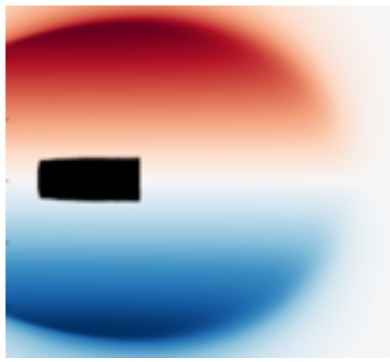
$$\boxed{\frac{\partial^2 X_c}{\partial\xi^2} + \frac{k_p^2}{2}\left[c_c(\xi)X_c - c_b(\xi)X_b\right] = 0}$$



Saturation of the beam-hosing instability with a betatron chirp in the quasi-linear regime

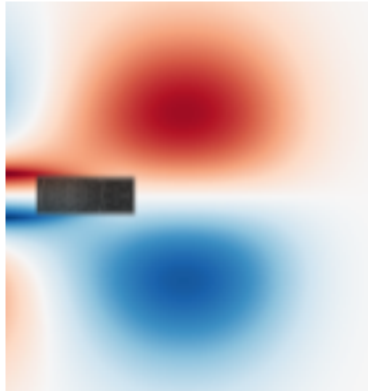
A varying betatron frequency across the bunch ("betatron chirp") can lead to a **saturation** of the beam-hosing instability.

Blow-out regime



Focusing strength is constant across the bunch.
Betatron chirp **requires an energy spread**.

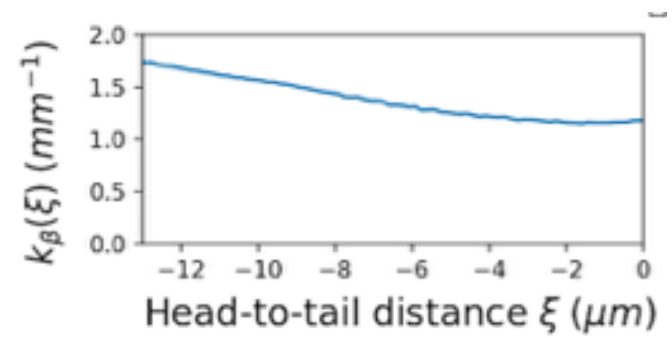
Quasi-linear regime



Focusing strength naturally varies across bunch.
No energy spread required.

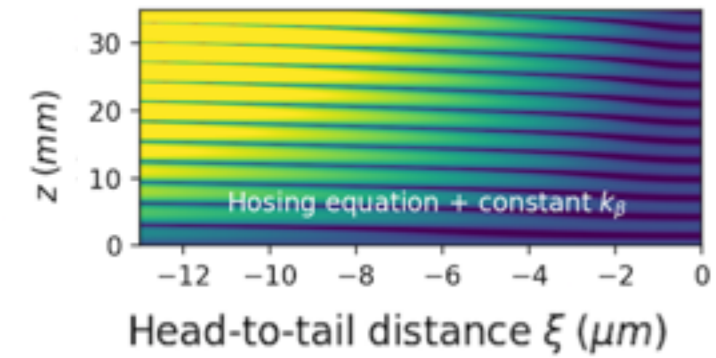
Confirmation in PIC simulations: Monoenergetic beam in quasi-linear regime

Betatron chirp is observed in the simulation:

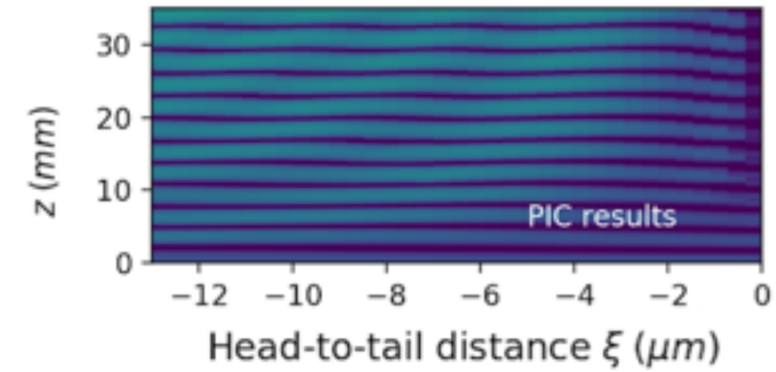


Standard hosing scalings (which **neglect** betatron chirp) predict high instability:

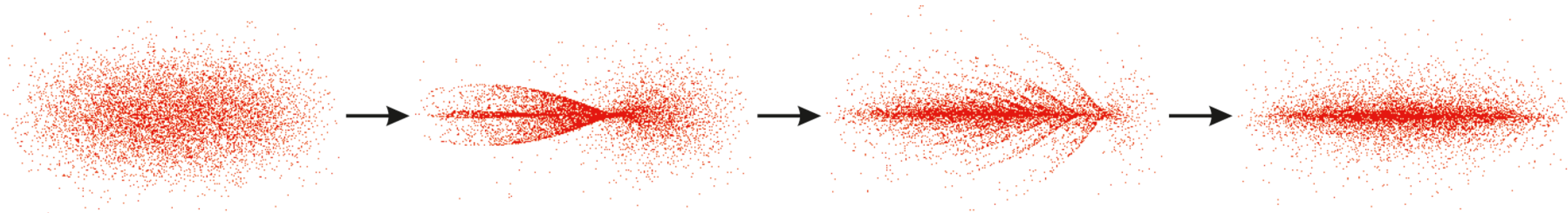
(Colormap=instability level)

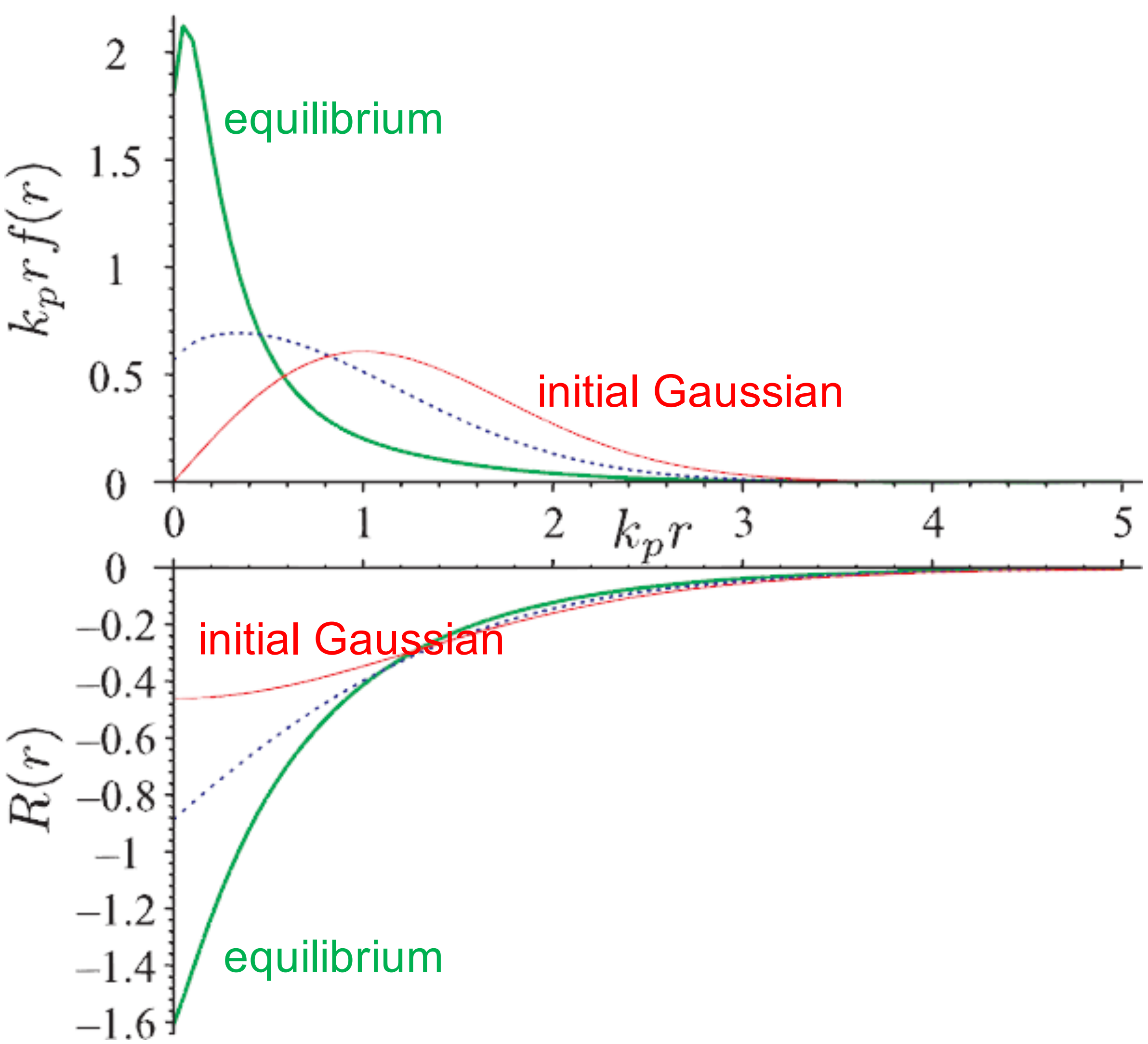


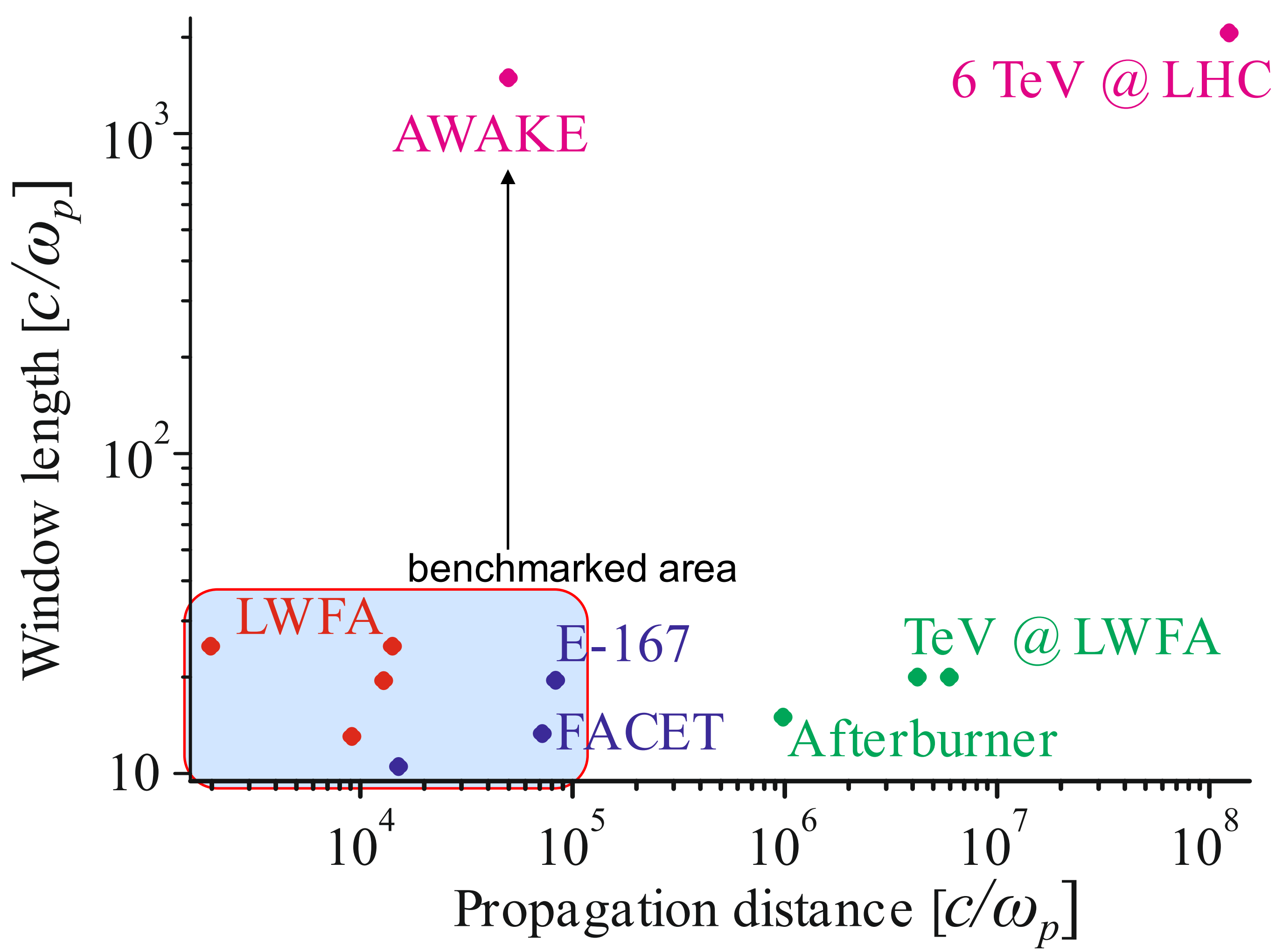
But **actual** hosing level **saturates** at a much lower level:



Transverse bunch evolution







Development of an analytical model for emittance calculation in external injection scenarios

- Using a single particle DGL and applying a momentum approach, e.g.

$$\langle x^2\rangle(t) = \int_{-\infty}^{\infty}(x^2(t))f_0\mathrm{d}x_0\mathrm{d}p_{x,0}\mathrm{d}\delta\gamma,\ f_0 = f_\perp(x_0,p_{x,0})f_\gamma(\gamma_0),\ \int f_0\mathrm{d}x_0\mathrm{d}p_{x,0}\mathrm{d}\gamma_0 = 1$$

- Two scenarios were analyzed
  - Single witness beam slice without energy gain (E_z zero crossing)
  - Single witness beam slice with energy gain (positioned at defined E_z)
- Formulas for emittance evolution of a single beam slice were derived, e.g. for a scenario without energy gain:

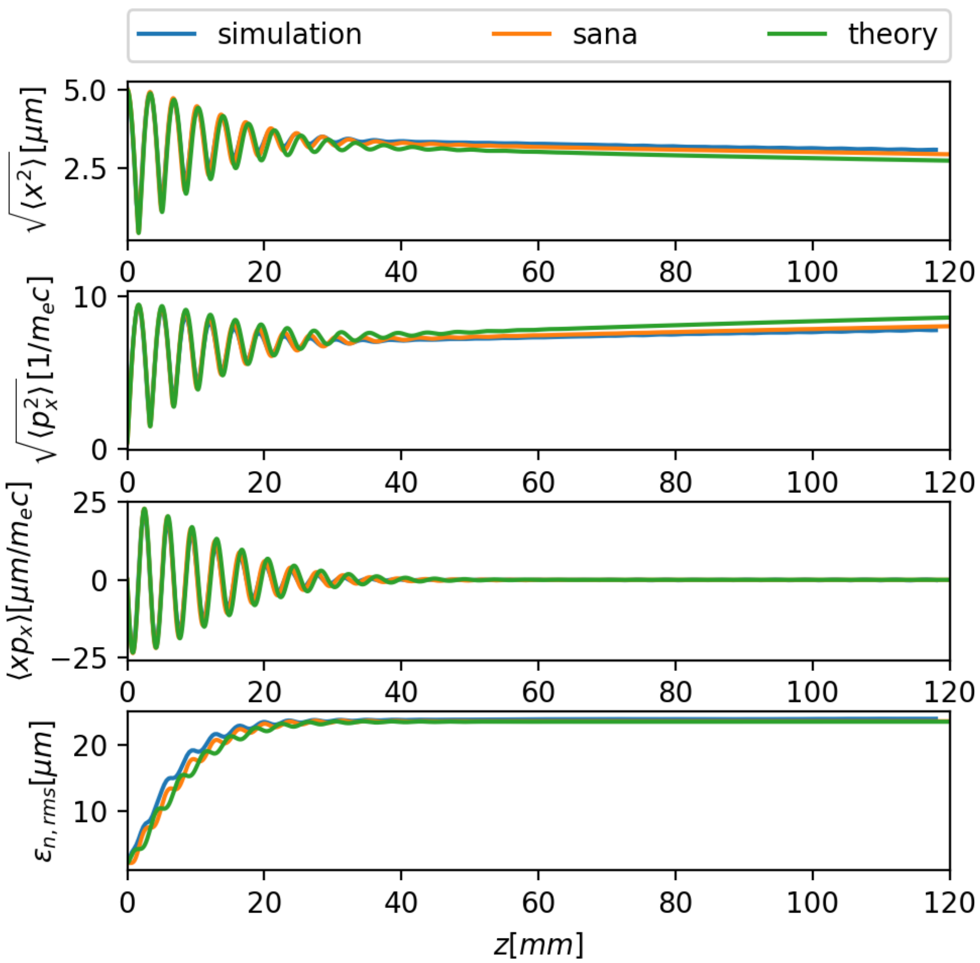
$$\frac{\epsilon^2_{n,rms}(\tilde{t})}{\epsilon_0^2} = \frac{1}{4}\left(\left(\frac{\langle x_0^2\rangle}{\langle x^2\rangle_m}\right)^2 + \left(\frac{\langle u_{x,0}^2\rangle}{\langle u_x^2\rangle_m}\right)^2\right)\left(1-e^{-b\tilde{t}^2}\right) + \frac{1}{2}\frac{\langle x_0^2\rangle}{\langle x^2\rangle_m}\frac{\langle u_{x,0}^2\rangle}{\langle u_x^2\rangle_m}\left(1+e^{-b\tilde{t}^2}\right) - \frac{\langle xu_{x,0}\rangle^2}{\epsilon_0^2}e^{-b\tilde{t}^2}$$

- With (index 'm' denoting beam moments under matching conditions)

$$b = \Delta\gamma^2/2\gamma_0,\ \Delta\gamma = \sigma_\gamma/\gamma,\ \langle xu_x\rangle_m = 0,\ \langle x^2\rangle_m = \epsilon_0\sqrt{2/\overline{\gamma_0}},\ \langle u_x^2\rangle_m = \epsilon_0\sqrt{\overline{\gamma_0}/2}$$

- Also providing the final emittance as

$$\lim_{t\to\infty}\epsilon^2_{n,rms}(\tilde{t}) = \frac{\overline{\gamma_0}}{8}\langle x_0^2\rangle^2 + \frac{1}{2\overline{\gamma_0}}\langle u_{x,0}^2\rangle^2 + \frac{1}{2}\langle x_0^2\rangle\langle u_{x,0}^2\rangle$$

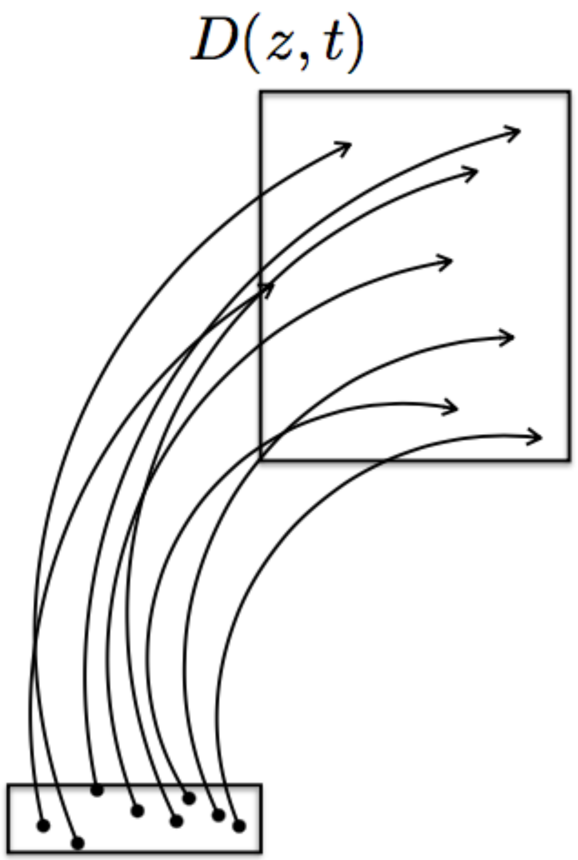


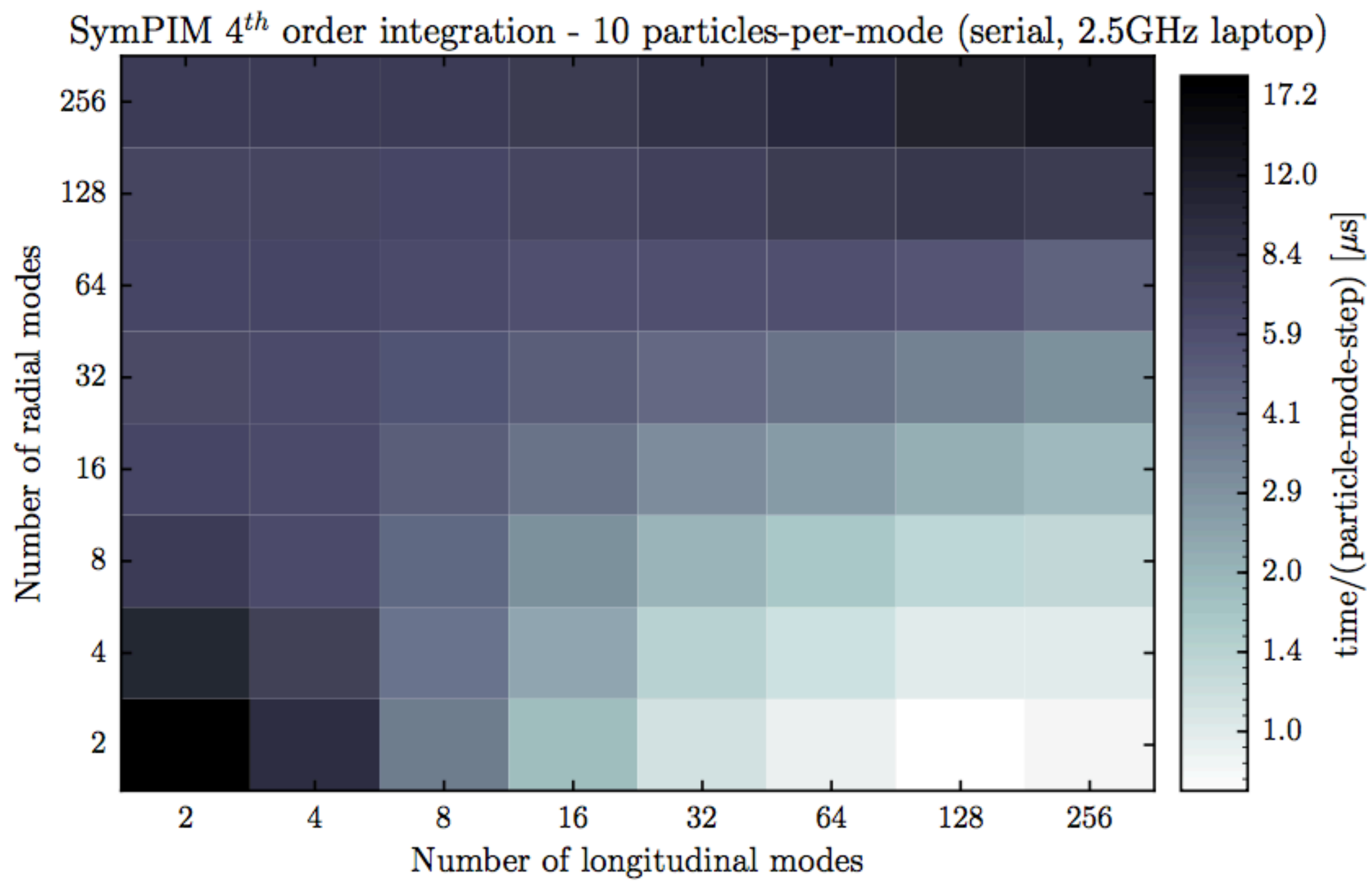
Comparison between analytical, a semi-analytic numerical (SANA) and Particle-in-Cell approaches

Symplectic approach

$$D(z,t) = D(\mathscr{M}_{-t} \circ z_0, t=0)$$

$$\underbrace{\mathbb{M}^t \; J \; \mathbb{M}}_{2D \times 2D} = J \rightarrow \dim_{\mathbb{M}} = 2D^2 + D$$

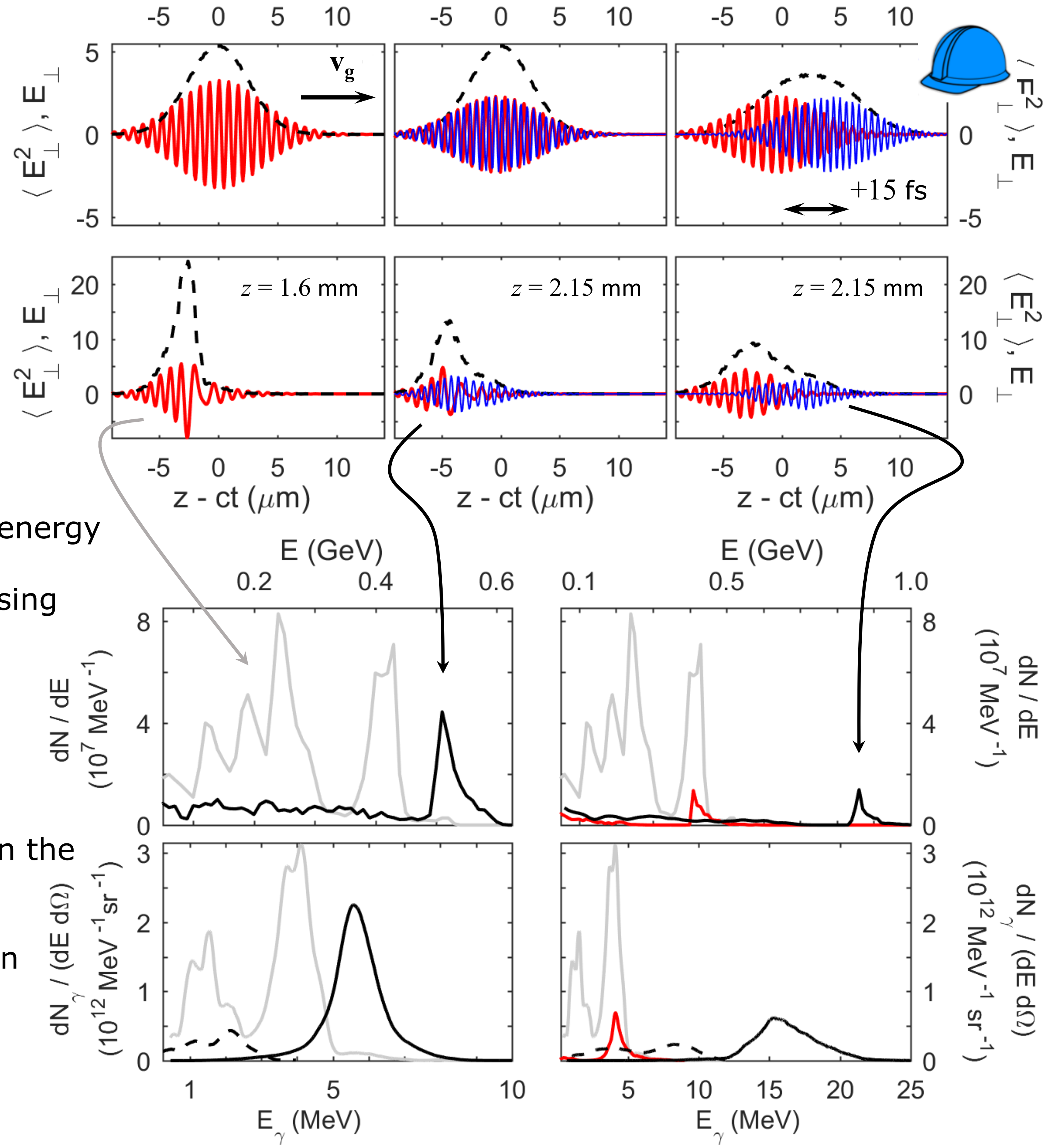




Optically controlled laser-plasma electron accelerators for compact γ - ray sources

- Bi-color stack of sub-Joule pulses is resilient to degradation of the dense plasma ($n_0 \sim 10^{19}$ cm^{-3})
- Electron beam quality is preserved
- Electron energy is doubled vs. predictions of scaling

Production of ultra-bright ($B_n > 10^{17}$ A/m²), GeV-scale



Electron energy spectra at dephasing

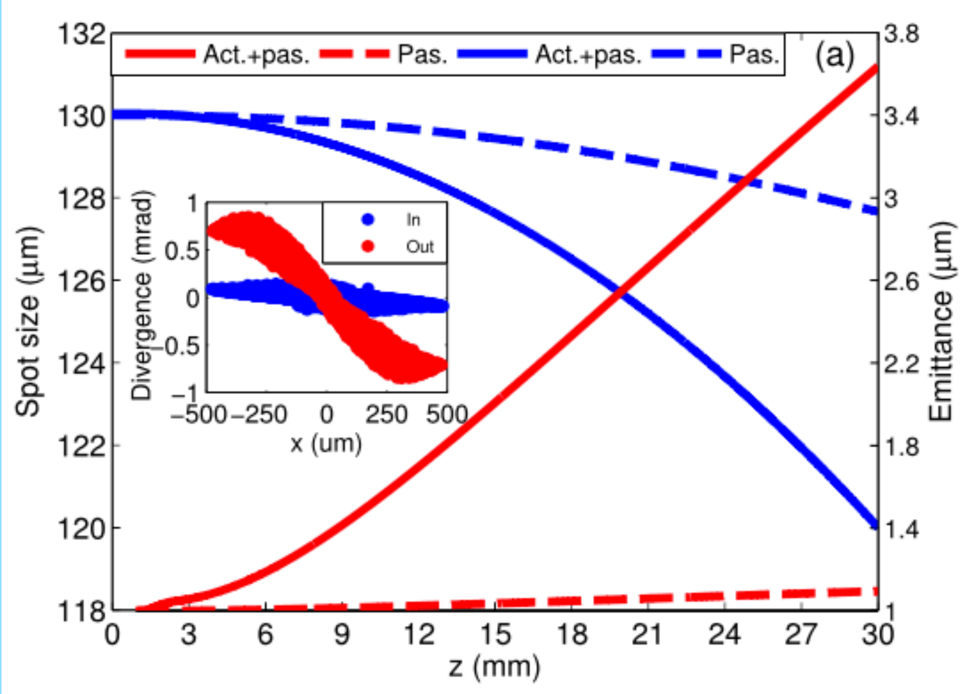
Stack-driven LPA produces perfect e-beams for a Thomson scattering-based γ-ray source:

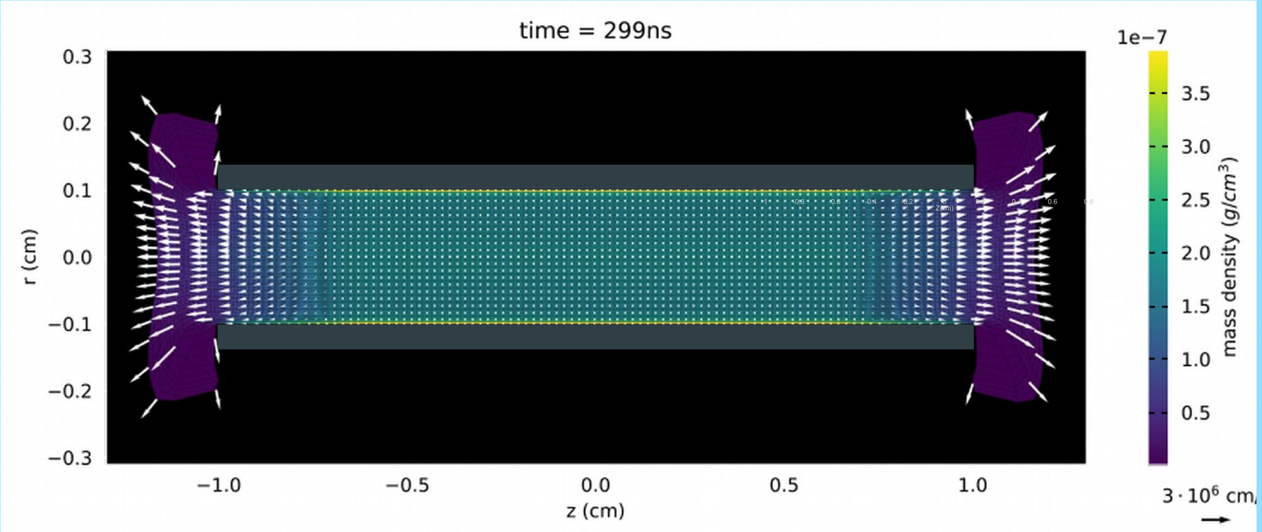
γ-ray flux in the direction of e-beam propagation

- Photon signal to background ratio exceeds 4:1
- Photon yield in a μsr observation solid angle $\Omega_d = (\pi/2)\langle \gamma_e \rangle^{-2}$: up to 5×10^6 in full bandwidth
- Photon energy is tunable from 4 to 16 MeV, while preserving the yield

Plasma lens simulations

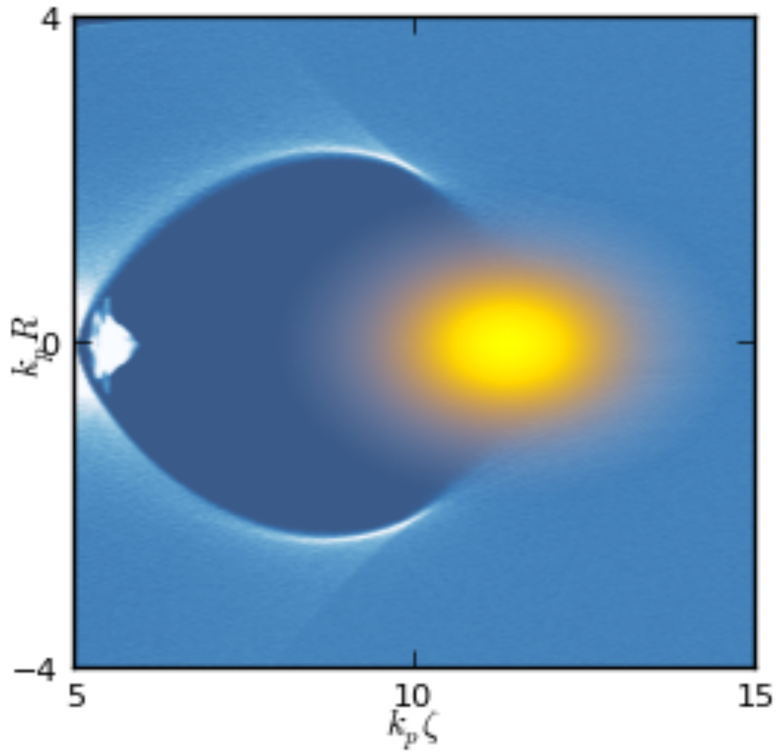
active and passive lens sims

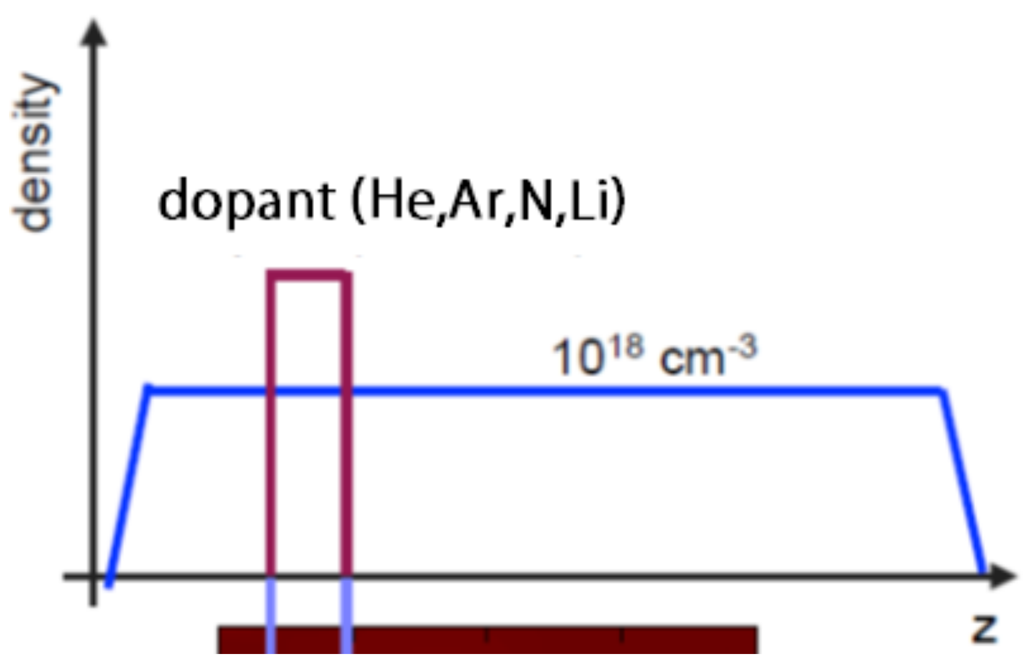




- start-to-end simulations
- GPT + Architect
- Hydro simulations

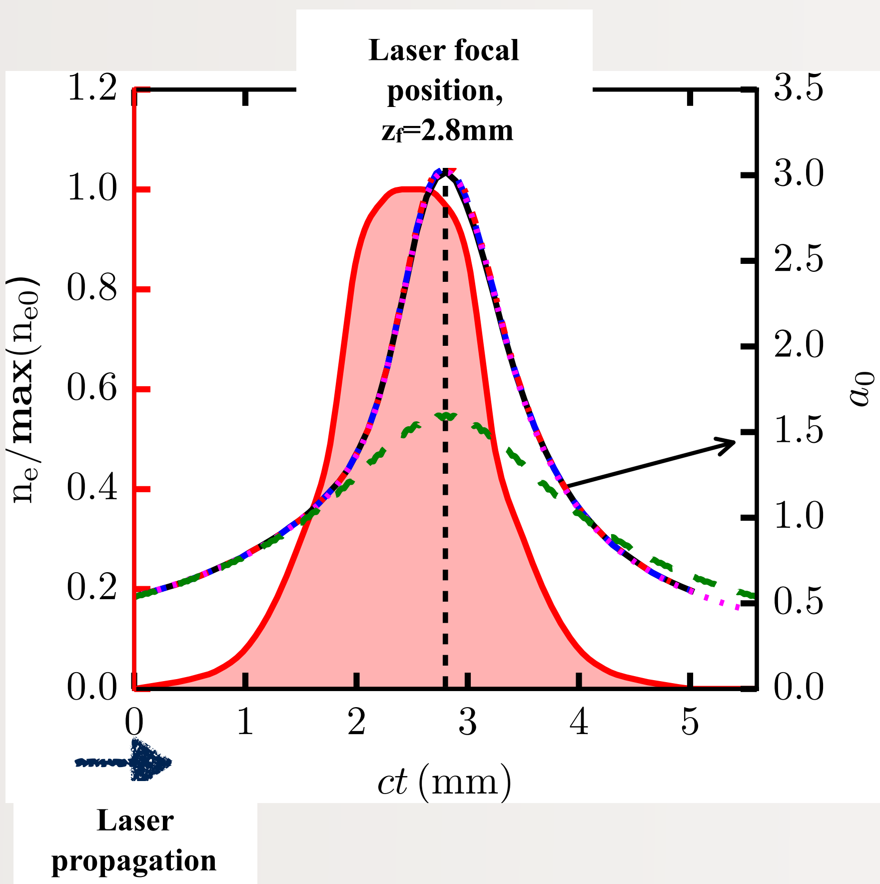
ionisation injection for PWFA

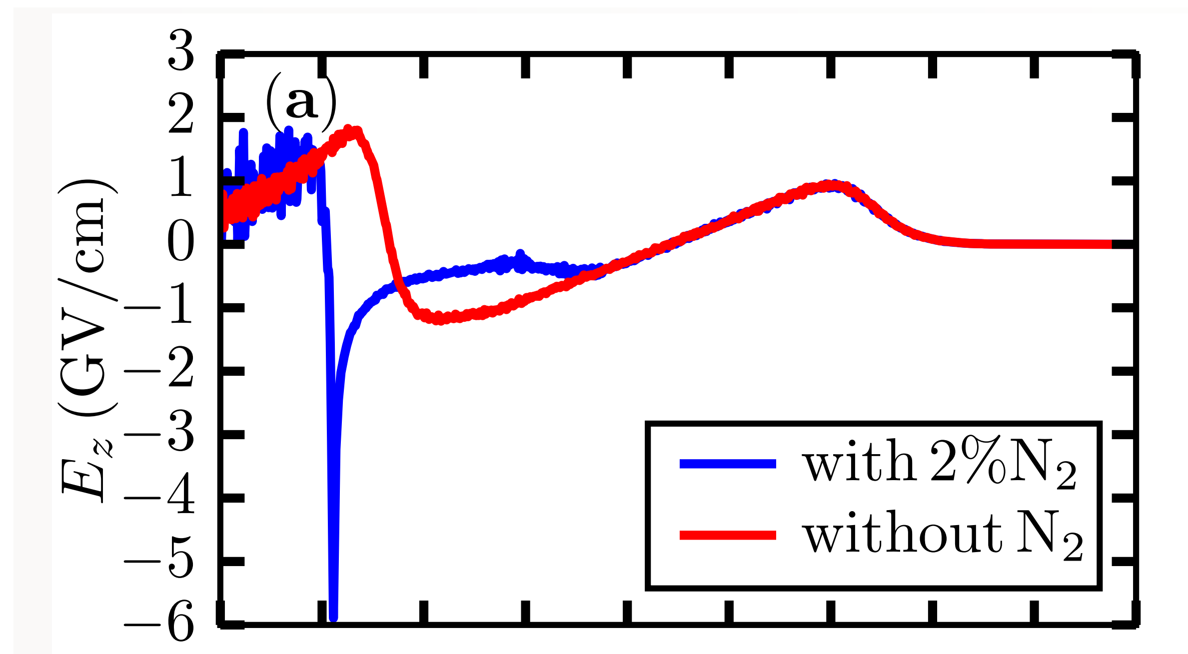




600 µm **pagation**	Q[pC]	σ_γ/γ[%]	ε_(n,rms) [µm]
N^{1+}	22.2	2.9	0.96
Ar^{1+}	26.7	3.3	0.87
Ne	22.5	3.9	1.2

ionisation injection
for LWFA





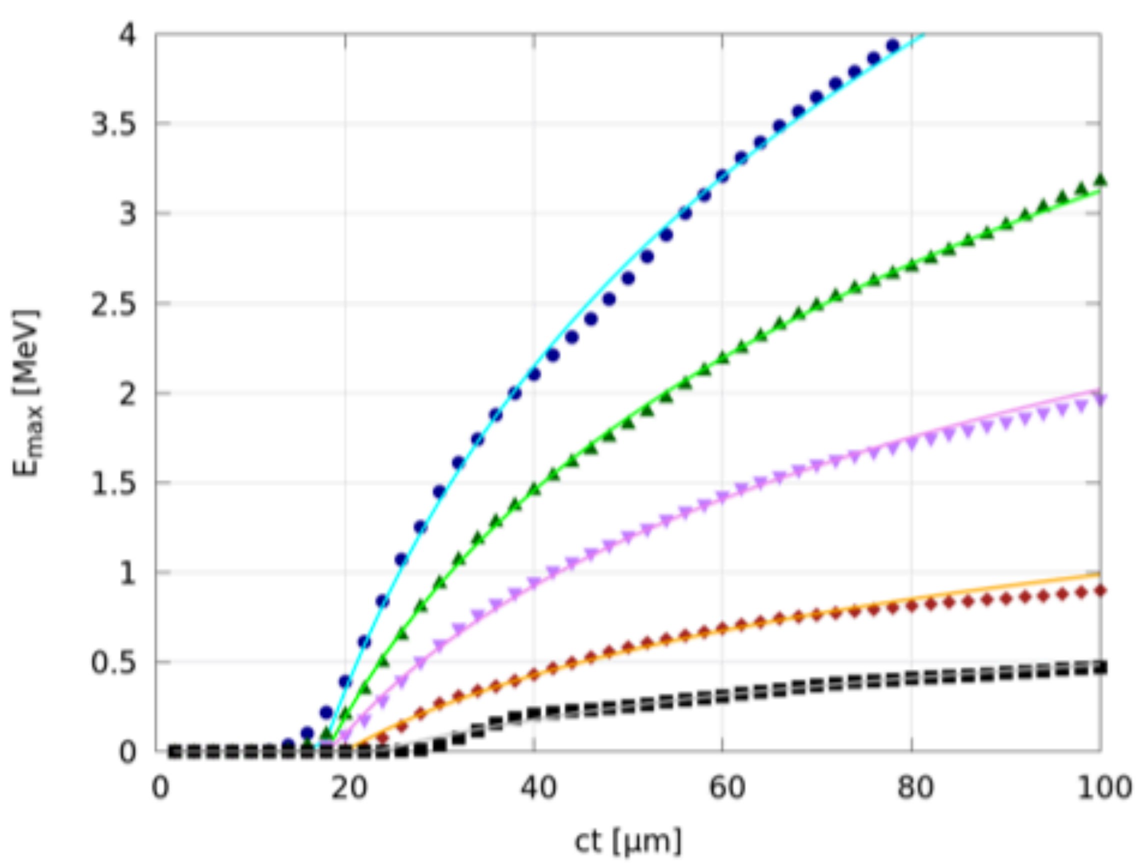
C_{N_2} (%)	Q (pC)	$\langle\mathcal{E}\rangle$ (MeV)	$\Delta\mathcal{E}_{rms}/\langle\mathcal{E}\rangle$ (%)	θ_x (mrad)	θ_y (mrad)	$\varepsilon_{x,n}$ (mm.mrad)	$\varepsilon_{y,n}$ (mm.mrad)
0.35	27	142	3.8	2.1	2.9	0.8	1.8
0.5	37	135	5.0	2.8	3.1	1.1	1.9
1.0	72	113	14.7	3.7	4.0	1.8	2.2
2.0	107	93	29.1	4.6	5.6	2.5	3.8

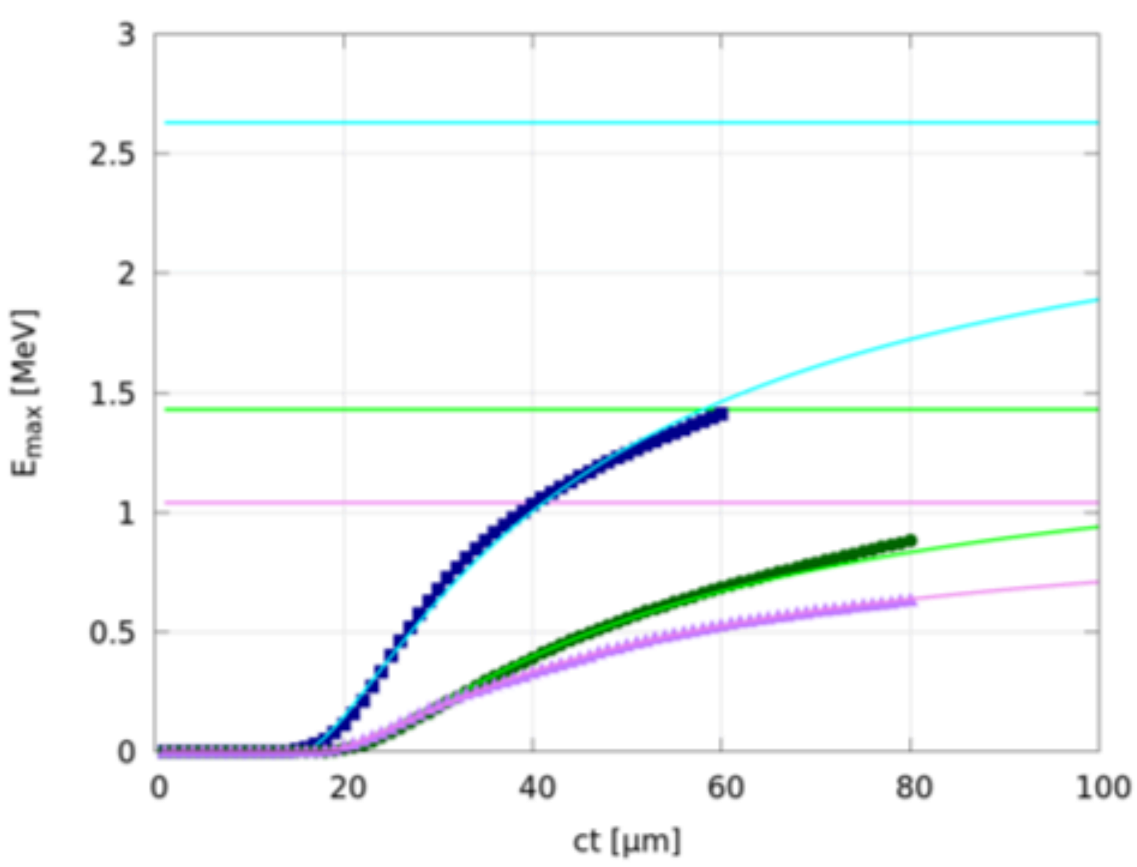
} optimal values

TNSA max-Energy estimation laws

$$\begin{cases} E_{\max}^{(2D)}(ct) = 0 & \text{for } t < t^{*(2D)} \\ E_{\max}^{(2D)}(ct) = E_{\infty}^{(2D)} \log \dfrac{ct}{ct^*} & \text{for } t > t^{*(2D)} \end{cases}$$

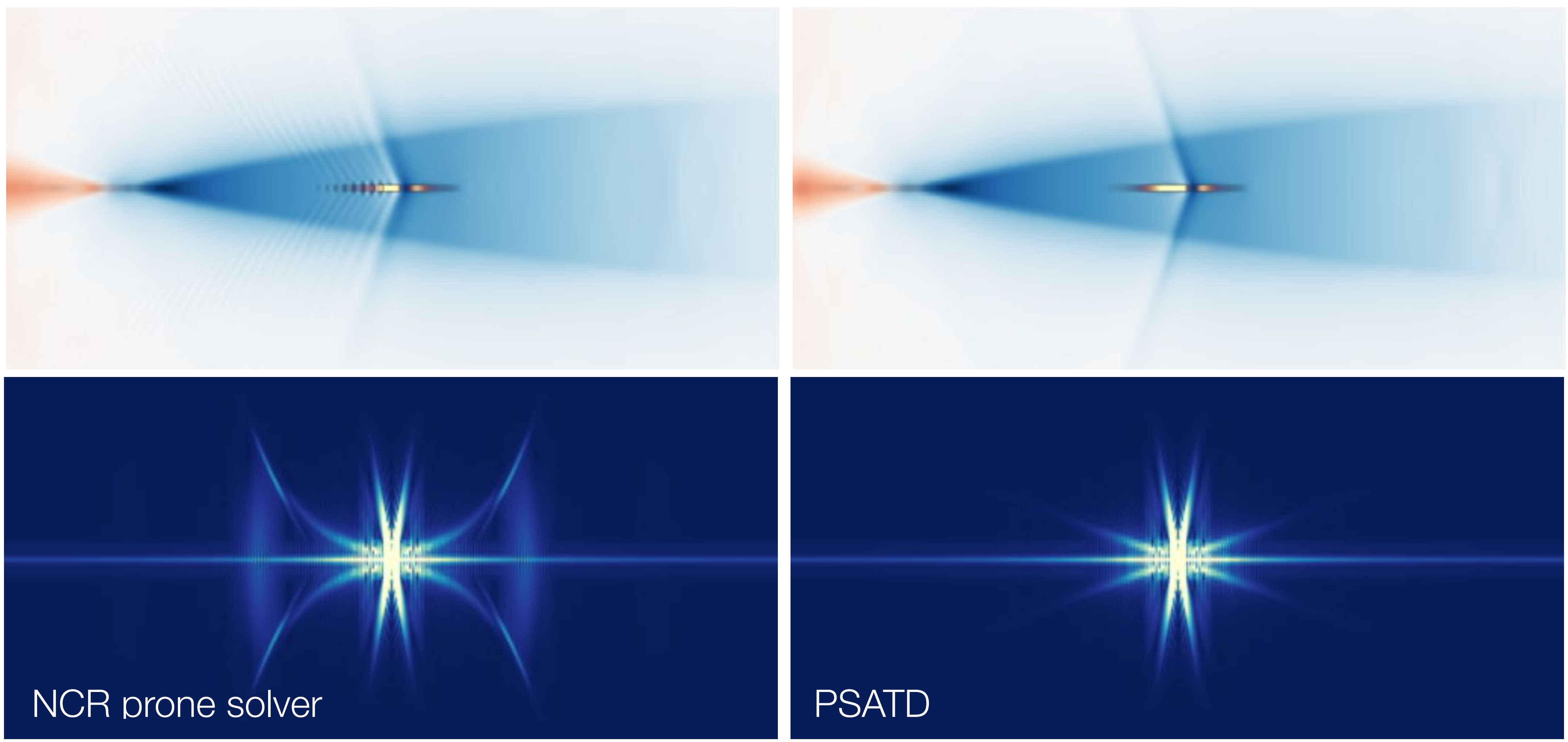
$$\begin{cases} E_{\max}^{(3D)}(ct) = 0 & \text{for } t < t^{*(3D)} \\ E_{\max}^{(3D)}(ct) = E_{\infty}^{(3D)} \left(1 - \dfrac{ct^{*(3D)}}{ct}\right)^2 & \text{for } t > t^{*(3D)} \end{cases}$$





PSATD Cherenkov Reduction

Pseudo-Spectral-Analytic-Time-Domain (PSATD)

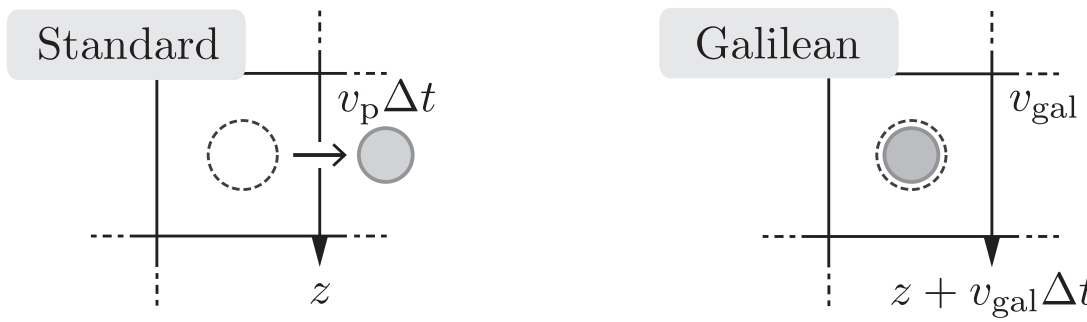


Intrinsic elimination of NCI in Lorentz-boosted frame simulations

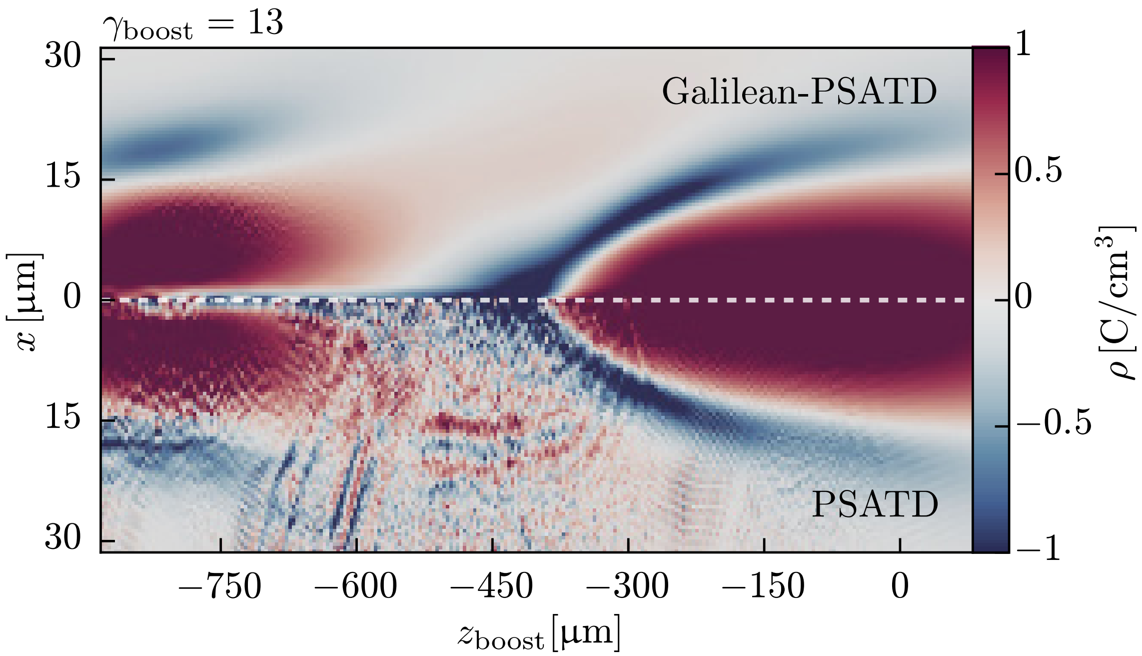
Concept & applications: Physics of Plasmas 23, 100704 (2016)
Math & stability analysis: Phys. Rev. E 94, 053305 (2016)
or checkout **lux.cfel.de/publications/**

Galilean-PSATD

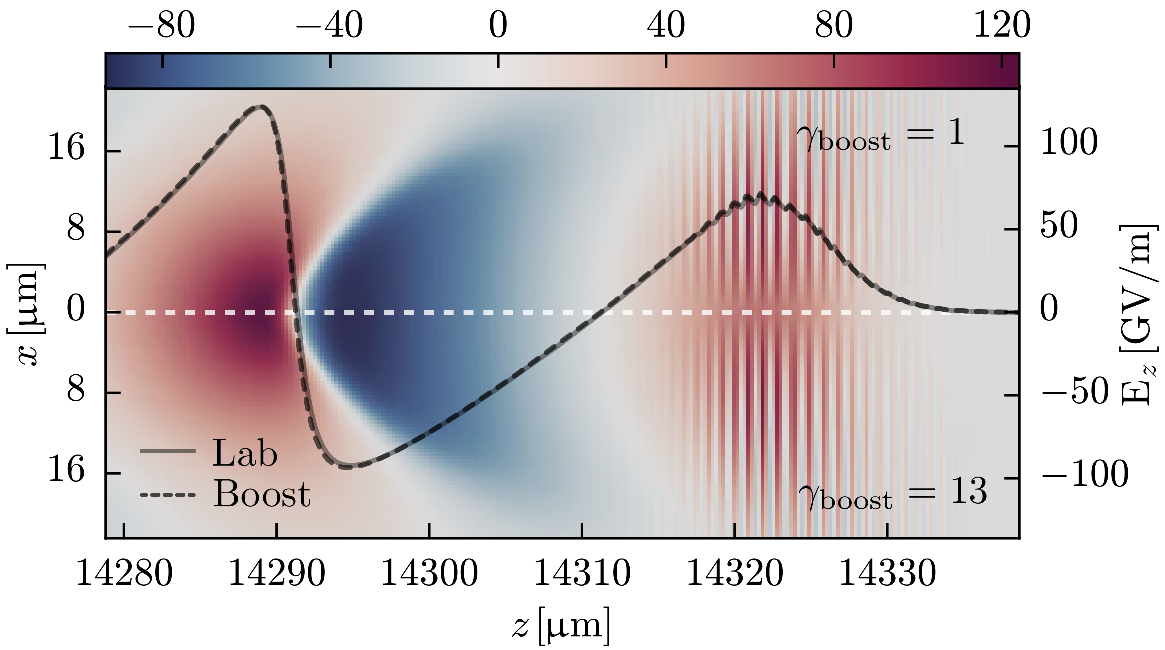
- Solves PIC in co-propagating *Galilean* frame
- No artificial numerical corrections required
- Independent of geometry
- **Intrinsically free of NCI for drifting plasma**



Comparison PSATD / Galilean-PSATD in the boosted frame



Comparison to lab frame simulation



Exascale computing

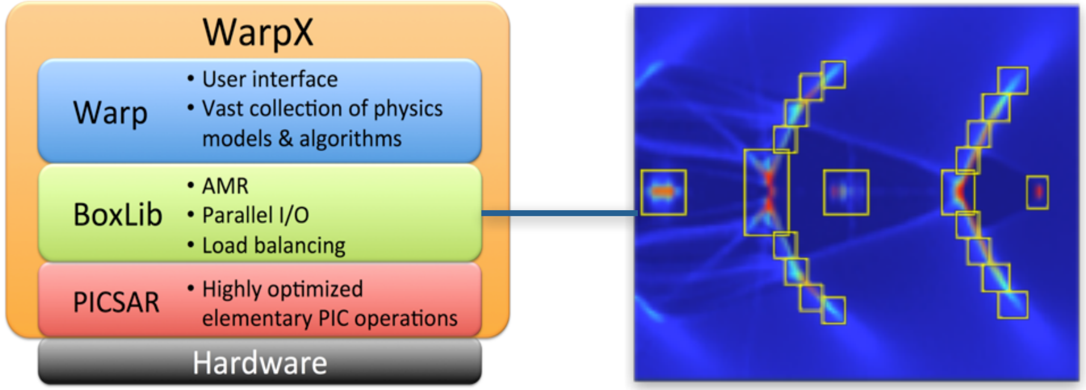
present and future for WarpX - Mesh Refinement

ECP Project WarpX: Exascale Modeling of Advanced Particle Accelerators

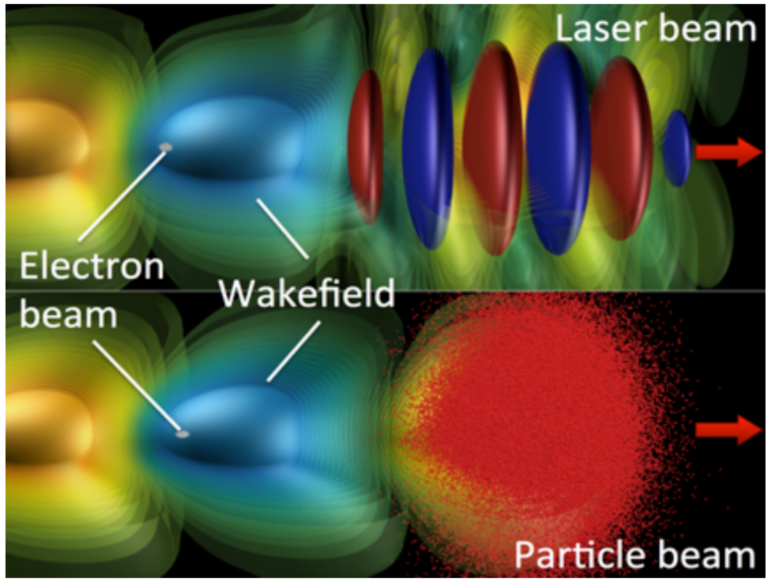
Goal (4 years): Convergence study in 3-D of 10 consecutive multi-GeV stages in linear and bubble regime, for laser- & beam-driven plasma accelerators.

How: ➔ Combination of most advanced algorithms

➔ Coupling of Warp+BoxLib/AMReX+PICSAR



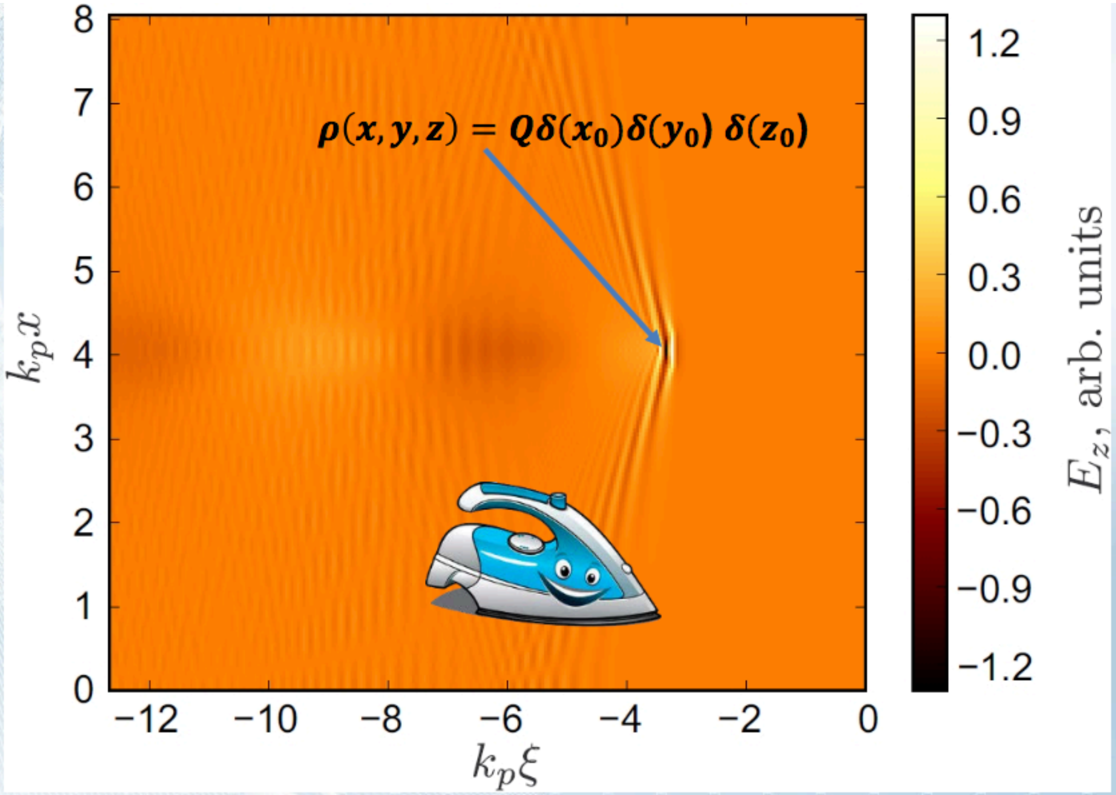
➔ Port to emerging architectures (Xeon Phi, GPU)

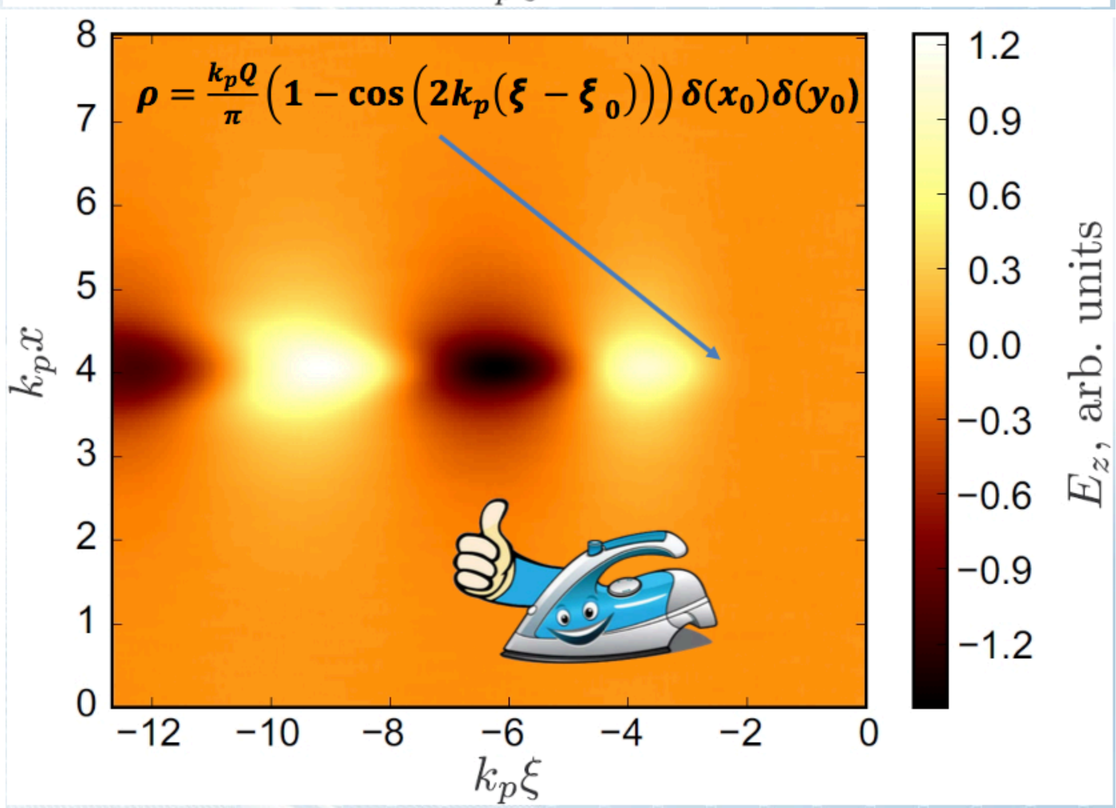


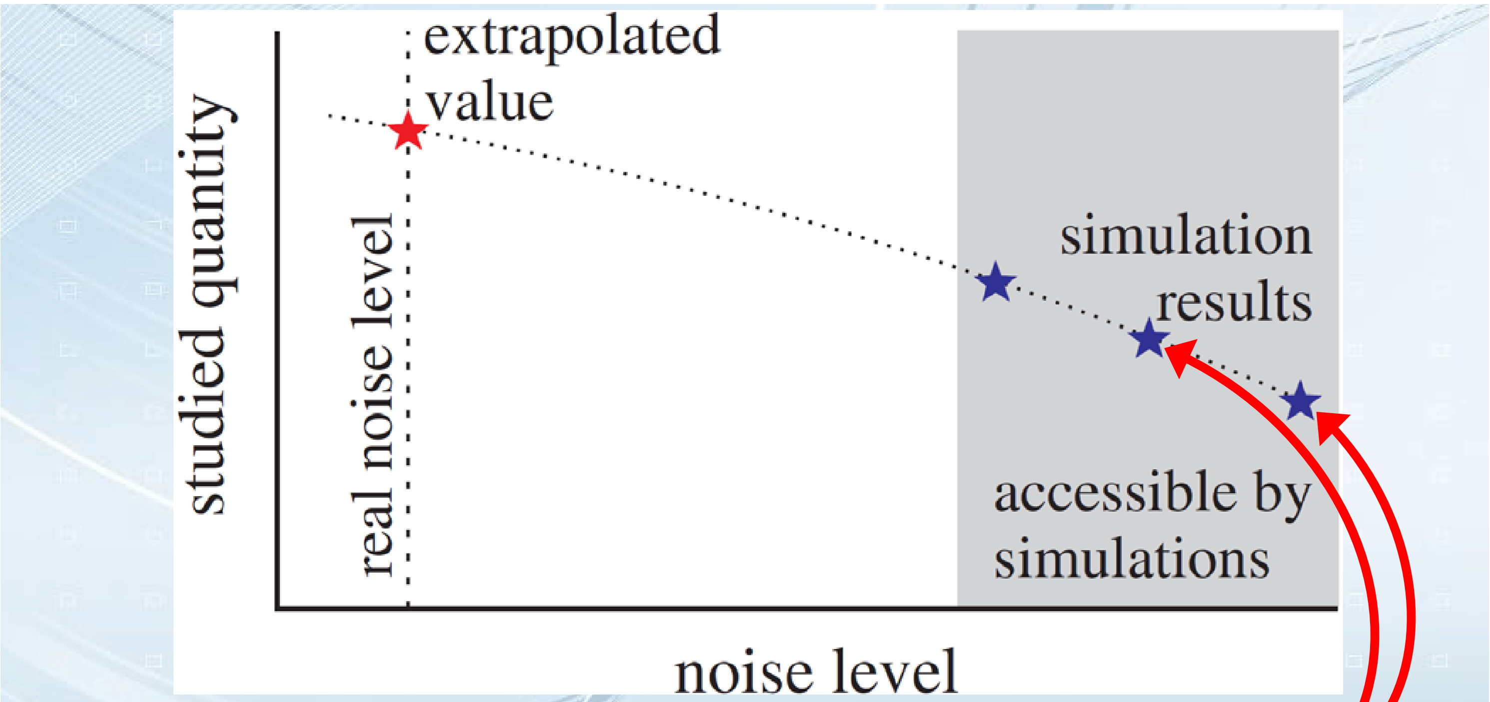
Team: LBNL ATAP (accelerators) + LBNL CRD (computing science) + SLAC + LLNL

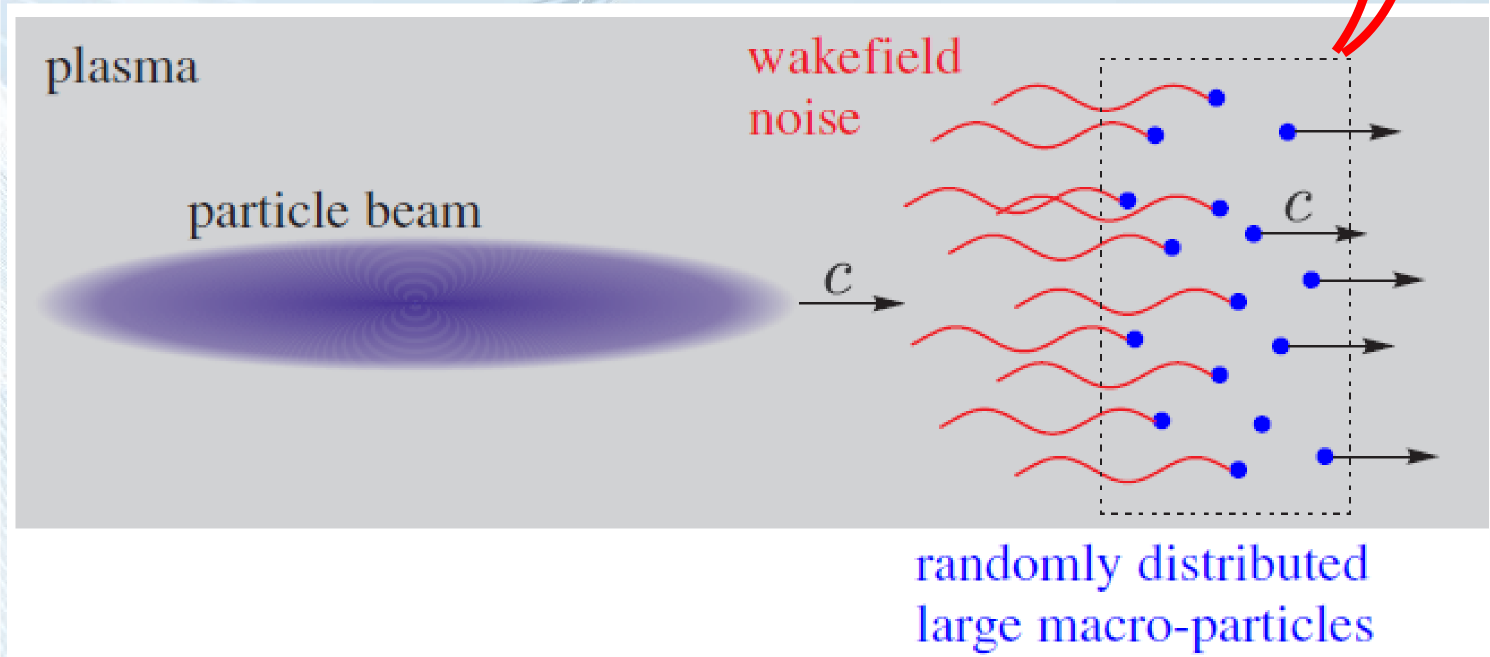
Ultimate goal: enable modeling of 100 stages by 2025 for 1 TeV collider design!

Noise control



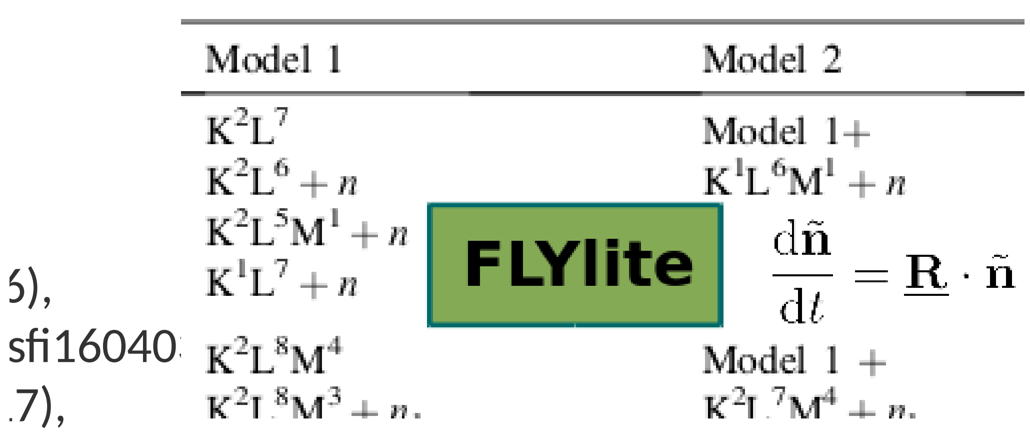




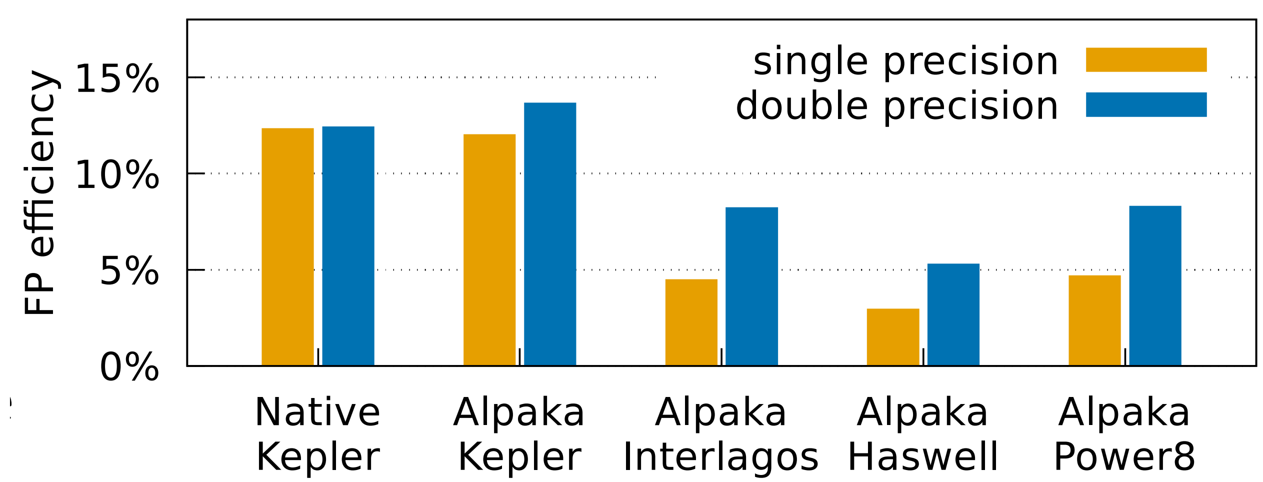


PICon GPU on all Platforms & XFEL-Plasma Modeling

- *Got no GPUs?* Now runs also on: **CPU, KNL, ARM, Power, ...!**
- **open** software stack towards exascale **3D3V PIC** simulations
- **single-source**, performance portable C++ (27k LOC)



Upcoming: Non-LTE Atomic Physics

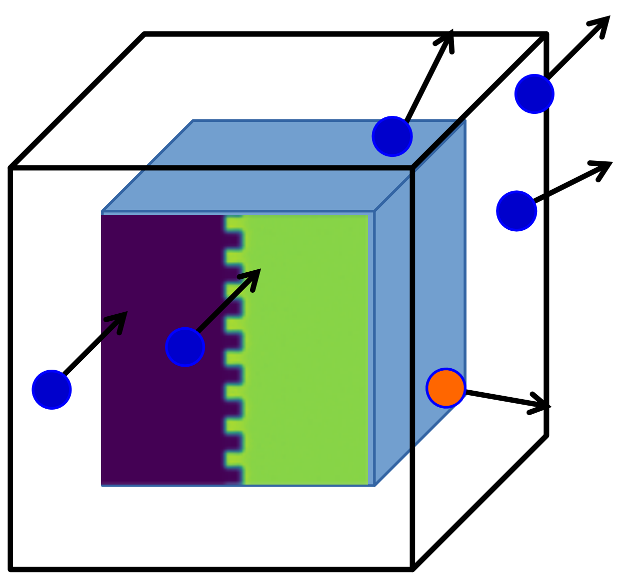


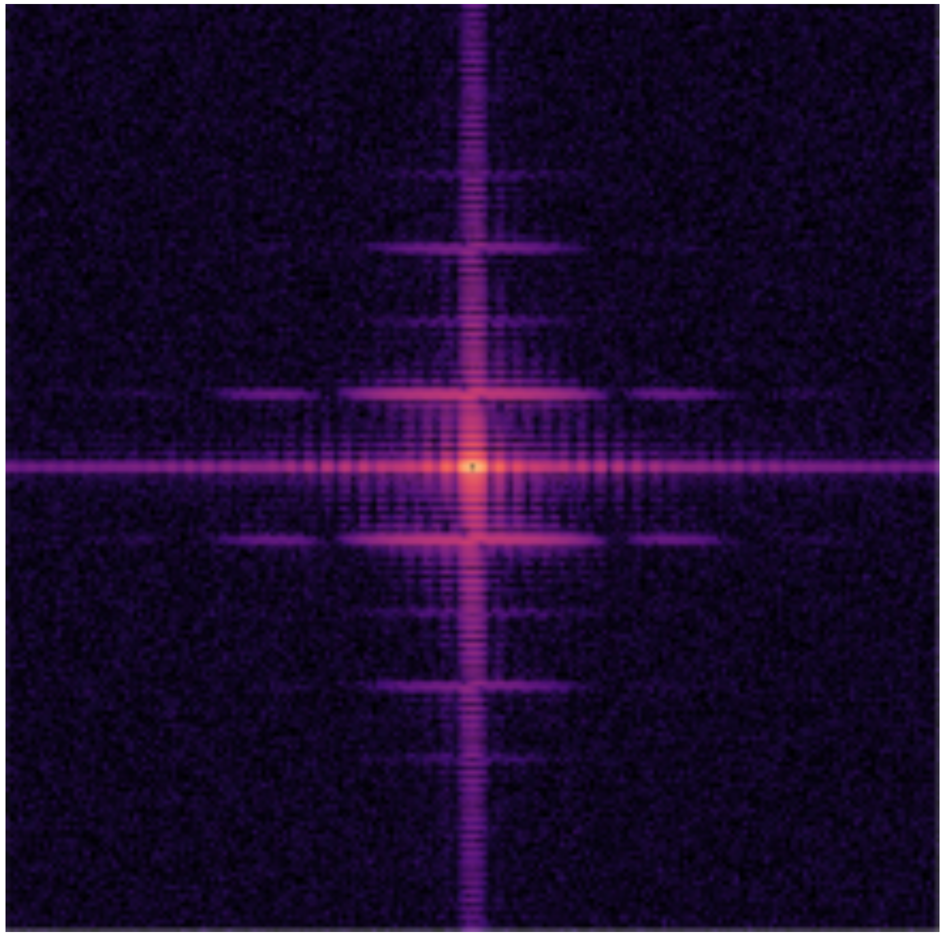
Photon Scattering in Solid-Density Plasmas

Massive Monte-Carlo X-ray photon scattering

- arbitrarily complex 3D density distributions from PIC simulations
- multiple scattering, arbitrary atomic physics

PIConGPU openPMD ParaTAXIS

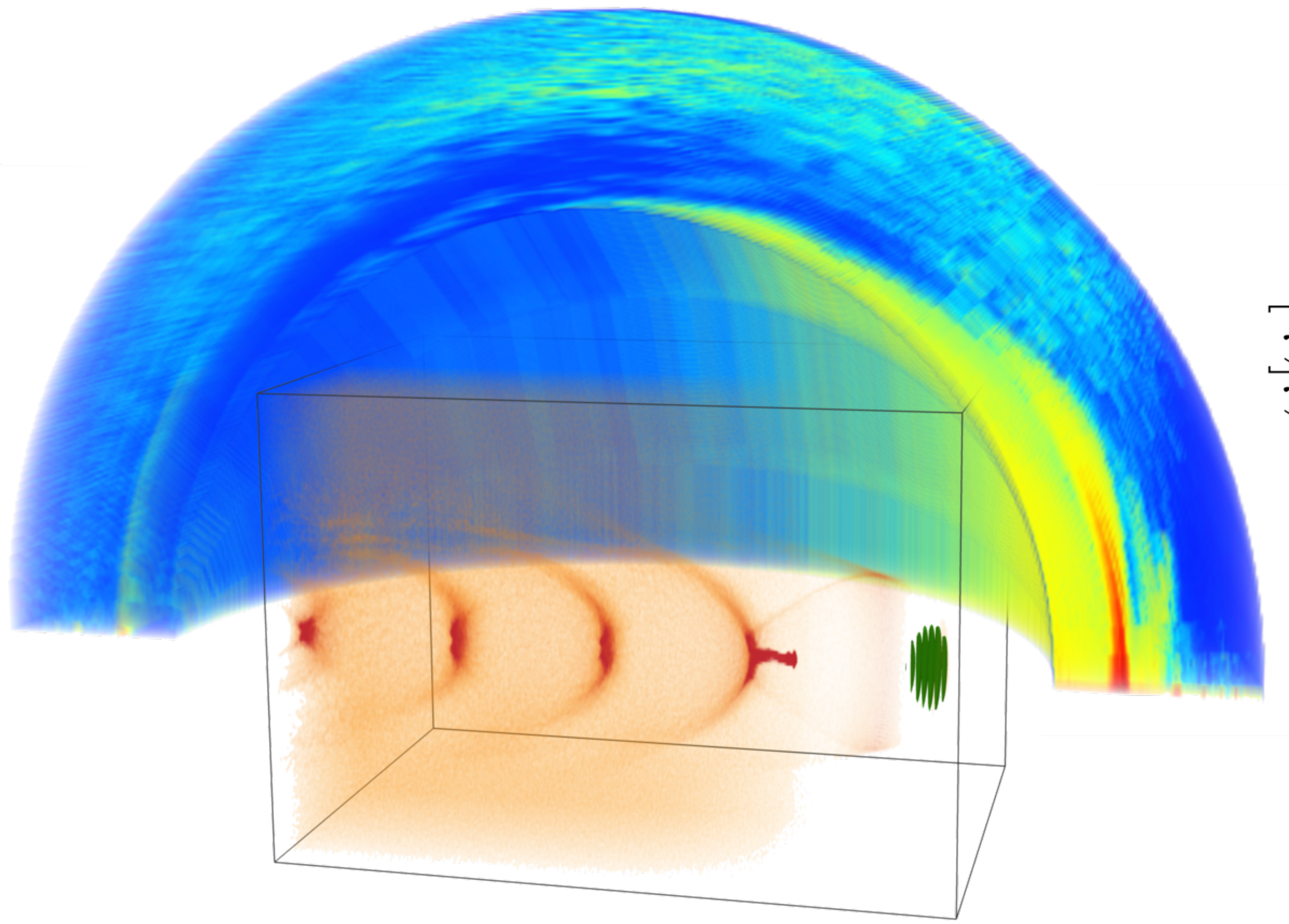


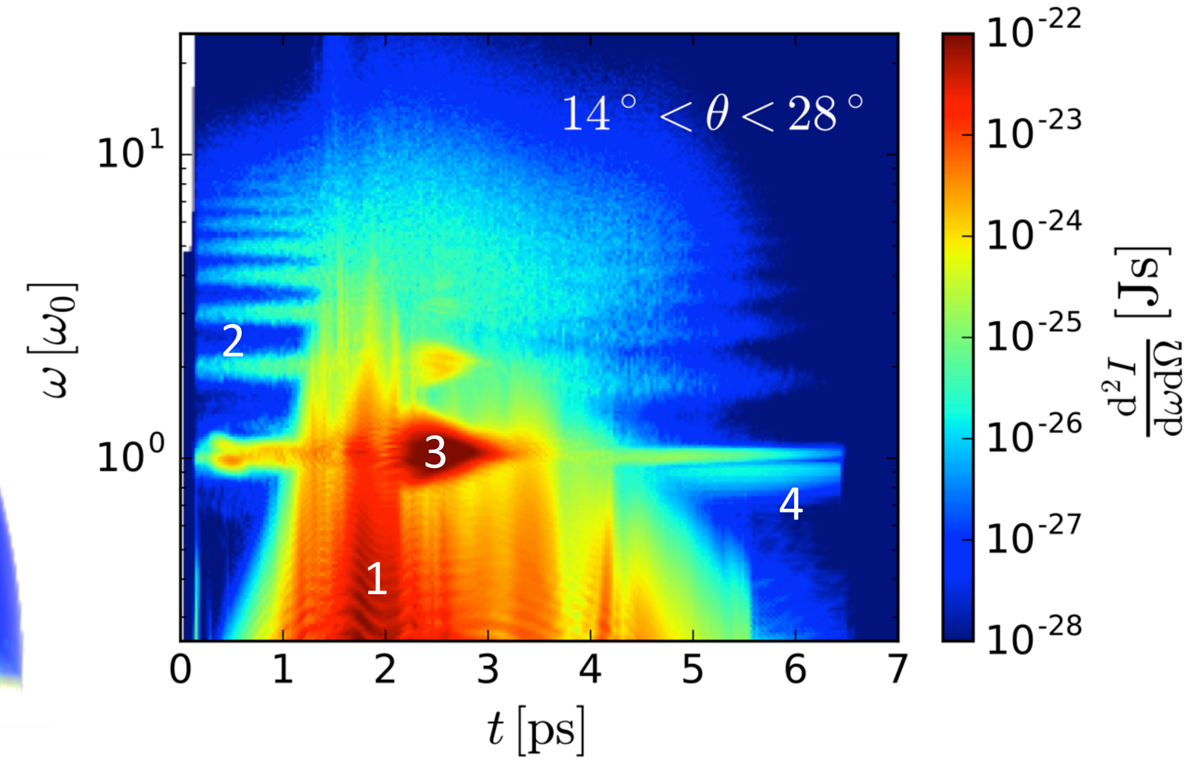


Part of complete start-to-end simulation framework for pump-probe experiments EUCALL SIMEX_platform

How can one observe the plasma dynamics?

Using radiation as synthetic radiation diagnostics





The first 3D LWFA radiation simulation linking spectral signatures to laser and plasma dynamics.

Radiation signatures allow to determine:

1. wave breaking
2. laser intensity
3. laser-bunch interaction
4. self-phase modulation

PIConGPU

MATTER AND TECHNOLOGIES · GPU CENTER OF EXCELLENCE · DRESDEN concept · HZDR

Rise of the open source

- Codes
  - Epoch
  - PiconGPU
  - Aladyn / Architect
  - Smilei
  - FBPIC
  - WarpX (2018)
- Libraries
  - PICSAR (soon)
  - PMacc
  - Alpaka
  - ADIOS
- Standards
  - openPMD
  - Where are the other standards ?

Exascale approaches : future of PIC codes

Numerical methods

- Improvements of (pseudo) spectral solvers implementation
- Fighting Cherenkov radiation and instability
- Adaptative Mesh Refinement (AMR)
- Dynamic Load Balancing
- Reduced models (envelope, symplectic, hybrid ...)
- Continuous integration, robustness tests

Diagnostics and data

- In situ visualization
- Radiation diagnostics
- Data reduction

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